IBM

Application Program

GH20-0586-0

System/360 Scientific Subroutine Package (PL/I)

(360A-CM-07X)

Program Description and Operations Manual

The System/360 Scientific Subroutine Package (SSP) (PL/I) is a collection of mathematical and statistical subroutines (or procedures) written in the PL/I language. It provides the PL/I user with most of the basic capabilities in earlier FORTRAN versions of SSP/360. It also has the same basic characteristics as the FORTRAN versions, in that it consists of input/output-free computational building blocks, written completely in PL/I, which may be combined with a user's input, output, or computational routines as needed. The package may be applied to the solution of many problems in industry, science, and engineering.

This manual contains sufficient information to permit the reader to understand and use all of the subroutines in the Scientific Subroutine Package.

Note: This programming package has been developed with the cooperation and assistance of IBM Germany and IBM France.

First Edition (January 1968)

Significant changes or additions to the specifications contained in this publication will be reported in subsequent revisions or Technical Newsletters.

This edition applies to Version 1, Modification Level 0 of System/360 Scientific Subroutine Package (PL/I) (360A-CM-07X) and to all subsequent versions and modifications until otherwise indicated in new editions or Technical Newsletters.

Changes are continually made to the specifications herein. Therefore, before using this publication, consult the latest System/360 SRL Newsletter (N20-0360) for the editions that are applicable and current.

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CONTENTS

Introduction 1
Areas of Application 1
Mathematics 1
Statistics 1
IBM Reference Material 1
Characteristics 1
Required Systems 2
Programming Systems 2
Machine Configuration 2
Overall Rules of Usage 3
General Rules 3
Error Codes 4
Matrix Operations 4
Variable Dimensioning 4
Storage Compression 4
Double Precision 4
Format of the Documentation 5
Subroutine Descriptions 5
Sample Program Descriptions 5
Operating Notes 5
Categorical Guide to Subroutines and Sample Programs 6
Mathematics 6
Matrix Operations 6
Polynomial Operations 7
Numerical Quadrature 7
Numerical Differentiation 7
Interpolation of Tabulated Functions . . . 8
Approximation of Tabulated Functions . . 8
Smoothing of Tabulated Functions 8
Roots and Extrema of Functions 8
Systems of Ordinary Differential Equations 8
Special Mathematical Functions 8
Statistics 8
Data Screening and Analysis 8
Elementary Statistics 9
Correlation and Regression Analysis . . . 9
Analysis of Variance 9
Discriminant Analysis 9
Principal Components Analysis 9
Nonparametric Statistics 9
Distribution Functions 9
Guide to Sample Programs 9
Data Screening 9
Multiple Linear Regression 9
Stepwise Multiple Regression 10
Canonical Correlation 10
Analysis of Variance 10
Discriminant Analysis 10
Principal Components Analysis 10
Kolmogorov-Smirnov Test 10
Triple Exponential Smoothing 10
Allocation of Overhead Costs 10
Alphabetic Guide to Subroutines and Sample Programs 11
Subroutine Descriptions and Listings 13
Mathematics 13
Matrix Operations 13
Polynomial Operations 77
Numerical Quadrature 92
Numerical Differentiations 107
Interpolation of Tabulated Functions . . 118
Approximation of Tabulated Functions 129
Smoothing of Tabulated Functions 147
Roots and Estrema of Functions 153
Systems of Ordinary Differential Equations 167
Special Mathematical Functions 172
Statistics 181
Data Screening and Analysis 181
Elementary Statistics 191
Correlation and Regression Analysis . . 194
Analysis of Variance 206
Discriminant Analysis 209
Principal Components Analysis 212
Nonparametric Statistics 218
Distribution Functions 239
Appendix A: Accuracy of Subroutines 248
Appendix B: Sample Program Descriptions 255

INTRODUCTION

The Scientific Subroutine Package (SSP) for Operating System/360 PL/I is a set of basic computational subroutines intended to help the user develop his own PL/I program library. The user may supplement or modify the subroutines to meet his needs. This package includes a wide variety of subroutines to perform the functions listed below but is not intended to be exhaustive in terms of either functions performed or methods used. As with all tools, the user should understand their capabilities and their application to his functional requirements before deciding to use them.

AREAS OF APPLICATION

Individual subroutines or a combination of them can be used for the general areas listed here.

Mathematics

- Matrix operations
  - Elementary
  - Linear equations
  - Eigenvalues
- Polynomial operations
  - Orthogonal polynomials
  - Polynomial economization
  - Polynomial roots
- Numerical quadrature
  - Tabulated functions
  - Nontabulated functions
- Numerical differentiation
  - Tabulated functions
  - Nontabulated functions
- Interpolation of tabulated functions
- Approximation of tabulated functions
- Smoothing of tabulated functions
- Roots and extrema of functions
- Systems of ordinary differential equations
- Special mathematical functions

Statistics

- Data screening and analysis
- Elementary statistics
- Correlation and regression analysis
  - Correlation
  - Multiple linear regression
  - Stepwise multiple regression
  - Canonical correlation
- Analysis of variance
- Discriminant analysis
- Principal components analysis
- Nonparametric statistics
- Distribution functions

IBM REFERENCE MATERIAL

System/360 Scientific Subroutine Package (360A-CM-03X) Version III Programmer's Manual (H20-0205)

IBM System/360 Operating System PL/I (F) Reference Manual (C28-8201)

IBM System/360 Operating System PL/I (F) Programmer's Guide (C28-6594)

Preface to PL/I Programming in Scientific Computing (E20-0312)

CHARACTERISTICS

Some of the characteristics of SSP/360 (PL/I) are as follows:

- All subroutines are free of input/output statements.
- All subroutines are written in OS/360 PL/I (F).
- Most of the subroutines provide a double-precision option.
- The use of certain subroutines (or groups of them) is illustrated in the program documentation by sample main programs with input/output.
- All subroutines are documented uniformly.

An example of a sample main program that uses several of the subroutines is the statistical function called Principal Components Analysis (FACT).* It uses five separate subroutine capabilities, as follows:

- Computation of means, standard deviations, and correlation matrix (CORR)
- Computation of eigenvalues and eigenvectors of the correlation matrix (MSDU)
- Selection of eigenvalues (TRAC)
- Computation of factor matrix (LOAD)
- Varimax rotation of the factor matrix (VRMX)

This is one of the sample main programs included in the program documentation.

*This program performs the same functions as the program that was called Factor Analysis in the FORTRAN versions of SSP. The name Principal Components Analysis more aptly describes the function of this program than the name Factor Analysis. For a discussion of the distinction between Factor Analysis and Principal Components Analysis see Section 2.2 of 1130 Statistical System (1130-CA-06X) User's Manual (H20-0333).

REQUIRED SYSTEMS

Programming Systems

The subroutines are written in the PL/I language, using the 48-character set and the facilities provided by the PL/I (F) compiler, which functions under Operating System/360.

Machine Configuration

A minimum requirement is a System/360 suitable for the OS/360 PL/I (F) compiler. The machine configuration required for any given problem depends on the number of subroutines used, the size of the compiled subroutines, the size of the compiled main program, the size of the control program, and the data storage requirements.

OVERALL RULES OF USAGE

GENERAL RULES

All subroutines in SSP are entered by means of the standard PL/I CALL statement. The subroutines are purely computational in nature and do not contain any references to input/output devices. The user must therefore furnish, as part of his program, the input/output and other operations necessary for the total solution of his problem. He must also define by DECLARE statements all matrices to be operated on by SSP subroutines as well as those matrices utilized in his program. The subroutines contained in SSP are used like any user-supplied subroutine. All of the normal rules of PL/I concerning subroutines must therefore be followed. Note that the subroutines have been written using the 48-character set, so the programmer should be familiar with its use.

All variables in the calling program must be declared with the proper attributes. Those variables appearing as parameters in the call statement of the calling program should not have attributes conflicting with those of the called program.

The CALL statement transfers control to the subroutine and replaces the dummy variables in that subroutine with the value of the actual arguments that appear in the CALL statement. When the argument is an array, the address and size of the array are transmitted to the called subroutine.

The arguments in a CALL statement should agree in order, number, and type with the corresponding arguments in the subroutine. In SSP, all arguments in a CALL statement must be variable names. Constants are not acceptable. For example, if the user wishes to invert a matrix A, which is 10 by 10, using the SSP subroutine MINV, and if the constant for testing the condition of the matrix is 10^{-8}, these constants must be defined as variables before calling MINV, as illustrated below:

```
N = 10, .

CON = 1.0 E - 8, .

CALL MINV (A, N, D, CON), .
```

where D is the determinant.

Some of the subroutines in SSP require the name of a user function subprogram or a PL/I-supplied function name as part of the argument list in the CALL statement. If the user's program contains such a CALL, the function name appearing in the argument list must be declared as ENTRY in the user's calling program.

For example, the SSP routine SBST calls a user-supplied subroutine. The user must, therefore, prepare a subroutine, with the proper argument list, to perform the desired tasks. He must declare the name of this subroutine as ENTRY in his calling program and supply the name of that subroutine to SBST as the appropriate parameter in his CALL statement to subroutine SBST. The subroutine SBST need not be modified by the user. The dummy argument B in the subroutine SBST is replaced by the user's subroutine name at execution time.

The following illustrates these procedures:

SSP Subroutine SBST (need not be altered)

```
SBST. .
   PROCEDURE (A, C, R, B, S, NO, NV, NC), .
   DECLARE
         B ENTRY, .
      .
      .
      .
   CALL B (R, TR), .
      .
      .
      .
   RETURN, .
   END, .
```

User's Calling Program

```
USER. .
   PROCEDURE OPTIONS (MAIN), .
   DECLARE
         BOOL ENTRY, .
      .
      .
      .
   CALL SBST (A, C, R, BOOL, S, NO, NX,
   NC), .
      .
      .
      .
   RETURN, .
   END, .
```

User's Function Subprogram

```
BOOL..
  PROCEDURE (R, T), .
       .
       .
       .
  RETURN, .
  END, .
```

ERROR CODES

In the Scientific Subroutine Package most of the subroutines use an error indicator to warn the user that a certain condition exists. The user, in his calling program, should check the error indicator when returning from a called program. If the user wishes to use the error indicator as an aid, he should, in his calling program, declare ERROR EXTERNAL CHARACTER(1). In this way he has available in the calling program the value of the error indicator (ERROR).

If, in using a subroutine, an error is detected, some of the output areas may contain invalid data. Generally, however, output areas are set to appropriate values (for example, zero or $\pm 10^{75}$).

MATRIX OPERATIONS

Special consideration must be given to the subroutines that perform matrix operations. These subroutines have two characteristics that affect the size and format of the data in storage: variable dimensioning and data storage compression.

Variable Dimensioning

Those subroutines that deal with matrices can operate on any size array, limited in most cases only by the available core storage and numerical analysis considerations. The subroutines do not contain fixed maximum dimensions for data arrays named in their calling sequence. The variable dimension capability has been implemented in SSP by using the asterisk notation. Under this approach, where a called subroutine needs to declare an array of the same dimensions as a calling program, the dimension specifications are replaced by asterisks. Thus, the user does not need to modify the subroutines so long as he has declared adequate dimensions for arrays in the calling program or main program.

One way to ensure that arrays have adequate dimensions for various problems is to declare them with variable notations. For example, if matrix R contains intercorrelation coefficients among M variables, the DECLARE statement appears as follows:

```
DECLARE R(M,M), .
```

If M is 10, then 100 locations will be allocated for matrix R.

If M is 20, then 400 locations will be allocated automatically.

Storage Compression

When working with symmetric matrices it is often advantageous to use a compressed (vector) storage form. This means that only the upper or lower triangular part of the matrix need be stored, which for an N by N matrix reduces the core requirements from N^2 locations to N(N+1)/2 locations. A subroutine, MSCS, is provided in this package which stores a symmetric matrix in compressed form and at the same time tests the matrix for symmetry. The element stored is the average of each pair of symmetric elements of an n by n matrix Q, i.e.,

$$S_{ik} = \frac{Q_{ik} + Q_{ki}}{2} \qquad \begin{matrix} i = 1, \ldots, n. \\ k = 1, \ldots, i. \end{matrix}$$

At the same time the difference $Q_{ik} - Q_{ki}$ is tested against a user-supplied tolerance. If this test fails, an ERROR indication is given but in any case the results S_{ik} are supplied in the vector form:

$$S_{11}, S_{21}, S_{22}, S_{31}, S_{32}, S_{33} \ldots S_{nn}$$

Another subroutine, MSCG, is provided which converts this vector (compressed) form back to the general two-dimensional form.

Some of the subroutines of SSP-- for example, MMSS and MAGS--accept input in this compressed form.

DOUBLE PRECISION

The accuracy of the computations in many of the SSP subroutines is highly dependent upon the number of significant digits available for arithmetic operations. Matrix inversion, integration, and many of the statistical subroutines fall into this category. The user may, therefore, wish to use double-precision versions of these subroutines. Most of the SSP/360 (PL/I) subroutines provide a double-precision option. PL/I double-precision statements have been included in each of these subroutines in

the form of a comments card. The double-precision version of the subroutine can be obtained by removing/* from cc 3 and 4 of the double-precision statement card(s) and by removing the corresponding single-precision cards (or making them comments cards) before compilation. The use of double-precision subroutines requires a detailed knowledge of the PL/I rules concerning double precision. Two of the more basic rules are as follows:

1. Any real variable, vector, or array name contained in the argument list of a CALL to a double-precision subroutine must be declared as double precision in the calling program.
2. Any user-supplied function named in the CALL statement for a double-precision SSP subroutine must be programmed as a double-precision function.

FORMAT OF THE DOCUMENTATION

The major portion of this manual consists of the documentation for the individual subroutines and sample programs.

SUBROUTINE DESCRIPTIONS

Subroutines and sample program guides, both categorical and alphabetic, designed to help locate particular subroutines are given in the pages that follow.

The subroutine descriptions, in general, consist of purpose, usage, remarks, method, mathematical background, programming considerations, and a program listing. References to books and periodicals will be found under the method section of the description. The mathematical description pages do not, in all cases, indicate the derivation of the mathematics. They are intended to indicate what mathematical operations are actually being performed in the subroutines.

SAMPLE PROGRAM DESCRIPTIONS

A sample program, in general, consists of a description of the problem, program, input, output, program modification, operating instructions, error messages, timing, machine listing of the program, sample input data, and output results. In some cases (for example, as a part of developing the data screening sample program) a special sample subroutine has been implemented that may prove useful to the programmer. One such subroutine, called HIST, prints a histogram of frequencies. The listing of these subroutines is included after the sample program documentation in this manual.

Instructions for modifying the sample programs for different data formats are included in the documentation. In addition, those sample programs that illustrate potentially double-precision subroutines include double-precision statements in the form of comment cards. These comment cards are contained in the sample program source decks.

OPERATING NOTES

It is recommended that those SSP subroutines that will be frequently used in an installation be compiled and that the relocatable programs be placed on the PL/I systems residence device. In the case of Operating System/360, this will be the PL/I library portion of the system disk pack. Information on the method for updating the system to include user-supplied subroutines appears in the appropriate PL/I programmer's guide. SSP subroutines are handled in the same manner as user-supplied subroutines. If the subroutines are not placed in the PL/I library, those required by a particular program will have to be included in that program each time it is run. As noted earlier, the subroutines have been written using the 48-character set.

CATEGORICAL GUIDE TO SUBROUTINES AND SAMPLE PROGRAMS

MATHEMATICS

Matrix Operations

Elementary Operations

		Page
MSCS	Storage conversion — two-dimensional to compressed	13
MSCG	Storage conversion — compressed to two-dimensional	14
MAGS	Add-subtract general and symmetric matrices	14
MMGG	Product of two general matrices	15
MMSS	Product of two symmetric matrices	16
MMGS	Product of a general matrix and a symmetric matrix	17
MMGT	Product of a general matrix and its transpose	18
MPRM	Permutation of rows or columns of a matrix	19
MTPI	Calculation of permutations from transpositions	20
MPTT	Calculation of inverse permutation and transpositions	21

Linear Equations and Related Topics

MFG	Triangular factorization of a general nonsingular matrix	23
MFS	Triangular factorization of a symmetric positive definite matrix	25
MFSB	Triangular factorization of a symmetric positive definite band matrix	27
MFGR	Factorization and rank determination of a general rectangular matrix	29
MDLS/MDRS	Dividing a matrix by a triangular matrix that has been factored from a symmetric positive definite matrix	35
MDSB	Dividing a matrix by a triangular matrix that has been factored from a symmetric positive definite band matrix	37
MDLG	Dividing a matrix by a lower or upper triangular matrix that has been factored from a general nonsingular matrix	39
MIG	Inverting a general nonsingular matrix that has been factored into upper and lower triangular factors	40
MIS	Inverting a symmetric positive definite matrix that has been factored into a triangular matrix and its transpose	42
MINV	Inverting a general square matrix	44
MLSQ	Solution of a system of linear equations, the least squares solution being obtained in case of an overdetermined system	45
MGB1/MGB2	Solution of simultaneous linear equations with band matrix of coefficients	49

Eigenvalues and Related Topics

MATE	Reduction of a real matrix to upper almost-triangular form by elementary transformations	56
MATU	Reduction of a real matrix to upper almost-triangular form by orthogonal transformations	58
MSTU	Reduction of a symmetric matrix to tridiagonal form by orthogonal transformations	59
MEAT	Eigenvalues of a real upper almost-triangular matrix	61
MEST	Eigenvalues of a real symmetric tridiagonal matrix	63
MEBS	Bounds for the eigenvalues of a real symmetric matrix	66
MVST	Eigenvector of a symmetric tridiagonal matrix, corresponding to a given eigenvalue	67
MSDU	Eigenvalues and eigenvectors of a real symmetric matrix	69

		Page
MGDU	Eigenvalues and eigenvectors of a special real nonsymmetric matrix	71
MVAT	Eigenvector of a complex almost-triangular matrix, corresponding to a given eigenvalue	72
MVSU	Eigenvector of a symmetric matrix from the corresponding eigenvector of the associated tridiagonal form	74
MVUB	Eigenvector of a real matrix from the corresponding eigenvector of the associated almost-triangular matrix, which has been developed using MATU	75
MVEB	Eigenvector of a real matrix from the corresponding eigenvector of the associated almost-triangular matrix, which has been developed using MATE	76

Polynomial Operations

POV	Values of orthogonal polynomials (Chebyshev, Legendre, Laguerre and Hermite)	77
POSV	Value of series expansion in orthogonal polynomials (Chebyshev, Legendre, Laguerre and Hermite)	78
PEC/PTC	Economization of a polynomial for symmetric and asymmetric range, transformation of polynomial to expansion in Chebyshev or shifted Chebyshev polynomials	81
POST	Transformation of orthogonal polynomial expansion to a polynomial	86
PRTC	Roots of a complex polynomial by Nickel's method based on a method of Newton	87

Numerical Quadrature

Quadrature of Tabulated Functions

QTFG/QTFE	Integration of monotonically or equidistantly tabulated function by trapezoidal rule	92
QSF	Integration of equidistantly tabulated function by Simpson's rule	93
QHFG/QHSG/ QHFE/QHSE	Integration of monotonically or equidistantly tabulated function with first (and second) derivatives by Hermitian formula of the first (and second) order	94

Quadrature of Nontabulated Functions

QATR	Integration of a given function by the trapezoidal rule together with Romberg's extrapolation method	97
QG2, QG4, QG8, QG16, QG24, QG32, QG48	Integration of a given function by Gaussian quadrature formulas	99
QL2, QL4, QL8, QL12, QL16, QL24	Integration of a given function by Gaussian-Laguerre quadrature formulas	101
QH2, QH4, QH8, QH16, QH24, QH32, QH48	Integration of a given function by Gaussian-Hermite quadrature formulas	103
QA2, QA4, QA8, QA12, QA16, QA24	Integration of a given function by associated Gaussian-Laguerre quadrature formulas	105

Numerical Differentiation

Differentiation of Tabulated Functions

DGT3	Differentiation of a tabulated function by Lagrangian interpolation	107
DET3	Differentiation of an equidistantly tabulated function using Lagrangian interpolation formulas	108
DET5	Differentiation of an equidistantly tabulated function using Lagrangian interpolation formulas	110

Differentiation of Nontabulated Functions

DFEC	Derivative of a function at the center of an interval by Richardson's and Romberg's extrapolation method	112

		Page
DFEO	Derivative of a function at the end of an interval by Richardson's and Romberg's extrapolation method	115

Interpolation of Tabulated Functions

ALIM/ALIE	Aitken-Lagrange interpolation, monotonic and equidistant tables	118
AHIM/AHIE	Aitken-Hermite interpolation, monotonic and equidistant tables	122
ACFM/ACFE	Continued fraction interpolation, monotonic and equidistant tables	126

Approximation of Tabulated Functions

FFT	Fast Fourier transform for real or complex one-dimensional array	129
FFTM	Fast Fourier transform for real or complex multidimensional array	134
APLL	Setting up normal equations for least squares polynomial approximation	139
APC1/APC2	Setting up normal equations for least squares Chebyshev polynomial approximation	140
ASN	Solving normal equations for least squares fit	143

Smoothing of Tabulated Functions

SG13/SE13	Local least squares smoothing of a tabulated function using a linear fit relative to three points	147
SE15	Local least-squares smoothing of an equidistantly tabulated function using a linear fit relative to five points	149
SE35	Local least-squares smoothing of an equidistantly tabulated function using a cubic fit relative to five points	150
EXSM	Triple exponential smoothing of a given series	152

		Page

Roots and Extrema of Functions

FMFP	Minimization of a function of several variables without constraints	153
RTF	Root of a function using linear, quadratic, or hyperbolic interpolation	159
RTFD	Root of a function with given derivatives, by linear, inverse, quadratic, or hyperbolic interpolation	163

Systems of Ordinary Differential Equations

DERE	Performing one integration step on a system of first-order ordinary differential equations	167

Special Mathematical Functions

CEL1/CEL2	Complete elliptic integral of first and second kind	172
ELI1/ELI2	Incomplete elliptic integral of first and second kind	174
JELF	Jacobian elliptic functions	177
LGAM	Log of the gamma function	180

STATISTICS

Data Screening and Analysis

TALY	Totals, means, standard deviations, minima, and maxima	181
BOUN	Selection of observations over, under, and within bounds	182
ABST	Detection of missing data	183
SBST	Subset selection from observation matrix satisfying certain conditions	184
TAB1	Tabulation of data (one variable) including frequencies, over class intervals, mean, standard deviation, minimum, and maximum	185
TAB2	Tabulation of data (two variables)	187

		Page
SUBM	Copying a subset matrix that satisfies certain conditions from an observation matrix	190

Elementary Statistics

MOMN	First four moments for grouped data on equal class intervals	191
TTST	Certain t-statistics on the means of populations	192

Correlation and Regression Analysis

CORR	Means, standard deviations, and correlation coefficients	194
ORDR	Selection of submatrix from matrix of correlation coefficients for multiple linear regression analysis	196
MLTR	Multiple linear regression analysis	197
STRG	Stepwise multiple linear regression analysis	200
CANC	Canonical correlation between two sets of variables	204

Analysis of Variance

AVAR	Analysis of variance for a complete factorial design	206

Discriminant Analysis

DMTX	Means and dispersion matrix for all groups	209
DSCR	Discriminant functions	210

Principal Components Analysis

TRAC	Cumulative percentage of eigenvalues	213
LOAD	Factor loading	214
VRMX	Varimax rotation	215

Nonparametric Statistics

KLMO	Kolmogorov-Smirnov one-sample test	218
KLM2	Kolmogorov-Smirnov two-sample test	221
SMIR	Kolmogorov-Smirnov limiting distribution values	223
CHSQ	Chi-square test for contingency tables	224
KRNK	Kendall rank correlation	227
QTST	Cochran Q-test	229
RANK	Rank observation	230
SRNK	Spearman rank correlation	231
TIE	Calculation of correction factor due to ties	233
TWAV	Friedmann two-way analysis of variance statistic	234
UTST	Mann-Whitney U-test	235
WTST	Kendall coefficient of concordance	236
HTES	Kruskal-Wallis H-test	238

Distribution Functions

NDTR	Normal distribution function	239
BDTR	Beta distribution function	240
CDTR	Chi-square distribution function	243
NDTI	Inverse of normal distribution function	246

GUIDE TO SAMPLE PROGRAMS

Data Screening

DACR	Sample main program	255
Illustrates use of:		
SBST	Subset selection from observation matrix	184
TAB1	Tabulation of data (one variable)	185

Special sample subroutines are:

BOOL	Boolean expression	259
HIST	Histogram printing	259
DAT1	Sample data read	259

Multiple Linear Regression

REGR	Sample main program	260
Illustrates use of:		
CORR	Means, standard deviations, and correlations	194
ORDR	Rearrangement of intercorrelations	196
MINV	Matrix inversion	44
MLTR	Multiple regression	197
Special sample subroutines are:		
DAT2	Sample data read	265
IDT1	Sample binary fixed data read	265

Page

Stepwise Multiple Regression

STEP	Sample main program	265
Illustrates use of:		
CORR	Means, standard deviations, and correlations	194
STRG	Stepwise multiple regression	200
Special sample subroutines are:		
DAT2	Sample data read subroutine	270
IDT2	Sample binary fixed data read	270
SOUT	Sample stepwise regression output subroutine	270

Canonical Correlation

CANO	Sample main program	270
Illustrates use of:		
CORR	Means, standard deviations, and correlations	194
CANC	Canonical correlation	204
MINV	Matrix inversion	44
MGDU	Eigenvalues and eigenvectors of a special general matrix	71
MSDU	Eigenvalues and eigenvectors of a symmetric matrix	69
Special sample subroutine is:		
DAT2	Sample data read	274

Analysis of Variance

ANOV	Sample main program	274
Illustrates the use of:		
AVAR	Analysis of variance	206
Special sample subroutine is:		
DAT3	Sample data read	277

Discriminant Analysis

MDSC	Sample main program	277
Illustrates the use of:		
DMTX	Means and dispersion matrix	209
MINV	Matrix inversion	44
DSCR	Discriminant analysis	210
Special sample subroutine is:		
DAT2	Sample data read	281

Page

Principal Components Analysis

FACT	Sample main program	281
Illustrates the use of:		
CORR	Means, standard deviations, and correlations	194
MSDU	Eigenvalues and eigenvectors of a real symmetric matrix	69
TRAC	Cumulative percentage of eigenvalues	213
LOAD	Factor loading	214
VRMX	Varimax rotation	215
Special sample subroutine is:		
DAT2	Sample data read	286

Kolmogorov-Smirnov Test

KOLM	Sample main program	286
Illustrates the use of:		
KLMO	One sample test	218
KLM2	Two sample test	221
SMIR	Kolmogorov-Smirnov limiting distribution function	223
NDTR	Normal distribution function	239

Triple Exponential Smoothing

EXPN	Sample main program	291
Illustrates the use of:		
EXSM	Triple exponential smoothing	152
Special sample subroutine is:		
DAT3	Sample data read	293

Allocation of Overhead Costs

COST	Sample main program	294
Illustrates the use of:		
MFG	Matrix triangular factorization	23
MDLG	Division by triangular matrices	39

ALPHABETIC GUIDE TO SUBROUTINES AND SAMPLE PROGRAMS, WITH STORAGE REQUIREMENTS

The following table lists the number of bytes of storage for the program control section required by each of the subroutines in the Scientific Subroutine Package. The storage requirements were obtained by using Version 4 of PL/I and Release 16 of OS. The use of other versions and releases may cause deviations from these figures.

The double-precision version storage requirements of the subroutines in the Scientific Subroutine Package are included in parentheses.

Name	Math. Description Page Number	Storage Required Bytes
ABST	183	610
ACFM	126	2,826 (2,696)
ACFE	126	
AHIM	122	2,946 (2,950)
AHIE	122	
ALIM	118	2,306 (2,310)
ALIE	118	
ANOV	274	4,482
APC1	140	1,766 (1,766)
APC2	140	
APLL	139	986 (986)
ASN	143	1,902 (1,874)
AVAR	206	4,174 (4,174)
BDTR	240	3,830
BOOL	259	266
BOUN	182	1,102
CANC	204	4,718 (4,718)
CANO	270	5,478
CDTR	243	3,962
CEL1	172	858 (854)
CEL2	172	
CHSQ	224	3,882
CORR	194	4,352 (4,408)
COST	294	3,206
DACR	255	4,294
DAT1	259	1,098
DAT2	265	1,098
DAT3	277	850
DERE	167	2,762 (2,738)
DET3	108	658 (658)
DET5	110	890 (890)
DFEC	112	1,142 (1,142)
DFEO	115	1,118 (1,118)
DGT3	107	894 (894)
DMTX	209	2,498 (2,510)
DSCR	210	3,090 (3,110)
ELI1	174	1,458 (1,454)
ELI2	174	
EXPN	291	2,430
EXSM	152	1,030
FACT	281	7,116
FFT	129	3,166 (3,166)
FFTM	134	4,040 (4,040)
FMFP	153	4,174 (4,040)
HIST	259	2,674
HTES	238	1,122
IDT1	265	614
IDT2	270	614
JELF	177	1,270 (1,270)
KLMO	218	2,010
KLM2	221	1,998
KOLM	286	6,828
KRNK	227	2,010
LGAM	180	750
LOAD	214	666 (666)
MAGS	14	638 (638)
MATE	56	1,706
MATU	58	1,918
MDLG	39	1,314
MDLS	35	1,426 (1,414)
MDRS	35	
MDSB	37	1,202 (1,186)
MDSC	277	6,482
MEAT	61	5,638
MEBS	66	1,066
MEST	63	1,890
MFG	23	1,882 (1,858)
MFGR	29	2,730 (2,714)
MFS	25	886 (874)
MFSB	27	1,158 (1,142)
MGB1	49	3,562 (3,550)
MGB2	49	
MGDU	71	2,274 (2,274)
MIG	40	1,894 (1,858)
MINV	44	3,014 (3,014)
MIS	42	1,198 (1,182)
MLSQ	45	3,622 (3,558)
MLTR	197	2,098 (2,098)
MMGG	15	630 (622)
MMGS	17	1,062 (1,058)
MMGT	18	858 (846)
MMSS	16	718 (710)
MOMN	191	2,078
MPRM	19	1,078 (1,078)
MPIT	21	730
MSCG	14	474 (474)
MSCS	13	626 (626)
MSDU	69	3,538 (3,538)
MSTU	59	2,426
MTPI	20	674

Name	Math. Description Page Number	Storage Required Bytes
MVAT	72	5,782
MVEB	76	1,294
MVST	67	3,254
MVSU	74	1,182
MVUB	75	1,518
NDTI	246	834
NDTR	239	450
ORDR	196	1,238 (1,238)
PEC	81	2,082 (2,090)
PTC	81	
POST	86	1,322 (1,322)
POSV	78	798 (790)
POV	77	722 (714)
PRTC	87	2,686 (2,718)
QA2	105	362 (354)
QA4	105	510 (490)
QA8	105	398 (398)
QA12	105	402 (402)
QA16	105	402 (402)
QA24	105	398 (394)
QATR	97	1,318 (1,318)
QG2	99	422 (422)
QG4	99	574 (554)
QG8	99	534 (526)
QG16	99	538 (530)
QG24	99	538 (530)
QG32	99	538 (530)
QG48	99	530 (522)
QH2	103	346 (342)
QH4	103	474 (466)
QH8	103	454 (450)
QH16	103	458 (454)
QH24	103	458 (454)
QH32	103	458 (454)
QH48	103	450 (446)
QHFG	94	
QHFE	94	
QHSG	94	1,178 (1,178)
QHSE	94	

Name	Math. Description Page Number	Storage Required Bytes
QL2	101	362 (354)
QL4	101	510 (490)
QL8	101	398 (398)
QL12	101	402 (402)
QL16	101	402 (402)
QL24	101	398 (394)
QSF	93	710 (710)
QTFG	92	702 (702)
QTFE	92	
QTST	229	1,462
RANK	230	962
REGR	260	7,930
RTF	159	1,878 (1,882)
RTFD	163	1,762 (1,762)
SBST	184	1,562
SE13	147	1,118 (1,118)
SG13		
SE15	149	730 (730)
SE35	150	774 (774)
SMIR	223	710
SRNK	231	1,558
SOUT	270	3,458
STEP	265	5,494
STRG	200	4,914 (4,950)
SUBM	190	790
TAB1	185	2,642
TAB2	187	4,894
TALY	181	2,090
TIE	233	926
TRAC	213	818 (818)
TTST	192	2,562
TWAV	234	1,562
UTST	235	1,302
VRMX	215	3,970 (3,852)
WTST	236	1,986

MATHEMATICS

Matrix Operations

Elementary Operations

- Subroutine MSCS

```
MSCS..                                                              MSCS  10
/*******************************************************************/MSCS  20
/*                                                                 */MSCS  30
/*      CONVERT THE STORAGE ALLOCATION OF A SYMMETRIC MATRIX       */MSCS  40
/*      FROM A TWO-DIMENSIONAL ARRAY TO A LINEAR ARRAY             */MSCS  50
/*                                                                 */MSCS  60
/*******************************************************************/MSCS  70
   PROCEDURE(Q,N,EPS,S),.                                           MSCS  80
   DECLARE                                                          MSCS  90
         (Q(*,*),EPS,S(*),Q1,Q2,M)                                  MSCS 100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MSCS 110
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MSCS 120
         (N,I,K,L)BINARY FIXED,                                     MSCS 130
         ERROR EXTERNAL CHARACTER(1),.                              MSCS 140
   ERROR='0',.                         /*PRESET ERROR INDICATOR    */MSCS 150
   L    =0,.                                                        MSCS 160
   IF N GT 0                           /*TEST SPECIFIED DIMENSION  */MSCS 170
   THEN DO I =1 TO N,.                                              MSCS 180
           DO K =1 TO I,.                                           MSCS 190
           L    =L+1,.                                              MSCS 200
           Q1   =Q(I,K),.              /*REPLACE Q1 BY Q(I,K)      */MSCS 210
           Q2   =Q(K,I),.              /*REPLACE Q2 BY Q(K,I)      */MSCS 220
           S(L),M=(Q1+Q2)*0.5,.        /*SET RES. S(L) =(Q1+Q2)/2  */MSCS 230
           IF ABS(Q1-Q2) GT            /*TEST FOR SYMMETRY OF Q    */MSCS 240
                EPS*MAX(1,ABS(M))                                   MSCS 250
           THEN ERROR='S',.            /*Q IS NOT SYMMETRIC        */MSCS 260
           END,.                                                    MSCS 270
        END,.                                                       MSCS 280
   ELSE ERROR='D',.                    /*ERROR IN SPECIFIED DIMENSION */MSCS 290
   END,.                               /*END OF PROCEDURE MSCS     */MSCS 300
```

Purpose:

MSCS compresses the storage allocation of a symmetric two-dimensional matrix to a one-dimensional array.

Usage:

CALL MSCS (Q, N, EPS, S);

Q(N, N) - BINARY FLOAT [(53)]
Given N by N symmetric matrix.

N - BINARY FIXED
Given order of matrices Q and S.

EPS - BINARY FLOAT [(53)]
Given relative tolerance for test on symmetry.

S(N*(N+1)/2) - BINARY FLOAT [(53)]
Resultant symmetric matrix in one-dimensional compressed form.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='D' means N is less than 1.

ERROR='S' means given matrix Q does not pass the specified symmetry test. Nonetheless, all of the elements S_{ik} are computed as shown below and stored in S.

Method:

$$S_{ik} = \frac{Q_{ik} + Q_{ki}}{2} \quad \text{for } i=1,2,\ldots,n \quad k=1,\ldots,i$$

Symmetry-test:

$Q_{ik} - Q_{ki}$ must be absolutely less than

$$\text{Max } (1, \frac{|Q_{ki} + Q_{ik}|}{2}) * \text{EPS}$$

- Subroutine MSCG

```
MSCG..                                                              MSCG  10
/*******************************************************************/MSCG  20
/*                                                                 */MSCG  30
/*      CONVERT THE STORAGE ALLOCATION OF A SYMMETRIC MATRIX       */MSCG  40
/*      FROM A LINEAR ARRAY TO A TWO-DIMENSIONAL ARRAY             */MSCG  50
/*                                                                 */MSCG  60
/*******************************************************************/MSCG  70
   PROCEDURE(S,N,Q),.                                               MSCG  80
   DECLARE                                                          MSCG  90
        (S(*),Q(*,*))                                               MSCG 100
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MSCG 110
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MSCG 120
        (N,I,K,L)BINARY FIXED,.                                     MSCG 130
   L    =0,.                                                        MSCG 140
   IF N GT 0                          /*TEST SPECIFIED DIMENSION    */MSCG 150
   THEN DO I =1 TO N,.                                              MSCG 160
             DO K =1 TO I,.                                         MSCG 170
             L    =L+1,.                                            MSCG 180
             Q(I,K),Q(K,I)=S(L),.     /*STORE Q(I,K) AND Q(K,I)     */MSCG 190
             END,.                                                  MSCG 200
        END,.                                                       MSCG 210
   END,.                              /*END OF PROCEDURE MSCG       */MSCG 220
```

Purpose:

MSCG expands the compressed one-dimensional storage allocation of a symmetric matrix to general two-dimensional form.

Usage:

CALL MSCG (S, N, Q);

S(N*(N+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array representing a symmetric N by N matrix in compressed form.

N - BINARY FIXED
Given order of matrices S and Q.

Q(N, N) - BINARY FLOAT [(53)]
Resultant two-dimensional general representation of given symmetric matrix S.

Remarks:

Operation is bypassed in case of a nonpositive value of N. The elements of given S are assumed to be stored in compressed form -- that is:

$(S_{11}, S_{21}, S_{22}, S_{31}, S_{32}, S_{32}, \ldots, S_{n1}, \ldots, S_{nn})$

Method:

For the elements of resultant Q:

$$Q_{ik} = Q_{ki} = S_{ik} \text{ for } \begin{matrix} i = 1, 2, \ldots, n \\ k = 1, 2, \ldots, i \end{matrix}$$

- Subroutine MAGS

```
MAGS..                                                              MAGS  10
/*******************************************************************/MAGS  20
/*                                                                 */MAGS  30
/*      ADD OR SUBTRACT A SQUARE AND A SYMMETRIC MATRIX            */MAGS  40
/*                                                                 */MAGS  50
/*******************************************************************/MAGS  60
   PROCEDURE(A,B,N,OPT,C),.                                         MAGS  70
   DECLARE                                                          MAGS  80
        (A(*,*),B(*),C(*,*),AL,BL)                                  MAGS  90
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MAGS 100
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MAGS 110
        (N,I,K,L,LI)BINARY FIXED,                                   MAGS 120
        OPT CHARACTER(1),.                                          MAGS 130
   IF N GT 0                          /*IS N GREATER THAN ZERO      */MAGS 140
   THEN DO,.                                                        MAGS 150
        LI,I =1,.                                                   MAGS 160
NEXTI..                                                             MAGS 170
        L    =LI,.                                                  MAGS 180
        K    =1,.                                                   MAGS 190
NEXTK..                                                             MAGS 200
        AL   =A(I,K),.             /*REPLACE AL BY A(I,K)        */MAGS 210
        BL   =B(L),.               /*SET BL CORRESPONDING TO AL  */MAGS 220
        IF K LT I                                                   MAGS 230
        THEN L    =L+1,.                                            MAGS 240
        ELSE L    =L+K,.                                            MAGS 250
        IF OPT='2'                 /*SHOULD A-B BE CALCULATED    */MAGS 260
        THEN BL   =-BL,.           /*THEN CONVERT SIGN OF BL     */MAGS 270
        ELSE IF OPT='3'            /*SHOULD B-A BE CALCULATED    */MAGS 280
        THEN AL   =-AL,.           /*THEN CONVERT SIGN OF AL     */MAGS 290
        C(I,K)=AL+BL,.             /*SET RESULTANT C(I,K) TO AL+BL*/MAGS 300
        IF K LT N                                                   MAGS 310
        THEN DO,.                  /*INCREMENT K                 */MAGS 320
             K    =K+1,.                                           MAGS 330
             GO TO NEXTK,.                                         MAGS 340
             END,.                                                 MAGS 350
        ELSE IF I LT N                                             MAGS 360
        THEN DO,.                  /*INCREMENT I                 */MAGS 370
             LI   =LI+I,.                                          MAGS 380
             I    =I+1,.                                           MAGS 390
             GO TO NEXTI,.                                         MAGS 400
             END,.                                                 MAGS 410
        END,.                                                      MAGS 420
   END,.                           /*END OF PROCEDURE MAGS       */MAGS 430
```

Purpose:

MAGS computes C = A + B if OPT = '1'
C = A - B if OPT = '2'
C = B - A if OPT = '3'

for given matrices A and B which are general and symmetric respectively.

Usage:

CALL MAGS (A, B, N, OPT, C);

A(N, N) - BINARY FLOAT [(53)]
Given general N by N matrix.

B(N*(N+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array containing the lower triangular part of symmetric matrix B stored rowwise in compressed form.

N - BINARY FIXED
Given order of matrices A, B and C.

OPT - CHARACTER(1)
Given option for selection of operation.

C(N, N) - BINARY FLOAT [(53)]
Resultant general N by N matrix, which may be overlaid with A.

Remarks:

Operation is bypassed in case of a nonpositive value of N. A value of OPT different from '2' and '3' is treated as if it were '1'.

Method:

The sum or difference of matrices A and B is calculated elementwise. The elements of the symmetric matrix B are accessed only once.

- Subroutine MMGG

```
MMGG..                                                                  MMGG  10
/*************************************************************************/MMGG  20
/*                                                                       */MMGG  30
/*      MULTIPLY TWO GENERAL MATRICES                                    */MMGG  40
/*                                                                       */MMGG  50
/*************************************************************************/MMGG  60
   PROCEDURE(A,B,K,L,M,C),.                                              MMGG  70
   DECLARE                                                               MMGG  80
         (A(*,*),B(*,*),C(*,*))                                          MMGG  90
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MMGG 100
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MMGG 110
         S BINARY FLOAT(53),                                             MMGG 120
         (K,L,M,I,J,N)                                                   MMGG 130
         BINARY FIXED,                                                   MMGG 140
         ERROR EXTERNAL CHARACTER(1),.                                   MMGG 150
   ERROR='D',.                         /*PRESET ERROR INDICATOR       */MMGG 160
   IF K GT 0                           /*TEST SPECIFIED DIMENSIONS    */MMGG 170
   THEN IF L GT 0                                                        MMGG 180
   THEN IF M GT 0                                                        MMGG 190
   THEN DO,.                                                             MMGG 200
         I    =0,.                                                       MMGG 210
NEXTI..                                /*COMPUTE THE I-TH ROW OF C    */MMGG 220
         I    =I+1,.                                                     MMGG 230
         J    =0,.                                                       MMGG 240
NEXTJ..                                /*COMPUTE THE J-TH ELEMENT     */MMGG 250
         J    =J+1,.                                                     MMGG 260
         S    =0,.                                                       MMGG 270
              DO N =1 TO L,.           /*PERFORM SCALAR PRODUCT       */MMGG 280
              S    =S+MULTIPLY(A(I,N),                                   MMGG 290
                   B(N,J),53),.                                          MMGG 300
              END,.                                                      MMGG 310
         C(I,J)=S,.                    /*STORE RESULTANT C(I,J)       */MMGG 320
         IF J LT M                                                       MMGG 330
         THEN GO TO NEXTJ,.            /*INCREMENT J                  */MMGG 340
         ELSE IF I LT K                                                  MMGG 350
         THEN GO TO NEXTI,.            /*INCREMENT I                  */MMGG 360
         ERROR='0',.                   /*SUCCESSFUL OPERATION         */MMGG 370
         END,.                                                           MMGG 380
   END,.                               /*END OF PROCEDURE MMGG        */MMGG 390
```

Purpose:

MMGG computes the standard matrix product $C = A \cdot B$.

Usage:

CALL MMGG (A, B, K, L, M, C);

A(K, L) - BINARY FLOAT [(53)]
Given K by L matrix A (left-hand factor).

B(L, M) - BINARY FLOAT [(53)]
Given L by M matrix B (right-hand factor).

K - BINARY FIXED
Given row dimension of A and C.

L - BINARY FIXED
Given column dimension of A and row dimension of B.

M - BINARY FIXED
Given column dimension of B and C.

C(K, M) - BINARY FLOAT [(53)]
Resultant K by M product matrix.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='D' means errors in specified dimensions K, L, M. Accumulation of scalar products is performed in double-precision arithmetic. C must be different from A and B.

Method:

Standard multiplication means that the element C_{ik} is the scalar product of the i-th row of A with the k-th column of B.

- Subroutine MMSS

```
MMSS..                                                                  MMSS  10
/*************************************************************************/MMSS  20
/*                                                                       */MMSS  30
/*      MULTIPLY TWO SYMMETRIC MATRICES STORED IN LINEAR ARRAYS          */MMSS  40
/*                                                                       */MMSS  50
/*************************************************************************/MMSS  60
   PROCEDURE(A,B,N,P),.                                                 MMSS  70
   DECLARE                                                              MMSS  80
         (A(*),B(*),P(*,*))                                             MMSS  90
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MMSS 100
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MMSS 110
         S BINARY FLOAT(53),                                            MMSS 120
         (N,L1,L2,LI,LK,I,K,J)                                          MMSS 130
         BINARY FIXED,.                                                 MMSS 140
   IF N GT 0                                                            MMSS 150
   THEN DO,.                                                            MMSS 160
         LI,I =1,.                                                      MMSS 170
NEXTI..                                                                 MMSS 180
         LK,K =1,.                                                      MMSS 190
NEXTK..                                                                 MMSS 200
         L1   =LI,.                                                     MMSS 210
         L2   =LK,.                                                     MMSS 220
         S    =0,.                     /*COMPUTE VECTOR PRODUCT OF TWO*/MMSS 230
              DO J =1 TO N,.           /*CORRESP. SUBARRAYS OF A AND B*/MMSS 240
              S    =S+MULTIPLY(A(L1),                                   MMSS 250
                   B(L2),53),.                                          MMSS 260
              IF J LT I                                                 MMSS 270
              THEN L1   =L1+1,.                                         MMSS 280
              ELSE L1   =L1+J,.                                         MMSS 290
              IF J LT K                                                 MMSS 300
              THEN L2   =L2+1,.                                         MMSS 310
              ELSE L2   =L2+J,.                                         MMSS 320
              END,.                                                     MMSS 330
         P(I,K)=S,.                    /*STORE RESULTANT ELEMENT OF P */MMSS 340
         IF K LT N                                                      MMSS 350
         THEN DO,.                     /*INCREMENT K                */MMSS 360
              LK   =LK+K,.                                              MMSS 370
              K    =K+1,.                                               MMSS 380
              GO TO NEXTK,.                                             MMSS 390
              END,.                                                     MMSS 400
         ELSE IF I LT N                                                 MMSS 410
         THEN DO,.                     /*INCREMENT I                */MMSS 420
              LI   =LI+I,.                                              MMSS 430
              I    =I+1,.                                               MMSS 440
              GO TO NEXTI,.                                             MMSS 450
              END,.                                                     MMSS 460
         END,.                                                          MMSS 470
   END,.                               /*END OF PROCEDURE MMSS      */MMSS 480
```

Purpose:

MMSS computes the standard product P = A · B of two symmetric matrices.

Usage:

CALL MMSS (A, B, N, P);

A(N*(N+1)/2) - BINARY FLOAT [(53)]
Given symmetric N by N matrix, stored in compressed form (left-hand factor).

B(N*(N+1)/2) - BINARY FLOAT [(53)]
Given symmetric N by N matrix, stored in compressed form (right-hand factor).

N - BINARY FIXED
Given order of matrices A, B, P.

P(N, N) - BINARY FLOAT [(53)]
Resultant N by N general product matrix.

Remarks:

Operation is bypassed in case of a nonpositive value of N. The symmetric matrices A and B must be stored in compressed form. Accumulation of scalar products is performed in double-precision arithmetic.

Method:

Standard multiplication means that the element P_{ik} is the scalar product of the i-th row of A with the k-th column of B.

- Subroutine MMGS

```
MMGS..                                                                  MMGS  10
/*************************************************************************/MMGS  20
/*                                                                       */MMGS  30
/*      MULTIPLY A GENERAL WITH A SYMMETRIC MATRIX                       */MMGS  40
/*                                                                       */MMGS  50
/*************************************************************************/MMGS  60
   PROCEDURE(G,S,M,N,OPT),.                                              MMGS  70
   DECLARE                                                               MMGS  80
        (G(*,*),S(*),H(MAX(N,M)))                                        MMGS  90
        BINARY FLOAT,                    /*SINGLE PRECISION VERSION  /*S*/MMGS 100
 /*     BINARY FLOAT(53),                /*DOUBLE PRECISION VERSION  /*D*/MMGS 110
        T BINARY FLOAT(53),                                              MMGS 120
        (M,N,MM,NN,I,J,K,L,LI,LJ,RN,CN)                                  MMGS 130
        BINARY FIXED,                                                    MMGS 140
        (OPT,ERROR EXTERNAL)CHARACTER(1),.                               MMGS 150
   NN   =N,.                        /*SET NN TO NUMBER OF COLUMNS  */MMGS 160
   MM   =M,.                        /*SET MM TO NUMBER OF ROWS OF G*/MMGS 170
   ERROR='0',.                      /*PRESET ERROR INDICATOR       */MMGS 180
   IF NN GT 0                       /*TEST SPECIFIED DIMENSIONS    */MMGS 190
   THEN IF MM GT 0                                                       MMGS 200
   THEN DO,.                                                             MMGS 210
        IF OPT='2'                                                       MMGS 220
        THEN DO,.                   /*IN CASE OF MULTIPL. S*G      */MMGS 230
             NN   =MM,.             /*INTERCHANGE NN AND MM        */MMGS 240
             MM   =N,.                                                   MMGS 250
             END,.                                                       MMGS 260
        K    =0,.                                                        MMGS 270
NEXTK..                                                                  MMGS 280
        RN,CN,K=K+1,.                                                    MMGS 290
             DO I =1 TO NN,.        /*REPLACE H(*) BY CURRENT ROW  */MMGS 300
             IF OPT='2'             /*RESP. COLUMN VECTOR OF G     */MMGS 310
             THEN RN    =I,.                                             MMGS 320
             ELSE CN    =I,.                                             MMGS 330
             H(I) =G(RN,CN),.                                            MMGS 340
             END,.                                                       MMGS 350
        LI,I =1,.                                                        MMGS 360
NEXTI..                             /*FOR CURRENT ROW RESP. COLUMN */MMGS 370
        L    =LI,.                  /*VECTOR COMPUTE I-TH ELEMENT  */MMGS 380
        T    =0,.                                                        MMGS 390
             DO J =1 TO NN,.        /*PERFORM SCALAR PRODUCT       */MMGS 400
             T    =T+MULTIPLY(H(J),                                      MMGS 410
                  S(L),53),.                                             MMGS 420
             IF J LT I                                                   MMGS 430
             THEN L    =L+1,.                                            MMGS 440
             ELSE L    =L+J,.                                            MMGS 450
             END,.                                                       MMGS 460
        IF OPT='2'                  /*TEST SPECIFIED MULTIPLICATION*/MMGS 470
        THEN RN    =I,.                                                  MMGS 480
        ELSE CN    =I,.                                                  MMGS 490
        G(RN,CN)=T,.                /*STORE RESULTANT ELEMENT      */MMGS 500
        LI   =LI+I,.                                                     MMGS 510
        I    =I+1,.                                                      MMGS 520
        IF I LE NN                                                       MMGS 530
        THEN GO TO NEXTI,.          /*INCREMENT I                  */MMGS 540
        ELSE IF K LT MM                                                  MMGS 550
        THEN GO TO NEXTK,.          /*INCREMENT K                  */MMGS 560
        ERROR='0',.                 /*SUCCESSFUL OPERATION         */MMGS 570
        END,.                                                            MMGS 580
   END,.                            /*END OF PROCEDURE MMGS        */MMGS 590
```

Purpose:

MMGS calculates G · S if OPT='1'
S · G if OPT='2'
where G is a general and S a symmetric matrix.

Usage:

CALL MMGS (G, S, M, N, OPT);

G(M, N) - BINARY FLOAT [(53)]
Given general M by N matrix.
Resultant product matrix G · S or S · G.

S(dimension) - BINARY FLOAT [(53)]
Given symmetric N by N or M by M matrix stored in compressed form in a one-dimensional array, lower triangular part rowwise.

M - BINARY FIXED
Given row dimension of matrix A.

N - BINARY FIXED
Given column dimension of matrix A.

OPT - CHARACTER (1)
Given option for selection of operation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR ='D' means errors in specified dimensions M, N. Any value of OPT different from '2' is treated as if it were '1'.

Scalar products are accumulated in double-precision arithmetic.

Method:

Standard multiplication is performed; the general product is generated in the storage locations occupied by G.

- Subroutine MMGT

```
MMGT..                                                                  MMGT  10
/*************************************************************************/MMGT  20
/*                                                                       */MMGT  30
/*      MULTIPLY A GENERAL MATRIX WITH ITS TRANSPOSE                     */MMGT  40
/*                                                                       */MMGT  50
/*************************************************************************/MMGT  60
   PROCEDURE(A,M,N,OPT,S),.                                             MMGT  70
   DECLARE                                                              MMGT  80
        (A(*,*),S(*))                                                   MMGT  90
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/MMGT 100
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/MMGT 110
        T BINARY FLOAT(53),                                             MMGT 120
        (M,N,I,II,J,JJ,K,L)                                             MMGT 130
        BINARY FIXED,                                                   MMGT 140
        (OPT,ERROR EXTERNAL)CHARACTER(1),.                              MMGT 150
   II   =M,.                                                            MMGT 160
   JJ   =N,.                                                            MMGT 170
   ERROR='D',.                     /*PRESET ERROR INDICATOR       */MMGT 180
   IF II GT 0                      /*TEST SPECIFIED DIMENSIONS    */MMGT 190
   THEN IF JJ GT 0                                                      MMGT 200
   THEN DO,.                                                            MMGT 210
        IF OPT='2'                 /*CHECK SPECIFIED MULTIPLIC.   */MMGT 220
        THEN DO,.                                                       MMGT 230
             JJ   =II,.            /*INTERCHANGE II AND JJ IN CASE*/MMGT 240
             II   =N,.             /*OF PRODUCT TRANSPOSE(A)*A    */MMGT 250
             END,.                                                      MMGT 260
        L,I  =1,.                                                       MMGT 270
NEXTI..                                                                 MMGT 280
        K    =1,.                                                       MMGT 290
NEXTK..                                                                 MMGT 300
        T    =0,.                                                       MMGT 310
        IF OPT='2'                 /*CHECK SPECIFIED MULTIPLIC.   */MMGT 320
        THEN DO J =1 TO JJ,.       /*TRANSPOSE(A)*A IS PERFORMED  */MMGT 330
             T    =T+MULTIPLY(A(J,I),                                   MMGT 340
                  A(J,K),53),.                                          MMGT 350
             END,.                                                      MMGT 360
        ELSE DO J =1 TO JJ,.       /*A*TRANSPOSE(A) IS PERFORMED  */MMGT 370
             T    =T+MULTIPLY(A(I,J),                                   MMGT 380
                  A(K,J),53),.                                          MMGT 390
             END,.                                                      MMGT 400
        S(L) =T,.                  /*STORE RESULTANT ELEMENT S(L) */MMGT 410
        L    =L+1,.                                                     MMGT 420
        IF K LT I                                                       MMGT 430
        THEN DO,.                  /*INCREMENT K                  */MMGT 440
             K    =K+1,.                                                MMGT 450
             GO TO NEXTK,.                                              MMGT 460
             END,.                                                      MMGT 470
        ELSE IF I LT II                                                 MMGT 480
        THEN DO,.                  /*INCREMENT I                  */MMGT 490
             I    =I+1,.                                                MMGT 500
             GO TO NEXTI,.                                              MMGT 510
             END,.                                                      MMGT 520
        ERROR='C',.                /*SUCCESSFUL OPERATION         */MMGT 530
        END,.                                                           MMGT 540
   END,.                           /*END OF PROCEDURE MMGT        */MMGT 550
```

Purpose:

MMGT calculates $A \cdot A^T$ if OPT='1'
$A^T \cdot A$ if OPT='2'

Usage:

CALL MMGT (A, M, N, OPT, S);

A(M, N) - BINARY FLOAT [(53)]
Given M by N matrix.

M - BINARY FIXED
Given row dimension of A.

N - BINARY FIXED
Given column dimension of A.

OPT - CHARACTER(1)
Given option for selection of operation

S(dimension) - BINARY FLOAT [(53)]
Resultant symmetric product matrix, stored in compressed form in a one-dimensional array.
Dimension is M·(M+1)/2 if OPT='1' and N·(N+1)/2 if OPT='2'.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='D' means errors in specified dimensions M, N. Any value of OPT different from '2' is treated as if it were '1'.

Scalar products are accumulated in double-precision arithmetic.

Method:

Standard multiplication is performed; $A \cdot A^T$ is symmetric M by M, while $A^T \cdot A$ is symmetric N by N.

- Subroutine MPRM

```
MPRM..                                                                  MPRM  10
/*************************************************************************/MPRM  20
/*                                                                       */MPRM  30
/*      PERMUTE THE ROWS OR, IF OPT = 'C', THE COLUMNS OF A              */MPRM  40
/*      MATRIX                                                           */MPRM  50
/*                                                                       */MPRM  60
/*************************************************************************/MPRM  70
   PROCEDURE(A,M,N,T,OPT,INV),.                                         MPRM  80
   DECLARE                                                              MPRM  90
         (A(*,*),AJ)                                                    MPRM 100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MPRM 110
/*       BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MPRM 120
         (M,N,T(*),IE,TI,I,J,IA,DI,IT)                                  MPRM 130
         BINARY FIXED,                                                  MPRM 140
         (OPT,INV,ERROR EXTERNAL)CHARACTER(1),.                         MPRM 150
   ERROR='D',.                   /*PRESET ERROR INDICATOR          */MPRM 160
   IF M GT C                     /*TEST SPECIFIED DIMENSIONS       */MPRM 170
   THEN IF N GT C                                                       MPRM 180
   THEN DO,.                                                            MPRM 190
         ERROR='C',.                                                    MPRM 200
         IF OPT='C'              /*IF COLUMNS SHOULD BE MOVED      */MPRM 210
         THEN IE   =N,.          /*SET IE TO NUMBER OF COLUMNS     */MPRM 220
         ELSE IE   =M,.          /*RESP. NUMBER OF ROWS IF NOT     */MPRM 230
         IT   =IE,.                                                     MPRM 240
         DI,IA=1,.                                                      MPRM 250
         IF INV='1'                                                     MPRM 260
         THEN DO,.                                                      MPRM 270
               IA   =IE,.                                               MPRM 280
               IE   =DI,.                                               MPRM 290
               DI   =-DI,.                                              MPRM 300
               END,.                                                    MPRM 310
               DO I =IA TO IE BY DI,.                                   MPRM 320
               TI   =T(I),.          /*SET TI TO T(I)                */MPRM 330
               IF TI NE I            /*IS INTERCHANGE STEP NEEDED    */MPRM 340
               THEN DO,.                                                MPRM 350
                     IF TI GT 0      /*IS ELEMENT OF T VALID         */MPRM 360
                     THEN IF TI LE IT                                   MPRM 370
                     THEN DO,.                                          MPRM 380
                           IF OPT='C'  /*CHECK SPECIFIED OPERATION    */MPRM 390
                                       /*INTERCHANGE COLUMNS I AND TI */MPRM 400
                           THEN DO J =1 TO M,.                          MPRM 410
                                 AJ   =A(J,I),.                         MPRM 420
                                 A(J,I)=A(J,TI),.                       MPRM 430
                                 A(J,TI)=AJ,.                           MPRM 440
                                 END,.                                  MPRM 450
                                       /*INTERCHANGE ROWS I AND TI     */MPRM 460
                           ELSE DO J =1 TO N,.                          MPRM 470
                                 AJ   =A(I,J),.                         MPRM 480
                                 A(I,J)=A(TI,J),.                       MPRM 490
                                 A(TI,J)=AJ,.                           MPRM 500
                                 END,.                                  MPRM 510
                           GOTO END,.                                   MPRM 520
                           END,.                                        MPRM 530
                     ERROR='T',.         /*T CONTAINS INVALID ELEMENTS */MPRM 540
END,.                                                                   MPRM 550
               END,.                                                    MPRM 560
         END,.                                                          MPRM 570
   END,.                                                                MPRM 580
                               /*END OF PROCEDURE MPRM               */MPRM 590
```

Purpose:

MPRM permutes rows (if OPT='R') or columns (if OPT='C') of a given matrix A according to the permutation P (if INV='0') or its inverse P^{-1} (if INV='1'). The permutation P is given in the form of its transposition vector T.

Usage:

CALL MPRM (A, M, N, T, OPT, INV);

A(M, N) - BINARY FLOAT [(53)]
Given M by N matrix.
Resultant matrix.

M - BINARY FIXED
Given number of rows of A.

N - BINARY FIXED
Given number of columns of A.

T(range) - BINARY FIXED
Given transposition vector. Its dimension range equals M if OPT='R' and N if OPT='C'.

OPT - CHARACTER(1)
Given option specifying row or column permutation.

INV - CHARACTER(1)
Given option specifying whether permutation P or inverse permutation P^{-1} is applied.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='D' means error in specified dimensions.
ERROR='T' means invalid transposition vector.

If some element t_i of T does not satisfy $1 \leq t_i \leq$ range (invalid transposition vector), then the value of this element is interpreted as if it were equal to i (no interchange).

Any value of OPT different from 'C' is interpreted as if it were 'R'.

Any value of INV different from '1' is interpreted as if it were '0'.

Method:

Permutation of A is performed by successively interchanging rows (if OPT='R') or columns (if OPT='C'), i and t_i for i = 1 up to range if INV='0' and for i = range down to 1 if INV ='1'.

In case $i = t_i$ no interchange takes place.

Mathematical Background:

The resultant A is calculated as the product

$$I_{m,t_m} \cdot I_{m-1,t_{m-1}} \cdots I_{1,t_1} \cdot A$$

if OPT='R', INV='0'

$$I_{1,t_1} \cdot I_{2,t_2} \cdots I_{m,t_m} \cdot A$$

if OPT='R', INV='1'

$$A \cdot I_{1,t_1} \cdot I_{2,t_2} \cdots I_{n,t_n}$$

if OPT='C', INV='0'

$$A \cdot I_{n,t_n} \cdot I_{n-1,t_{n-1}}, \cdots I_{1,t_1}$$

if OPT='C', INV='1'

For notational details see MPIT.

- Subroutine MTPI

```
MTPI..                                                                  MTPI  10
/*********************************************************************/MTPI  20
/*                                                                   */MTPI  30
/*      CALCULATE PERMUTATION VECTOR (OR ITS INVERSE IF INV ='1')    */MTPI  40
/*      CORRESPONDING TO GIVEN TRANSPOSITION VECTOR                  */MTPI  50
/*                                                                   */MTPI  60
/*********************************************************************/MTPI  70
   PROCEDURE(T,N,INV,P),.                                               MTPI  80
   DECLARE                                                              MTPI  90
        (T(*),N,P(*),I,II,PI,TI,LN)                                     MTPI 100
        BINARY FIXED,                                                   MTPI 110
        (INV,ERROR EXTERNAL)CHARACTER(1),.                              MTPI 120
   I    =0,.                                                            MTPI 130
   II   =1,.                                                            MTPI 140
   LN   =N,.                                                            MTPI 150
   IF LN GT 0                          /*TEST SPECIFIED DIMENSION     */MTPI 160
   THEN DO,.                                                            MTPI 170
NEXTI,.                                /*PRESET PERMUTATION VECTOR    */MTPI 180
        I    =I+1,.                    /*TO IDENTITY PERMUTATION      */MTPI 190
        P(I) =I,.                                                       MTPI 200
        IF I LT N                                                       MTPI 210
        THEN GO TO NEXTI,.                                              MTPI 220
        IF INV NE '1'                  /*SHOULD THE INVERSE PERMUTAT. */MTPI 230
        THEN I    =1,.                 /*VECTOR BE GENERATED          */MTPI 240
        ELSE II   =-II,.                                                MTPI 250
        ERROR='0',.                    /*PRESET ERROR INDICATOR       */MTPI 260
REP,.                                                                   MTPI 270
        TI   =T(I),.                   /*REPLACE TI BY T(I)           */MTPI 280
        IF TI GT 0                     /*IF (I,TI) IS A VALID         */MTPI 290
        THEN IF TI LE LN               /*TRANSPOSITION THEN           */MTPI 300
        THEN DO,.                      /*INTERCHANGE P(I) AND P(TI)   */MTPI 310
             PI   =P(I),.                                               MTPI 320
             P(I) =P(TI),.                                              MTPI 330
             P(TI)=PI,.                                                 MTPI 340
        GOTO STEP,.                                                     MTPI 350
             END,.                                                      MTPI 360
        ERROR='T',.                    /*MARK INVALID TRANSPOSITION   */MTPI 370
STEP,.                                                                  MTPI 380
        I    =I+II,.                                                    MTPI 390
        IF I LE N                      /*HAS I ITS FINAL VALUE        */MTPI 400
        THEN IF I GE 1                                                  MTPI 410
        THEN GO TO REP,.                                                MTPI 420
        END,.                                                           MTPI 430
   ELSE ERROR='D',.                    /*ERROR IN SPECIFIED DIMENSION */MTPI 440
   END,.                               /*END OF PROCEDURE MTPI        */MTPI 450
```

Purpose:

MTPI calculates the permutation vector if INV='0' and the inverse permutation vector if INV='1' from a given transposition vector.

Usage:

CALL MTPI (T, N, INV, P);

T(N) - BINARY FIXED
Given transposition vector.

N - BINARY FIXED
Given dimension of vectors T and P.

INV - CHARACTER(1)
Given option for selection of operation.

P(N) - BINARY FIXED
Resultant vector containing the permutation vector of permutation or inverse permutation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='D' means N is less than 1.
ERROR='T' means T contains elements outside the range (1, N).

A value of INV different from '1' is interpreted as if it were '0'.

Method:

Vector P is preset to the identity permutation $P=(1,\ldots,N)$. Interchanging successively the components i and t_i within P results in the permutation vector belonging to T if i runs from 1 up to N and to the inverse permutation if i runs backward from N down to 1.

Mathematical Background:

See MPIT for notation and definitions on permutation and transposition vectors.

The permutation vector $P=(p_1,\ldots,p_n)$ corresponding to the transposition vector $T=(t_1,\ldots,t_n)$ is defined through:

$$I[k,\ p_k] = I_{n,t_n} \cdot I_{n-1,t_{n-1}} \cdots I_{1,t_1} \cdot I$$

The elementary matrices I_{jk} are symmetric and orthogonal, that is,

$$I_{jk} = I_{jk}^{T} = I_{jk}^{-1}$$

Therefore, the inverse permutation vector is defined by:

$$I[k,q_k] = I_{1,t_1} \cdot I_{2,t_2} \cdots I_{n,t_n} \cdot I$$

Programming Considerations:

For valid transposition vectors it is necessary that $1 \le t_i \le n$ for all $i = 1,2,\ldots,n$. As soon as a given transposition vector is detected nonvalid, the error indicator is set to T and further calculation is bypassed.

• Subroutine MPIT

```
MPIT..                                                                  MPIT  10
/*************************************************************************/MPIT  20
/*                                                                       */MPIT  30
/*      CALCULATE THE INVERSE PERMUTATION VECTOR OR, IF OPT = 'T',       */MPIT  40
/*      THE TRANSPOSITION VECTORS OF THE GIVEN AND INVERSE               */MPIT  50
/*      PERMUTATIONS                                                     */MPIT  60
/*                                                                       */MPIT  70
/*************************************************************************/MPIT  80
   PROCEDURE(P,N,OPT,PI),.                                              MPIT  90
   DECLARE                                                              MPIT 100
         (P(*),N,PI(*),LN,J,P1,P2)                                      MPIT 110
         BINARY FIXED,                                                  MPIT 120
         (OPT,ERROR EXTERNAL)CHARACTER(1),.                             MPIT 130
   LN,J =N,.                                                            MPIT 140
   IF LN GT 0                          /*TEST SPECIFIED DIMENSION      */MPIT 150
   THEN DO,.                                                            MPIT 160
REP..                                                                   MPIT 170
         PI(J)=0,.                     /*PRESET RESULTING VALUES IN    */MPIT 180
         J    =J-1,.                   /*ORDER TO CHECK PERMUTATION    */MPIT 190
         IF J GT 0                                                      MPIT 200
         THEN GO TO REP,.                                               MPIT 210
         ERROR='P',.                   /*PRESET ERROR INDICATOR        */MPIT 220
NEXTJ..                                                                 MPIT 230
         J    =J+1,.                                                    MPIT 240
         P1   =P(J),.                  /*SET P1 TO P(J)                */MPIT 250
         IF P1 LE LN                   /*FEASIBILITY TEST..            */MPIT 260
         THEN IF P1 GT 0               /*IS 1 LE P1 LE N, AND IS       */MPIT 270
         THEN IF PI(P1)=0              /*P1 DIFF. FROM PREVIOUS VALUES */MPIT 280
         THEN DO,.                                                      MPIT 290
              PI(P1)=J,.               /*SET P1-TH ELEMENT OF PI TO J  */MPIT 300
              IF J LT LN               /*HAS J ITS FINAL VALUE         */MPIT 310
              THEN GO TO NEXTJ,.                                        MPIT 320
              ERROR='0',.              /*VALID PERMUTATION VECTOR      */MPIT 330
              IF OPT='T'               /*IF SPECIFIED THEN TRANSPOS.   */MPIT 340
              THEN DO J =1 TO LN,.     /*VECTORS ARE CALCULATED        */MPIT 350
                   P1   =P(J),.                                         MPIT 360
                   P2   =PI(J),.                                        MPIT 370
                   P(P2)=P1,.                                           MPIT 380
                   PI(P1)=P2,.                                          MPIT 390
                   END,.                                                MPIT 400
              END,.                                                     MPIT 410
         END,.                                                          MPIT 420
   ELSE ERROR='D',.                    /*ERROR IN SPECIFIED DIMENSION  */MPIT 430
   END,.                               /*END OF PROCEDURE MPIT         */MPIT 440
```

Purpose:

MPIT calculates the permutation vector corresponding to the inverse of a given permutation if OPT='I' and the transposition vectors of the given permutation and of its inverse if OPT='T'.

Usage:

CALL MPIT (P, N, OPT, PI);

P(N) - BINARY FIXED
Given permutation vector of given permutation.
Resultant transposition vector of given permutation if OPT='T'; otherwise, unchanged.

N - BINARY FIXED
Given dimension of vectors P and PI.

OPT - CHARACTER(1)
Given option for selection of operation.

PI(N) - BINARY FIXED
Resultant permutation vector of inverse permutation if OPT='I' or transposition vector of inverse permutation if OPT='T'.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='D' means N is less than 1.

ERROR='P' means given permutation vector P is not a valid permutation vector. A value of OPT different from 'T' is treated as if it were "I". PI cannot coincide with P in case OPT='I'.

Method:

In case OPT='I' as well as OPT='T' the first step is calculation of the inverse permutation vector PI combined with a check on the feasibility of given permutation vector P.

If OPT='T' a second step is performed which replaces the permutation vectors by the corresponding transposition vectors simultaneously.

Mathematical Background:

Elementary matrices I_{kl}

The elementary matrix I_{kl} is obtained from the identity matrix I by interchanging rows k and l. Multiplication of a matrix A on the left by an I_{kl} of compatible dimensions results in an interchange of rows k and l of A, while multiplication on the right interchanges columns k and l. An interchange of two elements is also called a transposition. Note that I_{kl} is symmetric and orthogonal:

$$I_{kl} = I_{kl}^{T} = I_{kl}^{-1}$$

Permutation vector

Let N* denote the set of integers $\{1, 2, \ldots, n\}$. A permutation is a one-to-one function that maps N* onto N*. It is fully described by the ordered n-tuple $(s_1, s_2, \ldots, s_n)$ called a permutation vector, where $s_i \in N^*$ is the function value corresponding to argument $i \in N^*$. Applying the permutation $(s_1, \ldots, s_n)$ on the rows of the n by n identity matrix I results in an orthogonal matrix $I[k, s_k]$. The notation indicates that the k-th row is identical with the s_k-th row of I for all $k = 1, 2, \ldots, n$.

If an n by n matrix A is multiplied on the left by $I[k, s_k]$, its rows get permuted according to the permutation vector $(s_1, s_2, \ldots, s_n)$.

Permutation of columns is similarly performed multiplying by the permutation matrix $I^T[k, s_k] = I[s_k, k]$ on the right-hand side.

Transposition vector

An n-term product $I_{n,t_n} \cdot I_{n-1,t_{n-1}} \cdots I_{1,t_1}$ corresponds uniquely to a permutation matrix $I[k, s_k]$. The ordered n-tuple $(t_1, t_2, \ldots, t_n)$, which fully describes the above transposition product, is called a transposition vector. The correspondence between permutation vectors and transposition vectors is not one to one: a given permutation vector $(s_1, s_2, \ldots, s_n)$ corresponds to several different transposition vectors if $n > 2$. A uniquely determined transposition vector is obtained under the additional restriction $t_i \geq i$.

The transposition vector comes in naturally when pivoting is used with Gaussian elimination technique. If, at the j-th elimination step, rows j and t_j must be interchanged for $j=1, \ldots, n$, then $(t_1, t_2, \ldots t_n)$ is the transposition vector of the permutation that was applied to the rows of the original matrix. This transposition vector is uniquely determined since $t_i \geq i$.

Permutation vector of the inverse permutation

The inverse P^{-1} of a permutation $P = (p_1, \ldots, p_n)$ has function value i corresponding to argument p_i. Let $Q = (q_1, \ldots, q_n)$ be the permutation vector of P^{-1}. $I[k, p_k]$ is orthogonal -- that is, $I^{-1}[k, p_k] = I^T[k, p_k]$. Therefore, $I[k, q_k] = I[p_k, k]$. Since $I[k, q_k] = I[p_k, q_{p_k}]$, it follows by comparison $q_{p_k} = k$.

Transposition vector of permutation

The calculation of the transposition vector $T = (t_1, t_2, \ldots, t_n)$ corresponding to the permutation vector $P = (p_1, p_2, \ldots, p_n)$ is based on the identity

$$I[k, p_k] \cdot I_{i,\, q_i} = I[k, p_k'] \qquad (1)$$

with $P' = (p_1', \ldots, p_n') = (p_1, \ldots, p_{i-1}, i,$

$$p_{i+1}, \ldots, p_{q_i - 1}, q_i, p_{q_i + 1}, \ldots, p_n)$$

Applying identity (1) successively for $i = 1, 2, \ldots, n$ leads to

$$I[k, p_k] \cdot I_{1,\, t_1} \cdot I_{2,\, t_2} \cdots I_{n,\, t_n} = I$$

or

$$I[k, p_k] = I_{n,t_n} \cdot I_{n-1,t_{n-1}} \cdots I_{2,\, t_2} \cdot I_{1,t_1}$$

It is interesting to note that combining the calculation of transposition vectors of P and P^{-1} greatly improves the efficiency.

Programming Considerations:

The check on validity of the given permutation vector is performed so that all components of the

vector PI are preset to zero. At the i-th step of the calculation of the inverse permutation vector, p_i is checked for $1 \leq p_i \leq n$, and q_{p_i} is checked for zero. If both restrictions are met q_{p_i} is reset to i. Otherwise, the error indicator is set to 'P' and further calculation is bypassed.

- Subroutine MFG

```
MFG..                                                                  MFG   10
/*********************************************************************/MFG   20
/*                                                                   */MFG   30
/*      FACTORIZE A GENERAL NON-SINGULAR MATRIX A INTO A PRODUCT      */MFG   40
/*      OF A LOWER TRIANGULAR MATRIX L AND AN UPPER TRIANGULAR       */MFG   50
/*      MATRIX U OVERWRITTEN ON A, OMITTING UNIT DIAGONAL OF U       */MFG   60
/*                                                                   */MFG   70
/*********************************************************************/MFG   80
  PROCEDURE(A,IPER,N,EPS),.                                            MFG   90
  DECLARE                                                              MFG  100
       ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MFG  110
       EPS BINARY FLOAT,                                               MFG  120
       W BINARY FLOAT(53),                                             MFG  130
       (A(*,*),H,R)                                                    MFG  140
       BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MFG  150
/*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MFG  160
       (IPER(*),I,IND,J,K,L,LN,M,N)                                    MFG  170
       BINARY FIXED,.                                                  MFG  180
  LN   =N,.                                                            MFG  190
  IF LN LE 0                         /*TEST SPECIFIED DIMENSION     */MFG  200
  THEN DO,.                                                            MFG  210
       ERROR='P',.                   /*P MEANS WRONG PARAMETER      */MFG  220
       GO TO RETURN,.                                                  MFG  230
       END,.                                                           MFG  240
  ERROR='0',.                        /*PRESET ERROR INDICATOR       */MFG  250
                                     /*****************************/MFG  260
       DO L =1 TO LN,.               /*CALCULATE SCALING FACTORS    */MFG  270
       R    =0,.                     /*****************************/MFG  280
            DO J =1 TO LN,.          /*COMPUTE ABSOLUTELY GREATEST  */MFG  290
            H    =ABS(A(L,J)),.      /*ELEMENT R IN EACH ROW OF A   */MFG  300
            IF H GT R                                                  MFG  310
            THEN R    =H,.                                             MFG  320
            END,.                                                      MFG  330
       IF R = 0                      /*TEST FOR ZEROS IN ANY ROW    */MFG  340
       THEN DO,.                                                       MFG  350
            ERROR='S',.              /*ANY ROW IN GIVEN MATRIX A    */MFG  360
            GO TO RETURN,.           /*IS ZERO                      */MFG  370
            END,.                                                      MFG  380
                                     /*STORE R IN AN INTEGER VECTOR */MFG  390
       ELSE UNSPEC(IPER(L))=UNSPEC(R),.                                MFG  400
       END,.                         /*****************************/MFG  410
                                     /*GAUSS  ELIMINATION           */MFG  420
       DO L =1 TO LN,.               /*****************************/MFG  430
       UNSPEC(M)='1'B,.              /*PRESET M AS SMALLEST INTEGER */MFG  440
            DO J =L TO LN,.          /*MODIFY COLUMN, SEARCH PIVOT  */MFG  450
            W,H  =A(J,L),.           /*SAVE ELEMENT                 */MFG  460
                 DO K =1 TO L-1,.    /*COMPUTE SCALAR PRODUCTS      */MFG  470
                 W    =W-MULTIPLY(A(J,K),A(K,L),53),.                  MFG  480
                 END,.                                                 MFG  490
            A(J,L)=W,.               /*UPDATE ELEMENT               */MFG  500
            W    =ABS(W),.                                             MFG  510
            UNSPEC(I)=UNSPEC(W),.                                      MFG  520
            I    =I-IPER(J),.        /*DIFFERENCE OF EXPONENTS      */MFG  530
            IF I GT M                /*SEARCH FOR LARGEST DIFFERENCE*/MFG  540
            THEN DO,.                                                  MFG  550
                 IND  =J,.           /*STORE ROW-INDEX              */MFG  560
                 M    =I,.                                             MFG  570
                 R    =H,.           /*SAVE ORIGINAL ELEMENT FOR    */MFG  580
                 END,.               /*TEST ON LOSS OF SIGNIFICANCE */MFG  590
            END,.                                                      MFG  600
       IF IND GT L                   /*IS INTERCHANGE NECESSARY     */MFG  610
       THEN DO,.                                                       MFG  620
            IPER(IND)=IPER(L),.      /*RESTORE PERMUTATION VECTOR   */MFG  630
                 DO J =1 TO LN,.     /*INTERCHANGE ROWS OF MATRIX A */MFG  640
                 H    =A(L,J),.                                        MFG  650
                 A(L,J)=A(IND,J),.                                     MFG  660
                 A(IND,J)=H,.                                          MFG  670
                 END,.                                                 MFG  680
            END,.                                                      MFG  690
       IPER(L)=IND,.                 /*STORE ROW NUMBER             */MFG  700
       H    =A(L,L),.                /*H CONTAINS THE PIVOT         */MFG  710
       IF ABS(H) LE ABS(EPS*R)       /*TEST PIVOT ELEMENT FOR LOSS  */MFG  720
       THEN IF H NE 0                /*OF SIGNIFICANCE AND FOR ZERO */MFG  730
       THEN ERROR='W',.              /*W MEANS WARNING              */MFG  740
       ELSE IF R = 0                 /*IS ORIGINAL ELEMENT ZERO     */MFG  750
       THEN DO,.                                                       MFG  760
            ERROR='S',.              /*CALCULATED PIVOT AND THE     */MFG  770
            GO TO RETURN,.           /*ORIGINAL ELEMENT ARE ZERO    */MFG  780
            END,.                                                      MFG  790
       ELSE DO ,.                    /*CORRECT ZERO PIVOT           */MFG  800
            H    =R*1E-7,.           /*SINGLE PRECISION CORRECTION  */MFG  810
/*          H =R*1E-16,.             /* DOUBLE PRECISION CORRECTION */MFG  820
            ERROR='C',.              /*WARNING AND CORRECTION       */MFG  830
            END,.                                                      MFG  840
            DO J =L+1 TO LN,.        /*EXECUTE LOOP OVER L-TH ROW   */MFG  850
            W    =0,.                                                  MFG  860
                 DO K =1 TO L-1,.    /*CALCULATE SCALAR PRODUCTS    */MFG  870
                 W    =W+MULTIPLY(A(L,K),A(K,J),53),.                  MFG  880
                 END,.                                                 MFG  890
            A(L,J)=(A(L,J)-W)/H,.    /*COMPUTE NEW ELEMENT          */MFG  900
            END,.                                                      MFG  910
       END,.                                                           MFG  920
RETURN,.                                                               MFG  930
  END,.                              /*END OF PROCEDURE MFG         */MFG  940
```

Purpose:

MFG factorizes a general nonsingular matrix A into a product of a lower triangular matrix L and an upper triangular matrix U overwritten on A, omitting the unit diagonal of U.

Usage:

CALL MFG (A, IPER, N, EPS);

A(N, N) - BINARY FLOAT [(53)]
Given two-dimensional array. Resultant calculated triangular factors L and U, where unit diagonal of U is not stored.

IPER(N) - BINARY FIXED
Resultant vector containing the permutations of rows of the matrix.

N - BINARY FIXED
Given order of matrix A.

EPS - BINARY FLOAT
Given relative tolerance for test on loss of significant digits.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' means error in specified dimension $N \leq 0$

ERROR='S' means that any row in the given matrix A is zero or that any calculated pivot and the corresponding original elements are zero; this implies that the given matrix A is singular.

ERROR='G' indicates correction. Any calculated zero pivot is modified to $R \cdot 10^{-7}$ in single precision ($R \cdot 10^{-16}$ in double precision if the corresponding original element R is nonzero).

ERROR='W' indicates a warning. A possible loss of significance may occur.

If at any factorization step the calculated pivot is equal to zero, the corresponding original element R is tested for zero. The given matrix A is interpreted as being singular if R is zero. MFG sets error indicator ERROR to 'S' and further calculation is bypassed. If R is not zero, pivot is corrected to $R \cdot 10^{-7}$ (in double precision $R \cdot 10^{-16}$) and ERROR is set to 'G'.

Method:

Calculation of the triangular factors L and U is done using the standard Gaussian elimination technique. Columnwise pivoting is built in, combined with scaling of rows (equilibration). The upper triangular matrix U is normalized so that the diagonal contains all ones, which are not stored. The given matrix A is overwritten by the resulting triangular factors L and U, omitting the unit diagonal of U.

For reference, see:

H.J. Bowdler, R.S. Martin, G. Peters, J.H. Wilkinson, "Solution of Real and Complex Systems of Linear Equations", Numerische Mathematik, Vol. 8, 1966, pp. 217-234.
A. Ralston and H.S. Wilf, Mathematical Methods for Digital Computers, Vol. 2, 1967, pp. 69-71.

Mathematical Background:

Let A be a nonsingular real matrix of order n. In general, it can be factorized into a product

$$A = L \cdot U$$

where L and U are lower and upper triangular matrices respectively; U is chosen so that it has a unit diagonal.

The elements l_{ik} and u_{ik} of the factor matrices L and U are computed using the following recursive formulas:

$$l_{ik} = a_{ik} - \sum_{m=1}^{k-1} l_{im} \cdot u_{mk} \qquad \begin{Bmatrix} i = 1, 2, \ldots, N \\ k = 1, 2, \ldots, i \end{Bmatrix}$$

$$u_{ik} = \frac{1}{l_{ii}} \left(a_{ik} - \sum_{m=1}^{i-1} l_{im} \cdot u_{mk}\right) \qquad \begin{Bmatrix} i = 1, 2, \ldots, N-1 \\ k = i+1, \ldots, N \end{Bmatrix}$$

Programming Considerations:

Even if the given matrix A is nonsingular and well conditioned, the process can fail when a leading principal submatrix of A is singular; furthermore, the process is numerically unstable whenever a leading principal submatrix is ill conditioned.

In order to avoid these inconveniences, a technique of partial pivoting with an equilibration of the matrix has been introduced in MFG. Initially, the element with greatest absolute value -- say,

W_i (i=1, 2, ..., N), of each row of A is computed. The scaling factors W_i are used as weights for pivoting.

The p-th factorization step is as follows:

1. Computation of the p-th column of L:

$$l_{ip} = a_{ip} - \sum_{m=1}^{p-1} l_{im} \cdot u_{mp}$$

and overwrite l_{ip} on a_{ip} (i = p, p+1, ..., N)

2. Equilibrated partial pivoting:

Choose k so that

$$\frac{|l_{kp}|}{W_k} = \underset{i \geq p}{\text{MAX}} \left\{ \frac{|l_{ip}|}{W_i} \right\}$$

Store the integer k in the vector $IPER_p$ and, if k > p, interchange the k-th and p-th rows. Then l_{pp} is the next pivot.

3. Computation of the p-th row of U:

$$u_{pi} = \frac{1}{l_{pp}} \left(a_{pi} - \sum_{m=1}^{p-1} l_{pm} \cdot u_{mi}\right)$$

and overwrite u_{pi} on a_{pi} (i = p+1, p+2, ..., N)

The diagonal terms of U, which are 1, are not stored. For economy of storage, the scaling weights W_i are initially stored in the vector IPER. This is done using the PL/I function UNSPEC, which stores W_i in internal coded representation. This allows substituting subtractions for divisions in the choice of pivots.

If at factorization step p the pivot l_{pp} becomes zero, the corresponding original element a_{pp} is tested for zero. The given matrix A is interpreted as being singular if a_{pp} is also zero. MFG sets error indicator ERROR to 'S' and further calculation is bypassed. In other cases zero pivot is modified to:

$$l_{pp} = a_{pp} * \left\{ \begin{array}{l} 10^{-7} \text{ in the single precision version} \\ 10^{-16} \text{ in the double precision version} \end{array} \right\}$$

- Subroutine MFS

```
MFS..                                                                  MFS   10
/*********************************************************************/MFS   20
/*                                                                   */MFS   30
/*          FACTORIZE SYMMETRIC POSITIVE DEFINITE MATRIX             */MFS   40
/*                                                                   */MFS   50
/*********************************************************************/MFS   60
   PROCEDURE(A,N,EPS),.                                                MFS   70
   DECLARE                                                             MFS   80
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MFS   90
        EPS BINARY FLOAT,                                              MFS  100
        SUM BINARY FLOAT(53),                                          MFS  110
        A(*)                                                           MFS  120
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MFS  130
/*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MFS  140
        (IND,IB,K,KL,L,N)                                              MFS  150
        BINARY FIXED,.                                                 MFS  160
   IF N LE 0                          /*TEST SPECIFIED DIMENSION     */MFS  170
   THEN DO,.                                                           MFS  180
        ERROR='P',.                   /*P MEANS WRONG PARAMETER      */MFS  190
        GO TO RETURN,.                                                 MFS  200
        END,.                                                          MFS  210
   ERROR='0',.                        /*PRESET ERROR INDICATOR       */MFS  220
   IND  =0,.                          /*INITIALIZE ROW-LOOP          */MFS  230
   IB   =1,.                                                           MFS  240
        DO K =1 TO N,.                /*EXECUTE LOOP OVER ALL ROWS   */MFS  250
        KL   =0,.                                                      MFS  260
LOOP..                                /*PERFORM LOOP WITHIN K-TH ROW */MFS  270
        SUM  =0,.                                                      MFS  280
             DO L =IB TO IND,.        /*CALCULATE SCALAR PRODUCT     */MFS  290
             KL   =KL+1,.                                              MFS  300
             SUM  =SUM+MULTIPLY(A(L),A(KL),53),.                       MFS  310
             END,.                                                     MFS  320
        KL   =KL+1,.                                                   MFS  330
        IND  =IND+1,.                                                  MFS  340
        SUM  =A(IND)-SUM,.                                             MFS  350
        IF IND GT KL                  /*IS A(IND) ON DIAGONAL        */MFS  360
        THEN DO,.                                                      MFS  370
             A(IND)=SUM/A(KL),.       /*CALCULATE NON-DIAGONAL TERM  */MFS  380
             GO TO LOOP,.                                              MFS  390
             END,.                                                     MFS  400
        IF SUM GT 0                   /*TEST SIGN OF RADICAND        */MFS  410
        THEN DO,.                     /*POSITIVE RADICAND            */MFS  420
             IF SUM LE ABS(EPS*A(IND))/*TEST ON LOSS OF SIGNIFICANCE */MFS  430
             THEN ERROR='W',.         /*W MEANS WARNING              */MFS  440
             A(IND)=SQRT(SUM),.       /*CALCULATE NEW DIAGONAL TERM  */MFS  450
             END,.                                                     MFS  460
        ELSE DO,.                     /*NEGATIVE RADICAND            */MFS  470
             ERROR='S',.              /*S MEANS MATRIX A IS NOT      */MFS  480
             N    =K-1,.              /*POSITIVE DEFINITE            */MFS  490
             GO TO RETURN,.           /*REDUCE DIMENSION OF LOWER    */MFS  500
             END,.                    /*TRIANGULAR FACTOR            */MFS  510
        IB   =IB+K,.                                                   MFS  520
        END,.                                                          MFS  530
RETURN..                                                               MFS  540
   END,.                              /*END OF PROCEDURE MFS         */MFS  550
```

Purpose:

MFS computes a triangular factorization of a symmetric positive definite matrix using the square root method of Cholesky.

Usage:

CALL MFS (A, N, EPS);

A(N*(N+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array containing the matrix A stored rowwise in compressed form.
Resultant calculated lower triangular factor T stored rowwise in compressed form.

N - BINARY FIXED
Given order of matrix A.
Resultant order of the triangular factor T.

EPS - BINARY FLOAT
Given relative tolerance for test on loss of significant digits.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The

following constitutes the possible error conditions that may be detected:

ERROR= 'P'	means error in specified dimension: $N \leq 0$
ERROR='S'	means given matrix A is not positive definite, possibly because of severe loss of significance.
ERROR='W'	is a warning. A possible loss of significance could occur.

The lower part of the given symmetric matrix, A, is assumed to be stored in compressed form -- that is, rowwise in N*(N+ 1)/2 successive storage locations. On return the lower triangular factor T is stored in the same way.

Method:

Factorization is done using the square root method of Cholesky, which generates a lower triangular factor matrix T such that

$$T \cdot \text{transpose } (T) = A$$

The given matrix, A, is replaced in core by the resultant matrix, T.

For reference, see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.
A. Ralston and H.S. Wilf, Mathematical Methods for Digital Computers, Vol. 2, 1967, pp. 71-72.

Mathematical Background:

The elements t_{ij} of the lower triangular matrix T are computed using the following recursive formulas:

$$t_{kk} = \sqrt{a_{kk} - \sum_{m=1}^{k-1} t_{km}^2}$$

$$t_{ik} = \frac{a_{ik} - \sum_{m=1}^{k-1} t_{im}\, t_{km}}{t_{kk}},$$

$i = k+1, \ldots, N, \; k=1, \ldots, N$

($\sum_{m=1}^{j}$ is to be interpreted as zero when $j < 1$.)

The determinant of A may be computed by the formula:

$$\det(A) = \prod_{k=1}^{N} t_{kk}^2$$

Programming Considerations:

The given symmetric matrix A is assumed to be stored in compressed form. The resultant lower triangular factor T is returned in the locations of A.

If at factorization step k (k=1, 2, ..., N) the radicand is not positive, the error parameter ERROR is set to 'S', N to k-1, and further calculation is bypassed.

The error parameter ERROR is set to 'W' if any calculated radicand $\bar{r} = r - SUM$ is not greater than $| EPS \cdot r |$, where r is the original diagonal term and SUM a scalar product sum.

It should be noted that Cholesky factorization is done without pivoting.

- Subroutine MFSB

```
MFSB..                                                                  MFSB  10
/*************************************************************************/MFSB  20
/*                                                                       */MFSB  30
/*      FACTORIZE A GIVEN POSITIVE DEFINITE N BY N MATRIX A              */MFSB  40
/*      WITH SYMMETRIC BAND STRUCTURE (NUD UPPER CODIAGONALS)            */MFSB  50
/*                                                                       */MFSB  60
/*************************************************************************/MFSB  70
   PROCEDURE(A,N,NUD,EPS),.                                             MFSB  80
   DECLARE                                                              MFSB  90
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR       */MFSB 100
         EPS BINARY FLOAT,                                              MFSB 110
         SUM BINARY FLOAT(53),                                          MFSB 120
         (A(*,*),PIV)                                                   MFSB 130
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MFSB 140
/*       BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MFSB 150
         (I,ID,J,JEND,K,KK,KEND,                                        MFSB 160
         LN,LNUD,M,N,NC,NR,NUD)                                         MFSB 170
         BINARY FIXED,.                                                 MFSB 180
   LN    =N,.                                                           MFSB 190
   LNUD =NUD,.                                                          MFSB 200
   ERROR='P',.                         /*P MEANS WRONG PARAMETER       */MFSB 210
   IF LNUD LT 0                        /*TEST SPECIFIED NUMBER OF      */MFSB 220
   THEN GO TO RETURN,.                 /*UPPER CODIAGONALS             */MFSB 230
   IF LN LE LNUD                       /*TEST SPECIFIED DIMENSION N    */MFSB 240
   THEN GO TO RETURN,.                                                  MFSB 250
   NR    =LN-LNUD,.                    /*INITIALIZE PARAMETERS         */MFSB 260
   NC,JEND=LNUD+1,.                                                     MFSB 270
         DO I =1 TO LN,.               /*EXECUTE LOOP OVER ALL ROWS    */MFSB 280
         IF I GT NR                    /*MODIFY JEND AT THE END OF     */MFSB 290
         THEN JEND =JEND-1,.           /*THE BAND STRUCTURE            */MFSB 300
         KEND =NC,.                    /*INITIALIZE KEND AND M         */MFSB 310
         M     =NC-I,.                                                  MFSB 320
         IF M GT 0                     /*MODIFY KEND AT THE START OF   */MFSB 330
         THEN KEND =KEND-M,.           /*THE BAND STRUCTURE            */MFSB 340
              DO J =1 TO JEND,.        /*EXECUTE LOOP OVER I-TH ROW    */MFSB 350
              ID   =J-1,.              /*CALULATE INCREMENT ID         */MFSB 360
              KK   =I,.                /*INITIALIZE KK AND SUM         */MFSB 370
              SUM  =0,.                                                 MFSB 380
                   DO K =J+1 TO KEND,. /*COMPUTE SCALAR PRODUCT SUM     */MFSB 390
                   KK   =KK-1,.                                         MFSB 400
                   SUM  =SUM+MULTIPLY(A(KK,K),A(KK,K-ID),53),.          MFSB 410
                   END,.                                                MFSB 420
              SUM  =A(I,J)-SUM,.                                        MFSB 430
              IF J = 1                 /*IS A(I,J) DIAGONAL ELEMENT    */MFSB 440
              THEN IF SUM GT 0         /*TEST FOR LOSS OF SIGNIFICANT  */MFSB 450
              THEN DO,.                /*DIGITS AND COMPUTE NEW TERM   */MFSB 460
                   IF SUM LE ABS(EPS*A(I,J))                            MFSB 470
                   THEN ERROR='W',.                                     MFSB 480
                   PIV,A(I,J)=SQRT(SUM),.                               MFSB 490
                   END,.                                                MFSB 500
              ELSE DO,.                                                 MFSB 510
                   ERROR='S',.         /*A IS NOT POSITIVE DEFINITE    */MFSB 520
                   N     =I-1,.        /*RESET INPUT DIMENSION N       */MFSB 530
                   GO TO RETURN,.                                       MFSB 540
                   END,.                                                MFSB 550
              ELSE A(I,J)=SUM/PIV,.    /*MODIFY NON-DIAGONAL ELEMENT   */MFSB 560
              IF J LE M                                                 MFSB 570
              THEN KEND =KEND+1,.      /*UPDATE KEND IF NECESSARY      */MFSB 580
              END,.                                                     MFSB 590
         END,.                                                          MFSB 600
   ERROR='0',.                         /*SUCCESSFUL OPERATION          */MFSB 610
RETURN,.                                                                MFSB 620
   END,.                               /*END OF PROCEDURE MFSB         */MFSB 630
```

Purpose:

MFSB computes a triangular factorization of a symmetric positive definite band matrix using the square root method of Cholesky.

Usage:

CALL MFSB (A, N, NUD, EPS);

A(N, NUD+1) - BINARY FLOAT [(53)]
Given two-dimensional array containing the upper part of a symmetric band matrix A with NUD upper codiagonals.
Each row starts with its diagonal element.
Resultant calculated upper band factor T.

N - BINARY FIXED
Given number of rows of matrix A.
Resultant number of rows of upper band factor T.

NUD - BINARY FIXED
Given number of upper codiagonals of A.

EPS - BINARY FLOAT
Given relative tolerance for test on loss of significant digits.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' - means error in specified dimensions:
$NUD < 0$ or $N \leq NUD$

ERROR='S' - means any calculated pivot is not positive -- that is, given matrix A is not positive definite. This is possibly due to a severe loss of significance.

ERROR='W' - is a warning indicating possible loss of significance.

The upper part of symmetric band matrix A, consisting of the main diagonal and NUD upper codiagonals, is assumed to be stored rowwise in array A(N, NUD+1) starting with its diagonal elements. Thus, A(i, 1) are the diagonal elements of the given band matrix A (i = 1, 2, ..., N). On return, the upper band factor T is stored in the same way in the locations of A.

Input parameters N and NUD should satisfy the following restrictions:

$0 \leq NUD < N$

Method:

Factorization is done using the square root method of Cholesky. This generates the upper band factor T such that

T · transpose (T) = A

The given A is replaced by the resultant T.

For reference see:

H. Rutishauser, "Algorithmus 1 - Lineares Gleichungssystem mit symmetrischer positiv-definiter Bandmatrix nach Cholesky", Computing (Archives for Electronic Computing), Vol. 1, iss. 1, 1966, pp. 77-78.

Mathematical Background:

For the elements a_{ik} of a symmetric band matrix with NUD upper codiagonals, the following is true:

$$a_{ik} = 0 \quad \text{if} \quad |i - k| > NUD$$

The elements t_{ik} of the upper factorized matrix T are computed using the following recursive formula:

$$t_{ik} = \frac{1}{t_{ii}} \left[a_{ik} - \sum_{m=m_0}^{i-1} t_{mi} \cdot t_{mk} \right]$$

$$m_0 = \max (1, k-NUD) \quad i=1, 2, \ldots, N$$
$$k=i+1, \ldots,$$
$$\min (i + NUD, N)$$

(any symbol $\sum_{m=m_0}^{r} X_m$ is to be interpreted as zero if $r < m_0$)

In the special case i = k (diagonal elements), the above equation may be written:

$$t_{kk} = \sqrt{a_{kk} - \sum_{m=m_0}^{k-1} t_{mk}^2} \; ;$$

$$k = 1, 2, \ldots, N \quad m_0 = \max (1, k-NUD)$$

The resultant upper factor T has band structure again, because the following is true:

$$t_{ik} = 0 \quad \text{if} \quad k > i + NUD$$

Programming Considerations:

The upper part of the symmetric positive definite band matrix A, consisting of the main diagonal and NUD upper codiagonals, is assumed to be stored rowwise in the two-dimensional array A(N, NUD+1) such that A(i, 1) are the diagonal elements (i=1, 2, ..., N). Therefore, the elements A(i, k) of array A with i+k > N are irrelevant; they are not touched within MFSB. The resultant upper band factor T is returned in the locations of A.

If, at factorization step m(m=1, 2, ..., N), the radicand is not positive, error parameter ERROR is set to 'S', dimension N to m - 1, and further calculation is bypassed.

The error character is set to 'W' if any calculated radicand $\bar{r} = r -$ SUM is positive but no longer greater than $|EPS \cdot r|$, where r means the original diagonal term and SUM a scalar product sum.

The input parameters N and NUD must satisfy the restriction:

$$0 \leq NUD < N$$

Otherwise, ERROR is set to 'P'.

It should be noted that Cholesky's factorization is done without pivoting.

• Subroutine MFGR

```
MFGR..                                                              MFGR  10
/*******************************************************************/MFGR  20
/*                                                                 */MFGR  30
/*      FOR A GIVEN M BY N MATRIX A THE FOLLOWING CALCULATIONS     */MFGR  40
/*      ARE PERFORMED                                              */MFGR  50
/*      (1) DETERMINE RANK AND LINEARLY INDEPENDENT ROWS AND       */MFGR  60
/*          COLUMNS  (BASIS)                                       */MFGR  70
/*      (2) FACTORIZE A SUBMATRIX OF MAXIMAL RANK                  */MFGR  80
/*      (3) EXPRESS NON-BASIC ROWS IN TERMS OF BASIC ONES          */MFGR  90
/*      (4) EXPRESS BASIC VARIABLES IN TERMS OF FREE ONES          */MFGR 100
/*                                                                 */MFGR 110
/*******************************************************************/MFGR 120
   PROCEDURE(A,M,N,EPS,IRANK,IROW,ICOL),.                           MFGR 130
   DECLARE                                                          MFGR 140
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR    */MFGR 150
        EPS BINARY FLOAT,                                           MFGR 160
        SUM BINARY FLOAT(53),                                       MFGR 170
        (A(*,*),HOLD,PIV,SAVE,TOL,WORK)                             MFGR 180
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MFGR 190
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MFGR 200
        (ICOL(*),IROW(*),I,IC,IR,                                   MFGR 210
        IND,IRANK,J,K,LM,LN,M,N)                                    MFGR 220
        BINARY FIXED,.                                              MFGR 230
   LM   =M,.                                                        MFGR 240
   LN   =N,.                                                        MFGR 250
   ERROR='P',.                        /*P MEANS WRONG INPUT       */MFGR 260
   IF LM LT 1                         /*TEST OF DIMENSION M       */MFGR 270
   THEN GO TO RETURN,.                                              MFGR 280
   IF LN LT 1                         /*TEST OF DIMENSION N       */MFGR 290
   THEN GO TO RETURN,.                                              MFGR 300
   ERROR='0',.                        /*PRESET ERROR INDICATOR    */MFGR 310
                                      /*INIT. COLUMN INDEX VECTOR */MFGR 320
   PIV  =0,.                          /*SEARCH FIRST PIVOT ELEMENT*/MFGR 330
        DO J =1 TO LN,.               /*EXECUTE LOOP OVER COLUMNS */MFGR 340
        ICOL(J)=J,.                                                 MFGR 350
             DO I =1 TO LM,.          /*EXECUTE LOOP OVER ALL ROWS*/MFGR 360
             HOLD =A(I,J),.                                         MFGR 370
             IF ABS(HOLD) GT ABS(PIV)                               MFGR 380
             THEN DO,.                                              MFGR 390
                  PIV  =HOLD,.        /*SAVE VALUE AND INDEX OF THE*/MFGR 400
                  IR   =I,.           /*ABSOLUTELY GREATEST ELEMENT*/MFGR 410
                  IC   =J,.                                         MFGR 420
                  END,.                                             MFGR 430
             END,.                                                  MFGR 440
        END,.                                                       MFGR 450
        DO I =1 TO LM,.               /*INITIALIZE ROW INDEX VECTOR*/MFGR 460
        IROW(I)=I,.                                                 MFGR 470
        END,.                                                       MFGR 480
   TOL  =ABS(EPS*PIV),.               /*SET UP INTERNAL TOLERANCE */MFGR 490
   IRANK=0,.                          /*********************************/MFGR 500
        DO J =1 TO LN,.               /*GAUSS  ELIMINATION        */MFGR 510
        IF ABS(PIV) LE TOL            /*********************************/MFGR 520
        THEN GO TO ROW,.              /*PIVOT IS NOT FEASIBLE     */MFGR 530
        IRANK=J,.                     /*UPDATE RANK               */MFGR 540
        IF IR GT IRANK                /*SHOULD ROWS BE INTERCHANGED*/MFGR 550
        THEN DO,.                                                   MFGR 560
                  DO I =1 TO LN,.     /*INTERCHANGE ROWS          */MFGR 570
                  SAVE =A(IRANK,I),.                                MFGR 580
                  A(IRANK,I)=A(IR,I),.                              MFGR 590
                  A(IR,I)=SAVE,.                                    MFGR 600
                  END,.                                             MFGR 610
             IND  =IROW(IR),.         /*UPDATE ROW INDEX VECTOR   */MFGR 620
             IROW(IR)=IROW(IRANK),.                                 MFGR 630
             IROW(IRANK)=IND,.                                      MFGR 640
             END,.                                                  MFGR 650
        IF IC GT IRANK                /*SHOULD COLUMNS BE INTER-  */MFGR 660
        THEN DO,.                     /*CHANGED                   */MFGR 670
                  DO I =1 TO LM,.     /*INTERCHANGE COLUMNS       */MFGR 680
                  SAVE =A(I,IRANK),.                                MFGR 690
                  A(I,IRANK)=A(I,IC),.                              MFGR 700
                  A(I,IC)=SAVE,.                                    MFGR 710
                  END,.                                             MFGR 720
             IND  =ICOL(IC),.         /*UPDATE COLUMN INDEX VECTOR*/MFGR 730
             ICOL(IC)=ICOL(IRANK),.                                 MFGR 740
             ICOL(IRANK)=IND,.                                      MFGR 750
             END,.                                                  MFGR 760
        IND  =IRANK+1,.               /*INITIALIZE LOOP FOR TRANS-*/MFGR 770
        SAVE =PIV,.                   /*FORMING CURRENT SUBMATRIX */MFGR 780
        PIV  =0,.                     /*AND SEARCHING NEXT PIVOT  */MFGR 790
             DO I =IND TO LM,.                                      MFGR 800
             HOLD,A(I,IRANK)=A(I,IRANK)/SAVE,.                      MFGR 810
                  DO K =IND TO LN,.                                 MFGR 820
                  WORK,A(I,K)=A(I,K)-HOLD*A(IRANK,K),.              MFGR 830
                                      /*SEARCH NEXT PIVOT ELEMENT */MFGR 840
                  IF ABS(WORK) GT ABS(PIV)                          MFGR 850
                  THEN DO,.                                         MFGR 860
                       PIV  =WORK,.   /*SAVE VALUE AND INDEX OF THE*/MFGR 870
                       IR   =I,.      /*ABSOLUTELY GREATEST ELEMENT*/MFGR 880
                       IC   =K,.                                    MFGR 890
                       END,.                                        MFGR 900
                  END,.                                             MFGR 910
             END,.                                                  MFGR 920
        END,.                         /*********************************/MFGR 930
ROW..                                 /*COMPUTE ROW DEPENDENCIES  */MFGR 940
   IF IRANK= LM                       /*********************************/MFGR 950
   THEN GO TO HOM,.                   /*ALL ROWS ARE BASIC ONES   */MFGR 960
        DO J =IRANK-1 TO 1 BY -1,.    /*SET UP MATRIX EXPRESSING  */MFGR 970
        IR   =J+1,.                   /*ROW DEPENDENCIES          */MFGR 980
             DO I =IND TO LM,.        /*LOOP FOR NON-BASIC ROWS   */MFGR 990
             SUM  =0,.                                              MFGR1000
                  DO K =IR TO IRANK,. /*CALCULATE SCALAR PRODUCTS */MFGR1010
                  SUM  =SUM+MULTIPLY(A(I,K),A(K,J),53),.            MFGR1020
                  END,.                                             MFGR1030
             A(I,J)=A(I,J)-SUM,.      /*MODIFY ELEMENT            */MFGR1040
             END,.                                                  MFGR1050
        END,.                         /*********************************/MFGR1060
HOM..                                 /*COMPUTE HOMOGENEOUS SOLUTION */MFGR1070
   IF IRANK= LN                       /*********************************/MFGR1080
   THEN GO TO RETURN,.                /*ALL COLUMNS ARE BASIC ONES*/MFGR1090
                                      /*SET UP MATRIX EXPRESSING  */MFGR1100
        DO J =IRANK TO 1 BY -1,.      /*BASIC VARIABLES IN TERMS OF*/MFGR1110
        IR   =J+1,.                   /*FREE PARAMETERS           */MFGR1120
             DO I =IND TO LN,.        /*LOOP FOR FREE COLUMNS     */MFGR1130
             SUM  =0,.                                              MFGR1140
                  DO K =IR TO IRANK,. /*CALCULATE SCALAR PRODUCTS */MFGR1150
                  SUM  =SUM+MULTIPLY(A(J,K),A(K,I),53),.            MFGR1160
                  END,.                                             MFGR1170
             A(J,I)=-(A(J,I)+ SUM)/A(J,J),.                         MFGR1180
             END,.                                                  MFGR1190
        END,.                                                       MFGR1200
RETURN..                                                            MFGR1210
   END,.                              /*END OF PROCEDURE MFGR     */MFGR1220
```

Purpose:

For a given general rectangular matrix, MFGR performs the following:

1. Determines rank and linearly independent rows and columns (basis)
2. Factorizes a submatrix of maximal rank
3. Expresses nonbasic rows in terms of basic rows
4. Expresses basic variables in terms of free variables

Usage:

CALL MFGR(A, M, N, EPS, IRANK, IROW, ICOL);

A(M, N) - BINARY FLOAT [(53)]
Given general matrix with M rows and N columns.
Resultant calculated triangular factors L, U and submatrices C, H, D.

M - BINARY FIXED
Given number of rows of matrix A.

N - BINARY FIXED
Given number of columns of matrix A.

EPS - BINARY FLOAT
Given relative tolerance for test on zero.

IRANK - BINARY FIXED
Resultant rank of given matrix.

IROW(M) - BINARY FIXED
Resultant vector containing the subscripts of basic rows in IROW(1) up to IROW(IRANK).

ICOL(N) - BINARY FIXED
Resultant vector containing the subscripts of basic columns in ICOL(1) up to ICOL(IRANK).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='P' means error in specified dimensions: $M \leq 0$ and/or $N \leq 0$

Calculation of the rank of given matrix A is most critical. It is not claimed that MFGR will give the correct rank in all cases, because of the intrinsic difficulty caused by performing calculations with a finite number of digits.

Suggested range for values of EPS is (10^{-4}, 10^{-6}) in single precision and (10^{-8}, 10^{-15}) in double precision.

Method:

Calculation of the rank IRANK and of the triangular factors L and U is done using the standard Gaussian elimination technique with complete pivoting. The lower triangular matrix L is normalized so that the diagonal contains all ones, which are not stored. The subdiagonal part of L and the upper triangular factor U are stored in the locations of the given matrix A.

In case A is singular, the triangular factors L and U only of a submatrix of maximal rank are retained. The remaining parts of the resultant matrix give the dependencies of rows and columns and the solution of the homogeneous matrix equation $A \cdot X = 0$.

For reference see:

A. S. Householder, The Theory of Matrices in Numerical Analysis, 1965, pp. 125-130.

Mathematical Background:

Interchange information

Gauss elimination with complete pivoting implies that the rows and columns of the given M by N matrix A are interchanged at each elimination step if necessary. The interchange information is recorded in two integer vectors IROW and ICOL:

The i-th $\left\{\begin{matrix}\text{row}\\\text{column}\end{matrix}\right\}$ of the interchanged matrix corresponds

to the $\left\{\begin{matrix}\text{IROW(i)-th row}\\\text{ICOL(i)-th column}\end{matrix}\right\}$ in the original matrix, where initially

$$\text{IROW(i)=i and ICOL(i)=i for i} = \left\{\begin{matrix}1,2,\ \ldots,\ M\\1,2,\ \ldots,\ N\end{matrix}\right\}$$

At the i-th elimination step the interchanged matrix is denoted by A^i.

First elimination step

After pivoting, the interchanged matrix A^1 is uniquely expressed as:

$$A^1 = L^1 \cdot D^1 \cdot U^1$$

by imposing the following conditions:

1. U^1 is the N by N identity matrix except for the first row.
2. L^1 is the M by M identity matrix except for the first column. The first diagonal element has a value of one.
3. D^1 is an M by N matrix with first diagonal element equal to one, while all remaining elements of the first row and column are equal to zero.

Partitioning of matrices A^1, L^1, D^1, U^1 leads to:

$$\begin{pmatrix} a^1_{11} & A^1_{12} \\ A^1_{21} & A^1_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ L^1_{21} & I \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & D^1_{22} \end{pmatrix} \cdot \begin{pmatrix} u^1_{11} & U^1_{12} \\ 0 & I \end{pmatrix}$$

where:

$$a^1_{11} = u^1_{11}$$

$$A^1_{12} = U^1_{12}$$

$$A^1_{21} = L^1_{21} \cdot u^1_{11}$$

$$A^1_{22} = L^1_{21} \cdot U^1_{12} + D^1_{22}$$

This implies the following:

1. The elements of the first column of U^1 are

$$u^1_{1k} = a^1_{1k} \quad (k = 1, 2, 3, \ldots, N)$$

2. The elements of the first column of L^1 are

$$l^1_{11} = 1 \ ; \ l^1_{i1} = \frac{a^1_{i1}}{a^1_{11}} \quad (i = 2, 3, \ldots, M)$$

3. The elements of submatrix D^1_{22} of D^1 are

$$d^1_{ik} = a^1_{ik} - l^1_{i1} \cdot u^1_{1k} = a^1_{ik} - \frac{a^1_{i1} \cdot a^1_{ik}}{a^1_{11}}$$

$i = 2, 3, \ldots, M$
$k = 2, 3, \ldots, N$

Note that it is possible to record all nontrivial information about L^1, D^1, U^1 in the storage locations originally occupied by A, storing only:

$$\begin{pmatrix} u^1_{11} & U^1_{12} \\ L^1_{21} & D^1_{22} \end{pmatrix}$$

Second elimination step

Assume D^1_{22} is not zero in the sense that all its elements are absolutely greater than an internal tolerance TOL. The complete pivoting in D^1_{22} implies that matrix A^1 possibly is interchanged, giving A^2:

$$A^2 = \begin{pmatrix} 1 & 0 \\ L^2_{21} & I \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & D^2_{22} \end{pmatrix} \cdot \begin{pmatrix} u^1_{11} & U^2_{12} \\ 0 & I \end{pmatrix}$$

Now D^2_{22} may be expressed uniquely in the form:

$$D^2_{22} = \begin{pmatrix} 1 & 0 \\ L^2_{32} & I \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & D^2_{33} \end{pmatrix} \cdot \begin{pmatrix} u^2_{22} & U^2_{23} \\ 0 & I \end{pmatrix}$$

It is easily seen that

$$A^2 = L^2 \cdot D^2 \cdot U^2$$

where

$$L^2 = \begin{pmatrix} 1 & 0 & 0 \\ l^2_{21} & 1 & 0 \\ L^2_{31} & L^2_{32} & I \end{pmatrix}$$

$$D^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & D^2_{33} \end{pmatrix}$$

$$U^2 = \begin{pmatrix} u^1_{11} & u^2_{12} & U^2_{13} \\ 0 & u^2_{22} & U^2_{23} \\ 0 & 0 & I \end{pmatrix}$$

Final elimination step

At the next step D^2_{33} is factorized, and so on. Now assume that $D^r_{r+1,\ r+1}$ equals zero -- that is, that all its elements are absolutely less than or equal to TOL. This is interpreted as matrix A has the rank r and the result is the factorization:

$$A^r = L^r \cdot D^r \cdot U^r$$

Neglecting the small elements in $D^r_{r+1,\ r+1}$ this may be written as:

$$A^r = \begin{pmatrix} L \\ LR \end{pmatrix} \cdot (U,\ UR)$$

with

$$L = \begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & 0 \\ l^2_{21} & 1 & & & & 0 \\ \cdot & \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ l^r_{r1} & l^r_{r2} & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} u^1_{11} & u^2_{12} & \cdot & \cdot & \cdot & u^r_{1r} \\ 0 & u^2_{22} & \cdot & & & u^r_{2r} \\ \cdot & \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & u^r_{rr} \end{pmatrix}$$

$$LR = (L^r_{r+1,\ 1},\ L^r_{r+1,\ 2},\ \ldots,\ L^r_{r+1,\ r})$$

$$UR = \begin{pmatrix} U^r_{1,\,r+1} \\ U^r_{2,\,r+1} \\ \cdot \\ \cdot \\ \cdot \\ U^r_{r,\,r+1} \end{pmatrix}$$

L is a lower triangular matrix of order r with unit diagonal.

U is an r by r upper triangular matrix.

LR is an (M-r) by r matrix; if the given matrix A is row regular (that is, r=M), LR is absent in the final factorization.

UR is an r by (N-r) matrix; if the given matrix A is column regular (that is, r = N), UR is absent in the final factorization.

Further calculations

The problem of matrix factorization arises in connection with the solution of systems of equations $A \cdot X = R$. Three different cases must be distinguished:

1. $r = M = N$

   A is nonsingular, and $A \cdot X = R$ has a unique solution.

2. $r < M$

   A is not row regular; solutions of $A \cdot X = R$ exist only if the linear combinations among the rows of A are also valid among the rows of R.

3. $r < N$

   A is not column regular; $A \cdot X = 0$ has nontrivial solutions.

The cases (2) and (3) may occur together. The solution, if it exists, is uniquely determined for r=N; otherwise, it contains N-r free parameters. It is quite natural to ask for the linear combinations among the rows and columns of given matrix A and for the linear forms expressing basic variables in terms of free variables. Therefore, instead of LR and UR, matrices C and H, containing linear combinations, are returned.

Observe carefully that the calculated factorization belongs to the interchanged matrix A^r. Therefore, we use $A^r \cdot X^r = R^r$ instead of $A \cdot X = R$.

Let X^r, R^r be partitioned into $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ and $\begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$.

Then, from $A^r \cdot X^r = R^r$ is obtained:

$$\begin{pmatrix} L \\ LR \end{pmatrix} \cdot (U,\ UR) \cdot \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$$

More explicitly:

$$L \cdot U \cdot X_1 + L \cdot UR \cdot X_2 = R_1$$

$$LR \cdot U \cdot X_1 + LR \cdot UR \cdot X_2 = R_2$$

Since L and U are nonsingular, this implies that:

$$X_1 = U^{-1} \cdot L^{-1} R_1 - U^{-1} \cdot UR \cdot X_2$$

$$R_2 = LR \cdot L^{-1} \cdot R_1$$

For the user's convenience:

LR is replaced by $C_1 = LR \cdot L^{-1}$

UR is replaced by $H = -U^{-1} \cdot UR$

while L and U remain unchanged.

For consistency it is necessary to set $R_2 = C_1 \cdot R_1$ and to obtain homogeneous solutions from the equation:

$$X_1 = H \cdot X_2$$

In case of a consistent system of equations $A^r \cdot X^r = R^r$, the general solution is:

$$X^r = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \text{ with } X_1 = U^{-1} \cdot L^{-1} \cdot R_1 + H \cdot X_2$$

while the values of the free variables contained in X_2 may be chosen arbitrarily.

Programming Considerations:

Let a_{ik} be the absolutely greatest element of the original matrix A, which is found first in column-wise scan. The internal tolerance TOL is set equal to $|\,EPS \cdot a_{ik}\,|$.

If, at the m-th elimination step, the absolutely greatest element of $D^{m-1}_{m,m}$ is less than or equal to TOL, the submatrix $D^{m-1}_{m,m}$ is interpreted as being

the zero matrix. Then m-1 is returned as rank of the given matrix A and further factorization is bypassed.

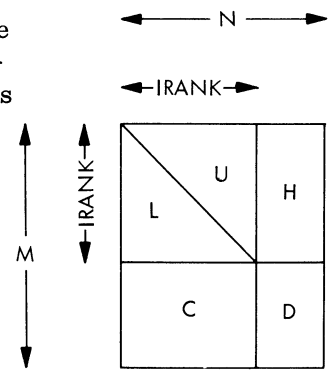
The calculated factorization belongs to the interchanged matrix A^r. Therefore, we deal with $A^r \cdot X^r = R^r$ instead of $A \cdot X = R$, where:

$\begin{Bmatrix} X^r \\ R^r \end{Bmatrix}$ is obtained from $\begin{Bmatrix} X \\ R \end{Bmatrix}$ using the

$\begin{Bmatrix} ICOL(k) \\ IROW(i) \end{Bmatrix}$ element of $\begin{Bmatrix} X \\ R \end{Bmatrix}$ as $\begin{Bmatrix} k\text{-th} \\ i\text{-th} \end{Bmatrix}$ element of $\begin{Bmatrix} X^r \\ R^r \end{Bmatrix}$

with k = 1, 2, ..., N and i = 1, 2, ..., M.

Within the storage area originally occupied by the input matrix A, procedure MFGR returns, in a compact scheme, the matrices L, U, C, H, and D (see diagram).



Numerical example

$$\text{Let } A = \begin{pmatrix} 1 & 2 & 1 \\ 2 & 2 & 4 \\ 2 & 4 & 2 \\ 1 & 4 & -1 \end{pmatrix}, \quad EPS = 1E\text{-}5$$

Procedure MFGR returns L, U, C, H, and D:

$$L = \begin{pmatrix} 1 & 0 \\ 0.5 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 4 & 2 \\ 0 & 3 \end{pmatrix},$$

$$C = \begin{pmatrix} 0.5 & 0 \\ 1.5 & -1 \end{pmatrix}, \quad H = \begin{pmatrix} -0.33333325 \\ -0.33333331 \end{pmatrix}, \quad D = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and combines them in the following compact scheme:

$$\begin{pmatrix} 4 & 2 & -0.33333325 \\ 0.5 & 3 & -0.33333331 \\ 0.5 & 0 & 0 \\ 1.5 & -1 & 0 \end{pmatrix}$$

and IRANK = 2
IROW = (3, 2, 1, 4)
ICOL = (2, 3, 1)

From information in C, IRANK, IROW we get the linear dependencies among rows:

row(1) = 0.5 · row(3) + 0 · row(2)
row(4) = 1.5 · row(3) - 1 · row(2)

From information in H, IRANK, ICOL we get the homogeneous solution of $A \cdot X = 0$: $X_1 = H \cdot X_2$:

$x_2 = -0.33333325\ x_1$
$x_3 = -0.33333331\ x_1$

and with

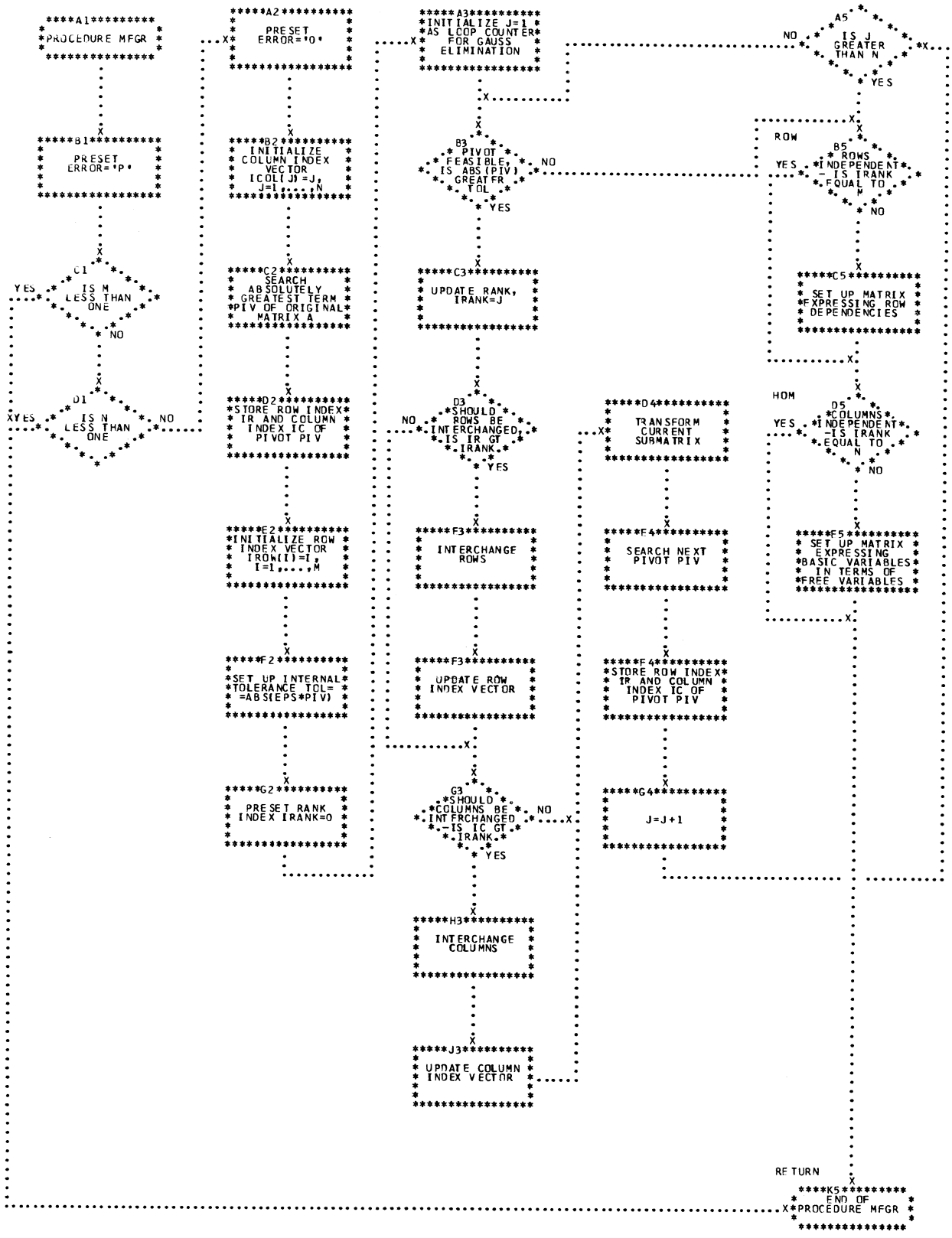
column (1) · x_1 + column (2) · x_2 + column (3) · x_3 = 0, the linear dependencies among columns:

column (1) = 0.33333325 · column (2)
+0.33333331 · column (3).

Multiplying the triangular factors L, U we get:

$$L \cdot U = \begin{pmatrix} a_{32} & a_{33} \\ a_{22} & a_{23} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 4 \end{pmatrix}$$

FOR A GIVEN GENERAL RECTANGULAR MATRIX MFGR PERFORMS THE FOLLOWING
DETERMINES RANK AND LINEARLY INDEPENDENT ROWS AND COLUMNS (BASIS), FACTORIZES A SUBMATRIX OF MAXIMAL RANK,
EXPRESSES NONBASIC ROWS IN TERMS OF BASIC ROWS, EXPRESSES BASIC VARIABLES IN TERMS OF FREE VARIABLES.



- Subroutine MDLS/MDRS

```
MDLS..                                                                  MDLS  10
/*************************************************************************/MDLS  20
/*                                                                       */MDLS  30
/*      FOR AN EQUATION SYSTEM  A*X=R  WITH SYMMETRIC POSITIVE           */MDLS  40
/*      DEFINITE MATRIX  A=T*TRANSPOSE(T)  CALCULATE OPTIONALLY          */MDLS  50
/*           SOLUTION X                                                  */MDLS  60
/*           INVERSE(T) * R                                              */MDLS  70
/*           TRANSPOSE(INVERSE(T)) * R                                   */MDLS  80
/*      FOR GIVEN TRIANGULAR FACTOR T AND RIGHT HAND SIDE MATRIX R       */MDLS  90
/*                                                                       */MDLS 100
/*************************************************************************/MDLS 110
   PROCEDURE(F,M,N,A,OPT),.                                             MDLS 120
   DECLARE                                                              MDLS 130
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MDLS 140
         (OPT,COPT) CHARACTER(1),      /*OPTION PARAMETER              */MDLS 150
         SUM BINARY FLOAT(53),                                          MDLS 160
         (R(*,*),A(*))                                                  MDLS 170
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION   /*S*/MDLS 180
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION   /*D*/MDLS 190
         (I,IEND,II,IIA,IID,IIST,IK,                                    MDLS 200
         IKA,IKD,IKST,J,JEND,K,L,LD,                                    MDLS 210
         LX,LDX,M,MSTA,MDEL,MX,N)                                       MDLS 220
         BINARY FIXED,.                                                 MDLS 230
                                       /*****************************/MDLS 240
   IID,IKA=1,.                         /*INITIALIZE PARAMETERS FOR     */MDLS 250
   IKD,IIA=0,.                         /*DIVISION FROM LEFT            */MDLS 260
   IEND =N,.                           /*****************************/MDLS 270
   JEND =M-1,.                                                          MDLS 280
   GO TO BOTH,.                                                         MDLS 290
MDRS..                                                                  MDLS 300
/*************************************************************************/MDLS 310
/*                                                                       */MDLS 320
/*      FOR AN EQUATION SYSTEM  X*A=R  WITH SYMMETRIC POSITIVE           */MDLS 330
/*      DEFINITE MATRIX  A=T*TRANSPOSE(T)  CALCULATE OPTIONALLY          */MDLS 340
/*           SOLUTION X                                                  */MDLS 350
/*           R * TRANSPOSE(INVERSE(T))                                   */MDLS 360
/*           R * INVERSE(T)                                              */MDLS 370
/*      FOR GIVEN TRIANGULAR FACTOR T AND RIGHT HAND SIDE MATRIX R       */MDLS 380
/*                                                                       */MDLS 390
/*************************************************************************/MDLS 400
   ENTRY(R,M,N,A,OPT),.                                                 MDLS 410
                                       /*****************************/MDLS 420
   IID,IKA=0,.                         /*INITIALIZE PARAMETERS FOR     */MDLS 430
   IKD,IIA=1,.                         /*DIVISION FROM RIGHT           */MDLS 440
   IEND =M,.                           /*****************************/MDLS 450
   JEND =N-1,.                                                          MDLS 460
BOTH..                                                                  MDLS 470
   ERROR='P',.                         /*P MEANS WRONG PARAMETER       */MDLS 480
   IF IEND LE 0                        /*TEST INPUT DIMENSIONS M AND N*/MDLS 490
   THEN GO TO RETURN,.                                                  MDLS 500
   IF JEND LT 0                                                         MDLS 510
   THEN GO TO RETURN,.                                                  MDLS 520
   IIST,IKST=1,.                                                        MDLS 530
   COPT =OPT,.                                                          MDLS 540
   IF COPT= '2'                        /*TEST SPECIFIED OPERATION      */MDLS 550
   THEN GO TO NEW,.                                                     MDLS 560
                                       /*****************************/MDLS 570
   LX   =0,.                           /*INITIALIZATION FOR  A*X = R   */MDLS 580
   MSTA,MDEL,MX,LD=1,.                 /*AND FOR  X*TRANSPOSE(A) = R   */MDLS 590
                                       /*****************************/MDLS 600
MAIN..                                 /*EXECUTE DIVISION PROCESS      */MDLS 610
         DO J =0 TO JEND,.                                              MDLS 620
         II   =IIST,.                  /*INITIALIZE ADDRESSING VALUES */MDLS 630
         IK   =IKST,.                                                   MDLS 640
              DO I =1 TO IEND,.        /*EXECUTE LOOP OVER COLUMNS     */MDLS 650
              SUM  =0,.                /*OR ROWS OF MATRIX R           */MDLS 660
              L    =MSTA,.                                             MDLS 670
              LDX  =LD,.                                               MDLS 680
                   DO K =1 TO J,.      /*COMPUTE SCALAR PRODUCT SUM    */MDLS 690
                   SUM  =SUM+MULTIPLY(A(L),R(II,IK),53),.               MDLS 700
                   L    =L+LDX,.                                        MDLS 710
                   LDX  =LDX+LX,.      /*UPDATE ADDRESSING PARAMETERS */MDLS 720
                   II   =II+IID,.                                       MDLS 730
                   IK   =IK+IKD,.                                       MDLS 740
                   END,.                                                MDLS 750
              IF A(L)= 0               /*IS DIAGONAL TERM IN A ZERO    */MDLS 760
              THEN DO,.                                                 MDLS 770
                   ERROR='S',.         /*S MEANS ZERO DIAGONAL TERM    */MDLS 780
                   GO TO RETURN,.      /*IN TRIANGULAR FACTOR A        */MDLS 790
                   END,.                                                MDLS 800
                                       /*CALCULATE NEW ELEMENT         */MDLS 810
              ELSE R(II,IK)=(R(II,IK)-SUM)/A(L),.                       MDLS 820
              II   =IIST+IIA*I,.                                        MDLS 830
              IK   =IKST+IKA*I,.       /*UPDATE ADDRESSING PARAMETERS */MDLS 840
              END,.                                                     MDLS 850
         MSTA =MSTA+MDEL,.             /*MODIFY START PARAMETERS       */MDLS 860
         MDEL =MDEL+MX,.                                                MDLS 870
         END,.                                                          MDLS 880
   IF COPT NE '1'                      /*TEST END OF OPERATION         */MDLS 890
   THEN                                                                 MDLS 900
NEW..                                  /*****************************/MDLS 910
         DO,.                          /*INITIALIZATION FOR  X*A = R   */MDLS 920
         COPT ='1',.                   /*AND FOR  TRANSPOSE(A)*X = R   */MDLS 930
         MX   =0,.                     /*****************************/MDLS 940
         LX   =1,.                                                      MDLS 950
         MDEL =-1,.                                                     MDLS 960
         LD   =-JEND,.                                                  MDLS 970
         MSTA =(JEND+1)*(JEND+2)/2,.                                    MDLS 980
         IID  =-IID,.                                                   MDLS 990
         IKD  =-IKD,.                                                   MDLS1000
         IF IIA= 0                     /*SHOULD DIVISION FROM LEFT     */MDLS1010
         THEN IIST =M,.                /*BE EXECUTED                   */MDLS1020
         ELSE IKST =N,.                                                 MDLS1030
         GO TO MAIN,.                  /*GO TO MAIN PART OF MDLS       */MDLS1040
         END,.                                                          MDLS1050
   ERROR='0',.                         /*SUCCESSFUL OPERATION          */MDLS1060
RETURN..                                                                MDLS1070
   END,.                               /*END OF PROCEDURE MDLS         */MDLS1080
```

Purpose:

For a system of equations AX = R with symmetric positive definite matrix A = T • T^T, MDLS performs the following calculations depending on the character of the input parameter OPT:

OPT = '1'	R is replaced by T^{-1} • R
OPT = '2'	R is replaced by $(T^{-1})^T$ • R
otherwise	R is replaced by $(T \cdot T^T)^{-1}$ • R

Usage:

CALL MDLS (R, M, N, A, OPT);

R(M,N) - BINARY FLOAT [(53)]
Given general right-hand-side matrix with M rows and N columns.
Resultant solution depending on the option parameter OPT.

M - BINARY FIXED
Given number of rows of matrix R and the order of matrix A.

N - BINARY FIXED
Given number of columns of matrix R.

A(M*(M+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array containing lower triangular matrix T stored rowwise in compressed form (possibly resultant array A of SSP procedure MFS).

OPT - CHARACTER (1)
Given option parameter for selection of operation. (See "Purpose" above.)

Purpose:

For a system of equations XA = R with symmetric positive definite matrix A = T • T^T, MDRS performs the following calculations, depending on the character of an input parameter OPT:

OPT = '1'	R is replaced by R • $(T^{-1})^T$
OPT = '2'	R is replaced by R • T^{-1}
otherwise	R is replaced by R • $(T \cdot T^T)^{-1}$

Usage:

CALL MDRS (R, M, N, A, OPT);

R(M, N) - BINARY FLOAT [(53)]
Given general right-hand-side matrix with M rows and N columns.
Resultant solution depending on the option parameter OPT.

M - BINARY FIXED
Given number of rows of matrix R

N - BINARY FIXED
Given number of columns of matrix R and the order of matrix A.

A(N*(N+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array containing lower triangular matrix T stored rowwise in compressed form (possibly resultant array A of SSP procedure MFS).

OPT - CHARACTER (1)
Given option parameter for selection of operation (see "Purpose", above).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' - means error in specified dimensions: $M \leq 0$ and/or $N \leq 0$

ERROR='S' - means given triangular factor T has at least one diagonal term (pivot) equal to zero -- that is, matrix A is not positive definite.

The given lower triangular factor T is assumed to be stored in compressed form, that is, rowwise in successive K*(K+1)/2 storage locations, where K is the number of rows (or columns) implied by compatibility:

K = M in procedure MDLS
K = N in procedure MDRS

During calculation the lower triangular matrix T is not changed. The right-hand-side matrix R is replaced by the solution depending on the character of parameter OPT.

Method:

It is supposed that the symmetric positive definite matrix A is given in the factored form (Cholesky):

$$A = T \cdot T^T$$

where T is the lower triangular factor (possibly calculated by SSP procedure MFS) and T^T the transpose of T.

The required calculations are done using forward and/or backward substitutions.

Mathematical Background:

Calculation of $X = T^{-1} \cdot R$ is done using forward substitution to obtain X from $T \cdot X = R$.

Calculation of $Y = (T^{-1})^T \cdot R$ is done using backward substitution to obtain Y from $T^T \cdot Y = R$.

Calculation of $Z = (T \cdot T^T)^{-1} \cdot R$ is done by first solving $T \cdot X = R$ and then solving $T^T \cdot Z = X$.

Calculation of $X = R(T^{-1})^T$ is done using forward substitution to obtain X from $X \cdot T^T = R$.

Calculation of $Y = R \cdot T^{-1}$ is done using backward substitution to obtain Y from $Y \cdot T = R$.

Calculation of $Z = R \cdot (T \cdot T^T)^{-1}$ is done by first solving $X \cdot T^T = R$ and then solving $Z \cdot T = X$.

Programming Considerations:

The given lower triangular matrix T is assumed to be stored rowwise in successive storage locations. During calculation, T is not changed, while the right-hand-side matrix R is replaced by the solution depending on parameter OPT. If any diagonal element (pivot) of T is zero, the error parameter ERROR is set to 'S' and further calculation is bypassed. Any zero pivot in T means that the matrix $A = T \cdot T^T$ is not positive definite, possibly because of severe loss of significance in the factorization routine.

- Subroutine MDSB

```
MDSB..                                                                  MDSB  10
/*************************************************************************/MDSB  20
/*                                                                       */MDSB  30
/*      FOR AN EQUATION SYSTEM  A*X=R  WITH SYMMETRIC POSITIVE           */MDSB  40
/*      DEFINITE  BAND  MATRIX   A=TRANSPOSE(T)*T   CALCULATE            */MDSB  50
/*      OPTIONALLY                                                       */MDSB  60
/*           SOLUTION X                                                  */MDSB  70
/*           TRANSPOSE(INVERSE(T)) * R                                   */MDSB  80
/*           INVERSE(T) * R                                              */MDSB  90
/*      FOR GIVEN UPPER BAND FACTOR T AND GENERAL RIGHT HAND             */MDSB 100
/*      SIDE MATRIX R                                                    */MDSB 110
/*                                                                       */MDSB 120
/*************************************************************************/MDSB 130
   PROCEDURE(A,R,N,NUD,M,OPT),.                                         MDSB 140
   DECLARE                                                              MDSB 150
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MDSB 160
         (OPT,COPT) CHARACTER(1),      /*OPTION PARAMETER              */MDSB 170
         SUM BINARY FLOAT(53),                                          MDSB 180
         (A(*,*),R(*,*),H)                                              MDSB 190
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MDSB 200
/*       BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MDSB 210
         (I,ISTA,IEND,INCR,J,K,                                         MDSB 220
         KEND,KI,KINC,KK,L,LM,                                          MDSB 230
         LN,LNUD,M,N,NC,NR,NUD)                                         MDSB 240
         BINARY FIXED,.                                                 MDSB 250
   LN    =N,.                        /*STORE VARIABLES N, NUD, M,    */MDSB 260
   LNUD =NUD,.                       /*OPT FROM CALLING SEQUENCE     */MDSB 270
   LM    =M,.                        /*INTO LOCAL PARAMETERS         */MDSB 280
   COPT =OPT,.                                                          MDSB 290
   ERROR='P',.                       /*P MEANS WRONG INPUT           */MDSB 300
   IF LNUD LT 0                      /*TEST SPECIFIED INPUT PARA-    */MDSB 310
   THEN GO TO RETURN,.               /*METERS NUD, N, M              */MDSB 320
   IF LN LE LNUD                                                        MDSB 330
   THEN GO TO RETURN,.               /*PROCEDURE RETURNS IF AT       */MDSB 340
   IF LM LT 0                        /*LEAST ONE OF THE PARAMETERS   */MDSB 350
   THEN GO TO RETURN,.               /*NUD, N, M IS WRONG            */MDSB 360
                                     /*                              */MDSB 370
   NC    =LNUD+1,.                   /*NC AND NR ARE MARKS FOR BEGIN*/MDSB 380
   NR    =LN-LNUD,.                  /*AND END OF THE BAND STRUCTURE*/MDSB 390
   IF COPT= '2'                      /*SHOULD R BE DIVIDED BY T ONLY*/MDSB 400
   THEN GO TO UPPER,.                /*****************************/MDSB 410
   ISTA,INCR=1,.                     /*INITIALIZATION FOR            */MDSB 420
   IEND =LN,.                        /*TRANSPOSE(T) * X = R          */MDSB 430
   KINC =-1,.                        /*****************************/MDSB 440
MAIN..                                                                  MDSB 450
         DO I =ISTA TO IEND BY INCR,. /*EXECUTE LOOP OVER ALL ROWS   */MDSB 460
         H     =A(I,1),.             /*STORE I-TH DIAGONAL ELEMENT   */MDSB 470
         IF H = 0                    /*AND TEST IT FOR ZERO          */MDSB 480
         THEN DO,.                                                      MDSB 490
              ERROR='S',.            /*S MEANS ANY PIVOT IS ZERO     */MDSB 500
              GO TO RETURN,.                                            MDSB 510
              END,.                                                     MDSB 520
         KEND =NC,.                 /*KEND IS END VALUE OF THE      */MDSB 530
         IF INCR= 1                 /*INNERMOST DO-COUNTER K        */MDSB 540
         THEN L     =NC-I,.         /*L IF DIVISION BY TRANSP(T)    */MDSB 550
         ELSE L     =I-NR,.         /*L IF DIVISION BY MATRIX T     */MDSB 560
         IF L GT 0                                                      MDSB 570
         THEN KEND =KEND-L,.        /*MODIFY KEND                   */MDSB 580
              DO J =1 TO LM,.       /*LOOP OVER THE M COLUMNS OF R  */MDSB 590
              SUM  =R(I,J),.        /*INITIALIZE SUM                */MDSB 600
              KI,KK=I,.                                                 MDSB 610
                   DO K =2 TO KEND,. /*COMPUTE SCALAR PRODUCT SUM   */MDSB 620
                   KI    =KI+KINC,.                                   MDSB 630
                   KK    =KK-INCR,.                                   MDSB 640
                   SUM   =SUM-MULTIPLY(A(KI,K),R(KK,J),53),.          MDSB 650
                   END,.                                              MDSB 660
              R(I,J)=SUM/H,.        /*DIVIDE SUM BY DIAGONAL TERM   */MDSB 670
              END,.                 /*AND STORE IT BACK             */MDSB 680
         END,.                                                          MDSB 690
   IF COPT= '1'                     /*TEST END OF OPERATION         */MDSB 700
   THEN DO,.                                                            MDSB 710
         ERROR='0',.                /*SUCCESSFUL DIVISION           */MDSB 720
         GO TO RETURN,.                                                 MDSB 730
         END,.                                                          MDSB 740
UPPER..                             /*****************************/MDSB 750
   COPT ='1',.                      /*INITIALIZATION FOR  T * X = R*/MDSB 760
   ISTA =LN,.                       /*****************************/MDSB 770
   INCR =-1,.                                                           MDSB 780
   IEND =1,.                                                            MDSB 790
   KINC =0,.                                                            MDSB 800
   GO TO MAIN,.                     /*BRANCH TO THE MAIN LOOPS      */MDSB 810
RETURN..                                                                MDSB 820
   END,.                            /*END OF PROCEDURE MDSB         */MDSB 830
```

Purpose:

Depending on the character of the input parameter OPT, MDSB performs the following operations on a system of equations A • X = R with symmetric positive definite band matrix:

$A = T^T \cdot T$

OPT = '1' R is replaced by $(T^{-1})^T \cdot R$

OPT = '2' R is replaced by $T^{-1} \cdot R$

otherwise R is replaced by $(T^T \cdot T)^{-1} \cdot R$

Usage:

CALL MDSB (A, R, N, NUD, M, OPT);

A(N, NUD+1) - BINARY FLOAT [(53)]
Given two-dimensional array containing the upper band factor T stored rowwise such that A(i, 1) are the diagonal elements (i = 1, 2, ... N). This could be the resultant array A from SSP procedure MFSB.

R(N, M) - BINARY FLOAT [(53)]
Given general right-hand-side matrix with N rows and M columns. Resultant solution depending on option parameter OPT.

N - BINARY FIXED
Given number of rows of matrices R and A.

NUD - BINARY FIXED
Given number of upper codiagonals of symmetric matrix A.

M - BINARY FIXED
Given number of columns of matrix R.

OPT - CHARACTER (1)
Given option parameter for selection of operation (see "Purpose").

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' - Indicates an error in specified dimension: NUD <0 or N ≤ NUD

ERROR='S' - means the given band factor T has at least one diagonal term (pivot) equal to zero -- that is, matrix A is not positive definite.

Upper factor matrix T, consisting of main diagonal and NUD upper codiagonals, is assumed to be stored rowwise in array A(N, NUD+1) such that A(i, 1) are the diagonal elements of T (i=1,2,...,N). SSP procedure MFSB provides upper band factor T in its resultant array A, which may be used directly for input in MDSB.

During calculation in MDSB, the band matrix T is not changed. The right-hand-side matrix R is replaced by a solution depending on the input

character of parameter OPT. Input values N and NUD should satisfy the restriction

$$0 \leq NUD < N$$

Method:

Depending on the actual character of OPT, division of R by T^T and/or T is performed using forward and/or backward substitutions. The result is returned in the locations of R.

For reference see:

R. S. Martin and J. H. Wilkinson, "Solution of Symmetric and Unsymmetric Band Equations and the Calculation of Eigenvectors of Band Matrices", Numerische Mathematik, Vol. 9, iss. 4, 1967, pp. 279-301.

H. Rutishauser, "Algorithmus 1-Lineares Gleichungssystem mit symmetrischer positiv-definiter Bandmatrix nach Cholesky", Computing (Archives for Electronic Computing), Vol. 1, iss. 1, 1966, pp. 77-78.

Mathematical Background:

The given elements of the upper factor matrix T are to be stored rowwise in array A so that A(i, 1) are the diagonal elements of T (i = 1, 2, ..., N).

Calculation of $X = (T^{-1})^T \cdot R$ is done using forward substitution to obtain X from $T^T \cdot X = R$ and satisfying the following recursive scheme:

$$x_{ik} = \frac{1}{a_{ik}} \left[r_{ik} - \sum_{m=m_0}^{i-1} a_{m,i+1-m} \cdot x_{mk} \right]$$

$$m_0 = \max (1, i - NUD); \quad \begin{matrix} i = 1, 2, \ldots, N \\ k = 1, 2, \ldots, M \end{matrix}$$

(Any symbol $\sum_{m=m_0}^{r} c_m$ is to be interpreted as zero if $r < m_0$.)

After each x_{ik} is computed, it is stored in the location r_{ik}. Analogously, computing $Y = T^{-1} \cdot R$ is the same as solving the equation $T \cdot Y = R$ for Y. This is done using backward substitution in a similar recursive scheme:

$$y_{ik} = \frac{1}{a_{ik}} \left[r_{ik} - \sum_{m=2}^{m_0} a_{im} \cdot y_{i-1+m,k} \right]$$

$$m_0 = \min (NUD + 1, N + 1 - i)$$

$$\begin{matrix} i = N, N-1, \ldots, 1 \\ k = 1, 2, \ldots, M \end{matrix}$$

Calculation of $Z = A^{-1} \cdot R = (T^T \cdot T)^{-1} \cdot R$ is done by first computing X from $T^T \cdot X = R$ and overwriting on R, then solving $T \cdot Z = X$, again in the locations of R. If R is equal to the unit matrix, this process replaces R with the inverse A^{-1} of A. It should be noted that in general A^{-1} is no longer a band matrix.

Programming Considerations:

The upper band factor matrix T is assumed to be stored rowwise in the two-dimensional array A(N, NUD+1) such that A(i, 1) are the diagonal elements of T (i = 1, 2, ..., N). Therefore, the elements A(i,k) of array A with i + k > N are irrelevant and not used within MDSB.

During calculation, the upper band factor T is not changed, while the right-hand-side matrix R is replaced by a solution depending on the character of parameter OPT.

If any diagonal element A(i, 1) of factor T is zero, the error parameter ERROR is set to 'S' and further calculation is bypassed. Any zero pivot of T means that matrix $A = T^T \cdot T$ is not positive definite. This is possibly due to severe loss of significance in the factorization routine.

If the SSP procedure MFSB provides the factor matrix T directly as input for MDSB, the resultant error indicator ERROR from MFSB should be tested.

- Subroutine MDLG

```
MDLG..                                                                  MDLG  10
/*************************************************************************/MDLG  20
/*                                                                       */MDLG  30
/*      FOR AN EQUATION SYSTEM  A*X=R  WITH GENERAL NON-SINGULAR         */MDLG  40
/*      MATRIX  A=L*U  CALCULATE OPTIONALLY                              */MDLG  50
/*           SOLUTION X                                                  */MDLG  60
/*           INVERSE(L) * R                                              */MDLG  70
/*           INVERSE(U) * R                                              */MDLG  80
/*      FOR GIVEN TRIANGULAR FACTORS L, U AND RIGHT HAND SIDE R          */MDLG  90
/*                                                                       */MDLG 100
/*************************************************************************/MDLG 110
   PROCEDURE(A,R,IPER,N,M,OPT),.                                         MDLG 120
   DECLARE                                                               MDLG 130
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR        */MDLG 140
        OPT CHARACTER(1),             /*OPTION PARAMETER                 */MDLG 150
        SUM BINARY FLOAT(53),                                            MDLG 160
        (A(*,*),R(*,*),H)                                                MDLG 170
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MDLG 180
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MDLG 190
        (IPER(*),I,IS,J,                                                 MDLG 200
        K,LM,LN,M,N)                                                     MDLG 210
        BINARY FIXED,.                                                   MDLG 220
   LM   =M,.                                                             MDLG 230
   LN   =N,.                                                             MDLG 240
   ERROR='P',.                        /*P MEANS WRONG INPUT            */MDLG 250
   IF LN LE 0                         /*TEST SPECIFIED PARAMETER N     */MDLG 260
   THEN GO TO RETURN,.                                                   MDLG 270
   IF LM LE 0                         /*TEST SPECIFIED PARAMETER M     */MDLG 280
   THEN GO TO RETURN,.                                                   MDLG 290
   ERROR='0',.                        /*PRESET ERROR INDICATOR         */MDLG 300
   IF OPT= '2'                        /*SHOULD R BE DIVIDED BY U ONLY  */MDLG 310
   THEN GO TO UPPER,.                 /*******************************/MDLG 320
                                      /*LOOP FOR DIVISION BY LOWER     */MDLG 330
        DO I =1 TO LN,.               /*TRIANGULAR MATRIX L            */MDLG 340
        H    =A(I,I),.                /*******************************/MDLG 350
        IF H = 0                      /*IS ANY DIAGONAL ELEMENT ZERO   */MDLG 360
        THEN DO,.                                                        MDLG 370
             ERROR='S',.              /*S MEANS ANY PIVOT IS ZERO      */MDLG 380
             GO TO RETURN,.                                              MDLG 390
             END,.                    /*FOR PERMUTATION OF ROWS OF     */MDLG 400
        IS   =IPER(I),.               /*RIGHT HAND SIDE ARRAY R        */MDLG 410
             DO K =1 TO LM,.          /*LOOP OVER THE M COLUMNS OF R   */MDLG 420
             SUM  =R(IS,K),.          /*INITIALIZE SUM                 */MDLG 430
             R(IS,K)=R(I,K),.         /*RESTORE ROWS OF ARRAY R        */MDLG 440
                  DO J =1 TO I-1,.    /*COMPUTE SCALAR PRODUCT SUM     */MDLG 450
                  SUM  =SUM-MULTIPLY(A(I,J),R(J,K),53),.                 MDLG 460
                  END,.                                                  MDLG 470
             R(I,K)=SUM/H,.           /*DIVIDE SUM BY DIAGONAL TERM    */MDLG 480
             END,.                    /*AND STORE RESULT               */MDLG 490
        END,.                                                            MDLG 500
   IF OPT= '1'                        /*TEST END OF OPERATION          */MDLG 510
   THEN GO TO RETURN,.                /*******************************/MDLG 520
                                      /*LOOP FOR DIVISION BY UPPER     */MDLG 530
UPPER..                               /*TRIANGULAR MATIX U             */MDLG 540
        DO I =LN-1 TO 1 BY -1,.       /*******************************/MDLG 550
             DO K =1 TO LM,.          /*LOOP OVER THE M COLUMNS OF R   */MDLG 560
             SUM  =R(I,K),.           /*INITIALIZE SUM                 */MDLG 570
                  DO J =I+1 TO LN,.   /*COMPUTE SCALAR PRODUCT SUM     */MDLG 580
                  SUM  =SUM-MULTIPLY(A(I,J),R(J,K),53),.                 MDLG 590
                  END,.                                                  MDLG 600
             R(I,K)=SUM,.             /*STORE RESULT                   */MDLG 610
             END,.                                                       MDLG 620
        END,.                                                            MDLG 630
RETURN..                                                                 MDLG 640
   END,.                              /*END OF PROCEDURE MDLG          */MDLG 650
```

Purpose:

For a system of equations $A \cdot X = R$, where $A = L \cdot U$ is a general nonsingular matrix, MDLG performs the following calculations, depending on the character of an input parameter OPT:

OPT = '1'	R is replaced by $L^{-1} \cdot R$
OPT = '2'	R is replaced by $U^{-1} \cdot R$
otherwise	R is replaced by $(L \cdot U)^{-1} \cdot R$

Usage:

CALL MDLG (A, R, IPER, N, M, OPT);

A(N, N) - BINARY FLOAT [(53)]
Given two-dimensional array containing lower and upper triangular matrices L and U where the unit diagonal of U is omitted.

R(N, M) - BINARY FLOAT [(53)]
Given general right-hand-side matrix with N rows and M columns.
Resultant solution depending on the option parameter OPT.

IPER(N) - BINARY FIXED
Given integer vector containing the permutations of rows of the matrix A in factorization steps.

N - BINARY FIXED
Given order of matrix A and number of rows of matrix R.

M - BINARY FIXED
Given number of columns of matrix R.

OPT - CHARACTER (1)
Given option parameter for selection of operation (see "Purpose").

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' - means error in specified dimensions: $M \leq 0$ and/or $N \leq 0$

ERROR='S' - means that a diagonal element (pivot) in the given lower triangular matrix L is zero; further calculation is bypassed.

The given matrix A is assumed to be factorized into a product of a lower triangular matrix L and an upper triangular matrix U using partial pivoting with row interchanges, where L and U are overwritten on A, omitting the unit diagonal of U. Details of the row interchanges are to be stored in the vector IPER. This required factorization may be obtained using the SSP procedure MFG. The resulting arrays A and IPER are used as input for MDLG.

During calculation in MDLG the arrays A and IPER are not changed. The right-hand-side matrix R is replaced by a solution depending on the character of parameter OPT.

Method:

The required calculations are performed using forward and/or backward substitutions, where the interchange information is combined with the lower triangular matrix L.

Mathematical Background:

Suppose a general nonsingular matrix A of order n is factored into the form:

$$A = P \cdot L \cdot U$$

where L is the lower triangular matrix, U the upper triangular matrix with unit diagonal, and P the permutation matrix corresponding to the integer vector

IPER. Then $X = L^{-1} \cdot P^{-1} \cdot R = L^{-1} \cdot \bar{R}$ is calculated using forward substitution to obtain X from $L \cdot X = P^{-1} \cdot R = \bar{R}$. $\bar{R}$ is obtained from R by interchanging rows in the same way as the rows of matrix A are interchanged during partial pivoting in any factorization routine (for example, MFG).

To calculate $Y = U^{-1} \cdot R$ backward substitution is used in obtaining Y from $U \cdot Y = R$. Calculation of $Z = U^{-1} \cdot L^{-1} \cdot P^{-1} \cdot R = U^{-1} \cdot L^{-1} \cdot \bar{R}$ is done by first solving $L \cdot X = \bar{R}$ and then solving $U \cdot Z = X$.

Programming Considerations:

Matrix A is assumed to be given in the factored form:

$$A = P \cdot L \cdot U$$

where the lower triangular matrix L and the upper triangular matrix U are overwritten on A, omitting the unit diagonal of U. The permutation matrix P is obtained by interchanging the rows of an n by n unit matrix according to information stored in the vector IPER.

- Subroutine MIG

```
MIG..                                                                  MIG   10
/*********************************************************************/MIG   20
/*                                                                   */MIG   30
/*      INVERT A FACTORIZED GENERAL MATRIX A.                        */MIG   40
/*      A MUST BE FACTORIZED INTO THE FORM A = L*U, WHERE THE        */MIG   50
/*      UPPER TRIANGULAR MATRIX U CONTAINS THE UNIT DIAGONAL         */MIG   60
/*      WHICH IS NOT STORED.                                         */MIG   70
/*                                                                   */MIG   80
/*********************************************************************/MIG   90
   PROCEDURE(A,IPER,N),.                                               MIG  100
   DECLARE                                                             MIG  110
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR     */MIG  120
         SUM BINARY FLOAT(53),                                         MIG  130
         (A(*,*),PIV)                                                  MIG  140
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MIG  150
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MIG  160
         (IPER(*),I,J,K,LN,M,MN,N)                                     MIG  170
         BINARY FIXED,.                                                MIG  180
   LN    =N,.                                                          MIG  190
   MN    =LN-1,.                                                       MIG  200
   IF LN LE 0                          /*TEST SPECIFIED PARAMETER N   */MIG  210
   THEN DO,.                                                           MIG  220
         ERROR='P',.                   /*P MEANS WRONG INPUT          */MIG  230
         GO TO RETURN,.                                                MIG  240
         END,.                         /*****************************/MIG  250
                                       /*INVERT LOWER TRIANG. MATRIX L*/MIG  260
         DO I =0 TO MN,.               /*****************************/MIG  270
         M    =I+1,.                                                   MIG  280
         PIV  =A(M,M),.                                                MIG  290
         IF PIV= 0                     /*IS ANY DIAGONAL ELEMENT ZERO */MIG  300
         THEN DO,.                                                     MIG  310
               ERROR='S',.             /*S MEANS NEXT PIVOT ELEMENT   */MIG  320
               GO TO RETURN,.          /*IS ZERO                      */MIG  330
               END,.                                                   MIG  340
         PIV,A(M,M)=1/PIV,.            /*CALCULATE NEW DIAGONAL TERM  */MIG  350
               DO J =1 TO I,.          /*EXECUTE LOOP IN M-TH ROW     */MIG  360
               SUM  =0,.                                               MIG  370
                     DO K =J TO I,.    /*COMPUTE SCALAR PRODUCT SUM   */MIG  380
                     SUM  =SUM+MULTIPLY(A(M,K),A(K,J),53),.            MIG  390
                     END,.                                             MIG  400
               A(M,J)=-SUM*PIV,.       /*CALCULATE AND STORE NEW TERM */MIG  410
               END,.                                                   MIG  420
         END,.                         /*****************************/MIG  430
                                       /*INVERT UPPER TRIANG. MATRIX U*/MIG  440
         DO I =MN TO 1 BY -1,.         /*****************************/MIG  450
         M    =I+1,.                                                   MIG  460
               DO J =LN TO M BY -1,.   /*EXECUTE LOOP IN I-TH ROW     */MIG  470
               SUM  =A(I,J),.                                          MIG  480
                     DO K =M TO J-1,.  /*COMPUTE SCALAR PRODUCT SUM   */MIG  490
                     SUM  =SUM+MULTIPLY(A(I,K),A(K,J),53),.            MIG  500
                     END,.                                             MIG  510
               A(I,J)=-SUM,.           /*STORE NEW VALUE              */MIG  520
               END,.                                                   MIG  530
         END,.                         /*****************************/MIG  540
                                       /*MULTIPLY  INVERSE(U)*INV(L)  */MIG  550
         DO I =1 TO MN,.               /*****************************/MIG  560
         M    =I+1,.                                                   MIG  570
               DO J =1 TO LN,.         /*EXECUTE LOOP IN I-TH ROW     */MIG  580
               IF J LE I                                               MIG  590
               THEN SUM  =A(I,J),.     /*FOR LOWER TRIANGULAR PART    */MIG  600
               ELSE DO,.                                               MIG  610
                     SUM  =0,.         /*IF ELEMENT A(I,J) BELONGS TO */MIG  620
                     M    =J,.         /*THE UPPER TRIANGULAR PART OF */MIG  630
                     END,.             /*MATRIX A                     */MIG  640
                                       /*COMPUTE SCALAR PRODUCT SUM   */MIG  650
                     DO K =M TO LN,.   /*OF I-TH ROW WITH J-TH COLUMN */MIG  660
                     SUM  =SUM+MULTIPLY(A(I,K),A(K,J),53),.            MIG  670
                     END,.                                             MIG  680
               A(I,J)=SUM,.            /*STORE RESULT                 */MIG  690
               END,.                                                   MIG  700
         END,.                         /*****************************/MIG  710
                                       /*RE-INTERCHANGE COLUMNS OF A  */MIG  720
         DO I =MN TO 1 BY -1,.         /*****************************/MIG  730
         M    =IPER(I),.                                               MIG  740
         IF M GT I                     /*SHOULD RE-INTERCHANGE BE DONE*/MIG  750
         THEN DO,.                                                     MIG  760
               DO J =1 TO LN,.         /*INTERCHANGE COLUMN I WITH    */MIG  770
               PIV  =A(J,I),.          /*COLUMN IPER(I)               */MIG  780
               A(J,I)=A(J,M),.                                         MIG  790
               A(J,M)=PIV,.                                            MIG  800
               END,.                                                   MIG  810
         END,.                                                         MIG  820
      END,.                                                            MIG  830
RETURN..                                                               MIG  840
   END,.                             /*END OF PROCEDURE MIG         */MIG  850
```

Purpose:

MIG inverts a general nonsingular matrix A, which is given in the factored form:

$$A = L \cdot U$$

where the upper triangular matrix U contains the unit diagonal, which is not stored.

Usage:

CALL MIG (A, IPER, N);

A(N, N) - BINARY FLOAT [(53)]
Given two-dimensional array containing lower and upper triangular factors L and

U, where the unit diagonal of U is not stored (possibly resultant array A of SSP procedure MFG).
Resultant calculated inverse of matrix A.

IPER(N) - BINARY FIXED
Given vector contains the permutations of rows of the matrix in factorization steps.

N - BINARY FIXED
Given order of matrix A.

Remarks:

ERROR='P' - means error in specified dimension: $N \leq 0$

ERROR='S' - means that a diagonal element (pivot) in the given lower triangular matrix L is zero; further calculation is bypassed.

Method:

It is required that the general nonsingular matrix A be given in the factored form:

$$A = L \cdot U$$

where L means the lower triangular matrix and U the upper triangular matrix with unit diagonal. L and the superdiagonal part of U are stored in the storage locations of A, which may be factored by SSP procedure MFG.

In the first step MIG inverts L, giving L^{-1}, which is overwritten on L. In the second step U^{-1} is calculated and stored in U. Then U^{-1} is multiplied by L^{-1}, giving, in an order determined by pivoting, the columns of A^{-1}. These, finally, are reordered to produce A^{-1}.

For reference see:

A. S. Householder, The Theory of Matrices in Numerical Analysis, 1965, pp. 125-130.
A. Ralston and H. S. Wilf, Mathematical Methods for Digital Computers, Vol. 2, 1967, pp. 69-71.
R. Zurmühl, Matrizen, 1964, pp. 75-77.

Mathematical Background:

Suppose A, a general nonsingular matrix of order N, is factored into the form:

$$A = P \cdot L \cdot U$$

where L is the lower triangular matrix, U the upper triangular matrix with unit diagonal, and P the row-permutation matrix (unit matrix with interchanged rows) resulting from partial pivoting in any factorization routine. Then A^{-1} is calculated in four steps:

1. The elements $\bar{l}_{ik}$ of L^{-1} are computed from the elements l_{ik} of L with the following recursive formulas:

$$\bar{l}_{ik} = -\frac{1}{l_{ii}} \sum_{m=k}^{i-1} l_{im} \cdot \bar{l}_{mk} \qquad i>k$$

$$\bar{l}_{ik} = \frac{1}{l_{ii}} \qquad i=k$$

$$\bar{l}_{ik} = 0 \qquad i<k$$

2. The elements $\bar{u}_{ik}$ of U^{-1} are computed from the elements u_{ik} of U with the following recurrsive formulas:

$$\bar{u}_{ik} = -u_{ik} - \sum_{m=i+1}^{k-1} u_{im} \cdot \bar{u}_{mk} \qquad i<k$$

(any symbol $\sum_{m=k}^{k-1} x_m$ is to be interpreted as zero)

$$\bar{u}_{ik} = 1 \qquad i=k$$

$$\bar{u}_{ik} = 0 \qquad i>k$$

3. The elements $\bar{a}_{ik}$ of the product $U^{-1} \cdot L^{-1}$ are computed with the formulas:

$$\bar{a}_{ik} = \bar{l}_{ik} + \sum_{m=i+1}^{N} \bar{u}_{im} \cdot \bar{l}_{mk} \qquad i \geq k$$

$$\bar{a}_{ik} = \sum_{m=k}^{N} \bar{u}_{im} \cdot \bar{l}_{mk} \qquad i<k$$

4. The resultant product $U^{-1} \cdot L^{-1}$ is multiplied on the right by the inverse permutation matrix P^{-1} giving:

$$A^{-1} = U^{-1} \cdot L^{-1} \cdot P^{-1}$$

That is, the columns of the product $U^{-1} \cdot L^{-1}$ are rearranged according to the interchanges performed during the factorization of the matrix.

Programming Considerations:

Matrix A is required in the factored form:

$$A = P \cdot L \cdot U$$

where L is the lower triangular matrix, U the upper triangular matrix with unit diagonal, and P the permutation matrix corresponding to the integer vector IPER. L and the superdiagonal part of U are to be stored in the two-dimensional array A.

If the required factorization is done using the SSP procedure MFG, the resulting arrays A and IPER may be directly used as input for MIG. The inverse matrix A^{-1} is calculated by MIG in the storage locations of array A.

- Subroutine MIS

```
MIS..                                                                  MIS   10
/*********************************************************************/MIS   20
/*                                                                   */MIS   30
/*          INVERT SYMMETRIC POSITIVE DEFINITE MATRIX                */MIS   40
/*                                                                   */MIS   50
/*********************************************************************/MIS   60
   PROCEDURE(A,N),.                                                    MIS   70
   DECLARE                                                             MIS   80
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MIS   90
        SUM BINARY FLOAT(53),                                          MIS  100
        (A(*),PIV)                                                     MIS  110
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MIS  120
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MIS  130
        (ICOL,IPIV,IROW,J,K,L,LN,M,N)                                  MIS  140
        BINARY FIXED,.                                                 MIS  150
                                      /*****************************/MIS  160
                                      /*INVERT TRIANGULAR MATRIX    */MIS  170
   LN   =N,.                          /*****************************/MIS  180
   J    =0,.                                                           MIS  190
   IF LN LE 0                         /*TEST SPECIFIED PARAMETER N  */MIS  200
   THEN DO,.                                                           MIS  210
        ERROR='P',.                   /*P MEANS WRONG INPUT         */MIS  220
        GO TO RETURN,.                                                 MIS  230
        END,.                                                          MIS  240
                                      /*PERFORM LOOP OVER ALL ROWS  */MIS  250
        DO K =0 TO LN-1,.                                              MIS  260
        IPIV =0,.                                                      MIS  270
        J    =J+1,.                                                    MIS  280
        PIV  =A(J+K),.                                                 MIS  290
        IF PIV= 0                     /*IS ANY DIAGONAL ELEMENT ZERO*/MIS  300
        THEN DO,.                                                      MIS  310
             ERROR='S',.              /*S MEANS MATRIX IS NOT       */MIS  320
             GO TO RETURN,.           /*POSITIVE DEFINITE           */MIS  330
             END,.                                                     MIS  340
        PIV,A(J+K)=1/PIV,.                                             MIS  350
             DO L =1 TO K,.           /*EXECUTE LOOP IN (K+1)-TH ROW*/MIS  360
             SUM  =0,.                                                 MIS  370
             IROW =J,.                                                 MIS  380
             ICOL,IPIV=IPIV+L,.                                        MIS  390
                  DO M =L TO K,.      /*CALCULATE SCALAR PRODUCTS   */MIS  400
                  SUM  =SUM+MULTIPLY(A(IROW),A(ICOL),53),.             MIS  410
                  ICOL =ICOL+M,.                                       MIS  420
                  IROW =IROW+1,.                                       MIS  430
                  END,.                                                MIS  440
             A(J) =-SUM*PIV,.         /*CALCULATE NEW ELEMENT       */MIS  450
             J    =J+1,.                                              MIS  460
             END,.                                                     MIS  470
        END,.                         /*****************************/MIS  480
                                      /*MULTIPLY WITH TRANSPOSE     */MIS  490
                                      /*****************************/MIS  500
        =0,.                                                           MIS  510
        DO K =1 TO LN,.               /*PERFORM LOOP OVER ALL ROWS  */MIS  520
        IROW =K,.                                                      MIS  530
             DO L =1 TO K,.           /*EXECUTE LOOP WITHIN K-TH ROW*/MIS  540
             SUM  =0,.                                                 MIS  550
             ICOL,J=J+1,.                                              MIS  560
             IROW =IROW-1,.                                            MIS  570
                  DO M =K TO LN,.     /*CALCULATE SCALAR PRODUCTS   */MIS  580
                  SUM  =SUM+MULTIPLY(A(ICOL),A(ICOL+IROW),53),.        MIS  590
                  ICOL =ICOL+M,.                                       MIS  600
                  END,.                                                MIS  610
             A(J) =SUM,.                                               MIS  620
             END,.                                                     MIS  630
   END,.                                                               MIS  640
RETURN..                                                               MIS  650
   END,.                              /*END OF PROCEDURE MIS        */
```

Purpose:

MIS inverts a symmetric positive definite matrix A, which is given in factored form (Cholesky):

$$A = T \cdot \text{transpose } (T)$$

Usage:

CALL MIS (A, N);

A(N*(N+1)/2) - BINARY FLOAT [(53)]
Given one-dimensional array containing the lower triangular factor T of matrix A stored rowwise in compressed form (possibly resultant array A of SSP procedure MFS). Resultant lower triangular part of calculated inverse (A) stored rowwise in compressed form.

N - BINARY FIXED
Given order of matrices A and T.

Remarks:

ERROR='P'	means error in specified dimension: N ≤ 0
ERROR='S'	means given triangular factor T has at least one pivot equal to zero -- that is, matrix A is not positive definite.

The given lower triangular factor T is assumed to be stored in compressed form -- that is, rowwise in N*(N+1)/2 successive storage locations. On return the lower triangular part of the inverse of A is stored in the same way.

Method:

It is supposed that the symmetric positive definite matrix A is given in the factored form (Cholesky):

A = T · transpose (T)

where T is the lower triangular factor, possibly calculated by SSP procedure MIS.

In the first step MIS inverts the given triangular matrix T in the storage locations of T. Using

inverse (transpose (T)) = transpose (inverse (T))

in the second step MIS multiplies inverse (T) with its transpose on the same storage locations, giving

inverse (A) = transpose (inverse (T))

· inverse (T)

Thus, the given lower triangular factor T is replaced by the lower part of the resultant inverse (A).

For reference see:

A. S. Householder, The Theory of Matrices in Numerical Analysis, 1965, pp. 125-130.
R. Zurmühl, Matrizen, 1964, pp. 77-79.

Mathematical Background:

Suppose the symmetric positive definite matrix A is factored in the form:

A = T · transpose (T)

where T is a lower triangular factor matrix. Then:

inverse (A) = transpose (inverse (T))

· inverse (T)

1. The elements $\bar{t}_{ik}$ of inverse (T) are computed from the elements t_{ik} of T using the following recursive formulas:

$$\bar{t}_{ik} = -\frac{\sum_{m=k}^{i-1} \bar{t}_{mk} \cdot t_{im}}{t_{ii}} \qquad i>k$$

$$\bar{t}_{ik} = \frac{1}{t_{ii}} \qquad i=k$$

$$\bar{t}_{ik} = 0 \qquad i<k$$

2. From inverse (T) the elements $\bar{a}_{ik}$ of inverse (A) are calculated as follows:

$$\bar{a}_{ik} = \sum_{m=i}^{N} \bar{t}_{mk} \cdot \bar{t}_{mi} \qquad i \geq k$$

with $\bar{a}_{ik} = \bar{a}_{ki}$

Programming Considerations:

The given lower triangular matrix T is assumed to be stored in compressed form -- that is, rowwise in N · (N+1)/2 successive storage locations. The lower triangular part of the resultant inverse (A) is returned in these locations of T.

If any pivot of the input matrix T is equal to zero, the error parameter ERROR is set to 'S' and further calculation is bypassed. Any zero pivot in T means that matrix A = T · transpose (T) is not positive definite, possibly because of severe loss of significance in the factorization routine.

- Subroutine MINV

```
MINV..                                                                  MINV  10
/*************************************************************************/MINV  20
/*                                                                       */MINV  30
/*      TO INVERT A MATRIX                                               */MINV  40
/*                                                                       */MINV  50
/*************************************************************************/MINV  60
   PROCEDURE (A,N,D,CON),.                                               MINV  70
   DECLARE                                                               MINV  80
         ERROR EXTERNAL CHARACTER(1),                                    MINV  90
         (I,J,K,N,L(N),M(N))                                             MINV 100
         FIXED BINARY,                                                   MINV 110
         (A(*,*),BIGA,HOLD,D,CON,S)                                      MINV 120
         BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/MINV 130
/*       BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/MINV 140
/*                                                                       */MINV 150
   ERROR='0',.                                                           MINV 160
   IF N LE 0                                                             MINV 170
   THEN DO,.                                                             MINV 180
         ERROR='1',.                 /* ORDER OF MATRIX = 0.          */MINV 190
         GO TO FIN,.                                                     MINV 200
         END,.                                                           MINV 210
   IF CON= 0                                                             MINV 220
   THEN S    =1.0E-5,.               /* SINGLE PRECISION VERSION /*S*/MINV 230
/*THEN S    =1.0E-15,.              /* DOUBLE PRECISION VERSION /*D*/MINV 240
   ELSE S    =CON,.                                                      MINV 250
   IF N = 1                        /* INVERT A SCALAR               */MINV 260
   THEN DO,.                                                           MINV 270
         D    =A(1,1),.                                                MINV 280
         IF ABS(D) LE S                                                MINV 290
         THEN DO,.                                                     MINV 300
               ERROR='2',.                                             MINV 310
               END,.                                                   MINV 320
         ELSE A(1,1) = 1/D,.                                           MINV 330
         GO TO FIN,.                                                   MINV 340
         END,.                                                         MINV 350
   D    =1.0,.                     /* SEARCH FOR LARGEST ELEMENT    */MINV 360
         DO K = 1 TO N,.                                               MINV 370
         L(K) =K,.                                                     MINV 380
         M(K) =K,.                                                     MINV 390
         BIGA =A(K,K),.                                                MINV 400
               DO I=K TO N,.                                           MINV 410
                     DO J=K TO N,.                                     MINV 420
                     IF ABS(BIGA) LT ABS(A(I,J))                       MINV 430
                     THEN DO,.                                         MINV 440
                           BIGA =A(I,J),.                              MINV 450
                           L(K) =I,.                                   MINV 460
                           M(K) =J,.                                   MINV 470
                           END,.                                       MINV 480
                     END,.                                             MINV 490
               END,.                                                   MINV 500
         J    =L(K),.                    /* INTERCHANGE ROWS       */MINV 510
         IF L(K) GT K                                                  MINV 520
         THEN DO,.                                                     MINV 530
                     DO I = 1 TO N,.                                   MINV 540
                     HOLD =-A(K,I),.                                   MINV 550
                     A(K,I)=A(J,I),.                                   MINV 560
                     A(J,I)=HOLD,.                                     MINV 570
                     END,.                                             MINV 580
               END,.                                                   MINV 590
         I    =M(K),.                    /* INTERCHANGE COLUMNS    */MINV 600
         IF M(K) GT K                                                  MINV 610
         THEN DO,.                                                     MINV 620
                     DO J = 1 TO N,.                                   MINV 630
                     HOLD =-A(J,K),.                                   MINV 640
                     A(J,K)=A(J,I),.                                   MINV 650
                     A(J,I)=HOLD,.                                     MINV 660
                     END,.                                             MINV 670
               END,.                                                   MINV 680
         IF ABS(BIGA) LE S                                             MINV 690
         THEN DO,.                                                     MINV 700
               D    =0.0,.                                             MINV 710
               GO TO COMP,.                                            MINV 720
               END,.                                                   MINV 730
/*                                                                     */MINV 740
/*       DIVIDE COLUMNS BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS      */MINV 750
/*       CONTAINED IN BIGA)                                            */MINV 760
               DO I = 1 TO N,.                                         MINV 770
               IF I NE K                                               MINV 780
               THEN A(I,K)=A(I,K)/(-A(K,K)),.                          MINV 790
               END,.                                                   MINV 800
               DO I = 1 TO N,.           /* REDUCE MATRIX           */MINV 810
               IF I NE K                                               MINV 820
               THEN DO,.                                               MINV 830
                           DO J = 1 TO N,.                             MINV 840
                           IF J NE K                                   MINV 850
                           THEN A(I,J)=A(I,K)*A(K,J)+A(I,J),.          MINV 860
                           END,.                                       MINV 870
                     END,.                                             MINV 880
               END,.                                                   MINV 890
               DO J = 1 TO N,.                                         MINV 900
               IF J NE K                 /* DIVIDE BY ROW PIVOT     */MINV 910
               THEN A(K,J)=A(K,J)/A(K,K),.                             MINV 920
               END,.                                                   MINV 930
         D    =D*A(K,K),.               /* COMPUTE DETERMINANT     */MINV 940
COMP..                                                                  MINV 950
         IF ABS(D) LE S                                                MINV 960
         THEN DO,.                                                     MINV 970
               ERROR='2',.               /* DETERMINANT IS ZERO     */MINV 980
               GO TO FIN,.                                             MINV 990
               END,.                                                   MINV1000
         A(K,K)=1.0/A(K,K),.             /* REPLACE PIVOT BY RECIPROCAL */MINV1010
         END,.                                                         MINV1020
/*                                                                     */MINV1030
/*       FINAL ROW AND COLUMN INTERCHANGE                              */MINV1040
/*                                                                     */MINV1050
   K    =N,.                                                          MINV1060
LOOP..                                                                 MINV1070
   K    =K-1,.                                                        MINV1080
   IF K GT 0                                                          MINV1090
   THEN DO,.                                                          MINV1100
         I    =L(K),.                                                 MINV1110
         IF I GT K                                                    MINV1120
         THEN DO,.                                                    MINV1130
                     DO J = 1 TO N,.                                  MINV1140
                     HOLD =A(J,K),.                                   MINV1150
                     A(J,K)=-A(J,I),.                                 MINV1160
                     A(J,I)=HOLD,.                                    MINV1170
                     END,.                                            MINV1180
               END,.                                                  MINV1190
         J    =M(K),.                                                 MINV1200
         IF J GT K                                                    MINV1210
         THEN DO,.                                                    MINV1220
                     DO I = 1 TO N,.                                  MINV1230
                     HOLD =A(K,I),.                                   MINV1240
                     A(K,I)=-A(J,I),.                                 MINV1250
                     A(J,I)=HOLD,.                                    MINV1260
                     END,.                                            MINV1270
               END,.                                                  MINV1280
         GO TO LOOP,.                                                 MINV1290
         END,.                                                        MINV1300
FIN..                                                                 MINV1310
   RETURN,.                                                          MINV1320
   END,.                           /*END OF PROCEDURE MINV          */MINV1330
```

Purpose:

MINV inverts a general square matrix.

Usage:

CALL MINV (A, N, D, CON);

A(N, N) - BINARY FLOAT [(53)]
Given matrix.
Resultant inverse of given matrix.

N - BINARY FIXED
Given order of matrix A.

D - BINARY FLOAT [(53)]
Resultant determinant.

CON - BINARY FLOAT [(53)]
Given constant with which the determinant is compared. If the given value of CON is zero, the program assigns the value 10^{-5} in single precision and 10^{-15} is double precision.

Remarks:

A must be a general square matrix.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - means that the order of the matrix is less than or equal to zero.

ERROR=2 - means that the absolute value of the determinant is less than or equal to the specified constant CON (see description of parameters for explanation).

Method:

The standard Gauss-Jordan method is used and the determinant is calculated.

- Subroutine MLSQ

```
MLSQ..                                                                  MLSQ  10
/*************************************************************************/MLSQ  20
/*                                                                       */MLSQ  30
/*      LINEAR LEAST SQUARES PROBLEM SOLVED USING HOUSEHOLDER TRANSF.*/MLSQ  40
/*                                                                       */MLSQ  50
/*************************************************************************/MLSQ  60
   PROCEDURE(A,B,M,N,K),.                                               MLSQ  70
   DECLARE                                                              MLSQ  80
         (A(*,*),B(*,*),PIVR,MAXA)                                      MLSQ  90
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/MLSQ 100
/*       BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/MLSQ 110
         (AUX(N),H,SIG,BETA)                                            MLSQ 120
         BINARY FLOAT(53),                                              MLSQ 130
         (TOL,PIV(N))                                                   MLSQ 140
         BINARY FLOAT,                                                  MLSQ 150
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MLSQ 160
         (I,J,K,L,M,N,PIVI,LM,LN,LK)                                    MLSQ 170
         BINARY FIXED,.                                                 MLSQ 180
   LM    =M,.                                                           MLSQ 190
   LN    =N,.                                                           MLSQ 200
   LK    =K,.                                                           MLSQ 210
   SIG   =0,.                                                           MLSQ 220
   ERROR='D',.                  /*PRESET ERROR INDICATOR              */MLSQ 230
   IF LM GE LN                  /*IF M LESS THAN N                    */MLSQ 240
   THEN IF LN GE 0              /*OR IF N NOT POSITIVE                */MLSQ 250
   THEN IF LK GT 0              /*OR IF K NOT POSITIVE                */MLSQ 260
   THEN DO,.                    /*THEN BYPASS OPERATION               */MLSQ 270
            DO L = 1 TO LN,.    /*CALCULATE SCALARPRODUCTS OF         */MLSQ 280
            H    =0,.           /*COLUMNS                             */MLSQ 290
                 DO I = 1 TO LM,.                                       MLSQ 300
                 H    =H+MULTIPLY(A(I,L),A(I,L),53),.                   MLSQ 310
                 END,.                                                  MLSQ 320
            IF H GE SIG                                                 MLSQ 330
            THEN DO,.                                                   MLSQ 340
                 SIG  =H,.      /*SAVE MAXIMAL SCALARPRODUCT          */MLSQ 350
                 PIVI =L,.      /*SAVE SUBSCRIPT OF PIVOTCOLUMN       */MLSQ 360
                 END,.                                                  MLSQ 370
            AUX(L),PIV(L)=H,.                                           MLSQ 380
            END,.               /*******************************/     MLSQ 390
                                /*DECOMPOSITION LOOP                  */MLSQ 400
      ERROR='0',.               /*******************************/     MLSQ 410
            DO L = 1 TO LN,.                                            MLSQ 420
            TOL  =PIV(PIVI),.   /*ORIGINAL LENGTH OF PIVOTCOL. */MLSQ 430
            IF PIVI GT L        /*SHOULD COLUMN BE INTERCHANGED*/MLSQ 440
            THEN DO,.                                                   MLSQ 450
                 H    =AUX(L),.  /*INTERCHANGE SCALARPRODUCTS        */MLSQ 460
                 AUX(L)=AUX(PIVI),.                                     MLSQ 470
                 PIV(PIVI)=PIV(L),.                                     MLSQ 480
                 AUX(PIVI)=H,.                                          MLSQ 490
                      DO J=L TO LM,. /*INTERCHANGE LOWER PART OF     */MLSQ 500
                      PIVR =A(J,L),. /*COLUMNS OF A                  */MLSQ 510
                      A(J,L)=A(J,PIVI),.                                MLSQ 520
                      A(J,PIVI)=PIVR,.                                  MLSQ 530
                      END,.                                             MLSQ 540
                 END,.                                                  MLSQ 550
            IF L GT 1           /*RECALCULATE COLUMN LENGTH         */MLSQ 560
            THEN DO,.           /*TO AVOID ROUND-OFF PROBLEMS       */MLSQ 570
                 SIG  =0,.                                              MLSQ 580
                 DO I = L TO LM,.                                       MLSQ 590
                 SIG  =SIG+MULTIPLY(A(I,L),A(I,L),53),.                 MLSQ 600
                 END,.                                                  MLSQ 610
            END,.                                                       MLSQ 620
            IF TOL= 0                                                   MLSQ 630
            THEN DO,.                                                   MLSQ 640
                 IF ERROR NE 'B'                                        MLSQ 650
                 THEN IF ERROR NE 'W'                                   MLSQ 660
                 THEN ERROR='S',.   /*GIVEN A HAS ZERO-COLUMN(S)    */MLSQ 670
                 ELSE ERROR='B',.                                       MLSQ 680
                 TOL  =1,.                                              MLSQ 690
                 END,.                                                  MLSQ 700
            BETA =TOL*1E-10,.       /*SINGLE PRECISION VERSION  /*S*/MLSQ 710
/*          BETA =TOL*1E-2C,.       /*DOUBLE PRECISION VERSION  /*D*/MLSQ 720
            IF SIG LE BETA                                              MLSQ 730
            THEN DO,.               /*INDICATE LOSS OF SIGNIFICANCE*/MLSQ 740
                 IF ERROR NE 'B'                                        MLSQ 750
                 THEN IF ERROR NE 'S'                                   MLSQ 760
                 THEN ERROR='W',.                                       MLSQ 770
                 ELSE ERROR='B',.                                       MLSQ 780
                 IF SIG LE 0                                            MLSQ 790
                 THEN SIG  =BETA,.  /*MODIFY ZERO VALUE             */MLSQ 800
                 END,.                                                  MLSQ 810
            SIG  =SQRT(SIG),.                                           MLSQ 820
            H    =A(L,L),.                                              MLSQ 830
            IF H LT 0                                                   MLSQ 840
            THEN SIG  =-SIG,.       /*FORCE SIGN(SIG) TO SIGN(H)   */MLSQ 850
            PIV(L)=PIVI,.           /*SAVE INTERCHANGE INFORMATION */MLSQ 860
            A(L,L),BETA=H*SIG,.     /*TRANSFORM DIAGONAL ELEMENT   */MLSQ 870
            AUX(L)=-SIG,.           /*SAVE DIAGONAL ELEMENT        */MLSQ 880
            BETA =SIG*BETA,.                                            MLSQ 890
                                    /*TRANSFORM SUBMATRIX OF A     */MLSQ 900
            PIVR =0,.                                                   MLSQ 910
                 DO J = L+1 TO LN,. /*TRANSFORM LOWER PART OF A     */MLSQ 920
                 H    =0,.          /*COLUMNS L+1 UP TO N ONLY     */MLSQ 930
                      DO I = L TO LM,.                                  MLSQ 940
                      H    =H+MULTIPLY(A(I,L),A(I,J),53),.              MLSQ 950
                      END,.                                             MLSQ 960
                 SIG  =H/BETA,.     /*MODIFY J-TH COLUMN           */MLSQ 970
                      DO I = LM TO L BY -1,.                            MLSQ 980
                      H    =A(I,J),.                                    MLSQ 990
                      A(I,J)=H-A(I,L)*SIG,.                             MLSQ1000
                      END,.         /*NEXT UPDATE COLUMN LENGTH    */MLSQ1010
                 H    =A(L,J),.                                         MLSQ1020
                 AUX(J),H=AUX(J)-H*H,.                                  MLSQ1030
                 IF H GE PIVR       /*SEARCH NEXT PIVOTCOLUMN      */MLSQ1040
                 THEN DO,.                                              MLSQ1050
                      PIVR =H,.                                         MLSQ1060
                      PIVI =J,.                                         MLSQ1070
                      END,.                                             MLSQ1080
                 END,.                                                  MLSQ1090
                                    /*TRANSFORM LOWER PART OF      */MLSQ1100
                 DO J = 1 TO LK,.   /*RIGHT HAND SIDE MATRIX B     */MLSQ1110
                 H    =0,.                                             MLSQ1120
                      DO I = L TO LM,.                                  MLSQ1130
                      H    =H+MULTIPLY(A(I,L),B(I,J),53),.              MLSQ1140
                      END,.                                             MLSQ1150
                 MAXA =H/BETA,.     /*MODIFY J-TH COLUMN           */MLSQ1160
                      DO I = L TO LM,.                                  MLSQ1170
                      B(I,J)=B(I,J)-A(I,L)*MAXA,.                       MLSQ1180
                      END,.                                             MLSQ1190
                 END,.                                                  MLSQ1200
            END,.               /*END OF DECOMPOSITION LOOP    */MLSQ1210
                                /*******************************/MLSQ1220
            DO J = LN TO 1 BY -1,.  /*BACKSUBSTITUTION,INTERCHANGE */MLSQ1230
                 DO I = 1 TO LK,.   /*******************************/MLSQ1240
                 H    =B(J,I),.                                         MLSQ1250
                      DO L = J+1 TO LN,.                                MLSQ1260
                      H    =H-MULTIPLY(A(J,L),B(L,I),53),.              MLSQ1270
                      END,.                                             MLSQ1280
                 PIVI =PIV(J),.                                         MLSQ1290
                 B(J,I)=B(PIVI,I),.                                     MLSQ1300
                 B(PIVI,I)=H/AUX(J),.                                   MLSQ1310
                 END,.                                                  MLSQ1320
            END,.                                                       MLSQ1330
      IF LN LT LM                   /*COMPUTE LEAST SQUARES        */MLSQ1340
      THEN DO J = 1 TO LK,.         /*IN CASE OF AN OVERDETERMINED */MLSQ1350
           H    =0,.                /*EQUATION SYSTEM ONLY         */MLSQ1360
                DO I = LN+1 TO LM,.                                     MLSQ1370
                H    =H+MULTIPLY(B(I,J),B(I,J),53),.                    MLSQ1380
                END,.                                                   MLSQ1390
           B(LM,J)=H,.                                                  MLSQ1400
           END,.                                                        MLSQ1410
      END,.                         /*END OF OPERATION             */MLSQ1420
   END,.                            /*END OF PROCEDURE MLSQ        */MLSQ1430
```

Purpose:

MLSQ calculates X satisfying AX=B, that is, the solution of a system of linear equations using Householder transformations. The least squares solution is obtained in case of an overdetermined system of equations.

Usage:

CALL MLSQ (A, B, M, N, K);

A(M, N) - BINARY FLOAT [(53)]
Given coefficient matrix of equation system.
A gets destroyed.

B(M, K) - BINARY FLOAT [(53)]
Given matrix of right-hand sides.
Resultant solution of A·X=B stored in upper N rows of B, and if M>N resultant square sum of residuals for I-th right-hand side stored in elements B(M, I) for I = 1, 2, ..., K.

M - BINARY FIXED
Given number of equations, that is, number of rows of matrices A and B.

N - BINARY FIXED
Given number of unknowns, that is, number of columns of matrix A and number of rows of resultant X, which is overlaid with B.

K - BINARY FIXED
Given number of right-hand sides, that is, number of columns of B.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='D' means incorrect dimension(s); not all of the conditions $M \geq N > 0$, $K > 0$ are satisfied. Operation is bypassed.

ERROR='W' means warning, indicating possible loss of significance in resultant X.

ERROR='S' means A has at least one zero-column. Resultant X is a least squares solution (not necessarily of minimal norm).

ERROR='B' implies both ERROR='S' and ERROR='W'; that is, resultant X is a least squares solution, but possibly affected by loss of significance.

The internal relative tolerance for test on loss of significance is set to 10^{-5} in single precision and to 10^{-10} in double precision. In the single precision version, scalar products are accumulated using double precision arithmetic.

Method:

A is reduced to upper triangular form, using Householder transformations successively. The same sequence of transformations is applied to given right-hand-side matrix B. Solution X is then obtained using backsubstitution.

For reference see:

G. Golub, "Numerical Methods for Solving Linear Least Squares Problems", Numerische Mathematik, vol. 7, 1965, pp. 206-216.

Mathematical Background:

Notation

The transpose of a matrix A is written as A^T. The kth column vector of A is written as $A_{*,k}$ and the ith row vector as $A_{i,*}$. The Euclidean norm of the vector $R = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix}$ is abbreviated:

$$\| R \| = \sqrt{R^T R} = \sqrt{\sum_{i=1}^{n} r_i^2}$$

Problem

For a given m by n coefficient matrix A with $m \geq n$ and an m by k matrix B of right-hand sides, an n by k matrix X must be calculated that solves AX = B in the least squares sense, that is:

$$\left\| B_{*j} - A X_{*j} \right\| = \min, \text{ for } j = 1, 2, \ldots, k$$

The determination of X is based on the reduction of the matrix A to an m by n matrix R of the form

$$R = \begin{pmatrix} U \\ O \end{pmatrix}$$

by means of an orthogonal transformation Q, so that U is an upper trangular matrix of order n.

$$QA = R$$

Then, the given equation AX = B can be solved as follows:

$$\begin{aligned} QAX &= QB \\ RX &= QB \\ X &= [U^{-1} O]\, QB \end{aligned}$$

if U is of maximal rank (otherwise, see "Programming Considerations"). It is interesting to note that U is the triangular factor provided by the Cholesky factorization of A^TA.

$$A^TA = U^TU$$

Householder's transformations

The reduction of the given matrix A to the matrix R can be achieved by means of a sequence of (n-1) orthogonal transformations the product of which will be Q. This can be written as

$$A^{(0)} = A$$

$$A^{(i)} = P^{(i)}\, A^{(i-1)}, \quad i = 1, \ldots, n-1$$

where $A^{(i)}$ is supposed to have the same form as R in its first i columns, and where $P^{(i)}$ is an orthogonal matrix. Then:

$$R = A^{(n-1)}$$

Among the possible matrices $P^{(i)}$, let us consider those of the form

$$P^{(i)} = I + \alpha^{(i)}\, W^{(i)}\, W^{(i)\,T}$$

where I is the unit matrix and w a vector of order m related to the scalar $\alpha^{(i)} \neq 0$ by

$$< W^{(i)}, W^{(i)} > = -\frac{2}{\alpha^{(i)}}$$

It is easy to see that these matrices are orthogonal and symmetric. By definition of $A^{(i)}$, $P^{(i)}$ can be written as

$$P^{(i)} = I + \frac{1}{g^{(i)}\,(v_i^{(i)} - g^{(i)})}\,(v^{(i)} - g^{(i)} e_i)\,(v^{(i)} - g^{(i)} e_i)^T$$

where:

$$v^{(i)T} = (v_1^{(i)}, v_2^{(i)}, \ldots, v_m^{(i)})$$

$$v_j^{(i)} = 0 \text{ for } j < i$$

$$v_j^{(i)} = a_{ji}^{(i-1)} \text{ for } j \geq i$$

$$g^{(i)} = -\,\text{sign}\,(v_i^{(i)}) \left\| v^{(i)} \right\|$$

and where e_i is a vector of order m whose components are zero except for the i-th, which is one.

Actually, neither matrices $P^{(i)}$ nor matrix $Q = P^{(n-1)} \ldots P^{(1)}$ is computed explicitly.

Each column k of $A^{(i)}$, k = i, ..., n, is calculated from column k of $A^{(i-1)}$ as follows

$$A_{*k}^{(i)} = A_{*k}^{(i-1)} + \frac{1}{g^{(i)}\,(v_i^{(i)} - g^{(i)})} < v^{(i)}$$

$$- g^{(i)} e_i,\ A_{*k}^{(i-1)} > (v^{(i)} - g^{(i)} e_i)$$

The columns of matrix B are modified in the same manner.

Pivoting

To keep roundoff errors as small as possible, an interchange of columns is performed before the i-th transformation, so that the i-th column of $A^{(i-1)}$ gets permuted with the k-th for which $\left\| v^{(i)} \right\|$ is maximum. k is determined by:

$$s_k^{(i)} = \max_{i \leq j \leq n} (s_j^{(i)})$$

where:

$$s_j^{(i)} = \sum_{q=i}^{m} \left[a_{qj}^{(i-1)} \right]^2$$

Back substitution

When the matrix is reduced to the triangular form, the solution is obtained by back substitution. The interchange of rows determined by the pivoting is applied to the solution as soon as any component is computed.

Programming Considerations:

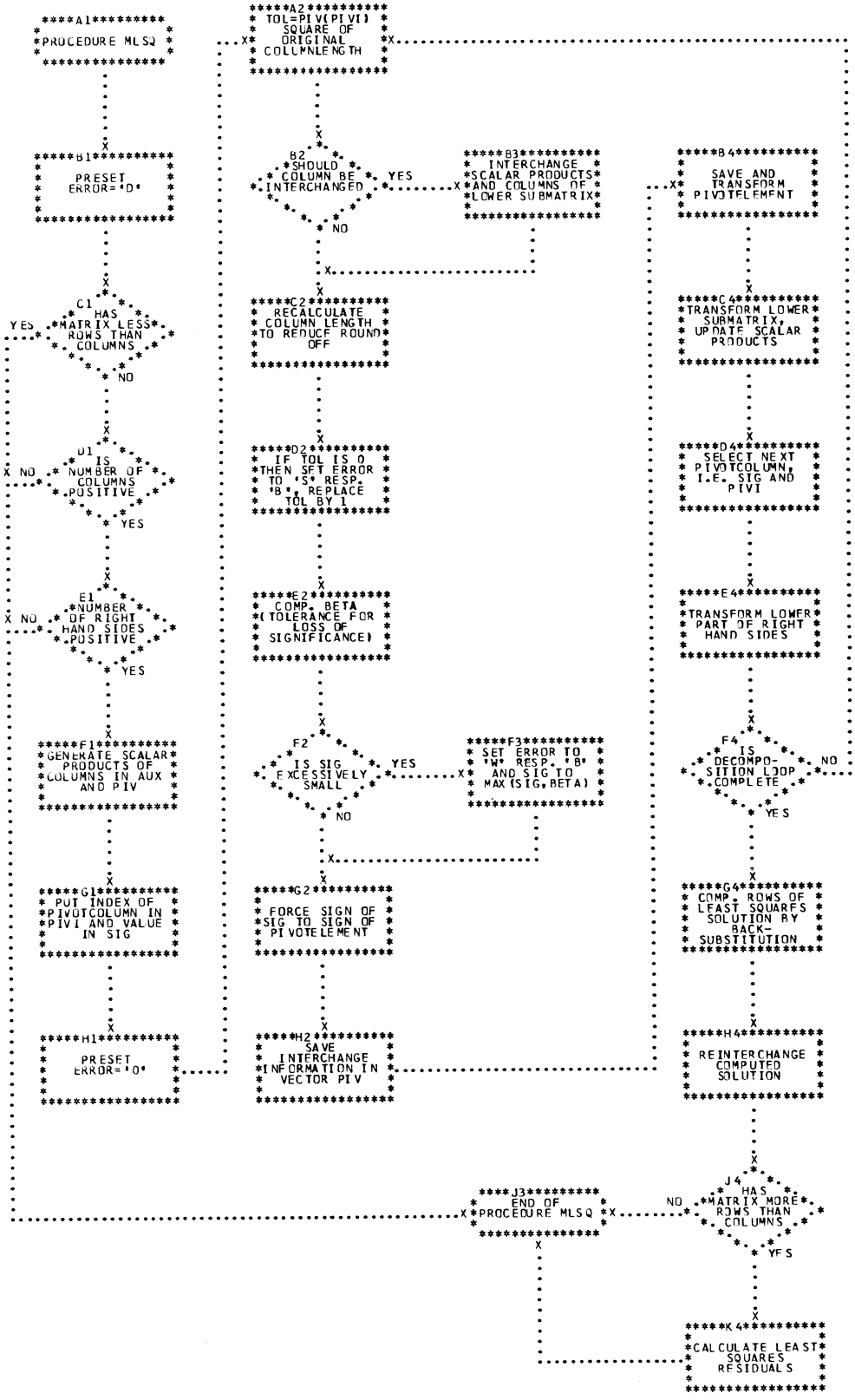
The procedure may fail if, at any intermediate step i, no column with nonzero parameter $g^{(i)}$ can be found -- that is, if no nonzero main diagonal element in U can be generated. In this case, the rank of the matrix A is less than n. Because of roundoff errors this situation may even occur if the rank of the given matrix A equals n. In order to indicate this ill-conditioned case, with its possible loss of significance, each $\left| g^{(i)} \right|$ is compared against a tolerance TOL_i. TOL_i is the product of the norm of the corresponding column in the original matrix A times the internal tolerance EPS (10^{-5} in single precision and 10^{-10} in double precision).

1. If the relative tolerances TOL_i are all positive (no zero columns in original A), then ERROR = 'W' if $\left| g^{(i)} \right| > TOL_i$ does not hold true for all i = 1, 2, ..., n. Zero elements $g^{(i)}$ get replaced by $TOL_i \cdot 10^{-10}$ ($TOL \cdot 10^{-20}$ in double precision).
2. If A has zero columns (corresponding $TOL_i = 0$), then ERROR = 'S'. The corresponding $g^{(i)}$ is set to $1E^{-10}$ or $1E^{-20}$.
3. If cases 1 and 2 occur combined, ERROR = 'B'.

Case 1 indicates possible loss of significance in resultant solution X. Case 2 means that X is a least squares solution but possibly not the uniquely determined one of minimal norm.

For full understanding of the procedure note that:

1. The $g^{(i)}$'s are recalculated to avoid roundoff problems.
2. The resultant X is overlaid with the given right-hand sides.
3. Least squares deviations are calculated only in case m > n, and stored in the last row of the given right-hand-side matrix.


A1
PROCEDURE MLSQ
B1
PRESET ERROR='0'
C1
HAS MATRIX LESS ROWS THAN COLUMNS
YES
NO
D1
IS NUMBER OF COLUMNS POSITIVE
NO
YES
E1
NUMBER OF RIGHT HAND SIDES POSITIVE
NO
YES
F1
GENERATE SCALAR PRODUCTS OF COLUMNS IN AUX AND PIV
G1
PUT INDEX OF PIVOTCOLUMN IN PIVI AND VALUE IN SIG
H1
PRESET ERROR='0'
A2
TOL=PIV(PIVI) SQUARE OF ORIGINAL COLUMNLENGTH
B2
SHOULD COLUMN BE INTERCHANGED
YES
NO
B3
INTERCHANGE SCALAR PRODUCTS AND COLUMNS OF LOWER SUBMATRIX
C2
RECALCULATE COLUMN LENGTH TO REDUCE ROUND OFF
D2
IF TOL IS 0 THEN SET ERROR TO 'S' RESP. 'B', REPLACE TOL BY 1
E2
COMP. BETA (TOLERANCE FOR LOSS OF SIGNIFICANCE)
F2
IS SIG EXCESSIVELY SMALL
YES
NO
F3
SET ERROR TO 'W' RESP. 'B' AND SIG TO MAX(SIG,BETA)
G2
FORCE SIGN OF SIG TO SIGN OF PIVOTELEMENT
H2
SAVE INTERCHANGE INFORMATION IN VECTOR PIV
J3
END OF PROCEDURE MLSQ
B4
SAVE AND TRANSFORM PIVOTELEMENT
C4
TRANSFORM LOWER SUBMATRIX, UPDATE SCALAR PRODUCTS
D4
SELECT NEXT PIVOTCOLUMN, I.E. SIG AND PIVI
E4
TRANSFORM LOWER PART OF RIGHT HAND SIDES
F4
IS DECOMPOSITION LOOP COMPLETE
NO
YES
G4
COMP. ROWS OF LEAST SQUARES SOLUTION BY BACK-SUBSTITUTION
H4
REINTERCHANGE COMPUTED SOLUTION
J4
HAS MATRIX MORE ROWS THAN COLUMNS
NO
YES
K4
CALCULATE LEAST SQUARES RESIDUALS

- Subroutine MGB1/MGB2

```
MGB1..                                                                  MGB   10
/*********************************************************************/MGB   20
/*                                                                   */MGB   30
/*      FOR AN EQUATION SYSTEM  A*X=R  WITH BAND MATRIX  A=L*U       */MGB   40
/*      CALCULATE OPTIONALLY                                         */MGB   50
/*           UPPER TRIANGULAR FACTOR U AND SOLUTION X,               */MGB   60
/*           UPPER TRIANGULAR FACTOR U AND INVERSE(L)*R,             */MGB   70
/*           INVERSE(U)*R FOR GIVEN U,R.                             */MGB   80
/*                                                                   */MGB   90
/*********************************************************************/MGB  100
   PROCEDURE(A,R,N,NLD,NUD,M,EPS,OPT),.                                 MGB  110
   DECLARE                                                              MGB  120
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */MGB  130
        (OPT,COPT) CHARACTER(1),                                        MGB  140
        EPS BINARY FLOAT,                                               MGB  150
        SUM BINARY FLOAT(53),                                           MGB  160
        (A(*,*),R(*,*),L(*),SL(N),PIV,W)                                MGB  170
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/MGB  180
/*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/MGB  190
        (IPER(*),I,IBAC,IND,INL,IPIV,                                   MGB  200
        J,K,KL,LM,LLM,LN,LNLD,LNUD,M,                                   MGB  210
        N,NB,NLD,NUD)                                                   MGB  220
        BINARY FIXED,.                                                  MGB  230
   IND  =1,.                                                            MGB  240
   GO TO BOTH,.                                                         MGB  250
MGB2..                                                                  MGB  260
/*********************************************************************/MGB  270
/*                                                                   */MGB  280
/*      FOR AN EQUATION SYSTEM  A*X=R  WITH BAND MATRIX  A=L*U       */MGB  290
/*      COMPUTE OPTIONALLY                                           */MGB  300
/*           TRIANGULAR FACTORS L,U  POSSIBLY COMBINED WITH          */MGB  310
/*           CALCULATION OF X OR INVERSE(L)*R,                       */MGB  320
/*           INVERSE(L)*R OR INVERSE(A)*R FOR GIVEN L,U,R.           */MGB  330
/*                                                                   */MGB  340
/*********************************************************************/MGB  350
   ENTRY(A,R,L,IPER,N,NLD,NUD,M,EPS,OPT),.                              MGB  360
   IND  =2,.                                                            MGB  370
BOTH,.                                                                  MGB  380
   LN   =N,.                          /*STORE VARIABLES N, M, NUD,   */MGB  390
   LM,LLM=M,.                         /*NLD FROM CALLING SEQUENCE    */MGB  400
   LNUD =NUD,.                        /*INTO LOCAL PARAMETERS        */MGB  410
   LNLD =NLD,.                                                          MGB  420
   ERROR='P',.                        /*P MEANS WRONG INPUT          */MGB  430
   IF LM LE 0                         /*VALUE M MUST BE POSITIVE     */MGB  440
   THEN GO TO RETURN,.                                                  MGB  450
   IF LNLD LT 0                       /*NUMBER OF LOWER CODIAGONALS  */MGB  460
   THEN GO TO RETURN,.                /*NLD MAY NOT BE NEGATIVE AND  */MGB  470
   IF LNLD GE LN                      /*EQUAL TO OR GREATER THAN N   */MGB  480
   THEN GO TO RETURN,.                                                  MGB  490
   IF LNUD LT 0                       /*NUMBER OF UPPER CODIAGONALS  */MGB  500
   THEN GO TO RETURN,.                /*NUD MAY NOT BE NEGATIVE AND  */MGB  510
   IF LNUD GE LN                      /*EQUAL TO OR GREATER THAN N   */MGB  520
   THEN GO TO RETURN,.                                                  MGB  530
   ERROR='0',.                        /*PRESET ERROR INDICATOR       */MGB  540
   NB   =LNUD+LNLD+1,.                /*CALCULATE THE MAXIMUM WIDTH  */MGB  550
   IF NB GT LN                        /*OF BAND MATRIX               */MGB  560
   THEN NB   =LN,.                                                      MGB  570
   IBAC =1,.                          /*IBAC IS AN INDICATOR FOR     */MGB  580
   KL   =0,.                          /*BACKSUBSTITUTION             */MGB  590
   COPT =OPT,.                                                          MGB  600
   IF COPT= 'A'                       /*CALCULATE  INVERSE(L) * R    */MGB  610
   THEN DO,.                          /*FOR GIVEN  L, U, R           */MGB  620
        IND  =0,.                                                       MGB  630
        IBAC =0,.                                                       MGB  640
        GO TO GAUSS,                                                    MGB  650
        END,.                                                           MGB  660
   IF COPT= 'B'                       /*CALCULATE  INVERSE(U) * R    */MGB  670
   THEN GO TO BACK,.                  /*FOR GIVEN  U, R              */MGB  680
   IF COPT= 'C'                                                         MGB  690
   THEN DO,.                          /*CALCULATE  INVERSE(A) * R    */MGB  700
        IND  =0,.                     /*FOR GIVEN  L, U, R           */MGB  710
        GO TO GAUSS,.                                                   MGB  720
        END,.                                                           MGB  730
   IF COPT= 'L'                       /*COMPUTE TRIANGULAR FACTOR U  */MGB  740
   THEN DO,.                          /*AND OPTIONALLY  L  AND       */MGB  750
        IBAC =0,.                     /*CALCULATE  INVERSE(L) * R    */MGB  760
        GO TO SCAL,.                  /*FOR GIVEN  A, R              */MGB  770
        END,.                                                           MGB  780
   IF COPT= 'F'                       /*COMPUTE TRIANGULAR FACTORS   */MGB  790
   THEN DO,.                          /*L AND U  FOR GIVEN MATRIX A  */MGB  800
        IBAC =0,.                                                       MGB  810
        LLM  =0,.                                                       MGB  820
        GO TO SCAL,.                                                    MGB  830
        END,.                         /*COMPUTE TRIANGULAR FACTOR U  */MGB  840
   IF COPT= 'U'                       /*AND INVERSE(U)*R FOR GIVEN   */MGB  850
   THEN LLM  =0,.                     /*A, R                         */MGB  860
                                      /*                             */MGB  870
SCAL..                                /*CALCULATE SCALING FACTORS    */MGB  880
                                      /*                             */MGB  890
   K    =LNUD,.                       /*K IS AN END INDICATOR FOR    */MGB  900
   INL  =LNLD+LN-NB+1,.               /*EACH ROW OF MATRIX A         */MGB  910
   IPIV =NB-LNUD,.                                                      MGB  920
        DO I =1 TO LN,.               /*EXECUTE LOOP OVER ALL ROWS   */MGB  930
        IF I LE IPIV                                                    MGB  940
        THEN K    =K+1,.              /*IN I-TH ROW THE ELEMENTS     */MGB  950
        IF I GT INL                   /*A(I,K+1) TO A(I,NB) ARE      */MGB  960
        THEN K    =K-1,.              /*FILLED UP WITH ZEROS         */MGB  970
        PIV  =0,.                                                       MGB  980
             DO J =1 TO NB,.          /*EXECUTE LOOP OVER I-TH ROW   */MGB  990
             IF J GT K                                                  MGB 1000
             THEN A(I,J)=0,.          /*FILL UP WITH ZEROS           */MGB 1010
             ELSE DO,.                                                  MGB 1020
                  W    =ABS(A(I,J)),./*COMPUTE ABSOLUTELY GREATEST   */MGB 1030
                  IF W GT PIV         /*ELEMENT PIV IN I-TH ROW OF A */MGB 1040
                  THEN PIV  =W,.                                        MGB 1050
                  END,.                                                 MGB 1060
             END,.                                                      MGB 1070
        IF PIV= 0                     /*TEST FOR ZERO-ROW            */MGB 1080
        THEN DO,.                     /*ALL ELEMENTS IN I-TH ROW OF  */MGB 1090
             ERROR='S',.              /*GIVEN MATRIX A ARE ZERO      */MGB 1100
             GO TO RETURN,.                                             MGB 1110
             END,.                    /*STORE THE RECIPROCAL IN THE  */MGB 1120
        SL(I)=1/PIV,.                 /*VECTOR SL                    */MGB 1130
        END,.                         /*****************************/MGB 1140
GAUSS..                               /*GAUSS ELIMINATION            */MGB 1150
        DO I =1 TO LN-1,.             /*****************************/MGB 1160
        INL  =I+LNLD,.                /*INVERSE(L)*R                 */MGB 1170
        IF INL GT LN                                                    MGB 1180
        THEN INL  =LN,.                                                 MGB 1190
        IF IND= 0                     /*NO FACTORIZATION             */MGB 1200
        THEN DO,.                     /*CALCULATE INVERSE(L) * R     */MGB 1210
             IPIV =IPER(I),.          /*FOR GIVEN L, U, R            */MGB 1220
             GO TO INTR,.                                               MGB 1230
             END,.                                                      MGB 1240
        W    =0,.                     /*INITIALIZE W FOR PIVOTING    */MGB 1250
             DO J =I TO INL,.                                           MGB 1260
             PIV  =ABS(A(J,1))*SL(J),./*MULTIPLY ELEMENTS WITH SCALE  */MGB 1270
             IF PIV GT W              /*FACTORS AND SEARCH GREATEST  */MGB 1280
             THEN DO,.                /*PRODUCT                      */MGB 1290
                  W    =PIV,.                                           MGB 1300
                  IPIV =J,.           /*STORE ROW INDEX              */MGB 1310
                  END,.                                                 MGB 1320
             END,.                                                      MGB 1330
        IF W LE ABS(EPS)              /*TEST FOR LOSS OF SIGNIFICANCE*/MGB 1340
        THEN IF W = 0                 /*AND FOR ZERO                 */MGB 1350
        THEN DO,.                                                       MGB 1360
             ERROR='S',.              /*NEXT PIVOT IS ZERO POSSIBLY  */MGB 1370
             GO TO RETURN,.           /*DUE TO LOSS OF SIGNIFICANCE  */MGB 1380
             END,.                                                      MGB 1390
        ELSE ERROR='W',.              /*W MEANS WARNING              */MGB 1400
        PIV  =A(IPIV,1),.             /*PIV CONTAINS THE PIVOT       */MGB 1410
        IF IND= 2                     /*STORE INFORMATION FOR ROW-   */MGB 1420
        THEN IPER(I)=IPIV,.           /*PERMUTATIONS                 */MGB 1430
        IF IPIV= I                    /*IS INTERCHANGE NECESSARY     */MGB 1440
        THEN GO TO FSUB,.                                               MGB 1450
        SL(IPIV)=SL(I),.              /*RESTORE SCALING ELEMENTS     */MGB 1460
             DO J =1 TO NB,.                                            MGB 1470
             W    =A(I,J),.           /*INTERCHANGE ROWS IN GIVEN    */MGB 1480
             A(I,J)=A(IPIV,J),.       /*MATRIX A                     */MGB 1490
             A(IPIV,J)=W,.                                              MGB 1500
             END,.                                                      MGB 1510
                                                                        MGB 1520
INTR..                                                                  MGB 1530
             DO J =1 TO LLM,.         /*INTERCHANGE ROWS IN RIGHT    */MGB 1540
             W    =R(I,J),.           /*HAND SIDE MATRIX R           */MGB 1550
             R(I,J)=R(IPIV,J),.                                         MGB 1560
             R(IPIV,J)=W,.                                              MGB 1570
             END,.                                                      MGB 1580
FSUB..                                /*MODIFY OPTIONALLY ROWS IN    */MGB 1590
             DO J =I+1 TO INL,.       /*MATRIX A AND IN RIGHT HAND   */MGB 1600
             IF IND= 0                /*SIDE MATRIX R                */MGB 1610
             THEN DO,.                                                  MGB 1620
                  KL   =KL+1,.                                          MGB 1630
                  W    =L(KL),.                                         MGB 1640
                  GO TO DIVL,.                                          MGB 1650
                  END,.                                                 MGB 1660
             W    =A(J,1)/PIV,.       /*W IS AN ELEMENT OF THE LOWER */MGB 1670
             IF IND= 2                /*TRIANGULAR FACTOR L          */MGB 1680
             THEN DO,.                                                  MGB 1690
                  KL   =KL+1,.                                          MGB 1700
                  L(KL)=W,.           /*STORE W INTO L IF REQUESTED  */MGB 1710
                  END,.                                                 MGB 1720
                  DO K =2 TO NB,.     /*MODIFY AND SHIFT ROWS OF A   */MGB 1730
                  A(J,K-1)=A(J,K)-W*A(I,K),.                            MGB 1740
                  END,.                                                 MGB 1750
             A(J,NB)=0,.              /*LAST TERM IS SET TO ZERO     */MGB 1760
DIVL..                                /*MODIFY ROWS OF R TO COMPUTE  */MGB 1770
                  DO K =1 TO LLM,.    /*INVERSE(L)*R                 */MGB 1780
                  R(J,K)=R(J,K)-W*R(I,K),.                              MGB 1790
                  END,.                                                 MGB 1800
             END,.                                                      MGB 1810
        END,.                                                           MGB 1820
   IF IND= 2                                                            MGB 1830
   THEN IPER(LN)=LN,.                                                   MGB 1840
   IF IBAC NE 1                                                         MGB 1850
   THEN GO TO RETURN,.                /*********************************/MGB 1860
BACK..                                /*BACKSUBSTITUTION             */MGB 1870
        DO I =LN TO 1 BY -1,.         /*********************************/MGB 1880
        PIV  =A(I,1),.                                                  MGB 1890
        IF PIV= 0                     /*TEST FOR ZERO PIVOT          */MGB 1900
        THEN DO,.                                                       MGB 1910
             ERROR='S',.              /*PIVOT ELEMENT IS ZERO        */MGB 1920
             GO TO RETURN,.                                             MGB 1930
             END,.                                                      MGB 1940
        INL  =I-1,.                                                     MGB 1950
             DO J =1 TO LM,.          /*LOOP OVER ALL COLUMNS OF R   */MGB 1960
             SUM  =R(I,J),.                                             MGB 1970
                  DO K =2 TO IBAC,.   /*CALCULATE SCALAR PRODUCT     */MGB 1980
                  SUM  =SUM-MULTIPLY(A(I,K),R(INL+K,J),53),.            MGB 1990
                  END,.                                                 MGB 2000
             R(I,J)=SUM/PIV,.         /*COMPUTE NEW ELEMENT IN R     */MGB 2010
             END,.                                                      MGB 2020
        IF IBAC LT NB                                                   MGB 2030
        THEN IBAC =IBAC+1,.           /*UPDATE END OF INNERMOST LOOP */MGB 2040
        END,.                                                           MGB 2050
RETURN..                                                                MGB 2060
   END,.                              /*END OF PROCEDURE MGB         */MGB 2070
```

Purpose:

MGB1 performs the following operations on an equation system $A \cdot X = R$ with general band matrix $A = L \cdot U$, depending on the character of an input parameter OPT:

OPT = 'L'	U replaces A and $L^{-1}R$ replaces R
OPT = 'U'	U replaces A and $U^{-1}R$ replaces R
OPT = 'B'	$U^{-1}R$ replaces R for a given U on storage locations of A
otherwise	U replaces A and the solution $X = A^{-1}R$ replaces R

The following table shows input and output depending on OPT:

MGB1 - OPT	'L'		'U'		'B'		otherwise	
INPUT	A	R	A	R	U	R	A	R
OUTPUT	U	$L^{-1} \cdot R$	U	$U^{-1} \cdot R$	U	$U^{-1} \cdot R$	U	$A^{-1} \cdot R$

Usage:

CALL MGB1 (A, R, N, NLD, NUD, M, EPS, OPT);

A(N, NB) - BINARY FLOAT [(53)]
Given N by N band matrix A consisting of the main diagonal, NLD lower codiagonals, and NUD upper codiagonals. A is stored rowwise and left-adjusted so that A(i, 1) contains the first nontrivial element in the i-th row of matrix A, i=1, 2, ..., N. Thus, the maximum number of elements in the rows of array A is:
NB = min (N, NLD + NUD + 1)
Resultant upper band factor U stored rowwise and left-adjusted so that A(i, 1) contains the diagonal element in the i-th row of the upper factor U, i=1, 2, ..., N. If OPT = 'B', A contains U.

R(N, M) - BINARY FLOAT [(53)]
Given right-hand-side matrix with N rows and M columns, which implies that M sets of right-hand-side vectors are given.
Resultant solution depending on the option parameter OPT (see "Purpose").

N - BINARY FIXED
Given row dimension of matrix A and number of rows of right-hand side R.

NLD - BINARY FIXED
Given number of lower codiagonals of matrix A.

NUD - BINARY FIXED
Given number of upper codiagonals of matrix A.

M - BINARY FIXED
Given number of columns of R, that is, number of right-hand-side vectors.

EPS - BINARY FLOAT
Given relative tolerance for test on loss of significant digits.

OPT - CHARACTER(1)
Given option parameter for selection of operation (see "Purpose").

Purpose:

MGB2 performs the following operations on an equation system $A \cdot X = R$ with general band matrix $A = L \cdot U$, depending on the character of an input parameter OPT:

OPT = 'L' A is replaced by upper band factor U, R is replaced by $L^{-1} \cdot R$, and lower band factor L is stored in a one-dimensional array L omitting the unit diagonal.

OPT = 'F' A is replaced by the upper band factor U and the lower band factor L is stored in the array L. The right-hand side R remains unchanged.

OPT = 'A' R is replaced by $L^{-1} \cdot R$ for the given upper factor U in array A and the lower factor L in vector L.

OPT = 'C' R is replaced by the solution $X = A^{-1} \cdot R$ for given U and L.

otherwise A is replaced by the upper factor U. The lower factor L is calculated and stored in L, and R is replaced by the solution $X = A^{-1} \cdot R$.

The following table shows input and output depending on OPT:

MGB2 - OPT	'L'			'F'			'A'			'C'			otherwise		
INPUT	A		R	A		R	U	L	R	U	L	R	A		R
OUTPUT	U	L	$L^{-1} \cdot R$	U	L	R	U	L	$L^{-1} \cdot R$	U	L	$A^{-1} \cdot R$	U	L	$A^{-1} \cdot R$

Usage:

CALL MGB2 (A, R, L, IPER, N, NLD, NUD, M, EPS, OPT);

A(N, NB) - BINARY FLOAT [(53)]
Given an N by N band matrix A consisting of the main diagonal, NLD lower codiagonals, and NUD upper codiagonals. A is stored rowwise and left-adjusted so that A(i, 1) contains the first nontrivial element in the i-th row of matrix A. Thus, the maximum number of elements in the rows of the array A is:
NB = min (N, NLD + NUD + 1)
Resultant upper band factor U stored rowwise and left-adjusted so that A(i, 1) contains the diagonal element in i-th row of U, i = 1, 2, ..., N. If OPT = 'A' or 'C', the array A contains U.

R(N, M) - BINARY FLOAT [(53)]
Given right-hand-side matrix with N rows and M columns, which implies that M sets of right-hand-side vectors are given.
Resultant solution depending on the option parameter OPT (see "Purpose").

L(N·NLD-NLD·(NLD+1)/2)
BINARY FLOAT [(53)]
Resultant one-dimensional array containing the lower factor L. If OPT = 'A' or 'C', array L contains the lower factor L, obtained by subroutine MGB2 with any other option parameter.

IPER(N) - BINARY FIXED
Resultant integer vector containing the permutations of rows of the matrix A in the factorization steps. If OPT = 'A' or 'C', permutation vector IPER must be given, obtained by MGB2 with OPT = 'A', 'C'.

N - BINARY FIXED
Given row dimension of matrix A and number of rows of right-hand side R.

NLD - BINARY FIXED
Given number of lower codiagonals of the matrix A.

NUD - BINARY FIXED
Given number of upper codiagonals of the matrix A.

M - BINARY FIXED
Given number of columns of R, that is, number of right-hand-side vectors.

EPS - BINARY FLOAT
Given relative tolerance for test on loss of significant digits.

OPT - CHARACTER(1)
Given option parameter for selection of operation (see "Purpose").

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='P' means error in specified parameters: M ≤ 0 or NLD < 0 or N ≤ NLD or NUD < 0 or N ≤ NUD

ERROR='S' means all elements in a row of the given matrix A are zero, or the calculated pivot in a factorization step is zero. This is possibly due to an ill-conditioned or singular matrix A.

ERROR='W' is a warning indicating possible loss of significance.

The storage mode for band matrices is a natural generalization of the normal two-dimensional storage scheme: any row is stored with NB=min (N, NLD+1+NUD) elements, but only the nontrivial elements (that is, those within the band) must be specified. The remaining elements are set to zero automatically within procedure MGB1/MGB2.

Note that a fully populated N by N matrix would require exactly N · N storage locations if stored as band matrix in compressed form. However, the unit lower triangular factor L would need additional N · (N-1)/2 storage locations.

Method:

Calculations of the lower and upper band factors L, U are done using a standard Gaussian elimination technique. Columnwise pivoting is built in, combined with scaling of rows (equilibration).

The lower band factor L is normalized such that the diagonal contains all ones, which are not stored (Doolittle factorization).

The procedure gets the required solutions by means of forward and/or backward substitutions, where the interchange information is combined with the lower band factor L.

For reference see:

R. S. Martin and J. H. Wilkinson, "Solution of Symmetric and Unsymmetric Band Equations on the

Calculation of Eigenvectors of Band Matrices", Numerische Mathematik, vol. 9, 1967, pp. 279-301.

Mathematical Background:

Let A be an N by N nonsingular real band matrix with NLD lower codiagonals and NUD upper codiagonals. In general, it can be factorized into a product

$$A = P \cdot L \cdot U$$

where L and U are lower and upper band factors respectively. L can be normalized so that it has a unit diagonal. P means the row-permutation matrix, that is, an N by N unit matrix with interchanged rows resulting from partial pivoting in the factorization steps.

Then $X = L^{-1} \cdot P^{-1} \cdot R = L^{-1} \bar{R}$ is calculated using forward substitution to obtain X from $L \cdot X = P^{-1} \cdot R = \bar{R}$, where $\bar{R}$ is obtained from R by interchanging rows in the same way that rows of matrix A are interchanged during columnwise pivoting in factorization.

Calculation of $Y = U^{-1} \cdot R$ is done using backward substitution to obtain Y from $U \cdot Y = R$.

Calculation of $Z = U^{-1} \cdot L^{-1} \cdot P^{-1} \cdot R = U^{-1} \cdot L^{-1} \cdot \bar{R}$ is done by first solving $L \cdot X = \bar{R}$ and then solving $U \cdot Z = X$.

Programming Considerations:

1. Storage Mode

The following is an example of a 7 by 7 matrix with two lower and three upper codiagonals which shows the storage compression of band matrices and the storage allocation of upper and lower triangular factors U and L.

Fully stored matrix:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} & 0 \\ 0 & a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ 0 & 0 & a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \\ 0 & 0 & 0 & a_{61} & a_{62} & a_{63} & a_{64} \\ 0 & 0 & 0 & 0 & a_{71} & a_{72} & a_{73} \end{pmatrix}$$

Compressed stored band matrix:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & x & x \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & x \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & x \\ a_{61} & a_{62} & a_{63} & a_{64} & x & x \\ a_{71} & a_{72} & a_{73} & x & x & x \end{pmatrix}$$

Elements marked X need not be specified. They get filled up with zeros automatically.

Resultant upper triangular factor U and unit lower triangular factor L:

$$U = \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} & u_{15} & u_{16} \\ u_{22} & u_{23} & u_{24} & u_{25} & u_{26} & u_{27} \\ u_{33} & u_{34} & u_{35} & u_{36} & u_{37} & 0 \\ u_{44} & u_{45} & u_{46} & u_{47} & 0 & 0 \\ u_{55} & u_{56} & u_{57} & 0 & 0 & 0 \\ u_{66} & u_{67} & 0 & 0 & 0 & 0 \\ u_{77} & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$L = \begin{pmatrix} l_{21} & & & & & \\ l_{31} & l_{32} & & & & \\ & l_{42} & l_{43} & & & \\ & & l_{53} & l_{54} & & \\ & & & l_{64} & l_{65} & \\ & & & & l_{75} & l_{76} \end{pmatrix}$$

The band-shaped upper triangular factor U is stored rowwise and left-adjusted, so that A(i, 1) contains the diagonal element for i = 1, 2, ..., N. The band-shaped lower unit triangular factor L is stored in a one-dimensional array. Only the non-trivial subdiagonal elements are stored columnwise in successive storage locations.

2. Computational remarks

In order to improve numerical stability, partial pivoting is used combined with an equilibration of rows. In each row i of the given matrix A the element a_{ij_i} of greatest absolute value is found. The absolute values $v_i = 1/\left|a_{ij_i}\right|$ are used as weights for pivoting:

At the first step of Gaussian elimination that element a_{kl} is used as pivot element piv for which

$$\left|a_{k1}\right| \cdot v_k = \max_{i=1,\ldots,NLD+1} \left(\left|a_{il}\right| \cdot v_i\right)$$

If necessary, rows k and l are interchanged in A, R and $V = \begin{pmatrix} v_1 \\ \cdot \\ \cdot \\ \cdot \\ v_N \end{pmatrix}$ and IPER(1) is set to k.

The elements in the first NLD rows are transformed by means of

$$l_{i1} = \frac{a_{i1}}{piv} \qquad i = 2,\ldots,NLD+1$$

$$a_{ij}^{(1)} = a_{ij} - l_{i1} \cdot a_{1j} \qquad j = 2,\ldots,NB$$

$$r_{ik}^{(1)} = r_{ik} - l_{i1} \cdot r_{1k} \qquad k = 1,\ldots,M$$

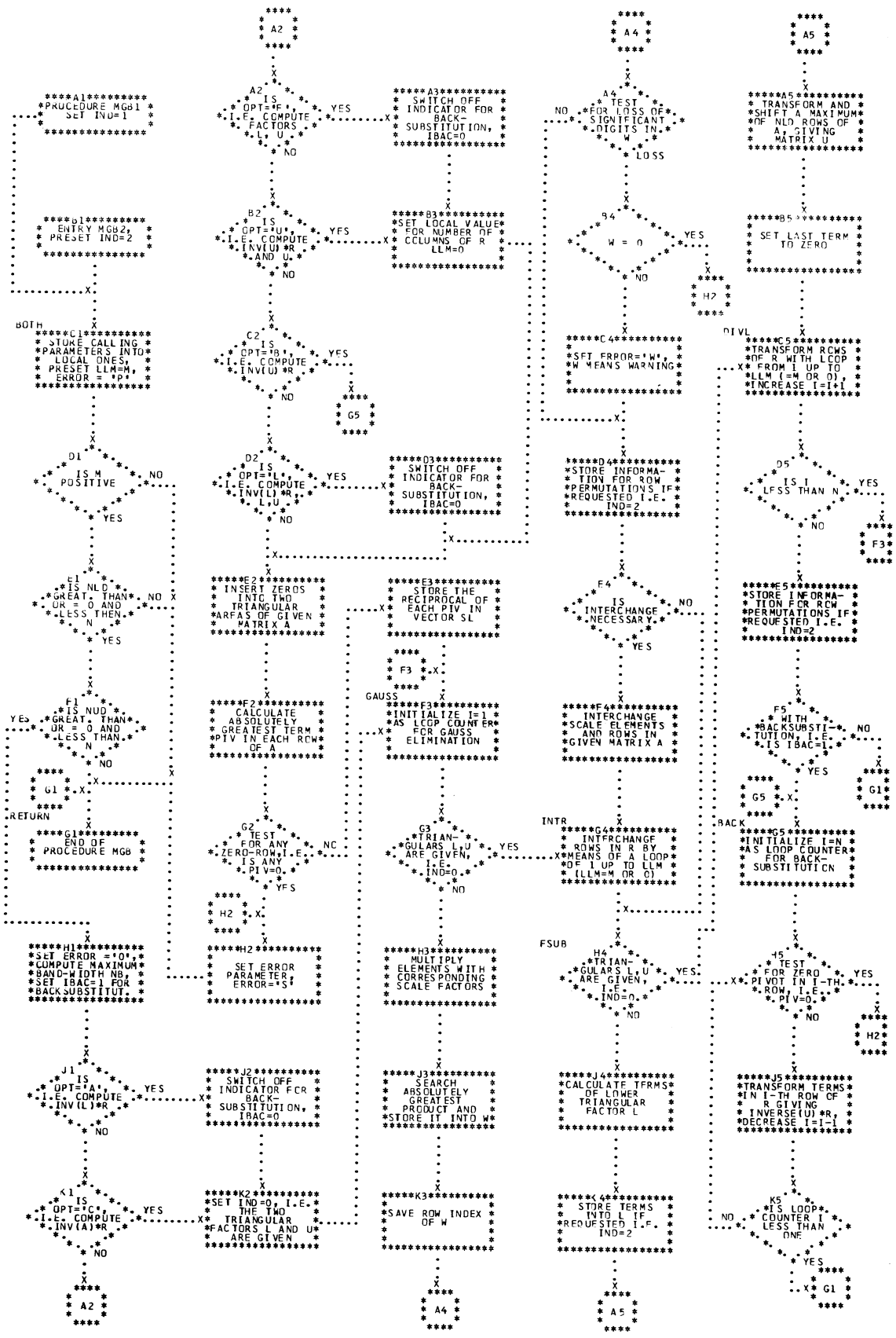
If specified, the elements l_{i1} are stored in successive locations within L.

Transformed rows of A get shifted to the left by one position, and zero is inserted in the last location.

Repeating this process (N-1) times gives triangular factors U and L and the product $L^{-1}R$, in permuted form.

If at an elimination step the value of piv becomes zero, then ERROR is set to 'S' and further calculation is bypassed.

ERROR is set to 'W' if, at elimination step j, $v_j \cdot piv \leq EPS$.


FOR AN EQUATION SYSTEM A*X=R WITH BAND MATRIX A=L*U
MGB1 OPTIONALLY COMPUTES X, U, INVERSE(L)*R, INVERSE(U)*R
MGB2 OPTIONALLY COMPUTES X, U, INVERSE(L)*R, AND L
A1 PROCEDURE MGB1 SET IND=1
B1 ENTRY MGB2, PRESET IND=2
BOTH
C1 STORE CALLING PARAMETERS INTO LOCAL ONES, PRESET LLM=M, ERROR = 'P'
D1 IS M POSITIVE
E1 IS NLD GREAT. THAN OR = 0 AND LESS THEN N
F1 IS NUD GREAT. THAN OR = 0 AND LESS THAN N
G1
RETURN
G1 END OF PROCEDURE MGB
A2
A2 IS OPT='F', I.E. COMPUTE FACTORS L, U
B2 IS OPT='U', I.E. COMPUTE INV(U)*R AND U
C2 IS OPT='B', I.E. COMPUTE INV(U)*R
G5
D2 IS OPT='L', I.E. COMPUTE INV(L)*R, L, U
E2 INSERT ZEROS INTO TWO TRIANGULAR ARFAS OF GIVEN MATRIX A
F2 CALCULATE ABSOLUTELY GREATEST TERM IN EACH ROW OF A
G2 TEST FOR ANY ZERO-ROW, I.E. IS ANY PIV=0
H2
H1 SET ERROR =10, COMPUTE MAXIMUM BAND-WIDTH NB, SET IBAC=1 FOR BACKSUBSTITUT.
H2 SET ERROR PARAMETER ERROR='S'
J1 IS OPT='A', I.E. COMPUTE INV(L)*R
J2 SWITCH OFF INDICATOR FOR BACK- SUBSTITUTION, IBAC=0
K1 IS OPT='C', I.E. COMPUTE INV(A)*R
K2 SET IND=0, I.E. THE TWO TRIANGULAR FACTORS L AND U ARE GIVEN
A2
A3 SWITCH OFF INDICATOR FOR BACK- SUBSTITUTION, IBAC=0
B3 SET LOCAL VALUE FOR NUMBER OF CCLUMNS OF R LLM=0
D3 SWITCH OFF INDICATOR FOR RECIPROCAL OF EACH PIV IN VECTOR SL
E3 STORE THE RECIPROCAL OF EACH PIV IN VECTOR SL
F3
GAUSS
F3 INITIALIZE I=1 AS LOOP COUNTER FOR GAUSS ELIMINATION
G3 TRIANGULARS L, U ARE GIVEN, I.E. IND=0
H3 MULTIPLY ELEMENTS WITH CORRESPONDING SCALE FACTORS
J3 SEARCH ABSOLUTELY GREATEST PRODUCT AND STORE IT INTO W
K3 SAVE ROW INDEX OF W
A4
A4 TEST FOR LOSS OF SIGNIFICANT DIGITS IN W
LOSS
B4 W = 0
H2
C4 SET ERROR='W', W MEANS WARNING
D4 STORE INFORMATION FOR ROW PERMUTATIONS IF REQUESTED I.E. IND=2
E4 IS INTERCHANGE NECESSARY
F4 INTERCHANGE SCALE ELEMENTS AND ROWS IN GIVEN MATRIX A
INTR
G4 INTERCHANGE ROWS IN R BY MEANS OF A LOOP OF L UP TO LLM (LLM=M OR 0)
FSUB
H4 TRIANGULARS L, U ARE GIVEN, I.E. IND=0
J4 CALCULATE TERMS OF LOWER TRIANGULAR FACTOR L
K4 STORE TERMS INTO L IF REQUESTED I.E. IND=2
A5
A5 TRANSFORM AND SHIFT A MAXIMUM OF NLD ROWS OF A, GIVING MATRIX U
B5 SET LAST TERM TO ZERO
DIVL
C5 TRANSFORM ROWS OF R WITH LOOP FROM I UP TO LLM (=M OR 0), INCREASE I=I+1
D5 IS I LESS THAN N
F3
E5 STORE INFORMATION FOR ROW PERMUTATIONS IF REQUESTED I.E. IND=2
F5 WITH BACKSUBSTITUTION, I.E. IS IBAC=1
G1
BACK
G5 INITIALIZE I=N AS LOOP COUNTER FOR BACK- SUBSTITUTION
H5 TEST FOR ZERO PIVOT IN I-TH ROW, I.E. PIV=0
H2
J5 TRANSFORM TERMS IN I-TH ROW OF R GIVING INVERSE(U)*R, DECREASE I=I-1
K5 IS LOOP COUNTER I LESS THAN ONE
G1

Eigenvalues and Related Topics

Note: The following example illustrates a way to link subroutines MATE, MEAT, MVAT, MVEB (which follow) for the computation of the eigenvalues and eigenvectors of a real nonsymmetric matrix. (Subroutines MATE and MVEB can be replaced with MATU and MVUB.)

Description of the parameters used:

A - Real array containing the given matrix (this matrix is not preserved)

N - Order of the matrix

H - Real array in which the Hessenberg matrix will be saved together with the elements of the transformations involved in subroutine MATE

CH - Complex array containing the Hessenberg matrix for the computation of the eigenvectors

EV - Complex array where the eigenvectors are stored

The other parameters are defined in the descriptions of the subroutines.

All the eigenvalues are assumed to be complex in this example, so that only N/2 eigenvectors are computed.

```
. . . . . .                                  / *              MAIN PROGRAM          * /
    N = 50, .
        BEGIN, .                             / *              BEGIN BLOCK           * /
        DECLARE
            (A(N, N), RR(N), RI(N), H(N, N))          BINARY,
            (CH(N, N), EIG, EV(N, N/2))               COMPLEX BINARY,
            (IP(N), I, J, K, M)                       BINARY FIXED,
            ANA(N)                                    BIT(1), .
        CALL GEN(A, N), .                    / *        GENERATE THE MATRIX        * /
        CALL MATE(A, N, IP), .               / *   REDUCTION TO HESSENBERG FORM    * /
        H = A, .                             / *       SAVE HESSENBERG MATRIX       * /
        CALL MEAT(A, N, RR, RI, ANA), .      / *      COMPUTE THE EIGENVALUES       * /
        I = 0, .
            DO M = 1 TO N BY 2, .            / *      COMPUTE N/2 EIGENVECTORS      * /
            I = I + 1, .
            EIG=COMPLEX(RR(M), RI(M)), .
            CH(1, *) = H (1, *), .           / *     PUT THE HESSENBERG MATRIX      * /
                DO J = 2 TO N, .             / *       INTO A COMPLEX ARRAY         * /
                    DO K=J - 1 TO N, .
                    CH(J, K) = H (J, K), .
                    END, .
                END, .
            CALL MVAT (CH, N, EIG, EV(*, I)), . / * EIGENVECTORS OF THE              * /
                                             / *   HESSENBERG MATRIX                 * /
            CALL MVEB(H, N, IP, EV(*, I)), . / * VECTORS OF THE GIVEN MATRIX         * /
            END, .
        PUT EDIT . . . . .                   / *   PRINT THE RESULTS                 * /
        END, .                               / *    END BEGIN BLOCK                  * /
. . . . . .                                  / *     MAIN PROGRAM
```

Note that the eigenvalues of the original matrix A are equal to the eigenvalues of the corresponding Hessenberg matrix, so that no back transformation of the eigenvalues is required.

- Subroutine MATE

```
MATE..
/*********************************************************************/
/*                                                                   */
/*          REDUCE A REAL MATRIX TO HESSENBERG FORM                  */
/*                    ELIMINATION TECHNIQUES                         */
/*                                                                   */
/*********************************************************************/
   PROCEDURE(A,N,IP),.
   DECLARE
        (A(*,*),C,U,V)
        BINARY,
        S
        BINARY(53),
        (N,IP(*),K,KP1,K1,M,I,J,N1)
        BINARY FIXED,.
   IF N LT 3 THEN GO TO EMATE,.
   IP(N)=N,.
   N1=N-1,.
        DO K=N1 TO 1 BY -1,.
        KP1=K+1,.
        K1=K-1,.
        M=K,.
        U=ABS(A(KP1,K)),.
             DO I=1 TO K1,.          /*          PIVOTING          */
             V=ABS(A(KP1,I)),.
             IF V GT U
             THEN DO,.
                  U=V,.
                  M=I,.
                  END,.
             END,.
        IP(K)=M,.
        IF M NE K
        THEN DO,.                    /*        INTERCHANGES        */
                  DO I=1 TO N,.      /*           COLUMNS          */
                  C=A(I,K),.
                  A(I,K)=A(I,M),.
                  A(I,M)=C,.
                  END,.
                  DO I=1 TO N,.      /*            ROWS            */
                  C=A(K,I),.
                  A(K,I)=A(M,I),.
                  A(M,I)=C,.
                  END,.
             END,.
        IF A(KP1,K) NE 0
        THEN DO I=1 TO K1,.          /* COEFFICIENTS OF ELIMINATION */
             A(KP1,I)=A(KP1,I)/A(KP1,K),.
             END,.
             DO I=N TO 1 BY -1,.     /*  K-TH ROW OF THE HESSENBERG */
             S=A(K,I),.              /*            MATRIX          */
                  DO J=1 TO K1,.
                  S=S+MULTIPLY(A(KP1,J),A(J,I),53),.
                  END,.
                  DO J=MAX(I+1,K) TO N1,.
                  S=S-MULTIPLY(A(K,J),A(J+1,I),53),.
                  END,.
             A(K,I)=S,.
             END,.
        END,.
EMATE..
   RETURN,.
   END,.                             /*    END OF PROCEDURE MATE    */
```

Purpose:

MATE reduces a given real matrix to upper almost triangular (Hessenberg) form by means of a sequence of similarities.

Usage:

CALL MATE (A, N, IP);

A(N, N) - BINARY FLOAT
Given real matrix.
Resultant upper almost triangular matrix.

N - BINARY FIXED
Given order of the matrix.

IP(N) - BINARY FIXED
Resultant vector containing information about the interchanges operated on rows and columns of the matrix.

Remarks:

The elements defining the transformations applied to the matrix are stored in place of the lower triangular part of the matrix on return. These elements and the vector IP will be used in the computation of the eigenvectors of the original matrix (Procedure MVEB).

Method:

Each row of the matrix is reduced in turn, starting from the last one, by applying a suitable elimination, and similarity is achieved by applying the left inverse transformation. A Crout-like algorithm is used to take advantage of the accumulation of the inner products in double precision.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical Background:

Let us consider a matrix A of order n and the similarity

$$TAT^{-1} = H \tag{1}$$

where H is a Hessenberg matrix associated with A, and T a lower triangular matrix with unit diagonal. Equation (1) can be written as

$$TA = HT \tag{2}$$

Matrices H and T will be determined row by row, according to the algorithm described below.

If rows (k+1) to n of H and rows k to n of T are assumed to be known, row k of H and row (k-1) of T will be determined as follows.

From equation (2) we get

$$a_{ki} = \sum_{j=1}^{k-1} t_{kj}\, a_{ji} = h_{ki} + \sum_{j=i+1}^{n} h_{kj}\, t_{ji}$$

and

$$h_{ki} = a_{ki} + \sum_{j=1}^{k-1} t_{kj}\, a_{ji} - \sum_{j=i+1}^{n} h_{kj}\, t_{ji} \tag{3}$$

If we apply equation (3) for i = n, n-1, . . ., k, we will obtain recursively the terms of the k-th row of H, excepting the subdiagonal term. (When the upper bound of a summation is less than the lower bound, the value of the sum is taken as zero.)

Let us determine now the (k-1)st row of T and the subdiagonal term

$$h_{k\,k-1} \text{ of H.}$$

From equation (2) we get

$$a_{ki} + \sum_{j=1}^{k-1} t_{kj}\, a_{ji} = \sum_{j=k-1}^{n} h_{kj}\, t_{ji}, \quad 1 \le i \le k-1$$

Defining

$$m_{ki} = a_{ki} + \sum_{j=1}^{k-1} t_{kj}\, a_{ji} - \sum_{j=k}^{n} h_{kj}\, t_{ji}, \quad 1 \le i \le k-1 \qquad (4)$$

we finally obtain

$$h_{k\,k-1} = m_{k\,k-1}, \quad t_{k-1\,i} = \frac{m_{ki}}{h_{k\,k-1}}, \quad 1 \le i \le k-2 \qquad (5)$$

To ensure stability, a technique of pivoting is incorporated in this algorithm.

After the computation of the m_{ki}'s, the subscript j is determined for which

$$\left| m_{kj} \right| \ge \left| m_{ki} \right|, \quad 1 \le i \le k-1$$

Then the elements m_{kj} and $m_{k\,k-1}$ are interchanged. So are columns j and (k-1) of T. Similarly, the columns and the rows of matrix A are also interchanged. Then equations (4) and (5) are applied.

The algorithm is initialized by taking

$$h_{nn} = a_{nn}$$

$$\left.\begin{aligned} m_{ni} &= a_{ni} \\ t_{ni} &= 0 \end{aligned}\right\} \quad 1 \le i \le n-1$$

$$t_{nn} = 1$$

When $m_{ki} = 0$ for $i = 1, \ldots, k-1$, $h_{k\,k-1} = 0$ and $t_{k-1\,i} = 0$ for $i = 1, \ldots, k-2$.

Programming considerations:

1. The interchanges determined by the pivoting are stored in vector IP. This vector will be used in the computation of the eigenvectors (subroutine MVEB).

2. The matrix T is stored in the lower part of the array A, overwriting the terms of the original matrix:

$$t_{I,J} \rightarrow A\,(I+1,\ J), \qquad 2 \le I \le N-1, \quad 1 \le J \le I-1$$

These elements $t_{I,J}$ will be used in the computation of the eigenvectors (subroutine MVEB). The last row and the diagonal of T are not stored.

3. The inner products involved in equations (3) and (4) are computed in double precision.

- Subroutine MATU

```
MATU..                                                                  MATU  10
/*********************************************************************/MATU  20
/*                                                                   */MATU  30
/*          REDUCE A REAL MATRIX TO HESSENBERG FORM                  */MATU  40
/*               HOUSEHOLDER'S TRANSFORMATIONS                       */MATU  50
/*                                                                   */MATU  60
/*********************************************************************/MATU  70
   PROCEDURE (A,N,B),.                                                  MATU  80
   DECLARE                                                              MATU  90
        (A(*,*),B(*),EPS,T,C,U) BINARY,                                 MATU 100
        S BINARY(53),                                                   MATU 110
        (I,J,K,KP1,KP2,N) BINARY FIXED,.                                MATU 120
   EPS=1.0E-14,.                                                        MATU 130
   B(1) =0,.                                                            MATU 140
        DO K=1 TO N-2,.                                                 MATU 150
        KP1  =K+1,.                                                     MATU 160
        KP2  =KP1+1,.                                                   MATU 170
        S    =0,.                    /* PREPARE K-TH TRANSFORMATION */MATU 180
             DO I=KP2 TO N,.                                            MATU 190
             S=S+MULTIPLY(A(I,K),A(I,K),53),.                           MATU 200
             END,.                                                      MATU 210
        T    =A(KP1,K)*A(KP1,K),.                                       MATU 220
        IF S GT EPS*T                                                   MATU 230
        THEN DO,.                                                       MATU 240
        S    =SQRT(S+T),.                                               MATU 250
             T    =S,.                /*  CHOOSE SIGN FOR STABILITY  */MATU 260
             IF A(KP1,K) GT 0 THEN T=-T,.                               MATU 270
             C    =A(KP1,K)-T,.                                         MATU 280
                  DO J=KP1 TO N,.     /*        ROW OPERATION        */MATU 290
                  S    =0,.                                            MATU 300
                       DO I=KP1 TO N,.                                  MATU 310
                       S=S+MULTIPLY(A(I,J),A(I,K),53),.                 MATU 320
                       END,.                                            MATU 330
                  U    =A(KP1,J),.                                     MATU 340
                  A(KP1,J)=S/T,.                                        MATU 350
                  U    =(A(KP1,J)-U)/C,.                               MATU 360
                       DO I=KP2 TO N,.                                  MATU 370
                       A(I,J)=A(I,J)+U*A(I,K),.                         MATU 380
                       END,.                                            MATU 390
                  END,.                                                 MATU 400
                  DO J=1 TO N,.       /*      COLUMN OPERATION       */MATU 410
                  S    =0,.                                            MATU 420
                       DO I=KP1 TO N,.                                  MATU 430
                       S=S+MULTIPLY(A(J,I),A(I,K),53),.                 MATU 440
                       END,.                                            MATU 450
                  U    =A(J,KP1),.                                     MATU 460
                  A(J,KP1)=S/T,.                                        MATU 470
                  U    =(A(J,KP1)-U)/C,.                               MATU 480
                       DO I=KP2 TO N,.                                  MATU 490
                       A(J,I)=A(J,I)+U*A(I,K),.                         MATU 500
                       END,.                                            MATU 510
                  END,.                                                 MATU 520
             B(KP1)=A(KP1,K),.                                          MATU 530
             A(KP1,K)=T,.             /*  TRANSFORM SUBDIAGONAL TERM */MATU 540
             END,.                                                      MATU 550
        ELSE B(KP1)=0,.               /*  BYPASS K-TH TRANSFORMATION */MATU 560
        END,.                                                           MATU 570
   RETURN,.                                                             MATU 580
   END,.                              /*    END OF PROCEDURE MATU    */MATU 590
```

Purpose:

MATU reduces a given real matrix to upper almost triangular (Hessenberg) form by means of a sequence of orthogonal transformations.

Usage:

CALL MATU (A, N, B);

A(N, N) - BINARY FLOAT
Given real matrix.
Resultant upper almost triangular matrix.

N - BINARY FIXED
Given order of the matrix.

B(N) - BINARY FLOAT
Resultant vector containing information about the transformations applied to the original matrix.

Remarks:

Other elements defining the transformations are stored in place of the lower triangular part of the matrix on return. These elements and the vector B will be used in the computation of the eigenvectors of the original matrix (Procedure MVUB).

Method:

Each column of the matrix is reduced in turn by means of orthogonal similarities (Householder's transformations).

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical Background:

For a given real matrix A of order n, let us consider the sequence of similarities

$$A^{(i+1)} = P_i A^{(i)} P_i^{-1} \quad i = 1, 2, \ldots, n-2$$

$$\text{with } A^{(1)} = A \tag{1}$$

Assuming that $A^{(i)}$ is of almost triangular form in its first (i-1) columns, we will determine a transformation P_i such that $A^{(i+1)}$ is of almost triangular form in its first i columns. Among the matrices P_i, let us consider those of the form

$$P_i = I - 2 u u^T \quad \text{(Householder's matrices)} \tag{2}$$

where I is the unit matrix and u a vector of order n such that

$$< u, u > = 1 \tag{3}$$

These matrices are orthogonal and symmetric, and equation (1) can be written as

$$A^{(i+1)} = P_i A^{(i)} P_i \tag{4}$$

Let us now define a vector v by

$$v^T = (v_1, v_2, \ldots, v_n),$$

with

$$v_k = 0 \text{ for } k = 1, 2, \ldots, i$$

$$v_k = a^{(i)}_{k,\,i} \text{ for } k = i + 1, \ldots, n$$

and try to determine the transformation P_i so that

$$P_i v = be_{i+1} \quad \text{where } b = \pm \langle v, v \rangle^{1/2} \qquad (5)$$

e_{i+1} is a vector whose components are zero, except for the (i+1) st which is one.

The combination of equations (2) and (5) gives

$$P_i v = v - 2\langle u, v \rangle u$$

$$= be_{i+1}$$

Putting $\langle u, v \rangle = s$, u is given by

$$u = \frac{v - be_{i+1}}{2s}$$

From equation (3) we get

$$s^2 = b(b - v_{i+1})/2$$

Then the matrix P_i can be written as

$$P_i = I + \frac{1}{b(v_{i+1} - b)} (v - be_{i+1})(v - be_{i+1})^T$$

The sign of b will be such that the magnitude of the denominator is maximum, that is,

$$\text{sign } (b) = - \text{ sign } (v_{i+1})$$

in order to ensure stability.

If we now form the product $P_i A^{(i)}$, the resulting matrix, according to (5), will have zeros in positions (k, i), k = 1 + 2, ..., n, and the term in position (i+1, i) will be b. The (i-1) first columns and rows remain unaltered.

The right transformation $(P_i A^{(i)}) P_i$, completing the similarity, will leave this structure unchanged. Thus, after (n-2) transformations according to (1) and (4), the matrix will be reduced to almost triangular form.

When the matrix is symmetric, it is interesting to note that the resulting almost triangular form is symmetric also (that is, tridiagonal).

Programming Considerations:

A transformation P_i for which $|v_{i+1} + b| < 10^{-7}|b|$ is bypassed. All the scalar products involved in the computation are calculated in double precision.

- Subroutine MSTU

```
MSTU..                                                                  MSTU  10
/*********************************************************************/MSTU  20
/*                                                                   */MSTU  30
/* REDUCE A COMPRESSED SYMMETRIC MATRIX TO SYMMETRIC TRIDIAGONAL FORM*/MSTU  40
/*                                                                   */MSTU  50
/*********************************************************************/MSTU  60
   PROCEDURE (A,N,D,CD),.                                               MSTU  70
   DECLARE                                                              MSTU  80
        (A(*),D(*),CD(*),T,EPS) BINARY,                                 MSTU  90
        (N,N2,ICD,MP2,M,MP,J,I,L,LK,K) BINARY FIXED,                    MSTU 100
        (S,DT) BINARY(53),.                                             MSTU 110
   N2   =N-2,.                                                          MSTU 120
   IF N2 LE 0 THEN GO TO EMSTU,.                                        MSTU 130
   D(1) =A(1),.                                                         MSTU 140
   EPS  =1.0E-14,.                                                      MSTU 150
   ICD  =0,.                                                            MSTU 160
   MP2  =2,.                                                            MSTU 170
        DO M=1 TO N2,.              /* COMPUTE NEW SUBDIAGONAL TERM*/MSTU 180
        MP   =MP2,.                                                     MSTU 190
        MP2  =MP+1,.                                                    MSTU 200
        ICD  =ICD+MP,.                                                  MSTU 210
        J    =ICD,.                                                     MSTU 220
        S    =0,.                                                       MSTU 230
             DO I=MP2 TO N,.                                            MSTU 240
             J    =J+I-1,.                                              MSTU 250
             D(I) =A(J),.                                               MSTU 260
             S=S+MULTIPLY(D(I),D(I),53),.                               MSTU 270
             END,.                                                      MSTU 280
        T    =A(ICD)*A(ICD),.                                           MSTU 290
        IF S GT T*EPS THEN GO TO TRANS,.                                MSTU 300
        CD(M)=A(ICD),.              /*    BYPASS TRANSFORMATION    */MSTU 310
        GO TO BYPASS,.                                                  MSTU 320
TRANS..                                                                 MSTU 330
        CD(M)=SQRT(S+T),.                                               MSTU 340
        IF A(ICD) GT 0 THEN CD(M)=-CD(M),.                              MSTU 350
        D(MP)=A(ICD)-CD(M),.                                            MSTU 360
        J    =ICD-M,.                                                   MSTU 370
        DT   =0,.                   /*   COMPUTE VECTORS DEFINING  */MSTU 380
             DO L=MP TO N,.         /*      THE TRANSFORMATION     */MSTU 390
             J    =J+L-1,.                                              MSTU 400
             S    =0,.                                                  MSTU 410
             LK   =J,.                                                  MSTU 420
                  DO K=MP TO L,.                                        MSTU 430
                  LK   =LK+1,.                                          MSTU 440
                  S=S+MULTIPLY(A(LK),D(K),53),.                         MSTU 450
                  END,.                                                 MSTU 460
                  DO K=L+1 TO N,.                                       MSTU 470
                  LK   =LK+K-1,.                                        MSTU 480
                  S=S+MULTIPLY(A(LK),D(K),53),.                         MSTU 490
                  END,.                                                 MSTU 500
             DT   =DT+S*D(L),.                                          MSTU 510
             CD(L)=S,.                                                  MSTU 520
             END,.                                                      MSTU 530
        DT   =0.5*DT,.                                                  MSTU 540
        T    =D(MP)*CD(M),.                                             MSTU 550
             DO L=MP TO N,.                                             MSTU 560
             D(L) =D(L)/T,.                                             MSTU 570
             CD(L)=CD(L)+DT*D(L),.                                      MSTU 580
             END,.                                                      MSTU 590
        J    =ICD-M,.               /*      PERFORM SIMILARITY     */MSTU 600
             DO K=MP TO N,.                                             MSTU 610
             J    =J+K-1,.                                              MSTU 620
             LK   =J,.                                                  MSTU 630
                  DO L=MP TO K,.                                        MSTU 640
                  LK   =LK+1,.                                          MSTU 650
                  S    =A(LK),.                                         MSTU 660
                  S=S+MULTIPLY(D(L),CD(K),53)+MULTIPLY(D(K),CD(L),53),.MSTU 670
                  A(LK)=S,.                                             MSTU 680
                  END,.                                                 MSTU 690
             END,.                                                      MSTU 700
BYPASS..                                                                MSTU 710
        D(MP)=A(ICD+1),.                                                MSTU 720
        END,.                                                           MSTU 730
   ICD  =ICD+N,.                                                        MSTU 740
   CD(N)=A(ICD),.                                                       MSTU 750
   D(N) =A(ICD+1),.                                                     MSTU 760
        DO J=N-1 TO 2 BY -1,.                                           MSTU 770
        CD(J)=CD(J-1),.                                                 MSTU 780
        END,.                                                           MSTU 790
   CD(1)=0,.                                                            MSTU 800
EMSTU..                                                                 MSTU 810
   RETURN,.                                                             MSTU 820
   END,.                            /*   END OF PROCEDURE MSTU    */MSTU 830
```

Purpose:

MSTU reduces a given real symmetric matrix to tridiagonal form by means of a sequence of orthogonal transformations.

Usage:

CALL MSTU (A, N, D, CD);

A(N*(N+1)/2) - BINARY FLOAT
Given matrix in compressed storage mode.

N - BINARY FIXED
Given order of the matrix.

D(N) - BINARY FLOAT
Resultant vector containing the diagonal terms of the tridiagonal matrix.

CD(N) - BINARY FLOAT
Resultant vector containing the co-diagonal terms of the tridiagonal matrix in positions 2, 3, ..., N.

Remarks:

The elements defining the transformations applied to the matrix will replace the given matrix in array A. These elements will be used in the computation of the eigenvectors of the original matrix (subroutine MVSU).

Method:

Each row and column of the matrix is reduced in turn by means of orthogonal similarities (Householder's transformations).

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.

Mathematical Background:

We know that a matrix A of order n can be reduced to almost triangular form by means of (n-2) successive unitary similarities (see description of subroutine MATU). Furthermore, when A is symmetric, these transformations preserve the property of symmetry, and the resulting matrix is symmetric and tridiagonal. Let us consider the sequence of such similarities that reduces A to the tridiagonal form $A^{(n-1)}$.

$$A^{(i+1)} = P_i A^{(i)} P_i, \quad A^{(1)} = A,$$

$$i = 1, 2, \ldots, n-2$$

where $A^{(i)}$ is assumed to be of tridiagonal form in its first (i-1) rows and symmetric, and where P_i is the Householder matrix such that $A^{(i+1)}$ is of tridiagonal form in its first i rows. We know that P_i is defined by

$$P_i = I + \frac{1}{b(v_{i+1}-b)} (v - be_{i+1}) (v - be_{i+1})^T$$

where:

$$v^T = (v_1, v_2, \ldots, v_n)$$

$$v_k = 0, \text{ for } k = 1, 2, \ldots, i$$

$$v_k = a^{(i)}_{k,i}, \text{ for } k = i+1, \ldots, n$$

$$b = \pm < v, v >^{1/2}, \text{ sign } (b) = - \text{ sign } (v_{i+1})$$

and where e_{i+1} is a vector whose (i+1)st component is one, the others being zero (see mathematical description of subroutine MATU).

Putting $x = v - be_{i+1}$ and $\alpha = \left[b (v_{i+1} - b)\right]^{-1}$, we have

$$\begin{aligned} P_i A^{(i)} P_i &= A^{(i)} + \alpha A^{(i)} xx^T + \alpha xx^T A^{(i)} \\ &\quad + \alpha^2 < x, A^{(i)} x > xx^T \\ &= A^{(i)} + \left[A^{(i)} x + 1/2 < x, A^{(i)} x> \right. \\ &\quad \left. \alpha x\right] \alpha x^T \\ &\quad + \alpha x \left[x^T A^{(i)} + 1/2 \right. \\ &\quad \left. < x, A^{(i)} x > \alpha x^T\right] \end{aligned}$$

Since $A^{(i)} = A^{(i)T}$, this can be written as

$$P_i A^{(i)} P_i = A^{(i)} + YZ^T + ZY^T \qquad (1)$$

where

$$Y = \left[A^{(i)} + \frac{\alpha}{2} < x, A^{(i)} x > I\right] x \qquad (2)$$

$$Z = \alpha x$$

Programming Considerations:

In the subroutine each similarity is performed on the upper part of the matrix according to equations (1) and (2).

The scalar products needed by the process are computed in double precision.

- Subroutine MEAT

```
MEAT..                                                                  MEAT  10
/*********************************************************************/MEAT  20
/*                                                                   */MEAT  30
/*          EIGENVALUES OF A REAL HESSENBERG MATRIX                  */MEAT  40
/*                                                                   */MEAT  50
/*********************************************************************/MEAT  60
   PROCEDURE (A,M,RR,RI,ANA),.                                          MEAT  70
   DECLARE                                                              MEAT  80
        ANA(*) BIT(1),                                                  MEAT  90
        (A(*,*),RR(*),RI(*),PRR(2),PRI(2),PAN(2),R,S,EPS,E6,E7,E12,H,T,MEAT 100
         U,V,G1,G2,G3,PSI1,PSI2,PHI,ETA) BINARY,                        MEAT 110
        (I,I1,I2,IP1,IP2,IP3,IT,ITMAX,J,K,N,N1,N2,P,Q,M) BINARY FIXED,.MEAT 120
   E6   =1.0E-6,.                    /*          CONSTANTS            */MEAT 130
   E7   =1.0E-7,.                                                       MEAT 140
   E12  =1.0E-12,.                                                      MEAT 150
   H    =0.5,.                                                          MEAT 160
   ITMAX=30,.                                                           MEAT 170
   N    =M,.                                                            MEAT 180
BEG..                                 /*        INITIALIZATION        */MEAT 190
   N1   =N-1,.                                                          MEAT 200
   IF N1=0 THEN GO TO ONE,.                                             MEAT 210
   R,S  =0,.                                                            MEAT 220
        DO I=1,2,.                                                      MEAT 230
        PAN(I),PRR(I),PRI(I)=0,.                                        MEAT 240
        END,.                                                           MEAT 250
   N2   =N1-1,.                                                        MEAT 260
        DO IT=1 TO ITMAX,.              /*   START LOOP FOR ITERATION  */MEAT 270
        IF ABS(A(N,N1)) LE E12*ABS(A(N,N)) THEN GO TO ONE,.             MEAT 280
        T     =A(N1,N1)-A(N,N),.        /*   ROOTS OF THE LOWER MAIN   */MEAT 290
        U     =T*T,.                    /*    SUBMATRIX OF ORDER TWO   */MEAT 300
        V     =4*A(N1,N)*A(N,N1),.                                      MEAT 310
        IF ABS(V) LT U*E7                                               MEAT 320
        THEN DO,.                                                       MEAT 330
             RR(N1)=A(N1,N1),.                                          MEAT 340
             RR(N) =A(N,N),.                                            MEAT 350
             GO TO ZIM,.                                                MEAT 360
             END,.                                                      MEAT 370
        ELSE DO,.                                                       MEAT 380
             T    =U+V,.                                                MEAT 390
             IF ABS(T) LT E6*MAX(U,ABS(V)) THEN T=0,.                   MEAT 400
             U    =(A(N1,N1)+A(N,N))/2,.                                MEAT 410
             V    =SQRT(ABS(T))/2,.                                     MEAT 420
             IF T LT 0                                                  MEAT 430
             THEN DO,.                  /*        COMPLEX ROOTS       */MEAT 440
                  RR(N),RR(N1)=U,.                                      MEAT 450
                  RI(N)=-V,.                                            MEAT 460
                  RI(N1)=V,.                                            MEAT 470
                  END,.                                                 MEAT 480
             ELSE DO,.                  /*         REAL ROOTS         */MEAT 490
                  RR(N)=U+V,.                                           MEAT 500
                  RR(N1)=U-V,.                                          MEAT 510
ZIM..                                                                   MEAT 520
                  RI(N),RI(N1)=0,.                                      MEAT 530
                  IF ABS(RR(N1)) LT ABS(RR(N))                          MEAT 540
                  THEN DO,.                                             MEAT 550
                       T    =RR(N1),.                                   MEAT 560
                       RR(N1)=RR(N),.                                   MEAT 570
                       RR(N)=T,.                                        MEAT 580
                       END,.                                            MEAT 590
                  END,.                                                 MEAT 600
             END,.                                                      MEAT 610
        IF N2=0 THEN GO TO TWO,.        /*     TESTS OF CONVERGENCE   */MEAT 620
        EPS  =E12*(RI(N1)+ABS(RR(N1))),.                                MEAT 630
        IF ABS(A(N1,N2)) LE EPS THEN GO TO TWO,.                        MEAT 640
        IF ABS(A(N1,N2)-PAN(1)) LT ABS(A(N1,N2))*E6 THEN GO TO CMP,.    MEAT 650
        IF ABS(A(N,N1)-PAN(2)) LT ABS(A(N,N1))*E6 THEN GO TO CMP,.      MEAT 660
        K    =0,.                                                       MEAT 670
             DO I=1,2,.                 /*     DETERMINE THE SHIFT    */MEAT 680
             J=I+N2,.                                                   MEAT 690
             IF ABS(RR(J)-PRR(I))+ABS(RI(J)-PRI(I))                     MEAT 700
                LT H*(ABS(RR(J))+ABS(RI(J))) THEN K=K+I,.               MEAT 710
             PRR(I)=RR(J),.                                             MEAT 720
             PRI(I)=RI(J),.                                             MEAT 730
             PAN(I)=A(J,J-1),.                                          MEAT 740
             END,.                                                      MEAT 750
        IF K=0                                                          MEAT 760
        THEN R,S  =0,.                                                  MEAT 770
        ELSE IF K=3                                                     MEAT 780
             THEN DO,.                                                  MEAT 790
                  S    =A(N,N)+A(N1,N1),.                               MEAT 800
                  R    =A(N,N)*A(N1,N1)-A(N1,N)*A(N,N1),.               MEAT 810
                  END,.                                                 MEAT 820
             ELSE DO,.                                                  MEAT 830
                  R    =PRR(K)*PRR(K),.                                 MEAT 840
                  S    =PRR(K)+PRR(K),.                                 MEAT 850
                  END,.                                                 MEAT 860
        IF N LT 4                       /*    SEARCH FOR A PARTITION  */MEAT 870
        THEN P,Q  =1,.                                                  MEAT 880
        ELSE DO,.                                                       MEAT 890
                  DO Q=N2 TO 2 BY -1,.                                  MEAT 900
                  IF ABS(A(Q,Q-1)) LE EPS THEN GO TO FDP,.              MEAT 910
                  END,.                                                 MEAT 920
             Q    =1,.                                                  MEAT 930
FDP..                                                                   MEAT 940
             IF Q LT N2                                                 MEAT 950
             THEN DO P=N2 TO Q+1 BY -1,.                                MEAT 960
                  IP1  =P+1,.                                           MEAT 970
                  IF (ABS(A(P,P)+A(IP1,IP1)-S)+ABS(A(IP1+1,IP1)))       MEAT 980
                      *ABS(A(P,P-1)*A(IP1,P))                           MEAT 990
                     LT EPS*ABS(A(P,P)*(A(P,P)-S)+A(P,IP1)*A(IP1,P)+R) MEAT1000
                  THEN GO TO QRT,.                                      MEAT1010
                  END,.                                                 MEAT1020
             P    =Q,.                                                  MEAT1030
             END,.                                                      MEAT1040
QRT..                                                                   MEAT1050
        DO I=P TO N1,.                  /*   START QR TRANSFORMATION  */MEAT1060
        IP1  =I+1,.                                                     MEAT1070
        IP2  =IP1+1,.                                                   MEAT1080
        I1   =I-1,.                                                     MEAT1090
        IF I=P                                                          MEAT1100
        THEN DO,.                       /*  INITIALIZE TRANSFORMATION */MEAT1110
             G1   =A(I,I)*(A(I,I)-S)+A(I,IP1)*A(IP1,I)+R,.              MEAT1120
             G2   =A(IP1,I)*(A(IP1,IP1)+A(I,I)-S),.                     MEAT1130
             G3   =A(IP1,I)* A(IP2,IP1),.                               MEAT1140
             A(IP2,I)=0,.                                               MEAT1150
             END,.                                                      MEAT1160
        ELSE DO,.                                                       MEAT1170
             G1   =A(I,I1),.                                            MEAT1180
             G2   =A(IP1,I1),.                                          MEAT1190
             IF I GT N2                                                 MEAT1200
             THEN G3   =0,.                                             MEAT1210
             ELSE G3   =A(IP2,I1),.                                     MEAT1220
             END,.                                                      MEAT1230
        U    =SQRT(G1*G1+G2*G2+G3*G3),.                                 MEAT1240
        IF U=0                                                          MEAT1250
        THEN DO,.                                                       MEAT1260
             PHI  =2,.                                                  MEAT1270
             PSI1,PSI2=0,.                                              MEAT1280
             END,.                                                      MEAT1290
        ELSE DO,.                                                       MEAT1300
             IF G1 LT 0 THEN U=-U,.                                     MEAT1310
             T    =G1+U,.                                               MEAT1320
             PSI1 =G2/T,.                                               MEAT1330
             PSI2 =G3/T,.                                               MEAT1340
             PHI  =2/(1+PSI1*PSI1+PSI2*PSI2),.                          MEAT1350
             END,.                                                      MEAT1360
        IF I=Q THEN GO TO ROW,.                                         MEAT1370
        IF I=P THEN A(I,I1)=-A(I,I1),.                                  MEAT1380
               ELSE A(I,I1)=-U,.                                        MEAT1390
ROW..                                                                   MEAT1400
             DO J=I TO N,.              /*        ROW OPERATION       */MEAT1410
             T    =PSI1*A(IP1,J),.                                      MEAT1420
             IF I LT N1 THEN T=T+PSI2*A(IP2,J),.                        MEAT1430
             ETA  =PHI*(T+A(I,J)),.                                     MEAT1440
             A(I,J)=A(I,J)-ETA,.                                        MEAT1450
             A(IP1,J)=A(IP1,J)-PSI1*ETA,.                               MEAT1460
             IF I LT N1 THEN A(IP2,J)=A(IP2,J)-PSI2*ETA,.               MEAT1470
             END,.                                                      MEAT1480
        IF I LT N1                      /*        COLUMN OPERATION    */MEAT1490
        THEN K    =IP2,.                                                MEAT1500
        ELSE K    =N,.                                                  MEAT1510
             DO J=Q TO K,.                                              MEAT1520
             T    =PSI1*A(J,IP1),.                                      MEAT1530
             IF I LT N1 THEN T=T+PSI2*A(J,IP2),.                        MEAT1540
             ETA  =PHI*(T+A(J,I)),.                                     MEAT1550
             A(J,I)=A(J,I)-ETA,.                                        MEAT1560
             A(J,IP1)=A(J,IP1)-ETA*PSI1,.                               MEAT1570
             IF I LT N1 THEN A(J,IP2)=A(J,IP2)-ETA*PSI2,.               MEAT1580
             END,.                                                      MEAT1590
        IF I LT N2                                                      MEAT1600
        THEN DO,.                                                       MEAT1610
             IP3  =IP2+1,.                                              MEAT1620
             ETA  =PHI*PSI2*A(IP3,IP2),.                                MEAT1630
             A(IP3,I)=-ETA,.                                            MEAT1640
             A(IP3,IP1)=-ETA*PSI1,.                                     MEAT1650
             A(IP3,IP2)=A(IP3,IP2)-ETA*PSI2,.                           MEAT1660
             END,.                                                      MEAT1670
        END,.                           /*    END QR TRANSFORMATION   */MEAT1680
        END,.                           /*    END LOOP OF ITERATION   */MEAT1690
CMP..                                                                   MEAT1700
   IF ABS(A(N,N1)) GT ABS(A(N1,N2))                                     MEAT1710
   THEN                                                                 MEAT1720
TWO..                                                                   MEAT1730
        DO,.                            /*  TWO EIGENVALUES HAVE BEEN */MEAT1740
        ANA(1)='1'B,.                   /*          FOUND             */MEAT1750
        ANA(N)='0'B,.                                                   MEAT1760
        N    =N2,.                                                      MEAT1770
        END,.                                                           MEAT1780
   ELSE                                                                 MEAT1790
ONE..                                                                   MEAT1800
        DO,.                            /*ONE EIGENVALUE HAS BEEN FOUND*/MEAT1810
        ANA(N)='1'B,.                                                   MEAT1820
        RR(N)  =A(N,N),.                                                MEAT1830
        RI(N)  =0,.                                                     MEAT1840
        N    =N1,.                                                      MEAT1850
        END,.                                                           MEAT1860
   IF N GT 0 THEN GO TO BEG,.                                           MEAT1870
   RETURN,.                                                             MEAT1880
   END,.                            /*    END OF PROCEDURE MEAT     */MEAT1890
```

Purpose:

MEAT computes the eigenvalues of a real upper almost triangular matrix (Hessenberg form -- see subroutines MATE and MATU) using the double QR iteration.

Usage:

CALL MEAT (A, M, RR, RI, ANA);

A(M, M) - BINARY FLOAT
Given almost triangular matrix.

M - BINARY FIXED
Given order of the matrix.

RR(M) - BINARY FLOAT
Resultant vector containing the real parts of the eigenvalues.

RI(M) - BINARY FLOAT
Resultant vector containing the imaginary parts of the eigenvalues.

ANA(M) - BIT(1)
Resultant vector containing information for checking the results (see "Programming Considerations", below).

Remarks:

The original matrix is destroyed.

Method:

Double QR iteration of J. G. F. Francis

For reference see:

J. G. F. Francis, Computer Journal, October 1961, 4-3; January 1962, 4-4.
J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical Background:

1. Definition of the QR iteration

Let A be a real or complex nonsingular matrix of order n. Then a decomposition of A exists of the form

$$A = Q\,R$$

where Q is unitary and R is upper triangular. If the diagonal elements of R are real and positive, Q is unique. Consider now the sequence of matrices $A^{(p)}$ defined recursively by

$$A^{(o)} = A,\ A^{(p)} = Q^{(p)}\,R^{(p)},\ A^{(p+1)} = R^{(p)}Q^{(p)} p \geq 0.$$

Note that $A^{(p+1)} = Q^{(p)*}\,A^{(p)}\,Q^{(p)}$ for $p \geq 0$; hence, $A^{(p)}$ is similar to A for all p.

Furthermore, if A satisfies certain conditions, it can be proved that $A^{(p)}$ tends to an upper triangular matrix as $p \to \infty$; thus the eigenvalues of A are the diagonal elements of this limit matrix.

2. Convergence

If the moduli of the eigenvalues are distinct, the elements $a_{ij}^{(p)}$ below the main diagonal of $A^{(p)}$ tend to zero, as do $|\lambda_i|^p/|\lambda_j|^p$, the eigenvalues being subscripted so that $|\lambda_i| > |\lambda_{i+1}|$.

Thus, in general, the eigenvalues appear on the main diagonal, starting from the last position, in increasing order of moduli.

So, when the smallest eigenvalue λ_n has been found, we can reduce the order of the matrix by neglecting the last row and column and find λ_{n-1} by the same process, without any special deflation.

Note that the speed of convergence is considerably improved when the origin of the eigenvalues is shifted close to λ_n.

Such a shift -- say, $s^{(p)}$ -- can be introduced before an iteration and the opposite one afterwards. Then the iteration can be written as:

$$A^{(p)} - s^{(p)}\,I = Q^{(p)}\,R^{(p)}$$

$$A^{(p+1)} = R^{(p)}\,Q^{(p)} + s^{(p)}\,I$$

In general, $A_{n,n}^{(p)}$, for p large enough, can provide an efficient value for $s^{(p)}$.

3. Use of the Hessenberg form

The Hessenberg form is preserved under the QR iteration. Thus, a reduction of the initial matrix to the Hessenberg form can give a significant saving of computation in each iteration for the QR decomposition, the lower part of the matrix consisting only of the codiagonal terms.

Before each iteration, the codiagonal terms will be inspected. If some of these are zero, the matrix will be split according to this occurrence, and the iteration will be applied to the lower main submatrix only.

4. The double QR iteration

Let A be a diagonalizable real upper Hessenberg matrix. Such a matrix must be expected to have complex conjugate pairs of eigenvalues. If these pairs are the only eigenvalues of equal modulus, it can be shown that they will appear as the latent roots of main submatrices of order 2. In this case, if a shift is close to one of these roots, it will be complex, and we will have to deal with complex matrices, although the initial one is real. The use of the double QR iteration avoids this inconvenience.

Taking $s^{(p+1)} = \bar{s}^{(p)}$, consider the transformation giving $A^{(p+2)}$ from $A^{(p)}$:

$$A^{(p+2)} = Q^{(p+1)*}\,Q^{(p)*}\,A^{(p)}\,Q^{(p)}\,Q^{(p+1)}$$

It can be proved that the product $Q^{(p)}Q^{(p+1)}$ derives from the QR decomposition of the matrix $M = (A^{(p)} - s^{(p)}\,I)\,(A^{(p)} - s^{(p+1)}\,I)$, which is real.

In fact, Francis (1961, 1962) showed that only the first column m_1 of M is necessary for determining the transformation which gives $A^{(p+2)}$ from $A^{(p)}$, if they both have the Hessenberg form.

Practically, the first part of the double iteration consists of the application of an initial transformation $N_1^*\,A^{(p)}\,N_1$ where N_1 is unitary and such that $N_1^*\,m_1 = \pm \|m_1\|\,e_1$. This leads to a matrix that no longer has the Hessenberg form.

Thus, the remaining part of the iteration will involve the application of (n-1) successive transformations, which have the same form as the initial one whose matrices N_i are such that the resulting matrix $A^{(p+2)}$ has the Hessenberg form.

This process can fail when a subdiagonal term of the given matrix is zero. In this case, the matrix can be split, and the iteration is performed on the lower main submatrix only.

In the subroutine, N_i are Householder's matrices.

Programming Considerations:

At each iteration, the latent roots x_1 and x_2 of the lower main submatrix of order 2 are computed. Then the following situations can occur:

1. The term $a_{n-1,n-2}$ can be taken as zero. Then x_1 and x_2 are eigenvalues of the original matrix, and the order of the matrix is reduced by 2. ANA(N) and ANA(N-1) are set to 0 and 1 respectively.

2. The term $a_{n,n-1}$ can be taken as zero. In this case, $a_{n,n}$ is an eigenvalue of the original matrix, and the order of the matrix is reduced by 1. ANA(N) is set to 1.

3. One of the last two subdiagonal terms is stable through one iteration. Then the smaller one is considered as zero. The corresponding components of ANA are set to 0 or 1, according to situation 1 or 2.

4. The maximum number of iterations is reached. In this case the smaller of the last two subdiagonal elements is taken as zero. The corresponding components of ANA are set to 0 or 1, according to situation 1 or 2.

The user can check the results by inspecting the subdiagonal terms of the matrix on return from the subroutine, according to the vector ANA, in the following way: If, for each ANA(I) containing 1,

$$|A(I,I-1)| \leq 10^{-7} \left(|RR(I)| + |RI(I)| \right),$$

$$i = 2, \ldots, M$$

then RR(I) and RI(I) were computed with a satisfactory accuracy.

- Subroutine MEST

```
MEST..                                                                  MEST  10
/*********************************************************************/MEST  20
/*                                                                   */MEST  30
/*        EIGENVALUES OF A SYMMETRIC TRIDIAGONAL MATRIX              */MEST  40
/*                                                                   */MEST  50
/*********************************************************************/MEST  60
   PROCEDURE (A,B,M,D,NEIG),.                                           MEST  70
   DECLARE                                                              MEST  80
        (MIT,M,N,NEIG,NR,I,K,IT,J,IP) BINARY FIXED,                     MEST  90
        (C1,C2,CD(N),CDJ,D(*),E7,E10,G,H,P,PD,S,SH,T,U,A(*),B(*))       MEST 100
        BINARY,.                                                        MEST 110
   E10  =1.E-2C,.                    /*          CONSTANTS          */MEST 120
   E7   =1.E-7,.                                                        MEST 130
   MIT  =30,.                                                           MEST 140
   H    =0.5,.                                                          MEST 150
   N    =M,.                         /*        INITIALIZATION       */MEST 160
   IF NEIG GE N                                                         MEST 170
   THEN DO,.                                                            MEST 180
        NEIG =N,.                                                       MEST 190
        NR   =N-1,.                                                     MEST 200
        END,.                                                           MEST 210
   ELSE NR   =NEIG,.                                                    MEST 220
   B(1)=C,.                                                             MEST 230
        DO I=1 TO N,.                                                   MEST 240
        D(I)=A(I),.                                                     MEST 250
        CD(I)=B(I)*B(I),.                                               MEST 260
        END,.                                                           MEST 270
        DO K=1 TO NR,.               /*   LOOP FOR NR EIGENVALUES   */MEST 280
        N1   =N-1,.                                                     MEST 290
        PD   =C,.                                                       MEST 300
             DO IT=1 TO MIT,.        /*   START LOOP FOR ITERATION  */MEST 310
             C1   =ABS(D(N)),.                                          MEST 320
             C2   =C1*C1,.           /*       TEST CONVERGENCE      */MEST 330
             IF CD(N) LE E10*C2 THEN GO TO DEC,.                        MEST 340
             S    =ABS(D(N)-PD),.                                       MEST 350
             IF S LE E7*C1 THEN GO TO DEC,.                             MEST 360
             IF S GT H*C1            /*  TEST FOR APPLYING A SHIFT  */MEST 370
             THEN SH   =0,.                                             MEST 380
             ELSE SH   =D(N),.                                          MEST 390
             PD   =D(N),.                                               MEST 400
                  DO J=N1 TO 2 BY -1,./*TEST FOR SPLITTING THE MATRIX*/MEST 410
                  IF CD(J) LE E10*C2 THEN GO TO SIT,.                   MEST 420
                  END,.                                                 MEST 430
             J    =1,.                                                  MEST 440
SIT..                                                                   MEST 450
             S,U  =C,.               /*INITIALIZE THE TRANSFORMATION*/MEST 460
             C2   =1,.                                                  MEST 470
             G    =D(J)-SH,.                                            MEST 480
             P    =G*G,.                                                MEST 490
             CDJ  =CD(J),.                                              MEST 500
                  DO I=J TO N1,.     /*      QR TRANSFORMATION      */MEST 510
                  IP   =I+1,.                                           MEST 520
                  T    =P+CD(IP),.                                      MEST 530
                  CD(I)=S*T,.                                           MEST 540
                  S    =CD(IP)/T,.                                      MEST 550
                  C1   =C2,.                                            MEST 560
                  C2   =P/T,.                                           MEST 570
                  D(IP)=D(IP)-SH,.                                      MEST 580
                  U    =S*(G+D(IP)),.                                   MEST 590
                  D(I) =G+U+SH,.                                        MEST 600
                  G    =D(IP)-U,.                                       MEST 610
                  IF C2=0                                               MEST 620
                  THEN P    =CD(IP)*C1,.                                MEST 630
                  ELSE P    =G*G/C2,.                                   MEST 640
                  END,.                                                 MEST 650
             CD(J)=CDJ,.                                                MEST 660
             CD(N)=S*P,.                                                MEST 670
             D(N) =G+SH,.                                               MEST 680
             END,.                  /*   END LOOP FOR ITERATION    */MEST 690
DEC..                                                                   MEST 700
        N    =N1,.                  /* DEFLATE ORDER OF THE MATRIX */MEST 710
        END,.                                                           MEST 720
   IF NEIG LT M                                                         MEST 730
   THEN DO,.                                                            MEST 740
        J=M-NEIG,.                                                      MEST 750
             DO I=1 TO NEIG,.                                           MEST 760
             J=J+1,.                                                    MEST 770
             D(I)=D(J),.                                                MEST 780
             END,.                                                      MEST 790
        END,.                                                           MEST 800
   RETURN,.                                                             MEST 810
   END,.                            /*   END OF PROCEDURE MEST     */MEST 820
```

Purpose:

MEST computes the eigenvalues of a real symmetric tridiagonal matrix (see subroutine MSTU).

Usage:

CALL MEST (A, B, M, D, NEIG);

A(M) - BINARY FLOAT
Given vector containing the diagonal terms of the matrix.

B(M) - BINARY FLOAT
Given vector containing in positions 2, 3, ..., M, the codiagonal terms of the matrix.

M - BINARY FIXED
Given order of the matrix.

D(M) - BINARY FLOAT
Resultant vector containing the eigenvalues.

NEIG - BINARY FIXED
Given number of eigenvalues required (see "Remarks").

Remarks:

When the eigenvalues are well separated, this procedure generally gives the NEIG eigenvalues of smallest moduli in the first NEIG positions of vector D.

Vectors A and B are preserved.

Method:

QR iteration modified by Kaiser and Ortega.

For reference see:

J. M. Ortega and H. F. Kaiser, "The LL^T and QR methods for symmetric tridiagonal matrices", Computer Journal, Volume 6, 1963, pp. 99-101.

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical Background:

The general properties of the QR algorithm are given in the description of subroutine MEAT ("Mathematical Background", items 1 and 2). We recall them briefly here.

For a given diagonalizable matrix A of order n, the QR iteration is defined by:

$$A^{(0)} = A,\ A^{(p)} = Q^{(p)}\ R^{(p)},\ A^{(p+1)} = R^{(p)}\ Q^{(p)}$$

where $Q^{(p)}\ R^{(p)}$ is a unitary-triangular factorization of $A^{(p)}$. A condition on $R^{(p)}$ is assumed to ensure the uniqueness of the factorization. If the eigenvalues have distinct moduli, for example, $|\lambda_i| > |\lambda_{i+1}|$ for i = 1, ..., n-1, then we have the following properties:

1. When p tends to infinity, $A^{(p)}$ tends to a triangular matrix and the eigenvalues of A appear on the main diagonal of $A^{(p)}$, starting from the last position in increasing order of moduli.

2. The symmetry and the tridiagonal structure of a matrix are preserved under the QR iteration.

3. If the origin of the eigenvalues is shifted close to λ_n before an iteration and shifted back afterwards, then the rate of convergence of $a^{(p)}_{n,n}$ to λ_n -- that is, the rate of convergence of $a^{(p)}_{n,i}$ to zero for i = 1, ..., n-1, can be considerably improved.

From the second property we can see that a preliminary reduction of a symmetric matrix to a similar tridiagonal form will give a significant saving of computation for each QR iteration.

From the first property we note that no special deflation is needed when λ_n has been found to sufficient accuracy; the last row and column of the matrix are neglected and the iteration is applied to the reduced matrix to obtain λ_{n-1}.

Let us consider a step of the iteration, denoted by

$$A = QR\ ,\ A' = RQ$$

where A' is the iterate of A, the iteration superscript being dropped for clarity of notation. A and A' are symmetric tridiagonal matrices of order n. A will be fully defined by its diagonal terms a_i, i = 1, ..., n and its subdiagonal terms b_i, i = 2, ... , n. The terms of A' will be denoted by a'_i, i = 1 ... , n and b'_i, i = 2, ..., n.

The reduction of A to R can be completed by premultiplication by (n-1) orthogonal matrices (Plane Rotations) Q_i, i = 1, ..., n-1 of the form

$$Q_i = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c_i & s_i & & \\ & & & -s_i & c_i & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{bmatrix} \qquad i = 1, \ldots, n-1$$

c_i and s_i are the cosine and sine of an angle such that

$$R = Q_{n-1} \ldots Q_1\ A$$

Then:

$$Q = Q_1^t \ldots Q_{n-1}^t$$

c_i and s_i are given by

$$c_i = \frac{p_i}{(p_i^2 + b_{i+1}^2)^{1/2}}$$

$$s_i = \frac{b_{i+1}}{(p_i^2 + b_{i+1})^{1/2}}$$

$$i = 1, \ldots, n-1 \qquad (1)$$

with

$$p_i = c_{i-1}\, a_i - s_{i-1}\, c_{i-2}\, b_{i+1}$$

and

$$c_{-1} = 0\ ,\ c_0 = 1\ ,\ s_0 = 0$$

R will be defined by:

$$r_{i,i} = c_i\, p_i + s_i\, b_{i+1}\ ,\ i = 1, \ldots, n-1$$

$$r_{n,n} = p_n$$

$$r_{1,2} = c_1 b_2 + s_1 a_2 \qquad (2)$$

$$r_{i,\,i+1} = c_i\, c_{i-1}\, b_{i+1} + s_i\, a_{i+1}\ ,$$

$$i = 2, \ldots, n-1$$

$$r_{i,\,i+2} = s_i\, b_{i+2},\ i = 1, \ldots, n-2$$

$$r_{i,j} = 0 \quad \text{for} \quad j > i+2$$

The post-multiplication of R by Q will provide A', according to:

$$a_1' = c_1\, r_{1,1} + s_1\, r_{1,2}$$

$$a_i' = c_{i-1}\, c_i\, r_{i,i} + s_i\, r_{i,i+1}$$

$$i = 2, \ldots, n-1$$

$$a_n' = c_{n-1}\, r_{n,n} \qquad (3)$$

$$b_{i+1}' = s_i\, r_{i+1,i+1}$$

$$i = 1, \ldots, n-1$$

Formulas (2) and (3) can be combined in order to get A' directly from A. This avoids the computation of the square roots appearing in the expressions of c_i and s_i.

Then the final algorithm can be expressed as follows:

$$u_0 = 0,\ c_0 = 1,\ b_{n+1} = 0,\ a_{n+1} = 0$$

$$g_i = a_i - u_{i-1}$$

$$p_1^2 = g_i^2 \,/\, c_{i-1}^2 \quad \text{when } c_{i-1} \neq 0$$

$$= c_{i-2}^2\, b_i^2 \quad \text{when } c_{i-1} = 0$$

$$b_i'^2 = s_{i-1}^2\, (p_i^2 + b_{i+1}^2) \quad \text{for } i > 1 \qquad (4)$$

$$s_i^2 = b_{i+1}^2 \,/\, (p_i^2 + b_{i+1}^2)$$

$$c_i^2 = p_i^2 \,/\, (p_i^2 + b_{i+1}^2)$$

$$u_i = s_i^2\, (g_i + a_{i+1})$$

$$a_i' = g_i + u_i$$

$$i = 1, 2, \ldots, n$$

Programming Considerations:

The iteration is performed according to equations (4). A shift of the origin of the eigenvalues is introduced in order to accelerate convergence. This shift is based on the last diagonal term of the matrix; it is applied only when convergence begins appearing.

When several eigenvalues are of same magnitude, codiagonal terms are close to zero. Then the matrix is split according to this occurrence and the iteration is performed on the lower main submatrix only. The iteration is stopped and the last diagonal term is taken as an eigenvalue when one of the following situations occurs:

1. The last subdiagonal term can be taken as zero.
2. The last subdiagonal term is stable through one iteration.
3. The maximum number of iterations is reached.

Then the order of the matrix is reduced by one and the process is repeated on the resulting matrix.

- Subroutine MEBS

```
MEBS..
/*****************************************************************/MEBS
/*                                                               */MEBS
/*        BOUNDS FOR THE EIGENVALUES OF A SYMMETRIC MATRIX       */MEBS
/*                                                               */MEBS
/*****************************************************************/MEBS
   PROCEDURE (A,N,B1,B2),.
   DECLARE
        (I,J,K,L,N) BINARY FIXED,
        (A(*),B1,B2,P,SQ) BINARY,
        (S,S1,S2) BINARY(53),.
   J    =2,.
   S1   =A(1),.
   S2   =0,.
   S    =S1*S1,.
   I    =1,.
        DO K=2 TO N,.
        I    =I+K,.
        S1   =S1+A(I),.                /*        SUM OF THE ROOTS    */MEBS
        S=S+MULTIPLY(A(I),A(I),53),.
             DO L=J TO I-1,.
             S2=S2+MULTIPLY(A(L),A(L),53),.
             END,.
        J    =I+1,.
        END,.
   S2   =2*S2+S,.                      /* SUM OF THE SQUARES OF ROOTS */MEBS
   SQ   =SQRT((N-1)*ABS(N*S2-S1*S1)),./*    ITERATE FROM INFINITY    */MEBS
   P    =(1-N)*S2+S1*S1,.
   IF S1 LT 0
   THEN DO,.
        B1   =S1-SQ,.
        B2   =P/B1,.
        B1   =B1/N,.
        END,.
   ELSE DO,.
        B2   =S1+SQ,.
        B1   =P/B2,.
        B2   =B2/N,.
        END,.
   RETURN,.
   END,.                              /*    END OF PROCEDURE MEBS   */MEBS
```

Purpose:

MEBS computes a lower and an upper bound for the eigenvalues of a real symmetric matrix.

Usage:

CALL MEBS (A, N, B1, B2);

A (N*(N+1) /2) -	BINARY FLOAT Given real symmetric matrix in compressed storage mode.
N -	BINARY FIXED Given order of the matrix.
B1 -	BINARY FLOAT Resultant lower bound.
B2 -	BINARY FLOAT Resultant upper bound.

Method:

Laguerre's iteration is applied to the points at infinity.

For reference see:

B. Parlett, "Laguerre's Method Applied to the Matrix Eigenvalue Problem", Mathematics of Computation, 18, 1964.

Mathematical Background:

1. Laguerre's iteration.
   Let P(x) be a polynomial of degree n. The Laguerre iterate of a point x for the polynomial P can be expressed by

$$L_P(x) = x - \frac{n\,P(x)}{P'(x) \pm \sqrt{(n-1)\left[(n-1)\,P'(x)^2 - n\,P(x)\,P''(x)\right]}} \qquad (1)$$

Letting

$$S_1(x) = \frac{P'(x)}{P(x)} = \sum_{i=1}^{n} \frac{1}{x-x_i}$$

$$S_2(x) = \frac{P'(x)^2 - P(x)\,P''(x)}{P(x)^2}$$

$$= \sum_{i=1}^{n} \frac{1}{(x-x_i)^2}$$

where $x_1, \ldots, x_n$ are the roots of P(x), formula (1) can be written as

$$L_P(x) = x - \frac{n}{s_1 \pm \sqrt{(n-1)\,(nS_2 - S_1^2)}} \qquad (2)$$

The sign of the square root is chosen so that the magnitude of the denominator is maximum.
When P(x) has real roots, we have the following properties:

a. Let us consider a partition of the real line defined by the points at infinity and the zeros of $P'(x)$. Starting from an initial point in any interval of the partition, the successive Laguerre iterates converge monotonically to the root therein. If the root is simple, convergence is asymptotically cubic.

b. Laguerre's iterations are invariant under Möbius transformations.

2. Iterates of the points at infinity.
   From the first property of monotonic convergence, we can see that the iterates of the points at infinity will provide bounds for the roots. The second property gives the relation.

$$L_P(x) = \frac{1}{L_Q\left(\frac{1}{x}\right)} \qquad (3)$$

where Q is the polynomial reciprocal of P, the roots of which are

$$\frac{1}{x_i}, \quad i = 1, \ldots, n.$$

Thus

$$L_P(\infty) = \frac{1}{L_Q(0)} \tag{4}$$

Now, if we combine equations (2) and (4), we can obtain the final formula

$$L_P(\infty) = \frac{1}{n}\left[\sigma_1 \pm \sqrt{(n-1)\ (n\,\sigma_2 - \sigma_1^2)}\right] \tag{5}$$

where σ_1 is the sum of the roots and σ_2 the sum of the squares of the roots of polynomial P.

Programming Considerations:

We can note that equation (5) does not require the coefficients of polynomial P but only the values of σ_1 and σ_2. If we apply this formula to the characteristic polynomial of a symmetric matrix (real roots), σ_1 will be obtained by computing the trace of the matrix and σ_2 the sum of the squares of the terms of the matrix. Then, equation (5) will give the bounds of the eigenvalues.

- Subroutine MVST

```
MVST..                                                                  MVST  10
/*********************************************************************/MVST  20
/*                                                                   */MVST  30
/*         EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX            */MVST  40
/*                                                                   */MVST  50
/*********************************************************************/MVST  60
  PROCEDURE (D,CD,N,EIG,Y),.                                            MVST  70
  DECLARE                                                               MVST  80
       (D(*),CD(*),EIG,Y(*),E7,T,EPS,W,                                 MVST  90
        X(N),P(N),Q(N),A(N),R(N),U,V,S,CI,CIP) BINARY,                  MVST 100
       (N,I,IP1,N1,IT,II) BINARY FIXED,                                 MVST 110
       CH(N) BIT(1),.                                                   MVST 120
  N1=N-1,.                                                              MVST 130
  E7=1.0E-7,.                                                           MVST 140
  T=ABS(D(1)),.                        /*    NORM OF THE MATRIX       */MVST 150
       DO I=2 TO N,.                                                    MVST 160
       W=MAX(ABS(D(I)),ABS(CD(I))),.                                    MVST 170
       IF W GT T THEN T=W,.                                             MVST 180
       END,.                                                            MVST 190
  EPS=T*E7,.                                                            MVST 200
  U=D(1)-EIG,.                                                          MVST 210
  IF ABS(CD(2)) LT EPS                                                  MVST 220
  THEN V,CIP=EPS,.                                                      MVST 230
  ELSE V,CIP=CD(2),.                                                    MVST 240
       DO I=1 TO N1,.                  /*    START FACTORIZATION       */MVST 250
       IP1=I+1,.                                                        MVST 260
       CI=CIP,.                                                         MVST 270
       IF I = N1                                                        MVST 280
       THEN CIP=0,.                                                     MVST 290
       ELSE IF ABS(CD(IP1+1)) LT EPS                                    MVST 300
            THEN CIP=EPS,.                                              MVST 310
            ELSE CIP=CD(IP1+1),.                                        MVST 320
       IF ABS(CI) GE ABS(U)            /*       PIVOTING              */MVST 330
       THEN DO,.                       /*      INTERCHANGE            */MVST 340
            IF U NE 0                                                   MVST 350
            THEN A(IP1)=U/CI,.                                          MVST 360
            ELSE IF CI=EPS                                              MVST 370
                 THEN A(IP1)=1,.                                        MVST 380
                 ELSE A(IP1)=0,.                                        MVST 390
            P(I)=CI,.                                                   MVST 400
            Q(I)=D(IP1)-EIG,.                                           MVST 410
            R(I)=CIP,.                                                  MVST 420
            U=V-A(IP1)*Q(I),.                                           MVST 430
            V= -A(IP1)*R(I),.                                           MVST 440
            CH(IP1)='1'B,.                                              MVST 450
            END,.                                                       MVST 460
       ELSE DO,.                       /*    NO INTERCHANGE           */MVST 470
            A(IP1)=CI/U,.                                               MVST 480
            P(I)=U,.                                                    MVST 490
            Q(I)=V,.                                                    MVST 500
            R(I)=0,.                                                    MVST 510
            U=D(IP1)-EIG-V*A(IP1),.                                     MVST 520
            V=CIP,.                                                     MVST 530
            CH(IP1)='0'B,.                                              MVST 540
            END,.                                                       MVST 550
       IF ABS(P(I)) LT EPS THEN P(I)=EPS,.                              MVST 560
       X(I)=1,.                        /* INITIAL GUESS OF EIGENVECTOR*/MVST 570
       END,.                                                            MVST 580
  IF ABS(U) LT EPS THEN U=EPS,.                                         MVST 590
  P(N)=U,.                             /*    END FACTORIZATION        */MVST 600
  X(N)=1,.                                                              MVST 610
       DO IT=1,2,.                     /*  START LOOP FOR ITERATION   */MVST 620
       IF IT GT 1                                                       MVST 630
       THEN DO,.                       /*  SOLVE WITH LOWER FACTOR    */MVST 640
            V=ABS(X(1)),.                                               MVST 650
                 DO I=2 TO N,.         /*       NORMALIZATION         */MVST 660
                 U=ABS(X(I)),.                                          MVST 670
                 IF U GT V THEN V=U,.                                   MVST 680
                 END,.                                                  MVST 690
            X(1)=X(1)/V,.                                               MVST 700
                 DO I=2 TO N,.                                          MVST 710
                 X(I)=X(I)/V,.                                          MVST 720
                 IF CH(I)                                               MVST 730
                 THEN DO,.                                              MVST 740
                      II=I-1,.                                          MVST 750
                      U=X(II),.                                         MVST 760
                      X(II)=X(I),.                                      MVST 770
                      X(I)=U-A(I)*X(II),.                               MVST 780
                      END,.                                             MVST 790
                 ELSE X(I)=X(I)-A(I)*X(I-1),.                           MVST 800
                 END,.                                                  MVST 810
            END,.                                                       MVST 820
       X(N)=X(N)/P(N),.                /*  SOLVE WITH UPPER FACTOR    */MVST 830
       X(N1)=(X(N1)-Q(N1)*X(N))/P(N1),.                                 MVST 840
            DO I=N-2 TO 1 BY -1,.                                       MVST 850
            X(I)=(X(I)-Q(I)*X(I+1)-R(I)*X(I+2))/P(I),.                  MVST 860
            END,.                                                       MVST 870
       END,.                           /*  END LOOP OF ITERATION      */MVST 880
  S=0,.                                                                 MVST 890
       DO I=1 TO N,.                   /*    NORMALIZE SOLUTION       */MVST 900
       S=S+X(I)*X(I),.                                                  MVST 910
       END,.                                                            MVST 920
  S=SQRT(S),.                                                           MVST 930
       DO I=1 TO N,.                                                    MVST 940
       Y(I)=X(I)/S,.                                                    MVST 950
       END,.                                                            MVST 960
  RETURN,.                                                              MVST 970
  END,.                                /*  END OF PROCEDURE MVST      */MVST 980
```

Purpose:

For a given symmetric tridiagonal matrix, MVST provides the eigenvector corresponding to a given eigenvalue.

Usage:

CALL MVST (D, CD, N, EIG, Y);

D(N) - BINARY FLOAT
Given vector containing the diagonal terms of the matrix.

CD(N) - BINARY FLOAT
Given vector containing in positions 2, 3, ..., N the codiagonal terms of the matrix.

N - BINARY FIXED
Given order of the matrix.

EIG - BINARY FLOAT
Given eigenvalue.

Y(N) - BINARY FLOAT
Resultant vector containing the eigenvector.

Remarks:

Vectors D and CD remain unaltered.

Method:

Wielandt's inverse iteration is applied to the matrix, using the given eigenvalue as a shift.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

J. H. Wilkinson, "Calculation of the eigenvectors of the symmetric tridiagonal matrix by inverse iteration", Numerische Mathematik, 4 (1962), pp. 368-376.

Mathematical Background:

Let us suppose that we know an approximation λ of an eigenvalue of a symmetric tridiagonal matrix A. A corresponding eigenvector V can be obtained by using Wielandt's inverse iteration (see the description of procedure MVAT), defined by the iterative process:

$$V^{(p+1)} = (A - \lambda I)^{-1} V^{(p)}$$

where $V^{(0)}$ is an arbitrary vector, not deficient in the eigenvector V.

Considering a triangular factorization of $A-\lambda I$,

$$A - \lambda I = LR,$$

$V^{(p+1)}$ will be provided by solving successively the following equations:

$$LW = V^{(p)} \qquad (1)$$

$$RV^{(p+1)} = W \qquad (2)$$

When λ is close to an eigenvalue of A, $V^{(p)}$ tends very rapidly to V. Most of the time, two iterations are quite sufficient to provide an accurate approximation of V.

Programming Considerations:

A technique of partial pivoting by row interchange is used for the triangular factorization. This factorization is performed before starting the iterative process.

The two iterations are then carried out according to formulas (1) and (2).

The initial vector $V^{(0)}$ is chosen so that $V^{(0)} = Le$, with $e^T = (1, 1, \ldots, 1)$. Then the first iteration will consist of solving equation (2) only:

$$RV^{(1)} = e$$

- Subroutine MSDU

```
MSDU..                                                                  MSDU  10
/*************************************************************************/MSDU  20
/*                                                                       */MSDU  30
/*      TO COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC      */MSDU  40
/*      MATRIX                                                           */MSDU  50
/*                                                                       */MSDU  60
/*************************************************************************/MSDU  70
   PROCEDURE (A,R,N,MV),.                                               MSDU  80
   DECLARE                                                              MSDU  90
         (I,IND,J,L,M,MV,N)                                             MSDU 100
         FIXED BINARY,                                                  MSDU 110
         ERROR EXTERNAL CHARACTER(1),                                   MSDU 120
         (A(*,*),R(*,*),ANORM,ANRMX,THR,U,Y,SINX,SINX2,COSX,COSX2,SINCS,MSDU 130
         FN)                                                            MSDU 140
         BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/MSDU 150
/*       BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/MSDU 160
/*                                                                       */MSDU 170
   ERROR='0',.                                                          MSDU 180
   IF N LE 1                       /* THE ORDER OF MATRIX A IS      */MSDU 190
   THEN DO,.                       /* LESS THAN OR EQUAL TO ONE.    */MSDU 200
         ERROR='1',.                                                    MSDU 210
         GO TO FIN,.                                                    MSDU 220
         END,.                                                          MSDU 230
   FN    =N,.                                                           MSDU 240
   IF MV= 0                                                             MSDU 250
   THEN DO,.                                                            MSDU 260
            DO I = 1 TO N,.        /* GENERATE IDENTITY MATRIX      */MSDU 270
               DO J = 1 TO N,.                                          MSDU 280
              R(I,J)=0,.                                                MSDU 290
               END,.                                                    MSDU 300
            R(I,I)=1,.                                                  MSDU 310
            END,.                                                       MSDU 320
         END,.                                                          MSDU 330
/*                                                                       */MSDU 340
/*      COMPUTE INITIAL AND FINAL NORM                                   */MSDU 350
/*                                                                       */MSDU 360
   ANORM=0,.                                                            MSDU 370
         DO I = 1 TO N-1,.                                              MSDU 380
            DO J = I+1 TO N,.                                           MSDU 390
            ANORM=ANORM+A(I,J)*A(I,J),.                                 MSDU 400
            END,.                                                       MSDU 410
         END,.                                                          MSDU 420
   IF ANORM LE C.0                                                      MSDU 430
   THEN GO TO SQRT,.                                                    MSDU 440
   ANORM=1.414*SQRT(ANORM),.                                            MSDU 450
   ANRMX=ANORM*1.0E-6/FN,.                                              MSDU 460
/*                                                                       */MSDU 470
/*      INITIALIZE INDICATOR AND COMPUTE THRESHOLD, THR                  */MSDU 480
/*                                                                       */MSDU 490
   IND  =0,.                                                            MSDU 500
   THR  =ANORM,.                                                        MSDU 510
S10..                                                                   MSDU 520
   THR  =THR/FN,.                                                       MSDU 530
S20..                                                                   MSDU 540
   L    =1,.                                                            MSDU 550
S30..                                                                   MSDU 560
   M    =L+1,.                                                          MSDU 570
S40..                                                                   MSDU 580
   IF ABS(A(L,M)) GE THR           /* COMPUTE SIN AND COS           */MSDU 590
   THEN DO,.                                                            MSDU 600
         IND  =1,.                                                      MSDU 610
         U    =0.5*(A(L,L)-A(M,M)),.                                    MSDU 620
         Y    =-A(L,M)/SQRT(A(L,M)*A(L,M)+U*U),.                        MSDU 630
         IF U LT 0.0                                                    MSDU 640
         THEN Y    =-Y,.                                                MSDU 650
         SINX =Y/SQRT(2.0*(1.0+(SQRT(1.0-Y*Y)))),.                      MSDU 660
         SINX2=SINX*SINX,.                                              MSDU 670
         COSX =SQRT(1.0-SINX2),.                                        MSDU 680
         COSX2=COSX*COSX,.                                              MSDU 690
         SINCS=SINX*COSX,.                                              MSDU 700
               DO I = 1 TO N,.       /* ROTATE L AND M COLUMNS        */MSDU 710
               IF I LT L                                                MSDU 720
               THEN DO,.                                                MSDU 730
                     IF I LT M                                          MSDU 740
                     THEN DO,.                                          MSDU 750
                           U    =A(I,L)*COSX-A(I,M)*SINX,.              MSDU 760
                           A(I,M)=A(I,L)*SINX+A(I,M)*COSX,.             MSDU 770
                           A(I,L)=U,.                                   MSDU 780
                           END,.                                        MSDU 790
                     END,.                                              MSDU 800
               ELSE IF I GT L                                           MSDU 810
               THEN DO,.                                                MSDU 820
                     IF I LT M                                          MSDU 830
                     THEN DO,.                                          MSDU 840
                           U    =A(L,I)*COSX-A(I,M)*SINX,.              MSDU 850
                           A(I,M)=A(L,I)*SINX+A(I,M)*COSX,.             MSDU 860
                           END,.                                        MSDU 870
                     ELSE IF I GT M                                     MSDU 880
                     THEN DO,.                                          MSDU 890
                           U    =A(L,I)*COSX-A(M,I)*SINX,.              MSDU 900
                           A(M,I)=A(L,I)*SINX+A(M,I)*COSX,.             MSDU 910
                           END,.                                        MSDU 920
                     IF I NE M                                          MSDU 930
                     THEN A(L,I)=U,.                                    MSDU 940
                     END,.                                              MSDU 950
               IF MV= 0                                                 MSDU 960
               THEN DO,.                                                MSDU 970
                     U    =R(I,L)*COSX-R(I,M)*SINX,.                    MSDU 980
                     R(I,M)=R(I,L)*SINX+R(I,M)*COSX,.                   MSDU 990
                     R(I,L)=U,.                                         MSDU1000
                     END,.                                              MSDU1010
               END,.                                                    MSDU1020
         U    =2.C*A(L,M)*SINCS,.                                       MSDU1030
         Y    =A(L,L)*COSX2+A(M,M)*SINX2-U,.                            MSDU1040
         U    =A(L,L)*SINX2+A(M,M)*COSX2+U,.                            MSDU1050
         A(L,M)=(A(L,L)-A(M,M))*SINCS+A(L,M)*(COSX2-SINX2),.            MSDU1060
         A(L,L)=Y,.                                                     MSDU1070
         A(M,M)=U,.                                                     MSDU1080
         END,.                                                          MSDU1090
   IF M NE N                       /* TEST FOR M = LAST COLUMN      */MSDU1100
   THEN DO,.                                                            MSDU1110
         M    =M+1,.                                                    MSDU1120
         GO TO S40,.                                                    MSDU1130
         END,.                                                          MSDU1140
/*                                                                       */MSDU1150
/*      TEST FOR L = SECOND FROM LAST COLUMN                             */MSDU1160
/*                                                                       */MSDU1170
   IF L NE N-1                                                          MSDU1180
   THEN DO,.                                                            MSDU1190
         L    =L+1,.                                                    MSDU1200
         GO TO S30,.                                                    MSDU1210
         END,.                                                          MSDU1220
   IF IND= 1                                                            MSDU1230
   THEN DO,.                                                            MSDU1240
         IND  =0,.                                                      MSDU1250
         GO TO S20,.                                                    MSDU1260
         END,.                                                          MSDU1270
/*                                                                       */MSDU1280
/*      COMPARE THRESHOLD WITH FINAL NORM                                */MSDU1290
/*                                                                       */MSDU1300
   IF THR GT ANRMX                                                      MSDU1310
   THEN GO TO S10,.                                                     MSDU1320
/*                                                                       */MSDU1330
/*      SORT EIGENVALUES AND EIGENVECTORS                                */MSDU1340
/*                                                                       */MSDU1350
SORT..                                                                  MSDU1360
         DO I = 1 TO N,.                                                MSDU1370
            DO J = I TO N,.                                             MSDU1380
            IF A(I,I) LT A(J,J)                                         MSDU1390
            THEN DO,.                                                   MSDU1400
                  U    =A(I,I),.                                        MSDU1410
                  A(I,I)=A(J,J),.                                       MSDU1420
                  A(J,J)=U,.                                            MSDU1430
                  IF MV= 0                                              MSDU1440
                  THEN DO,.                                             MSDU1450
                        DO L = 1 TO N,.                                 MSDU1460
                        U    =R(L,I),.                                  MSDU1470
                        R(L,I)=R(L,J),.                                 MSDU1480
                        R(L,J)=U,.                                      MSDU1490
                        END,.                                           MSDU1500
                     END,.                                              MSDU1510
               END,.                                                    MSDU1520
            END,.                                                       MSDU1530
         END,.                                                          MSDU1540
FIN..                                                                   MSDU1550
   RETURN,.                                                             MSDU1560
   END,.                           /*END OF PROCEDURE MSDU         */MSDU1570
```

Purpose:

MSDU computes eigenvalues and eigenvectors of a real symmetric matrix.

Usage:

CALL MSDU (A, R, N, MV);

A(N, N) - BINARY FLOAT [(53)]
Given matrix (symmetric), destroyed in computation.
Resultant eigenvalues are developed in the diagonal of matrix A in descending order.

R(N, N) - BINARY FLOAT [(53)]
Resultant matrix of eigenvectors (stored columnwise, in the same sequence as eigenvalues).

N - BINARY FIXED
Given order of matrix A and R.

MV - BINARY FIXED
Given code containing the following:
0--compute eigenvalues and eigenvectors.
1--compute eigenvalues only.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR=1 - The order of the matrix is one or less.

Note: If the initial norm is equal to zero, the matrix is diagonal.

Method:

Diagonalization method originated by Jacobi and adapted by Von Neumann for larger computers as found in Mathematical Methods for Digital Computers, edited by A. Ralston and H. S. Wilf, John Wiley and Sons, New York, 1962, Chapter 7.

Mathematical Background:

This subroutine computes the eigenvalues and eigenvectors of a real symmetric matrix.

Given a symmetric matrix A of order N, eigenvalues are to be developed in the diagonal elements of the matrix. A matrix of eigenvectors R is also to be generated.

An identity matrix is used as a first approximation of R.

The initial off-diagonal norm is computed:

$$\nu_I = \left(\sum_{i<k} 2A_{ik}^2 \right)^{1/2} \quad (1)$$

ν_I = initial norm

A = input matrix (symmetric)

This norm is divided by N at each stage to produce the threshold.

The final norm is computed:

$$\nu_F = \frac{\nu_I \times 10^{-6}}{N} \quad (2)$$

This final norm is set sufficiently small that the requirement for any off-diagonal element A_{lm} to be smaller than ν_F in absolute magnitude defines the convergence of the process.

An indicator is initialized. This indicator is later used to determine whether any off-diagonal elements have been found that are greater than the present threshold.

Each off-diagonal element is selected in turn and a transformation is performed to annihilate the off-diagonal (pivotal) element, as shown by the following equations:

$$\lambda = -A_{lm} \quad (3)$$

$$\mu = 1/2 \, (A_{ll} - A_{mm}) \quad (4)$$

$$\omega = \text{sign}\,(\mu) \frac{\lambda}{\sqrt{\lambda^2 + \mu^2}} \quad (5)$$

$$\sin\theta = \frac{\omega}{\sqrt{2(1 + \sqrt{1 - \omega^2})}} \quad (6)$$

$$\cos\theta = \sqrt{1 - \sin^2\theta} \quad (7)$$

$$B = A_{il}\cos\theta - A_{im}\sin\theta \quad (8)$$

$$C = A_{il}\sin\theta + A_{im}\cos\theta \quad (9)$$

$$B = R_{il}\cos\theta - R_{im}\sin\theta \quad (10)$$

$$R_{im} = R_{il}\sin\theta + R_{im}\cos\theta \quad (11)$$

$$R_{il} = B \quad (12)$$

$$A_{il} = A_{il}\cos^2\theta + A_{mm}\sin^2\theta - 2A_{lm}\sin\theta\cos\theta \quad (13)$$

$$A_{mm} = A_{ll}\sin^2\theta + A_{mm}\cos^2\theta + 2A_{lm}\sin\theta\cos\theta \quad (14)$$

$$A_{lm} = (A_{ll} - A_{mm})\sin\theta\cos\theta + A_{lm}(\cos^2\theta - \sin^2\theta) \quad (15)$$

The above calculations are repeated until all of the pivotal elements are less than the threshold.

Programming Considerations:

Matrix A cannot be in the same location as matrix R. If the eigenvectors are not calculated, the matrix R does not need to be dimensioned in the declare statement, but R must appear in the argument list of the procedure.

- Subroutine MGDU

```
MGDU..                                                                  MGDU  10
/*************************************************************************/MGDU  20
/*                                                                       */MGDU  30
/*      TO COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL NONSYMM-       */MGDU  40
/*      ETRIC MATRIX OF THE FORM B INVERSE TIMES A.                      */MGDU  50
/*                                                                       */MGDU  60
/*************************************************************************/MGDU  70
   PROCEDURE (M,A,B,XL,X),.                                               MGDU  80
   DECLARE                                                                MGDU  90
        (I,J,M,MV,K)                                                      MGDU 100
        FIXED BINARY,                                                     MGDU 110
        ERROR EXTERNAL CHARACTER(1),                                      MGDU 120
        (A(*,*),B(*,*),X(*,*),XL(*),SUMV)                                 MGDU 130
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/MGDU 140
 /*     BINARY FLOAT(53),.          /*DOUBLE PRECISION VERSION  /*D*/MGDU 150
/*                                                                       */MGDU 160
/*      COMPUTE EIGENVALUES AND EIGENVECTORS OF B                        */MGDU 170
/*                                                                       */MGDU 180
/*      THE MATRIX B IS A REAL SYMMETRIC MATRIX.                         */MGDU 190
/*                                                                       */MGDU 200
   MV   =0,.                                                              MGDU 210
   CALL MSDU (B,X,M,MV),.                                                 MGDU 220
   IF ERROR NE '0'                                                        MGDU 230
   THEN GO TO FIN,.                                                       MGDU 240
/*                                                                       */MGDU 250
/*      FORM RECIPROCALS OF SQUARE ROOT OF EIGENVALUES. THE RESULTS      */MGDU 260
/*      ARE PREMULTIPLIED BY THE ASSOCIATED EIGENVECTORS.                */MGDU 270
/*                                                                       */MGDU 280
        DO I = 1 TO M,.                                                   MGDU 290
        XL(I)=1.0/SQRT(ABS(B(I,I))),.                                     MGDU 300
             DO J = 1 TO M,.                                              MGDU 310
             B(J,I)=X(J,I)*XL(I),.                                        MGDU 320
             END,.                                                        MGDU 330
        END,.                                                             MGDU 340
/*                                                                       */MGDU 350
/*      FORM (B**(-1/2))PRIME * A * (B**(-1/2))                          */MGDU 360
/*                                                                       */MGDU 370
        DO I = 1 TO M,.                                                   MGDU 380
             DO J = 1 TO M,.                                              MGDU 390
             X(I,J)=0.0,.                                                 MGDU 400
                  DO K = 1 TO M,.                                         MGDU 410
                  X(I,J)=X(I,J)+B(K,I)*A(K,J),.                           MGDU 420
                  END,.                                                   MGDU 430
             END,.                                                        MGDU 440
        END,.                                                             MGDU 450
        DO I = 1 TO M,.                                                   MGDU 460
             DO J = 1 TO M,.                                              MGDU 470
             A(I,J)=0.0,.                                                 MGDU 480
                  DO K = 1 TO M,.                                         MGDU 490
                  A(I,J)=A(I,J)+X(I,K)*B(K,J),.                           MGDU 500
                  END,.                                                   MGDU 510
             END,.                                                        MGDU 520
        END,.                                                             MGDU 530
/*                                                                       */MGDU 540
/*      COMPUTE EIGENVALUES AND EIGENVECTORS OF A                        */MGDU 550
/*                                                                       */MGDU 560
   CALL MSDU (A,X,M,MV),.                                                 MGDU 570
        DO I = 1 TO M,.                                                   MGDU 580
        XL(I)=A(I,I),.                                                    MGDU 590
/*                                                                       */MGDU 600
/*      COMPUTE THE NORMALIZED EIGENVECTORS                              */MGDU 610
/*                                                                       */MGDU 620
             DO J = 1 TO M,.                                              MGDU 630
             A(I,J)=0.0,.                                                 MGDU 640
                  DO K = 1 TO M,.                                         MGDU 650
                  A(I,J)=A(I,J)+B(I,K)*X(K,J),.                           MGDU 660
                  END,.                                                   MGDU 670
             END,.                                                        MGDU 680
        END,.                                                             MGDU 690
        DO J = 1 TO M,.                                                   MGDU 700
        SUMV =0.0,.                                                       MGDU 710
             DO K = 1 TO M,.                                              MGDU 720
             SUMV =SUMV+A(K,J)*A(K,J),.                                   MGDU 730
             END,.                                                        MGDU 740
        SUMV =SQRT(SUMV),.                                                MGDU 750
             DO K = 1 TO M,.                                              MGDU 760
             X(K,J)=A(K,J)/SUMV,.                                         MGDU 770
             END,.                                                        MGDU 780
        END,.                                                             MGDU 790
FIN..                                                                     MGDU 800
   RETURN,.                                                               MGDU 810
   END,.                            /*END OF PROCEDURE MGDU              */MGDU 820
```

Purpose:

MGDU computes eigenvalues and eigenvectors of a real matrix of the form B-inverse times A, where A is symmetric and B is positive definite.

Usage:

CALL MGDU (M, A, B, XL, X);

M - BINARY FIXED
Given order of square matrices A, B, and X.

A(M,M) - BINARY FLOAT [(53)]
Given symmetric matrix.

B(M,M) - BINARY FLOAT [(53)]
Given positive definite matrix.

XL(M) - BINARY FLOAT [(53)]
Resultant vector containing eigenvalues of B-inverse times A.

X(M,M) - BINARY FLOAT [(53)]
Resultant matrix containing eigenvectors columnwise.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero by the called subroutine MSDU. The following constitutes the possible error condition that may be detected:

ERROR=1 MSDU has been called and an error has occurred (see MSDU).

Subroutines and function subroutines required:

MSDU

Both matrices A and B are destroyed.

Method:

Refer to W. W. Cooley and P. R. Lohnes, Multivariate Procedures for the Behavioral Sciences, John Wiley and Sons, 1962, Chapter 3.

Mathematical Background:

This subroutine calculates the eigenvalues and the matrix of eigenvectors of the matrix $B^{-1}A$.

First the subroutine MSDU is used to calculate the eigenvalues and eigenvectors of the matrix B. The eigenvalues b_{ii} are stored in the main diagonal of the original matrix B and the eigenvectors are stored columnwise in the matrix X. Next the square roots of the reciprocals of the eigenvalues b_{ii} are formed and stored in XL

$$XL_i = 1/\sqrt{b_{ii}}$$

Then each eigenvector stored in X is multiplied by the corresponding value XL_j. The matrix of results is again stored in B. Next the matrix B^TAB is generated and stored in A. Then the subroutine MSDU is used to calculate the eigenvalues and eigenvectors of B^TAB. The eigenvalues are stored in XL and the eigenvectors are stored in X. Next the matrix product BX is formed and stored in A. The eigenvectors are then normalized to the form $a_{ij}/\sqrt{SUM_j a_{ij}^2}$ to form the desired output matrix of eigenvectors.

- Subroutine MVAT

```
MVAT..                                                                  MVAT  10
/*************************************************************************/MVAT  20
/*                                                                       */MVAT  30
/*          EIGENVECTORS OF A COMPLEX HESSENBERG MATRIX                  */MVAT  40
/*                                                                       */MVAT  50
/*************************************************************************/MVAT  60
   PROCEDURE (A,N,EIG,V),.                                              MVAT  70
   DECLARE                                                              MVAT  80
         P(N)                                                           MVAT  90
         BIT(1),                                                        MVAT 100
         (E7,U,T,EPS)                                                   MVAT 110
         BINARY,                                                        MVAT 120
         (A(*,*),EIG,C,V(*)),                                           MVAT 130
         COMPLEX BINARY,                                                MVAT 140
         S                                                              MVAT 150
         COMPLEX BINARY(53),                                            MVAT 160
         (N,IS(N),I,I1,J,N1,K,K1,KP1,IT)                                MVAT 170
         BINARY FIXED,.                                                 MVAT 180
   E7=1.0E-7,.                                                          MVAT 190
   A(1,1)=A(1,1)-EIG,.                  /*   MODIFY DIAGONAL ELEMENTS  */MVAT 200
   IS(1)=1,.                                                            MVAT 210
   U=ABS(A(1,1)),.                      /*COMPUTE A NORM OF THE MATRIX */MVAT 220
         DO I=2 TO N,.                                                  MVAT 230
         I1=I-1,.                                                       MVAT 240
         IS(I)=I1,.                                                     MVAT 250
         A(I,I)=A(I,I)-EIG,.                                            MVAT 260
         T=ABS(A(1,I)),.                                                MVAT 270
         IF T GT U THEN U=T,.                                           MVAT 280
              DO J=I1 TO N,.                                            MVAT 290
              T=ABS(A(I,J)),.                                           MVAT 300
              IF T GT U THEN U=T,.                                      MVAT 310
              END,.                                                     MVAT 320
         END,.                                                          MVAT 330
   EPS=U*E7,.                                                           MVAT 340
   N1=N-1,.                             /*     START FACTORIZATION     */MVAT 350
   P(1)='0'B,.                                                          MVAT 360
   IF ABS(A(2,1)) GT ABS(A(1,1))        /*       INITIALIZATION        */MVAT 370
   THEN DO,.                                                            MVAT 380
         P(1)='1'B,.                                                    MVAT 390
              DO I=1 TO N,.                                             MVAT 400
              C=A(1,I),.                                                MVAT 410
              A(1,I)=A(2,I),.                                           MVAT 420
              A(2,I)=C,.                                                MVAT 430
              END,.                                                     MVAT 440
         END,.                                                          MVAT 450
   IF ABS(A(1,1)) LT EPS THEN A(1,1)=EPS,.                              MVAT 460
   A(2,1)=A(2,1)/A(1,1),.                                               MVAT 470
         DO K=2 TO N1,.                                                 MVAT 480
         KP1=K+1,.                                                      MVAT 490
         K1=K-1,.                                                       MVAT 500
         S=A(K,K),.                     /*   COMPUTE THE LOWER FACTOR  */MVAT 510
              DO I=IS(K) TO K1,.                                        MVAT 520
              S=S-MULTIPLY(A(K,I),A(I,K),53),.                          MVAT 530
              END,.                                                     MVAT 540
         A(K,K)=S,.                                                     MVAT 550
         IF ABS(A(K,K)) LT ABS(A(KP1,K))                                MVAT 560
         THEN DO,.                      /*          PIVOTING           */MVAT 570
              P(K)='1'B,.                                               MVAT 580
                   DO I=K TO N,.                                        MVAT 590
                   C=A(K,I),.                                           MVAT 600
                   A(K,I)=A(KP1,I),.                                    MVAT 610
                   A(KP1,I)=C,.                                         MVAT 620
                   END,.                                                MVAT 630
                   DO I=IS(K) TO K1,.                                   MVAT 640
                   A(KP1,I)=A(K,I),.                                    MVAT 650
                   END,.                                                MVAT 660
              I=IS(K),.                                                 MVAT 670
              IS(K)=IS(KP1),.                                           MVAT 680
              IS(KP1)=I,.                                               MVAT 690
              END,.                                                     MVAT 700
         ELSE DO,.                                                      MVAT 710
              P(K)='0'B,.                                               MVAT 720
                   DO J=KP1 TO N,.      /*   COMPUTE THE UPPER FACTOR  */MVAT 730
                   S=A(K,J),.                                           MVAT 740
                        DO I=IS(K) TO K1,.                              MVAT 750
                        S=S-MULTIPLY(A(I,J),A(K,I),53),.                MVAT 760
                        END,.                                           MVAT 770
                   A(K,J)=S,.                                           MVAT 780
                   END,.                                                MVAT 790
              END,.                                                     MVAT 800
                                        /*  NORMALIZE THE LOWER FACTOR */MVAT 810
         IF ABS(A(K,K)) LT EPS THEN A(K,K)=EPS,.                        MVAT 820
         A(KP1,K)=A(KP1,K)/A(K,K),.                                     MVAT 830
         END,.                                                          MVAT 840
   S=A(N,N),.                                                           MVAT 850
         DO I=IS(N) TO N1,.                                             MVAT 860
         S=S-MULTIPLY(A(N,I),A(I,N),53),.                               MVAT 870
         END,.                                                          MVAT 880
   A(N,N)=S,.                           /*      END FACTORIZATION      */MVAT 890
   IF ABS(A(N,N)) LT EPS THEN A(N,N)=EPS,.                              MVAT 900
         DO I=1 TO N,.                  /*      INVERSE ITERATION      */MVAT 910
         V(I)=1,.                       /*       STARTING VALUE        */MVAT 920
         END,.                                                          MVAT 930
         DO IT=1,2,.                                                    MVAT 940
         K=N,.                                                          MVAT 950
         IF IT GT 1                                                     MVAT 960
         THEN DO,.                                                      MVAT 970
                   DO I=1 TO N1,.       /*        INTERCHANGES         */MVAT 980
                   IF P(I)                                              MVAT 990
                   THEN DO,.                                            MVAT1000
                        I1=I+1,.                                        MVAT1010
                        C=V(I),.                                        MVAT1020
                        V(I)=V(I1),.                                    MVAT1030
                        V(I1)=C,.                                       MVAT1040
                        END,.                                           MVAT1050
                   END,.                                                MVAT1060
                   DO I=2 TO N,.        /*   SOLVE WITH LOWER FACTOR  */MVAT1070
                        S=V(I),.                                        MVAT1080
                             DO J=IS(I) TO I-1,.                        MVAT1090
                             S=S-MULTIPLY(A(I,J),V(J),53),.             MVAT1100
                             END,.                                      MVAT1110
                        V(I)=S,.                                        MVAT1120
                   END,.                                                MVAT1130
              END,.                                                     MVAT1140
         V(N)=V(N)/A(N,N),.             /*   SOLVE WITH UPPER FACTOR  */MVAT1150
         U=ABS(V(N)),.                                                  MVAT1160
              DO I=N1 TO 1 BY -1,.                                      MVAT1170
              S=V(I),.                                                  MVAT1180
                   DO J=I+1 TO N,.                                      MVAT1190
                   S=S-MULTIPLY(A(I,J),V(J),53),.                       MVAT1200
                   END,.                                                MVAT1210
              V(I)=S/A(I,I),.                                           MVAT1220
              T=ABS(V(I)),.                                             MVAT1230
              IF T GT U                                                 MVAT1240
              THEN DO,.                                                 MVAT1250
                   K=I,.                                                MVAT1260
                   U=T,.                                                MVAT1270
                   END,.                                                MVAT1280
              END,.                                                     MVAT1290
         C    =V(K),.                                                   MVAT1300
              DO I=1 TO N,.             /*  NORMALIZE RESULTING VECTOR */MVAT1310
              V(I) =V(I)/C,.                                            MVAT1320
              END,.                                                     MVAT1330
         END,.                          /*  END OF LOOP FOR ITERATION  */MVAT1340
   RETURN,.                                                             MVAT1350
   END,.                                /*    END OF PROCEDURE MVAT    */MVAT1360
```

Purpose:

For a given almost triangular complex matrix (Hessenberg), this procedure provides the eigenvector corresponding to a given eigenvalue.

Usage:

CALL MVAT (A, N, EIG, V);

A(N, N) - COMPLEX BINARY FLOAT
Given almost triangular matrix.

N - BINARY FIXED
Given order of the matrix.

EIG - COMPLEX BINARY FLOAT
Given eigenvalue.

V(N) - COMPLEX BINARY FLOAT
Resultant vector containing the eigenvector corresponding to EIG.

Remarks:

The original matrix is destroyed.

Method:

Wielandt's inverse iteration is applied to the matrix, using the given eigenvalue as a shift.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical Background:

For a given nonsingular matrix A, the inverse iteration is defined by the following process:

$$V^{(p+1)} = A^{-1} V^{(p)}$$

where $V^{(0)}$ is an arbitrary starting vector. We know that when $P \to \infty$, under certain conditions $V^{(p)}$ tends to an eigenvector V associated with the smallest eigenvalue λ_0 of the matrix A.

When converging to V, the speed of convergence can be substantially improved by shifting the origin

of the eigenvalues close to λ_0. Then the iteration can be written as

$$V^{(p+1)} = (A - \lambda I)^{-1} V^{(p)} \quad (1)$$

where λ is the value of the shift.

When we know an approximation λ of λ_0, the above properties of the inverse iteration can be used for finding the corresponding eigenvector V by means of equation (1).

The closer λ is to λ_0, the faster $V^{(p)}$ converges to V. If λ has been obtained with good accuracy, V can be obtained using only a few steps of inverse iteration.

Each step of iteration is equivalent to finding the solution of the equation

$$(A - \lambda I)\ V^{(p+1)} = V^{(p)} \quad (2)$$

Considering a triangular factorization of $A - \lambda I$, $A - \lambda I = LR$, the solution of equation (2) will be provided by solving successively

$$LW = V^{(p)} \quad (3)$$

$$RV^{(p+1)} = W \quad (4)$$

where L and R are lower and upper triangular matrices. The triangular decomposition has to be performed only once before starting the iterative process, and the iteration is carried out by solving equations (3) and (4).

Programming Considerations:

A technique of partial pivoting by row interchange is included in the process of triangular factorization. This pivoting is obviously convenient in two ways; it is economical and does not modify the special structure of the matrix. Thus, it will be possible to take advantage of this structure in the factorization of the matrix, as well as in the solution of equation (3).

Since the starting vector is arbitrary, we choose it so that

$$V^{(0)} = Le,\ W = e,$$

where:

$$e^T = (1, 1, \ldots, 1)$$

Then the first iteration will consist of solving equation (4) only:

$$RV^{(1)} = e$$

Only two iterations are performed. Most of the time they are quite sufficient to provide an accurate approximation of the eigenvector V.

- Subroutine MVSU

```
MVSU..                                                                  MVSU  10
/*************************************************************************/MVSU  20
/*                                                                       */MVSU  30
/*            BACK TRANSFORMATION OF THE EIGENVECTORS                    */MVSU  40
/*                        SYMMETRIC CASE                                 */MVSU  50
/*                                                                       */MVSU  60
/*************************************************************************/MVSU  70
   PROCEDURE (A,N,CD,V),.                                               MVSU  80
   DECLARE                                                              MVSU  90
        (A(*),CD(*),V(*),T,C) BINARY,                                   MVSU 100
        (M,N,ICD,K,KP1,KP2,J,I,L) BINARY FIXED,                         MVSU 110
        (S,DP) BINARY(53),.                                             MVSU 120
   ICD=(N*(N+1))/2-1,.                                                  MVSU 130
        DO K=N-1 TO 2 BY -1,.                                           MVSU 140
        KP1=K+1,.                                                       MVSU 150
        ICD=ICD-KP1,.                                                   MVSU 160
        C=A(ICD)-CD(K),.                                                MVSU 170
        IF C NE 0                                                       MVSU 180
        THEN DO,.                       /*  ORTHOGONAL TRANSFORMATION  */MVSU 190
             S=0,.                                                      MVSU 200
                  J=ICD-K+1,.                                           MVSU 210
                       DO I=K TO N,.                                    MVSU 220
                       J=J+I-1,.                                        MVSU 230
                       S=S+MULTIPLY(A(J),V(I),53),.                     MVSU 240
                       END,.                                            MVSU 250
                  S=S/CD(K),.                                           MVSU 260
                  T=(S-V(K))/C,.                                        MVSU 270
                  V(K)=S,.                                              MVSU 280
                  J=ICD,.                                               MVSU 290
                       DO I=KP1 TO N,.                                  MVSU 300
                       J=J+I-1,.                                        MVSU 310
                       V(I)=V(I)+T*A(J),.                               MVSU 320
                       END,.                                            MVSU 330
             END,.                                                      MVSU 340
        END,.                                                           MVSU 350
        S=0,.                           /*          NORMALIZE         */MVSU 360
             DO I=1 TO N,.                                              MVSU 370
             DP=V(I),.                                                  MVSU 380
             S=S+DP*DP,.                                                MVSU 390
             END,.                                                      MVSU 400
        S=SQRT(S),.                                                     MVSU 410
             DO I=1 TO N,.                                              MVSU 420
             V(I)=V(I)/S,.                                              MVSU 430
             END,.                                                      MVSU 440
   RETURN,.                                                             MVSU 450
   END,.                            /*    END OF PROCEDURE MVSU       */MVSU 460
```

Purpose:

For a given symmetric matrix M that has been reduced to a similar tridiagonal symmetric matrix H by procedure MSTU, MVSU gives the eigenvector of M corresponding to a given eigenvector of H.

Usage:

CALL MVSU (A, N, CD, V);

A(N*(N+1)/2) - BINARY FLOAT
Given vector whose elements are set up by procedure MSTU.

N - BINARY FIXED
Given order of the original matrix M.

CD(N) - BINARY FLOAT
Given vector containing in positions 2, 3, ..., N the codiagonal terms of the tridiagonal matrix.

V(N) - BINARY FLOAT
Given eigenvector of the tridiagonal matrix. Resultant eigenvector of the original matrix.

Remarks:

See procedure MSTU.

Method:

The eigenvector of the almost triangular matrix H is transformed according to the unitary similarities applied to matrix M in procedure MSTU.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical background:

For a symmetric matrix M of order n that has been reduced to the tridiagonal matrix H by similarities, we have a relation of the form

$$H = P^{-1} MP$$

and an eigenvector of M, X(M) corresponding to an eigenvector of H, X(H) according to

$$H(M) = P \cdot X(H) \qquad (1)$$

In procedure MSTU, P consists of the product of (n-2) Householder's matrices:

$$P = P_1 \cdot P_2 \cdots\cdots P_{n-2} \qquad (2)$$

$$P_i = I + \frac{1}{b(v_{i+1} - b)} (v - be_{i+1}) (v - be_{i+1})^T$$

where the vector v and the scalar b have been defined in the transformation of the i-th column of the given matrix in procedure MSTU.

P will thus be applied to X(H) by means of (n-2) successive transformations, P_{n-2}, P_{n-1}, ..., P_1, according to equations (1) and (2).

The elements v and b defining each P_i are transmitted to MVSU through the parameters A and B.

- Subroutine MVUB

```
MVUB..                                                              MVUB  10
/*******************************************************************/MVUB  20
/*                                                                 */MVUB  30
/*            BACK TRANSFORMATION OF THE EIGENVECTORS              */MVUB  40
/*                HOUSEHOLDER'S TRANSFORMATIONS                    */MVUB  50
/*                                                                 */MVUB  60
/*******************************************************************/MVUB  70
   PROCEDURE (A,N,B,V),.                                            MVUB  80
   DECLARE                                                          MVUB  90
        (A(*,*),B(*),T,U) BINARY,                                   MVUB 100
        (I,K,K1,KP1,N) BINARY FIXED,                                MVUB 110
        (V(*),X) COMPLEX BINARY,                                    MVUB 120
        S COMPLEX BINARY(53),.                                      MVUB 130
        DO K=N-1 TO 2 BY -1,.                                       MVUB 140
        IF B(K) NE 0                                                MVUB 150
        THEN DO,.                       /*  ORTHOGONAL TRANSFORMATION  */MVUB 160
             KP1=K+1,.                                              MVUB 170
             K1=K-1,.                                               MVUB 180
             S=MULTIPLY(B(K),V(K),53),.                             MVUB 190
                  DO I=KP1 TO N,.                                   MVUB 200
                  S=S+MULTIPLY(A(I,K1),V(I),53),.                   MVUB 210
                  END,.                                             MVUB 220
             S=S/A(K,K1),.                                          MVUB 230
             X=(S-V(K))/(B(K)-A(K,K1)),.                            MVUB 240
             V(K)=S,.                                               MVUB 250
                  DO I=KP1 TO N,.                                   MVUB 260
                  V(I)=V(I)+X*A(I,K1),.                             MVUB 270
                  END,.                                             MVUB 280
             END,.                                                  MVUB 290
        END,.                                                       MVUB 300
   K=1,.                                                            MVUB 310
   T=ABS(V(1)),.                        /*          NORMALIZE      */MVUB 320
        DO I=2 TO N,.                                               MVUB 330
        U=ABS(V(I)),.                                               MVUB 340
        IF U GT T                                                   MVUB 350
        THEN DO,.                                                   MVUB 360
             T=U,.                                                  MVUB 370
             K=I,.                                                  MVUB 380
             END,.                                                  MVUB 390
        END,.                                                       MVUB 400
   X    =V(K),.                                                     MVUB 410
        DO I=1 TO N,.                                               MVUB 420
        V(I) =V(I)/X,.                                              MVUB 430
        END,.                                                       MVUB 440
   RETURN,.                                                         MVUB 450
   END,.                                /*   END OF PROCEDURE MVUB  */MVUB 460
```

Purpose:

For a given matrix M that has been reduced to a similar almost triangular matrix H by procedure MATU, MVUB gives the eigenvector of M corresponding to a given eigenvector of H.

Usage:

CALL MVUB (A, N, B, V);

A(N, N) - BINARY FLOAT
Given two-dimensional array whose elements are set up by procedure MATU.

N - BINARY FIXED
Given order of the matrix.

B(N) - BINARY FLOAT
Given vector whose components are provided by procedure MATU.

V(N) - COMPLEX BINARY FLOAT
Given eigenvector of the almost triangular matrix.
Resultant eigenvector of the original matrix.

Remarks:

See procedure MATU.

Method:

The eigenvector of the tridiagonal matrix H is transformed according to the unitary similarities applied to the matrix M in procedure MATU.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical background:

For a matrix M of order n that has been reduced to the almost triangular matrix H by similarities, we have a relation of the form

$$H = P^{-1}MP$$

and an eigenvector of M, X(M) corresponding to an eigenvector of H, X(H) according to

$$X(M) = P \cdot X(H) \qquad (1)$$

In procedure MATU, P consists of a product of (n-2) Householder's matrices:

$$P = P_1 \cdot P_2 \cdots P_{n-2} \qquad (2)$$

$$P_i = I + \frac{1}{v(v_{i+1} - b)} (v - be_{i+1}) (v - be_{i+1})^t$$

where the vector v and the scalar b have been defined in the transformation of the i-th column of the given matrix in procedure MATU.

P will thus be applied to X(H) by means of (n-2) successive transformations, P_{n-2}, P_{n-1}, ..., P_1, according to equations (1) and (2).

The elements v and b defining each P_i are transmitted to MSTU through the parameters A and B.

- Subroutine MVEB

```
MVEB..                                                                  MVEB  10
/*********************************************************************/MVEB  20
/*                                                                   */MVEB  30
/*            BACK TRANSFORMATION OF THE EIGENVECTORS                */MVEB  40
/*                    ELIMINATION TECHNIQUES                         */MVEB  50
/*                                                                   */MVEB  60
/*********************************************************************/MVEB  70
   PROCEDURE (A,N,IP,V),.                                               MVEB  80
   DECLARE                                                              MVEB  90
        (A(*,*),T,U) BINARY,                                            MVEB 100
        (V(*),C) COMPLEX BINARY,                                        MVEB 110
        (IP(*),I,K,K1,N) BINARY FIXED,                                  MVEB 120
        S COMPLEX BINARY(53),.                                          MVEB 130
        DO K=2 TO N-1,.                                                 MVEB 140
        K1=K+1,.                                                        MVEB 150
        IF A(K1,K) NE 0                                                 MVEB 160
        THEN DO,.                       /*  ELEMENTARY TRANSFORMATION  */MVEB 170
             S=V(K),.                                                   MVEB 180
                DO I=1 TO K-1,.                                         MVEB 190
                S=S-MULTIPLY(A(K1,I),V(I),53),.                         MVEB 200
                END,.                                                   MVEB 210
             V(K)=S,.                                                   MVEB 220
             END,.                                                      MVEB 230
        END,.                                                           MVEB 240
        DO K=2 TO N-1,.                                                 MVEB 250
        IF IP(K) NE K                   /*        INTERCHANGES        */MVEB 260
        THEN DO,.                                                       MVEB 270
             I=IP(K),.                                                  MVEB 280
             C=V(K),.                                                   MVEB 290
             V(K)=V(I),.                                                MVEB 300
             V(I)=C,.                                                   MVEB 310
             END,.                                                      MVEB 320
        END,.                                                           MVEB 330
   K=1,.                                                                MVEB 340
   T=ABS(V(1)),.                        /*          NORMALIZE         */MVEB 350
        DO I=2 TO N,.                                                   MVEB 360
        U=ABS(V(I)),.                                                   MVEB 370
        IF U GT T                                                       MVEB 380
        THEN DO,.                                                       MVEB 390
             T=U,.                                                      MVEB 400
             K=I,.                                                      MVEB 410
             END,.                                                      MVEB 420
        END,.                                                           MVEB 430
   C    =V(K),.                                                         MVEB 440
        DO I=1 TO N,.                                                   MVEB 450
        V(I) =V(I)/C,.                                                  MVEB 460
        END,.                                                           MVEB 470
   RETURN,.                                                             MVEB 480
   END,.                                /*   END OF PROCEDURE MVEB    */MVEB 490
```

Purpose:

For a given matrix M that has been transformed to a similar almost triangular matrix H by procedure MATE, MVEB gives the eigenvector of M corresponding to a given eigenvector of H.

Usage:

CALL MVEB (A, N, IP, V);

A(N, N) - BINARY FLOAT
Given two-dimensional array whose elements are set up by procedure MATE.

N - BINARY FIXED
Given order of the almost triangular matrix.

IP(N) - BINARY FIXED
Given vector whose components are provided by procedure MATE.

V(N) - COMPLEX BINARY FLOAT
Given eigenvector of the almost triangular matrix.
Resultant eigenvector of the original matrix.

Remarks:

See procedures MATE and MVAT.

Method:

The eigenvector of the almost triangular matrix is transformed according to the similarities applied to the matrix M in procedure MATE.

For reference see:

J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

Mathematical background:

We know that a given matrix M of order n can be reduced by similarity to an almost triangular matrix H. This can be written as

$$H = SMS^{-1}$$

Then, for a given eigenvalue of both M and H, the corresponding eigenvectors V of M and W of H are related by the equation

$$V = S^{-1}W$$

The transformation S is defined here as the product of a triangular matrix T with unit diagonal by a permutation matrix P which was operating on the rows of M according to the pivoting used in procedure MATE.

The elements of the matrix T are transmitted to the procedure through the array A. The permutation matrix P is defined by the information contained in vector IP.

Then V is provided by

$$V = PX$$

where the vector X is the solution of the equation

$$TX = W$$

Polynomial Operations

- Subroutine POV

```
POV..                                                                  POV   10
/**********************************************************************/POV   20
/*                                                                    */POV   30
/*      CALCULATE VALUES OF FIRST N ORTHOGONAL POLYNOMIALS            */POV   40
/*                                                                    */POV   50
/**********************************************************************/POV   60
   PROCEDURE(X,N,OPT,Y),.                                              POV   70
   DECLARE                                                             POV   80
        (LX,H,HC,H1,H2,FN) BINARY FLOAT(53),                           POV   90
        (Y(*),X)                                                       POV  100
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/POV  110
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/POV  120
        (N,I) BINARY FIXED,                                            POV  130
        OPT CHARACTER(1),.                                             POV  140
   LX   =X,.                                                           POV  150
   IF N GE 1                          /*BYPASS OPERATION IF N LE 0   */POV  160
   THEN DO,.                                                           POV  170
        IF OPT='T'                    /*CHEBYSHEV POLYNOMIALS T(X)   */POV  180
        THEN H0   =LX,.               /*INIT. STARTING VALUE         */POV  190
        ELSE DO,.                                                      POV  200
             FN   =1,.                /*INIT. INTEGER FACTOR TERM    */POV  210
             H0   =0,.                /*INIT. STARTING VALUE         */POV  220
             END,.                                                     POV  230
        Y(1),H1=1,.                   /*STORE AND SAVE FIRST RESULT  */POV  240
             DO I = 2 TO N,.                                           POV  250
             H2   =LX*H1,.            /*PERFORM COMMON CALCULATION   */POV  260
             H    =H2-H0,.                                             POV  270
             IF OPT NE 'T'            /*CHEBYSHEV POLYNOMIALS T(X)   */POV  280
             THEN DO,.                                                 POV  290
                  IF OPT= 'H'         /*HERMITE POLYNOMIALS H(X)     */POV  300
                  THEN DO,.                                            POV  310
                       H2   =H2+FN*HC,.                                POV  320
                       FN   =FN-2,.   /*STEP INTEGER FACTOR          */POV  330
                       END,.                                           POV  340
                  ELSE DO,.                                            POV  350
                       IF OPT= 'L'    /*LAGUERRE POLYNOMIALS L(X)    */POV  360
                       THEN DO,.                                       POV  370
                            H2   =H1-(H+H1)/FN,.                       POV  380
                            H    =H1-H0,.                              POV  390
                            END,.                                      POV  400
                       ELSE H2   =H2  /*LEGENDRE POLYNOMIALS P(X)    */POV  410
                            -H/FN,.                                    POV  420
                       FN   =FN+1,.   /*STEP INTEGER DENOMINATOR     */POV  430
                       END,.                                           POV  440
                  END,.               /*CONTINUE COMMON CALCULATION  */POV  450
             H0   =H1,.               /*SAVE PRECEDING RESULT VALUE  */POV  460
             H1,Y(I)=H+H2,.           /*STORE AND SAVE I-TH RESULT   */POV  470
             END,.                                                     POV  480
        END,.                                                          POV  490
   END,.                             /*END OF PROCEDURE POV         */POV  500
```

Purpose:

POV computes the values of the first n orthogonal polynomials. The user has the choice of

Chebyshev polynomials (T_0, T_1, ..., T_{n-1}) with OPT = 'T'

Legendre polynomials (P_0, P_1, ..., P_{n-1}) with OPT = 'P'

Laguerre polynomials (L_0, L_1, ..., L_{n-1}) with OPT = 'L'

Hermite polynomials (H_0, H_1, ..., H_{n-1}) with OPT = 'H'

Usage:

CALL POV (X, N, OPT, Y);

X - BINARY FLOAT [(53)]
Given argument of the orthogonal polynomials

N - BINARY FIXED
Given number of orthogonal polynomials to be calculated.

OPT - CHARACTER (1)
Given parameter of choice (see "Purpose").

Y(N) - BINARY FLOAT [(53)]
Resultant vector containing the values of the first N orthogonal polynomials.

Remarks:

Operation is bypassed if N is not positive. Any input value of OPT other than 'T', 'L', or 'H' is treated as if it were 'P'. The values of the shifted polynomials of Chebyshev or Legendre for argument x are obtained as values of non-shifted polynomials for the argument (2 • x - 1).

Method:

Evaluation is based on the three-term recurrence relation for orthogonal polynomials.

For reference see:

Jahnke-Emde-Loesch, Tables of Higher Functions, B. G. Teubner, Stuttgart, 1960, pp. 96-114.
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Applied Mathematics Series 55, National Bureau of Standards, 1964, pp. 771-803.

Mathematical Background:

The orthogonal polynomials are defined by the following iteration scheme:

Chebyshev polynomials $T_k(x)$

$T_0(x) = 1$

$T_1(x) = x$

$T_{k+1}(x) = 2x\,T_k(x) - T_{k-1}(x)$, for k = 1, 2, ...

Laguerre polynomials $P_k(x)$

$P_0(x) = 1$

$P_1(x) = x$

$(k+1)P_{k+1}(x) = (2k+1)xP_k(x) - kP_{k-1}(x)$,

for k = 1, 2, ...

Laguerre polynomials $L_k(x)$

$L_0(x) = 1$

$L_1(x) = 1 - x$

$(k+1)L_{k+1}(x) = (2k+1 - x)\, L_k(x) - kL_{k-1}(x)$,

for k = 1, 2, . . .

Hermite polynomials $H_k(x)$

$H_0(x) = 1$

$H_1(x) = 2x$

$H_{k+1}(x) = 2xH_k(x) - 2kH_{k-1}(x)$, for k = 1, 2, . . .

Programming Considerations:

For reasons of programming efficiency and for diminishing roundoff errors, the recurrence relations are modified to the following forms:

Chebyshev polynomials

$T_{-1} = x,\ T_0 = 1,\ T_{k+1} = xT_k - T_{k-1} + xT_k$

for k = 0, 1, 2, . . . , n-2

Legendre polynomials

$P_{-1} = 0,\ P_0 = 1,$

$P_{k+1} = xP_k - P_{k-1} - (xP_k - P_{k-1})/(k+1) + xP_k$

for k = 0, 1, 2, . . . , n - 2

Laguerre polynomials

$L_{-1} = 0,\ L_0 = 1,$

$L_{k+1} = L_k - L_{k-1} + (L_k - (xL_k - L_{k-1} + L_k)/(k+1))$

for k = 0, 1, 2, . . . , n - 2

Hermite polynomials

$H_{-1} = 0,\ H_0 = 1,$

$H_{k+1} = xH_k - H_{k-1} - (2k-1)H_{k-1} + xH_k$

for k = 0, 1, 2, . . . , n-2

- Subroutine POSV

```
POSV..                                                                  POSV  10
/*********************************************************************/POSV  20
/*                                                                   */POSV  30
/*      EVALUATE N-TERM SERIES EXPANSION IN ORTHOGONAL POLYNOMIALS   */POSV  40
/*                                                                   */POSV  50
/*********************************************************************/POSV  60
   PROCEDURE(X,C,N,OPT,SUM),.                                           POSV  70
   DECLARE                                                              POSV  80
         (LX,H,HO,H1,H2,FN) BINARY FLOAT(53),                           POSV  90
         (X,C(*),SUM)                                                   POSV 100
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/POSV 110
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/POSV 120
         (N,I) BINARY FIXED,                                            POSV 130
         OPT CHARACTER(1),.                                             POSV 140
   I    =N,.                                                           POSV 150
   IF I GE 1                        /*BYPASS OPERATION IF N LE 0    */POSV 160
   THEN DO,.                                                            POSV 170
         LX   =X,.                                                      POSV 180
         IF OPT='L'                 /*LAGUERRE POLYNOMIALS L(X)     */POSV 190
         THEN LX   =1-LX,.                                              POSV 200
         H2,H1=0,.                  /*ZERO U(N+1), U(N+2) OR V(N+2) */POSV 210
         FN   =I,.                                                      POSV 220
ITER..                              /*LOOP OVER I = N TO 1 BY -1    */POSV 230
         IF OPT='T'                 /*CHEBYSHEV POLYNOMIALS T(X)    */POSV 240
         THEN DO,.                                                      POSV 250
              HO   =LX*H1,.                                             POSV 260
              H    =HO-H2+HO,.       /*H = 2*X*U(I+1)-U(I+2)         */POSV 270
              END,.                                                     POSV 280
         ELSE DO,.                                                      POSV 290
              IF OPT='H'            /*HERMITE POLYNOMIALS H(X)      */POSV 300
              THEN DO,.                                                 POSV 310
                   H    =LX*H1-FN*H2,.                                 POSV 320
                   H    =H+H,.       /*H = 2*(X*U(I+1)-I*U(I+2))     */POSV 330
                   END,.                                                POSV 340
              ELSE DO,.             /*LAGUERRE OR LEGENDRE POLYNOM. */POSV 350
                   HO   =H1,.       /*SAVE U(I+1)                   */POSV 360
                   H    =H1/FN,.                                       POSV 370
                   H1   =H1-H,.     /*COMPUTE V(I+1)                */POSV 380
                   IF OPT='L'       /*LAGUERRE POLYNOMIALS L(X)     */POSV 390
                   THEN H =H1+LX*H+H1,./*H = 2*V(I+1)+(1-X)*U(I+1)  */POSV 400
                   ELSE H =LX*(H1+HO),./*LEGENDRE POLYNOMIALS L(X)   */POSV 410
                        H    =H-H2,.  /*H = X*(V(I+1)+U(I+1))       */POSV 420
                   END,.             /*FOR BOTH H = H-V(I+2)         */POSV 430
              FN   =FN-1,.           /*DECREASE INTEGER FACTOR       */POSV 440
              END,.                                                     POSV 450
         H2   =H1,.                 /*SAVE U(I+1) RESP. V(I+1)      */POSV 460
         H1   =H+C(I),.             /*COMP. U(I) = H+C(I)           */POSV 470
         I    =I-1,.                /*DECREASE COUNTER I            */POSV 480
         IF I GT 0                                                      POSV 490
         THEN GO TO ITER,.          /*END OF LOOP OVER I            */POSV 500
         IF OPT='T'                                                     POSV 510
         THEN H1   =H1-HO,.         /*MODIFY U(1) IN CHEBYSHEV CASE */POSV 520
         SUM  =H1,.                 /*RETURN VALUE OF SERIES        */POSV 530
         END,.                                                          POSV 540
   END,.                            /*END OF PROCEDURE POSV         */POSV 550
```

Purpose :

POSV computes the value of the sum

$\sum_{k=1}^{N} c_k f_{k-1}(x)$ for a given vector $C = (c_1, c_2, \ldots, c_N)$,

and a specified set of orthogonal polynomials (f_k).

The user has the choice of

Chebyshev polynomials $(T_0, T_1, \ldots, T_{N-1})$
with OPT = 'T'

Legendre polynomials $(P_0, P_1, \ldots, P_{N-1})$
with OPT = 'P'

Laguerre polynomials $(L_0, L_1, \ldots, L_{N-1})$
with OPT = 'L'

Hermite polynomials $(H_0, H_1, \ldots, H_{N-1})$
with OPT = 'H'

Usage:

CALL POSV (X, C, N, OPT, SUM) ;

X - BINARY FLOAT [(53)]
Given argument of orthogonal polynomials.

C(N) - BINARY FLOAT [(53)]
Given coefficient vector of series expansion.

N - BINARY FIXED
Given dimension of coefficient vector.

OPT - CHARACTER (1)
Given parameter of choice (see "Purpose").

SUM - BINARY FLOAT [(53)]
Resultant value of series expansion for argument X.

Remarks:

Operation is bypassed if N is not positive. Any input value of OPT other than 'T', 'L', or 'H' is treated as if it were 'P'.

The sum of an expansion in shifted Chebyshev or Legendre polynomials for argument x is obtained as the value of the expansion in non-shifted polynomials for argument (2 • x - 1).

Method:

Evaluation is based on the three-term recurrence relation for orthogonal polynomials, using a backward iteration scheme.

For reference see:

M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Applied Mathematics Series 55, National Bureau of Standards, 1964, pp. 771-803.

Mathematical Background:

Evaluation is based on the following iteration schemes:

Chebyshev expansion

Set $U_{n+1} = U_{n+2} = 0$ and use the recurrence

relations:

$T_k = 2xT_{k-1} - T_{k-2}$, $U_k = c_k + 2xU_{k+1} - U_{k+2}$

successively for k = n, n-1, . . . , 2.

Then

$$\sum_{i=1}^{n} c_i T_{i-1} = \sum_{i=1}^{n} c_i T_{i-1} + U_{n+1} T_n - U_{n+2} \cdot T_{n-1}$$

$$= \sum_{i=1}^{n-1} c_i T_{i-1} + (c_n + 2xU_{n+1} - U_{n+2}) T_{n-1}$$

$$- U_{n+1} T_{n-2}$$

$$= \sum_{i=1}^{n-1} c_i T_{i-1} + U_n T_{n-1} - U_{n+1} T_{n-2}$$

$$\vdots$$

$$= c_1 T_0 + U_2 T_1 - U_3 T_0 = c_1 + xU_2 - U_3$$

Legendre expansion

Set $U_{n+1} = U_{n+2} = 0$ and use the recurrence relations

$$kP_k = x(2k-1)\, P_{k-1} - (k-1)P_{k-2}$$

$$(k-1)U_k = c_k + x(2k-1)\, U_{k+1} - kU_{k+2}$$

successively for k = n, n-1, . . . , 2. Then:

$$\sum_{i=1}^{n} c_i P_{i-1} = \sum_{i=1}^{n} c_i P_{i-1} + U_{n+1} \cdot nP_n - nU_{n+2} \cdot P_{n-1}$$

$$= \sum_{i=1}^{n-1} c_i P_{i-1} + (c_n + x(2n-1)U_{n+1} - nU_{n+2}) P_{n-1}$$

$$- U_{n+1}(n-1)P_{n-2}$$

$$= \sum_{i=1}^{n-1} c_i P_{i-1} + U_n(n-1)P_{n-1} - (n-1)$$

$$U_{n+1} \cdot P_{n-2}$$

$$= c_1 P_0 + U_2 \cdot P_1 - U_3 P_0 = c_1 + xU_2 - U_3$$

Laguerre expansion

Set $U_{n+1} = U_{n+2} = 0$ and use the recurrence

relations $kL_k = (2k-1-x)L_{k-1} - (k-1)L_{k-2}$

$(k-1)U_k = c_k + (2k-1-x)U_{k+1} - kU_{k+2}$

sucessively for k = n, n-1, . . . , 2. Then:

$$\sum_{i=1}^{n} c_i L_{i-1} = \sum_{i=1}^{n} c_i L_{i-1} + U_{n+1} \cdot nL_n - nU_{n+2} L_{n-1}$$

$$= \sum_{i=1}^{n-1} c_i L_{i-1} + (c_n + (2n-1-x)U_{n+1} - nU_{n+2}) L_{n-1} - (n-1)U_{n+1} L_{n-2}$$

$$= \sum_{i=1}^{n-1} c_i L_{i-1} + U_n \cdot (n-1)L_{n-1} - (n-1) U_{n+1} L_{n-2}$$

.
.
.

$$= c_1 L_0 + U_2 L_1 - U_3 L_0$$

$$= c_1 + U_2(1-x) - U_3$$

Hermite Expansion

Set $U_{n+1} = U_{n+2} = 0$ and use the recurrence relations $H_k = 2xH_{k-1} - 2(k-1)H_{k-2}$

$U_k = c_k + 2xU_{k+1} - 2kU_{k+2}$

successively for k = n, n-1, ..., 2. Then:

$$\sum_{i=1}^{n} c_i H_{i-1} = \sum_{i=1}^{n} c_i H_{i-1} + U_{n+1} H_n - 2nU_{n+2} \cdot H_{n-1}$$

$$= \sum_{i=1}^{n-1} c_i H_{i-1} + (C_n + 2xU_{n+1} - 2nU_{n+2}) H_{n-1} - 2(n-1)U_{n+1} \cdot H_{n-2}$$

$$= \sum_{i=1}^{n-1} c_i H_{i-1} + U_n \cdot H_{n-1} - 2(n-1) U_{n+1} H_{n-2}$$

.
.
.

$$= c_1 H_0 + U_2 \cdot H_1 - 2U_3 H_0$$

$$= c_1 + 2xU_2 - 2U_3$$

Programming Considerations:

For reasons of programming efficiency the following modifications of the backward iteration scheme are used for evaluations:

Chebyshev expansion

Set:

$$U_{n+1} = U_{n+2} = 0$$

$$U_i = xU_{i+1} - U_{i+2} + xU_{i+1} + c_i \text{ for } i = n, \ldots, 1$$

Then:

$$\sum_{i=1}^{n} c_i T_{i-1}(x) = U_1 - xU_2$$

Legendre expansion

Set:

$$U_{n+1} = V_{n+2} = 0$$

$$\left.\begin{aligned} V_{i+1} &= U_{i+1} - U_{i+1/i} \\ U_i &= x(V_{i+1} - U_{i+1}) - V_{i+2} \end{aligned}\right\} \text{for } i = n, \ldots, 1$$

Then:

$$\sum_{i=1}^{n} c_i P_{i-1}(x) = U_1$$

Laguerre expansion

Set:

$$U_{n+1} = V_{n+2} = 0$$

$$\left.\begin{aligned} V_{i+1} &= U_{i+1} - U_{i+1/i} \\ U_i &= V_{i+1} + (1-x)\, U_{i+1/i} + V_{i+1} - V_{i+2} + c_i \end{aligned}\right\}$$

for i = n, . . . , 1

Then:

$$\sum_{i=1}^{n} c_i L_{i-1}(x) = U_1$$

Hermite expansion

Set:

$$U_{n+1} = U_{n+2} = 0$$

$$U_i = (xU_{i+1} - i \cdot U_{i+2}) + (xU_{i+1} - iU_{i+2})$$

for i = n, . . . , 1

Then:

$$\sum_{i=1}^{n} c_i H_{i-1}(x) = U_1$$

- Subroutine PEC/PTC

```
PEC..                                                                  PEC   10
/*********************************************************************/PEC   20
/*                                                                   */PEC   30
/*      POLYNOMIAL ECONOMIZATION OVER THE RANGE (0,A) IF OPT ='S'    */PEC   40
/*      AND OVER THE RANGE (-A,A) IF OPT ='0'                        */PEC   50
/*                                                                   */PEC   60
/*********************************************************************/PEC   70
   PROCEDURE(C,N,M,TOL,EPS,A,OPT),.                                    PEC   80
   DECLARE                                                             PEC   90
        (C(*),A,FV,FX,FM,U,V,W)                                        PEC  100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/PEC  110
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/PEC  120
        (TOL,EPS)BINARY FLOAT,                                         PEC  130
        (N,M,NH,NT,JE,I,IC,NOD,JST,IST,J)                              PEC  140
        BINARY FIXED,                                                  PEC  150
        LN BINARY FIXED(31),                                           PEC  160
        (OPT,SW,ERROR EXTERNAL) CHARACTER(1),.                         PEC  170
   SW   ='E',.                     /*MARK ENTRY ECONOMIZATION     */PEC  180
   EPS,M = 0,.                                                         PEC  190
   GO TO COM,.                                                         PEC  200
PTC..                                                                  PEC  210
/*********************************************************************/PEC  220
/*                                                                   */PEC  230
/*      TRANSFORMATION OF POLYNOMIAL TO AN EXPANSION IN TERMS OF     */PEC  240
/*      CHEBYSHEV POLYNOMIALS OVER THE RANGE (-A,A) IF OPT='0' AND   */PEC  250
/*      SHIFTED CHEBYSHEV POLYNOMIALS OVER THE RANGE (0,A) IF OPT='S'*/PEC  260
/*                                                                   */PEC  270
/*********************************************************************/PEC  280
   ENTRY(C,N,A,OPT),.                                                  PEC  290
   SW   ='T',.                     /*MARK ENTRY TRANSFORMATION    */PEC  300
COM..                                                                  PEC  310
   LN   =N,.                                                           PEC  320
   IF LN LE 0                                                          PEC  330
   THEN GO TO EXIT,.               /*GIVEN N IS NOT POSITIVE      */PEC  340
   IF OPT NE 'S'                                                       PEC  350
   THEN DO,.                                                           PEC  360
        FV   =1,.                                                      PEC  370
        NH   =LN/10B,.                                                 PEC  380
        JST  =2,.                                                      PEC  390
        NOD  =LN-NH-NH,.                                               PEC  400
        END,.                                                          PEC  410
   ELSE DO,.                                                           PEC  420
        FV   =0.5,.                                                    PEC  430
        NH   =LN-1,.                                                   PEC  440
        JST,NOD=1,.                                                    PEC  450
        END,.                                                          PEC  460
   FM,FX=FV*ABS(A),.                                                   PEC  470
   IF FX=0                                                             PEC  480
   THEN GO TO EXIT,.               /*GIVEN A EQUALS ZERO,ERROR='P'*/PEC  490
   FV   =0.5*FX,.                                                      PEC  500
   NT   =NH*NH,.                   /*DIMENSION OF ARRAY T         */PEC  510
        BEGIN,.                                                        PEC  520
        DECLARE                                                        PEC  530
             T(NT)                                                     PEC  540
             BINARY FLOAT,.         /*SINGLE PRECISION VERSION  /*S*/PEC  550
 /*          BINARY FLOAT(53),.     /*DOUBLE PRECISION VERSION  /*D*/PEC  560
        ERROR='0',.                                                    PEC  570
        JE   =0,.                   /*INIT. CALCULATION OF T-ARRAY */PEC  580
        W    =2,.                                                      PEC  590
             DO I =1 TO NT BY NH,.                                     PEC  600
             U,V,T(I)=1,.           /*INSERT ONE IN DIAGONAL       */PEC  610
             IC   =I,.                                                 PEC  620
             JE   =JE+NH,.                                             PEC  630
             I    =I+1,.                                               PEC  640
                  DO J =I TO JE,.   /*INSERT REMAINING ELEMENTS OF */PEC  650
                  IF I GT 2         /*SUBROW AND SUBCOLUMN         */PEC  660
                  THEN W    =T(IC-1),.                                PEC  670
                  V,T(J)=V+W,.                                         PEC  680
                  IC   =IC+NH,.                                        PEC  690
                  U,T(IC)=U+V,.                                        PEC  700
                  END,.                                                PEC  710
             END,.                                                     PEC  720
             DO I =2 TO LN,.        /*SUBSTITUTION OF VARIABLE     */PEC  730
             C(I) =C(I)*FX,.                                           PEC  740
             FX   =FX*FV,.                                             PEC  750
             END,.                                                     PEC  760
        IC   =NT,.                  /*INIT. FIRST TELESCOPING STEP */PEC  770
TELE..                                                                 PEC  780
        IST  =1,.                                                      PEC  790
        I    =IC,.                                                     PEC  800
        IF NOD NE 1                                                    PEC  810
        THEN IST  =NH,.                                                PEC  820
        J    =LN,.                                                     PEC  830
        IF J =0                                                        PEC  840
        THEN GO TO END,.                                               PEC  850
        U    =C(LN),.                                                  PEC  860
        IF SW='E'                                                      PEC  870
        THEN DO,.                                                      PEC  880
             W    =EPS+ABS(U),.                                        PEC  890
             IF W GT ABS(TOL)                                          PEC  900
             THEN DO,.                                                 PEC  910
                  M    =LN,.         /*DIMENSION ECONOMIZED POLYNOM.*/PEC  920
                       DO I =2 TO LN,.                               PEC  930
                       C(I) =C(I)/FM,./*BACKSUBSTITUTION OF VARIABLE */PEC  940
                       FM   =FV*FM,.                                 PEC  950
                       END,.                                         PEC  960
                  GO TO END,.                                        PEC  970
                  END,.                                              PEC  980
             EPS  =W,.                                               PEC  990
             END,.                                                     PEC 1000
SUBT..                          /*SUBTRACT MULTIPLE OF CHEBY-  */PEC 1010
        I    =I-IST,.           /*SHEV POLYNOMIAL              */PEC 1020
        J    =J-JST,.                                                  PEC 1030
        IF J GT 1                                                      PEC 1040
        THEN DO,.                                                      PEC 1050
             C(J) =C(J)+U*T(I),.                                       PEC 1060
             U    =-U,.             /*ALTERNATE SIGNS IN T         */PEC 1070
             GO TO SUBT,.                                              PEC 1080
             END,.                                                     PEC 1090
        IF J = 1                                                       PEC 1100
        THEN C(1) =C(1)+U,.         /*ADJUST CONSTANT TERM         */PEC 1110
        IF OPT NE 'S'                                                  PEC 1120
        THEN NOD  =1-NOD,.          /*INIT. NEXT TELESCOPING STEP  */PEC 1130
        IF NOD=1                                                       PEC 1140
        THEN IC   =IC-NH-1,.                                           PEC 1150
        LN   =LN-1,.                                                   PEC 1160
        GO TO TELE,.                                                   PEC 1170
        END,.                                                          PEC 1180
EXIT..                                                                 PEC 1190
   ERROR='P',.                                                         PEC 1200
END..                                                                  PEC 1210
   END,.                            /*END OF PROCEDURE PEC         */PEC 1220
```

Purpose:

PEC approximates a given polynomial by a polynomial of lower degree, using a telescoping technique, so that the error does not exceed a user-specified tolerance TOL. Range of approximation is (-a, a) if OPT='0' and (0, a) if OPT='S'.

Usage:

CALL PEC (C, N, M, TOL, EPS, A, OPT);

C(N) - BINARY FLOAT [(53)]
Given coefficient vector of the polynomial $P(x) = c_1 + c_2x + ... + c_nx^{n-1}$
Resultant coefficient vector of the economized polynomial $P_{m-1}(x) = c_1 + c_2x + ... + c_mx^{m-1}$

N - BINARY FIXED
Given dimension of given coefficient vector.

M - BINARY FIXED
Resultant dimension of economized coefficient vector.

TOL - BINARY FLOAT
Given tolerance specified by the user.

EPS - BINARY FLOAT
Resultant bound for the absolute difference between the given and economized polynomial over the specified range.

A - BINARY FLOAT [(53)]
Given value defining the range of approximation.

OPT - CHARACTER(1)
Given option for selection of operation

Purpose:

PTC transforms a given polynomial into an expansion of Chebyshev polynomials if OPT = '0' and of shifted Chebyshev polynomials if OPT = 'S'.

Usage:

CALL PTC (C, N, A, OPT);

C(N) - BINARY FLOAT [(53)]
Given coefficient vector of the polynomial $P(x) = c_1 + c_2x + ... + c_nx^{n-1}$
Resultant coefficient vector of Chebyshev expansion
$P(x) = c_1 + c_2t_1(t) + ... + c_nt_{n-1}(t)$
with $t = x/A$
and $t_k(t) = \begin{cases} T_k(t) & \text{if OPT='0'} \\ T^*_k(t) & \text{if OPT='S'} \end{cases}$

N - BINARY FIXED
Given dimension of the coefficient vector.

A - BINARY FLOAT [(53)]
Given value defining the range of expansion.

OPT - CHARACTER (1)
Given option for selection of operation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR = 'P' means invalid parameters:
either $N \le 0$ or $A = 0$

A value of OPT different from 'S' is interpreted as if it were '0'.

On return from PEC the locations $c_{m+1}, ..., c_n$ contain the coefficients of the Chebyshev expansion of the difference between the given polynomial P(x) and the economized polynomial $P_{m-1}(x)$:

$$P(x) = P_{m-1}(x) + c_{m+1}t_m(t) + ... c_nt_{n-1}(t)$$

Therefore, using PEC with a very large tolerance TOL (say, 10^{75}) has the same effect as the application of PTC.

Method:

In the first telescoping step a multiple of the Chebyshev polynomial

$$t_{n-1}(x/a) = \begin{cases} T_{n-1}(x/a) & \text{if OPT = '0'} \\ T^*_{n-1}(x/a) & \text{if OPT = 'S'} \end{cases}$$

is subtracted from given P(x), so that the difference is a polynomial of degree n-2.
Set:

$$P_{n-1}(x) = P(x)$$

then:

$$P_{n-2}(x) = P_{n-1}(x) - b_nt_{n-1}(x/a) \qquad (1)$$

Telescoping $P_{n-2}(x)$ again results in a polynomial $P_{n-3}(x)$ of degree n-3, and by iteration

$$P(x) = b_1 + b_2t_1(x/a) + b_3t_2(x/a) + ... + b_nt_{n-1}(x/a) \qquad (2)$$

This means that calculated b's form the coefficient vector of the expansion in terms of Chebyshev polynomials. If telescoping steps are performed only as long as

$$\left| b_n \right| + \left| b_{n-1} \right| + \ldots + \left| b_{m+1} \right| \leq \left| \text{TOL} \right|$$

then $P_{m-1}(x)$ is the economized polynomial. For the Chebyshev polynomials

$$\left| t_k(x/a) \right| \leq 1 \text{ for } \left| x \right| \leq a$$

and for all values of k; therefore,

$$\begin{aligned} \left| P(x) - P_{m-1}(x) \right| &= \left| b_{m+1} t_m (x/a + \ldots \right. \\ &\quad \left. + b_n t_{n-1}(x/a) \right| \\ &\leq \left| b_{m+1} \right| + \left| b_{m+2} \right| \\ &\quad + \ldots + \left| b_n \right| \leq \left| \text{TOL} \right| \end{aligned} \tag{3}$$

Mathematical Background

Calculation of the coefficients of $T_k(t)$

Set $C_k(z) = 2T_k(z/2)$ or $T_k(t) = \frac{1}{2} C_k(2t)$, with $t = \frac{z}{2}$. (4)

Then $C_k(z) = S_k(z) - S_{k-2}(z)$ (5)

with $S_k(z) = \binom{k}{0} z^k - \binom{k-1}{1} z^{k-1} + - \ldots \pm \binom{0}{k}$. (6)

The binomial coefficients $\binom{k-v}{v}$ are easily generated using Pascal's triangle.

An analogous calculation scheme exists for the coefficients of $C_k(z)$:

$$C_k(z) = \frac{k}{k} \binom{k}{0} z^k - \frac{k}{k-1} \binom{k-1}{1} z^{k-z} + \frac{k}{k-2} \binom{k-2}{2} z^{k-4} - \ldots \tag{7}$$

The coefficients of successive $C_k(z)$ are easily found by the calculation scheme

2		$C_0(z) = 2$
1		$C_1(z) = z$
2	1	$C_2(z) = z^2 - 2$
3	1	$C_3(z) = z^2 - 3z$
2	4 1	$C_4(z) = z^4 - 4z^2 + 2$
5	(5) 1	$C_5(z) = z^5 - 5z^3 + 5z$
2	(9) 6 1	$C_6(z) = z^6 - 6z^4 + 9z^2 - 2$
7	(14) 7 1	. .
2	16 20 8 1	. .
.	. . . .	. .
.	. . . .	. .

(8)

The above calculation scheme means that the first column is all two's and the diagonal elements are all ones. The remaining elements are obtained by adding the two elements above in the same column and in the adjacent left-hand column. For example, circled element 14 is obtained by adding the two circled elements 9 and 5.

The shifted Chebyshev polynomials are reduced to ordinary ones using the identity

$$2T_k^*(u/4) = 2T_{2k}(\sqrt{u}/2) = C_{2k}(\sqrt{u}) \tag{9}$$

or

$$T_k^*(t) = \frac{1}{2} C_{2k}(2\sqrt{t}) \quad \text{with } t = u/4$$

Programming Considerations:

The triangle (8) may be stored more compactly in the rectangular scheme:

2	1	3	5	7	.
2	4	1	5	14	.
2	9	6	1	7	.
2	16	20	8	1	.
.	.	.	.	.	.

(10)

The coefficients of C_{2k-1} form subcolumns and those of C_{2k} corresponding subrows. In order to be able to use the coefficients of the auxiliary array (10), the given polynomial

$$P(x) = c_1 + c_2 x + \ldots + c_n x^{n-1} \qquad (11)$$

must first be transformed substituting $x = |a|\,t$, which gives

$$P(x) = b_1 + b_2 t + b_3 t^2 + \ldots + b_n t^{n-1} \qquad (12)$$

By this the argument range gets reduced to the standard interval (-1, +1) if OPT = '0' and (0, 1) if OPT = 'S'.

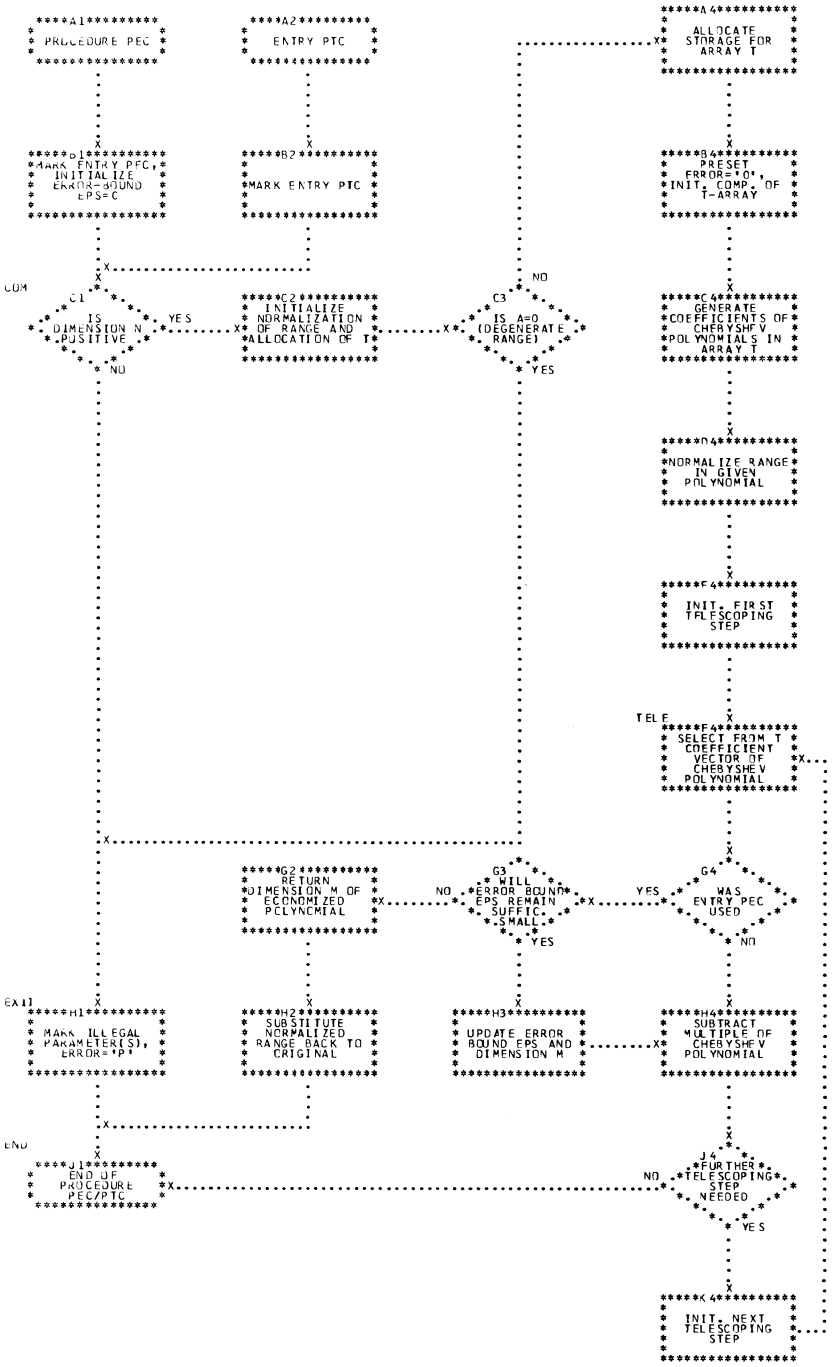
The next step is to introduce z=2t if OPT = '0' and u=4t if OPT = 'S' and to divide all coefficients so obtained by two, except the first one. Naturally the two substitutions may be applied simultaneously:

$$x = |a| \cdot t = \frac{|a|}{2} z = \frac{|a|}{4} u \qquad (13)$$

The sequence of calculations performed is as follows:

1. The auxiliary array (10) is set up calculating row and column simultaneously.
2. The given coefficient vector gets replaced by the coefficient vector with variable z or u.
3. In case PTC, performing n-1 successive telescoping steps gives the expansion in terms of Chebyshev polynomials. In case PEC, the iterative telescoping is stopped as soon as the tolerance TOL is exceeded.
4. The economized polynomial must be back-transformed to the original variable x.

PROCEDURE PEC ECONOMIZES A POLYNOMIAL USING TRUNCATION IN CORRESPONDING CHEBYSHEV EXPANSION
ENTRY PTC TRANSFORMS A POLYNOMIAL TO AN EXPANSION IN TERMS OF CHEBYSHEV POLYNOMIALS



- Subroutine POST

```
POST..                                                              POST  10
/*******************************************************************/POST  20
/*                                                                 */POST  30
/*      TRANSFORM N-TERM SERIES EXPANSION IN ORTHOGONAL POLYNOMIALS */POST  40
/*                                                                 */POST  50
/*******************************************************************/POST  60
   PROCEDURE(X0,X1,C,N,OPT,POL),.                                   POST  70
   DECLARE                                                          POST  80
        (X0,X1,C(*),POL(*),F,FI,AI,BI,CI,U,U1,U2,U3,H(N+N))         POST  90
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/POST 100
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/POST 110
        (N,I,J,K,KP1) BINARY FIXED,                                 POST 120
        OPT CHARACTER(1),.                                          POST 130
   IF N GE 1                          /*BYPASS OPERATION IF N LE 0  */POST 140
   THEN DO,.                          /*INITIALIZATION              */POST 150
        AI   =X0+X0,.                 /*INIT. CONSTANT MULTIPLIERS  */POST 160
        CI   =X1+X1,.                                               POST 170
        IF OPT='T'                    /*CHEBYSHEV POLYNOMIALS T(X)  */POST 180
        THEN BI   =0.5,.              /*MODIFY FIRST CHEB. POLYNOMIAL*/POST 190
        ELSE DO,.                                                   POST 200
             BI   =1,.                /*INIT. FIRST ORTH. POLYNOMIAL */POST 210
             FI   =0,.                /*INIT. INTEGER FACTOR        */POST 220
             END,.                                                  POST 230
        H(2) =BI,.                    /*STORE FIRST ORTH. POLYNOMIAL */POST 240
        H(1) =0,.                     /*INIT. PSEUDO POLYNOMIAL(-1) */POST 250
        POL(1)=C(1),.                 /*INIT. RESULTING POLYNOMIAL  */POST 260
             DO I = 2 TO N,.          /*CALCULATE COEFFICIENT VECTOR */POST 270
             F    =C(I),.             /*OF I-TH ORTHOGONAL POLYNOM. */POST 280
             IF OPT NE 'T'                                          POST 290
             THEN DO,.                /*MODIFY MULTIPLIERS AI,BI,CI  */POST 300
                  BI   =FI,.                                        POST 310
                  FI   =FI+1,.        /*FOR                         */POST 320
                  IF OPT NE 'H'       /*HERMITE POLYNOMIALS H(X)    */POST 330
                  THEN DO,.                                         POST 340
                       BI   =BI/FI,.  /*FOR                         */POST 350
                       IF OPT='L'     /*LAGUERRE POLYNOMIALS L(X)   */POST 360
                       THEN DO,.                                    POST 370
                            AI   =1-X0/FI+BI,.                      POST 380
                            CI   =-X1/FI,.                          POST 390
                            END,.     /*FOR                         */POST 400
                       ELSE DO,.      /*LEGENDRE POLYNOMIALS P(X)   */POST 410
                            AI   =X0+BI*X0,.                        POST 420
                            CI   =X1+BI*X1,.                        POST 430
                            END,.                                   POST 440
                  END,.                                             POST 450
             ELSE BI   =BI+BI,.                                     POST 460
             END,.                                                  POST 470
        ELSE IF I = 3                 /*READJUST CHEBYSHEV POLYNOMIAL*/POST 480
        THEN H(1) =1,.                                              POST 490
        U    =0,.                     /*INIT. PSEUDO TERM FOR RECURR.*/POST 500
        K    =1,.                                                   POST 510
        KP1  =2,.                                                   POST 520
             DO J = 1 TO I-1,.        /*APPLY RECURRENCE RELATION   */POST 530
             U1   =H(K),.                                           POST 540
             H(K),U2=H(KP1),.                                       POST 550
             IF OPT NE 'T'            /*IN CHEBYSHEV CASE           */POST 560
             THEN U1   =BI*U1,.       /*BYPASS MULTIPLICATION WITH 1 */POST 570
             H(KP1),U3=AI*U2-U1+CI*U,.                              POST 580
             U    =U2,.                                             POST 590
             POL(J)=POL(J)+F*U3,./*UPDATE POLYNOMIAL VECTOR         */POST 600
             K    =KP1+1,.                                          POST 610
             KP1  =K+1,.                                            POST 620
             END,.                                                  POST 630
        H(K) =0,.                     /*INIT. PSEUDO TERM FOR RECURR.*/POST 640
        U3,H(KP1)=U2*CI,.             /*COMPLETE I-TH ORTH.POLYNOMIAL*/POST 650
        POL(I)=F*U3,.                 /*INIT. I-TH TERM OF POLYNOMIAL*/POST 660
        END,.                         /*COEFFICIENT VECTOR          */POST 670
   END,.                                                            POST 680
END,.                                 /*END OF PROCEDURE POST       */POST 690
```

Purpose:

POST transforms a given series expansion in orthogonal polynomials to a polynomial. The independent variable of the given expansion is assumed to be $x_0 + x_1 x$; that is, a linear transformation of the range is built in. The coefficient vector $C = (c_1, \ldots, c_n)$ is given. Procedure POST calculates $POL = (pol_1, \ldots, pol_n)$ satisfying

$$\sum_{i=1}^{n} c_i f_{i-1}(x_0 + x_1 \cdot x) = \sum_{i=1}^{n} pol_i \cdot x^{i-1}$$

For the specified set of orthogonal polynomials (f_k) the user has the choice of:

Chebyshev polynomials $(T_0, T_1, \ldots, T_{n-1})$
with OPT = 'T'
Legendre polynomials $(P_0, P_1, \ldots, P_{n-1})$
with OPT = 'P'
Laguerre polynomials $(L_0, L_1, \ldots, L_{n-1})$
with OPT = 'L'
Hermite polynomials $(H_0, H_1, \ldots, H_{n-1})$
with OPT = 'H'

Usage:

CALL POST (X0, X1, C, N, OPT, POL);

X0 - BINARY FLOAT [(53)]
Given constant term of argument transformation.

X1 - BINARY FLOAT [(53)]
Given linear term of argument transformation.

C(N) - BINARY FLOAT [(53)]
Given coefficient vector of expansion, with coefficients ordered from low to high.

N - BINARY FIXED
Given dimension of coefficient vector.

OPT - CHARACTER (1)
Given parameter of choice (see "purpose").

POL(N) - BINARY FLOAT [(53)]
Resultant coefficient vector of resultant ordinary polynomial, with coefficients ordered from low to high.

Remarks:

N must be positive, or operation is bypassed.

Any input value of OPT other than 'T', 'L', or 'H' is treated as if it were 'P'.

Transformation of an expansion in shifted Chebyshev or Legendre polynomials is obtained using the linear transformation $(2x_0 - 1) + (2x_1)\, x$.

The resultant vector POL may occupy the same storage locations as the given vector C.

Method:

The coefficient vector POL is calculated from the coefficient vectors of the orthogonal polynomials, which are generated successively using the recurrence relation.

$$f_{k+1} = (a_k + c_k x) f_k - b_k f_{k-1} \quad \text{for } k \geq 0$$

with $f_{-1}=0$, $f_0=1$.

For reference see:

M. Abramowitz/I. A. Stegun, Handbook of Mathematical Functions, Applied Mathematics Series 55, National Bureau of Standards, 1964, pp. 771-803.

Mathematical Background:

The coefficient vectors of the orthogonal polynomials for argument $z = x_0 + x_1 x$ are generated using the three-term recurrence relation:

Chebyshev polynomials

$$T_{-1} = 0,\ T_0 = 1,\ T_1(z) = x_0 + x_1 x$$

$$T_{k+1}(z) = 2x_0 T_k(z) - T_{k-1}(z) + 2x_1 \cdot xT_k(z),$$

for $k \geq 1$

Legendre polynomials

$$P_{-1} = 0,\ P_0 = 1$$

$$P_{k+1}(z) = \left(1 + \frac{k}{k+1}\right) x_0 P_k(z) - \left(\frac{k}{k+1}\right) P_{k-1}(z) + \left(1 + \frac{k}{k+1}\right) x_1 x\, P_k(z),\ \text{for } k \geq 0$$

Laguerre polynomials

$$L_{-1} = 0,\ L_0 = 1$$

$$L_{k+1}(z) = \left(1 + \frac{k}{k+1} - \frac{x_0}{k+1}\right) L_k(z) - \left(\frac{k}{k+1}\right) L_{k-1}(z) - \left(\frac{x_1}{k+1}\right) xL_k(z),\ \text{for } k \geq 0$$

Hermite polynomials

$$H_{-1} = 0,\ H_0 = 1$$

$$H_{k+1} = 2x_0 H_k(z) - 2kH_{k-1}(z) + 2x_1 xH_k(z),$$

for $k \geq 0$

Programming Considerations:

Using $T_0/2$ instead of T_0, the above recurrence relation for Chebyshev polynomials is also valid for calculation of the coefficient vector of $T_1(z)$ with $k = 0$. The coefficient vectors of two successive orthogonal polynomials are combined in an auxiliary linear array H with coefficients of the lower polynomial in H(1), H(3), ..., and those of the higher polynomial in H(2), H(4), ...

Both coefficient vectors are ordered from low to high.

- Subroutine PRTC

```
(NOUNDERFLOW)..PRTC..                                                    PRTC  10
/*************************************************************************/PRTC  20
/*                                                                       */PRTC  30
/*      CALCULATE ALL RCCTS CF A COMPLEX PCLYNCMIAL                      */PRTC  40
/*                                                                       */PRTC  50
/*************************************************************************/PRTC  60
   PROCEDURE(C,N),.                                                      PRTC  70
   DECLARE                                                               PRTC  80
         C(*) COMPLEX                                                    PRTC  90
         BINARY FLCAT,                  /*SINGLE PRECISION VERSION  /*S*/PRTC 100
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/PRTC 110
         (D(N),B(N),Z,DZ,V,W,U,ZC) COMPLEX                               PRTC 120
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/PRTC 130
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/PRTC 140
         (N,LN,I,K,KD,J,JE)                                              PRTC 150
         BINARY FIXED,                                                   PRTC 160
         (I1,IN DEFINED R,ID DEFINED AW,IR,IR1,IR2)                      PRTC 170
         BINARY FIXED(31),                                               PRTC 180
         (AV,AVO,TCL,AZ,Ak,R,RD,RKM,ARG,ARGV)                            PRTC 190
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/PRTC 200
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/PRTC 210
         ERROR EXTERNAL CHARACTER(1),.                                   PRTC 220
                                                                         PRTC 230
   I1    =1091567616,.                                                   PRTC 240
   LN    =N,.                           /*NUMBER CF MISSING ROOTS     */PRTC 250
   Z     =C,.                                                            PRTC 260
   ERRCR='0',.                                                           PRTC 270
ZERO..                                                                   PRTC 280
   AVO   =1E75,.                        /*FORCE SHIFT CF ORIGIN       */PRTC 290
   IF LN LE 0                                                            PRTC 300
   THEN GO TO EXIT,.                    /*ALL RCCTS CALCULATED        */PRTC 310
   IF C(LN)=0                                                            PRTC 320
   THEN DO,.                            /*EXTRACT ZERO ROOT           */PRTC 330
         LN    =LN-1,.                                                   PRTC 340
         GO TO ZERC,.                                                    PRTC 350
         END,.                                                           PRTC 360
   CZ,Z =CONJG(Z),.                                                      PRTC 370
         DO I = 1 TO LN,.                                                PRTC 380
         D(I),B(I)=C(I),.               /*MOVE CCEFFICIEN: VECTOR     */PRTC 390
         END,.                                                           PRTC 400
VALUE..                                                                  PRTC 410
   TOL   =0.2,.                         /*INIT. RCUND CFF BOUND       */PRTC 420
   AZ    =ABS(Z),.                                                       PRTC 430
   V     =1,.                                                            PRTC 440
         DO I = 1 TO LN,.               /*CCMP. RCUND-CFF BOUNC       */PRTC 450
         W     =D(I),.                  /*AND PCLYNCMIAL VALUE        */PRTC 460
         V,C(I)=W+V*Z,.                                                  PRTC 470
         TOL   =ABS(W)+AZ*TCL,.                                          PRTC 480
         END,.                                                           PRTC 490
   TOL   =(TOL+4*(TOL-ABS(W)))                                           PRTC 500
         *1.0E-6,.,.                    /*SINGLE PRECISION VERSION  /*S*/PRTC 510
 /*      *0.25E-15,.                    /*DOUBLE PRECISION VERSION  /*D*/PRTC 520
   AV    =ABS(V),.                                                       PRTC 530
   IF AV= 0 THEN GO TC RCOT,.                                            PRTC 540
   IF AV LE TOL                                                          PRTC 550
   THEN IF AV GT AVO                                                     PRTC 560
   THEN DO,.                            /*STORE CALCULATED ROOT       */PRTC 570
ROOT..                                                                   PRTC 580
         C(LN)=Z,.                                                       PRTC 590
         LN    =LN-1,.                                                   PRTC 600
         GO TO ZERC,.                                                    PRTC 610
         END,.                                                           PRTC 620
   ARGV =ATAN(-IMAG(V),-REAL(V)),.                                       PRTC 630
   IF AV LT AVO                         /*HAS VALUE DECREASED         */PRTC 640
   THEN DO,.                                                             PRTC 650
         R     =AV,.                                                     PRTC 660
         RD,U =1,.                                                       PRTC 670
         IR    =(IN-I1)/LN,.                                             PRTC 680
         KD,JE=LN,.                                                      PRTC 690
SHIFT..                                                                  PRTC 700
         W     =1,.                                                      PRTC 710
               DO J=1 TO JE,.           /*SHIFT CF ORIGIN             */PRTC 720
               B(J),W=B(J)+W*DZ,.                                        PRTC 730
               END,.                                                     PRTC 740
         IF LN NE JE                                                     PRTC 750
         THEN DO,.                                                       PRTC 760
               AW    =ABS(W),.                                           PRTC 770
               K     =LN-JE,.                                            PRTC 780
               IR1   =(IN-ID)/K,.                                        PRTC 790
               IF IR1 LT IR                                              PRTC 800
               THEN DO,.                                                 PRTC 810
                     IR    =IR1,.                                        PRTC 820
                     RD    =AW,.                                         PRTC 830
                     U     =W,.                                          PRTC 840
                     KD    =K,.                                          PRTC 850
                     END,.                                               PRTC 860
               END,.                                                     PRTC 870
         JE    =JE-1,.                                                   PRTC 880
         IF JE GE 1                                                      PRTC 890
         THEN GO TC SHIFT,.                                              PRTC 900
         RKM   =1/FLOAT(KD),.                                           PRTC 910
         R     =(AV/RD)**RKM,.                                           PRTC 920
         ARG   =(ARGV-ATAN(IMAG(U),REAL(U)))*RKM,.                       PRTC 930
         ZO    =Z,.                                                      PRTC 940
         AVO   =AV,.                                                     PRTC 950
INCR..                                                                   PRTC 960
         REAL(DZ)=R*CCS(ARG),.                                           PRTC 970
         IMAG(DZ)=R*SIN(ARG),.                                           PRTC 980
         Z     =ZO+DZ,.                                                  PRTC 990
         IF ZO NE Z                                                      PRTC1000
         THEN GO TO VALUE,.                                              PRTC1010
         IF AV GT TOL                                                    PRTC1020
         THEN ERROR='C',.                                                PRTC1030
         GO TC ROOT,.                                                    PRTC1040
   ELSE DO,.                            /*MODIFY STEPSIZE TO DECREASE */PRTC1050
         R     =R/2,.                   /*PCLYNCMIAL VALUE            */PRTC1060
         IR2   =(IN-I1)/1C000C0000B,.                                    PRTC1070
         KD    =LN,.                                                     PRTC1080
         U     =1,.                                                      PRTC1090
         IR    =I1/10CCCCCCCCB,.                                         PRTC1100
         K     =0,.                                                      PRTC1110
               DO J = LN-1 TO 1 BY -1,.                                  PRTC1120
               K     =K+1,.                                              PRTC1130
               W     =B(J),.                                             PRTC1140
               AW    =ABS(W),.                                           PRTC1150
               IR1   =ID/10CC0C0C000B-(LN-K)*IR2,.                       PRTC1160
               IF IR LT IR1                                              PRTC1170
               THEN DO,.                                                 PRTC1180
                     KD    =K,.                                          PRTC1190
                     U     =W,.                                          PRTC1200
                     IR    =IR1,.                                        PRTC1210
                     END,.                                               PRTC1220
               END,.                                                     PRTC1230
```

```
      ARG =(ARGV-ATAN(IMAG(U),REAL(U)))/FLOAT(KD),.          PRTC1240
      GO TO INCR,.                                           PRTC1250
      END,.                                                  PRTC1260
EXIT..                                                       PRTC1270
   END,.                        /*END OF PROCEDURE PRTC      */PRTC1280
```

Purpose:

PRTC calculates all roots of a given complex polynomial.

Usage:

CALL PRTC (C, N);

C(N) - COMPLEX BINARY FLOAT [(53)]
Given coefficient vector of normalized polynomial

$$P(Z)=Z^N+C_1Z^{N-1}+\ldots+C_N$$

Resultant N complex roots of given polynomial.

N - BINARY FIXED
Given dimension of coefficient vector. N is also the degree of the polynomial and the number of roots to be calculated.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected.

ERROR='C' means that calculated roots are possibly inaccurate. The polynomial must be given in normalized form -- that is, the coefficient of Z^N should be one (and is not stored). The coefficient vector is replaced by the calculated roots, beginning with C(N). The coefficient vector must be complex. In the real polynomial case, the imaginary part of the coefficients must be set to zero before using PRTC. PRTC will compile with error message IEM 11051. However, the generated object code executes correctly.

Method:

The method used was proposed by K. Nickel. It is a generalization of Newton's method and is not sensitive to multiple roots.

For reference see:

K. Nickel, "Die numerische Berechnung der Wurzeln eines Polynoms", Numerische Mathematik, vol. 9 (1966), pp. 80-98.

K. Nickel, "Die Nullstellen eines Polynoms", Algorithmus 5, Computing, Vol. 2 (1967), iss. 3, pp. 284-290.

Mathematical Background:

Generalized Newton step

Let z_i be an approximation to a root of

$$P(z) = z^n + c_1 z^{n-1} + \ldots + c_n \tag{1}$$

The next approximation is calculated from the coefficients of the shifted polynomial:

$$P(z) = b_0 (z - z_i)^n + b_i (z - z_i)^{n-1} + \ldots + b_n \text{ with } b_0 = 1 \tag{2}$$

$$z_{i+1} = z_i + \sqrt[(n-k)]{\frac{-b_n}{b_k}} \tag{3}$$

where k is chosen so that

$$r_k = \min_{j = 0, 1, \ldots n-1} \sqrt[(n-j)]{\left|\frac{b_n}{b_j}\right|} = \sqrt[(n-k)]{\left|\frac{b_n}{b_k}\right|} \tag{4}$$

For k = n-1, (3) is the Newton iteration method, which requires $b_{n-1} \neq 0$. The above iteration method works in case of multiple roots.

Bisection step

The iteration method (3) does not guarantee monotonic convergence. If the condition

$$\left| P(z_{i+1}) \right| < \left| P(z_i) \right| \tag{5}$$

fails for some i, then a new approximation $\hat{z}_m$ is found such that

$$\left| P(\hat{z}_m) \right| < \left| P(z_i) \right| \tag{6}$$

The existence of a $\hat{z}_m$ satisfying (6) follows from $|P(z_i)| > 0$ and the maximum modulus principle. In fact, a suitable $\hat{z}_m$ can be found in the sequence

$$\hat{z}_m = z_i + 2^{-m} r_k \sqrt[(n-lm)]{\frac{-b_n}{b_{l_m}} \left| \frac{b_{l_m}}{b_n} \right|} \qquad m = 1, 2, \ldots \tag{7}$$

where l_m is chosen so that

$$\left| b_{l_m} \right| (2^{-m} r_k)^{n-l_m} = \max \left[\left| b_j \right| (2^{-m} r_k)^{n-j} \right]$$

$$l_{m-1} \le j \le n-1 \qquad (8)$$

The proof of this is given in the first reference above.

Stopping criterion

The iteration method (3) is terminated if, at some step, the polynomial value does not decrease and the value itself is already less than an estimate of the roundoff error. If the estimated roundoff bound cannot be met by the polynomial value because of failure of the bisection method, the iteration is stopped with error indication ERROR='C'.

Estimate for roundoff error

The polynomial value

$$P(Z) = \sum_{r=0}^{n} a_r z^{n-r} \qquad (9)$$

is evaluated using nested multiplication:

$$b_{-1} = 0, \quad b_k = z b_{k-1} = a_k \quad \text{for} \quad k = 0, 1, 2, \ldots, n \qquad (10)$$

with $P(z) = b_n$.

Since all arithmetic operations are performed with floating point arithmetic, instead of the numbers b_k, internal approximations $\hat{b}_k$ will be generated that do not satisfy $P(z) = b_n$.

The following calculation will give an estimate of

$$\left| P(Z) - \hat{b}_n \right| .$$

The approximate values

$$\hat{b}_k = \underline{\hat{rb}}_k + i\, \underline{\hat{cb}}_k,$$

where $\underline{\hat{rb}}_k$ and $\underline{\hat{cb}}_k$ are the real and imaginary parts of $\hat{b}_k$, satisfy the equations.

$$\underline{\hat{rb}}_k = \left[\xi \cdot \underline{\hat{rb}}_{k-1} (1 + \pi_{1,k}) - \eta\, \underline{\hat{cb}}_{k-1} (1 + \pi_{2,k}) \right] \left[(1 + \sigma_{1,k}) + \underline{ra}_k \right] / (1 + \sigma_{2,k})$$

$$\underline{\hat{cb}}_k = \left[\xi \cdot \underline{\hat{cb}}_{k-1} (1 + \pi_{3,k}) + \eta \cdot \underline{\hat{rb}}_{k-1} (1 + \pi_{4,k}) \right] \left[(1 + \sigma_{3,k}) + \underline{ca}_k \right] / (1 + \sigma_{4,k}) \qquad (11)$$

where $z = \xi + i\eta$, $Q_k = \underline{ra}_k + i\underline{ca}_k$, and $\sigma_{i,k}$, $\pi_{i,k}$ are relative errors of addition and multiplication respectively.

Solving (10) for a_k and inserting into

$$P(z) = \sum_{r=0}^{n} a_r z^{n-r}$$

gives

$$\begin{aligned} P(z) - \hat{b}_n = \sum_{k=0}^{n} z^{n-k} \Big(& \sigma_{2,k} \cdot \underline{\hat{rb}}_k + i\sigma_{4,k} \underline{\hat{cb}}_k \\ & - \xi\, \underline{\hat{rb}}_{k-1} (\pi_{1,k} + \sigma_{1,k} + \pi_{1,k}\, \sigma_{1,k}) \\ & + \eta \underline{\hat{cb}}_{k-1} (\pi_{2,k} + \sigma_{1,k} + \pi_{2,k}\, \sigma_{1,k}) \\ & - i\xi\, \underline{\hat{cb}}_{k-1} (\pi_{3,k} + \sigma_{3,k} + \pi_{3,k}\, \sigma_{3,k}) \\ & - i\eta\, \underline{\hat{rb}}_{k-1} (\pi_{4,k} + \sigma_{3,k} + \pi_{4,k}\, \sigma_{3,k}) \Big) \end{aligned} \qquad (12)$$

With $\left| \sigma_{i,k} \right| \le \sigma$, $\left| \pi_{i,k} \right| \le \pi$, $\left| \pi_{i,k} (1 + \sigma_{i,k}) \right| \le \pi$, and $b_{-1} = 0$

$$\left| P(z) - \hat{b}_n \right| \le \sum_{k=1}^{n-1} \left| z \right|^{n-k} \sigma \left| \hat{b}_k \right| + \left| z \right| \left| \hat{b}_{k-1} \right| (\sigma + 3\pi) + \sigma \left| b_0 \right| \left| z \right|^n \qquad (13)$$

or

$$\left| P(z) - \hat{b}_n \right| \le \sum_{k=1}^{n-1} \left| z \right|^{n-k} \left| \hat{b}_k \right| (2\sigma + 3\pi) + \sigma \left(\left| b_0 \right| \left| z \right|^n + \left| b_n \right| \right) = E$$

E may be generated using the iteration scheme

$$e_0 = \frac{\sigma}{2\sigma + 3\pi}\left| b_0 \right|, \quad e_k = \left|\hat{b}_k\right| + \left| z \right| e_{k-1} \text{ for}$$

$$k = 1, 2, \ldots, n$$

giving

$$E = (2\sigma + 3\pi)\, e_n - (\sigma + 3\pi)\left| b_n \right| \qquad (14)$$

In single precision, $\sigma = \pi = 10^{-6}$.

In double precision, $\sigma = \pi = 0.25 \cdot 10^{-15}$.

Programming Considerations:

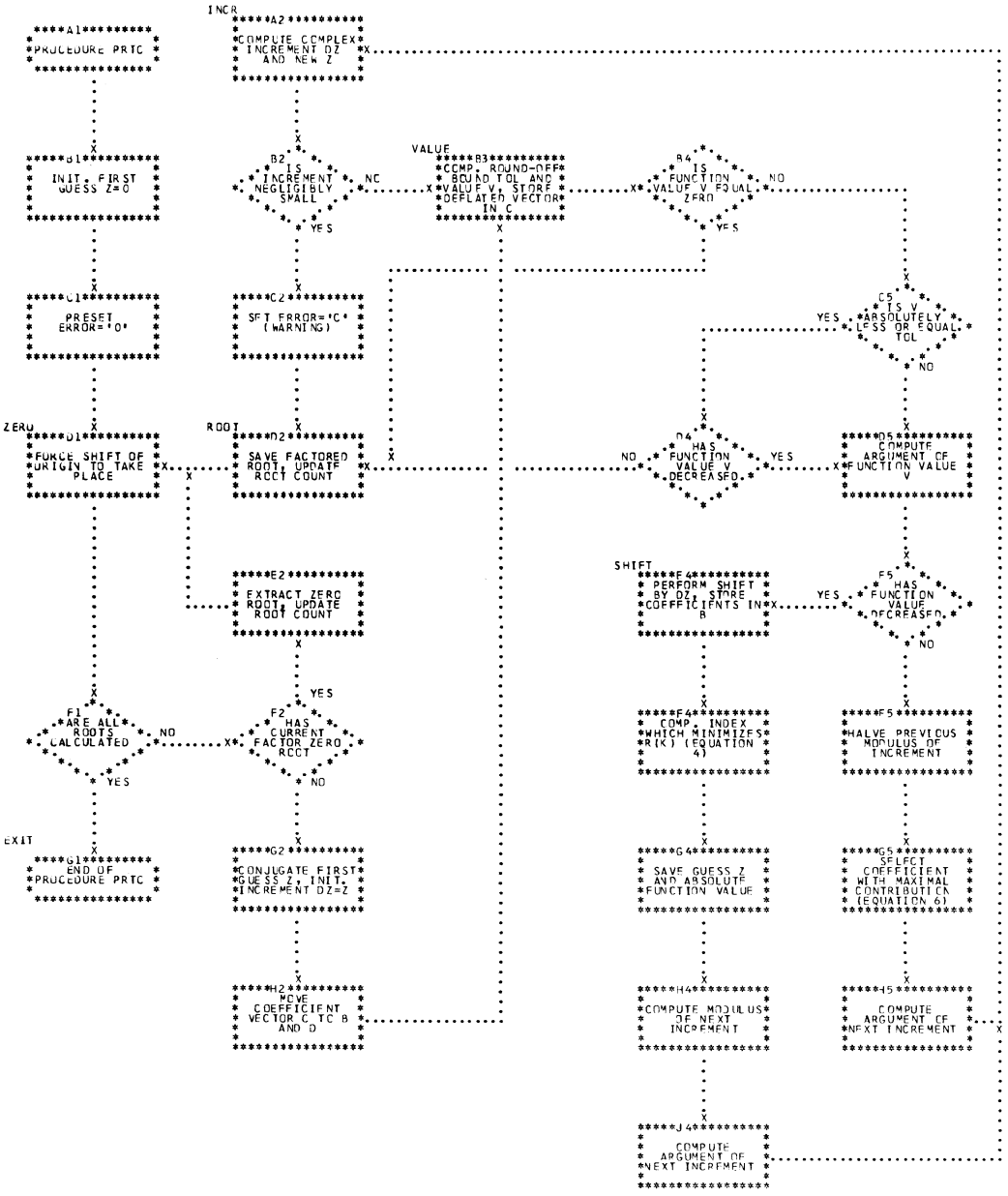
The polynomial must be given in normalized form; that is, the coefficient of z^n must be unity. Coefficients are ordered in decreasing order. Calculated zeros replace the coefficient vector; that is, the root stored in C(n) is calculated first and the root stored in C(1) is calculated last.

The iteration scheme starts with z = 0 initially.

As soon as the root z_1 has been calculated, P(z) is divided by $z - z_1$, giving $P_1(z)$. The complex conjugate $\overline{z}_1$ is used as the initial guess for a root of $P_1(z)$. Finally z_n is obtained as the root of $P_{n-1}(z)$, a linear polynomial.

No attempt is made to refine the approximated zeros with the original coefficient vector.

PROCEDURE PRTC CALCULATES ALL ROOTS OF A COMPLEX POLYNOMIAL



Numerical Quadrature

Quadrature of Tabulated Functions

- Subroutine QTFG/QTFE

```
QTFG..                                                              QTFG  10
/*******************************************************************/QTFG  20
/*                                                                 */QTFG  30
/*      INTEGRATION OF A MONOTONICALLY TABULATED FUNCTION BY       */QTFG  40
/*      TRAPEZOIDAL RULE                                           */QTFG  50
/*                                                                 */QTFG  60
/*******************************************************************/QTFG  70
   PROCEDURE(X,Y,Z,DIM),.                                           QTFG  80
   DECLARE                                                          QTFG  90
        (X(*),Y(*),Z(*),SUM,XC,XN,YO,YN,H,HH)                       QTFG 100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/QTFG 110
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/QTFG 120
        (DIM,I) BINARY FIXED,                                       QTFG 130
        (ERROR EXTERNAL,SW)CHARACTER(1),.                           QTFG 140
   SW   ='1',.                                                      QTFG 150
   XO   =X(1),.                                                     QTFG 160
   GOTO COM,.                                                       QTFG 170
QTFE..                                                              QTFG 180
/*******************************************************************/QTFG 190
/*                                                                 */QTFG 200
/*      INTEGRATION OF AN EQUIDISTANTLY TABULATED FUNCTION BY      */QTFG 210
/*      TRAPEZOIDAL RULE                                           */QTFG 220
/*                                                                 */QTFG 230
/*******************************************************************/QTFG 240
   ENTRY(H,Y,Z,DIM),.                                               QTFG 250
   SW   ='0',.                                                      QTFG 260
   HH   =0.5*H,.                                                    QTFG 270
COM..                                                               QTFG 280
   ERROR='1',.                         /*PRESET ERROR PARAMETER    */QTFG 290
   IF DIM GT 0                         /*NO ACTION IN CASE DIM LT 1 */QTFG 300
   THEN DO,.                                                        QTFG 310
        ERROR='0',.                                                 QTFG 320
        SUM  =0,.                                                   QTFG 330
        YO   =-Y(1),.                                               QTFG 340
        DO I=1 TO DIM,.                                             QTFG 350
        IF SW='1'                                                   QTFG 360
        THEN DO,.                      /*CALCULATE LENGTH OF INTERVAL */QTFG 370
             XN   =X(I),.                                           QTFG 380
             HH   =C.5*(XN-XO),.                                    QTFG 390
             XO   =XN,.                                             QTFG 400
             END,.                                                  QTFG 410
        YN   =Y(I),.                                                QTFG 420
        SUM  =SUM+HH*(YN+YO),.         /*ACCUMULATE INTEGRAL VALUE  */QTFG 430
        Z(I) =SUM,.                                                 QTFG 440
        YO   =YN,.                                                  QTFG 450
        END,.                                                       QTFG 460
      END,.                                                         QTFG 470
   END,.                               /*END OF PROCEDURE QTFG      */QTFG 480
```

Purpose:

QTFG computes a vector Z of integral values for a given vector X of argument values and a given vector Y of function values.

Usage:

CALL QTFG (X, Y, Z, DIM);

X(DIM) - BINARY FLOAT [(53)]
Given vector of argument values.

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.

DIM - BINARY FIXED
Given dimension of vectors X, Y, Z.

Purpose:

QTFE computes a vector Z of integral values for a given vector X of equidistantly tabulated argument values and a given vector Y of function values.

Usage:

CALL QTFE (H, Y, Z, DIM);

H - BINARY FLOAT [(53)]
Given difference of two successive arguments:
$H = x_i - x_{i-1}$

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.

DIM - BINARY FIXED
Given dimension of vectors Y, Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='1' - means DIM is less than 1.
The vectors Z and Y may be identically allocated, which means that the given function values are replaced by the resultant integral values.

Method:

The integral values are obtained by means of the trapezoidal rule.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 75.

Mathematical Background:

Let x_i, y_i be the given table of arguments and function values.

The vector of integral values

$$z_i = \int_{x_1}^{x_i} y(x)\,dx$$

is calculated using the trapezoidal rule

$$z_i = z_{i-1} + \frac{(x_i - x_{i-1})}{2}(y_i + y_{i-1})$$

for i = 2,..., DIM

with $z_1 = 0$.

In case of equidistant arguments: $x_i - x_{i-1} = h$.

The local truncation error at each step is

$$R_i = \frac{1}{12}(x_i - x_{i-1})^3 y''(\xi_i), \left(\xi_i \in [x_i, x_{i-1}]\right)$$

assuming that y(x) has continuous derivatives up to the second order.

The total truncation error is the accumulation of the local errors at the previous step.

- Subroutine QSF

```
QSF..                                                                  QSF   10
/*********************************************************************/QSF   20
/*                                                                   */QSF   30
/*      INTEGRATION OF AN EQUIDISTANTLY TABULATED FUNCTION BY        */QSF   40
/*      SIMPSON'S RULE                                               */QSF   50
/*                                                                   */QSF   60
/*********************************************************************/QSF   70
   PROCEDURE(H,Y,Z,DIM),.                                              QSF   80
   DECLARE                                                             QSF   90
        (H,Y(*),Z(*),AUX,SUM1,SUM2,HH,F1,F2)                           QSF  100
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/QSF  110
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/QSF  120
        ERROR EXTERNAL CHARACTER(1),                                   QSF  130
        (I,DIM) BINARY FIXED,.                                         QSF  140
   ERROR='1',.                        /*PRESET ERROR PARAMETER      */QSF  150
   IF DIM GE 4                        /*NO ACTION IN CASE DIM LT 4  */QSF  160
   THEN DO,.                                                           QSF  170
        ERROR='0',.                                                    QSF  180
        HH   =H/3,.                                                    QSF  190
        F1   =Y(1),.                                                   QSF  200
        F2   =Y(2),.                                                   QSF  210
        SUM1,Z(1)=0,.                                                  QSF  220
        SUM2,Z(2)=HH*0.125*(9*F1+     /*COMPUTE Z(2) BY COMBINATION  */QSF  230
             19*F2-5*Y(3)+Y(4)),.     /*OF SIMPSON'S WITH 3/8-RULE  */QSF  240
             DO I=3 TO DIM,.                                           QSF  250
             AUX  =F2+F2,.                                             QSF  260
             AUX  =AUX+AUX+F1,.                                        QSF  270
             F1   =F2,.                                                QSF  280
             F2   =Y(I),.                                              QSF  290
             AUX  =HH*(AUX+F2),.                                       QSF  300
             SUM1 =SUM1+AUX,.          /*ACCUMULATE INTEGRAL VALUE   */QSF  310
             AUX,Z(I)=SUM1,.                                           QSF  320
             SUM1 =SUM2,.                                              QSF  330
             SUM2 =AUX,.                                               QSF  340
             END,.                                                     QSF  350
        END,.                                                          QSF  360
   END,.                              /*END OF PROCEDURE QSF        */QSF  370
```

Purpose:

QSF computes a vector Z of integral values, given a vector Y of function values corresponding to a vector X of equidistantly tabulated arguments.

Usage:

CALL QSF (H, Y, Z, DIM);

H - BINARY FLOAT [(53)]
Given difference of two successive arguments:
$H = x_i - x_{i-1}$

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.

DIM - BINARY FIXED
Given dimension of vectors Y and Z.

REMARKS:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='1' - means DIM is less than four. Vectors Y and Z may be identically allocated, which means that the given function values are replaced by the resultant integral values.

Method:

The integral values z_i are obtained by Simpson's rule together with Newton's 3/8 rule.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 71-76.

R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 214-221.

Mathematical Background:

Let $Y = (y_1, y_2, \ldots, y_{DIM})$ be the given vector of function values corresponding to equidistant arguments x_i.

The vector of integral values

$$z_i = \int_{x_1}^{x_i} y(x)\, dx$$

is calculated from Simpson's rule

$$z_i = z_{i-2} + \frac{h}{3}(y_{i-2} + 4y_{i-1} + y_i) \text{ for } i = 3, \ldots, \text{DIM} \quad (1)$$

where the value of z_2 is obtained using a combination of Simpson's rule and Newton's 3/8 rule

$$z_i = z_{i-3} + 3/8\ h\ (y_{i-3} + 3y_{i-2} + 3y_{i-1} + y_i) \quad (2)$$

resulting in

$$z_2 = z_1 + \frac{h}{24}(9y_1 + 19y_2 - 5y_3 + y_4) \quad (3)$$

with $z_1 = 0$.

The local truncation errors of the above formulas are:

$$R_{1,i} = \frac{3}{90} h^5 y^{(4)}(\xi_i), \quad (\xi_i \in [x_{i-2}, x_i])$$

$$R_{2,i} = \frac{3}{80} h^5 y^{(4)}(\xi_i), \quad (\xi_i \in [x_{i-3}, x_i])$$

However, these truncation errors may accumulate.

- Subroutine QHFG/QHSG/QHFE/QHSE

```
QHFG..                                                                  QHFG  10
/*************************************************************************/QHFG  20
/*                                                                       */QHFG  30
/*      INTEGRATION OF A MONOTONICALLY TABULATED FUNCTION WITH           */QHFG  40
/*      FIRST DERIVATIVE BY A HERMITIAN FORMULA OF FIRST ORDER           */QHFG  50
/*                                                                       */QHFG  60
/*************************************************************************/QHFG  70
   PROCEDURE(X,Y,FDY,Z,DIM),                                            QHFG  80
   DECLARE                                                              QHFG  90
         (X(*),Y(*),Z(*),FDY(*),SDY(*),XC,XN,YC,YN,FDYO,FDYN,SDYO,SDYN, QHFG 100
         SUM1,SUM2,FACT,H,HH,HHH)                                       QHFG 110
         BINARY FLOAT,              /*SINGLE PRECISION VERSION  /*S*/QHFG 120
 /*      BINARY FLOAT(53),          /*DOUBLE PRECISION VERSION  /*D*/QHFG 130
         (I,DIM) BINARY FIXED,                                          QHFG 140
         (ERROR EXTERNAL,SW)CHARACTER(1),.                              QHFG 150
   SW   ='1',.                                                          QHFG 160
   GOTO MONO,.                                                          QHFG 170
QHSG..                                                                  QHFG 180
/*************************************************************************/QHFG 190
/*                                                                       */QHFG 200
/*      INTEGRATION OF A MONOTONICALLY TABULATED FUNCTION WITH           */QHFG 210
/*      FIRST AND SECOND DERIVATIVES BY A HERMITIAN FORMULA OF           */QHFG 220
/*      SECOND ORDER                                                     */QHFG 230
/*                                                                       */QHFG 240
/*************************************************************************/QHFG 250
   ENTRY(X,Y,FDY,SDY,Z,DIM),.                                           QHFG 260
   SW   ='2',.                                                          QHFG 270
MONO..                                                                  QHFG 280
   XC   =X(1),.                                                         QHFG 290
   GOTO MONEQ,.                                                         QHFG 300
QHFE..                                                                  QHFG 310
/*************************************************************************/QHFG 320
/*                                                                       */QHFG 330
/*      INTEGRATION OF AN EQUIDISTANTLY TABULATED FUNCTION WITH          */QHFG 340
/*      FIRST DERIVATIVE BY A HERMITIAN FORMULA OF FIRST ORDER           */QHFG 350
/*                                                                       */QHFG 360
/*************************************************************************/QHFG 370
   ENTRY(H,Y,FDY,Z,DIM),.                                               QHFG 380
   SW   ='3',.                                                          QHFG 390
   GOTO EQUI,.                                                          QHFG 400
QHSE..                                                                  QHFG 410
/*************************************************************************/QHFG 420
/*                                                                       */QHFG 430
/*      INTEGRATION OF AN EQUIDISTANTLY TABULATED FUNCTION WITH          */QHFG 440
/*      FIRST AND SECOND DERIVATIVES BY A HERMITIAN FORMULA OF           */QHFG 450
/*      SECOND ORDER                                                     */QHFG 460
/*                                                                       */QHFG 470
/*************************************************************************/QHFG 480
   ENTRY(H,Y,FDY,SDY,Z,DIM),.                                           QHFG 490
   SW   ='4',.                                                          QHFG 500
EQUI..                                                                  QHFG 510
   HH   =0.5*H,.                                                        QHFG 520
MONEQ..                                                                 QHFG 530
   ERROR='1',.                      /*PRESET ERROR PARAMETER        */QHFG 540
   FACT =3.333333333333333E-01,.                                        QHFG 550
   IF DIM GT 0                      /*NO ACTION IN CASE DIM LT 1    */QHFG 560
   THEN DO,.                                                            QHFG 570
        ERROR='0',.                                                     QHFG 580
        IF SW NE '1'                                                    QHFG 590
        THEN DO,.                                                       QHFG 600
             IF SW NE '3'                                               QHFG 610
             THEN DO,.                                                  QHFG 620
                  FACT =0.4,.                                           QHFG 630
                  SDYC =-SDY(1),.                                       QHFG 640
                  END,.                                                 QHFG 650
             END,.                                                      QHFG 660
        YO   =-Y(1),.                                                   QHFG 670
        FDYO =FDY(1),.                                                  QHFG 680
        SUM1,SUM2=0,.                                                   QHFG 690
             DO I=1 TO DIM,.                                            QHFG 700
             YN   =Y(I),.                                               QHFG 710
             FDYN =FDY(I),.                                             QHFG 720
             IF SW NE '3'                                               QHFG 730
             THEN DO,.                                                  QHFG 740
                  IF SW NE '4'          /*SW ='1' OR SW ='2'        */QHFG 750
                  THEN DO,.             /*FOR NONEQUIDISTANT ARGUMENTS*/QHFG 760
                       XN   =X(I),.     /*COMPUTE LENGTH OF INTERVAL  */QHFG 770
                       HH   =0.5*(XN-XO),.                              QHFG 780
                       XO   =XN,.                                       QHFG 790
                       END,.                                            QHFG 800
                  IF SW NE '1'          /*SW ='2' OR SW ='4'        */QHFG 810
                  THEN DO,.                                             QHFG 820
                       SDYN =SDY(I),.                                   QHFG 830
                       SUM2 =HH*HH*     /*MODIFY TO SECOND ORDER    */QHFG 840
                            (SDYC+      /*FORMULA                   */QHFG 850
                            SDYN)/15,.                                  QHFG 860
                       SDYO =SDYN,.                                     QHFG 870
                       END,.                                            QHFG 880
                  END,.                                                 QHFG 890
             HHH  =HH*FACT,.                                            QHFG 900
             SUM1 =SUM1+HH*(YC+YN+    /*ACCUMULATE INTEGRAL VALUE   */QHFG 910
                  HHH*(FDYO-FDYN)*SUM2),.                               QHFG 920
             Z(I) =SUM1,.                                               QHFG 930
             YO   =YN,.                                                 QHFG 940
             FDYO =FDYN,.                                               QHFG 950
             END,.                                                      QHFG 960
        END,.                                                           QHFG 970
   END,.                            /*END OF PROCEDURE QHFG       */QHFG 980
```

Purpose:

QHFG computes a vector Z of integral values for given vectors X, Y, and FDY of argument, function, and first derivative values respectively.

Usage:

CALL QHFG (X, Y, FDY, Z, DIM);

X(DIM) - BINARY FLOAT [(53)]
Given vector of argument values.
Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.
FDY(DIM) - BINARY FLOAT [(53)]
Given vector of first derivative values.
Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.
DIM - Given dimension of vectors X, Y, FDY, Z.

Purpose:

QHSG computes a vector Z of integral values for given vectors X, Y, FDY, and SDY of argument, function, first derivative, and second derivative values respectively.

Usage:

CALL QHSG (X, Y, FDY, SDY, Z, DIM);

X(DIM) - BINARY FLOAT [(53)]
Given vector of arguments.
Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.
FDY(DIM) - BINARY FLOAT [(53)]
Given vector of first derivative values.
SDY(DIM) - BINARY FLOAT [(53)]
Given vector of second derivative values.
Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.
DIM - BINARY FIXED
Given dimension of vectors X, Y, FDY, SDY, Z.

Purpose:

QHFE computes a vector Z of integral values for given vectors Y and FDY of function and first derivative values respectively, corresponding to a vector X of equidistantly tabulated argument values.

Usage:

CALL QHFE (H, Y, FDY, Z, DIM);

H - BINARY FLOAT [(53)]
Given difference of two arguments: $H = x_i - x_{i-1}$
Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.
FDY(DIM) - BINARY FLOAT [(53)]
Given vector of first derivative values.
Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.
DIM - BINARY FIXED
Given dimensions of vectors Y, FDY, Z.

Purpose:

QHSE computes a vector Z of integral values for given vectors Y, FDY, SDY of function values, first derivative values, and second derivative values respectively, corresponding to a vector X of equidistantly tabulated arguments.

Usage:

CALL QHSE (H, Y, FDY, SDY, Z, DIM);

H - BINARY FLOAT [(53)]
Given difference of two argument values: $H = x_i - x_{i-1}$
Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.
FDY(DIM) - BINARY FLOAT [(53)]
Given vector of first derivative values.
SDY(DIM) - BINARY FLOAT [(53)]
Given vector of second derivative values.
Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of integral values.
DIM - BINARY FIXED
Given dimensions of vectors Y, FDY, SDY, Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:
ERROR ='1' means DIM is less than 1.

The storage allocation of vector Z may be identical to one of the given vectors, which means that the given values are replaced by the resultant integral values.

Method:

The calculation of integral values is done using Hermitian formulas of the first and second order.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 314-319.

R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227-230.

Mathematical Background:

Let X, Y, FDY, SDY denote the vectors of arguments x_i, function values y_i, first derivative values y_i' and second derivative values y_i'' respectively.

The vector of integral values

$$z_i = \int_{x_1}^{x_i} y(x)\,dx$$

is calculated from one of the following:

Hermitian formula of first order:

$$z_i = z_{i-1} + \frac{x_i - x_{i-1}}{2}\left[y_{i-1} + y_i + \frac{x_i - x_{i-1}}{6}\,(y'_{i-1} - y'_i)\right] \qquad (1)$$

with $z_1 = 0$. $\qquad (i = 2,3, \ldots, DIM)$

Hermitian formula of second order:

$$z_i = z_{i-1} + \frac{x_i - x_{i-1}}{2}\left\{y_{i-1} + y_i + \frac{x_i - x_{i-1}}{5}\left[y_{i-1}' - y_i'\right. + \frac{x_i - x_{i-1}}{12}\,(y_{i-1}'' + y_i'')\right]\right\} \qquad (2)$$

$$(i = 2,3, \ldots, DIM)$$

with $z_1 = 0$.

Corresponding formulas for equidistant arguments (meaning $x_i - x_{i-1} = h$):

$$z_i = z_{i-1} + \frac{h}{2}\left[y_{i-1} + y_i + \frac{h}{6}\,(y'_{i-1} - y_i')\right] \qquad (1a)$$

$$(i = 2,3, \ldots, DIM)$$

with $z_1 = 0$, and

$$z_i = z_{i-1} + \frac{h}{2}\left\{y_{i-1} + y_i + \frac{h}{5}\left[y'_{i-1} - y'_i + \frac{h}{12}\,(y''_{i-1} + y_i'')\right]\right\} \qquad (2a)$$

$$(i = 2,3, \ldots, DIM)$$

with $z_1 = 0$.

Assuming that y(x) has continuous derivatives up to the sixth order, the local truncation error at each step is

$$R_{1,i} = \frac{(x_i - x_{i-1})^5}{120}\,y^{(4)}(\xi_i)$$

$$(\xi_i \in [x_{i-1}, x_i])$$

and

$$R_{2,i} = \frac{(x_i - x_{i-1})^7}{100800}\,y^{(6)}(\xi_i),$$

$$(\xi_i \in [x_{i-1}, x_i])$$

The total truncation error is the accumulation of the local errors at the previous step.

For equidistant arguments, this leads to:

$$R_{1n} = \frac{1}{120}\,h^4\,y^{(4)}(\xi),$$

$$(\xi \in [x_1, x_n])$$

and

$$R_{2n} = -\frac{1}{100800}\,h^6\,y^{(6)}(\xi),$$

$$(\xi \in [x_1, x_n])$$

where 1 is the length of the integration interval.

Quadrature of Nontabulated Functions

- Subroutine QATR

```
QATR..                                                                  QATR  10
/*************************************************************************/QATR  20
/*                                                                       */QATR  30
/*      INTEGRATION OF A GIVEN FUNCTION BY THE TRAPEZOIDAL RULE          */QATR  40
/*      TOGETHER WITH ROMBERG'S EXTRAPOLATION METHOD                     */QATR  50
/*                                                                       */QATR  60
/*************************************************************************/QATR  70
   PROCEDURE (XL,XU,EPS,DIM,FCT,Y),.                                    QATR  80
   DECLARE                                                              QATR  90
         (XL,XU,EPS,Y,AUX(DIM),H,HH,E,YY,                               QATR 100
         DELT1,DELT2,P,HD,X,SM,Q,AN,AO)                                 QATR 110
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/QATR 120
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/QATR 130
         ERROR EXTERNAL CHARACTER(1),                                   QATR 140
         (DIM,JJ,I,J) BINARY FIXED,                                     QATR 150
         FCT ENTRY                                                      QATR 160
         (BINARY FLOAT)                 /*SINGLE PRECISION VERSION  /*S*/QATR 170
 /*      (BINARY FLOAT(53))             /*DOUBLE PRECISION VERSION  /*D*/QATR 180
         RETURNS(BINARY FLOAT),.        /*SINGLE PRECISION VERSION  /*S*/QATR 190
 /*      RETURNS(BINARY FLOAT(53)),.    /*DOUBLE PRECISION VERSION  /*D*/QATR 200
   AN,YY,AUX(1)=0.5*(FCT(XL)+FCT(XU)),.                                 QATR 210
   H    =XU-XL,.                                                        QATR 220
   ERROR='0',.                          /*PRESET ERROR PARAMETER      */QATR 230
   IF DIM GT 1                                                          QATR 240
   THEN DO,.                                                            QATR 250
         IF H =0                                                        QATR 260
         THEN GOTO YEND,.                                               QATR 270
         HH   =H,.                      /*NORMAL CASE,DIM GREATER THAN */QATR 280
         E    =ABS(EPS/H),.             /*1 AND XL NOT EQUAL TO XU    */QATR 290
         DELT2=0,.                                                      QATR 300
         P    =1,.                                                      QATR 310
         JJ   =1,.                                                      QATR 320
              DO I=2 TO DIM,.                                           QATR 330
              DELT1=DELT2,.                                             QATR 340
              HD   =HH,.                                                QATR 350
              HH   =0.5*HH,.                                            QATR 360
              P    =0.5*P,.                                             QATR 370
              X    =XL+HH,.                                             QATR 380
              SM   =0,.                                                 QATR 390
                   DO J=1 TO JJ,.       /*REFINE STEPSIZE IN          */QATR 400
                   SM   =SM+FCT(X),.    /*TRAPEZOIDAL RULE            */QATR 410
                   X    =X+HD,.                                         QATR 420
                   END,.                                                QATR 430
              AN,AO,AUX(I)=0.5*AN+P*SM,.                                QATR 440
              Q    =1,.                /*APPLY ROMBERG'S EXTRAPOLATION*/QATR 450
                   DO J=1 TO I-1,.     /*METHOD                      */QATR 460
                   Q    =4*Q,.                                          QATR 470
                   AO,AUX(I-J)=AC+(AO-AUX(I-J))/(Q-1),.                 QATR 480
                   END,.                                                QATR 490
              DELT2=ABS(YY-AO),.        /*TEST ACCURACY               */QATR 500
              IF I GE 5                                                 QATR 510
              THEN DO,.                                                 QATR 520
                   IF DELT2 GE DELT1                                    QATR 530
                   THEN DO,.            /*TERMINATE SINCE LAST STEP   */QATR 540
                        IF DELT1 GT E   /*DID NOT IMPROVE             */QATR 550
                        THEN ERROR='1',.                                QATR 560
                        GOTO YEND,.                                     QATR 570
                        END,.                                           QATR 580
                   YY   =AC,.                                           QATR 590
                   IF DELT2 LE E                                        QATR 600
                   THEN GOTO YEND,.                                     QATR 610
                   END,.                                                QATR 620
              ELSE YY   =AO,.                                           QATR 630
              JJ   =JJ+JJ,.                                             QATR 640
              END,.                                                     QATR 650
         END,.                                                          QATR 660
   ERROR='2',.                                                          QATR 670
YEND..                                                                  QATR 680
   Y    =H*YY,.                                                        QATR 690
   END,.                                /*END OF PROCEDURE QATR       */QATR 700
```

Purpose:

QATR computes the integral value

$$Y = \int_{XL}^{XU} FCT(X)\, dX$$

for a given function FCT(X), defined in the closed interval [XL, XU], by the trapezoidal rule together with Romberg's extrapolation method.

Usage:

CALL QATR (XL, XU, EPS, DIM, FCT, Y);

XL - BINARY FLOAT [(53)]
Given lower bound of the interval.

XU - BINARY FLOAT [(53)]
Given upper bound of the interval.

EPS - BINARY FLOAT [(53)]
Given upper bound of the absolute error.

DIM - BINARY FIXED
Given maximum number of extrapolation steps +1 (for details see "Programming Considerations").

FCT - ENTRY
Given procedure for calculation of the function values, which must be supplied by the user.

Usage:
FCT(T)

T - BINARY FLOAT [(53)]
Given argument.

FCT(T) - BINARY FLOAT [(53)]
Resultant function value.

Y - BINARY FLOAT [(53)]
Resultant approximation for the integral value.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR = '1' means that it is impossible to reach the required accuracy because of rounding errors.

ERROR = '2' means that it was impossible to check accuracy because DIM is less than 5, or the required accuracy could not be reached within DIM-1 steps.

Method:

Evaluation of the approximation Y to the integral value is done by means of the trapezoidal rule combined with Romberg's extrapolation method.

For reference see:

S. Filippi, "Das Verfahren von Romberg-Stiefel-Bauer als Spezialfall des allgemeinen Prinzips von Richardson", Mathematik-Technik-Wirtschaft, vol. 11, iss. 2(1964), pp. 49-54.

Bauer, Algorithm 60, CACM, vol. 4, 155.6 (1961), pp. 255.

Mathematical Background:

The problem is to compute an approximation for

$$y = \int_a^b f(x)\,dx \qquad (1)$$

Successively dividing the interval [a,b] into 2^i equidistant subintervals (i = 0,1,2,...) and using the following notations:

$$h_i = \frac{b-a}{2^i} \; ; \; x_{i,k} = a + k \cdot h_i,$$

$$f_{i,k} = f(x_{i,k}) \quad (k = 0,1,2, \ldots, 2^i)$$

the trapezoidal rule gives approximations $T_{0,i}$ to the integral value y:

$$T_{0,i} = h_i \left\{ \sum_{k=0}^{2^i} f_{i,k} - \frac{1}{2}(f(a) + f(b)) \right\} \qquad (2)$$

Then the following can be written:

$$T_{0,i} = y + \sum_{r=1}^{\infty} C_{0,2r} \cdot h_i^{2r}$$

with unknown coefficients $C_{0,2r}$ that do not depend on i. Thus there is a truncation error of the order h_i^2.

Knowing two successive approximations, $T_{0,i}$ and $T_{0,i+1}$, we can generate an extrapolated value:

$$T_{1,i} = T_{0,i+1} + \frac{T_{0,i+1} - T_{0,i}}{2^2 - 1} \qquad (3)$$

This is a better approximation to y because:

$$T_{1,i} = y + \frac{1}{2^2 - 1} \sum_{r=1}^{\infty} C_{0,2r}(2^2 h_{i+1}^{2r} - h_i^{2r})$$

Noting that $2^2 h_{i+1}^2 - h_i^2 = 0$ and setting:

$$C_{1,2r} = \frac{1}{2^2 - 1} (2^2 - 2^{2r}) \cdot C_{0,2r}$$

$T_{1,i}$ becomes:

$$T_{1,i} = y + \sum_{r=2}^{\infty} C_{1,2r} h_{i+1}^{2r}$$

This gives a truncation error of the order h_{i+1}^4.

Knowing $T_{0,i+2}$ also, $T_{1,i+1}$ can be generated (equation 3), and:

$$T_{2,i} = T_{1,i+1} + \frac{T_{1,i+1} - T_{1,i}}{2^4 - 1} \qquad (4)$$

Thus:

$$T_{2,i} = y + \sum_{r=3}^{\infty} C_{2,2r} \cdot h_{i+2}^{2r}$$

with $C_{2,2r} = \frac{1}{2^4 - 1} (2^4 - 2^{2r}) C_{1,2r}$

with a truncation error of the order h_{i+2}^6. Observe that the order of truncation error increases by 2 at each new extrapolation step.

Programming Considerations:

The subroutine uses the scheme shown in Figure 1 for computation of T values and generates the upward diagonal in the one-dimensional storage array AUX, using the general formula:

$$T_{k,j} = T_{k-1,j+1} + \frac{T_{k-1,j+1} - T_{k-1,j}}{2^{2k} - 1} \qquad (5)$$

$$(k+j = i,\ j = i-1,\ i-2,\ \ldots,\ 2,1,0)$$

and storing:

$T_{0,i}$ into AUX (i+1)

$T_{1,i-1}$ into AUX (i)

.
.
.

$T_{k,0}$ into AUX (1)

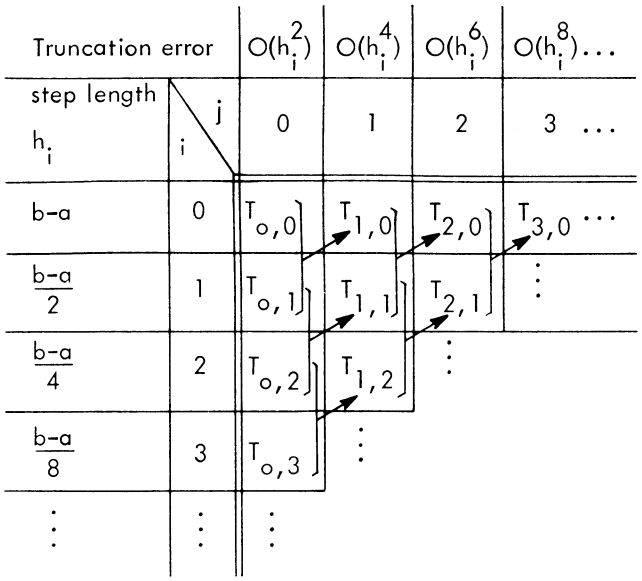


Figure 1. Computation of T-values (QATR)

The procedure stops if the difference between two successive values of AUX (1) is less than a given tolerance, or if the values of AUX (1) start oscillating, thus showing the influence of rounding errors.

- Subroutine QGn (n = 2, 4, 8, 16, 24, 32, 48)

```
QG2..                                                                  QG2   10
/**********************************************************************/QG2   20
/*                                                                    */QG2   30
/*      INTEGRATION OF GIVEN FUNCTION BY 2-POINT GAUSSIAN             */QG2   40
/*      QUADRATURE FORMULA                                            */QG2   50
/*                                                                    */QG2   60
/**********************************************************************/QG2   70
   PROCEDURE(XL,XU,FCT,Y),.                                            QG2   80
   DECLARE                                                             QG2   90
         (XL,XU,Y,A,B)                                                 QG2  100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/QG2  110
 /*      BINARY FLOAT (53),            /*DOUBLE PRECISION VERSION  /*D*/QG2  120
         FCT ENTRY RETURNS                                             QG2  130
         (BINARY FLOAT),.              /*SINGLE PRECISION VERSION  /*S*/QG2  140
 /*      (BINARY FLOAT (53)),.         /*DOUBLE PRECISION VERSION  /*D*/QG2  150
   A     =0.5*(XU+XL),.                                                QG2  160
   B     =XU-XL,.                                                      QG2  170
   Y     =2.886751345948128E-01*B,.                                    QG2  180
   Y     =0.5*B*(FCT(A+Y)+FCT(A-Y)),.                                  QG2  190
   END,.                           /*END OF PROCEDURE QG2            */QG2  200
```

```
QG4..                                                                  QG4   10
/**********************************************************************/QG4   20
/*                                                                    */QG4   30
/*      INTEGRATION OF A GIVEN FUNCTION BY 4-POINT GAUSSIAN           */QG4   40
/*      QUADRATURE FORMULA                                            */QG4   50
/*                                                                    */QG4   60
/**********************************************************************/QG4   70
   PROCEDURE (XL,XU,FCT,Y),.                                           QG4   80
   DECLARE                                                             QG4   90
         (XL,XU,Y,A,B,C)                                               QG4  100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/QG4  110
 /*      BINARY FLOAT (53),            /*DOUBLE PRECISION VERSION  /*D*/QG4  120
         FCT ENTRY RETURNS                                             QG4  130
         (BINARY FLOAT),.              /*SINGLE PRECISION VERSION  /*S*/QG4  140
 /*      (BINARY FLOAT (53)),.         /*DOUBLE PRECISION VERSION  /*D*/QG4  150
   A     =0.5*(XU+XL),.                                                QG4  160
   B     =XU-XL,.                                                      QG4  170
   C     =4.305681557577263E-01*B,.                                    QG4  180
   Y     =1.739274225687269E-01*(FCT(A+C)+FCT(A-C)),.                  QG4  190
   C     =1.699905217924281E-01*B,.                                    QG4  200
   Y     =B*(Y+3.260725774312731E-01*(FCT(A+C)+FCT(A-C))),.            QG4  210
   END,.                           /*END OF PROCEDURE QG4            */QG4  220
```

```
QG8..                                                                  QG8   10
/**********************************************************************/QG8   20
/*                                                                    */QG8   30
/*      INTEGRATION OF A GIVEN FUNCTION BY 8-POINT GAUSSIAN           */QG8   40
/*      QUADRATURE FORMULA                                            */QG8   50
/*                                                                    */QG8   60
/**********************************************************************/QG8   70
   PROCEDURE(XL,XU,FCT,Y),.                                            QG8   80
   DECLARE                                                             QG8   90
         (XL,XU,Y,A,B,C)                                               QG8  100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/QG8  110
 /*      BINARY FLOAT (53),            /*DOUBLE PRECISION VERSION  /*D*/QG8  120
         FCT ENTRY RETURNS                                             QG8  130
         (BINARY FLOAT),               /*SINGLE PRECISION VERSION  /*S*/QG8  140
 /*      (BINARY FLOAT (53)),          /*DOUBLE PRECISION VERSION  /*D*/QG8  150
         LY BINARY FLOAT (53),                                         QG8  160
         X( 8) BINARY FLOAT (53) STATIC INITIAL                        QG8  170
         (4.801449282487681E-01,     5.061426814518813E-02,            QG8  180
         3.983332387068134E-01,      1.111905172266872E-01,            QG8  190
         2.627662049581645E-01,      1.568533229389436E-01,            QG8  200
         9.171732124782495E-02,      1.813418916891810E-01),.          QG8  210
   A     =0.5*(XU+XL),.                                                QG8  220
   B     =XU-XL,.                                                      QG8  230
   LY    =0,.                                                          QG8  240
         DO I=1 TO  7 BY 2,.                                           QG8  250
         C     =X(I)*B,.                                               QG8  260
         LY    =LY+X(I+1)*(FCT(A+C)+FCT(A-C)),.                        QG8  270
         END,.                                                         QG8  280
   Y     =LY*B,.                                                       QG8  290
   END,.                           /*END OF PROCEDURE QG8            */QG8  300
```

```
QG16..                                                                 QG16  10
/**********************************************************************/QG16  20
/*                                                                    */QG16  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 16-POINT GAUSSIAN          */QG16  40
/*      QUADRATURE FORMULA                                            */QG16  50
/*                                                                    */QG16  60
/**********************************************************************/QG16  70
   PROCEDURE(XL,XU,FCT,Y),.                                            QG16  80
   DECLARE                                                             QG16  90
         (XL,XU,Y,A,B,C)                                               QG16 100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/QG16 110
 /*      BINARY FLOAT (53),            /*DOUBLE PRECISION VERSION  /*D*/QG16 120
         FCT ENTRY RETURNS                                             QG16 130
         (BINARY FLOAT),               /*SINGLE PRECISION VERSION  /*S*/QG16 140
 /*      (BINARY FLOAT (53)),          /*DOUBLE PRECISION VERSION  /*D*/QG16 150
         LY BINARY FLOAT (53),                                         QG16 160
         X(16) BINARY FLOAT (53) STATIC INITIAL                        QG16 170
         (4.947004674958625E-01,     1.357622570587705E-02,            QG16 180
         4.722875115366163E-01,      3.112676196932395E-02,            QG16 190
         4.328156011935159E-01,      4.757925584124639E-02,            QG16 200
         3.777022041775015E-01,      6.231448562776694E-02,            QG16 210
         3.089381222013219E-01,      7.479799440828837E-02,            QG16 220
         2.290088388286137E-01,      8.457825969750127E-02,            QG16 230
         1.408017753896255E-01,      9.130170752246179E-02,            QG16 240
         4.750625491881872E-02,      9.472530522753425E-02),.          QG16 250
   A     =0.5*(XU+XL),.                                                QG16 260
   B     =XU-XL,.                                                      QG16 270
   LY    =0,.                                                          QG16 280
         DO I=1 TO 15 BY 2,.                                           QG16 290
         C     =X(I)*B,.                                               QG16 300
         LY    =LY+X(I+1)*(FCT(A+C)+FCT(A-C)),.                        QG16 310
         END,.                                                         QG16 320
   Y     =LY*B,.                                                       QG16 330
   END,.                           /*END OF PROCEDURE QG16           */QG16 340
```

```
QG24..                                                                  QG24  10
/*********************************************************************/QG24  20
/*                                                                   */QG24  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 24-POINT GAUSSIAN         */QG24  40
/*      QUADRATURE FORMULA                                           */QG24  50
/*                                                                   */QG24  60
/*********************************************************************/QG24  70
   PROCEDURE(XL,XU,FCT,Y),.                                             QG24  80
   DECLARE                                                              QG24  90
        (XL,XU,Y,A,B,C)                                                 QG24 100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/QG24 110
 /*     BINARY FLOAT (53),             /*DOUBLE PRECISION VERSION  /*D*/QG24 120
        FCT ENTRY RETURNS                                               QG24 130
        (BINARY FLOAT),                /*SINGLE PRECISION VERSION  /*S*/QG24 140
 /*     (BINARY FLOAT (53)),           /*DOUBLE PRECISION VERSION  /*D*/QG24 150
        LY BINARY FLOAT (53),                                           QG24 160
        X(24) BINARY FLOAT (53) STATIC INITIAL                          QG24 170
        (4.975536C99585107E-01,    6.170614859993600E-03,               QG24 180
        4.873642779856547E-C1,    1.426569431446683E-02,                QG24 190
        4.691372760013664E-C1,    2.213871940870990E-02,                QG24 200
        4.432077635C22CC5E-C1,    2.964929245771839E-02,                QG24 210
        4.100009929865515E-01,    3.667324070554C15E-02,                QG24 220
        3.7C0620957892772E-C1,    4.309508076597664E-02,                QG24 230
        3.240468259E64878E-C1,    4.880932605205654E-02,                QG24 240
        2.727107356544158E-C1,    5.372213505798282E-02,                QG24 250
        2.16896753813C226E-C1,    5.775283402686280E-02,                QG24 260
        1.575213398848CE17E-01,    6.083523646390170E-02,               QG24 270
        5.555943373684C815E-02,    6.291872817341415E-02,               QG24 280
        3.202844643133C281E-C2,    6.396909767337608E-02),.             QG24 290
   A    =0.5*(XU+XL),.                                                  QG24 300
   B    =XU-XL,.                                                        QG24 310
   LY   =0,.                                                            QG24 320
        DO I=1 TO 23 BY 2,.                                             QG24 330
        C    =X(I)*B,.                                                  QG24 340
        LY   =LY+X(I+1)*(FCT(A+C)+FCT(A-C)),.                           QG24 350
        END,.                                                           QG24 360
   Y    =LY*B,.                                                         QG24 370
   END,.                          /*END OF PROCEDURE QG24        */QG24 380
```

```
QG32..                                                                  QG32  10
/*********************************************************************/QG32  20
/*                                                                   */QG32  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 32-POINT GAUSSIAN         */QG32  40
/*      QUADRATURE FORMULA                                           */QG32  50
/*                                                                   */QG32  60
/*********************************************************************/QG32  70
   PROCEDURE(XL,XU,FCT,Y),.                                             QG32  80
   DECLARE                                                              QG32  90
        (XL,XU,Y,A,B,C)                                                 QG32 100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/QG32 110
 /*     BINARY FLOAT (53),             /*DOUBLE PRECISION VERSION  /*D*/QG32 120
        FCT ENTRY RETURNS                                               QG32 130
        (BINARY FLOAT),                /*SINGLE PRECISION VERSION  /*S*/QG32 140
 /*     (BINARY FLOAT (53)),           /*DOUBLE PRECISION VERSION  /*D*/QG32 150
        LY BINARY FLOAT (53),                                           QG32 160
        X(32) BINARY FLOAT (53) STATIC INITIAL                          QG32 170
        (4.9863193092474C8E-01,    3.509305004735048E-03,               QG32 180
        4.928057557726342E-C1,    8.137197365452835E-03,                QG32 190
        4.823811277937532E-C1,    1.269603265463103E-02,                QG32 200
        4.674530379688658E-C1,    1.713693145651072E-02,                QG32 210
        4.481605778830261E-01,    2.141794901111334E-02,                QG32 220
        4.246838068662850E-C1,    2.549902963118809E-02,                QG32 230
        3.972418979835712E-01,    2.934204673926777E-02,                QG32 240
        3.666C91059370144BE-C1,    3.291111138818092E-02,               QG32 250
        3.315221334651C76E-01,    3.617289705442425E-02,                QG32 260
        2.936578786203812E-C1,    3.909694789353515E-02,                QG32 270
        2.534499544661147E-01,    4.165596211347338E-02,                QG32 280
        2.106756380653177E-C1,    4.382604650220191E-02,                QG32 290
        1.655343011410638E-01,    4.558693934788194E-02,                QG32 300
        1.196436811260685E-C1,    4.692219954040228E-02,                QG32 310
        7.223598079135825E-C2,    4.781936003963743E-02,                QG32 320
        2.415382843E65516E-C2,    4.827004425736390E-02),.              QG32 330
   A    =C.5*(XU+XL),.                                                  QG32 340
   B    =XU-XL,.                                                        QG32 350
   LY   =C,.                                                            QG32 360
        DO I=1 TO 31 BY 2,.                                             QG32 370
        C    =X(I)*B,.                                                  QG32 380
        LY   =LY+X(I+1)*(FCT(A+C)+FCT(A-C)),.                           QG32 390
        END,.                                                           QG32 400
   Y    =LY*B,.                                                         QG32 410
   END,.                          /*END OF PROCEDURE QG32        */QG32 420
```

```
QG48..                                                                  QG48  10
/*********************************************************************/QG48  20
/*                                                                   */QG48  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 48-POINT GAUSSIAN         */QG48  40
/*      QUADRATURE FORMULA                                           */QG48  50
/*                                                                   */QG48  60
/*********************************************************************/QG48  70
   PROCEDURE(XL,XU,FCT,Y),.                                             QG48  80
   DECLARE                                                              QG48  90
        (XL,XU,Y,A,B,C)                                                 QG48 100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/QG48 110
 /*     BINARY FLOAT (53),             /*DOUBLE PRECISION VERSION  /*D*/QG48 120
        FCT ENTRY RETURNS                                               QG48 130
        (BINARY FLOAT),                /*SINGLE PRECISION VERSION  /*S*/QG48 140
 /*     (BINARY FLOAT (53)),           /*DOUBLE PRECISION VERSION  /*D*/QG48 150
        LY BINARY FLOAT (53),.                                          QG48 160
   DECLARE                                                              QG48 170
        X(24) BINARY FLOAT(53) STATIC INITIAL (                         QG48 180
        4.993855036262131E-C1,   4.967650861331754E-01,                 QG48 190
        4.920622918614134E-C1,   4.852957962731236E-01,                 QG48 200
        4.764938515802154E-C1,   4.656933453532772E-01,                 QG48 210
        4.529395663577848E-C1,   4.38286C101371239E-01,                 QG48 220
        4.217941308121568E-C1,   4.035331020147213E-01,                 QG48 230
        3.835795162578 7C2E-C1,  3.620170654619073E-01,                 QG48 240
        3.389361898163 32CE-C1,  3.144336983882568E-01,                 QG48 250
        2.886123630415864E-01,   2.615804873611165E-01,                 QG48 260
        2.334514523754752E-C1,   2.043432405553584E-01,                 QG48 270
        1.743779431464C8C4E-C1,  1.436812436777278E-01,                 QG48 280
        1.123818951973445E-01,   8.061117803444586E-02,                 QG48 290
        4.852234960473135E-C2,   1.619008548143468E-02),.               QG48 300
   DECLARE                                                              QG48 310
        W(24) BINARY FLOAT(53) STATIC INITIAL (                         QG48 320
        1.576673026152919E-03,   3.663776950638131E-03,                 QG48 330
        5.738617269617 27CE-C3,  7.789657861471924E-03,                 QG48 340
        9.808080228677764E-C3,   1.178538041966219E-02,                 QG48 350
        1.371325465417847E-C2,   1.558361391639904E-02,                 QG48 360
        1.738861128238522E-C2,   1.912067553291535E-02,                 QG48 370
        2.077254147173237E-C2,   2.233728042834714E-02,                 QG48 380
        2.380832924624524E-C2,   2.517951777652724E-02,                 QG48 390
        2.644505474255683E-C2,   2.759975184999208E-02,                 QG48 400
        2.863866465022161E-02,   2.955741984915782E-02,                 QG48 410
        3.035221958246454E-C2,   3.1C1971157994633E-02,                 QG48 420
        3.155709614312701E-C2,   3.196211929232 4C9E-02,                QG48 430
        3.223306221797504E-C2,   3.236884840634196E-02),.               QG48 440
   A    =0.5*(XU+XL),.                                                  QG48 450
   B    =XU-XL,.                                                        QG48 460
   LY   =C,.                                                            QG48 470
        DO I=1 TO 24,.                                                  QG48 480
        C    =X(I)*B,.                                                  QG48 490
        LY   =LY+W(I)*(FCT(A+C)+FCT(A-C)),.                             QG48 500
        END,.                                                           QG48 510
   Y    =LY*B,.                                                         QG48 520
   END,.                          /*END OF PROCEDURE QG48        */QG48 530
```

Purpose:

QGn computes the integral value $Y = \int_{XL}^{XU} FCT(X)\,dX$ for a given function FCT (X) defined in the closed interval [XL, XU], using Gaussian quadrature formulas.

Usage:

CALL QGn (XL, XU, FCT, Y);

XL - BINARY FLOAT [(53)]
Given lower bound of the integral.

XU - BINARY FLOAT [(53)]
Given upper bound of the integral.

FCT - ENTRY
Given procedure for the computation of the function values, which must be supplied by the user.

Usage:

FCT(X)
FCT(X) - BINARY FLOAT [(53)]
Resultant function value.
X - BINARY FLOAT [(53)]
Given argument value.

Y - BINARY FLOAT [(53)]
Resultant integral value.

Remarks:

The number n within the procedure name QGn indicates the number of nodes used for calculation of Y.

Method:

Gaussian quadrature formulas are used for the evaluation of the integral values.

For reference see:

V. I. Krylow, Approximate Calculation of Integrals, Macmillan, New York-London, 1962, pp. 100-111 and 337-340.

Mathematical Background:

Set:

x_l = lower bound of integral
x_u = upper bound of integral
n = number of nodes used for the evaluation of the integral value.

By means of the linear transformation

$$x = t_0 + t_1 t$$

$$\text{with } t_0 = \frac{x_u + x_l}{2} \text{ and } t_1 = \frac{x_u - x_l}{2} \qquad (1)$$

the argument range $x_l \le x \le x_u$ is mapped onto

$$-1 \le t \le +1$$

and the integral

$$y = \int_{x_l}^{x_u} f(x)\,dx \qquad (2)$$

is reduced to standard form

$$y = \int_{-1}^{+1} \varphi(t)\,dt \qquad (3)$$

$$\text{with } \varphi(t) = t_1 f(t_0 + t_1 t).$$

Gaussian quadrature formulas are used to compute (3).

The integral value y is approximated by a weighted sum of function values:

$$y^{(n)} = 2t_1 \sum_{k=1}^{n} \left\{ \frac{A_k^{(n)}}{2} f(t_0 + t_1 t_k^{(n)}) \right\}$$

The value $y^{(n)}$ is exact whenever f(x) is a polynomial of degree less than or equal to 2n-1.

The weights $A_k^{(n)}$ and nodes $t_k^{(n)}$ are symmetric with respect to the origin t = 0:

$$A_k^{(n)} = A_{n-k+1}^{(n)}, \quad t_k^{(n)} = -t_{n-k+1}^{(n)}$$

- Subroutine QLn (n = 2, 4, 8, 12, 16, 24)

```
QL2..                                                                  QL2  10
/*********************************************************************/QL2  20
/*                                                                   */QL2  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 2-POINT GAUSSIAN-LAGUERRE */QL2  40
/*      QUADRATURE FORMULA                                           */QL2  50
/*                                                                   */QL2  60
/*********************************************************************/QL2  70
   PROCEDURE (FCT,Y),.                                                 QL2  80
   DECLARE                                                             QL2  90
         FCT ENTRY RETURNS                                             QL2 100
         (BINARY FLOAT),                 /*SINGLE PRECISION VERSION  /*S*/QL2 110
 /*      (BINARY FLOAT (53)),            /*DOUBLE PRECISION VERSION  /*D*/QL2 120
         (X,Y)                                                         QL2 130
         BINARY FLOAT,.                  /*SINGLE PRECISION VERSION  /*S*/QL2 140
 /*      BINARY FLOAT (53),.             /*DOUBLE PRECISION VERSION  /*D*/QL2 150
    X    =3.4142135623730950E+00,.                                     QL2 160
    Y    =1.4644660940672620E-01*FCT(X),.                              QL2 170
    X    =5.8578643762690500E-01,.                                     QL2 180
    Y    =Y+8.5355339059327380E-01*FCT(X),.                            QL2 190
    END,.                            /*END OF PROCEDURE QL2           */QL2 200
```

```
QL4..                                                                  QL4  10
/*********************************************************************/QL4  20
/*                                                                   */QL4  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 4-POINT GAUSSIAN-LAGUERRE */QL4  40
/*      QUADRATURE FORMULA                                           */QL4  50
/*                                                                   */QL4  60
/*********************************************************************/QL4  70
   PROCEDURE (FCT,Y),.                                                 QL4  80
   DECLARE                                                             QL4  90
         FCT ENTRY RETURNS                                             QL4 100
         (BINARY FLOAT),                 /*SINGLE PRECISION VERSION  /*S*/QL4 110
 /*      (BINARY FLOAT (53)),            /*DOUBLE PRECISION VERSION  /*D*/QL4 120
         (X,Y)                                                         QL4 130
         BINARY FLOAT,.                  /*SINGLE PRECISION VERSION  /*S*/QL4 140
 /*      BINARY FLOAT (53),.             /*DOUBLE PRECISION VERSION  /*D*/QL4 150
    X    =9.3950709123011330E+00,.                                     QL4 160
    Y    =5.3929470556132750E-04*FCT(X),.                              QL4 170
    X    =4.5366202969211280E+00,.                                     QL4 180
    Y    =Y+3.8887908515005380E-02*FCT(X),.                            QL4 190
    X    =1.7457611011583470E+00,.                                     QL4 200
    Y    =Y+3.5741869243779970E-01*FCT(X),.                            QL4 210
    X    =3.2255476896193923E-01,.                                     QL4 220
    Y    =Y+6.0315410434163360E-01*FCT(X),.                            QL4 230
    END,.                            /*END OF PROCEDURE QL4           */QL4 240
```

```
QL8..                                                                  QL8  10
/*********************************************************************/QL8  20
/*                                                                   */QL8  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 8-POINT GAUSSIAN-LAGUERRE */QL8  40
/*      QUADRATURE FORMULA                                           */QL8  50
/*                                                                   */QL8  60
/*********************************************************************/QL8  70
   PROCEDURE (FCT,Y),.                                                 QL8  80
   DECLARE                                                             QL8  90
         FCT ENTRY RETURNS                                             QL8 100
         (BINARY FLOAT),                 /*SINGLE PRECISION VERSION  /*S*/QL8 110
 /*      (BINARY FLOAT (53)),            /*DOUBLE PRECISION VERSION  /*D*/QL8 120
         (XX,Y)                                                        QL8 130
         BINARY FLOAT,                   /*SINGLE PRECISION VERSION  /*S*/QL8 140
 /*      BINARY FLOAT (53),              /*DOUBLE PRECISION VERSION  /*D*/QL8 150
         I BINARY FIXED,                                               QL8 160
         LY BINARY FLOAT (53),                                         QL8 170
         X(16) BINARY FLOAT (53) STATIC INITIAL                        QL8 180
         (2.2863131736889260E+01,     1.0480011748715100E-09,          QL8 190
         1.5740678641278000E+01,      8.4857467162725320E-07,          QL8 200
         1.0758516010181000E+01,      9.0765087733582130E-05,          QL8 210
         7.0459054023934660E+00,      2.7945362352256730E-03,          QL8 220
         4.2667001702876590E+00,      3.3343492261215650E-02,          QL8 230
         2.2510866298661310E+00,      1.7579498663717180E-01,          QL8 240
         9.0370177679937990E-01,      4.1878678081434300E-01,          QL8 250
         1.7027963230510100E-01,      3.6918858934163750E-01),.        QL8 260
    LY   =0,.                                                          QL8 270
         DO I=1 TO 15 BY 2,.                                           QL8 280
         XX   =X(I),.                                                  QL8 290
         LY   =LY+X(I+1)*FCT(XX),.                                     QL8 300
         END,.                                                         QL8 310
    Y    =LY,.                                                         QL8 320
    END,.                            /*END OF PROCEDURE QL8           */QL8 330
```

```
QL12..                                                                 QL12  10
/*********************************************************************/QL12  20
/*                                                                   */QL12  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 12-POINT GAUSSIAN-LAGUERRE*/QL12  40
/*      QUADRATURE FORMULA                                           */QL12  50
/*                                                                   */QL12  60
/*********************************************************************/QL12  70
   PROCEDURE (FCT,Y),.                                                 QL12  80
   DECLARE                                                             QL12  90
         (XX,Y)                                                        QL12 100
         BINARY FLOAT,                   /*SINGLE PRECISION VERSION  /*S*/QL12 110
 /*      BINARY FLOAT (53),              /*DOUBLE PRECISION VERSION  /*D*/QL12 120
         FCT ENTRY RETURNS                                             QL12 130
         (BINARY FLOAT),                 /*SINGLE PRECISION VERSION  /*S*/QL12 140
 /*      (BINARY FLOAT (53)),            /*DOUBLE PRECISION VERSION  /*D*/QL12 150
         I BINARY FIXED,                                               QL12 160
         LY BINARY FLOAT (53),                                         QL12 170
         X(24) BINARY FLOAT (53) STATIC INITIAL                        QL12 180
         (3.7099121044466920E+01,     8.1480774674262420E-16,          QL12 190
         2.8487967250984000E+01,      3.0616016350350210E-12,          QL12 200
         2.2151090379397010E+01,      1.3423910305150040E-09,          QL12 210
         1.7116855187462260E+01,      1.6684933765409100E-07,          QL12 220
         1.3006054993306350E+01,      8.3650558568197990E-06,          QL12 230
         9.6213168245686760E+00,      2.0323159266299940E-04,          QL12 240
         6.8445254531151770E+00,      2.6639735418653160E-03,          QL12 250
         4.5992276394183480E+00,      2.0102381154634100E-02,          QL12 260
         2.8337513377435070E+00,      9.0449222211680930E-02,          QL12 270
         1.5126102697764190E+00,      2.4408201131987760E-01,          QL12 280
         6.1175748451513070E-01,      3.7775927587313800E-01,          QL12 290
         1.5722117358020700E-01,      2.6473137105544320E-01),.        QL12 300
    LY   =0,.                                                          QL12 310
         DO I=1 TO 23 BY 2,.                                           QL12 320
         XX   =X(I),.                                                  QL12 330
         LY   =LY+X(I+1)*FCT(XX),.                                     QL12 340
         END,.                                                         QL12 350
    Y    =LY,.                                                         QL12 360
    END,.                            /*END OF PROCEDURE QL12          */QL12 370
```

```
QL16..                                                          QL16  10
/*****************************************************************/QL16  20
/*                                                               */QL16  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 16-POINT GAUSSIAN-LAGUERRE*/QL16  40
/*      QUADRATURE FORMULA                                       */QL16  50
/*                                                               */QL16  60
/*****************************************************************/QL16  70
   PROCEDURE (FCT,Y),.                                          QL16  80
   DECLARE                                                      QL16  90
         FCT ENTRY RETURNS                                      QL16 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QL16 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QL16 120
         (XX,Y)                                                 QL16 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QL16 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QL16 150
         I BINARY FIXED,                                        QL16 160
         LY BINARY FLOAT (53),                                  QL16 170
         X(32) BINARY FLOAT (53) STATIC INITIAL                 QL16 180
         (5.170116033954332E+01,     4.161462370372855E-22,     QL16 190
         4.194045264768833E+01,     5.050473700035513E-18,      QL16 200
         3.458339870228663E+01,     6.297967002517868E-15,      QL16 210
         2.857872974288214E+01,     2.127079033224103E-12,      QL16 220
         2.351596569399191E+01,     2.862350242973882E-10,      QL16 230
         1.918015685675313E+01,     1.8P1024841079673E-08,      QL16 240
         1.544152736878162E+01,     6.828319330871200E-07,      QL16 250
         1.221422336886616E+01,     1.484458687398130E-05,      QL16 260
         9.438314336391939E+00,     2.042719153C827B5E-04,      QL16 270
         7.070338535C48234E+00,     1.849070943526311E-03,      QL16 280
         5.078C18614549768E+00,     1.129990008033945E-02,      QL16 290
         3.437086633893207E+00,     4.732892869412522E-02,      QL16 300
         2.129283645098381E+00,     1.362969342963775E-01,      QL16 310
         1.141057774831227E+00,     2.657957776442142E-01,      QL16 320
         4.626963289150808E-01,     3.310578549508842E-01,      QL16 330
         8.764941047892784E-02,     2.061517149578010E-01),.    QL16 340
   LY    =0,.                                                   QL16 350
         DO I=1 TO 31 BY 2,.                                    QL16 360
         XX    =X(I),.                                          QL16 370
         LY    =LY+X(I+1)*FCT(XX),.                             QL16 380
         END,.                                                  QL16 390
   Y     =LY,.                                                  QL16 400
   END,.                              /*END OF PROCEDURE QL16    */QL16 410
```

```
QL24..                                                          QL24  10
/*****************************************************************/QL24  20
/*                                                               */QL24  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 24-POINT GAUSSIAN-LAGUERRE*/QL24  40
/*      QUADRATURE FORMULA                                       */QL24  50
/*                                                               */QL24  60
/*****************************************************************/QL24  70
   PROCEDURE (FCT,Y),.                                          QL24  80
   DECLARE                                                      QL24  90
         (XX,Y)                                                 QL24 100
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QL24 110
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QL24 120
         FCT ENTRY RETURNS                                      QL24 130
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QL24 140
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QL24 150
         I BINARY FIXED,                                        QL24 160
         LY BINARY FLOAT (53),.                                 QL24 170
   DECLARE                                                      QL24 180
         X(24) BINARY FLOAT(53) STATIC INITIAL (                QL24 190
         8.149827923394889E+01,   6.996224003510503E+01,        QL24 200
         6.105853144721876E+01,   5.360857454469507E+01,        QL24 210
         4.715310644515632E+01,   4.145172048487077E+01,        QL24 220
         3.635840580165162E+01,   3.177604135237472E+01,        QL24 230
         2.763593717433272E+01,   2.388732984816973E+01,        QL24 240
         2.049146008261642E+01,   1.741799266450898E+01,        QL24 250
         1.464273228959667E+01,   1.214610271172977E+01,        QL24 260
         9.912098015077706E+00,   7.927539247172152E+00,        QL24 270
         6.181535118736765E+00,   4.665083703467171E+00,        QL24 280
         3.370774264208998E+00,   2.292562058632190E+00,        QL24 290
         1.425597590803613E+00,   7.660969055459366E-01,        QL24 300
         3.112391461984837E-01,   5.9C1985218150798E-02),.      QL24 310
   DECLARE                                                      QL24 320
         W(24) BINARY FLOAT(53) STATIC INITIAL (                QL24 330
         5.575345788328357E-35,   4.088301593680658E-30,        QL24 340
         2.451818845878403E-26,   3.605765864552959E-23,        QL24 350
         2.010517464555503E-20,   5.350188813010038E-18,        QL24 360
         7.819800382459448E-16,   6.894181052958086E-14,        QL24 370
         3.917736515058451E-12,   1.507008226292585E-10,        QL24 380
         4.072858987550000E-09,   7.960812959133630E-08,        QL24 390
         1.151315812737280E-06,   1.254472197799333E-05,        QL24 400
         1.044612146552752E-04,   6.721625640935479E-04,        QL24 410
         3.369349058478304E-03,   1.322601940512016E-02,        QL24 420
         4.073247815140865E-02,   9.816627262991889E-02,        QL24 430
         1.833226889777780E-01,   2.588067072728698E-01,        QL24 440
         2.587741075174239E-01,   1.428119733347819E-01),.      QL24 450
   LY    =0,.                                                   QL24 460
         DO I=1 TO 24,.                                         QL24 470
         XX    =X(I),.                                          QL24 480
         LY    =LY+W(I)*FCT(XX),.                               QL24 490
         END,.                                                  QL24 500
   Y     =LY,.                                                  QL24 510
   END,.                              /*END OF PROCEDURE QL24    */QL24 520
```

Purpose:

QLn computes the integral value $Y = \int_0^\infty e^{-X} FCT(X)dX$ for a given function FCT(X), by Gaussian-Laguerre quadrature formulas.

Usage:

CALL QLn (FCT, Y);

FCT - ENTRY
Given procedure for the computation of the function values.
This procedure must be supplied by the user.

Usage:
FCT(X)
FCT(X) - BINARY FLOAT [(53)]
Resultant function value.
X - BINARY FLOAT [(53)]
Given argument value.

Y - BINARY FLOAT [(53)]
Resultant integral value.

Remarks:

The n in the name QLn indicates the number of nodes used for the calculation of Y.

Method:

Quadrature formulas of Gauss-Laguerre are used for the evaluation of the integral values.

For reference see:

H. E. Salzer, R. Zucker, "Table of Zeros and Weight Factors of the First Fifteen Laguerre Polynomials", Bul. Amer. Math. Soc., vol. 55 (1949), pp. 1004-1012.

V. I. Krylow, Approximate Calculation of Integrals, Macmillan, New York-London, 1962, pp 130-132 and 347-352.

Shao, Chen, Frank, "Tables of Zeros and Gaussian Weights of Certain Associated Laguerre Polynomials and the Related Generalized Hermite Polynomials", IBM Technical Report TR 00.1100, March 1964, pp. 24-25.

Mathematical Background:

Formulas of Gauss- Laguerre are used to compute

$$y = \int_0^\infty e^{-x} f(x)\,dx$$

Let n denote the number of nodes used for the calculation of the integral value y. The value y is approximated by a weighted sum of function values:

$$y^{(n)} = \sum_{k=1}^{n} [A_k^{(n)} \cdot f(x_k^{(n)})]$$

The value $y^{(n)}$ is exact whenever f(x) is a polynomial of degree less than or equal to 2n-1. The nodes $x_k^{(n)}$ are the roots of the Laguerre polynomials $L_n(x)$ of degree n.

- Subroutine QHn (n = 2, 4, 8, 16, 24, 32, 48)

```
QH2..                                                                  QH2   10
/*********************************************************************/QH2   20
/*                                                                   */QH2   30
/*      INTEGRATION OF A GIVEN FUNCTION BY 2-POINT GAUSSIAN-HERMITE  */QH2   40
/*      QUADRATURE FORMULA                                           */QH2   50
/*                                                                   */QH2   60
/*********************************************************************/QH2   70
   PROCEDURE (FCT,Y),.                                                 QH2   80
   DECLARE                                                             QH2   90
        FCT ENTRY RETURNS ,                                            QH2  100
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH2  110
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH2  120
        (X,Y,Z)                                                        QH2  130
        BINARY FLOAT,.               /*SINGLE PRECISION VERSION  /*S*/QH2  140
 /*     BINARY FLOAT(53),.           /*DOUBLE PRECISION VERSION  /*D*/QH2  150
   X    =7.071067811865475E-01,.                                       QH2  160
   Z    =-X,.                                                          QH2  170
   Y    =8.862269254527580E-01*(FCT(X)+FCT(Z)),.                       QH2  180
   END,.                             /*END OF PROCEDURE QH2          */QH2  190
```

```
QH4..                                                                  QH4   10
/*********************************************************************/QH4   20
/*                                                                   */QH4   30
/*      INTEGRATION OF A GIVEN FUNCTION BY 4-POINT GAUSSIAN-HERMITE  */QH4   40
/*      QUADRATURE FORMULA                                           */QH4   50
/*                                                                   */QH4   60
/*********************************************************************/QH4   70
   PROCEDURE (FCT,Y),.                                                 QH4   80
   DECLARE                                                             QH4   90
        FCT ENTRY RETURNS                                              QH4  100
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH4  110
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH4  120
        W BINARY FLOAT(53),                                            QH4  130
        (X,Y,Z)                                                        QH4  140
        BINARY FLOAT,.               /*SINGLE PRECISION VERSION  /*S*/QH4  150
 /*     BINARY FLOAT(53),.           /*DOUBLE PRECISION VERSION  /*D*/QH4  160
   X    =1.650680123885785E+00,.                                       QH4  170
   Z    =-X,.                                                          QH4  180
   W    =8.131283544724518E-02*(FCT(X)+FCT(Z)),.                       QH4  190
   X    =5.246476232752903E-01,.                                       QH4  200
   Z    =-X,.                                                          QH4  210
   Y    =W+8.049140900055128E-01*(FCT(X)+FCT(Z)),.                     QH4  220
   END,.                             /*END OF PROCEDURE QH4          */QH4  230
```

```
QH8..                                                                  QH8   10
/*********************************************************************/QH8   20
/*                                                                   */QH8   30
/*      INTEGRATION OF A GIVEN FUNCTION BY 8-POINT GAUSSIAN-HERMITE  */QH8   40
/*      QUADRATURE FORMULA                                           */QH8   50
/*                                                                   */QH8   60
/*********************************************************************/QH8   70
   PROCEDURE (FCT,Y),.                                                 QH8   80
   DECLARE                                                             QH8   90
        FCT ENTRY RETURNS                                              QH8  100
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH8  110
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH8  120
        (XX,Y)                                                         QH8  130
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QH8  140
 /*     BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QH8  150
        I BINARY FIXED,                                                QH8  160
        LY BINARY FLOAT (53),                                          QH8  170
        X( 8) BINARY FLOAT (53) STATIC INITIAL(                        QH8  180
        2.930637420257244E+00,     1.996040722113676E-04,              QH8  190
        1.981656756695843E+00,     1.707798300741348E-02,              QH8  200
        1.157193712446780E+00,     2.078023258148919E-01,              QH8  210
        3.811869902073221E-01,     6.611470125582413E-01),.            QH8  220
   LY   =0,.                                                           QH8  230
        DO I=1 TO  7 BY 2,.                                            QH8  240
        XX   =X(I),.                                                   QH8  250
        LY   =LY+X(I+1)*(FCT(XX)+FCT(-XX)),.                           QH8  260
        END,.                                                          QH8  270
   Y    =LY,.                                                          QH8  280
   END,.                             /*END OF PROCEDURE QH8          */QH8  290
```

```
QH16..                                                                 QH16  10
/*********************************************************************/QH16  20
/*                                                                   */QH16  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 16-POINT GAUSSIAN-HERMITE */QH16  40
/*      QUADRATURE FORMULA                                           */QH16  50
/*                                                                   */QH16  60
/*********************************************************************/QH16  70
   PROCEDURE (FCT,Y),.                                                 QH16  80
   DECLARE                                                             QH16  90
        FCT ENTRY RETURNS                                              QH16 100
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH16 110
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH16 120
        (XX,Y)                                                         QH16 130
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QH16 140
 /*     BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QH16 150
        I BINARY FIXED,                                                QH16 160
        LY BINARY FLOAT (53),                                          QH16 170
        X(16) BINARY FLOAT (53) STATIC INITIAL(                        QH16 180
        4.688738939305818E+00,     2.654807474011182E-10,              QH16 190
        3.869447904860123E+00,     2.320980844865211E-07,              QH16 200
        3.176999161979956E+00,     2.711860092537882E-05,              QH16 210
        2.546202157847481E+00,     9.322840086241805E-04,              QH16 220
        1.951787990916254E+00,     1.288031153550997E-02,              QH16 230
        1.380258539198881E+00,     8.381004139898583E-02,              QH16 240
        8.229514491446559E-01,     2.806474585285337E-01,              QH16 250
        2.734810461381525E-01,     5.079294790166137E-01),.            QH16 260
   LY   =0,.                                                           QH16 270
        DO I=1 TO 15 BY 2,.                                            QH16 280
        XX   =X(I),.                                                   QH16 290
        LY   =LY+X(I+1)*(FCT(XX)+FCT(-XX)),.                           QH16 300
        END,.                                                          QH16 310
   Y    =LY,.                                                          QH16 320
   END,.                             /*END OF PROCEDURE QH16         */QH16 330
```

```
QH24..                                                                  QH24  10
/*************************************************************************/QH24  20
/*                                                                       */QH24  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 24-POINT GAUSSIAN-HERMITE     */QH24  40
/*      QUADRATURE FORMULA                                               */QH24  50
/*                                                                       */QH24  60
/*************************************************************************/QH24  70
   PROCEDURE (FCT,Y),.                                                  QH24  80
   DECLARE                                                              QH24  90
         FCT ENTRY RETURNS,                                             QH24 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH24 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH24 120
         (XX,Y)                                                         QH24 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QH24 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QH24 150
         I BINARY FIXED,                                                QH24 160
         LY BINARY FLOAT (53),                                          QH24 170
         X(24) BINARY FLOAT (53) STATIC INITIAL(                        QH24 180
         6.015925561425740E+00,    1.664368496489109E-16,               QH24 190
         5.259382927668044E+00,    6.584620243078170E-13,               QH24 200
         4.625662756423787E+00,    3.046259269987566E-10,               QH24 210
         4.053664402448150E+00,    4.018971174941430E-08,               QH24 220
         3.520006813034525E+00,    2.158245704902334E-06,               QH24 230
         3.012546137565565E+00,    5.688691636404380E-05,               QH24 240
         2.523881017011427E+00,    8.236924826884175E-04,               QH24 250
         2.049003573661699E+00,    7.048355810072671E-03,               QH24 260
         1.584250010961694E+00,    3.744547050323075E-02,               QH24 270
         1.126768181611245E+00,    1.277396217845592E-01,               QH24 280
         6.741711070372122E-01,    2.861795353464430E-01,               QH24 290
         2.244145474725156E-01,    4.269311638686992E-01),.             QH24 300
   LY    =C,.                                                           QH24 310
         DO I=1 TO 23 BY 2,.                                            QH24 320
         XX    =X(I),.                                                  QH24 330
         LY    =LY+X(I+1)*(FCT(XX)+FCT(-XX)),.                          QH24 340
         END,.                                                          QH24 350
   Y     =LY,.                                                          QH24 360
   END,.                              /*END OF PROCEDURE QH24          */QH24 370
```

```
QH32..                                                                  QH32  10
/*************************************************************************/QH32  20
/*                                                                       */QH32  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 32-POINT GAUSSIAN-HERMITE     */QH32  40
/*      QUADRATURE FORMULA                                               */QH32  50
/*                                                                       */QH32  60
/*************************************************************************/QH32  70
   PROCEDURE (FCT,Y),.                                                  QH32  80
   DECLARE                                                              QH32  90
         FCT ENTRY RETURNS                                              QH32 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH32 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH32 120
         (XX,Y)                                                         QH32 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QH32 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QH32 150
         I BINARY FIXED,                                                QH32 160
         LY BINARY FLOAT (53),                                          QH32 170
         X(32) BINARY FLOAT (53) STATIC INITIAL(                        QH32 180
         7.125813909830728E+00,    7.310676427384162E-23,               QH32 190
         6.409498149269660E+00,    9.231736536518292E-19,               QH32 200
         5.812225949515914E+00,    1.197344017092849E-15,               QH32 210
         5.275550986515880E+00,    4.215010211326448E-13,               QH32 220
         4.771645033502596E+00,    5.933291463396639E-11,               QH32 230
         4.305547953351198E+00,    4.098832164770897E-09,               QH32 240
         3.853755485471445E+00,    1.574167792545594E-07,               QH32 250
         3.417167492818571E+00,    3.650585129562376E-06,               QH32 260
         2.992496825002374E+00,    5.416584061819983E-05,               QH32 270
         2.577249537732317E+00,    5.362683655279720E-04,               QH32 280
         2.169499183606112E+00,    3.654890326654428E-03,               QH32 290
         1.767654109463202E+00,    1.755342883157343E-02,               QH32 300
         1.370376410952872E+00,    6.045813095591261E-02,               QH32 310
         9.765004635896828E-01,    1.512697340766425E-01,               QH32 320
         5.849787654359324E-01,    2.774581423025299E-01,               QH32 330
         1.948407415693993E-01,    3.752383525928024E-01),.             QH32 340
   LY    =0,.                                                           QH32 350
         DO I=1 TO 31 BY 2,.                                            QH32 360
         XX    =X(I),.                                                  QH32 370
         LY    =LY+X(I+1)*(FCT(XX)+FCT(-XX)),.                          QH32 380
         END,.                                                          QH32 390
   Y     =LY,.                                                          QH32 400
   END,.                              /*END OF PROCEDURE QH32          */QH32 410
```

```
QH48..                                                                  QH48  10
/*************************************************************************/QH48  20
/*                                                                       */QH48  30
/*      INTEGRATION OF A GIVEN FUNCTION BY 48-POINT GAUSSIAN-HERMITE     */QH48  40
/*      QUADRATURE FORMULA                                               */QH48  50
/*                                                                       */QH48  60
/*************************************************************************/QH48  70
   PROCEDURE (FCT,Y),.                                                  QH48  80
   DECLARE                                                              QH48  90
         FCT ENTRY RETURNS                                              QH48 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QH48 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QH48 120
         (XX,Y)                                                         QH48 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QH48 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QH48 150
         I BINARY FIXED,                                                QH48 160
         LY BINARY FLOAT (53),.                                         QH48 170
   DECLARE                                                              QH48 180
         X(24) BINARY FLOAT(53) STATIC INITIAL (                        QH48 190
         8.975315081931687E+00,    8.310752190704784E+00,               QH48 200
         7.759295519765775E+00,    7.266046554164350E+00,               QH48 210
         6.810066578C74141E+00,    6.380564096186411E+00,               QH48 220
         5.971072225013545E+00,    5.577316981223729E+00,               QH48 230
         5.196287718792365E+00,    4.825757228133209E+00,               QH48 240
         4.464016546934459E+00,    4.109704603560590E+00,               QH48 250
         3.761726490228358E+00,    3.419165969363885E+00,               QH48 260
         3.081248988645106E+00,    2.747308624822383E+00,               QH48 270
         2.416760904873216E+00,    2.089C86660944276E+00,               QH48 280
         1.763817579895300E+00,    1.440525220137565E+00,               QH48 290
         1.118812152402157E+00,    7.983046277785622E-01,               QH48 300
         4.786463375944961E-01,    1.594929358488625E-01),.             QH48 310
   DECLARE                                                              QH48 320
         W(24) BINARY FLOAT(53) STATIC INITIAL (                        QH48 330
         7.935551460773997E-36,    5.984612693313878E-31,               QH48 340
         3.685036080150670E-27,    5.564577468902285E-24,               QH48 350
         3.188387323505138E-21,    8.730159601186677E-19,               QH48 360
         1.315159622658409E-16,    1.197589865479179E-14,               QH48 370
         7.046932581545889E-13,    2.815296537838169E-11,               QH48 380
         7.930467495165382E-10,    1.622514135895770E-08,               QH48 390
         2.468658993669750E-07,    2.847258691734848E-06,               QH48 400
         2.528599027748489E-05,    1.751504318011728E-04,               QH48 410
         9.563923198194153E-04,    4.153004911977552E-03,               QH48 420
         1.444496157498110E-02,    4.047967698460385E-02,               QH48 430
         9.182229707928518E-02,    1.692044719456411E-01,               QH48 440
         2.539615426647591E-01,    3.111001030377963lE-01),.            QH48 450
   LY    =0,.                                                           QH48 460
         DO I=1 TO 24,.                                                 QH48 470
         XX    =X(I),.                                                  QH48 480
         LY    =LY+W(I)*(FCT(XX)+FCT(-XX)),.                            QH48 490
         END,.                                                          QH48 500
   Y     =LY,.                                                          QH48 510
   END,.                              /*END OF PROCEDURE QH48          */QH48 520
```

Purpose:

QHn computes the integral value $Y = \int_{-\infty}^{+\infty} e^{-X^2} FCT(X)\,dX$ for a given function FCT(X), using Gaussian-Hermite quadrature formulas.

Usage:

CALL QHn (FCT, Y);

FCT - ENTRY
Given procedure for the computation of the function values, which must be supplied by the user.

Usage
FCT(X);
FCT(X) - BINARY FLOAT [(53)]
Resultant function value.
X - BINARY FLOAT [(53)]
Given argument value.

Y - BINARY FLOAT [(53)]
Resultant integral value.

Remarks:

The number n in the name QHn indicates the number of nodes used for the calculation of Y.

In case of an even function $f(x) = \varphi(x^2)$, f(x) may be changed by means of the transformation $t = x^2$ into:

$$y = \int_0^{\infty} \frac{e^{-t}\,\varphi(t)}{\sqrt{t}}\,dt$$

This is a form suitable to subroutines QAn, the use of which saves approximately half of the computation time.

Method:

Quadrature formulas of Gauss-Hermite are used for the computation of the integral values.

For reference see:

H. E. Salzer, R. Zucker, R. Capuano, Table of Zeros and Weight Factors of the First Twenty

Hermite Polynomials, F. Res. Nat. Bur. Standards, vol. 48 (1952), pp. 111-116.

V. I. Krylow, Approximate Calculation of Integrals, Macmillan, New York-London, 1962, pp. 129-130 and 343-346.

Mathematical Background:

Quadrature formulas of Gauss-Hermite are used to compute

$$y = \int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx$$

Let n denote the number of nodes used for the calculation of the integral value y. The value y is approximated by a weighted sum of function values:

$$y^{(n)} = \sum_{k=1}^{n} A_k^{(n)} f(x_k^{(n)})$$

The value $y^{(n)}$ is exact whenever f(x) is a polynomial of degree less than or equal to 2n-1.

The nodes $x_k^{(n)}$ are the roots of the Hermite polynomials $H_n(x)$ of degree n.

The weights $A_k^{(n)}$ and the nodes $x_k^{(n)}$ are symmetric with respect to the origin x=0:

$$A_k^{(n)} = A_{n-k+1}^{(n)}, \quad x_k^{(n)} = -x_{n-k+1}^{(n)}$$

• Subroutine QAn (n = 2, 4, 8, 12, 16, 24)

```
QA2..                                                                  QA2
/**********************************************************************/QA2
/*                                                                    */QA2
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 2-POINT         */QA2
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                          */QA2
/*                                                                    */QA2
/**********************************************************************/QA2
   PROCEDURE (FCT,Y),.                                                 QA2
   DECLARE                                                             QA2
        FCT ENTRY RETURNS                                              QA2
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA2
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA2
        (X,Y)                                                          QA2
        BINARY FLOAT,.               /*SINGLE PRECISION VERSION  /*S*/QA2
 /*     BINARY FLOAT (53),.          /*DOUBLE PRECISION VERSION  /*D*/QA2
   X    =2.724744871391589E+00,.                                       QA2
   Y    =1.626256708944903E-01*FCT(X),.                                QA2
   X    =2.752551286084109E-01,.                                       QA2
   Y    =Y+1.609828180011026E+00*FCT(X),.                              QA2
   END,.                             /*END OF PROCEDURE QA2          */QA2
```

```
QA4..                                                                  QA4
/**********************************************************************/QA4
/*                                                                    */QA4
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 4-POINT         */QA4
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                          */QA4
/*                                                                    */QA4
/**********************************************************************/QA4
   PROCEDURE (FCT,Y),.                                                 QA4
   DECLARE                                                             QA4
        FCT ENTRY RETURNS                                              QA4
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA4
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA4
        (X,Y)                                                          QA4
        BINARY FLOAT,.               /*SINGLE PRECISION VERSION  /*S*/QA4
 /*     BINARY FLOAT (53),.          /*DOUBLE PRECISION VERSION  /*D*/QA4
   X    =8.588635689012034E+00,.                                       QA4
   Y    =3.992081444227352E-04*FCT(X),.                                QA4
   X    =3.926963501358287E+00,.                                       QA4
   Y    =Y+3.415596601482695E-02*FCT(X),.                              QA4
   X    =1.339097288126361E+00,.                                       QA4
   Y    =Y+4.156046516297838E-01*FCT(X),.                              QA4
   X    =1.453035215033171E-01,.                                       QA4
   Y    =Y+1.322294025116483E+00*FCT(X),.                              QA4
   END,.                             /*END OF PROCEDURE QA4          */QA4
```

```
QA8..                                                                  QA8
/**********************************************************************/QA8
/*                                                                    */QA8
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 8-POINT         */QA8
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                          */QA8
/*                                                                    */QA8
/**********************************************************************/QA8
   PROCEDURE (FCT,Y),.                                                 QA8
   DECLARE                                                             QA8
        FCT ENTRY RETURNS                                              QA8
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA8
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA8
        (XX,Y)                                                         QA8
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QA8
 /*     BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QA8
        LY BINARY FLOAT (53),                                          QA8
        I BINARY FIXED,                                                QA8
        X(16) BINARY FLOAT (53) STATIC INITIAL                         QA8
        (2.198427284096265E+01,     5.309614948022364E-10,             QA8
        1.497262708842639E+01,     4.641961689730421E-07,              QA8
        1.009332367522134E+01,     5.423720185075763E-05,              QA8
        6.483145428627170E+00,     1.864568017248361E-03,              QA8
        3.809476361484907E+00,     2.576062307101995E-02,              QA8
        1.905113635031428E+00,     1.676200827979717E-01,              QA8
        6.772490876492892E-01,     5.612949170570674E-01,              QA8
        7.479188259681827E-02,     1.015858958033227E+00),.            QA8
   LY   =0,.                                                           QA8
        DO I=1 TO 15 BY 2,.                                            QA8
        XX   =X(I),.                                                   QA8
        LY   =LY+X(I+1)*FCT(XX),.                                      QA8
        END,.                                                          QA8
   Y    =LY,.                                                          QA8
   END,.                             /*END OF PROCEDURE QA8          */QA8
```

```
QA12..                                                                 QA12
/*********************************************************************/QA12
/*                                                                   */QA12
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 12-POINT       */QA12
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                         */QA12
/*                                                                   */QA12
/*********************************************************************/QA12
   PROCEDURE (FCT,Y),.                                                 QA12
   DECLARE                                                             QA12
        FCT ENTRY RETURNS                                              QA12
        (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA12
 /*     (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA12
        (XX,Y)                                                         QA12
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QA12
 /*     BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QA12
        LY BINARY FLOAT (53),                                          QA12
        I BINARY FIXED,                                                QA12
        X(24) BINARY FLOAT (53) STATIC INITIAL                         QA12
        (3.619136036061560E+01,     3.328736992978218E-16,             QA12
        2.766110877984609E+01,     1.316924048615634E-12,              QA12
        2.139675593616611E+01,     6.092508539975128E-10,              QA12
        1.643219508767531E+01,     8.037942349882859E-08,              QA12
        1.239044796380947E+01,     4.316491409804667E-06,              QA12
        9.075434230961203E+00,     1.137738327280876E-04,              QA12
        6.369975388030635E+00,     1.647384965376835E-03,              QA12
        4.198415644878413E+00,     1.409671162014534E-02,              QA12
        2.509848097232128E+00,     7.489094100646149E-02,              QA12
        1.269589940103961E+00,     2.554792435691183E-01,              QA12
        4.545066815637803E-01,     5.723590706928860E-01,              QA12
        5.036188911729395E-02,     8.538623277373985E-01),.            QA12
   LY   =0,.                                                           QA12
        DO I=1 TO 23 BY 2,.                                            QA12
        XX   =X(I),.                                                   QA12
        LY   =LY+X(I+1)*FCT(XX),.                                      QA12
        END,.                                                          QA12
   Y    =LY,.                                                          QA12
   END,.                             /*END OF PROCEDURE QA12        */QA12
```

```
QA16..                                                              QA16  10
/*******************************************************************/QA16  20
/*                                                                 */QA16  30
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 16-POINT     */QA16  40
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                       */QA16  50
/*                                                                 */QA16  60
/*******************************************************************/QA16  70
   PROCEDURE (FCT,Y),.                                              QA16  80
   DECLARE                                                          QA16  90
         FCT ENTRY RETURNS                                          QA16 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA16 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA16 120
         (XX,Y)                                                     QA16 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QA16 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QA16 150
         LY BINARY FLOAT (53),                                      QA16 160
         I BINARY FIXED,                                            QA16 170
         X(32) BINARY FLOAT (53) STATIC INITIAL                     QA16 180
         (5.C777223877537C8E+01,     1.462135285476832E-22,         QA16 190
         4.10816665254912CE+01,     1.846347307303658E-18,          QA16 200
         3.378197048822617E+01,     2.3946880341856976-15,          QA16 210
         2.783143821132868E+01,     8.4300204226528955-13,          QA16 220
         2.282130069352521E+01,     1.186658292679328E-10,          QA16 230
         1.853774317866669E+01,     8.1976643295417936-09,          QA16 240
         1.485143134180125E+01,     3.1483355850911886-07,          QA16 250
         1.167703367397596E+01,     7.3011702591247526-06,          QA16 260
         8.955001337723390E+00,     1.0833168123639976-04,          QA16 270
         6.642215179741444E+00,     1.0725367310559446-03,          QA16 280
         4.706726707667587E+00,     7.3097806533088566-03,          QA16 290
         3.124661050702144E+00,     3.5106857663146866-02,          QA16 300
         1.877931507696074E+00,     1.2091626191182526-01,          QA16 310
         9.535531553908655E-01,     3.0253946815328506-01,          QA16 320
         3.422001560109477E-01,     5.5491628460505986-01,          QA16 330
         3.796291457531345E-02,     7.5047670518560486-01),.        QA16 340
   LY    =0,.                                                       QA16 350
         DO I=1 TO 31 BY 2,.                                        QA16 360
         XX    =X(I),.                                              QA16 370
         LY    =LY+X(I+1)*FCT(XX),.                                 QA16 380
         END,.                                                      QA16 390
   Y     =LY,.                                                      QA16 400
   END,.                              /*END OF PROCEDURE QA16       */QA16 410
```

```
QA24..                                                              QA24  10
/*******************************************************************/QA24  20
/*                                                                 */QA24  30
/*      INTEGRATION OF A GIVEN FUNCTION BY ASSOCIATED 24-POINT     */QA24  40
/*      GAUSSIAN-LAGUERRE QUADRATURE FORMULA                       */QA24  50
/*                                                                 */QA24  60
/*******************************************************************/QA24  70
   PROCEDURE (FCT,Y),.                                              QA24  80
   DECLARE                                                          QA24  90
         FCT ENTRY RETURNS.                                         QA24 100
         (BINARY FLOAT),              /*SINGLE PRECISION VERSION  /*S*/QA24 110
 /*      (BINARY FLOAT (53)),         /*DOUBLE PRECISION VERSION  /*D*/QA24 120
         (XX,Y)                                                     QA24 130
         BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/QA24 140
 /*      BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/QA24 150
         LY BINARY FLOAT (53),                                      QA24 160
         I BINARY FIXED,.                                           QA24 170
   DECLARE                                                          QA24 180
         X(24) BINARY FLOAT(53) STATIC INITIAL (                    QA24 190
         8.055628C81995C41E+01,   6.906860197530437E+01,            QA24 200
         6.020666696305722E+01,   5.279543252728363E+01,            QA24 210
         4.637697955754013E+01,   4.071159818554311E+01,            QA24 220
         3.565370351632821E+01,   3.110646470904657E+01,            QA24 230
         2.7C01406C5647236E+01,   2.328793282487992E+01,            QA24 240
         1.992742587524246E+01,   1.688967192852711E+01,            QA24 250
         1.415058618728576E+01,   1.169069592605607E+01,            QA24 260
         9.494095330026488E+00,   7.547704680023454E+00,            QA24 270
         5.840733271323608E+00,   4.364283076935306E+00,            QA24 280
         3.111052455147713E+00,   2.075112909852381E+00,            QA24 290
         1.251740632362746E+00,   6.372902787326888E-01,            QA24 300
         2.291023164926243E-01,   2.543799658568936E-02),.          QA24 310
   DECLARE                                                          QA24 320
         W(24) BINARY FLOAT(53) STATIC INITIAL (                    QA24 330
         1.587110292154799E-35,   1.196922538662776E-30,            QA24 340
         7.370072160301340E-27,   1.112915493780457E-23,            QA24 350
         6.376774647C10277E-21,   1.746031920237335E-18,            QA24 360
         2.630319245316817E-16,   2.395179730958359E-14,            QA24 370
         1.4C9386516309178E-12,   5.630593075676338E-11,            QA24 380
         1.586093499C33076E-09,   3.245028271791540E-08,            QA24 390
         4.937317987339SC1E-07,   5.694517383469696E-06,            QA24 400
         5.057198C55496978E-05,   3.503C08636023457E-04,            QA24 410
         1.912784639638831E-03,   8.3C6009823955105E-03,            QA24 420
         2.888992314996220E-02,   8.095935396920770E-02,            QA24 430
         1.836445941585704E-01,   3.384089438912822E-01,            QA24 440
         5.079230853295182E-01,   6.220020607559262E-01),.          QA24 450
   LY    =0,.                                                       QA24 460
         DO I=1 TO 24,.                                             QA24 470
         XX    =X(I),.                                              QA24 480
         LY    =LY+W(I)*FCT(XX),.                                   QA24 490
         END,.                                                      QA24 500
   Y     =LY,.                                                      QA24 510
   END,.                              /*END OF PROCEDURE QA24       */QA24 520
```

Purpose:

QAn computes the integral value $Y = \int_0^\infty \frac{e^{-X}\,FCT(X)}{\sqrt{X}}\,dX$ for a given function FCT(X), using associated Gaussian-Laguerre quadrature formulas.

Usage:

CALL QAn (FCT, Y);

FCT - ENTRY
Given procedure for the computation of the function values. This procedure must be supplied by the user.

Usage
FCT(X);
FCT(X) - BINARY FLOAT [(53)]
Resultant function value.
X - BINARY FLOAT [(53)]
Given argument value.

Y - BINARY FLOAT [(53)]
Resultant integral value.

Remarks:

The n in the name QAn indicates the number of nodes used for the calculation of Y.

Method:

Quadrature formulas of Gauss- Laguerre are used for the evaluation of the integral value.

For reference see:

Concus, Cassatt, Jaehnig, Melby, "Tables for the Evaluation of $\int_0^\infty x^\beta e^{-x} f(x)\,dx$ by Gauss-Laguerre Quadrature, MTAC, vol. 17, No. 83 (1963), pp 245-256.

Shao, Chen, Frank, "Tables of Zeros and Gaussian Weights of Certain Associated Laguerre Polynomials and the Related Generalized Hermite Polynomials", IBM Technical Report TR 00.1100, March 1964, pp. 15-16.

Mathematical Background:

Formulas of Gauss-Laguerre are used to compute

$$y = \int_0^\infty \frac{e^{-x} f(x)}{\sqrt{x}}\,dx$$

Let n denote the number of nodes used for the calculation of the integral value y.

The value y is approximated by a weighted sum of function values:

$$y^{(n)} = \sum_{k=1}^{n} [A_k^{(n)} f(x_k^{(n)})]$$

The value $y^{(n)}$ is exact whenever f(x) is a polynomial of degree less than or equal to 2n-1.

The nodes $x_k^{(n)}$ are the roots of the associated Laguerre polynomials $L_n^{(-1/2)}(x)$ of degree n.

Differentiation of Tabulated Functions

- Subroutine DGT3

```
DGT3..                                                              DGT3  10
/*******************************************************************/DGT3  20
/*                                                                 */DGT3  30
/*      DIFFERENTIATE A TABLED FUNCTION USING LAGRANGIAN           */DGT3  40
/*      INTERPOLATION FORMULA, DEGREE 2                            */DGT3  50
/*                                                                 */DGT3  60
/*******************************************************************/DGT3  70
   PROCEDURE(X,Y,Z,DIM),.                                           DGT3  80
   DECLARE                                                          DGT3  90
        (X(*),Y(*),Z(*),XA,XB,XC,                                   DGT3 100
        XBA,XCB,YA,YB,YC,QBA,QCB)                                   DGT3 110
        BINARY FLOAT,               /*SINGLE PRECISION VERSION  /*S*/DGT3 120
 /*     BINARY FLOAT(53),           /*DOUBLE PRECISION VERSION  /*D*/DGT3 130
        (DIM,I)BINARY FIXED,                                        DGT3 140
        LERR CHARACTER(1),                                          DGT3 150
        ERROR EXTERNAL CHARACTER(1),.                               DGT3 160
   IF DIM GE 3                  /*TEST SPECIFIED DIMENSION      */DGT3 170
   THEN DO,.                                                        DGT3 180
        LERR ='0',.             /*INIT. LOCAL ERROR INDICATOR   */DGT3 190
        XB   =X(3),.                                                DGT3 200
        YB   =Y(3),.                                                DGT3 210
        XC   =X(1),.                                                DGT3 220
        YC   =Y(1),.                                                DGT3 230
        XCB  =XB-XC,                                                DGT3 240
        IF XCB=0                /*TEST MONOTONY OF ARGUMENTS    */DGT3 250
        THEN DO,.                                                   DGT3 260
             LERR ='1',.        /*NON-MONOTONIC ARGUMENTS       */DGT3 270
             XCB  =1E-30,.      /*CHANGE XCB TO 10**(-30)       */DGT3 280
             END,.                                                  DGT3 290
        QCB  =(YB-YC)/XCB,.     /*COMPUTE DIVIDED DIFFERENCE    */DGT3 300
             DO I =2 TO DIM,.                                       DGT3 310
             QBA  =QCB,.        /*SAVE DIVIDED DIFFERENCE       */DGT3 320
             XBA  =XCB,.        /*REPLACE XBA BY X(I-1)-X(I-2)  */DGT3 330
             XA   =XB,.         /*REPLACE XA  BY X(I-2)         */DGT3 340
             XB   =XC,.         /*REPLACE XB BY X(I-1)          */DGT3 350
             XC   =X(I),.       /*SET     XC  TO X(I)           */DGT3 360
             YA   =YB,.         /*REPLACE YA BY Y(I-2)          */DGT3 370
             YB   =YC,.         /*REPLACE YB  BY Y(I-1)         */DGT3 380
             YC   =Y(I),.       /*SET     YC  BY Y(I)           */DGT3 390
             XCB  =XC-XB,.      /*REPLACE XCB BY X(I)-X(I-1)    */DGT3 400
             IF XCB*XBA LE 0                                        DGT3 410
             THEN LERR ='1',.   /*MARK NON-MONOTONIC ARGUMENTS  */DGT3 420
             IF XCB=0                                               DGT3 430
             THEN XCB  =1E-30,. /*CHANGE XCB TO 10**(-30)        */DGT3 440
             QCB  =(YC-YB)/XCB,. /*COMPUTE DIVIDED DIFFERENCE    */DGT3 450
             XA   =XC-XA,.      /*REPLACE XA BY X(I)-X(I-1)     */DGT3 460
             IF XA=0                                                DGT3 470
             THEN XA   =1E-30,. /*CHANGE XA TO 10**(-30)         */DGT3 480
             YA   =(YC-YA)/XA,. /*COMPUTE DIVIDED DIFFERENCE    */DGT3 490
             Z(I-1)=QBA-YA+QCB,. /*STORE DERIVATIVE VALUE Z(I-1)*/DGT3 500
             END,.                                                  DGT3 510
        Z(DIM)=QCB-QBA+YA,.     /*STORE DERIVATIVE VALUE Z(DIM)*/DGT3 520
        END,.                                                       DGT3 530
   ELSE LERR ='2',.             /*ERROR IN SPECIFIED DIMENSION  */DGT3 540
   ERROR=LERR,.                                                     DGT3 550
   END,.                        /*END OF PROCEDURE DGT3         */DGT3 560
```

Purpose:

DGT3 computes a vector $Z = (z_1, \ldots, z_{DIM})$ of derivative values, when vectors $X = (x_1, \ldots, x_{DIM})$ of argument values and $Y = (y_1, y_2, \ldots, y_{DIM})$ of corresponding function values are given.

Usage:

CALL DGT3 (X, Y, Z, DIM);

X(DIM) - BINARY FLOAT [(53)]
Given vector of argument values.

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of derivative values.

DIM - BINARY FIXED
Given dimension of vectors X, Y and Z.

Remarks:

If no errors are detected in the processing of data, the data indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='1' means non-monotonic argument values; that is, for some i, $(x_i - x_{i-1}) \cdot (x_{i+1} - x_i)$ is less than or equal to zero.

ERROR='2' means DIM is less than three.

Vectors Z and Y may be identically allocated, which means that the given function values are replaced by the resultant derivative values.

Method:

The resultant value z_i is calculated as the derivative of the Lagrangian interpolation polynomial passing through points i-1, i, i+1, at argument x_i.

$$z_i = \frac{y_i - y_{i-1}}{x_i - x_{i-1}} + \frac{y_{i+1} - y_i}{x_{i+1} - x_i} - \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$$

for i = 2, 3, ..., DIM-1, and corresponding formulas for z_1, z_{DIM}.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York-Toronto-London, 1956, pp. 64-68.

Mathematical background:

For i = 1,..., n-2 we must find a_i, b_i, and c_i such that

$$\bar{y}_i(x) = a_i x^2 + b_i x + c_i$$

passes through (x_i, y_i), (x_{i+1}, y_{i+1}), and (x_{i+2}, y_{i+2}).

The desired derivative values z_i are given by:

$$z_i = \begin{cases} y'_1(x_1) = 2a_1x_1 + b_1 & \text{if } i = 1 \\ y'_{i-1}(x_i) = 2a_{i-1}x_i + b_{i-1} & \text{if } i = 2, \ldots, n-1 \\ y'_{n-2}(x_n) = 2a_{n-2}x_n + b_{n-2} & \text{if } i = n \end{cases}$$

An easy computation yields:

$$z_i = \begin{cases} \dfrac{y_2-y_1}{x_2-x_1} + \dfrac{y_3-y_1}{x_3-x_1} - \dfrac{y_3-y_2}{x_3-x_2} & \text{if } i=1 \\[2ex] \dfrac{y_i-y_{i-1}}{x_i-x_{i-1}} + \dfrac{y_{i+1}-y_i}{x_{i+1}-x_i} - \dfrac{y_{i+1}-y_{i-1}}{x_{i+1}-x_{i-1}} & \text{if } i=2,\ldots,n-1 \\[2ex] \dfrac{y_n-y_{n-1}}{x_n-x_{n-1}} + \dfrac{y_n-y_{n-2}}{x_n-x_{n-2}} - \dfrac{y_{n-1}-y_{n-2}}{x_{n-1}-x_{n-2}} & \text{if } i=n \end{cases} \qquad (1)$$

Assuming that the vectors X and Y represent a portion of a three-times-differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{1}{6}(x_1-x_2)(x_1-x_3)y'''(\xi_1) & \text{if } i=1 \\[2ex] \frac{1}{6}(x_i-x_{i-1})(x_i-x_{i+1})y'''(\xi_i) & \text{if } i=2,\ldots,n-1 \\[2ex] \frac{1}{6}(x_n-x_{n-2})(x_n-x_{n-1})y'''(\xi_n) & \text{if } i=n \end{cases}$$

and ξ_i is in the closed interval determined by the three argument values used in computing z_i, $i = 1,\ldots,n$.

Programming Considerations:

The given table should represent a single-valued function. Non-monotonic arguments may cause dubious derivative values. If any difference (x_i-x_{i-1}), $(x_{i+1}-x_i)$, $(x_{i+1}-x_{i-1})$ is zero, it is replaced by 10^{-30}.

- Subroutine DET3

```
DET3..                                                                  DET3  10
/*********************************************************************/DET3  20
/*                                                                   */DET3  30
/*      DIFFERENTIATE AN EQUIDISTANTLY TABLED FUNCTION USING         */DET3  40
/*      LAGRANGIAN INTERPOLATION FORMULA, DEGREE 2                   */DET3  50
/*                                                                   */DET3  60
/*********************************************************************/DET3  70
   PROCEDURE(H,Y,Z,DIM),.                                              DET3  80
   DECLARE                                                             DET3  90
        (H,Y(*),Z(*),YA,YB,YC,HH)                                      DET3 100
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/DET3 110
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/DET3 120
        (DIM,I)BINARY FIXED,                                           DET3 130
        ERROR EXTERNAL CHARACTER(1),.                                  DET3 140
   IF DIM GE 3                         /*TEST SPECIFIED DIMENSION     */DET3 150
   THEN DO,.                                                           DET3 160
        IF H NE 0                      /*TEST SPECIFIED INCREMENT     */DET3 170
        THEN DO,.                                                      DET3 180
             HH   =H+H,.                                               DET3 190
             YC   =Y(1),.                                              DET3 200
             YA   =YC-Y(2),.                                           DET3 210
             YB   =Y(3)+YA+YA+YA,.    /*MODIFICATION  YB = Y(0)      */DET3 220
                  DO I =2 TO DIM,.                                     DET3 230
                  YA   =YB,.          /*REPLACE YA BY Y(I-2)         */DET3 240
                  YB   =YC,.          /*REPLACE YB BY Y(I-1)         */DET3 250
                  YC   =Y(I),.        /*SET YC TO Y(I)               */DET3 260
                  Z(I-1)=(YC-YA)/HH,. /*SET Z(I-1) TO (Y(I)-Y(I-2)/2H*/DET3 270
                  END,.                                                DET3 280
             YC   =YC-YB,.                                             DET3 290
             Z(DIM)=(YA-YB+YC         /*Z(DIM)=(Y(DIM-2)-4*Y(DIM-1)  */DET3 300
                  +YC+YC)/HH,.        /*+3*Y(DIM))2*H                */DET3 310
             ERROR='0',.              /*SUCCESSFUL OPERATION         */DET3 320
             END,.                                                     DET3 330
        ELSE ERROR='1',.              /*ERROR IN SPECIFIED INCREMENT */DET3 340
        END,.                                                          DET3 350
   ELSE ERROR='2',.                   /*ERROR IN SPECIFIED DIMENSION */DET3 360
   END,.                              /*END OF PROCEDURE DET3        */DET3 370
```

Purpose:

DET3 computes a vector $Z = (z_1, z_2, \ldots, z_{DIM})$ of derivative values, given a vector $Y = (y_1, y_2, \ldots, y_{DIM})$ of function values whose components y_i correspond to DIM equidistantly spaced argument values x_i with $x_i-x_{i-1} = h$ for $i = 2, \ldots,$ DIM.

Usage:

CALL DET3 (H, Y, Z, DIM);

H - BINARY FLOAT [(53)]
Given increment of argument values.

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of derivative values.

DIM - BINARY FIXED
Given dimension of vector Y and Z.

Remarks:

If no errors are detected in the processing of data, the data indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='1' means DIM is less than three.
ERROR='2' means H is equal to zero.

Storage allocation for the vectors Z and Y may be identical, which means that the given function values are replaced by the resultant derivative values.

Method:

The resultant value z_i is calculated as the derivative of the Lagrangian interpolation polynomial passing through the points i-1, i, i+1 at argument x_i.

$$z_i = \frac{1}{2h}(y_{i+1} - y_{i-1}) \text{ for } i = 2, 3, \ldots, \text{DIM}-1$$

and corresponding formulas for z_1, z_{DIM}.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 82-84.

Mathematical Background:

The procedure is described under subroutine DGT3, but here we have the additional relation $x_i - x_{i-1} = h$, a constant, for i = 2, ..., n. This leads to the following expression for z_i:

$$z_i = \begin{cases} \frac{1}{2h}(-y_3 + 4y_2 - 3y_1) & \text{if } i=1 \\ \frac{1}{2h}(y_{i+1} - y_{i-1}) & \text{if } i=2,\ldots,n-1 \\ \frac{1}{2h}(3y_n - 4y_{n-1} + y_{n-2}) & \text{if } i=n \end{cases} \quad (1)$$

Assuming that the vector Y represents the function values of a portion of a three-times-differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{h^2}{3} y'''(\xi_1), \ \xi_1 \in [x_1, x_3] & \text{if } i=1 \\ \frac{-h^2}{6} y'''(\xi_i), \ \xi_i \in [x_{i-1}, x_{i+1}] & \text{if } i=2,\ldots,n-1 \\ \frac{h^2}{3} y'''(\xi_n), \ \xi_n \in [x_{n-2}, x_n] & \text{if } i=n \end{cases}$$

In addition to these truncation errors, roundoff errors may be of considerable magnitude. Supposing that each of the ordinates y_i can be in error by $\pm \epsilon$, $\epsilon > 0$, the magnitude $|R_i|$ of the corresponding error R_i in the calculation of z_i can be as large as:

$$|R_i| = \begin{cases} \frac{4\epsilon}{|h|} & \text{if } i=1, n \\ \frac{\epsilon}{|h|} & \text{if } i=2,\ldots,n-1 \end{cases}$$

Since small truncation errors generally require small $|h|$, while small roundoff errors generally require large $|h|$, it is reasonable to choose h so that $|T_i| \approx |R_i|$.

If $M = \sup y'''(\xi)$, where $\xi \in [x_1, x_n]$, and if we regard only the inner points $x_2, \ldots, x_{n-1}$, we find that

$$h_{\text{optimum}} \approx \pm 1.8 \sqrt[3]{\epsilon/M}$$

and the magnitude $|E_i|$ of the total possible error E_i in z_i is given by:

$$|E_i| \approx \begin{cases} 3.3 \sqrt[3]{\epsilon^2 M} & \text{if } i=1, n \\ 1.1 \sqrt[3]{\epsilon^2 M} & \text{if } i=2,\ldots,n-1 \end{cases}$$

- Subroutine DET5

```
DET5..                                                                  DET5  10
/*********************************************************************/DET5  20
/*                                                                   */DET5  30
/*      DIFFERENTIATE AN EQUIDISTANTLY TABLED FUNCTION USING         */DET5  40
/*      LAGRANGIAN INTERPOLATION FORMULA, DEGREE 4                   */DET5  50
/*                                                                   */DET5  60
/*********************************************************************/DET5  70
   PROCEDURE(H,Y,Z,DIM),.                                             DET5  80
   DECLARE                                                            DET5  90
        (H,Y(*),Z(*),YA,YB,YC,YD,YE,HH)                               DET5 100
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/DET5 110
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/DET5 120
        (DIM,I)BINARY FIXED,                                          DET5 130
        ERROR EXTERNAL CHARACTER(1),.                                 DET5 140
   IF DIM GE 5                        /*TEST SPECIFIED DIMENSION     */DET5 150
   THEN DO,.                                                          DET5 160
        IF H NE 0                     /*TEST SPECIFIED INCREMENT     */DET5 170
        THEN DO,.                                                     DET5 180
             HH   =12*H,.                                             DET5 190
             YD   =Y(1),.                                             DET5 200
             YE   =Y(2),.                                             DET5 210
             YA   =Y(3)-YE,.                                          DET5 220
             YB   =Y(4),.                                             DET5 230
             YC   =Y(5)                /*MODIFICATION  YC = Y(0)      */DET5 240
                  +5*(YD-YB+YA+YA),.                                  DET5 250
             YB   =5*(YC-YD+YE-YD-YA) /*MODIFICATION  YB = Y(-1)     */DET5 260
                  +YB,.                                               DET5 270
                  DO I =3 TO DIM,.                                    DET5 280
                  YA   =YB,.          /*REPLACE YA BY Y(I-4)         */DET5 290
                  YB   =YC,.          /*REPLACE YB BY Y(I-3)         */DET5 300
                  YC   =YD,.          /*REPLACE YC BY Y(I-2)         */DET5 310
                  YD   =YE,.          /*REPLACE YD BY Y(I-1)         */DET5 320
                  YE   =Y(I),.        /*SET YE TO Y(I)               */DET5 330
                  Z(I-2)=(YA-YE+      /*Z(I-2)=(Y(I-4)-Y(I)+         */DET5 340
                       (YD-YB)*8)/HH,./**8*(Y(I-1)-Y(I-3))/12H        */DET5 350
                  END,.                                               DET5 360
             YA   =YA-6*(YB-YC                                        DET5 370
                  +YD-YC+YD-YC),.                                     DET5 380
             Z(DIM-1)=(YE-YD+YE-YD    /*COMPUTE LAST TWO DERIVATIVE  */DET5 390
                  +YE-YA)/HH,.        /*VALUES                       */DET5 400
             Z(DIM)=(YA+YA+YA+YB+YB                                   DET5 410
                  +YE-6*YC+12*(YE                                     DET5 420
                  -YD+YE-YC))/HH,.                                    DET5 430
             ERROR='0',.              /*SUCCESSFUL OPERATION         */DET5 440
             END,.                                                    DET5 450
        ELSE ERROR='1',.              /*ERROR IN SPECIFIED INCREMENT */DET5 460
        END,.                                                         DET5 470
   ELSE ERROR='2',.                   /*ERROR IN SPECIFIED DIMENSION */DET5 480
   END,.                              /*END OF PROCEDURE DET5        */DET5 490
```

Purpose:

DET5 computes a vector $Z = (z_1, z_2, \ldots, z_{DIM})$ of derivative values, given $Y = (y_1, y_2, \ldots, y_{DIM})$ of function values whose components correspond to DIM equidistantly spaced argument values x_i, with $x_i - x_{i-1} = h$.

Usage:

CALL DET5 (H, Y, Z, DIM);

H - BINARY FLOAT [(53)]
Given increment for argument values.

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of derivative values.

DIM - BINARY FIXED
Given dimension of vectors Y and Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR='1' means H is equal to zero.
ERROR='2' means DIM is less than five.

Storage allocation for vectors Z and Y may be identical, which means that the given function values are replaced by the resultant derivative values.

Method:

The resultant value z_i is calculated as the derivative of the Lagrangian interpolation polynomial passing through the points i-2, i-1, i, i+1, i+2 at argument x_i.

$$z_i = \frac{1}{2h}(y_{i+1} - y_{i-1}) \quad \text{for } i = 3, 4, \ldots, DIM-2$$

and corresponding formulas for z_1, z_2, z_{DIM-1}, z_{DIM}

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 82-84.

Mathematical Background:

For $i = 1, \ldots, n-4$ we must find a_i, b_i, c_i, d_i, and e_i such that

$$\bar{y}_i(x) = a_i x^4 + b_i x^3 + c_i x^2 + d_i x + e_i$$

passes through (x_{i+k}, y_{i+k}) for $k = 0, \ldots, 4$.
The desired derivative values z_i are given by:

$$z_i = \begin{cases} \bar{y}'_1(x_i) = 4a_1 x_i^3 + 3b_1 x_i^2 + 2c_1 x_i + d_1 \\ \qquad \text{if } i = 1, 2 \\ \bar{y}'_{i-2}(x_i) = 4a_{i-2} x_i^3 + 3b_{i-2} x_i^2 + 2c_{i-2} x_i + d_{i-2} \\ \qquad \text{if } i = 3, \ldots, n-2 \\ \bar{y}'_{n-4}(x_i) = 4a_{n-4} x_i^3 + 3b_{n-4} x_i^2 + 2c_{n-4} x_i + d_{n-4} \\ \qquad \text{if } i = n-1, n \end{cases}$$

Using the fact that $x_i - x_{i-1} = h$, a constant, for $i = 2, \ldots, n$, we get:

$$z_i = \begin{cases} \frac{1}{12h}(-25y_1 + 48y_2 - 36y_3 + 16y_4 - 3y_5) \\ \qquad \text{if } i = 1 \\ \frac{1}{12h}(-3y_1 - 10y_2 + 18y_3 - 6y_4 + y_5) \\ \qquad \text{if } i = 2 \\ \frac{1}{12h}(y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2}) \\ \qquad \text{if } i = 3, \ldots, n-2 \\ \frac{1}{12h}(-y_{n-4} + 6y_{n-3} - 18y_{n-2} + 10_{n-1} + 3y_n) \\ \qquad \text{if } i = n-1 \\ \frac{1}{12h}(3y_{n-4} - 16y_{n-3} + 36y_{n-2} - 48y_{n-1} + 25y_n) \\ \qquad \text{if } i = n \end{cases} \tag{1}$$

Assuming that the vector Y represents the function values of a portion of a five-times-differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{h^4}{5} y^{v}(\xi_1), & \xi_1 \epsilon [x_1, x_5] & \text{if } i = 1 \\ -\frac{h^4}{20} y^{v}(\xi_2), & \xi_2 \epsilon [x_1, x_5] & \text{if } i = 2 \\ \frac{h^4}{30} y^{v}(\xi_i), & \xi_i \epsilon [x_{i-2}, x_{i+2}] & \text{if } i = 3, \ldots, n-2 \\ -\frac{h^4}{20} y^{v}(\xi_{n-1}), & \xi_{n-1} \epsilon [x_{n-4}, x_n] & \text{if } i = n-1 \\ \frac{h^4}{5} y^{v}(\xi_n), & \xi_n \epsilon [x_{n-4}, x_n] & \text{if } i = n \end{cases}$$

In addition to the truncation errors, roundoff errors may be of considerable magnitude. Supposing that the ordinates y_i can be in error by $\pm \epsilon$, $\epsilon > 0$, the magnitude $|R_i|$ of the corresponding error R_i in the computation of z_i can be as large as:

$$|R_i| = \begin{cases} \frac{32\epsilon}{3|h|} & \text{if } i = 1, n \\ \frac{19\epsilon}{6|h|} & \text{if } i = 2, n-1 \\ \frac{3\epsilon}{2|h|} & \text{if } i = 3, \ldots, n-2 \end{cases}$$

Since small truncation errors generally require small $|h|$, while small roundoff errors generally require large $|h|$, it is reasonable to choose h so that $|T_i| \approx |R_i|$.

If $M = \sup_{\xi \epsilon [x_1, x_n]} y^{v}(\xi)$

and if we regard only the inner points $x_3, \ldots, x_{n-2}$, we find that

$$h_{optimum} \approx 2.1 \sqrt[5]{\epsilon / M}$$

and the magnitude $|E_i|$ of the total possible error E_i in z_i is given by:

$$|E_i| \simeq \begin{cases} 9 \sqrt[5]{\epsilon^4 M} & \text{if } i = 1, n \\ 2.5 \sqrt[5]{\epsilon^4 M} & \text{if } i = 2, n-1 \\ 1.4 \sqrt[5]{\epsilon^4 M} & \text{if } i = 3, \ldots, n-2 \end{cases}$$

Differentiation of Nontabulated Functions

- Subroutine DFEC

```
DFEC..                                                                  DFEC  10
/*************************************************************************/DFEC  20
/*                                                                       */DFEC  30
/*      COMPUTE DERIVATIVE VALUE OF A FUNCTION USING EXTRAPOLATION       */DFEC  40
/*      METHOD ON CENTRAL DIVIDED DIFFERENCES                            */DFEC  50
/*                                                                       */DFEC  60
/*************************************************************************/DFEC  70
   PROCEDURE(X,H,OPT,FCT,Z),.                                           DFEC  80
   DECLARE                                                              DFEC  90
         (X,Z,H,HH,HK,V,LZ,H1,                                          DFEC 100
         DA,DB,DZ,AUX(5))                                               DFEC 110
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/DFEC 120
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/DFEC 130
         (K,M)BINARY FIXED,                                             DFEC 140
         FCT ENTRY                                                      DFEC 150
         (BINARY FLOAT)                 /*SINGLE PRECISION VERSION  /*S*/DFEC 160
 /*      (BINARY FLOAT(53))             /*DOUBLE PRECISION VERSION  /*D*/DFEC 170
         RETURNS(BINARY FLOAT),         /*SINGLE PRECISION VERSION  /*S*/DFEC 180
 /*      RETURNS(BINARY FLOAT(53)),     /*DOUBLE PRECISION VERSION  /*D*/DFEC 190
         (ERROR EXTERNAL,OPT)CHARACTER(1),.                             DFEC 200
   IF H NE 0                            /*TEST SPECIFIED INTERVAL     */DFEC 210
   THEN DO,.                                                            DFEC 220
         HK,H1=ABS(H),.                 /*SET H1 TO ABS(H)            */DFEC 230
         IF OPT NE '0'                  /*SHOULD OPTIMUM STEPSIZE H1  */DFEC 240
         THEN DO,.                      /*BE GENERATED                */DFEC 250
              V    =5E-1,.              /*SINGLE PRECISION VERSION  /*S*/DFEC 260
 /*           V    =5E-3,.              /*DOUBLE PRECISION VERSION  /*D*/DFEC 270
              IF HK GT V                                                DFEC 280
              THEN HK   =V,.            /*SET HK =MIN(V,ABS(H))       */DFEC 290
              DB   =1,.                                                 DFEC 300
              DA   =ABS(FCT(X+HK)                                       DFEC 310
                   -FCT(X-HK))/2,.                                      DFEC 320
              IF DA GT HK                                               DFEC 330
              THEN DB   =DA/HK,.        /*SET DB TO MAX(1,ABS(T))     */DFEC 340
              IF DA LT 1                                                DFEC 350
              THEN DA   =1,.            /*SET DA TO MAX(1,ABS(Y)      */DFEC 360
              HK   =V*DA/DB,.                                           DFEC 370
              IF HK LT H1                                               DFEC 380
              THEN H1   =HK,.           /*SET H1 TO MIN(V*DA/DB,ABS(H))*/DFEC 390
              END,.                                                     DFEC 400
         V    =5,.                                                     DFEC 410
              DO K =1 TO 5,.                                            DFEC 420
              HK   =(V/5)*H1,.          /*SET HK TO H1*(6-K)/5        */DFEC 430
              LZ,AUX(K)=(FCT(X+HK)-     /*SET AUX(K) TO T(0,K)        */DFEC 440
                   FCT(X-HK))/(HK+HK),.                                 DFEC 450
              HH   =1/V,.                                               DFEC 460
              HK   =0,.                                                 DFEC 470
              DA   =1E30,.                                              DFEC 480
                   DO M =K-1 TO 1 BY -1,.                               DFEC 490
                   DB   =DA,.                                           DFEC 500
                   HK   =HK+HH,.                                        DFEC 510
                   DZ   =(LZ-AUX(M))/  /*SET DZ TO INCREMENT           */DFEC 520
                        (HK*(2+HK)),.                                   DFEC 530
                   DA   =ABS(DZ),.                                      DFEC 540
                   IF DB LT DA          /*TEST FOR DECR. INCREMENTS   */DFEC 550
                   THEN GOTO NEWK,.                                     DFEC 560
                   LZ,AUX(M)=LZ+DZ,.    /*SET Z,AUX(M) TO T(K-M  ,M)  */DFEC 570
                   END,.                                                DFEC 580
NEWK..                                                                  DFEC 590
              V    =V-1,.                                               DFEC 600
              END,.                                                     DFEC 610
         Z    =LZ,.                                                    DFEC 620
         ERROR='0',.                    /*SUCCESSFUL OPERATION        */DFEC 630
         END,.                                                          DFEC 640
   ELSE ERROR='1',.                     /*ERROR IN SPECIFIED INTERVAL */DFEC 650
   END,.                                /*END OF PROCEDURE DFEC       */DFEC 660
```

Purpose:

Given the argument X and the function FCT(X), defined in the closed interval [X-|H| , X+|H|]. DFEC computes an approximation Z to the derivative of the function FCT(X).

Usage:

CALL DFEC (X, H, OPT, FCT, Z);

X - BINARY FLOAT [(53)]
Given argument value.

H - BINARY FLOAT [(53)]
Given radius of closed interval about X.

OPT - CHARACTER (1)
Given option for calculation of the stepsize.

FCT - ENTRY
Given procedure for calculating of function values, which must be supplied by the user.

Usage:
FCT(T)

FCT(T) - BINARY FLOAT [(53)]
Resultant function value.

T - BINARY FLOAT [(53)]
Given argument value.

Z - BINARY FLOAT [(53)]
Resultant approximation to $\frac{d}{dx}$ FCT(X).

Remarks:

OPT = '0' means maximum stepsize is set equal to H; otherwise, it will be calculated within procedure DFEC (for details see "Mathematical Background").

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR = '1' means given H is equal to zero.

Method:

The approximation Z of the derivative is obtained by applying Richardson's and Romberg's extrapolation method to successively computed central divided differences, using function values in the closed interval [X-|H|, X+|H|].

For reference see:

S. Fillipi and H. Engels, "Altes und Neues zur numerischen Differentiation", Elektronische Datenverarbeitung, iss. 2 (1966), pp. 57 - 65.

Mathematical Background:

Suppose, first, that y = y(t) is analytic at x; that is, y has a Taylor series expansion about the point x with radius of convergence R > 0. Let h be such that $0 < |h| < R$. For each positive integer n a step size h_1 with $0 < h_1 \leq |h|$ is computed as described below, and a sequence h_k of increments is generated, where

$$h_k = \frac{n-k+1}{n} h_1 \qquad \text{for } k=2,\ldots,n$$

From the sequence $(x-h_k, x+h_k)$ of point pairs $(k=1,\ldots,n)$, the sequence of central divided differences

$$T_{0,k} = \frac{y(x+h_k) - y(x-h_k)}{2h_k} \quad \text{for } k=1,\ldots,n \qquad (1)$$

is computed, which forms the first column of the triangular Romberg scheme. The central divided

differences $T_{0,k}$ represent the slopes of the secants s_k in Figure 2.

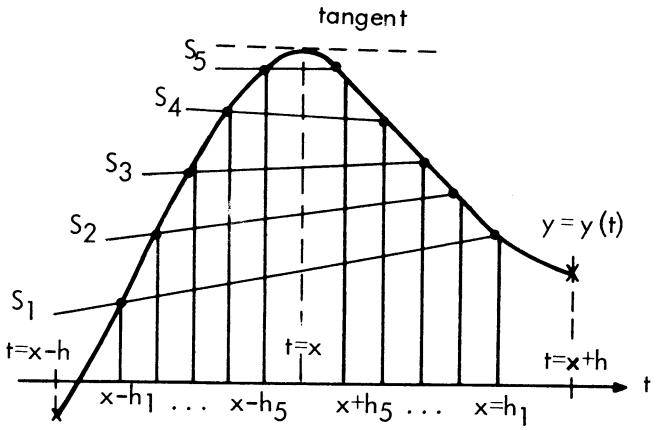


Figure 2. A sequence of secants for a given function y=y(t) and a given argument t=x for the case n=5, h > 0

From the Taylor series expansions of $y(x+h_k)$ and $y(x-h_k)$ it follows that

$$T_{0,k} = y'(x) + \frac{h_k^2}{3!} y'''(x) + \frac{h_k^4}{5!} y^{v}(x) + \ldots$$

for $k = 1, \ldots, n$

so that, as an approximation to $y'(x)$, $T_{0,k}$ involves a truncation error of order h_k^2.

Knowing the two divided differences $T_{0,k}$ and $T_{0,k+1}$, we are able to generate the extrapolated value

$$T_{1,k} = T_{0,k+1} + \frac{T_{0,k+1} - T_{0,k}}{a_{1,k} - 1}$$

where (2)

$$a_{1,k} = \left(1 + \frac{1}{n-k}\right)^2$$

$T_{1,k}$ is a better approximation to $y'(x)$ since

$$T_{1,k} = y'(x) - \frac{1}{5!} \frac{1}{a_{1,k}} h_k^4 y^{v}(x) - \frac{1}{7!} \frac{1}{a_{1,k}} \left(1 + \frac{1}{a_{1,k}}\right) h_k^6 y^{vii}(x) - \ldots$$

which involves a truncation error of order h_k^4.

If we also know $T_{0,k+2}$, we can generate $T_{1,k+1}$ using equation (2), and further, we can compute the extrapolated value

$$T_{2,k} = T_{1,k+1} + \frac{T_{1,k+1} - T_{1,k}}{a_{2,k} - 1}$$

where

$$a_{2,k} = \left(1 + \frac{2}{n-(k+1)}\right)^2$$

which involves a truncation error of order h_k^6.

Generally, the order of the truncation error is increased by 2 with each new extrapolation step; in particular, $T_{i,j}$ will involve a truncation error of order

$$h_j^{2i+2}, \quad i = 0, \ldots, n-1, \quad j = 1, \ldots, n.$$

Figure 3 shows the arrangement of the T values in the triangular Romberg scheme. The T values are computed following the upward diagonals, using the general formula:

$$T_{m,k-m} = T_{m-1,k-m+1} + \frac{T_{m-1,k-m+1} - T_{m-1,k-m}}{\frac{m}{n-(k+1)}\left(2 + \frac{m}{n-(k+1)}\right)} \qquad (4)$$

for $m = 1, \ldots, k-1$ for fixed k, $k=2, \ldots, n$

Truncation error		$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$	$O(h_k^{10})$
Stepsize	k \ m	0	1	2	3	4
h_1	1	$T_{0,1}$	$T_{1,1}$	$T_{2,1}$	$T_{3,1}$	$T_{4,1}$
$h_2=0.8h_1$	2	$T_{0,2}$	$T_{1,2}$	$T_{2,2}$	$T_{3,2}$	
$h_2=0.6h_1$	3	$T_{0,3}$	$T_{1,3}$	$T_{2,3}$		
$h_4=0.4h_1$	4	$T_{0,4}$	$T_{1,4}$			
$h_5=0.2h_1$	5	$T_{0,5}$				

Figure 3. The triangular Romberg scheme of T-values for the case n=5

Numerical experience shows that the accuracy of the results depends heavily on roundoff errors in the central divided differences $T_{0,k}$. Therefore, the choice of the absolutely smallest step size, h_n, is based on the following considerations.
Let:

$$v = \begin{cases} 1 \text{ in single-precision computation} \\ 3 \text{ in double-precision computation} \end{cases}$$

$$h_0 = \min (n \cdot 10^{-v}, |h|)$$

Set:

$$Y = \frac{1}{2}(y(x+h_0) + y(x-h_0))$$

and

$$T = \frac{1}{2}(y(x+h_0) - y(x-h_0))/h_0$$

Y and T are approximations to y(x) and y'(x), respectively.

Assuming that the errors in the function values y(t) for $t \in [x-|h|, x+|h|]$ are bounded by

$$\epsilon = \begin{cases} Y \cdot 10^{-D} & \text{if } |Y| > 1 \\ 10^{-D} & \text{if } |Y| \leq 1 \end{cases}$$

formula (1) shows that the roundoff error in the computation of $T_{0,n}$ is bounded by

$$R(T_{0,n}) = \frac{\epsilon}{h_n} = \begin{cases} \frac{Y \cdot 10^{-D}}{h_n} & \text{if } |Y| > 1 \\ \frac{10^{-D}}{h_n} & \text{if } |Y| \leq 1 \end{cases}$$

where D is the number of significant digits in the floating-point representation of numbers. Suppose, also, that we are willing to tolerate a roundoff error

$$R'(T_{0,n}) = \begin{cases} T \cdot 10^{-D+v} & \text{if } |T| > 1 \\ 10^{-D+v} & \text{if } |T| \leq 1 \end{cases}$$

Then we must have $R(T_{0,n}) \leq R'(T_{0,n})$, which is satisfied when

$$h_n = \frac{\max(1, |Y|)}{\max(1, |T|)} \cdot 10^{-v} \qquad (5)$$

Finally we set

$$h_1 = \min(n \cdot h_n, |h|) \qquad (6)$$

guaranteeing that the evaluation of the function y = y(t) is restricted to the closed interval $[x-|h|, x+|h|]$.

Programming Considerations:

Numerical experience shows that, because of increasing roundoff errors, it is generally fruitless to perform more than five extrapolations. Thus, the subroutine uses n = 5, and it is therefore necessary only that y = y(t) be eleven-times differentiable, rather than analytic. It is easy to see that in the case n = 5, y = y(t) must be evaluated at twelve points in the closed interval $[x-|h|, x+|h|]$.

As previously explained, the computation of the T values is performed along the upward diagonals of the triangular Romberg scheme. Therefore, only a one-dimensional internal storage vector, named AUX, with five storage locations is necessary. Figure 4 shows the storage administration and the sequence of computations (numbers in parentheses).

AUX(1)	$T_{0,5}^{(11)}$				
AUX(2)	$T_{0,4}^{(7)}$	$T_{1,4}^{(12)}$			
AUX(3)	$T_{0,3}^{(4)}$	$T_{1,3}^{(8)}$	$T_{2,3}^{(13)}$		
AUX(4)	$T_{0,2}^{(2)}$	$T_{1,2}^{(5)}$	$T_{2,2}^{(9)}$	$T_{3,2}^{(14)}$	
AUX(5)	$T_{0,1}^{(1)}$	$T_{1,1}^{(3)}$	$T_{2,1}^{(6)}$	$T_{3,1}^{(10)}$	$T_{4,1}^{(15)}$

Figure 4. Storage administration and order of computation

Each extrapolation loop, the computation of the elements on an upward diagonal, is terminated as soon as the absolute values of the differences between adjacent diagonal elements stop decreasing, showing the influence of roundoff errors. The computed T value that differs least in absolute value from its immediately preceding diagonal neighbor is the desired value Z.

- Subroutine DFEO

```
DFEO..                                                                  DFEO  10
/**********************************************************************/DFEO  20
/*                                                                    */DFEO  30
/*      COMPUTE DERIVATIVE VALUE OF A FUNCTION USING EXTRAPOLATION    */DFEO  40
/*      METHOD ON ONE-SIDED DIVIDED DIFFERENCES                       */DFEO  50
/*                                                                    */DFEO  60
/**********************************************************************/DFEO  70
   PROCEDURE(X,H,OPT,FCT,Z),.                                           DFEO  80
   DECLARE                                                              DFEO  90
         (X,Z,H,HK,HH,V,Y,H1,                                           DFEO 100
         DA,DB,DZ,AUX(10))                                              DFEO 110
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/DFEO 120
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/DFEO 130
         (K,M)BINARY FIXED,                                             DFEO 140
         FCT ENTRY                                                      DFEO 150
         (BINARY FLOAT)                 /*SINGLE PRECISION VERSION  /*S*/DFEO 160
 /*      (BINARY FLOAT(53))             /*DOUBLE PRECISION VERSION  /*D*/DFEO 170
         RETURNS(BINARY FLOAT),         /*SINGLE PRECISION VERSION  /*S*/DFEO 180
 /*      RETURNS(BINARY FLOAT(53)),     /*DOUBLE PRECISION VERSION  /*D*/DFEO 190
         (ERROR EXTERNAL,OPT)CHARACTER(1),.                             DFEO 200
   IF H NE 0                            /*TEST SPECIFIED INTERVAL      */DFEO 210
   THEN DO,.                                                            DFEO 220
         H1   =H,.                                                      DFEO 230
         Y    =FCT(X),.                                                 DFEO 240
         IF OPT NE 'C'                  /*SHOULD OPTIMUM STEPSIZE H1   */DFEO 250
         THEN DO,.                      /*BE GENERATED                 */DFEO 260
              V    =5E-1,.              /*SINGLE PRECISION VERSION  /*S*/DFEO 270
 /*           V    =5E-3,.              /*DOUBLE PRECISION VERSION  /*D*/DFEO 280
              IF H1 LT 0                                                DFEO 290
              THEN V    =-V,.                                           DFEO 300
              IF ABS(V) GT ABS(H1)                                      DFEO 310
              THEN HH   =H1,.           /*SET HH=SIGN(H)*MIN(V,ABS(H)) */DFEO 320
              ELSE HH   =V,.                                            DFEO 330
              DB   =ABS((FCT(X+HH)                                      DFEO 340
                   -Y)/HH),.                                            DFEO 350
              IF DB LT 1                                                DFEO 360
              THEN DB   =1,.            /*SET DB TO MAX(1,ABS(T))      */DFEO 370
              HK   =(V+V)/DB,.                                          DFEO 380
              IF ABS(Y) GT 1                                            DFEO 390
              THEN HK   =HK*ABS(Y),.    /*SET HK=2*V*MAX(1,ABS(Y))/DB  */DFEO 400
              IF ABS(HK) LT ABS(H1)                                     DFEO 410
              THEN H1   =HK,.           /*SET H1=SIGN(H)*MIN(HK,ABS(H))*/DFEO 420
              END,.                                                     DFEO 430
         V    =10,.                                                     DFEO 440
              DO K =1 TO 10,.                                           DFEO 450
              HK   =(V/10)*H1,.         /*SET HK TO H1*(11-K)/10       */DFEO 460
              Z,AUX(K)=(FCT(X+HK)-Y)    /*SET AUX(K) TO T(0,K)         */DFEO 470
                   /HK,.                                                DFEO 480
              HH   =1/V,.                                               DFEO 490
              HK   =C,.                                                 DFEO 500
              DA   =1E30,.                                              DFEO 510
                   DO M =K-1 TO 1 BY -1,.                               DFEO 520
                   HK   =HK+HH,.                                        DFEO 530
                   DZ   =(Z-AUX(M))                                     DFEO 540
                        /HK,.           /*SET DZ TO INCREMENT          */DFEO 550
                   DB   =DA,.                                           DFEO 560
                   DA   =ABS(DZ),.                                      DFEO 570
                   IF DB LT DA          /*TEST FOR DECREASING INCREMENT*/DFEO 580
                   THEN GOTO NEWK,.                                     DFEO 590
                   Z,AUX(M)=Z+DZ,.      /*SET Z,AUX(M) TO T(K-M,M)     */DFEO 600
                   END,.                                                DFEO 610
NEWK,.                                                                  DFEO 620
              V    =V-1,.                                               DFEO 630
              END,.                                                     DFEO 640
         ERROR='0',.                    /*SUCCESSFUL OPERATION         */DFEO 650
         END,.                                                          DFEO 660
   ELSE ERROR='1',.                     /*ERROR IN SPECIFIED INTERVAL  */DFEO 670
   END,.                                /*END OF PROCEDURE DFEO        */DFEO 680
```

Purpose:

Given argument X and function FCT(X), defined in the one-sided interval [X, X+H], DFEO computes an approximation Z to the derivative.

Usage:

CALL DFEO (X, H, OPT, FCT, Z);

X - BINARY FLOAT [(53)]
Given argument value.

H - BINARY FLOAT [(53)]
Given length of interval.

OPT - CHARACTER (1)
Given option for calculation of the stepsize.

FCT - ENTRY
Given procedure for calculation of function values, which must be supplied by the user.
Usage:
FCT(T)

FCT(T) - BINARY FLOAT [(53)]
Resultant function value.

T - BINARY FLOAT [(53)]
Given argument value.

Z - BINARY FLOAT [(53)]
Resultant approximation to $\frac{d}{dx}$ FCT(X).

Remarks:

OPT = '0' means maximum stepsize is set equal to H; otherwise, it will be calculated within procedure DFEO (for details see "Mathematical Background").

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR = '1' means H is equal to zero.

Method:

The approximation Z of the derivative is obtained by applying Richardson's and Romberg's extrapolation method to successively computed one-sided divided differences, using function values in the closed interval [X, X+H].

For reference see:

S. Fillipi and Engels, "Altes und Neues zur numerischen Differentiation", Elektronische Datenverarbeitung, iss. 2 (1966), pp. 57-65.

Mathematical Background:

Suppose, first, that y=y(t) is analytic at x; that is, y has a Taylor series expansion about the point x with radius of convergence R > 0. Let h be such that $0 < |h| < R$. For each positive integer n, a stepsize h_1 with $0 < |h_1| \leq |h|$ is computed as described below, and a sequence h_k of increments is generated, where

$$h_k = \frac{n-k+1}{n} h_1$$

for k = 2, ..., n.

From the sequence $(x, x+h_k)$ of point pairs (k = 1,..., n), the sequence of one-sided divided differences

$$T_{0,k} = \frac{y(x+h_k) - y(x)}{h_k} \quad \text{for } k = 1,\ldots, n \qquad (1)$$

is computed, which forms the first column of the triangular Romberg scheme. These one-sided divided differences $T_{0,k}$ represent the slopes of the secants s_k in Figure 5 in the case $h > 0$.

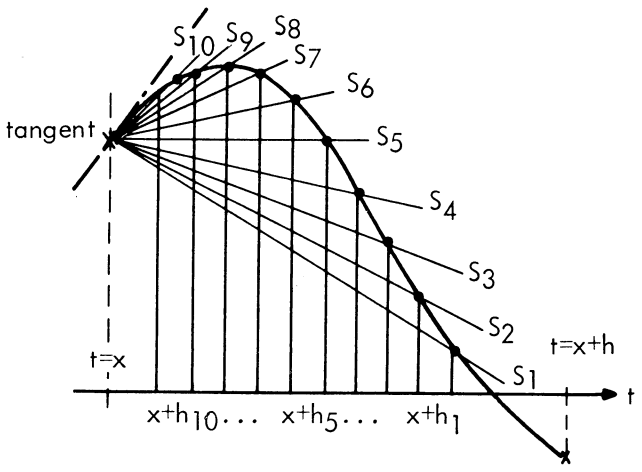


Figure 5. A sequence of secants for a given function $y=y(t)$ and a given argument $t=x$ for the case $n=10, h > 0$

From the Taylor series expansion of $y(x+h_k)$ it follows that

$$T_{0,k} = y'(x) + \frac{h_k}{2} y''(x) + \frac{h_k^2}{3!} y'''(x) + \ldots$$

for $k=1, \ldots, n$

so that, as an approximation to $y'(x)$, $T_{0,k}$ involves a truncation error of order h_k. Knowing the two divided differences $T_{0,k}$ and $T_{0,k+1}$, we are able to generate the extrapolated value

$$T_{1,k} = T_{0,k+1} + \frac{T_{0,k+1} - T_{0,k}}{a_{1,k}^{-1}} \qquad (2)$$

where

$$a_{1,k} = \left(1 + \frac{1}{n-k}\right)$$

$T_{1,k}$ is a better approximation to $y'(x)$ since

$$T_{1,k} = y'(x) - \frac{1}{3!} \frac{1}{a_{i,k}^{-1}} h_k^2 y'''(x)$$

$$- \frac{1}{4!} \frac{1}{a_{i,k}} \left(1 + \frac{1}{a_{i,k}}\right) h_k^3 y^{iv}(x) - \ldots$$

which involves a truncation error of order h_k^2.

If we also know $T_{0,k+2}$, we can generate $T_{1,k+1}$ using equation (2), and further, we can compute the extrapolated value

$$T_{2,k} = T_{1,k+1} + \frac{T_{1,k+1} - T_{1,k}}{a_{2,k}^{-1}}$$

where

$$a_{2,k} = \left(1 + \frac{2}{n-(k+1)}\right)$$

which involves a truncation error of order h_k^3.

Generally, the order of the truncation error is increased by 1 with each new extrapolation step; in particular, $T_{i,j}$ will involve a truncation error of order

$$h_j^{i+1}, \quad i = 0, \ldots, n-1, \quad j = 1, \ldots, n.$$

Figure 6 shows the arrangement of the T values in the triangular Romberg scheme. The T values are computed following the upward diagonals, using the general formula

$$T_{m,k-m} = T_{m-1,k-m+1} + \frac{T_{m-1,k-m+1} - T_{m-1,k-m}}{\frac{m}{n-k+1}} \qquad (3)$$

for $m = 1, \ldots, k-1$ for fixed k, $k=2, \ldots, n$

Truncation error		$O(h_k)$	$O(h_k^2)$	$O(h_k^3)$	$O(h_k^4)$	$O(h_k^5)$	$O(h_k^6)$	$O(h_k^7)$	$O(h_k^8)$	$O(h_k^9)$	$O(h_k^{10})$
Stepsize	k \ m	0	1	2	3	4	5	6	7	8	9
h_1	1	$T_{0,1}$	$T_{1,1}$	$T_{2,1}$	$T_{3,1}$	$T_{4,1}$	$T_{5,1}$	$T_{6,1}$	$T_{7,1}$	$T_{8,1}$	$T_{9,1}$
$h_2=0.9h_1$	2	$T_{0,2}$	$T_{1,2}$	$T_{2,2}$	$T_{3,2}$	$T_{4,2}$	$T_{5,2}$	$T_{6,2}$	$T_{7,2}$	$T_{8,2}$	
$h_3=0.8h_1$	3	$T_{0,3}$	$T_{1,3}$	$T_{2,3}$	$T_{3,3}$	$T_{4,3}$	$T_{5,3}$	$T_{6,3}$	$T_{7,3}$		
$h_4=0.7h_1$	4	$T_{0,4}$	$T_{1,4}$	$T_{2,4}$	$T_{3,4}$	$T_{4,4}$	$T_{5,4}$	$T_{6,4}$			
$h_5=0.6h_1$	5	$T_{0,5}$	$T_{1,5}$	$T_{2,5}$	$T_{3,5}$	$T_{4,5}$	$T_{5,5}$				
$h_6=0.5h_1$	6	$T_{0,6}$	$T_{1,6}$	$T_{2,6}$	$T_{3,6}$	$T_{4,6}$					
$h_7=0.4h_1$	7	$T_{0,7}$	$T_{1,7}$	$T_{2,7}$	$T_{3,7}$						
$h_8=0.3h_1$	8	$T_{0,8}$	$T_{1,8}$	$T_{2,8}$							
$h_9=0.2h_1$	9	$T_{0,9}$	$T_{1,9}$								
$h_{10}=0.1h_1$	10	$T_{0,10}$									

Figure 6. The triangular Romberg scheme of T values for the case $n=10$

Numerical experience shows that the accuracy of the results depends heavily on roundoff errors in

the one-sided divided differences $T_{0,k}$. Therefore, the choice of the absolutely smallest step size, h_n, is based on the following considerations.
Let:

$$v = \begin{cases} 1 \text{ in single-precision computation} \\ 3 \text{ in double-precision computation} \end{cases}$$

Set:

$$h_0 = \text{sgn}(h) \cdot \min\left(\frac{n}{2} \cdot 10^{-v}, |h|\right)$$

$$T = (y(x+h_0) - y(x))/h_0$$

T is an approximation to y'(x).

Assuming that the errors in the function values y(t) for $t_\epsilon [x, x+h]$ are bounded by

$$\epsilon = \begin{cases} |y(x)| \cdot 10^{-D} & \text{if } |y(x)| > 1 \\ 10^{-D} & \text{if } |y(x)| \le 1 \end{cases}$$

equation (1) shows that the roundoff error in the computation of $T_{0,n}$ is bounded by

$$R(T_{0,n}) = \frac{2\epsilon}{|h_n|} = \begin{cases} \frac{2|y(x)|\ 10^{-D}}{|h_n|} & \text{if } |y(x)| > 1 \\ 2\frac{10^{-D}}{|h_n|} & \text{if } |y(x)| \le 1 \end{cases}$$

where D is the number of significant digits in the floating-point representation of numbers. If we are also willing to tolerate a roundoff error

$$R'(T_{0,n}) = \begin{cases} 2T \cdot 10^{-D+v} & \text{if } |T| > 1 \\ 2 \cdot 10^{-D+v} & \text{if } |T| \le 1 \end{cases}$$

we must have $R(T_{0,n}) \le R'(T_{0,n})$, which is satisfied when

$$h_n = \frac{\max(1, |y(x)|)}{\max(1, |T|)} \cdot 10^{-v} \qquad (4)$$

Finally, we set

$$h_1 = \text{sgn}(h) \cdot \min(n \cdot |h_n|, |h|) \qquad (5)$$

guaranteeing that the evaluation of the function y = y(t) is restricted to the closed interval [x, x+h].

Programming Considerations:

Numerical experience shows that, because of increasing roundoff errors, it is generally fruitless to perform more than ten extrapolations. Thus, the subroutine uses n = 10, and it is therefore necessary only that y = y(t) be eleven-times differentiable, rather than analytic. It is easy to see that in the case n = 10, y = y(t) must be evaluated at twelve points in the closed interval [x, x+h].

As previously explained, the computation of the T values is performed along the upward diagonals of the triangular Romberg scheme. Therefore, only a one-dimensional internal storage vector, named AUX, with ten storage locations is necessary. Figure 7 shows the storage administration and the sequence of computations (numbers in parentheses).

AUX(1)	$T_{0,10}$(46)						
AUX(2)	$T_{0,9}$(37)	$T_{1,9}$(47)					
AUX(3)	$T_{0,8}$(29)	$T_{1,8}$(38)	$T_{2,8}$(48)				
AUX(4)	$T_{0,7}$(22)	$T_{1,7}$(30)	$T_{2,7}$(39)	...			
AUX(5)	$T_{0,6}$(16)	$T_{1,6}$(23)	$T_{2,6}$(31)	...			
AUX(6)	$T_{0,5}$(11)	$T_{1,5}$(17)	$T_{2,5}$(24)	...			
AUX(7)	$T_{0,4}$(7)	$T_{1,4}$(12)	$T_{2,4}$(18)	...			
AUX(8)	$T_{0,3}$(4)	$T_{1,3}$(8)	$T_{2,3}$(13)	...	$T_{7,3}$(53)		
AUX(9)	$T_{0,2}$(2)	$T_{1,2}$(5)	$T_{2,2}$(9)	...	$T_{7,2}$(44)	$T_{8,2}$(54)	
AUX(10)	$T_{0,1}$(1)	$T_{1,1}$(3)	$T_{2,1}$(6)	...	$T_{7,1}$(36)	$T_{8,1}$(45)	$T_{9,1}$(55)

Figure 7. Storage administration and sequence of calculations

Each extrapolation loop, the computation of the elements on an upward diagonal, is terminated as soon as the absolute values of the differences between adjacent diagonal elements stop decreasing, showing the influence of roundoff errors. The computed T value that differs least in absolute value from its immediately preceding diagonal neighbor is the desired value Z.

- Subroutine ALIM/ALIE

```
ALIM..
/*************************************************************   ********/
/*                                                                      */
/*      AITKEN SCHEME FOR INTERPOLATION OF FUNCTION VALUE               */
/*      FROM GIVEN MONOTONIC TABLE                                      */
/*                                                                      */
/************************************************************************/
   PROCEDURE (X,Y,DIM,ORDER,EPS,XVAL,YVAL),.
   DECLARE
        (DIM,I,J,K,N,II,JL,JR,JJL,JJR,DIMS,ORDER)
        BINARY FIXED,
        (X(*),Y(*),ARG(MIN(DIM,ORDER)),VAL(MIN(DIM,ORDER)),XVAL,
        YVAL,XST,DX,EPS,XS,Z1,Z2,D,DD,VALI,VALI1,A,DIST,DIST1,
        H,DELT1,DELT2,FACT,ARGI)
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/
 /*     BINARY FLOAT (53),           /*DOUBLE PRECISION VERSION  /*D*/
        (ERROR EXTERNAL,SW)
        CHARACTER (1),.
   SW   ='M',.                       /*MONOTONIC ARGUMENTS            */
   J    =1,.
   D    =1E75,.
        DO I = 1 TO DIM,.            /*COMPUTE STARTING SUBSCRIPT J */
        DD   =ABS(XVAL-X(I)),.
        IF DD LE D
        THEN DO,.
             D    =DD,.
             J    =I,.
             END,.
        END,.
   A,ARG(1)=X(J),.
   GO TO COM,.
ALIE..
/************************************************************************/
/*                                                                      */
/*      AITKEN SCHEME FOR INTERPOLATION OF FUNCTION VALUE               */
/*      FROM GIVEN EQUIDISTANT TABLE                                    */
/*                                                                      */
/************************************************************************/
   ENTRY (XST,DX,Y,DIM,ORDER,EPS,XVAL,YVAL),.
   SW   ='E',.
   Z1   =XST,.                       /*EQUIDISTANT ARGUMENTS          */
   Z2   =DX,.
   J    =1,.
   A,ARG(1)=Z1,.
   IF Z2= 0
   THEN GO TO COM,.
   J    =MAX(1,(XVAL-Z1)/Z2+1.5),.   /*COMPUTE STARTING SUBSCRIPT J */
   J    =MIN(DIM,J),.
   A,ARG(1)=Z1+FLOAT(J-1)*Z2,.
COM..
   ERROR='2',.
   XS   =XVAL,.
   DIMS =DIM,.
   N    =MIN(DIMS,ORDER),.
   DELT1,JL,JR=0,.
   VALI1,VAL(1)=Y(J),.
   FACT =XS-A,.
   DIST1=ABS(FACT),.
   N    =MAX(N,1),.
        DO I =2 TO N,.               /*TABLE SELECTION                */
        JJR  =J+JR,.                 /*TEST IF SUBSCRIPT IS GREATER   */
        IF JJR GE DIMS               /*THAN DIM OR LESS THAN ONE      */
        THEN GO TO LAB2,.
        JJL  =J-JL,.
        IF JJL LE 1
        THEN GO TO LAB3,.
        IF SW= 'E'
        THEN A     =-FACT*Z2,.       /*A=(ARG(I-1)-XVAL)*DX           */
        ELSE A     =ABS(X(JJR+1)-XS)
             -ABS(X(JJL-1)-XS),.
        IF A LE 0                    /*TEST IF THE NEXT STEP IS TO    */
        THEN GO TO LAB3,.            /*THE RIGHT OR TO THE LEFT       */
LAB2..                               /*STEP TO THE LEFT               */
        JL   =JL+1,.
        K    =J-JL,.
        GO TO CONT,.
LAB3..                               /*STEP TO THE RIGHT              */
        JR   =JR+1,.
        K    =J+JR,.
CONT..
        IF SW= 'E'
        THEN A     =Z1+FLOAT(K-1)*Z2,.
        ELSE A     =X(K),.
        FACT =XS-A,.
        IF SW='M'
        THEN DO,.
             DIST =ABS(FACT),.
             IF DIST LT DIST1
             THEN GO TO IDENT,.      /*ARGUMENTS NOT MONOTONIC        */
             DIST1=DIST,.
             END,.
        ARG(I)=A,.
        VALI,VAL(I)=Y(K),.
             DO II     =1 TO I-1,.   /*COMPUTE VAL(I)                 */
             ARGI =ARG(II),.
             H    =ARGI-A,.
             IF H =0
             THEN GO TO IDENT,.
             VALI =(VAL(II)*FACT-VALI
                  *(XS-ARGI))/H,.
             END,.
        DELT2=ABS(VALI-VALI1),.
        VALI1,VAL(I)=VALI,.
        IF I GT 2
        THEN DO,.
             IF DELT2 LE EPS         /*TEST ON ACCURACY               */
             THEN GO TO STOP,.
             IF I GE 5               /*SINGLE PRECISION VERSION  /*S*/
 /*          IF I GE 8               /*DOUBLE PRECISION VERSION  /*D*/
             THEN IF DELT2 GE DELT1  /*TEST ON OSCILLATION            */
             THEN GO TO OSCIL,.
             END,.
        DELT1=DELT2,.
        END,.                        /*END OF AITKEN-LOOP             */
   I    =N,.
   GO TO RETURN,.
OSCIL..
   ERROR='1',.
   GO TO IDENT1,.
IDENT..
   ERROR='3',.
IDENT1..
   I    =I-1,.
   GO TO RETURN,.
STOP..
   ERROR='C',.
RETURN..
   YVAL =VAL(I),.
   END,.                  /*END OF PROCEDURE ALI                */
```

Purpose:

ALIM interpolates the function value YVAL for a given argument value XVAL using a given table (X, Y) of argument and function values.

Usage:

CALL ALIM (X, Y, DIM, ORDER, EPS, XVAL, YVAL);

X - BINARY FLOAT [(53)]
Given vector of monotonic argument values.

Y - BINARY FLOAT [(53)]
Given vector of table-function values.

DIM - BINARY FIXED
Given dimension of vector X and Y.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y)

EPS - BINARY FLOAT [(53)]
Given constant used as upper bound for the absolute error.

XVAL - BINARY FLOAT [(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT [(53)]
Resultant interpolated function value.

Purpose:

ALIE interpolates the function value YVAL for a given argument value XVAL using XST, the starting value of the arguments, DX, the increment of the argument values, and the vector Y of function values.

Usage:

CALL ALIE (XST, DX, Y, DIM, ORDER, EPS, XVAL, YVAL);

XST - BINARY FLOAT [(53)]
Given starting value of arguments.

DX - BINARY FLOAT [(53)]
Given increment of argument values.

Y - BINARY FLOAT [(53)]
Given vector of table-function values.

DIM - BINARY FIXED
Given dimension of vector X and Y.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y).

EPS - BINARY FLOAT [(53)]
Given constant used as upper bound for the absolute error.

XVAL - BINARY FLOAT [(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT [(53)]
Resultant interpolated function value.

Remarks:

ERROR='0' - means required accuracy could be reached.

ERROR='1' - means required accuracy could not be reached because of rounding errors.

ERROR='2' - means accuracy could not be checked because MIN (DIM; ORDER) is less than 2, or the required accuracy could not be reached by means of the given table (X, Y). ORDER should be increased.

ERROR='3' - means two arguments in the argument vector X are identical, or the arguments are not monotonic.

In case ERROR='0' and ERROR='2' the last interpolated value for YVAL is returned. In case ERROR='1' and ERROR='3' the value prior to the last interpolated value for YVAL is returned. If, by a user error, ORDER is greater than DIM, the procedure selects only a maximum table of DIM points. In order to avoid errors, the user should check the correspondence between the selected table and its dimension by comparison of DIM and ORDER.

Method:

Interpolation is done by means of Aitken's scheme of Lagrange interpolation.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 49-50.

Mathematical Background:

Before starting Lagrange interpolation, a table (ARG, VAL) must be selected out of the given monotonic or equidistant table. This selection is done in two parts. In the first part, the subscript J of the argument next to the search argument XVAL is computed, using the following formulas:

In case of equidistant table -

$$\text{Subscript } J = \text{integer part of } \left(\frac{XVAL-XST}{DX} + 1.5\right)$$

In case of monotonic table -
Subscript J is searched for such that

$$\left| XVAL - X(J) \right| \leq \left| XVAL - X(I) \right|, \quad 1 \leq I \leq DIM$$

At each of the N = MIN (DIM, ORDER) interpolation steps, the procedure decides by comparison of distances whether the next step has to go to the right or to the left within the dimension of the given table.

It is assumed that $|X(I) - XVAL| > |X(J) - XVAL|$ for all $I > J$. Otherwise, ERROR='3' is returned.

y_i means VAL(i); x_i means ARG(i).
Using the formulas

$$y_{i,n} = \frac{y_i (x_n - XVAL) - y_n (x_1 - XVAL)}{x_n - x_1}$$

and

$$y_{1,2,\ldots,m,n} = y_{1,2,\ldots,m} (x_n - XVAL) - y_{1,2,\ldots,m-1,n} (x_m - XVAL) / (x_n - x_m)$$

it is possible to generate, by row, the following triangular Aitken scheme:

$$x_1 \; y_1$$

$$x_2 \; y_2 \; y_{1,2}$$

$$x_3 \; y_3 \; y_{1,3} \; y_{1,2,3}$$

$$\begin{array}{ccccccc} x_4 & y_4 & y_{1,4} & y_{1,2,4} & y_{1,2,3,4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n & y_n & y_{1,n} & y_{1,2,n} & y_{1,2,3,n} & \cdots & y_{1,2,3,\ldots,n} \end{array}$$

All resultant values of row I are stored in VAL(i):

VAL(i) = VAL(ii) * (XVAL - ARG(i))
- VAL(i) (XVAL - ARG(ii)) / (ARG(ii) - ARG(i))

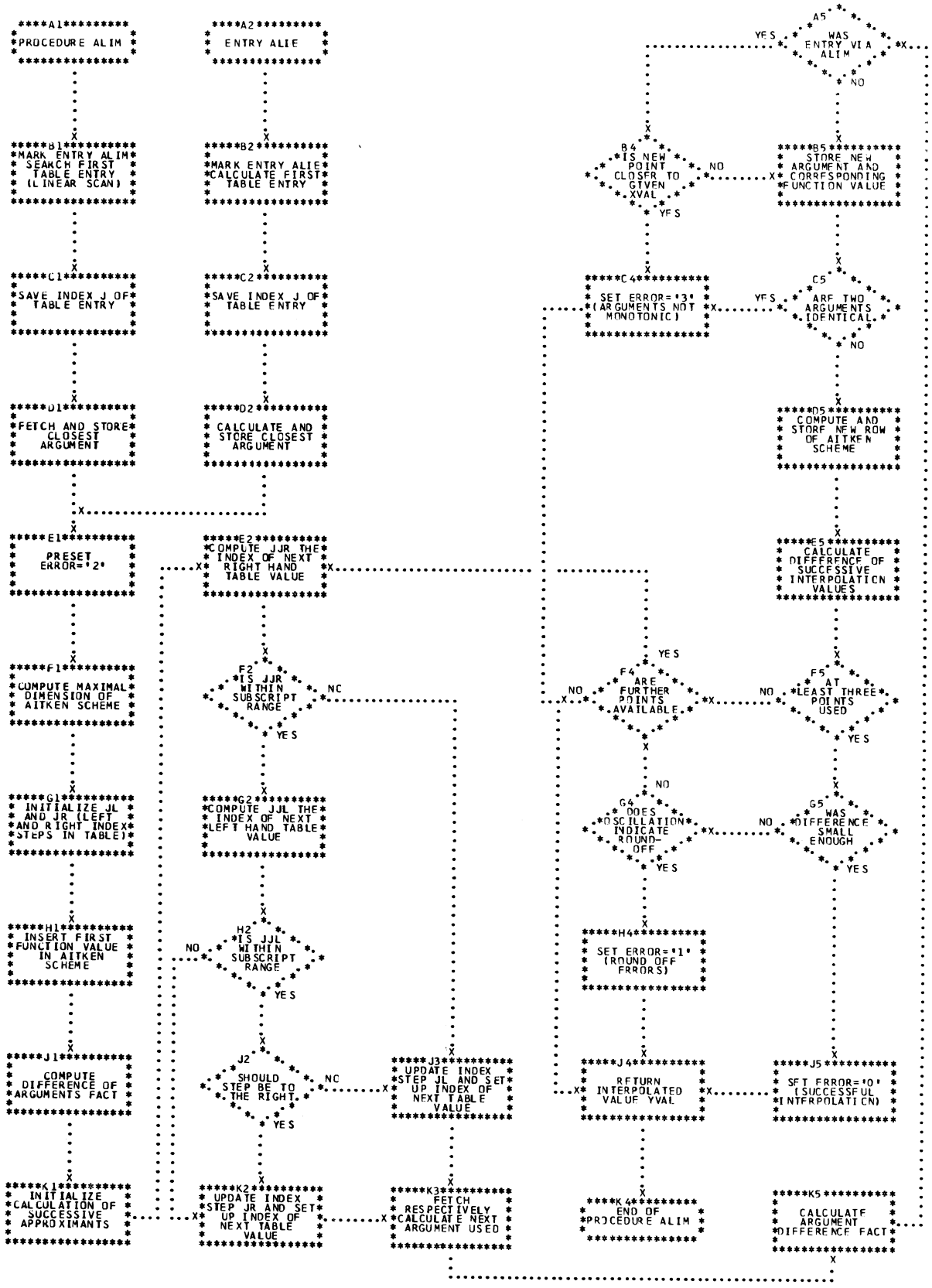
(ii = 1,2,..., i - 1) for i = 2, 3, ..., MIN(DIM, ORDER).

Programming Considerations:

The procedure stops under the following conditions:

1. If the difference | (VAL(i-1) - VAL (i))|, with i ≥ 3, of two successive values is less then a given tolerance EPS, ERROR='0' is returned.
2. If the absolute value of this difference stops diminishing, thus showing the influence of rounding errors, ERROR='1' is returned. (Test starts at step i = 5 for single precision, step i = 8 for double precision.)
3. If the procedure has worked through the whole triangular Aitken scheme, ERROR='2' is returned.
4. If the procedure discovers that the arguments are not monotonic or that two arguments are identical, ERROR='3' is returned.

PROCEDURE ALIM USES AITKEN'S SCHEME FOR INTERPOLATION IN GIVEN MONOTONIC TABLE
ENTRY ALIE INTERPOLATES IN EQUIDISTANT TABLE



- Subroutine AHIM/AHIE

```
AHIM..                                                                  AHI   10
/*********************************************************************/AHI   20
/*                                                                   */AHI   30
/*      AITKEN HERMITE SCHEME FOR INTERPOLATION OF FUNCTION VALUE    */AHI   40
/*      FROM GIVEN MONOTONIC TABLE                                   */AHI   50
/*                                                                   */AHI   60
/*********************************************************************/AHI   70
   PROCEDURE (X,Y,DY,DIM,ORDER,EPS,XVAL,YVAL),.                        AHI   80
   DECLARE                                                             AHI   90
        (DIM,DIMS,I,II,J,JJL,JJR,JL,JR,K,N,ORDER)                      AHI  100
        BINARY FIXED,                                                  AHI  110
        (X(*),Y(*),DY(*),ARG(MIN(DIM,ORDER)),VAL(2*MIN(DIM,ORDER)),    AHI  120
        EPS,XVAL,YVAL,XST,DX,A,D,DD,DELT1,DELT2,DIST,DIST1,H,          AHI  130
        H1,H2,VALI,VALII,VALJ,VALJL,XS,Y1,YS,Z1,Z2)                    AHI  140
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/AHI  150
 /*     BINARY FLOAT (53),            /*DOUBLE PRECISION VERSION  /*D*/AHI  160
        (ERROR EXTERNAL,SW)                                            AHI  170
        CHARACTER(1),.                                                 AHI  180
   SW   ='M',.                        /*MONOTONIC ARGUMENTS          */AHI  190
   J    =1,.                                                           AHI  200
   D    =1E75,.                                                        AHI  210
        DO I = 1 TO DIM,.             /*COMPUTE STARTING SUBSCRIPT J */AHI  220
        DD   =ABS(XVAL-X(I)),.                                         AHI  230
        IF DD LE D                                                     AHI  240
        THEN DO,.                                                      AHI  250
             D    =DD,.                                                AHI  260
             J    =I,.                                                 AHI  270
             END,.                                                     AHI  280
        END,.                                                          AHI  290
   ARG(1)=X(J),.                                                       AHI  300
   GO TO COM,.                                                         AHI  310
AHIE..                                                                 AHI  320
/*********************************************************************/AHI  330
/*                                                                   */AHI  340
/*      AITKEN HERMITE SCHEME FOR INTERPOLATION OF FUNCTION VALUE    */AHI  350
/*      FROM GIVEN EQUIDISTANT TABLE                                 */AHI  360
/*                                                                   */AHI  370
/*********************************************************************/AHI  380
   ENTRY (XST,DX,Y,DY,DIM,ORDER,EPS,XVAL,YVAL),.                       AHI  390
   SW   ='E',.                                                         AHI  400
   Z1   =XST,.                        /*EQUIDISTANT ARGUMENTS        */AHI  410
   Z2   =DX,.                                                          AHI  420
   J    =1,.                                                           AHI  430
   ARG(1)=Z1,.                                                         AHI  440
   IF Z2= 0                                                            AHI  450
   THEN GO TO COM,.                                                    AHI  460
   J    =MAX(1,(XVAL-Z1)/Z2+1.5),.    /*COMPUTE STARTING SUBSCRIPT J */AHI  470
   J    =MIN(DIM,J),.                                                  AHI  480
   ARG(1)=Z1+FLOAT(J-1)*Z2,.                                           AHI  490
COM..                                                                  AHI  500
   ERROR='2',.                                                         AHI  510
   XS   =XVAL,.                                                        AHI  520
   YS   =YVAL,.                                                        AHI  530
   DIMS =DIM,.                                                         AHI  540
   N    =MIN(DIMS,ORDER),.                                             AHI  550
   JL,JR=0,.                                                           AHI  560
   VALI,VAL(1)=Y(J),.                                                  AHI  570
   VALJ,VAL(2)=DY(J),.                                                 AHI  580
   H2   =XS-ARG(1),.                                                   AHI  590
   DIST1=ABS(H2),.                                                     AHI  600
   IF N LE 1                                                           AHI  610
   THEN DO,.                                                           AHI  620
        IF N = 1                                                       AHI  630
        THEN VAL(1)=VAL(I)+VAL(J)*H2,.                                 AHI  640
        ELSE VAL(1)=YS,.                                               AHI  650
        GO TO RETURN,.                                                 AHI  660
        END,.                                                          AHI  670
        DO I =2 TO N,.                /*TABLE SELECTION              */AHI  680
        JJR  =J+JR,.                                                   AHI  690
        IF JJR GE DIMS                                                 AHI  700
        THEN GO TO LAB2,.                                              AHI  710
        JJL  =J-JL,.                                                   AHI  720
        IF JJL LE 1                                                    AHI  730
        THEN GO TO LAB3,.                                              AHI  740
        IF SW= 'E'                                                     AHI  750
        THEN A    =(ARG(I-1)-XS)*Z2,. /*A=(ARG(I-1)-XVAL)*DX         */AHI  760
        ELSE A    =ABS(X(JJR+1)-XS)                                    AHI  770
             -ABS(X(JJL-1)-XS),.                                       AHI  780
        IF A LE C                                                      AHI  790
        THEN GO TO LAB3,.                                              AHI  800
LAB2..                                                                 AHI  810
        JL   =JL+1,.                  /*STEP TO THE LEFT             */AHI  820
        K    =J-JL,.                                                   AHI  830
        GO TO CONT,.                                                   AHI  840
LAB3..                                                                 AHI  850
        JR   =JR+1,.                  /*STEP TO THE RIGHT            */AHI  860
        K    =J+JR,.                                                   AHI  870
CONT..                                                                 AHI  880
        IF SW= 'E'                                                     AHI  890
        THEN A    =Z1+FLOAT(K-1)*Z2,.                                  AHI  900
        ELSE DO,.                                                      AHI  910
             A    =X(K),.                                              AHI  920
             DIST =ABS(XS-A),.                                         AHI  930
             IF DIST LT DIST1                                          AHI  940
             THEN GO TO IDENT,.       /*ARGUMENTS NOT MONOTONIC      */AHI  950
             DIST1=DIST,.                                              AHI  960
             END,.                                                     AHI  970
        II   =I+I,.                                                    AHI  980
        VALJ1=DY(K),.                 /*VAL(2*I)=DY(K)               */AHI  990
        VALI1=Y(K),.                  /*VAL(2*I-1)=Y(K)              */AHI 1000
        ARG(I)=A,.                                                     AHI 1010
        VAL(II-3)=VALI+VALJ*H2,.                                       AHI 1020
        H1   =H2,.                                                     AHI 1030
        H2   =XS-A,.                                                   AHI 1040
        H    =H1-H2,.                                                  AHI 1050
        IF H = 0                                                       AHI 1060
        THEN GO TO IDENT,.            /*TWO IDENTICAL ARGUMENTS      */AHI 1070
        VAL(II-2)=VALI+(VALI1                                          AHI 1080
             -VALI)*H1/H,.                                             AHI 1090
        VALI =VALI1,.                                                  AHI 1100
        VALJ =VALJ1,.                                                  AHI 1110
        END,.                         /*END OF TABLE SELECTION       */AHI 1120
   VAL(II-1)=VALI+VALJ*H2,.                                            AHI 1130
   DELT2=0,.                          /*PREPARE AITKEN-SCHEME        */AHI 1140
   Y1   =VAL(1),.                                                      AHI 1150
        DO I = 1 TO N+N-2,.           /*START AITKEN-LOOP            */AHI 1160
        YS   =Y1,.                                                     AHI 1170
        DELT1=DELT2,.                                                  AHI 1180
        H1   =ARG((I+3)/2),.                                           AHI 1190
        Y1   =VAL(I+1),.                                               AHI 1200
        DO K = I TO 1 BY -1,.                                          AHI 1210
        H2   =ARG((K+1)/2),.                                           AHI 1220
        H    =H2-H1,.                                                  AHI 1230
        IF H = 0                      /*COMPUTE DIAGONALS OF AITKEN- */AHI 1240
        THEN GO TO IDENT,.            /*SCHEME                       */AHI 1250
        Y1,VAL(K)=(VAL(K)*(XS-H1)                                      AHI 1260
             -Y1*(XS-H2))/H,.                                          AHI 1270
        END,.                                                          AHI 1280
        DELT2=ABS(YS-Y1),.            /*TEST ON ACCURACY             */AHI 1290
        IF DELT2 LE EPS                                                AHI 1300
        THEN GO TO STOP,.                                              AHI 1310
        IF I GE 5                     /*SINGLE PRECISION VERSION  /*S*/AHI 1320
 /*     IF I GE 8                     /*DOUBLE PRECISION VERSION  /*D*/AHI 1330
        THEN IF DELT2 GE DELT1                                         AHI 1340
        THEN GO TO OSCIL,.                                             AHI 1350
        END,.                         /*END OF AITKEN-LOOP           */AHI 1360
   GO TO RETURN,.                                                      AHI 1370
OSCIL..                               /*DELT2 STARTS OSCILLATING     */AHI 1380
   ERROR='1',.                                                         AHI 1390
   VAL(1)=YS,.                                                         AHI 1400
   GO TO RETURN,.                                                      AHI 1410
IDENT..                                                                AHI 1420
   VAL(1)=YS,.                                                         AHI 1430
   ERROR='3',.                                                         AHI 1440
   GO TO RETURN,.                                                      AHI 1450
STOP..                                                                 AHI 1460
   ERROR='0',.                                                         AHI 1470
RETURN..                                                               AHI 1480
   YVAL =VAL(1),.                                                      AHI 1490
   END,.                              /*END OF PROCEDURE AHI         */AHI 1500
```

Purpose:

AHIM interpolates the function value YVAL for a given argument value XVAL using a given table (X, Y, DY) of argument values, function values, and their derivatives.

Usage:

CALL AHIM(X, Y, DY, DIM, ORDER, EPS, XVAL, YVAL);

X - BINARY FLOAT[(53)]
Given vector of monotonic arguments.

Y - BINARY FLOAT[(53)]
Given vector of table-function values.

DY - BINARY FLOAT[(53)]
Given vector of derivative values.

DIM - BINARY FIXED
Given dimension of vector X, Y, DY.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y, DY).

EPS - BINARY FLOAT[(53)]
Given constant used as upper bound for the absolute error.

XVAL - BINARY FLOAT[(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT[(53)]
Resultant interpolated function value.

Purpose:

AHIE interpolates the function value YVAL for a given argument value XVAL using XST, the starting value of the argument, DX, the increment of the argument values, vector Y of the function values, and vector DY of the function derivative values.

Usage:

CALL AHIE (XST, DX, Y, DY, DIM, ORDER, EPS, XVAL, YVAL);

XST - BINARY FLOAT [(53)]
Given starting value of the arguments.

DX - BINARY FLOAT [(53)]
Given increment of the argument values.

Y - BINARY FLOAT [(53)]
Given vector of table-function values.

DY - BINARY FLOAT [(53)]
Given vector of function derivative values.

DIM - BINARY FIXED
Given dimension of the vector X, Y, DY.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y, DY).

EPS - BINARY FLOAT [(53)]
Given constant used as the upper bound for the absolute error.

XVAL - BINARY FLOAT [(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT [(53)]
Resultant interpolated function value.

Remarks:

ERROR='0' means required accuracy could be reached.

ERROR='1' means required accuracy could not be reached because of rounding errors.

ERROR='2' means accuracy could not be checked because MIN(DIM, ORDER) is less than 2, or the required accuracy could not be reached by means of the given table (X, Y, DY). ORDER should be increased.

ERROR='3' means two arguments in argument vector X are identical or the arguments are not monotonic.

In the case ERROR='0' and ERROR='2' the last interpolated value of YVAL is returned. The value prior to the last interpolated value for YVAL is returned.

If, by a user error, ORDER is greater than DIM, the procedure selects only a maximum table of DIM points. In order to avoid errors, the user should check the correspondence between the selected table and its discussion by comparison of DIM and ORDER.

Method:

Interpolation is done by means of Aitken's scheme of Hermite interpolation.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, 11. 314-317.

Gershinsky and Levine, "Aitken-Hermite Interpolation" JACM, vol. 11, issue 3 (1964), pp. 352-356.

Mathematical Background:

Before starting Hermite interpolation, a table (ARG, VAL) must be selected out of the given monotonic or equidistant table. This selection is done in two parts. In the first part, the subscript J of the argument next to the search argument XVAL is computed, using the following formulas:

In case of the equidistant table -

Subscript J = the integer part of

$$\left(\frac{XVAL-XST}{DX} + 1.5\right)$$

In case of the monotonic table -

Subscript J is searched for such that

$$\left|XVAL - X(J)\right| \leq \left|XVAL - X(I)\right|, \quad 1 \leq I \leq DIM$$

At each of the N = MIN(DIM, ORDER) selection steps, the procedure decides, by comparison of distances, whether the next step in vector X has to go to the right or to the left within the dimension of the given table, and replaces the components of vector VAL (that is, function and derivative values) by interpolation values Z_i of the first order (see Figure 8, third column). This is done by the following formulas:

$$VAL(i) = y_i + VAL(i+1) \cdot H1 \quad (i=1,3,\ldots,2n-1)$$

$$VAL(i+1) = y_i + (VAL(i+2) - y) \cdot \frac{H1}{H1-H2} \quad (i=1,3,\ldots,2n-3)$$

with

$$n = MIN(DIM, ORDER), \quad y_i = VAL(i)$$

H1 = XVAL - ARG(j-1), H2 = XVAL - ARG(j)

and

$$j = \frac{i+1}{2} + 1$$

Now it is possible to generate successively the upward diagonals of the triangular Aitken scheme, using the following formulas:

$$z_{1,2} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_1 & x_1 - XVAL \\ z_2 & x_2 - XVAL \end{vmatrix}$$

$$z_{2,3} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_2 & x_1 - XVAL \\ z_3 & x_2 - XVAL \end{vmatrix}$$

$$z_{1,2,3} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_{1,2} & x_1 - XVAL \\ z_{2,3} & x_2 - XVAL \end{vmatrix}$$

$$z_{3,4} = \frac{1}{x_3 - x_2} \cdot \begin{vmatrix} z_3 & x_2 - XVAL \\ z_4 & x_3 - XVAL \end{vmatrix}$$

with

x_i = ARG (i).

All resultant values of an upward diagonal can be stored in positions of vector VAL with decreasing subscripts: VAL(k) =

$$\frac{VAL(k) \cdot (XVAL - H1) - VAL(k+1) \cdot (XVAL - ARG(l))}{ARG(l) - H1}$$

for

$j = 1, 2, \ldots, i,$

where

$$k = i-j+1, \quad m = \left[\frac{i+3}{2}\right],$$

$$l = \left[\frac{k+1}{2}\right]$$

and H1 = ARG (m)

for i = 1, 2, ... , 2n-2.

ARG(1) = x_1	VAL(1) = y_1	VAL(1) = z_1	$z_{1,2}$	$z_{1,2,3}$	$z_{1,2,3,4}$ ..
	VAL(2) = y'_1	VAL(2) = z_2	$z_{2,3}$	$z_{2,3,4}$	.
ARG(2) = x_2	VAL(3) = y_2	VAL(3) = z_3	$z_{3,4}$	$z_{3,4,5}$	.
.	VAL(4) = y'_2	VAL(4) = z_4	.		
.	.	.	.		
.	.	.	.		
.	.	.	.		
.	.	.	.		
.	.	.	.		
ARG(n) = x_n	VAL(2n-1) = y_n	VAL(2n-1)			
	VAL(2n) = y'_n	= z_{2n-1}			

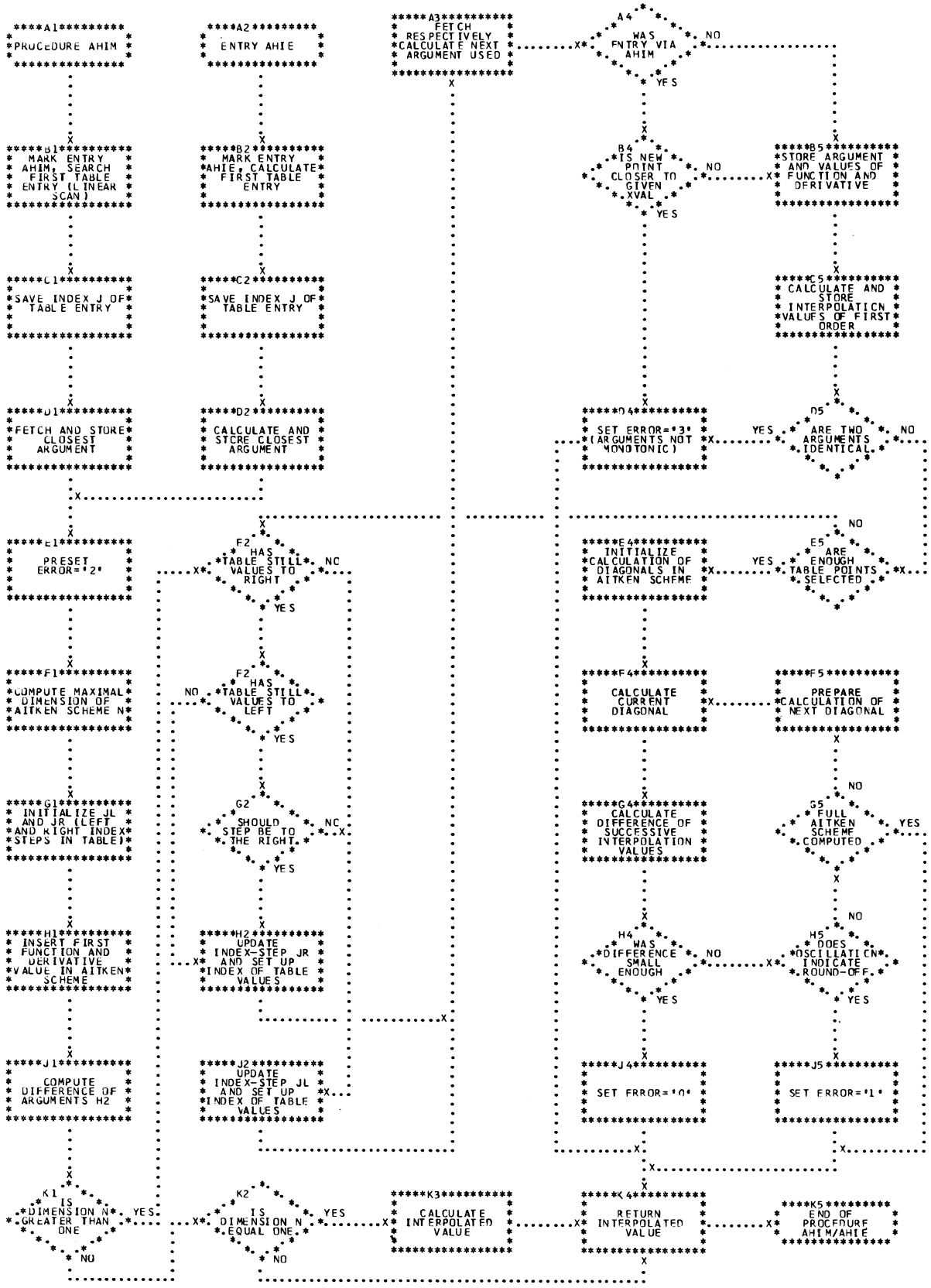
Figure 8. Triangular scheme for Aitken-Hermite interpolation

Programming Considerations

The procedure stops under the following conditions:

1. If the absolute value of the difference between two successive interpolated values VAL(1) is less than a given tolerance EPS, ERROR='0' is returned.
2. If the absolute value of this difference stops diminishing (thus showing the influence of rounding errors), ERROR='1' is returned. (Test starts at step i = 5 for single precision, i = 8 for double precision.)
3. If the procedure has worked through the whole triangular scheme, ERROR='2' is returned (see "Remarks", above).
4. If the procedure discovers two table points with identical arguments or the arguments are not monotonic, ERROR='3' is returned.

PROCEDURE AHIM USES AITKEN-HERMITE SCHEME FOR INTERPOLATION IN GIVEN MONOTONIC TABLE
ENTRY AHIE INTERPOLATES IN EQUIDISTANT TABLE



• Subroutine ACFM/ACFE

```
ACFM..
/************************************************************************/
/*                                                                      */
/*      CONTINUED FRACTION SCHEME FOR INTERPOLATION OF FUNCTION VALUE*/
/*      FROM GIVEN MONOTONIC TABLE                                      */
/*                                                                      */
/************************************************************************/
   PROCEDURE (X,Y,DIM,ORDER,EPS,XVAL,YVAL),.
   DECLARE
        (DIM,I,J,K,N,II,III,JL,JR,JJL,JJR,DIMS,ORDER)
        BINARY FIXED,
        (X(*),Y(*),ARG(MIN(DIM,ORDER)),VAL(MIN(DIM,ORDER)),XVAL,A1,
        YVAL,XST,DX,EPS,XS,Z1,Z2,D,DD,VALI,ARGI,A,DIST,DIST1,H,DELT1,
        DELT2,ARGJ,P1,P2,P3,Q1,Q2,Q3,ZS,YS,ARGI1,VALI1,EPS1)
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/
 /*     BINARY FLOAT (53),             /*DOUBLE PRECISION VERSION  /*D*/
        (ERROR EXTERNAL,SW)
        CHARACTER (1),.
   SW   ='M',.                         /*MONOTONIC ARGUMENTS           */
   J    =1,.
   D    =1E75,.
        DO I = 1 TO DIM,.
        DD   =ABS(XVAL-X(I)),.
        IF DD LE D
        THEN DO,.
             D    =DD,.
             J    =I,.
             END,.
        END,.
   ARGI,ARG(1)=X(J),.
   GO TO COM,.
ACFE..
/************************************************************************/
/*                                                                      */
/*      CONTINUED FRACTION SCHEME FOR INTERPOLATION OF FUNCTION VALUE*/
/*      FROM GIVEN EQUIDISTANT TABLE                                    */
/*                                                                      */
/************************************************************************/
   ENTRY (XST,DX,Y,DIM,ORDER,EPS,XVAL,YVAL),.
   SW   ='E',.
   Z1   =XST,.
   Z2   =DX,.
   J    =1,.
   ARGI,ARG(1)=Z1,.
   IF Z2= 0
   THEN GO TO COM,.
   J    =MAX(1,(XVAL-Z1)/Z2+1.5),.     /*COMPUTE STARTING SUBSCRIPT J */
   J    =MIN(DIM,J),.
   ARGI,ARG(1)=Z1+FLOAT(J-1)*Z2,.
COM..
   EPS1 =1E-6,.                        /*SINGLE PRECISION VERSION  /*S*/
 /*EPS1 =1E-13,.                       /*DOUBLE PRECISION VERSION  /*D*/
   ERROR='2',.
   XS   =XVAL,.
   DIMS =DIM,.
   N    =MIN(DIMS,ORDER),.
   Q2,DELT2,JL,JR=0,.
   P3,YS,VAL(1)=Y(J),.
   P2,Q3=1,.
   A1   =XS-ARGI,.
   DIST1=ABS(A1),.
        DO I = 2 TO N,.                /*START TABLE SELECTION         */
        JJR  =J+JR,.
        IF JJR GE DIMS                 /*TABLE SELECTION               */
        THEN GO TO LAB2,.
        JJL  =J-JL,.
        IF JJL LE 1
        THEN GO TO LAB3,.
        IF SW= 'E'
        THEN A     =-A1*Z2,.           /*A=(ARG(I-1)-XVAL)*DX          */
        ELSE A     =ABS(X(JJR+1)
             -XS)-ABS(X(JJL
             -1)-XS),.
        IF A LE 0
        THEN GO TO LAB3,.
LAB2..
        JL   =JL+1,.                   /*STEP TO THE LEFT              */
        K    =J-JL,.
        GO TO CONT,.
LAB3..
        JR   =JR+1,.                   /*STEP TO THE RIGHT             */
        K    =J+JR,.
CONT..
        IF SW= 'E'
        THEN A     =Z1+FLOAT(K-1)*Z2,.
        ELSE A     =X(K),.
        A1   =XS-A,.
        IF SW='M'
        THEN DO,.
             DIST =ABS(A1),.
             IF DIST LT DIST1
             THEN GO TO IDENT,.        /*ARGUMENTS NOT MONOTONIC       */
             DIST1=DIST,.
             END,.
        ARG(I)=A,.
        VAL(I)=Y(K),.
        END,.                          /*END OF TABLE SELECTION        */
   A1   =XS-ARG(1),.
        DO I = 2 TO N,.                /*START INTERPOLATION LOOP      */
        II   =0,.
        P1   =P2,.                     /*MOVE PARAMETERS P2,P3,Q2,Q3   */
        Q1   =Q2,.
        P2   =P3,.
        Q2   =Q3,.
        ZS   =YS,.
        DELT1=DELT2,.
        ARGI =ARG(I),.
        VALI =VAL(I),.
INVERT..                               /*COMPUTE INVERTED DIFFERENCES */
        ARGI1=ARGI,.
        VALI1=VALI,.
             DO J = 1 TO I-1,.
             ARGJ =ARG(J),.
             H    =VALI-VAL(J),.
             IF ABS(H) LE ABS(VALI)*EPS1
             THEN DO,.
                  IF ARGI= ARGJ        /*ERROR RETURNS,IF TWO          */
                  THEN GO TO IDENT,.   /*IDENTICAL ARGUMENTS EXIST     */
                  IF J GE I-1
```

```
                  THEN DO,.
                       II   =II+1,.    /*INTERCHANGE ROW I WITH        */
                       III  =I+II,.    /*ROW I+II                      */
                       IF III GT N
                       THEN GO TO RETURN,.
                       VALI =VAL(III),.
                       VAL(III)=VALI1,.
                       ARGI =ARG(III),.
                       ARG(III)=ARGI1,.
                       GO TO INVERT,.
                       END,.
                  VALI =1E75,.         /*VAL(I) = VAL(J), J LT I-1     */
                  END,.
             ELSE VALI =(ARGI          /*VAL(I) NE VAL(J)              */
                  -ARGJ)/H,.
             END,.
        P3   =VALI*P2+A1*P1,.          /*COMPUTE INVERTED DIFFERENCES */
        Q3   =VALI*Q2+A1*Q1,.          /*BY WALLIS-EULER SCHEME        */
        VAL(I)=VALI,.                  /*GENERATE NEW VAL(I),ARG(I)    */
        ARG(I)=ARGI,.
        A1   =XS-ARGI,.
        IF Q3= 0
        THEN YS    =1E75,.             /*Q3 = 0                        */
        ELSE YS    =P3/Q3,.            /*Q3 NE 0                       */
        DELT2=ABS(ZS-YS),.
        IF DELT2 LE EPS                /*TEST ON ACCURACY              */
        THEN GO TO STOP,.
        IF I GE 8                      /*SINGLE PRECISION VERSION  /*S*/
 /*     IF I GE 10                     /*DOUBLE PRECISION VERSION  /*D*/
        THEN IF DELT2 GE DELT1
        THEN GO TO OSCIL,.
        END,.                          /*END OF INTERPOLATION LOOP     */
   GO TO RETURN,.
IDENT..                                /*ARG(I) = ARG(J) FOR I NE J    */
   ERROR='3',.
   GO TO RETURN,.
OSCIL..                                /*DELT2 STARTS OSCILLATING      */
   YS   =ZS,.
   ERROR='1',.
   GO TO RETURN,.
STOP..
   ERROR='0',.
RETURN..
   YVAL =YS,.
   END,.                               /*END OF PROCEDURE ACFI         */
```

Purpose:

ACFM interpolates the function value YVAL for a given argument value XVAL using a given table (X, Y) of arguments and function values.

Usage:

CALL ACFM (X, Y, DIM, ORDER, EPS, XVAL, YVAL);

X - BINARY FLOAT [(53)]
Given vector of monotonic arguments.

Y - BINARY FLOAT [(53)]
Given vector table-function values.

DIM - BINARY FIXED
Given dimension of vector X and Y.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y).

EPS - BINARY FLOAT [(53)]
Given constant used as upper bound for the absolute error.

XVAL - BINARY FLOAT [(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT [(53)]
Resultant interpolated function value.

Purpose:

ACFE interpolates the function value YVAL for a given argument value XVAL using XST, the starting value of the arguments, DX, the increment of the argument values, and vector Y of function values.

Usage:

CALL ACFE (XST, DX, Y, DIM, ORDER, EPS, XVAL, YVAL);

XST - BINARY FLOAT [(53)]
Given the starting value of the arguments.

DX - BINARY FLOAT [(53)]
Given increment of the argument values.

Y - BINARY FLOAT [(53)]
Given vector of table-function values.

DIM - BINARY FIXED
Given dimension of vector X and Y.

ORDER - BINARY FIXED
Given number of points to be selected out of the given table (X, Y).

EPS - BINARY FLOAT [(53)]
Given constant used as upper bound for the absolute error.

XVAL - BINARY FLOAT [(53)]
Given argument to be interpolated.

YVAL - BINARY FLOAT [(53)]
Resultant interpolated function value.

Remarks:

See AHIM/AHIE, ALIM, ALIE

Method:

Interpolation is done by a continued fraction and inverted differences scheme.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 395-406.

Mathematical Background:

Before starting continued fraction interpolation, a table (ARG, VAL) must be selected out of the given monotonic or equidistant table. This selection is done before the continued fraction interpolation in the same way as in ALIM/ALIE.

It is assumed that $|x(i) - XVAL| > |x(j) - XVAL|$ for all $i > j$; otherwise, ERROR='3' is returned.

Using the following formulas:

$$y_{1,n} = \frac{x_n - x_1}{y_n - y_1}$$

$$y_{1,2,\ldots,m,n} = \frac{x_n - x_m}{y_{1,2,\ldots,m-1,n} - y_{1,2,\ldots,m}}$$

with x_i = ARG(i), y_i = VAL(i)

the triangular scheme of inverted differences shown in Figure 9 can be generated by row for the table (ARG, VAL). All resultant values of row i can be stored in VAL(i). Thus, it is possible to generate the downward diagonal of the inverted differences scheme in vector VAL:

$$VAL(i) = \frac{ARG(i) - ARG(j)}{VAL(i) - VAL(j)} (j = 1, 2, \ldots, i-1)$$

for i = 2, 3, ..., MIN(DIM, ORDER).

If for j = i-1, VAL(i) is equal to the infinity element, table point ARG(i), VAL(i) is interchanged with a table point ahead.

Now, after computation of each new component VAL(i), continued fraction interpolation generates the following parameters using Wallis-Euler formula:

$$P3 = VAL(i) \cdot P2 + (XVAL - ARG(i-1)) \cdot P1$$

$$Q3 = VAL(i) \cdot Q2 + (XVAL - ARG(i-1)) \cdot Q1$$

and YVAL = P3/Q3,

starting with P1 = 1, P2 = VAL(1), Q1 = 0, Q2 = 1. After each step, P1 = P2, P2 = P3, Q1 = Q2, Q2 = Q3 are set.

$ARG(1) = x_1$	$VAL(1) = y_1$			
$ARG(2) = x_2$	$VAL(2) = y_2$	$y_{1,2}$		
$ARG(3) = x_3$	$VAL(3) = y_3$	$y_{1,3}$	$y_{1,2,3}$	
.	.	.	.	
.	.	.	.	
.	.	.	.	
.	.	.	.	
.	.	.	.	
$ARG(n) = x_n$	$VAL(n) = y_n$	$y_{1,n}$	$y_{1,2,n}$	$y_{1,2,3,\ldots,n}$

Figure 9. Triangular scheme for fraction interpolation

Programming Considerations:

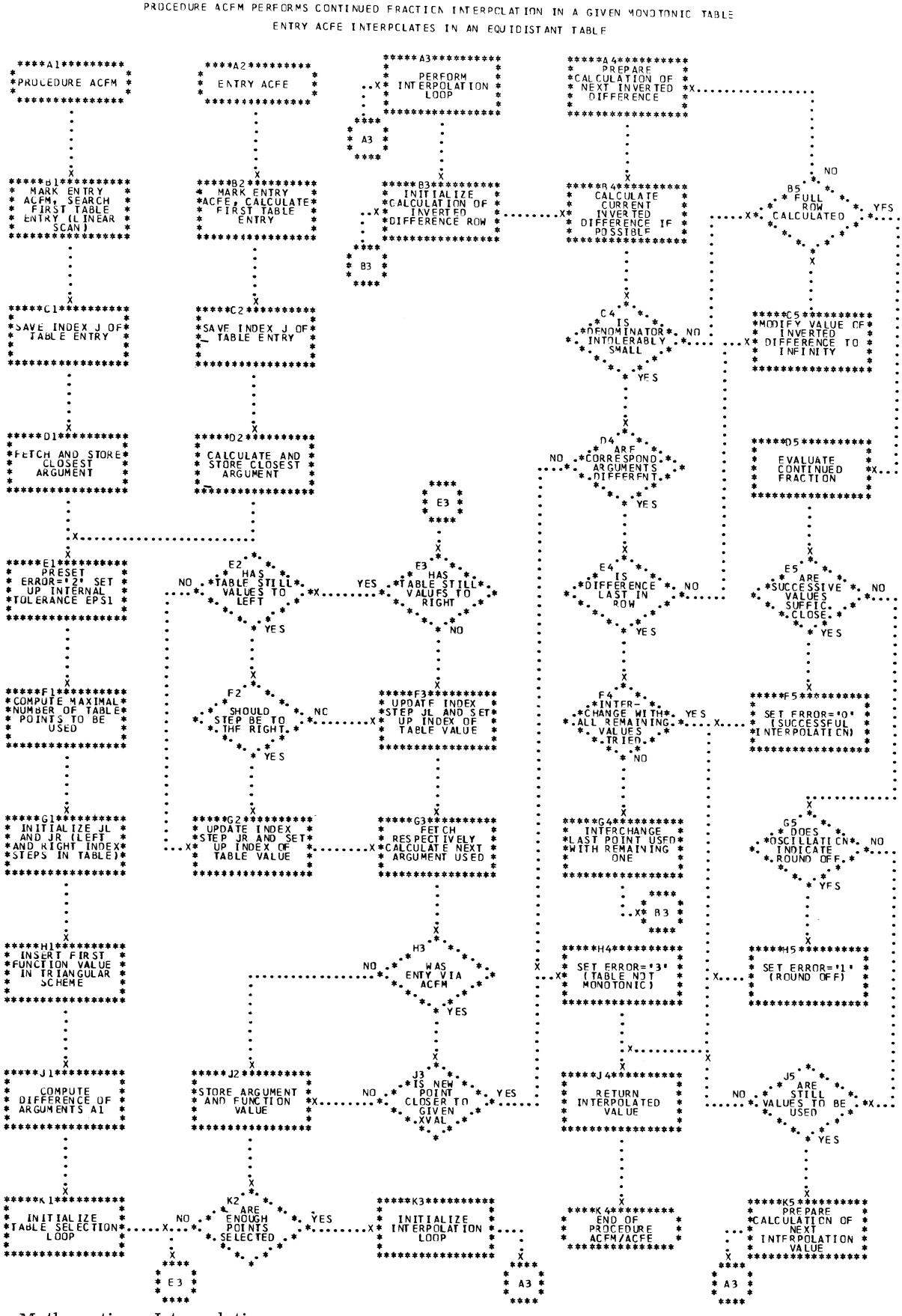
The procedure stops under the following conditions:

1. If the absolute value of the difference between two successive values of YVAL is less than a given tolerance EPS, ERROR='0' is returned.

2. If the absolute value of this difference starts oscillating, ERROR='1' is returned. (Test starts at step i = 8 for single precision, i = 10 for double precision.)

3. If the number of interpolation steps has become MIN(DIM, ORDER), ERROR='2' is returned.

4. If the procedure discovers that two table points have identical argument values or that the arguments are not monotonic, ERROR='3' is returned.



- Subroutine FFT

```
FFT..                                                                  FFT   10
/*********************************************************************/FFT   20
/*                                                                   */FFT   30
/*      FAST  FOURIER  TRANSFORM  FOR ANY ONE-DIMENSIONAL ARRAY      */FFT   40
/*                                                                   */FFT   50
/*********************************************************************/FFT   60
   PROCEDURE(A,M,OPT),.                                                FFT   70
   DECLARE                                                             FFT   80
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR      */FFT   90
        (OPT,COPT) CHARACTER(1),                                       FFT  100
        (DA,DB,DC,DH,DS,RI)                                            FFT  110
        BINARY FLOAT(53),                                              FFT  120
        (A(*),S(2**(M-2)+1),AAR,                                       FFT  130
        AAI,ABR,ABI,AW,CO,SI)                                          FFT  140
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/FFT  150
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/FFT  160
        (I,ID,IND,IR,IST,                                              FFT  170
        J,K,L,M,N,NH,NQ)                                               FFT  180
        BINARY FIXED,.                                                 FFT  190
   IF M LT 2                          /*TEST SPECIFIED DIMENSION M   */FFT  200
   THEN DO ,.                                                          FFT  210
        ERROR='P',.                   /*P MEANS WRONG PARAMETER      */FFT  220
        GO TO RETURN,.                                                 FFT  230
        END,.                                                          FFT  240
   ERROR='0',.                        /*PRESET ERROR INDICATOR       */FFT  250
   COPT =OPT,.                                                         FFT  260
   N    =2**M,.                       /*INITIALIZE PARAMETERS        */FFT  270
   NH   =N/10B,.                                                       FFT  280
   NQ   =N/100B+2,.                                                    FFT  290
   L    =NQ+1,.                                                        FFT  300
   RI   =3.141592653589793E+00/NH,.   /*RI MEANS  2*PI/N             */FFT  310
   DA,S(1)=0,.                        /*SET SINE FOR 0 AND PI/2      */FFT  320
   DB,S(NQ-1)=1,.                                                      FFT  330
   DS,S(2)=SIN(RI),.                                                   FFT  340
   DC   =COS(RI),.                    /*********************************/FFT  350
        DO I =3 TO N/1000B+1,.        /*CALCULATE SINE TERMS         */FFT  360
        RI   =DC*DB,.                 /*BETWEEN  0  AND  PI/2        */FFT  370
        S(L-I),DH=RI-DA,.             /*********************************/FFT  380
        DA   =DA,.                                                     FFT  390
        DB   =RI+DH,.                 /*CALCULATION IS DONE USING    */FFT  400
        S(I) =DB*DS,.                 /*DOUBLE PRECISION ARITHMETIC  */FFT  410
        END,.                                                          FFT  420
   IF COPT= '2'                       /*'2' MEANS CALCULATION OF     */FFT  430
   THEN GO TO REAL,.                  /*REAL FOURIER SERIES          */FFT  440
   IF COPT= '3'                       /*'3' MEANS CALCULATION OF     */FFT  450
   THEN GO TO INV,.                   /*COMPLEX FOURIER SERIES       */FFT  460
   AW   =1/NH,.                                                       FFT  470
        DO I =1 TO N,.                /*PREPARE VECTOR A FOR FINITE  */FFT  480
        A(I) =A(I)*AW,.               /*FOURIER TRANSFORM            */FFT  490
        END,.                         /*********************************/FFT  500
INV..                                 /*REORDER INITIAL TERMS A(I)   */FFT  510
   J    =1,.                          /*BY BIT REVERSAL TECHNIQUE    */FFT  520
        DO I =1 TO N BY 2,.           /*********************************/FFT  530
        IF J GT I                     /*IS BIT REVERSAL GREATER THAN */FFT  540
        THEN DO,.                     /*INIT. BINARY REPRESENTATION  */FFT  550
             AAR  =A(J),.                                              FFT  560
             AAI  =A(J+1),.           /*INTERCHANGE A(I) WITH A(J)   */FFT  570
             A(J) =A(I),.             /*AND  A(I+1)  WITH  A(J+1)    */FFT  580
             A(J+1)=A(I+1),.                                           FFT  590
             A(I) =AAR,.                                               FFT  600
             A(I+1)=AAI,.                                              FFT  610
             END,.                                                     FFT  620
        K    =NH,.                                                     FFT  630
             DO WHILE (J GT K),.      /*UPDATE  J  AND  K            */FFT  640
             J    =J-K,.                                               FFT  650
             K    =K/10B,.                                             FFT  660
             END,.                                                     FFT  670
        J    =J+K,.                   /*COMPUTE NEW BIT REVERSAL     */FFT  680
        END,.                                                          FFT  690
   IR,I =2,.                                                           FFT  700
   ID   =NH,.                         /*********************************/FFT  710
CPLX..                                /*COMPLEX FOURIER TRANSFORM    */FFT  720
                                      /*WITH  N/2  ELEMENTS          */FFT  730
   IST  =I+I,.                        /*********************************/FFT  740
   IND  =1,.                                                           FFT  750
        DO J =1 TO I BY 2,.                                            FFT  760
        SI   =-S(IND),.               /*STORE SINE VALUES IN SI      */FFT  770
        IF COPT= '3'                  /*CHANGE SIGN IN CASE OF       */FFT  780
        THEN SI   =-SI,.              /*FOURIER SERIES               */FFT  790
        CO   =S(NQ-IND),.             /*STORE COSINE VALUES IN CO    */FFT  800
        IF J GE IR                                                     FFT  810
        THEN DO,.                     /*MODIFY INDEX IND OF THE      */FFT  820
             IND  =IND-ID,.           /*SINE VECTOR S                */FFT  830
             CO   =-CO,.              /*COS(PI/2+B) = -SIN(B)        */FFT  840
             END,.                                                     FFT  850
        ELSE IND  =IND+ID,.                                            FFT  860
                                      /*EXECUTE TRANSFORMATION-LOOP  */FFT  870
             DO K =J TO N BY IST,.                                     FFT  880
             L    =K+I,.                                               FFT  890
             AAR  =CO*A(L)-SI*A(L+1),.                                 FFT  900
             AAI  =CO*A(L+1)+SI*A(L),.                                 FFT  910
             A(L) =A(K)-AAR,.         /*MODIFY AND RESTORE ELEMENTS  */FFT  920
             A(L+1)=A(K+1)-AAI,.                                       FFT  930
             A(K) =A(K)+AAR,.                                          FFT  940
             A(K+1)=A(K+1)+AAI,.                                       FFT  950
             END,.                                                     FFT  960
        END,.                                                          FFT  970
   IR   =I+1,.                        /*UPTATE PARAMETERS            */FFT  980
   I    =IST,.                                                         FFT  990
   ID   =ID/10B,.                                                      FFT 1000
   IF I LE NH                                                          FFT 1010
   THEN GO TO CPLX,.                  /*END OF OUTER LOOP            */FFT 1020
   IF COPT= '1'                       /*'1'  AND  '3'  MEAN COMPLEX  */FFT 1030
   THEN GO TO RETURN,.                /*FOURIER CALCULATIONS         */FFT 1040
   IF COPT= '3'                                                        FFT 1050
   THEN GO TO RETURN,.                /*********************************/FFT 1060
REAL..                                /*REAL VALUES FROM (FOR)       */FFT 1070
   I    =1,.                          /*COMPLEX FOURIER TRANSFORM    */FFT 1080
        DO K =3 TO NH-1 BY 2,.        /*********************************/FFT 1090
        J    =N-K+2,.                                                  FFT 1100
        AAR  =A(K)  +A(J),                                             FFT 1110
        AAI  =A(K+1)-A(J+1),.                                          FFT 1120
        ABR  =A(K+1)+A(J+1),.                                          FFT 1130
        ABI  =A(J)  -A(K),.                                            FFT 1140
        I    =I+1,.                                                    FFT 1150
        SI   =S(I),.                  /*STORE SINE AND COSINE        */FFT 1160
        CO   =S(NQ-I),.                                                FFT 1170
        AW   = ABR*CO+ABI*SI,.                                         FFT 1180
        ABI  =-ABI*CO+ABR*SI,.                                         FFT 1190
        A(K) =( AAR+AW )*1E-18,.                                       FFT 1200
        A(K+1)=(-AAI+ABI)*1E-18,.                                      FFT 1210
        A(J) =( AAR-AW )*1E-18,.                                       FFT 1220
        A(J+1)=( AAI+ABI)*1E-18,.                                      FFT 1230
        END,.                                                          FFT 1240
   AW   =A(1),.                                                        FFT 1250
   IF COPT= '2'                       /*PREPARE  A(1),A(2)  FOR      */FFT 1260
   THEN DO,.                          /*CALCULATION OF REAL FOURIER  */FFT 1270
        A(1) =(AW+A(N+1)),.           /*SERIES                       */FFT 1280
        A(2) =(AW-A(N+1)),.                                            FFT 1290
        COPT = '3',.                  /*CHANGE INTERNAL OPTION TERM  */FFT 1300
        GO TO INV,.                                                    FFT 1310
        END,.                                                          FFT 1320
   A(1) =(AW+A(2))*1E-18,.            /*CALCULATE VALUES             */FFT 1330
   A(N+1)=(AW-A(2))*1E-18,.           /*A(1),A(2),A(N+1),A(N+2)      */FFT 1340
   A(2) =0,.                                                           FFT 1350
   A(N+2)=0,.                                                          FFT 1360
RETURN..                                                               FFT 1370
   END,.                              /*END OF PROCEDURE FFT         */FFT 1380
```

Purpose:

FFT performs finite one-dimensional Fourier analysis and synthesis for a set of $N=2^M$ real data, or for a sequence of $\frac{N}{2} = 2^{M-1}$ complex data.

Depending on the character of the input parameter OPT, the following transformations can be done:

OPT	= '0'	real analysis
OPT	= '1'	complex analysis
OPT	= '2'	real synthesis
OPT	= '3'	complex synthesis

Usage:

CALL FFT (A, M, OPT);

A(2^M or 2^M+2) - BINARY FLOAT [(53)]
Given one-dimensional array with length

$$\left.\begin{matrix} N = 2^M \\ N+2=2^M+2 \end{matrix}\right\} \text{for} \left\{\begin{matrix} \text{complex} \\ \text{real} \end{matrix}\right\} \text{Fourier calculations.}$$

Resultant transform values are returned in the array A, replacing the input data.

The contents of the input and output array A depend on the option parameter OPT:

In cases OPT = '1' and OPT = '3' the complex data are located by pairs in N immediately adjacent storage locations. In the other cases the N function values are stored in N successive storage locations, while the Fourier coefficients a(n), b(n) need N+2 locations and they are stored as follows:

$$\frac{a_0}{2},\ b_0 = 0,\ a_1,\ b_1,\ a_2,\ b_2,\ \ldots,\ \frac{a_N}{2}-1,\ \frac{b_N}{2}-1,\ \frac{\frac{a_N}{2}}{2},\ \frac{b_N}{2} = 0$$

M - BINARY FIXED
Given integer that determines the size of vector A.
The size of A is $\left\{\begin{matrix}2^M \\ 2^M+2\end{matrix}\right\}$ for $\left\{\begin{matrix}\text{complex} \\ \text{real}\end{matrix}\right\}$ Fourier calculations.

OPT - CHARACTER(1)
Given option parameter for selection of operation (see "Purpose").

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='P' means error in specified parameter -- for example, M < 2. Any value of OPT different from '1', '2', '3' is treated as if it were '0'. The integer N in the given formulas (see "Purpose") must be a power of two:

$$N = 2^M$$

FFT is restricted to one-dimensional Fourier transformations.

Another procedure, called FFTM, is available in SSP-PL/I which operates on multidimensional arrays.

For real and complex applications of FFT the following is true: A forward transform (Fourier analysis) followed by an inverse transform (Fourier synthesis) returns the original data (except for roundoff errors).

Method:

Calculations depending on the option parameter OPT are done using the Cooley-Tukey Fast Fourier Transform.

For reference see:

J. W. Cooley, P. A. W. Lewis, P. D. Welch, "The Fast Fourier Transform Algorithm and its Applications", IBM Research, RC 1743, February 9, 1967, pp. 15-33.

N. M. Brenner, "Three Fortran Programs that Perform the Cooley-Tukey Fourier Transform", Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Technical Note ESD-TR-67-462, 1967.

J. W. Cooley and J. W. Tukey, "An Algorithm for the Machine Calculation of Complex Fourier Series", Mathematics of Computations, vol. 19, 1965, pp. 297-301.

Mathematical Background:

Complex Fourier calculations

Let X(k), k = 0, 1, 2,..., N-1, be a sequence of $N = 2^M$ complex numbers. The finite Fourier transform of X(k) is defined as

$$A(n) = \frac{1}{N}\sum_{k=0}^{N-1} X(k) \cdot W_N^{-n\cdot k}$$

$$n = 0, 1, \ldots, N-1 \qquad (1)$$

where

$$W_N = \exp\left(\frac{2\pi i}{N}\right) \text{ and } i = \sqrt{-1}$$

Similarly, X(k) can be expressed as the finite Fourier series of A(n)

$$X(k) = \sum_{n=0}^{N-1} A(n) \cdot W_N^{n\cdot k} \qquad (2)$$

Since $N = 2^M$ we express X(k) as a function of the M arguments $k_{M-1}, k_{M-2} \cdots k_1, k_0$ of the binary representation of k:

$$k = k_{M-1} \cdot 2^{M-1} + k_{M-2} \cdot 2^{M-2}$$

$$+ \ldots k_1 \cdot 2 + k_0; \; k_v = 0 \text{ or } 1. \qquad (3)$$

Analogously, if

$$n = n_{M-1} \cdot 2^{M-1} + n_{M-2} \cdot 2^{M-2} + \ldots n_1 \cdot 2$$

$$+ n_0 ; \; n_v = 0 \text{ or } 1, \qquad (4)$$

then equation (2) can be written:

$$X(k_{M-1}, k_{M-2}, \ldots, k_1, k_0)$$

$$= \sum_{n_0=0}^{1} \sum_{n_1=0}^{1} \cdots \sum_{n_{M-1}=0}^{1} A(n_{M-1}, n_{M-2},$$

$$\ldots n_1, n_0) \cdot W_N^{k(n_{M-1} \cdot 2^{M-1}}$$

$$+ \ldots + n_1 \cdot 2 + n_0) \qquad (5)$$

Using $W_N^{2^M} = W_N^N = 1$, we have

$$W_N^{k \cdot n_{M-1} \cdot 2^{M-1}} = W_N^{k_0 \cdot n_{M-1} \cdot 2^{M-1}}$$

Therefore the innermost sum in equation (5) yields an array:

$$A_1(k_0, n_{M-2}, \ldots, n_1, n_0) =$$

$$\sum_{n_{M-1}=0}^{1} A(n_{M-1}, n_{M-2}, \ldots, n_1, n_0) \cdot W_N^{k_0 n_{M-1} \cdot 2^{M-1}}$$

Then, summing over n_{M-2} to get an array A_2 from A_1, and so on, leads to the general formula ($L = 1, 2, 3, \ldots, M$):

$$A_L(k_0, \ldots, k_{L-1}, n_{M-L-1}, \ldots, n_1, n_0)$$

$$= \sum_{n_{M-L}=0}^{1} A_{L-1}(k_0, \ldots, k_{L-2}, n_{M-L}, n_{M-L-1}, \ldots, n_1, n_0) \cdot W_N^{(k_{L-1} \cdot 2^{L-1} + \ldots + k_0) \cdot n_{M-L} \cdot 2^{M-L}}$$

The final array will be the desired X. The storage indexing convention used here is to let the M arguments of $A_L(k_0, \ldots, n_0)$ be the binary representation of the index of the storage location for $A_L(k_0, \ldots, n_0)$. In this way, each step of the algorithm involves fetching from two storage locations and returning results in the same two locations, thereby saving storage. However, the elements of the final array are in wrong order:

$$X(k_{M-1}, k_{M-2}, \ldots, k_1, k_0) = A_M(k_0, k_1, \ldots, k_{M-1})$$

Now we must reverse the order of the bits in the binary representation of k. FFT does the reordering on the initial array so that the result is in the correct order.

Real Fourier calculations

Given 2N real data Y(j), $j = 0, 1, 2, \ldots, 2N-1$. The coefficients of the trigonometric series

$$Y(j) = \frac{a(0)}{2} + \sum_{n=1}^{N-1} \left(a(n) \cdot \cos\frac{\pi n j}{N} + b(n) \cdot \sin\frac{\pi n j}{N}\right) + (-1)^j \frac{a(N)}{2}$$

can be derived from the N-point complex Fourier transform

$$A(n) = \frac{1}{N} \sum_{K=0}^{N-1} X(k) \cdot W_N^{-n \cdot k} \qquad n = 0, 1, 2, \ldots, N-1$$

where $X(k) = Y(2k) + iY(2k+1)$; $k = 0, 1, 2, \ldots, N-1$.

Let (the bar is conjugation):

$$2C(0) = \text{Re } A(0) + \text{Im } A(0)$$
$$2C(N) = \text{Re } A(0) - \text{Im } A(0)$$
$$2C(\tfrac{N}{2}) = \bar{A}(\tfrac{N}{2})$$

Calculate for $m = 1, 2, \ldots, \frac{N}{2} - 1$:

$$A_1(m) = \frac{1}{2}(A(m) + \bar{A}(N-m))$$

$$\bar{A}_2(N-m) = \frac{1}{2i}(A(m) - \bar{A}(N-m))$$

$$2C(m) = A_1(m) + \bar{A}_2(N-m) \cdot W_{2N}^{-m}$$

$$2C(N-m) = A_1(m) - \bar{A}_2(N-m) \cdot W_{2N}^{-m}$$

Now, identify the a(n), b(n) coefficients by means of the relations

$$a(0) = 2C(0)$$
$$a(N) = 2C(N)$$
$$a(n) = 2\text{Re}C(n)$$
$$b(n) = -2\,\text{Im}C(n) \qquad n = 1, 2, \ldots, N-1.$$

Note: To compute the 2N real Y(j) (Fourier synthesis) when the coefficients a(n) and b(n) are given, the process described above is applied in reverse order.

Programming Considerations:

FFT accepts input data stored according to option parameter OPT:

OPT = '1' or OPT = '3': any set of $\frac{N}{2} = 2^{M-1}$ complex values whose real and imaginary parts are located by pairs in N adjacent storage locations.

OPT = '2': the coefficients

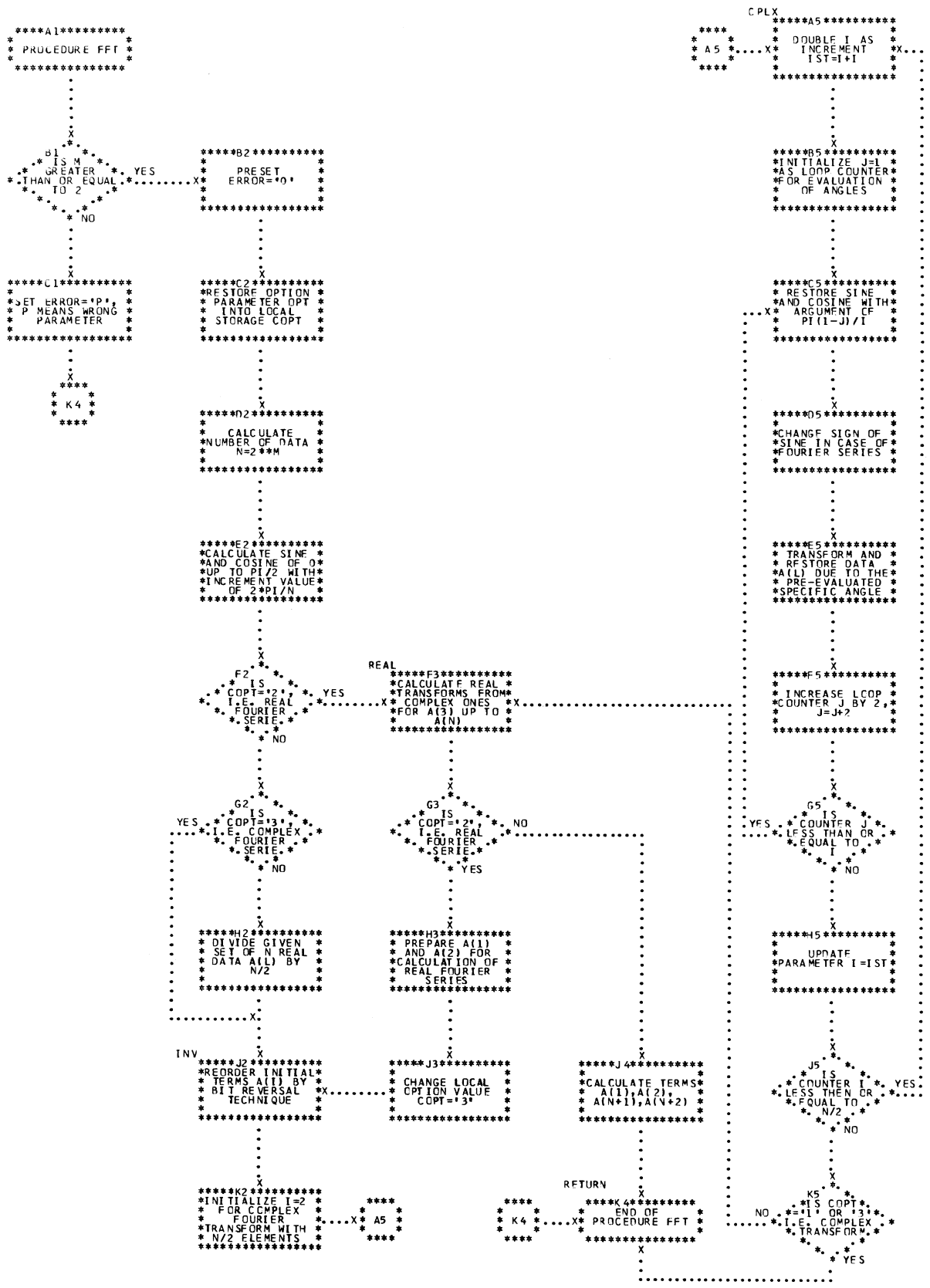
$$\frac{a_0}{2}, b_0 = 0, a_1, b_1, \ldots, a_{\frac{N}{2}-1}, b_{\frac{N}{2}-1}, a_{\frac{N}{2}}, b_{\frac{N}{2}} = 0$$

in N + 2 successive storage locations.

OPT = '0': N real elements in successive storage locations.

During calculation, input vector A is replaced by results depending on the character of parameter OPT. These results are stored in an analogous manner. For example, with OPT = '0', FFT calculates the N+2 Fourier coefficients a(n), b(n) and stores them into array A (with length N+2), overwriting the first N given real values.

PROCEDURE FFT PERFORMS FINITE, ONE-DIMENSIONAL FOURIER CALCULATIONS FOR A SET OF N=2**M REAL DATA A(L), L=1,2,...,N



- Subroutine FFTM

```
FFTM..                                                          FFTM  10
/*****************************************************************/FFTM  20
/*                                                               */FFTM  30
/*      FAST  FOURIER  TRANSFORM  FOR  MULTI-DIMENSIONAL  ARRAY  */FFTM  40
/*                                                               */FFTM  50
/*****************************************************************/FFTM  60
   PROCEDURE(A,M,NDIM,OPT),.                                    FFTM  70
   DECLARE                                                      FFTM  80
        ERROR CHARACTER(1),  /*EXTERNAL ERROR INDICATOR        */FFTM  90
        OPT CHARACTER(1),                                       FFTM 100
        (A(*),PI,RI,RTH,TR,T2R,T2I,                             FFTM 110
        T3R,T3I,T4R,T4I,U1R,U1I,U2R,                            FFTM 120
        U2I,U3R,U3I,U4R,U4I,WR,WI,                              FFTM 130
        W2R,W2I,W3R,W3I)                                        FFTM 140
        BINARY FLOAT,                /*SINGLE PRECISION VERSION  /*S*/FFTM 150
/*      BINARY FLOAT(53),            /*DOUBLE PRECISION VERSION  /*D*/FFTM 160
        (I,IND,J,JM,K,K2,K3,K4,KDIF,                            FFTM 170
        KINC,KM,KMIN,L,LJ,LMAX,M(*),                            FFTM 180
        MM,MMAX,N(NDIM),NA,NAD,NB,                              FFTM 190
        NBH,NDIM,NIN,NT)                                        FFTM 200
        BINARY FIXED,.                                          FFTM 210
   ERROR='P',.                  /*'P' MEANS WRONG PARAMETER     */FFTM 220
   IF NDIM LT 1                 /*TEST NUMBER OF DIMENSIONS     */FFTM 230
   THEN GO TO RETURN,.                                          FFTM 240
   NT   =2,.                                                    FFTM 250
        DO I =1 TO NDIM,.                                       FFTM 260
        N(I),K=10**M(I),.       /*COMPUTE AND TEST DIMENSION    */FFTM 270
        IF K LT 1                                               FFTM 280
        THEN GO TO RETURN,.     /*CALCULATE TOTAL NUMBER OF     */FFTM 290
        NT   =NT*K,.            /*ELEMENTS                      */FFTM 300
        END,.                                                   FFTM 310
                                /*COMPUTE  PI  AND  RTH         */FFTM 320
   PI   =3.14159265358979E+00,.                                 FFTM 330
   RTH  =7.07106781186547E-01,. /*RTH MEANS  SQRT(2)/2          */FFTM 340
   NA   =2,.                    /*****************************/FFTM 350
        DO IND =NDIM TO 1 BY -1,. /*LOOP FOR EACH DIMENSION     */FFTM 360
        NIN  =N(IND),.          /*****************************/FFTM 370
        NB   =NA*NIN,.                                          FFTM 380
        IF NIN= 1                                               FFTM 390
        THEN GO TO MULTI,.                                      FFTM 400
        NBH  =NB/100,.                                          FFTM 410
        J    =1,.               /*****************************/FFTM 420
        DO I =1 TO NB BY NA,.   /*BIT REVERSAL TECHNIQUE       */FFTM 430
        IF J LE I               /*****************************/FFTM 440
        THEN GO TO MOD1,.                                       FFTM 450
        KM   =I+NA-2,.                                          FFTM 460
        JM   =J-1,.                                             FFTM 470
             DO K =I TO KM BY 2,.                               FFTM 480
                  DO L =K TO NT BY NB,.                         FFTM 490
                  LJ   =L+JM,.                                  FFTM 500
                  WR   =A(L),.  /*INTERCHANGE  A(L)  WITH  A(LJ)  */FFTM 510
                  WI   =A(L+1),. /*AND  A(L+1)  WITH  A(LJ+1)   */FFTM 520
                  A(L) =A(LJ),.                                 FFTM 530
                  A(L+1)=A(LJ+1),.                              FFTM 540
                  A(LJ)=WR,.                                    FFTM 550
                  A(LJ+1)=WI,.                                  FFTM 560
                  END,.                                         FFTM 570
             END,.                                              FFTM 580
MOD1..                          /*MODIFY PARAMETER  J  AND  K   */FFTM 590
        K    =NBH,.                                             FFTM 600
        DO WHILE (J GT K),.                                     FFTM 610
        J    =J-K,.                                             FFTM 620
        K    =K/100,.                                           FFTM 630
        END,.                                                   FFTM 640
        J    =J+K,.             /*COMPUTE NEW BIT REVERSAL      */FFTM 650
        END,.                                                   FFTM 660
   NAD  =NA+NA,.                                                FFTM 670
ODD..                           /*TEST FOR ODD M(IND)           */FFTM 680
   IF NIN LT 2                                                  FFTM 690
   THEN GO TO LEN4,.            /*M(IND) IS EVEN,    NIN = 1    */FFTM 700
   IF NIN= 2                                                    FFTM 710
   THEN GO TO LEN2,.            /*M(IND) IS ODD,     NIN = 2    */FFTM 720
   NIN  =NIN/100,.                                              FFTM 730
   GO TO ODD,.                  /*****************************/FFTM 740
LEN2..                          /*TRANSFORM WITH LENGTH 2       */FFTM 750
        DO I =1 TO NA BY 2,.    /*****************************/FFTM 760
             DO K =I TO NT BY NAD,.                             FFTM 770
             L    =K+NA,.                                       FFTM 780
             WR   =A(L),.                                       FFTM 790
             WI   =A(L+1),.                                     FFTM 800
             A(L) =A(K)-WR,.    /*MODIFY AND RESTORE ELEMENTS   */FFTM 810
             A(L+1)=A(K+1)-WI,.                                 FFTM 820
             A(K) =A(K)+WR,.                                    FFTM 830
             A(K+1)=A(K+1)+WI,.                                 FFTM 840
             END,.                                              FFTM 850
        END,.                   /*****************************/FFTM 860
LEN4..                          /*FAST  FOURIER  TRANSFORMS     */FFTM 870
   MMAX =NA,.                   /*WITH  LENGTH  4               */FFTM 880
MAIN..                          /*****************************/FFTM 890
   IF MMAX GE NBH                                               FFTM 900
   THEN GO TO MULTI,.                                           FFTM 910
   MM   =MMAX+MMAX,.                                            FFTM 920
   LMAX =MAX(NAD,MMAX/10B),.                                    FFTM 930
        DO I =NA TO LMAX BY NAD,./*EXECUTE LOOP FOR CALCULATION */FFTM 940
        J    =I,.               /*OF ANGLES FOR SPECIFIC MMAX   */FFTM 950
        IF MMAX LE NA                                           FFTM 960
        THEN GO TO INITL,.                                      FFTM 970
        PI   =-PI*J/MM,.                                        FFTM 980
        IF OPT='1'                                              FFTM 990
        THEN PI   =-RI,.        /*CHANGE SIGN FOR CALCULATION   */FFTM1000
        WR   =COS(RI),.         /*OF FOURIER SERIES             */FFTM1010
        WI   =SIN(RI),.                                         FFTM1020
DOUBLE..                                                        FFTM1030
        W2R  =WR*WR-WI*WI,.     /*COMPUTE COSINE AND SINE       */FFTM1040
        W2I  =WR*WI*1.0E+00,.   /*FOR   2*RI   AND   3*RI       */FFTM1050
        W3R  =W2R*WR-W2I*WI,.                                   FFTM1060
        W3I  =W2R*WI+W2I*WR,.                                   FFTM1070
INITL..                         /*INITIALIZE L AS INDEX FOR     */FFTM1080
        L    =I,.               /*MULTIDIMENSIONAL CALCULATIONS*/FFTM1090
STRT..                                                          FFTM1100
        IF MMAX= NA             /*COMPUTE START VALUE KMIN FOR  */FFTM1110
        THEN KMIN =L,.          /*TRANSFORMATION LOOP           */FFTM1120
        ELSE KMIN =L+NIN*J,.                                    FFTM1130
        KDIF =NIN*MMAX,.                                        FFTM1140
INCR..                          /*COMPUTE INCREMENT FOR THE     */FFTM1150
        KINC =KDIF*100,.        /*TRANSFORMATION LOOP           */FFTM1160
             DO K =KMIN TO NT BY KINC,.                         FFTM1170
             K2   =K +KDIF,.                                    FFTM1180
             K3   =K2+KDIF,.    /*K,K2,K3,K4  ARE PARAMETERS    */FFTM1190
             K4   =K3+KDIF,.    /*FOR OPERATION WITH LENGTH 4   */FFTM1200
             IF MMAX= NA        /*WITHOUT MULTIPLICATIONS       */FFTM1210
             THEN DO,.                                          FFTM1220
                  U1R  =A(K)   +A(K2),.                         FFTM1230
                  U1I  =A(K+1) +A(K2+1),.                       FFTM1240
                  U2R  =A(K3)  +A(K4),.                         FFTM1250
                  U2I  =A(K3+1)+A(K4+1),.                       FFTM1260
                  U3R  =A(K)   -A(K2),.                         FFTM1270
                  U3I  =A(K+1) -A(K2+1),.                       FFTM1280
                  U4R  =A(K3+1)-A(K4+1),.                       FFTM1290
                  U4I  =A(K4)  -A(K3),.                         FFTM1300
                  END,.                                         FFTM1310
             ELSE DO,.                                          FFTM1320
                  T2R  =W2R*A(K2)  -W2I*A(K2+1),.               FFTM1330
                  T2I  =W2R*A(K2+1)+W2I*A(K2),.                 FFTM1340
                  T3R  =WR *A(K3)  -WI *A(K3+1),.               FFTM1350
                  T3I  =WR *A(K3+1)+WI *A(K3),.                 FFTM1360
                  T4R  =W3R*A(K4)  -W3I*A(K4+1),.               FFTM1370
                  T4I  =W3R*A(K4+1)+W3I*A(K4),.                 FFTM1380
                  U1R  =A(K)  +T2R,.                            FFTM1390
                  U1I  =A(K+1)+T2I,.                            FFTM1400
                  U2R  =T3R   +T4R,.                            FFTM1410
                  U2I  =T3I   +T4I,.                            FFTM1420
                  U3R  =A(K)  -T2R,.                            FFTM1430
                  U3I  =A(K+1)-T2I,.                            FFTM1440
                  U4R  =T3I   -T4I,.                            FFTM1450
                  U4I  =T4R   -T3R,.                            FFTM1460
                  END,.                                         FFTM1470
             IF OPT= '1'            /*IN CASE OF FOURIER SERIES  */FFTM1480
             THEN DO,.                                          FFTM1490
                  U4R  =-U4R,.                                  FFTM1500
                  U4I  =-U4I,.                                  FFTM1510
                  END,.                                         FFTM1520
             A(K) =U1R+U2R,.        /*COMPUTE AND STORE NEW VALUES */FFTM1530
             A(K+1)=U1I+U2I,.                                   FFTM1540
             A(K2)=U3R+U4R,.                                    FFTM1550
             A(K2+1)=U3I+U4I,.                                  FFTM1560
             A(K3)=U1R-U2R,.                                    FFTM1570
             A(K3+1)=U1I-U2I,.                                  FFTM1580
             A(K4)=U3R-U4R,.                                    FFTM1590
             A(K4+1)=U3I-U4I,.                                  FFTM1600
             END,.                                              FFTM1610
        KMIN =L+(KMIN-L)*100B,. /*UPDATE KMIN, KDIF AND IF NEC-*/FFTM1620
        KDIF =KINC,.            /*ESSARY REPEAT TRANSFORMATION  */FFTM1630
        IF KDIF LE NBH          /*LOOP IN ORDER TO GET FINAL    */FFTM1640
        THEN GO TO INCR,.       /*VALUES                        */FFTM1650
                                /*                              */FFTM1660
        L    =L+2,.             /*MODIFY L AND -IF NECESSARY-   */FFTM1670
        IF L LT NA              /*START ANOTHER TRANSFORM       */FFTM1680
        THEN GO TO STRT,.                                       FFTM1690
                                /*                              */FFTM1700
        J    =J+LMAX,.          /*MODIFY J AND -IF NECESSARY-   */FFTM1710
        IF J LE MMAX            /*THE ANGLE                     */FFTM1720
        THEN DO,.                                               FFTM1730
             TR   =WR,.         /*IF Z = COS(RI) + I*SIN(RI)    */FFTM1740
             WR   =(TR+WI)*RTH,. /*THEN Z IS SUBSTITUTED BY     */FFTM1750
             WI   =(WI-TR)*RTH,. /*Z  = Z * EXP(-PI/4 * I)      */FFTM1760
             IF OPT= '1'                                        FFTM1770
             THEN DO,.                                          FFTM1780
                  TR   =WR,.    /*Z IS SUBSTITUTED BY           */FFTM1790
                  WR   =-WI,.   /*Z  = Z * EXP(+PI/4 * I)       */FFTM1800
                  WI   =TR,.                                    FFTM1810
                  END,.                                         FFTM1820
             GO TO DOUBLE,.                                     FFTM1830
             END,.                                              FFTM1840
        END,.                                                   FFTM1850
   NIN  =3-NIN,.                /*UPDATE NIN AND DOUBLE MMAX    */FFTM1860
   MMAX =MM,.                                                   FFTM1870
   GO TO MAIN,.                                                 FFTM1880
MULTI..                                                         FFTM1890
   NA   =NB,.                                                   FFTM1900
   END,.                                                        FFTM1910
   ERROR='0',.                  /*SUCCESSFUL FOURIER TRANSFORM */FFTM1920
RETURN..                                                        FFTM1930
   END,.                        /*END OF PROCEDURE FFTM         */FFTM1940
```

Purpose:

FFTM performs finite, multidimensional Fourier forward or inverse transformations for complex arrays whose dimensions are powers of two.

Depending on the value of the input parameter OPT, the following transformations can be done:

OPT = '0' forward Fourier transform
OPT = '1' inverse Fourier transform

Usage:

CALL FFTM (A, M, NDIM, OPT);

A ($2^{1+M_1+M_2 \cdots M_{NDIM}}$) -

BINARY FLOAT [(53)]
Given one-dimensional real array used to hold the complex multidimensional array A(N_1, N_2,..., N_{NDIM}) to be transformed.
The real and the imaginary parts of a data element must be placed by pairs

into immediately adjacent locations in storage. Note that the last subscript increases most rapidly.
Resultant complex Fourier transform in the same storage order.
The number of elements of vector A is

$$2 \cdot N_1 \cdot N_2 \cdot \ldots N_{NDIM} = 2^{1+M_1+M_2} \ldots M_{NDIM}$$

M(NDIM) - BINARY FIXED
Given integer vector of length NDIM, which determines the extent of each dimension of complex array $A(N_1, N_2, N_{NDIM})$:

$$N_1 = 2^{M(1)},\ N_2 = 2^{M(2)},\ \ldots\ N_{NDIM} = 2^{M(NDIM)}$$

NDIM - BINARY FIXED
Given number of dimensions of multidimensional array A.

OPT - CHARACTER (1)
Given option parameter for selection of transform.

Remarks:

Procedure FFTM is to be used for Fourier transforms of complex, multidimensional arrays in which each dimension is a power of two:

$$N_\nu = 2^{M(\nu)} \text{ with } \nu = 1,2,\ldots,NDIM$$

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero.

Error parameter ERROR='P' is returned if NDIM < 1 or any $N_\nu < 1$.

A forward transform followed by an inverse transform, returns the original data multiplied by $N_1 \cdot N_2 \cdot \ldots N_{NDIM}$ (except for roundoff errors).

Method:

Calculations performed are based on the Cooley-Tukey Fast Fourier transform.

For reference see:

J. W. Cooley, P. A. W. Lewis, P. D. Welch, "The Fast Fourier Transform Algorithm and its Applications", IBM Research, RC 1743, February 9, 1967, pp. 15-30.

N. M. Brenner, "Three Fortran Programs that Perform the Cooley-Tukey Fourier Transform", Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Technical Note ESD-TR-67-462, 1967.

J. W. Cooley and J. W. Tukey, "An Algorithm for the Machine Calculation of Complex Fourier Series", Mathematics of Computations, vol. 19, 1965, pp. 297-301.

Mathematical Background

The normal algorithm

Let $B(n_1, n_2, \ldots, n_L)$ be a complex multidimensional array whose dimensions are powers of two:

$$N_\nu = 2^{M(\nu)},\ \nu = 1,2,\ldots,L$$

The finite Fourier forward transform of B is defined as

$$A(k_1,\ldots k_L) = \frac{1}{N_1 \cdot N_2 \cdot \ldots N_L} \sum_{n_1=0}^{N_1-1} \ldots \sum_{n_L=0}^{N_L-1} B(n_1,\ldots,n_L) \cdot W_1^{-n1 \cdot k_1} \cdot \ldots \cdot W_L^{-n_L \cdot k_L} \quad (1)$$

where:

$$W_\nu = \exp\left(\frac{2\pi i}{N_\nu}\right) \text{ and } I = \sqrt{-1}$$

Similarly, $B(n_1,\ldots,n_L)$ can be expressed as the finite Fourier inverse transform (or Fourier series) of $A(k_1,\ldots,k_L)$.

$$B(n_1,\ldots,n_L) = \sum_{k_1=0}^{N_1-1} \ldots \sum_{k_L=0}^{N_L-1} A(k_1,\ldots,k_L) \cdot W_1^{+k_1 \cdot n_1} \cdot \ldots \cdot W_L^{+k_L \cdot n_L} \quad (2)$$

The innermost sum yields an array

$$A_1(k_1,\ldots,k_{L-1},n_L) = \sum_{k_L=0}^{N_L-1} A(k_1,\ldots,k_L) \cdot W_L^{+k_L \cdot n_L} \quad (3)$$

Since equation (3) is equivalent to a one-dimensional problem, we discuss now the algorithm for one-dimensional complex Fourier transform.

$$X(n) = \sum_{k=0}^{N-1} A(k) \cdot W_N^{k \cdot n}, \quad W_N = \exp\left(\frac{2\pi i}{N}\right) \tag{4}$$

Since $N = 2^M$, we express X(n) as a function of the M arguments $n_{M-1}, n_{M-2}, \ldots n_1, n_0$ of the binary representation of n:

$$n = n_{M-1} \cdot 2^{M-1} + n_{M-2} \cdot 2^{M-2} + \ldots + n_1 \cdot 2 + n_0; \; n_\nu = 0 \text{ or } 1.$$

Analogously, if

$$k = k_{M-1} \cdot 2^{M-1} + k_{M-2} \cdot 2^{M-2} + \ldots + k_1 \cdot 2 + k_0 \; ; \; k_\nu = 0 \text{ or } 1$$

then equation (4) can be written:

$$X(n_{M-1}, n_{M-2}, \ldots n_1, n_0) = \sum_{k_0=0}^{1} \cdots \sum_{k_{M-1}=0}^{1} A(k_{M-1}, k_{M-2}, \ldots, k_1, k_0) \; W_N^{n \cdot (k_{M-1} \cdot 2^{M-1} + \ldots + k_1 \cdot 2 + k_0)} \tag{5}$$

Using $W_N^{2M} = W_N^N = 1$, we have

$$W_N^{n \cdot k_{M-1} \cdot 2^{M-1}} = W_N^{n_0 \cdot k_{M-1} \cdot 2^{M-1}}$$

Therefore the innermost sum in equation (5) yields an array:

$$A_1(n_0, k_{M-2}, \ldots, k_1, k_0) = \sum_{k_{M-1}=0}^{1} A(k_{M-1}, k_{M-2}, \ldots, k_1, k_0) \cdot W_N^{n_0 \cdot k_{M-1} \cdot 2^{M-1}}$$

Then, summation over k_{M-2}, to get an array A_2 from A_1, and so on, leads to the general formula (L = 1, 2, ..., M):

$$A_L(n_0, \ldots n_{L-1}, k_{M-L-1}, \ldots k_0) = \sum_{k_{M-L}=0}^{1} A_{L-1}(n_0, \ldots, n_{L-2}, k_{M-L}, k_{M-L-1}, \ldots, k_1, k_0) \cdot W_N^{(n_{L-1} \cdot 2^{L-1} + \ldots + n_1 \cdot 2 + n_0) \cdot k_{M-L} \cdot 2^{M-L}} \tag{6}$$

The final array will be the desired X. The storage indexing convention used here is to let the M arguments of $A_L(n_0, \ldots, k_0)$ be the binary representation of the index of the storage location for $A_L(n_0, \ldots, k_0)$. In this way, each step of the algorithm involves fetching from two storage locations and returning results in the same two locations, thereby saving storage. However, the elements of the final array are in wrong order:

$$X(n_{M-1}, n_{M-2}, \ldots, n_1, n_0) = A_M(n_0, n_1, \ldots, n_{M-1})$$

Now, we must reverse the order of the bits in the binary representation of n. FFT does the reordering on the initial array so that the result is in the correct order.

The two-step algorithm

A modification that achieves further economy at the expense of program complexity is to take two steps at a time when the A_L in equation (6) are calculated. Let us define J as the index given by the high-order L-2 bit positions of an index and let K be the low-order M-L bit positions:

$$A_L(\underbrace{n_0, \ldots, n_{L-3}}_{J}, n_{L-2}, n_{L-1}, \underbrace{k_{M-L-1}, \ldots, k_0}_{K}).$$

Let:

$$U = W_N^{(n_{L-3} \cdot 2^{L-3} + \ldots + n_1 2 + n_0) \cdot 2^{M-L}}$$

Then the step from L-2 to L-1, with

$$W_N^{2^{M-1}} = W_N^{\frac{N}{2}} = -1$$

is:

$$A_{L-1}(J,0,k_{M-L},K) = A_{L-2}(J,0,k_{M-L},K) + A_{L-2}(J,1,k_{M-L},K) \cdot U^2$$

$$A_{L-1}(J,1,k_{M-L},K) = A_{L-2}(J,0,k_{M-L},K) - A_{L-2}(J,1,k_{M-L},K) \cdot U^2 \quad (7)$$

for $k_{M-L} = 0,1$.

For the step from L-1 to L, we make use of the fact that

$W_N^{2^{M-2}} = W_N^{\frac{N}{4}} = i$ and get:

$$A_L(J,n_{L-2},0,K) = A_{L-1}(J,n_{L-2},0,K) + A_{L-1}(J,n_{L-2},1,K) \cdot i^{n_{L-2}} \cdot U$$

$$A_L(J,n_{L-2},1,K) = A_{L-1}(J,n_{L-2},0,K) - A_{L-1}(J,n_{L-2},1,K) \cdot i^{n_{L-2}} \cdot U \quad (8)$$

for $n_{L-2} = 0,1$.

Dropping J and K to simplify notation, we write equations (7) and (8) in a form that requires only three instead of four complex multiplications. To do this, let

$$\bar{A}_{L-1}(n_{L-2},1) = A_{L-1}(J,n_{L-2},1,K) \cdot U$$

Then, we have:

for $k_{M-L} = 0$

$$A_{L-1}(0,0) = A_{L-2}(0,0) + A_{L-2}(1,0) \cdot U^2$$

$$A_{L-1}(1,0) = A_{L-2}(0,0) - A_{L-2}(1,0) \cdot U^2$$

for $k_{M-L} = 1$

$$\bar{A}_{L-1}(0,1) = A_{L-2}(0,1) \cdot U + A_{L-2}(1,1) \cdot U^3$$

$$\bar{A}_{L-1}(1,1) = A_{L-2}(0,1) \cdot U - A_{L-2}(1,1) \cdot U^3$$

for $n_{L-2} = 0$ (9)

$$A_L(0,0) = A_{L-1}(0,0) + \bar{A}_{L-1}(0,1)$$

$$A_L(0,1) = A_{L-1}(0,0) - \bar{A}_{L-1}(0,1)$$

for $n_{L-2} = 1$

$$A_L(1,0) = A_{L-1}(1,0) + \bar{A}_{L-1}(1,1) \cdot i$$

$$A_L(1,1) = A_{L-1}(1,0) - \bar{A}_{L-1}(1,1) \cdot i$$

These equations are used for $L = 2,4,6,\ldots,M$, if M is even. If M is odd, a single step is taken with $L = 1$ and equations (9) are used with $L = 3,5,7,\ldots,M$.

The cases with $J = 0$ and $J = 1$ are programmed separately to avoid multiplications:

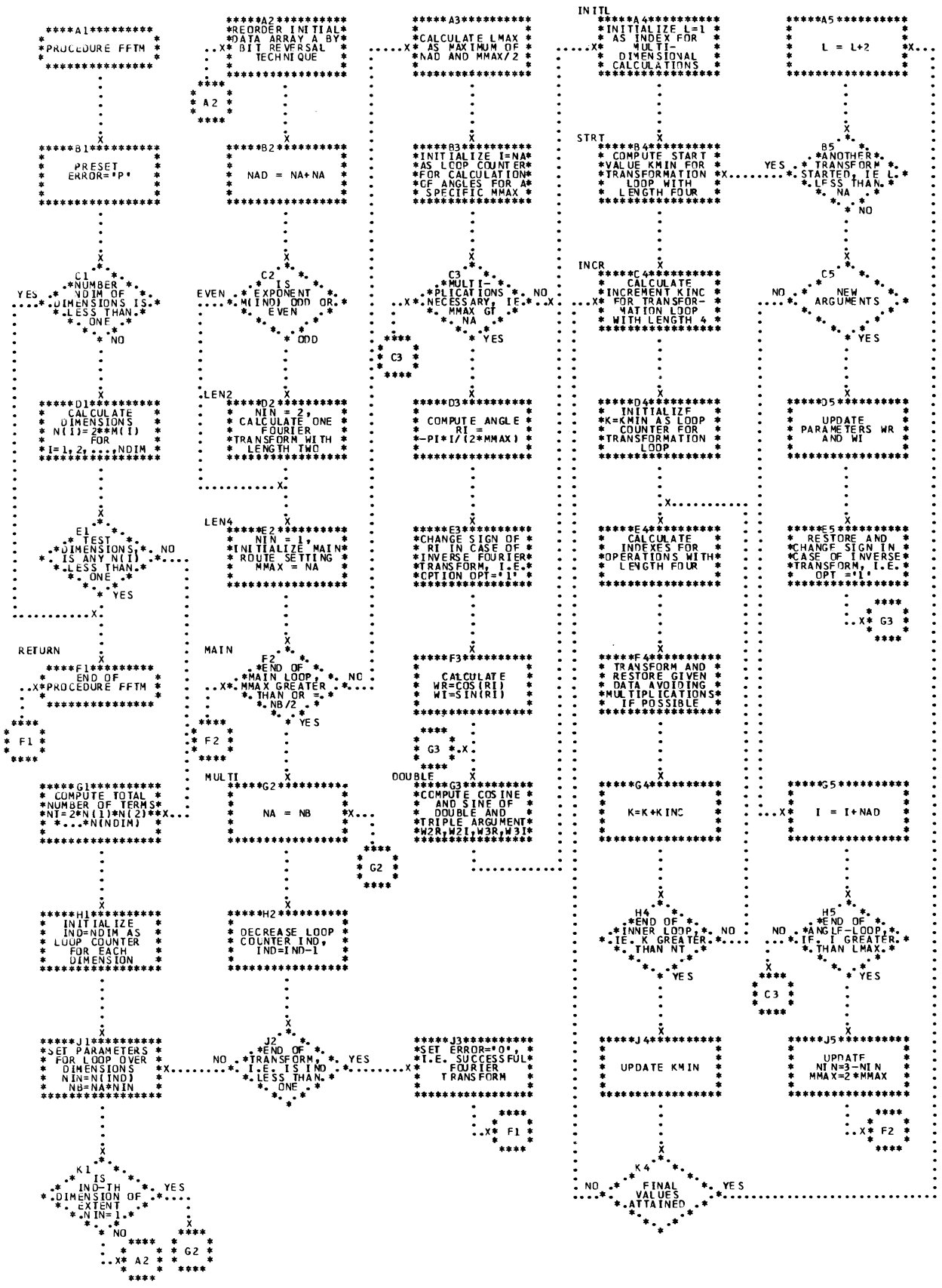
$J = 0$ gives $U = 1$

$J = 1$ gives $U = W_N^{2^{L-3} \cdot 2^{M-L}}$

$$= W_N^{\frac{N}{8}} = e^{\frac{\pi i}{4}} = \frac{1}{\sqrt{2}}(1+i)$$

and $U^2 = i$, $U^3 = \frac{1}{\sqrt{2}}(i-1)$.

FFTM PERFORMS FINITE, MULTIDIMENSIONAL FOURIER TRANSFORMS FOR COMPLEX ARRAYS, WHOSE DIMENSIONS ARE POWERS OF TWO



- Subroutine APLL

```
APLL..                                                                  APLL  10
/*********************************************************************/APLL  20
/*                                                                   */APLL  30
/*      SET UP NORMAL EQUATIONS FOR A LINEAR LEAST SQUARES           */APLL  40
/*      FIT TO A GIVEN DISCRETE FUNCTION                             */APLL  50
/*                                                                   */APLL  60
/*********************************************************************/APLL  70
   PROCEDURE(FCT,N,IP,WORK),.                                           APLL  80
   DECLARE                                                              APLL  90
         FCT ENTRY,                                                     APLL 100
         (WORK(*),P(IP+1),A,WGT)                                        APLL 110
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/APLL 120
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/APLL 130
         (N,IP,LIP,IP1,I,J,K,L,M)                                       APLL 140
         BINARY FIXED,                                                  APLL 150
         ERROR EXTERNAL CHARACTER(1),.                                  APLL 160
   ERROR='0',.                      /*SUCCESSFUL OPERATION          */APLL 170
   LIP  =IP,.                                                           APLL 180
   IP1  =LIP+1,.                                                        APLL 190
   M    =IP1*(IP1+1)/2,.                                                APLL 200
         DO I =1 TO M,.             /*INIT. RIGHT HAND SIDE AND     */APLL 210
         WORK(I)=0,.                /*COEFFICIENT MATRIX EQUAL ZERO*/APLL 220
         END,.                                                          APLL 230
   IF N GT 0                        /*TEST SPECIFIED DIMENSIONS     */APLL 240
   THEN IF LIP GT 0                                                    APLL 250
   THEN IF N GT LIP                                                    APLL 260
   THEN DO I =1 TO N,.              /*FOR I-TH ARGUMENT             */APLL 270
                                    /*PROVIDE VALUES OF GIVEN FCT.,*/APLL 280
         CALL FCT(I,N,LIP,P,WGT),.  /*WEIGHT AND FUNDAMENTAL FCT.  */APLL 290
         IF ERROR NE '0'                                                APLL 300
         THEN GO TO OUT,.           /*ERROR IN PROCEDURE FCT.       */APLL 310
         J    =0,.                                                      APLL 320
              DO K =1 TO IP1,.      /*COMPUTE COEFFICIENT MATRIX    */APLL 330
              A    =P(K)*WGT,.      /*AND RIGHT HAND SIDE           */APLL 340
                   DO L =1 TO K,.                                       APLL 350
                   J    =J+1,.                                          APLL 360
                   WORK(J)=WORK(J)+P(L)*A,.                             APLL 370
                   END,.                                                APLL 380
              END,.                                                     APLL 390
         END,.                                                          APLL 400
   ELSE ERROR='D',.                 /*ERROR IN SPECIFIED DIMENSIONS*/APLL 410
OUT,.                                                                   APLL 420
   END,.                            /*END OF PROCEDURE APLL         */APLL 430
```

Purpose:

APLL sets up the normal equations for a polynomial least squares fit to a given discrete function.

Usage:

CALL APLL (FCT, N, IP, WORK);

FCT - ENTRY
Given procedure supplying the values of the fundamental functions, of the function that is to be approximated and of the weights.
Usage:
CALL FCT (I, N, IP, P, WGT);

I - BINARY FIXED
Given subscript value for current point.

N - BINARY FIXED
Given number of points.

IP - BINARY FIXED
Given number of fundamental functions.

P(IP+1) - BINARY FLOAT [(53)]
Resultant vector containing values of fundamental functions, one up to IP, followed by value of function that must be approximated for the i-th argument.

WGT - BINARY FLOAT [(53)]
Resultant weight value for i-th argument.

N - BINARY FIXED
Given number of points.

IP - BINARY FIXED
Given number of fundamental functions.

WORK((IP+1)(IP+2)/2) - BINARY FLOAT [(53)]
Resultant vector containing the lower triangular part of symmetric coefficient matrix of normal equations, stored rowwise, followed by right-hand side and square sum of function values.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='D' means error in specified dimensions IP, N -- that is, IP is not less than N or N not greater than 1.

For solving the normal equations, ASN may be used.

If ERROR is set to a nonzero value within procedure FCT, control is returned to the calling program.

Method:

The normal equations stored in the vector WORK are obtained by minimizing

$$\sum_{k=1}^{N} w(X_k) \left[f(X_k) - p(X_k) \right]^2$$

where:

$w(X_k)$ is the weight value for argument X_k
$f(X_k)$ is the value of the function to be approximated
$p(X_k)$ is the value of the approximation function

Mathematical Background:

Let $f(x)$, $g_i(x)$, $i = 1, 2, .., IP$, and $w(x) > 0$ be functions defined for $x = x_1, x_2, .., x_N$ (the x_i may be vectors as well as scalars).

The problem is to determine the coefficients c_i of the linear combination $p(x) \sum_{i=1}^{IP} c_i g_i(x)$ such that

$$\sum_{k=1}^{N} w(x_k) \left(f(x_k) - p(x_k)\right)^2 = \min.$$

This problem leads to a system of linear equations AC = R, where C is the vector of unknown coefficients, A is the IP by IP symmetric positive definite matrix with elements

$$a_{jk} = \sum_{i=1}^{N} w(x_i)\, g_j(x_i)\, g_k(x_i)$$

and R is an IP dimensional vector with elements

$$r_j = \sum_{i=1}^{N} w(x_i) f(x_i) g_j(x_i)$$

(See ASN for details.)

Some remarks regarding polynomial approximation are in order. Use of monomials $g_i(x) = x^{i-1}$ as fundamental functions results in a very badly conditioned coefficient matrix A. If Chebyshev or Legendre polynomials are used instead, the condition of the normal equations is improved remarkably, provided the arguments have a sensible distribution (for example, equidistant in the interval -1 to +1).

Programming Considerations:

To allow for full flexibility in data handling, the user must provide a procedure, described under "Usage".

Coefficient matrix A and right-hand side R are stored adjacently. Within a linear array WORK, the lower triangular part of A is stored rowwise, followed by R, which is augmented by one element, ff, in which the weighted square sum of function values is returned.

WORK = (a_{11}, a_{12}, a_{22}, ..., a_{1IP}, ..., $a_{IP\,IP}$, r_1, ..., r_{IP}, ff) represents a triangular array.

The described storage allocation of WORK is required by procedure ASN. The user has full flexibility for handling of the data

$$x_i,\ f(x_i),\ w(x_i),\ g_1(x_i), \ldots, g_{IP}(x_i)$$

1. If he wishes to allocate

$$x_i,\ f(x_i),\ w(x_i),\ g_1(x_i), \ldots, g_{IP}(x_i)$$

in main storage he may use external declarations.

2. Calculation of some or all of the required quantities as functions of the subscript or as functions of the argument x_i is another convenient choice.

3. The needed data may be read in sequentially from one or more external devices.

The three cases listed above may occur in any sensible combination.

- Subroutine APC1/APC2

```
APC1..                                                                  APC   10
/*********************************************************************/APC   20
/*                                                                   */APC   30
/*      SET UP NORMAL EQUATIONS OF WEIGHTED LEAST SQUARES FIT IN     */APC   40
/*      TERMS OF CHEBYSHEV POLINOMIALS FOR A GIVEN DESCRETE FUNCTION */APC   50
/*                                                                   */APC   60
/*********************************************************************/APC   70
   PROCEDURE(X,Y,W,N,IP,XC,X1,WORK),.                                   APC   80
   DECLARE                                                              APC   90
         (X(*),Y(*),W(*),XC,X1,WORK(*),                                 APC  100
         A,B,C,TI,FI,SUM)                                               APC  110
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/APC  130
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/APC  120
         (N,IP,NN,LN,IP1,IPP,EP1,                                       APC  140
         EP,EPE,I,K,KK,L,LL)                                            APC  150
         BINARY FIXED,                                                  APC  160
         (TEST,ERROR EXTERNAL)CHARACTER(1),.                            APC  170
   TEST ='1',.                         /*WEIGHTS ARE GIVEN           */APC  180
   GO TO COMMON,.                                                       APC  190
APC2..                                                                  APC  200
/*********************************************************************/APC  210
/*                                                                   */APC  220
/*      SET UP NORMAL EQUATIONS OF LEAST SQUARES FIT IN TERMS OF     */APC  230
/*      CHEBYCHEV POLYNOMIALS FOR A GIVEN DISCRETE FUNCTION          */APC  240
/*                                                                   */APC  250
/*********************************************************************/APC  260
   ENTRY(X,Y,N,IP,XC,X1,WORK),.                                         APC  270
   TEST ='2',.                         /*CONSTANT WEIGHTING ASSUMED  */APC  280
COMMON..                                                                APC  290
   LN   =N,.                                                            APC  300
   NN   =LN+LN,.                                                        APC  310
   IPP  =IP+IP,.                                                        APC  320
   IP1  =IP+1,.                                                         APC  330
   EP   =(IP*IP1)/2,.                                                   APC  340
   EP1  =EP+1,.                                                         APC  350
   EPE  =EP+IP1,.                                                       APC  360
   ERROR='0',.                         /*PRESET ERROR INDICATOR      */APC  370
   IF LN GT 1                          /*TEST SPECIFIED DIMENSIONS   */APC  380
   THEN IF IP1 GE 1                                                     APC  390
   THEN IF LN GE IP1                                                    APC  400
   THEN DO,.                                                            APC  410
         A,B  =X(1),.                                                   APC  420
              DO I =2 TO N,.                                            APC  430
              C    =X(I),.                                              APC  440
              IF C LT A                                                 APC  450
              THEN A    =C,.          /*SET A TO INF(X(I))          */APC  460
              ELSE IF C GT B                                            APC  470
              THEN B    =C,.          /*SET B TO SUP(X(I))          */APC  480
              END,.                                                     APC  490
         X1   =B-A,.                                                    APC  500
         IF X1 LE 0                                                     APC  510
         THEN DO,.                                                      APC  520
              ERROR='A',.              /*ERROR RETURN FOR            */APC  530
              GO TO OUT,.              /*DEGENERATE ARGUMENT RANGE   */APC  540
              END,.                                                     APC  550
         X0   =-(A+B)/X1,.                                              APC  560
         X1   =2/X1,.                                                   APC  570
              DO I =1 TO IPP-1,        /*INIT. RIGHT HAND SIDE AND   */APC  580
                   EP1 TO EPE-1,.      /*WORKING STORAGE             */APC  590
              WORK(I)=0,.                                               APC  600
              END,.                                                     APC  610
         SUM  =0,.                     /*INIT. SQUARE SUM OF FCT.VAL.*/APC  620
              DO I =1 TO LN,.                                           APC  630
              TI   =X1*X(I)+XC,.       /*TRANSFORM ARGUMENT TO (-1,1)*/APC  640
              A    =1,.                                                 APC  650
              IF TEST='1'              /*SHOULD WEIGHTS BE USED, THEN*/APC  660
              THEN A    =W(I),.        /*SET A TO I-TH WEIGHT        */APC  670
              B    =TI*A,.                                              APC  680
              FI   =Y(I),.             /*SET FI TO FUNCTION VALUE    */APC  690
              SUM  =SUM+FI*FI*A,.      /*UPDATE SQUARES SUM          */APC  700
              FI   =FI+FI,.                                             APC  710
                   DO L =1 TO IPP-1,.  /*UPDATE RIGHT HAND SIDE AND  */APC  720
                   C    =A,.           /*WORKING STORAGE             */APC  730
                   LL   =L,.                                            APC  740
REP..                                                                   APC  750
                   WORK(LL)=WORK(LL)+C,.                                APC  760
                   IF LL LE IP                                          APC  770
                   THEN DO,.                                            APC  780
                        LL   =EP+LL,.                                   APC  790
                        C    =C*FI,.                                    APC  800
                        GO TO REP,.                                     APC  810
                        END,.                                           APC  820
                   C    =TI*B,.                                         APC  830
                   C    =C-A*C,.                                        APC  840
                   A    =B,.                                            APC  850
                   B    =C,.                                            APC  860
                   END,.                                                APC  870
              END,.                                                     APC  880
         LL   =EP1,.                                                    APC  890
              DO K =IPP TO 2 BY -2,.   /*COMPUTE COEFFICIENT MATRIX  */APC  900
              L    =1,.                                                 APC  910
              KK   =K,.                                                 APC  920
STORE..                                                                 APC  930
              LL   =LL-1,.                                              APC  940
              KK   =KK-1,.                                              APC  950
              WORK(LL)=WORK(KK)+WORK(L),.                               APC  960
              L    =L+1,.                                               APC  970
              IF KK GT L                                                APC  980
              THEN GO TO STORE,.                                        APC  990
              END,.                                                     APC 1000
         WORK(EPE)=SUM+SUM,.          /*INSERT SQUARE SUM OF FCT.VAL.*/APC 1010
         ERROR='0',.                  /*SUCCESSFUL OPERATION        */APC 1020
         END,.                                                          APC 1030
OUT..                                                                   APC 1040
   END,.                              /*END OF PROCEDURE APC        */APC 1050
```

Purpose:

APC1/APC2 sets up the normal equations for a polynomial least squares fit to a given discrete function, using Chebyshev polynomials as fundamental functions.

Usage:

CALL APC1 (X, Y, W, N, IP, X0, X1, WORK);

X(N) - BINARY FLOAT [(53)]
Given vector of argument values.

Y(N) - BINARY FLOAT [(53)]
Given vector of function values that are to be approximated.

W(N) - BINARY FLOAT [(53)]
Given vector of weighted values.

N - BINARY FIXED
Given number of argument values.

IP - BINARY FIXED
Given number of Chebyshev polynomials.

X0 - BINARY FLOAT [(53)]
Resultant additive constant for linear transformation of argument range.

X1 - BINARY FLOAT [(53)]
Resultant multiplicative constant for linear transformation of argument range.

WORK((IP+1)(IP+2)/2) - BINARY FLOAT [(53)]
Resultant vector containing the lower triangular part of symmetric coefficient matrix of normal equations, stored rowwise, followed by right-hand side and square sum of function values.

CALL APC2 (X, Y, N, IP, X0, X1, WORK);

X(N) - BINARY FLOAT [(53)]
Given vector of argument values.

Y(N) - BINARY FLOAT [(53)]
Given vector of function values that are to be approximated.

N - BINARY FIXED
Given number of argument values.

IP - BINARY FIXED
Given number of Chebyshev polynomials.

X0 - BINARY FLOAT [(53)]
Resultant additive constant for linear transformation of argument range.

X1 - BINARY FLOAT [(53)]
Resultant multiplicative constant for linear transformation of argument range.

WORK((IP+1)(IP+2)/2) - BINARY FLOAT [(53)]
Resultant vector containing the lower triangular part of symmetric coefficient matrix of normal equations, stored rowwise, followed by right-hand side and square sum of function values.

Remarks:

1. If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='D' means error in specified dimensions IP, N -- that is, for IP not less than N or N not greater than 1.

2. APC2 implies constant weighting (value one).

3. The use of Chebyshev polynomials instead of monomials results in a remarkable improvement of the condition of the normal equations, provided the arguments have a sensible distribution (for example, equidistant).

4. The given argument range is reduced by means of the linear transformation.

$$t(x) = x_1 \cdot x + x_0$$

to the reduced range $-1 \leq t(x) \leq +1$. The normal equations are set up for Chebyshev expansions in t(x) and the solution of these equations is determined by procedure ASN. This is no disadvantage, since the Chebyshev expansion may be evaluated effectively for a specified argument x using procedure POSV with argument $t = x \cdot x_1 + x_0$ and the calculated coefficient vector of the Chebyshev expansion.

5. The transformation of the calculated Chebyshev expansion to an ordinary polynomial may be accomplished using procedure POST.

Method:

The polynomial fit is calculated in the form of its Chebyshev expansion.

$$C_1 T_0(t) + C_2 T_1(t) + \ldots + C_{IP} T_{IP-1}(t)$$

where $T_k(t)$ is the Chebyshev polynomial of degree k.

The values of the Chebyshev polynomials for the argument t are calculated by means of the three-term recurrence equation:

$$T_k(t) = 2\,t\,T_{k-1}(t) - T_{k-2}(t); \quad k \geq 2$$

with starting values $T_0(t) = 1$, $T_1(t) = t$. In setting up the coefficient matrix, time is saved by using the identity

$$2\,T_j \cdot T_k = T_{j+k} + T_{|j-k|}$$

Mathematical Background:

Let x_L and x_R denote the leftmost and rightmost arguments respectively. By means of the linear transformation

$$t(x) = \frac{2x-(x_L + x_R)}{x_R - x_L} = x_1 \cdot x + x_0$$

the argument range $x_L \le x \le x_R$ is reduced to the argument range $-1 \le t(x) \le +1$.

The function f(x), given for $x = x_1, x_2, \ldots, x_N$, is to be approximated by an expansion in Chebyshev polynomials:

$$p(x) = \sum_{0}^{IP} C_i \, T_{i-1} \, (t(x))$$

so that

$$\sum_{i=1}^{N} w(x_i) \, [f(x_i) - p(x_i)]^2 = \min.$$

T_k (t) is the Chebyshev polynomial of degree k.

The vector C of unknown coefficients C_i is a solution of the matrix equation AC = R, where A is an IP by IP symmetric positive definite matrix with elements

$$a_{jk} = \sum_{i=1}^{N} w(x_i) \, T_{j-1} \, (t(x_i)) \, T_{k-1} \, (t(x_i))$$

and R is a vector of dimension IP with elements

$$r_j = \sum_{i=1}^{N} w(x_i) \, T_{j-1} \, (t(x_i)) \, f(x_i)$$

(See ASN for details.)

The Chebyshev expansion of the polynomial p(x) gives a much better indication of the accuracy of the approximation than the coefficient vector of the polynomial itself. If the specified degree of the polynomial is too high, the last terms of the Chebyshev expansion are uniformly small compared with the preceding coefficients. The degree might be reduced by the number of small trailing coefficients without unduly enlarging the overall error.

An upper bound for the error introduced by neglecting the last terms of the Chebyshev expansion is given by the sum of the absolute values of these terms. Normally, transformation of the Chebyshev expansion in t(x) to ordinary polynomials in x results in severe loss of accuracy. Therefore, no attempt is made to return the polynomial expansions.

Programming Considerations:

Only the lower triangular part of the symmetric coefficient matrix is generated and stored rowwise, followed immediately by the right-hand side and by the weighted square sum of function values.

This storage allocation scheme is required by subroutine ASN, which may be used for calculation of the normal equations.

- Subroutine ASN

```
ASN..                                                                  ASN   10
/*********************************************************************/ASN   20
/*                                                                   */ASN   30
/*      SOLUTION OF NORMAL-EQUATIONS UP TO SPECIFIED ORDER           */ASN   40
/*      OP PRECISION.                                                */ASN   50
/*      ALL FITS OF SMALLER ORDER ARE CALCULATED OPTIONALLY.         */ASN   60
/*                                                                   */ASN   70
/*********************************************************************/ASN   80
   PROCEDURE(WORK,IP,IRES,OPT,EPS,ETA),.                               ASN   90
   DECLARE                                                             ASN  100
        S BINARY FLOAT(53),                                            ASN  110
        (WORK(*),EPS,ETA,TOL,TEST,                                     ASN  120
        AUX(IP),WE,Q,R)                                                ASN  130
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/ASN  140
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/ASN  150
        (IP,IP1,RS,DG,DDG,L,LL,                                        ASN  160
        EPE,LLL,DL,IPR,IRES,K,EP,                                      ASN  170
        I,II,LL1,DLK)                                                  ASN  180
        BINARY FIXED,                                                  ASN  190
        (OPT,CHECK,ERROR EXTERNAL)                                     ASN  200
        CHARACTER(1),.                                                 ASN  210
   IF ETA NE 0                     /*PRESET ERROR INDICATOR          */ASN  220
   THEN CHECK='A',.                /*A= ACCURACY NOT REACHED         */ASN  230
   ELSE CHECK='0',.                /*0= SUCCESSFUL OPERATION         */ASN  240
   IP1 =IP+1,.                                                         ASN  250
   IF IP1 LE 1                                                         ASN  260
   THEN DO,.                                                           ASN  270
        CHECK='D',.                /*ERROR IN SPECIFIED DIMENSION    */ASN  280
        GO TO OUT,.                                                    ASN  290
        END,.                                                          ASN  300
   EP   =IP*IP1/2,.                /*SET UP ADDRESSING CONSTANTS     */ASN  310
   EPE  =EP+IP1,.                                                      ASN  320
   WE   =WORK(EPE),.                                                   ASN  330
   IF CHECK='A'                    /*SET TEST TO ABSOLUTE VALUE OF   */ASN  340
   THEN TEST =ABS(ETA*WE),.        /*SPEC. ACCURACY FOR WANTED FIT   */ASN  350
   IPR,LL=0,.                                                          ASN  360
   L,LL1=1,.                                                           ASN  370
                                   /*********************************/ASN  380
        DO I =1 TO IP,.            /*FACTORIZE GIVEN MATRIX          */ASN  390
        LL   =LL+I,.               /*********************************/ASN  400
        K    =0,.                                                      ASN  410
ITER..                             /*COMPUTE ELEMENTS OF I-TH ROW    */ASN  420
        S    =0,.                                                      ASN  430
             DO II=LL1 TO LL-1,.   /*MODIFY ELEMENTS IN I-TH         */ASN  440
             S    =S+MULTIPLY(     /*ROW BY SCALAR PRODUCT OF        */ASN  450
                  WORK(II),        /*ELEMENTS OF FACTORIZATION       */ASN  460
                  WORK(L),53),.    /*IN ROW AND COLUMN CROSSING      */ASN  470
             L    =L+1,.           /*AT CURRENT ELEMENT              */ASN  480
             END,.                                                     ASN  490
        R    =WORK(L),.                                               ASN  500
        S    =0-S,.                                                   ASN  510
        IF L =LL                   /*TEST FOR LOSS OF SIGNIFICANCE   */ASN  520
        THEN DO,.                  /*IN PIVOTAL DIVISOR              */ASN  530
             IF S LE ABS(EPS*R)                                        ASN  540
             THEN DO,.                                                 ASN  550
                  CHECK='P',.      /*MARK LOSS OF SIGNIFICANCE       */ASN  560
                  GO TO SOL,.      /*BYPASS FURTHER FACTORIZATION    */ASN  570
                  END,.                                                ASN  580
             Q,S  =SQRT(S),.       /*CALCULATE DIAGONAL ELEMENT      */ASN  590
             END,.                 /*OF FACTORIZATION                */ASN  600
        ELSE S    =S/Q,.                                               ASN  610
        WORK(L)=S,.                /*STORE FINAL ELEMENT             */ASN  620
        K    =K+1,.                /*OF FACTORIZATION                */ASN  630
        L    =L+K,.                                                   ASN  640
        IF K+1 LE IP1              /*TEST IF ALL ELEMENTS OF I-TH    */ASN  650
        THEN GO TO ITER,.          /*ROW ARE COMPUTED                */ASN  660
        LL1,L=LL+1,.                                                   ASN  670
        WE   =WE-S*S,.                                                 ASN  680
        AUX(I)=WE,.                /*STORE SQUARESUM OF RESIDUALS    */ASN  690
        IF CHECK='A'               /*TEST ON SPECIFIED PRECISION     */ASN  700
        THEN IF WE LT TEST                                             ASN  710
        THEN DO,.                                                      ASN  720
             CHECK='0',.           /*SUCCESSFUL OPERATION            */ASN  730
             GO TO SOL,.           /*RESP. ETA ACCURACY REACHED      */ASN  740
             END,.                                                     ASN  750
        IPR  =IPR+1,.                                                  ASN  760
        END,.                      /*END OF FACTORIZATION            */ASN  770
   IF OPT='F'                                                          ASN  780
   THEN GO TO OUT,.                                                    ASN  790
   LL   =EPE,.                     /*********************************/ASN  800
                                   /*COMPUTE LEAST SQUARE FIT(S)     */ASN  810
                                   /*********************************/ASN  820
SOL..                                                                  ASN  830
   RS   =EP+IPR,.                  /*INIT. ADDRESS RIGHT HAND SIDE   */ASN  840
   DG   =LL-1-IPR,.                /*INIT. ADDRESS DIAGONAL TERM     */ASN  850
        DO I =IPR TO 1 BY -1,.                                         ASN  860
        Q    =WORK(DG),.           /*SET Q TO I-TH DIAGONAL TERM     */ASN  870
        R    =WORK(RS),.           /*SET R TO I-TH RIGHT HAND SIDE   */ASN  880
        WORK(RS)=AUX(I),.          /*INSERT I-TH RESIDUAL            */ASN  890
        RS   =RS-1,.                                                   ASN  900
        DG   =DG-I,.                                                   ASN  910
        LL,L =LL-1,.                                                   ASN  920
        K    =IPR-I,.                                                  ASN  930
        DL,DLK=IPR,.                                                   ASN  940
REP..                              /*CALCULATE THE I-TH ELEMENT      */ASN  950
        L,LLL=L-DL,.               /*FOR THE HIGHEST FIT AND         */ASN  960
        DL,DLK=DL-1,.              /*OPTIONALLY OF ALL LOWER FITS    */ASN  970
        S    =0,.                                                      ASN  980
             DO II=L+K TO L+1 BY -1,. /*FORM SCALAR PRODUCTS NEEDED   */ASN  990
             S    =S+MULTIPLY(      /*WITH BACK SUBSTITUTION          */ASN 1000
                  WORK(LLL),                                           ASN 1010
                  WORK(II),53),.                                       ASN 1020
             LLL  =LLL-DLK,.                                           ASN 1030
             DLK  =DLK-1,.                                             ASN 1040
             END,.                                                     ASN 1050
        WORK(L)=(R-S)/Q,.                                              ASN 1060
        K    =K-1,.                                                    ASN 1070
        IF OPT='A'                 /*REPEAT IF ALL FITS SHOULD       */ASN 1080
        THEN IF K GE 0             /*BE CALCULATED                   */ASN 1090
        THEN GO TO REP,.                                               ASN 1100
        END,.                                                          ASN 1110
OUT..                                                                  ASN 1120
   IRES =IPR,.                                                         ASN 1130
   ERROR=CHECK,.                                                       ASN 1140
   END,.                           /*END OF PROCEDURE ASN            */ASN 1150
```

Purpose:

ASN computes the solution of normal equations set up by procedures APC1, APC2, and APLL.

Usage:

CALL ASN (WORK, IP, IRES, OPT, EPS, ETA);

WORK ((IP+1) (IP+2)/2) -
BINARY FLOAT [(53)]
Given vector, containing the lower triangular part of a symmetric coefficient matrix of normal equations, stored rowwise, followed by the right-hand side and the square sum of function values.
Resultant vector containing (sequentially) the coefficient vectors of computed least square fits, degree one up to IRES.
WORK((IP(IP+1)/2) + K), K=1, ..., IRES contains the residuals corresponding to the approximation fit of degree K.
If only the approximation fit of highest degree (that is, degree IRES) is calculated, the coefficient vector has the same storage allocation as if all fits were calculated (similarly for the corresponding residual vector).

IP - BINARY FIXED
Given number of fundamental functions.

IRES - BINARY FIXED
Resultant (highest) degree of approximation fit(s) with respect to the user-specified accuracy.

OPT - CHARACTER(1)
Given option for operations to be performed.

EPS - BINARY FLOAT [(53)]
Given relative tolerance for test on loss of significance.

ETA - BINARY FLOAT [(53)]
Given relative tolerance for tolerated square sum of residuals.

Remarks:

1. All operations are performed with respect to the user-specified tolerances EPS and ETA.

2. If OPT is not equal to 'A' or 'F', then ASN computes the least square fit of degree IRES only. OPT='A' means all fits of degree one up to IRES are calculated.
OPT='F' means the given coefficient matrix A is factored in the form T*T, in the linear array WORK. The triangular matrix T is allocated in the same way as the upper (lower) triangular part of A. The right-hand side R is replaced by $(T^*)^{-1}R$.

3. For EPS a sensible value is between 10^{-3} and 10^{-6} (10^{-10} and 10^{-15}) in single (double) precision. The absolute tolerance used internally for the test on loss of significance is ABS (EPS times current pivotal element).

For ETA a realistic value is between 1 and 10^{-6} (1 and 10^{-15}) in single (double) precision. Nevertheless, ETA may be set equal to zero. If no specification is made for ETA, it is equivalent to setting ETA=0. The absolute tolerance used internally for the square sum of residuals is ABS (ETA times square sum of function values).

4. Let:

n_1 = maximal dimension for which no loss of significance was indicated during factorization

n_2 = smallest dimension for which the square sum of residuals does not exceed the absolute tolerance ETA

IRES is given by MIN (n_1, n_2, IP). (n_2 = IP for ETA = 0).

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

5. ERROR='D' means IP is less than 1.
ERROR='A' means respective ETA accuracy is not reached.
ERROR='P' means loss of significance was detected.

Method:

Calculation of the least square fits is done using Cholesky's square root method for symmetric factorization.

Mathematical Background:

Let $f(x), g_i(x)$, $i = 1, 2, \ldots, m$, and $w(x) > 0$ be functions defined for $x = x_1, x_2, \ldots, x_n$. The problem is to determine the coefficients c_i of the linear combination

$$p(x) = \sum_{i=1}^{m} c_i g_i(x) \text{ such that}$$

$$e_m = \sum_{k=1}^{n} w(x_k)\,(f(x_k) - p(x_k))^2 = \min. \qquad (1)$$

The necessary conditions

$$\frac{\partial e_m}{\partial c_i} = 0,\ i = 1, 2, \ldots, m \qquad (2)$$

form a system of m linear equations in m unknowns c_i.

To simplify the notation we introduce the following matrices:

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad F = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix},$$

$$W = \begin{bmatrix} w(x_1) & & & \\ & w(x_2) & & \\ & & \ddots & \\ & & & w(x_n) \end{bmatrix},$$

$$c = \begin{bmatrix} c_1 \\ \vdots \\ c_m \end{bmatrix}, \quad G = \begin{bmatrix} g_1(x_1) & \cdots & g_1(x_n) \\ \vdots & & \vdots \\ g_m(x_1) & \cdots & g_m(x_n) \end{bmatrix}$$

Then we have

$$e_m = (F^T - C^T G)\, W(F - G^T C)$$

or, with $e_0 = F^T W F$,

$$e_m = e_0 - 2C^T GWF + C^T GWG^T C \qquad (1')$$

Using equation (1'), the equations (2) may be written

$$GWG^T C = GWF \qquad (2')$$

Combining (1') and (2') gives

$$e_0 - e_m = C^T GWG^T C \qquad (3)$$

The normal equations (2') for the unknown vector C may be solved using Cholesky's method since the coefficient matrix $A = GWG^T$ is obviously symmetric and it is positive definite if all the fundamental functions $g_i(x)$ are linearly independent for the arguments x_i -- that is, if the rows of G are linearly independent. Let R = GWF. Using Cholesky's method, A and R are replaced without additional storage requirements by T and $(T^T)^{-1}R$, where $A = T^T T$ and T is upper triangular.

An easy calculation shows

$$e_0 - e_m = \left\| (T^T)^{-1} R \right\|^2$$

Introducing additional fundamental functions in the linear combination p(x) will not affect the first m rows and columns of A or the first m elements of R. Therefore, Cholesky's method gives a decomposition of $e_0 - e_m$ into the separate components corresponding to individual degrees of freedom.

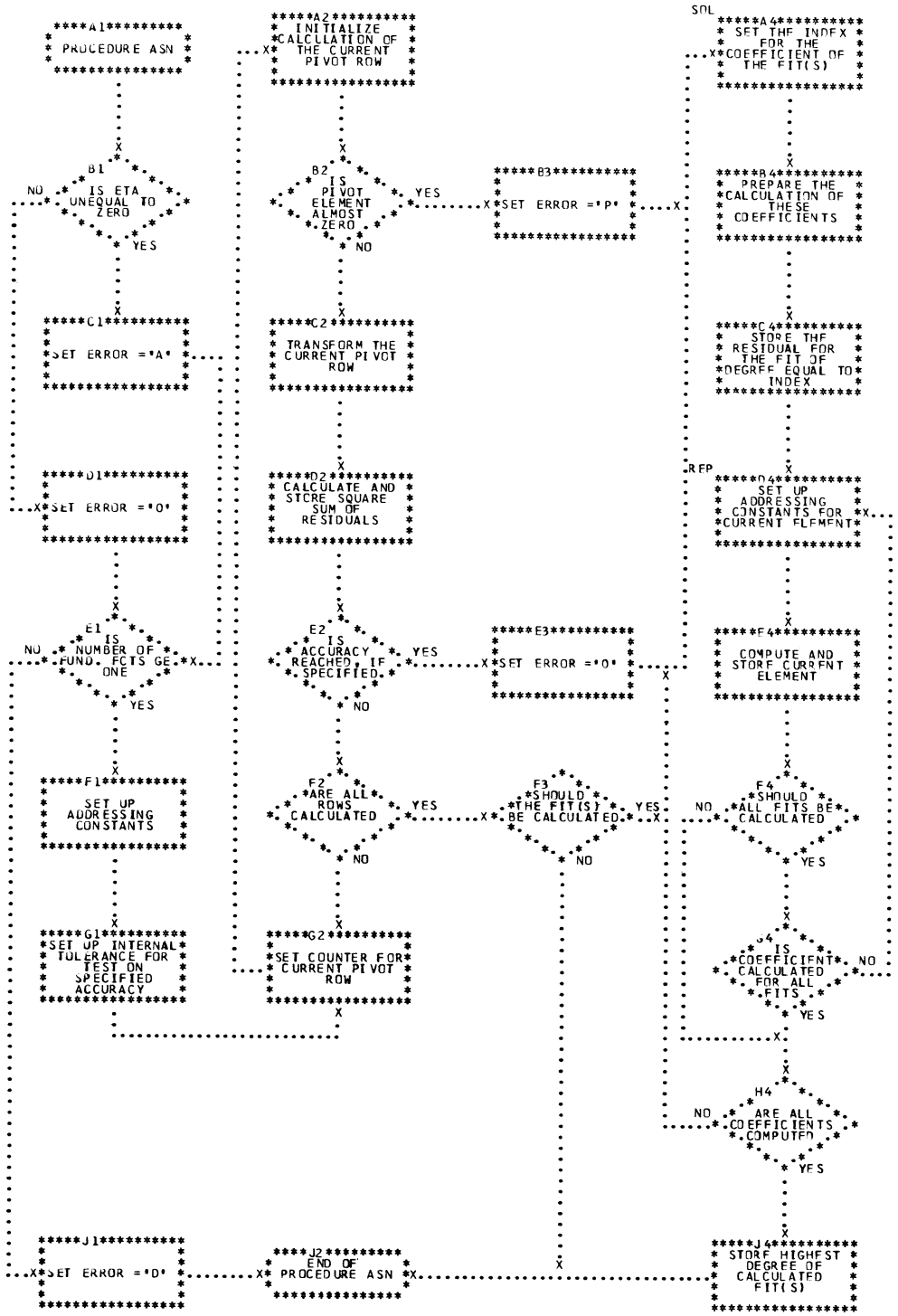
Programming Considerations:

All least squares fits of dimension 1, 2, ..., m may be computed from the reduced normal equations $TC = (T^T)^{-1}R$. If the solutions are generated in the storage locations of T, there is no additional storage requirement.

Using the decomposition of $e_0 - e_m$, the factorization may be terminated with dimension k if $e_k < \eta e_0$, giving the least squares fit of dimension k that satisfies the user-specified precision (relative tolerance η). Because of rounding errors this will work only if η is approximately between 1.0 and 1.0 E-6 in single precision, and between 1.0 and 1.0 E-15 in double precision. Nevertheless, the square sum of residuals corresponding to a least squares fit calculated in single (double) precision may be as small as $e_0\ 10^{-12}$ ($e_0\ 10^{-30}$).

Because of rounding errors the square root method may break down if very small or negative pivot elements indicate a loss of significance. Therefore, all pivot elements are tested against the absolute value of EPS times the current diagonal element of A. If the k-th pivot element is not greater than this internal test value, the normal equations are treated as if they had dimension k-1 only.

PROCEDURE ASN COMPUTES THE SOLUTION OF THE NORMAL EQUATIONS SET UP BY PROCEDURES APC1, APC2 AND APLL



Smoothing of Tabulated Functions

- Subroutine SG13/SE13

```
SG13..                                                              SG13  10
/*******************************************************************/SG13  20
/*                                                                 */SG13  30
/*      SMOOTH A TABLED FUNCTION USING                             */SG13  40
/*      A FIRST DEGREE POLYNOMIAL FIT RELEVANT TO THREE POINTS     */SG13  50
/*                                                                 */SG13  60
/*******************************************************************/SG13  70
   PROCEDURE(X,Y,Z,DIM),.                                           SG13  80
   DECLARE                                                          SG13  90
        (X(*),Y(*),Z(*),XA,XB,XC,                                   SG13 100
        YA,YB,YC,YM,TA,TB,TC,XM)                                    SG13 110
        BINARY FLOAT,               /*SINGLE PRECISION VERSION  /*S*/SG13 120
 /*     BINARY FLOAT(53),           /*DOUBLE PRECISION VERSION  /*D*/SG13 130
        (DIM,I)BINARY FIXED,                                        SG13 140
        SWITCH CHARACTER(1),                                        SG13 150
        ERROR EXTERNAL CHARACTER(1),.                               SG13 160
   SWITCH='G',.                     /*MARK GENERAL ARGUMENTS      */SG13 170
   GOTO INIT,.                                                      SG13 180
SE13..                                                              SG13 190
/*******************************************************************/SG13 200
/*                                                                 */SG13 210
/*      SMOOTH AN EQUIDISTANTLY TABLED FUNCTION USING              */SG13 220
/*      A FIRST DEGREE POLYNOMIAL FIT RELEVANT TO THREE POINTS     */SG13 230
/*                                                                 */SG13 240
/*******************************************************************/SG13 250
   ENTRY(Y,Z,DIM),.                                                 SG13 260
   SWITCH='E',.                     /*MARK EQUIDISTANT ARGUMENTS  */SG13 270
INIT..                                                              SG13 280
   IF DIM GE 3                      /*TEST SPECIFIED DIMENSION    */SG13 290
   THEN DO,.                                                        SG13 300
        YA   =Y(3),.                /*MODIFICATION  YA = Y(0)     */SG13 310
        YB   =Y(1),.                                                SG13 320
        IF SWITCH='G'               /*TEST GENERAL CASE           */SG13 330
        THEN DO,.                                                   SG13 340
             XA   =X(3),.           /*MODIFICATION  XA = X(0)     */SG13 350
             XB   =X(1),.                                           SG13 360
             END,.                                                  SG13 370
        ELSE YA   =YB+(YB-YA)/2,.   /*MODIFICATION  YA = Y(0)     */SG13 380
             DO I = 2 TO DIM,.                                      SG13 390
             YC   =Y(I),.                                           SG13 400
             YM   =(YA+YB+YC)/3,.   /*SET YM TO ARITHMETIC MEAN   */SG13 410
             IF SWITCH='G'          /*TEST GENERAL CASE           */SG13 420
             THEN DO,.                                              SG13 430
                  XC   =X(I),.                                      SG13 440
                  IF   (XB-XA)*                                     SG13 450
                       (XC-XB) LE 0                                 SG13 460
                  THEN ERROR='M',.  /*MARK NON-MONOTONIC TABLE    */SG13 470
                  XM   =(XA+XB+XC)/3,.                              SG13 480
                  TA   =XA-XM,.                                     SG13 490
                  TB   =XB-XM,.                                     SG13 500
                  TC   =XC-XM,.                                     SG13 510
                  XM   =TA*TA+TB*TB+TC*TC,.                         SG13 520
                  IF XM GT 0                                        SG13 530
                  THEN XM   =(TA*(YA-YB)+                           SG13 540
                       TB*(YB-YM)+                                  SG13 550
                       TC*(YC-YM))/XM,.                             SG13 560
                  XA   =XB,.                                        SG13 570
                  XB   =XC,.                                        SG13 580
                  YM   =XM*TB+YM,.  /*SET YM TO WEIGHTED MEAN     */SG13 590
                  END,.                                             SG13 600
             Z(I-1)=YM,.            /*REPLACE Z(I-1) BY YM        */SG13 610
             YA   =YB,.                                             SG13 620
             YB   =YC,.                                             SG13 630
             END,.                                                  SG13 640
        IF SWITCH='G'                                               SG13 650
        THEN Z(DIM)=XM*(TC-TB)+YM,. /*COMPUTE Z(DIM)  GENEPAL CASE */SG13 660
        ELSE Z(DIM)=YB+(YA-YM)/2,.  /*COMPUTE Z(DIM)  EQUID. CASE  */SG13 670
        ERROR='O',.                 /*SUCCESSFUL OPERATION        */SG13 680
        END,.                                                       SG13 690
   ELSE ERROR='D',.                 /*ERROR IN SPECIFIED DIMENSION*/SG13 700
   END,.                            /*END OF PROCEDURE S13        */SG13 710
```

Purpose:

SG13, SE13 computes a vector $Z = (z_1, \ldots, z_{DIM})$ of smoothed function values. SE13 requires a vector $Y = (y_1, \ldots, y_{DIM})$ and in the case of SG13 a vector $X = (x_1, \ldots, x_{DIM})$ of argument values must be given in addition. y_i corresponds to x_i, in the case of SE13 the y components correspond to equidistantly spaced argument values x_i, assuming $x_i - x_{i-1} = h$.

Usage:

CALL SG13 (X, Y, Z, DIM);

X(DIM) - BINARY FLOAT [(53)]
Given vector of argument values.

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of smoothed function values.

DIM - BINARY FIXED
Given dimension of vectors X, Y and Z.

CALL SE13 (Y, Z, DIM);

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of smoothed function values.

DIM - BINARY FIXED
Given dimension of vectors Y, Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR = 'D' means DIM is less than three.

ERROR = 'M' indicates a non-monotonic argument table, that is, for some i $(x_i - x_{i-1})(x_{i+1} - x_i)$, is less than or equal to zero. Vectors Z and Y may be identically allocated, which means that the given function values are replaced by the resultant smoothed function values.

Method:

The smoothed function values z_i are obtained by evaluating the least squares polynomial of degree one at x_i relevant to three successive points.

For references see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 258-311.

Mathematical Background:

For $i = 3, \ldots, n$ we must find m_i and b_i such that

$$w_i(x) = m_i x + b_i \qquad (1)$$

gives the least-squares fit to the points (x_{i-2}, y_{i-2}), (x_{i-1}, y_{i-1}), and (x_i, y_i). The problem, then, is to minimize

$$F(m_i, b_i) = \sum_{k=0}^{2} \left[w_i(x_{i-k}) - y_{i-k} \right]^2$$

This minimum will occur when

$$\frac{\partial F}{\partial b_i} = 0 \text{ and } \frac{\partial F}{\partial m_i} = 0 \tag{2}$$

Now

$$\left.\begin{aligned} \frac{\partial F}{\partial b_i} &= 2 \sum_{k=0}^{2} \left[w_i (x_{i-k}) - y_{i-k} \right] \\ \text{and} \\ \frac{\partial F}{\partial m_i} &= 2 \sum_{k=0}^{2} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \end{aligned}\right\} \tag{3}$$

Solving equations (2) and (3) yields:

$$m_i = \frac{\sum_{k=0}^{2} x_{i-k}\, y_{i-k} - 1/3 \left(\sum_{k=0}^{2} x_{i-k} \right) \left(\sum_{k=0}^{2} y_{i-k} \right)}{\sum_{k=0}^{2} x^2_{i-k} - 1/3 \left(\sum_{k=0}^{2} x_{i-k} \right)^2} \tag{4}$$

and

$$b_i = \frac{1}{3} \sum_{k=0}^{2} \left(y_{i-k} - m_i x_{i-k} \right) \tag{5}$$

Letting:

$$\left.\begin{aligned} \bar{y}_i &= \frac{1}{3} \sum_{k=0}^{2} y_{i-k} \\ \bar{x}_i &= \frac{1}{3} \sum_{k=0}^{2} x_{i-k} \\ t_{i,k} &= x_{i-k} - \bar{x}_i \text{ and } v_{i,k} = y_{i-k} - \bar{y}_i \end{aligned}\right\} \tag{6}$$

we may rewrite (4) and (5) as:

$$m_i = \frac{\sum_{k=0}^{2} t_{i,k}\, v_{i,k}}{\sum_{k=0}^{2} t^2_{i,k}} \tag{7}$$

and

$$b_i = \bar{y}_i - m_i \bar{x}_i \tag{8}$$

Using (8) in (1) gives

$$w_i(x) = m_i(x - \bar{x}_i) + \bar{y}_i$$

where m_i is as in (7).

The desired smoothed values z_i are given by:

$$z_i = \begin{cases} w_3(x_1) = m_3 t_{3,2} + \bar{y}_3 & \text{if } i=1 \\ w_{i+1}(x_i) = m_{i+1} t_{i+1,1} + \bar{y}_{i+1} & \text{if } i=2,\ldots,n-1 \\ w_n(x_n) = m_n t_{n,0} + \bar{y}_n & \text{if } i=n \end{cases} \tag{9}$$

for generally tabulated argument values -- that is, for SG13.

In the case of equidistantly spaced argument values (that is, in case of SE13) we have the additional relation $x_i - x_{i-1} = h$, a constant, for $i = 2, \ldots, n$. This leads to the following expressions for the z_i:

$$z_i = \begin{cases} \frac{1}{6}(5y_1 + 2y_2 - y_3) & \text{if } i=1 \\ \frac{1}{3}(y_{i-1} + y_i + y_{i+1}) & \text{if } i=2,\ldots,n-1 \\ \frac{1}{6}(-y_{n-2} + 2y_{n-1} + 5y_n) & \text{if } i=n \end{cases} \tag{1}$$

- Subroutine SE15

```
SE15..                                                              SE15  10
/*******************************************************************/SE15  20
/*                                                                 */SE15  30
/*      SMOOTH AN EQUIDISTANTLY TABLED FUNCTION USING              */SE15  40
/*      A FIRST DEGREE POLYNOMIAL FIT RELEVANT TO FIVE POINTS      */SE15  50
/*                                                                 */SE15  60
/*******************************************************************/SE15  70
   PROCEDURE(Y,Z,DIM),.                                             SE15  80
   DECLARE                                                          SE15  90
         (Y(*),Z(*),YA,YB,YC,YD,YE)                                 SE15 100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/SE15 110
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/SE15 120
         (DIM,I)BINARY FIXED,                                       SE15 130
         ERROR EXTERNAL CHARACTER(1),.                              SE15 140
   IF DIM GE 5                         /*TEST SPECIFIED DIMENSION     */SE15 150
   THEN DO,.                                                        SE15 160
         YA   =Y(4),.                                               SE15 170
         YE   =Y(2),.                                               SE15 180
         YD   =Y(1),.                                               SE15 190
         YC   =YD+(YE-YA)/2,.          /*MODIFICATION, SET YC TO Y(0) */SE15 200
         YB   =YC-Y(5)+YA,.            /*MODIFICATION, SET YB TO Y(-1)*/SE15 210
              DO I =3 TO DIM,.                                      SE15 220
              YA   =YB,.               /*REPLACE YA BY Y(I-4)        */SE15 230
              YB   =YC,.               /*REPLACE YB BY Y(I-3)        */SE15 240
              YC   =YD,.               /*REPLACE YC BY Y(I-2)        */SE15 250
              YD   =YE,.               /*REPLACE YD BY Y(I-1)        */SE15 260
              YE   =Y(I),.             /*SET YE TO Y(I)              */SE15 270
              Z(I-2)=(YA+YB+YC                                      SE15 280
                   +YD+YE)/5,.         /*SET Y(I-2) TO ARITHMETIC MEAN*/SE15 290
              END,.                                                 SE15 300
         YA   =YC+YD+YE+YE,.                                        SE15 310
         Z(DIM-1),YA=(YA+YA+YD+YB)/10,.                             SE15 320
         Z(DIM)=YA+YA-Z(DIM-2),.                                    SE15 330
         ERROR='0',.                  /*SUCCESSFUL OPERATION        */SE15 340
         END,.                                                      SE15 350
   ELSE ERROR='1',.                   /*ERROR IN SPECIFIED DIMENSION */SE15 360
   END,.                              /*END OF PROCEDURE S15        */SE15 370
```

Purpose:

SE15 computes a vector $Z = (z_1, z_2, \ldots, z_{DIM})$ of smoothed function values, given a vector $Y = (y_1, y_2, \ldots, y_{DIM})$ of function values whose components y_i correspond to DIM equidistantly spaced argument values x_i with $x_i - x_{i-1} = h$ for $i = 2, \ldots,$ DIM.

Usage:

CALL SE15 (Y, Z, DIM);

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of smoothed function values.

DIM - BINARY FIXED
Given dimension of vectors Y and Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR='1' means DIM is less than five.
Vectors Z and Y may be identically allocated, which means that the given function values are replaced by the resultant smoothed function values.

Method:

The smoothed function values are obtained by evaluation of the least squares polynomial of degree one relevant to five successive points.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 295-302.

Mathematical Background:

For $i = 5, \ldots, n$ we find m_i and b_i such that

$$w_i(x) = m_i x + b_i \tag{1}$$

gives the least-squares fit to the points (x_{i-k}, y_{i-k}), $k=0, \ldots, 4$. The problem, then, is to minimize

$$F(m_i, b_i) = \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]^2$$

This minimum will occur when

$$\frac{\partial F}{\partial b_i} = 0 \text{ and } \frac{\partial F}{\partial m_i} = 0 \tag{2}$$

Now

$$\frac{\partial F}{\partial b_i} = 2 \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]$$

and

$$\frac{\partial F}{\partial m_i} = 2 \sum_{k=0}^{4} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \tag{3}$$

Solving equations (2) and (3) yields:

$$m_i = \frac{\sum_{k=0}^{4} x_{i-k} y_{i-k} - \frac{1}{5} \left(\sum_{k=0}^{4} x_{i-k} \right) \left(\sum_{k=0}^{4} y_{i-k} \right)}{\sum_{k=0}^{4} x_{i-k}^2 - \frac{1}{5} \left(\sum_{k=0}^{4} x_{i-k} \right)^2} \tag{4}$$

and

$$b_i = \frac{1}{5} \sum_{k=0}^{4} \left[y_{i-k} - m_i x_{i-k} \right] \tag{5}$$

Using the fact that $x_j - x_{j-1} = h$, a constant, for $j = 2, \ldots, n$, equations (4) and (5) may be rewritten as

$$m_i = \frac{1}{10h}(2y_i + y_{i-1} - y_{i-3} - 2y_{i-4}) \qquad (6)$$

and

$$b_i = \frac{1}{5}\sum_{k=0}^{4} y_{i-k} - m_i x_{i-2} \qquad (7)$$

Using equation (7) in equation (1) yields

$$w_i(x) = m_i(x - x_{i-2}) + \frac{1}{5}(y_{i-4} + \ldots + y_i)$$

The desired smoothed function values z_i are given by:

$$z_i = \begin{cases} w_5(x_1) = \frac{1}{5}(3y_1 + 2y_2 + y_3 - y_5) & i=1 \\ w_5(x_2) = \frac{1}{10}(4y_1 + 3y_2 + 2y_3 + y_4) & i=2 \\ w_{i+2}(x_i) = \frac{1}{5}(y_{i-2} + y_{i-1} + y_i + y_{i+1} + y_{i+2}) & i=3,\ldots,n-2 \\ w_n(x_{n-1}) = \frac{1}{10}(y_{n-3} + 2y_{n-2} + 3y_{n-1} + 4y_n) & i=n-1 \\ w_n(x_n) = \frac{1}{5}(-y_{n-4} + y_{n-2} + 2y_{n-1} + 3y_n) & i=n \end{cases} \qquad (8)$$

- Subroutine SE35

```
SE35..                                                              SE35  10
/*******************************************************************/SE35  20
/*                                                                 */SE35  30
/*      SMOOTH AN EQUIDISTANTLY TABLED FUNCTION USING              */SE35  40
/*      A THIRD DEGREE POLYNOMIAL FIT RELEVANT TO FIVE POINTS      */SE35  50
/*                                                                 */SE35  60
/*******************************************************************/SE35  70
   PROCEDURE(Y,Z,DIM),.                                             SE35  80
   DECLARE                                                          SE35  90
         (Y(*),Z(*),YA,YB,YC,                                       SE35 100
         DA,DB,DAB,DBC)                                             SE35 110
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/SE35 120
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/SE35 130
         (DIM,I)BINARY FIXED,                                       SE35 140
         ERROR EXTERNAL CHARACTER(1),.                              SE35 150
   IF DIM GE 5                                                      SE35 160
   THEN DO,.                                                        SE35 170
         YA    =Y(4),.                                            SE35 180
         YB    =Y(1),.                                            SE35 190
         YC    =Y(2),.                                            SE35 200
         DBC   =YB-YC+YA-YC+YA-Y(5),.                             SE35 210
         DB    =(DBC+DBC                                          SE35 220
               +YA+YB+YB)/3-YC,.     /*MODIFICATION  DB =DELTA2(1)  */SE35 230
         DBC   =DBC/2,.              /*MODIFICATION  DBC=DELTA3(1/2)*/SE35 240
               DO I =3 TO DIM,.                                     SE35 250
               YA    =YB,.           /*REPLACE YA BY Y(I-2)       */SE35 260
               YB    =YC,.           /*REPLACE YB BY Y(I-1)       */SE35 270
               YC    =Y(I),.         /*SET YC TO Y(I)             */SE35 280
               DA    =DB,.           /*SAVE OLD SECOND DIFFERENCE */SE35 290
               DB    =(YA-YB)-(YB-YC),. /*COMPUTE DELTA2(I-1)     */SE35 300
               DAB   =DBC,.          /*SAVE OLD THIRD DIFFERENCE  */SE35 310
               DBC   =DA-DB,.        /*COMPUTE DELTA3(I-3/2)      */SE35 320
               Z(I-2)=YA             /*SET Z(I-2) TO              */SE35 330
                     -(DAB-DBC)*6/70,. /*Y(I-2)-DELTA4(I-2)*6/70   */SE35 340
               END,.                                                SE35 350
         DA    =(DAB-DBC)/35,.                                    SE35 360
         Z(DIM-1)=YB+DA+DA,.         /*COMPUTE LAST TWO SMOOTHED  */SE35 370
         Z(DIM)=YC-DA/2,.            /*VALUES                     */SE35 380
         ERROR='0',.                 /*SUCCESSFUL OPERATION       */SE35 390
         END,.                                                      SE35 400
   ELSE ERROR='1',.                  /*ERROR IN SPECIFIED DIMENSION */SE35 410
   END,.                             /*END OF PROCEDURE S35       */SE35 420
```

Purpose:

SE35 computes a vector $Z = (z_1, z_2, \ldots, z_{DIM})$ of smoothed function values, given a vector $Y = (y_1, y_2, \ldots, y_{DIM})$ of function values whose components y_i correspond to DIM equidistantly spaced argument values x_i with $x_i - x_{i-1} = h$ for $i = 2, \ldots,$ DIM.

Usage:

CALL SE35 (Y, Z, DIM);

Y(DIM) - BINARY FLOAT [(53)]
Given vector of function values.

Z(DIM) - BINARY FLOAT [(53)]
Resultant vector of smoothed function values.

DIM - BINARY FIXED
Given dimension of vector Y and Z.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected.

ERROR='1' means DIM is less than five.
Vectors Z and Y may be identically allocated, which means that the given function values are replaced by the resultant smoothed function values.

Method:

The smoothed function values z_i are obtained by evaluating at x_i the least squares polynomial of degree three relevant to five successive points.

For reference see:

F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York-Toronto-London, 1956, pp. 295-302.

Mathematical Background:

For $i = 5,\ldots,n$ we must find a_i, b_i, c_i, and d_i such that

$$w_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i \qquad (1)$$

gives the least-squares fit to the points (x_{i-k}, y_{i-k}), $k = 0,\ldots,4$.

The problem, thus, is to minimize

$$F(a_i, b_i, c_i, d_i) = \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]^2 \qquad (2)$$

The minimum will occur when

$$\frac{\partial F}{\partial a_i} = \frac{\partial F}{\partial b_i} = \frac{\partial F}{\partial c_i} = \frac{\partial F}{\partial d_i} = 0$$

Now:

$$\left.\begin{aligned} \frac{\partial F}{\partial a_i} &= 2\sum_{k=0}^{4} x_{i-k}^3 \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial b_i} &= 2\sum_{k=0}^{4} x_{i-k}^2 \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial c_i} &= 2\sum_{k=0}^{4} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial d_i} &= 2\sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right] \end{aligned}\right\} \qquad (3)$$

Solving (2) and (3) for a_i, b_i, c_i, and d_i, with $x_i - x_{i-1} = h$, we get:

$$a_i = A_i$$

$$b_i = -3A_i x_{i-2} + B_i$$

$$c_i = 3A_i x_{i-2}^2 - 2B_i x_{i-2} + C_i$$

$$d_i = -A_i x_{i-2}^3 + B_i x_{i-2}^2 - C_i x_{i-2} + D_i + \bar{y}_i$$

where:

$$\bar{y}_i = \frac{1}{5}\sum_{k=0}^{4} y_{i-k}$$

$$A_i = -\frac{1}{12h^3}(y_{i-4} - 2y_{i-3} + 2y_{i-1} - y_i)$$

$$B_i = \frac{1}{14h^2}(4y_{i-4} + y_{i-3} + y_{i-1} + 4y_i - 10\bar{y}_i)$$

$$C_i = \frac{1}{12h}(y_{i-4} - 8y_{i-3} + 8y_{i-1} - y_i)$$

$$D_i = -\frac{1}{7}(4y_{i-4} + y_{i-3} + y_{i-1} + 4y_i - 10\bar{y}_i)$$

Finally, the desired smoothed values z_i are given by:

$$z_i = \left\{\begin{array}{lll} w_5(x_1) = y_1 - \frac{1}{70}\delta^4 y_3 & & \text{if } i=1 \\ w_5(x_2) = y_2 + \frac{2}{35}\delta^4 y_3 & & \text{if } i=2 \\ w_{i+2}(x_i) = y_i - \frac{3}{35}\delta^4 y_i & & \text{if } i=3,\ldots,n-2 \\ w_n(x_{n-1}) = y_{n-1} + \frac{2}{35}\delta^4 y_{n-2} & & \text{if } i=n-1 \\ w_n(x_n) = y_n - \frac{1}{70}\delta^4 y_{n-2} & & \text{if } i=n \end{array}\right\} \qquad (4)$$

where:

$$\delta^4 y_i = y_{i-2} - 4y_{i-1} + 6y_i - 4y_{i+1} + y_{i+2}$$

for $i=3,\ldots,n-2$

- Subroutine EXSM

```
EXSM..
/*********************************************************************/
/*                                                                   */
/*      TO FIND THE TRIPLE EXPONENTIAL SMOOTHED SERIES S OF A GIVEN  */
/*      SERIES X.                                                    */
/*                                                                   */
/*********************************************************************/
   PROCEDURE (X,NX,AL,A,B,C,S),.
   DECLARE
        (X(*),S(*),AL,A,B,C,BE,ALCUB,BECUB,DIF)
        BINARY FLOAT,
        ERROR EXTERNAL CHARACTER(1),
        (I,NX)
        BINARY FIXED,.
/*                                                                   */
   ERROR='0',.
/*                                                                   */
/*      TEST THE VALUE OF ALPHA                                      */
/*                                                                   */
   IF AL LE 0 OR AL GE 1
   THEN DO,.
        ERROR='1',.
        GO TO FIN,.
        END,.
   IF NX LT 3
   THEN DO,.
        ERROR='2',.
        GO TO FIN,.
        END,.
/*      IF A=B=C=0.0, GENERATE INITIAL VALUES OF A, B, AND C         */
/*                                                                   */
        IF A = 0.0 AND B = 0.0 AND C = 0.0
   THEN DO,.
        C    =X(1)-2.0*X(2)+X(3),.
        B    =X(2)-X(1)-1.5*C,.
        A    =X(1)-B-0.5*C,.
        END,.
   BE   =1.0-AL,.
   BECUB=BE**3,.
   ALCUB=AL**3,.
/*                                                                   */
/*      DO THE FOLLOWING FOR I = 1 TO NX                             */
/*                                                                   */
        DO I = 1 TO NX,.
        S(I) =A+B+C.5*C,.              /* FIND S(I) FOR 1 PERIOD AHEAD*/
/*                                                                   */
/*      UPDATE COEFFICIENTS A, B, AND C                              */
/*                                                                   */
        DIF  =S(I)-X(I),.
        A    =X(I)+BECUB*DIF,.
        B    =B+C-1.5*AL*AL*(2.0-AL)*DIF,.
        C    =C-ALCUB*DIF,.
        END,.
FIN..
   RETURN,.
   END,.                              /*END OF PROCEDURE EXSM        */
```

Purpose:

EXSM develops the triple exponential smoothed series S of the given series X.

Usage:

CALL EXSM (X, NX, AL, A, B, C, S);

Description of parameters:

X(NX) - BINARY FLOAT
Given vector containing time series data to be exponentially smoothed.

NX - BINARY FIXED
Given number of elements in X.

AL - BINARY FLOAT
Given smoothing constant alpha. AL must be greater than zero and less than one.

A, B, C- BINARY FLOAT
Given coefficients of the prediction equation where S is predicted T periods hence by

$$A + B \cdot T + C \cdot T^2/_2$$

As input: If A=B=C=0, the program will provide initial values. If at least one of A, B, and C is not zero, the program will take given values as initial values.

As output: A, B, C, contain latest updated coefficients of prediction.

S(NX) - BINARY FLOAT
Resultant vector containing triple exponential smoothed time series.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error conditions that may be detected:

ERROR=1 - The specified smoothing constant, AL, is less than or equal to zero or is greater than or equal to one.

ERROR=2 - The number of data points is less than three.

Method:

Refer to R. G. Brown, Smoothing, Forecasting and Prediction of Discrete Time Series, Prentice-Hall, 1963, pp. 140 to 144.

Mathematical Background:

This procedure calculates a smoothed series S_1, S_2, ..., S_{NX}, given time series X_1, X_2, ..., X_{NX} and a smoothing constant α. Also, at the end of the computation, the coefficients A, B, and C are given for the expression $A + B(T) + C(T)^2/_2$. This expression can be used to find estimates of the smoothed series a given number of time periods, T, ahead.

The procedure has the following two stages for i = 1, 2, ..., NX, starting with A, B, and C either given by the user or provided automatically by the procedure (see below):

1. Finds S_i for one period ahead

$$S_i = A + B + 5C \tag{1}$$

2. Update coefficients A, B, and C

$$A = X_i + (1 - \alpha)^3 (S_i - X_i) \tag{2}$$

$$B = B + C - 1.5 (\alpha^2) (2 - \alpha) (S_i - X_i) \tag{3}$$

$$C = C - (\alpha^3) (S_i - X_i) \tag{4}$$

where α = smoothing constant specified by the user

$$(0.0 < \alpha < 1.0)$$

If coefficients A, B, and C are not all zero (0.0), take given values as initial values. However, if A=B=C=0.0, generate initial values of A, B, and C as follows:

$$C = X_1 - 2X_2 + X_3 \quad (5)$$

$$B = X_2 - X_1 - 1.5C \quad (6)$$

$$A = X_1 - B - 0.5C \quad (7)$$

- Subroutine FMFP

```
FMFP..                                                                  FMFP  10
/*********************************************************************/FMFP  20
/*                                                                   */FMFP  30
/*      FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES      */FMFP  40
/*      BY THE METHOD OF FLETCHER AND POWELL                         */FMFP  50
/*                                                                   */FMFP  60
/*********************************************************************/FMFP  70
   PROCEDURE (FUNCT,N,X,F,G,EST,EPS,LIMIT),.                            FMFP  80
   DECLARE                                                              FMFP  90
         (I,J,KOUNT,K,L,LIMIT,N,NS,N2,N3)                               FMFP 100
         BINARY FIXED,                                                  FMFP 110
         (X(*),G(*),H(N*(N+7)/2),ALFA,AMBDA,DALFA,DX,DY,GS,GNRM,FS,     FMFP 120
         EPS,EST,F,FX,FY,H1,H2,HNRM,OLDF,T,W,Z)                         FMFP 130
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/FMFP 140
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/FMFP 150
         FUNCT                                                          FMFP 160
         ENTRY,                                                         FMFP 170
         ERROR EXTERNAL                                                 FMFP 180
         CHARACTER(1),.                                                 FMFP 190
   NS    =N,.                                                           FMFP 200
   N2    =NS+NS,.                                                       FMFP 210
   N3    =N2+NS,.                                                       FMFP 220
   CALL FUNCT(X,FS,G),.                /*COMPUTE FUNCTION VALUE       */FMFP 230
   ERROR='0',.                         /*AND GRADIENT VECTOR          */FMFP 240
   KOUNT=0,.                                                            FMFP 250
CONT..                                                                  FMFP 260
   I     =N3,.                                                          FMFP 270
         DO J = NS-1 TO 0 BY -1,.      /*GENERATE IDENTITY MATRIX     */FMFP 280
         K     =I+1,.                                                   FMFP 290
         H(K) =1,.                                                      FMFP 300
         I     =K+J,.                                                   FMFP 310
               DO L = K+1 TO I,.                                        FMFP 320
               H(L) =0,.                                                FMFP 330
               END,.                                                    FMFP 340
         END,.                                                          FMFP 350
LOOP..                               /*START ITERATION LOOP         */FMFP 360
   KOUNT=KOUNT+1,.                                                      FMFP 370
   OLDF =FS,.                        /*SAVE FUNCTION VALUE,         */FMFP 380
   DY,HNRM,GNRM=0,.                  /*ARGUMENT VECTOR              */FMFP 390
         DO J = 1 TO NS,.            /*AND GRADIENT VECTOR          */FMFP 400
         H(NS+J),GS=G(J),.                                              FMFP 410
         H(N2+J)=X(J),.                                                 FMFP 420
         T     =0,.                                                     FMFP 430
         K     =N3+J,.                                                  FMFP 440
               DO L = 1 TO NS,.      /*DETERMINE DIRECTION VECTOR   */FMFP 450
               T     =T-G(L)*H(K),.                                     FMFP 460
               IF L LT J                                                FMFP 470
               THEN K     =K+NS-L,.                                     FMFP 480
               ELSE K     =K+1,.                                        FMFP 490
               END,.                                                    FMFP 500
         H(J) =T,.                                                      FMFP 510
         HNRM =HNRM+ABS(T),.           /*CALCULATE DIRECTIONAL        */FMFP 520
         GNRM =GNRM+ABS(GS),.          /*DERIVATIVE AND TESTVALUES    */FMFP 530
         DY    =DY+T*GS,.              /*FOR DIRECTION VECTOR H       */FMFP 540
         END,.                         /*AND GRADIENT VECTOR G.       */FMFP 550
   IF DY LT 0                          /*REPEAT SEARCH IN DIRECTION   */FMFP 560
   THEN IF HNRM/GNRM GT EPS            /*OF STEEPEST DESCENT IF       */FMFP 570
   THEN GO TO LAB1,.                   /*DIRECTIONAL DERIVATIVE       */FMFP 580
   GO TO REST,.                        /*APPEARS NOT NEGATIVE         */FMFP 590
LAB1..                                 /*SEARCH MINIMUM ALONG H       */FMFP 600
   FY    =FS,.                                                          FMFP 610
   AMBDA=MIN(1,2*(EST-FS)/DY),.                                         FMFP 620
   IF AMBDA LE 0                                                        FMFP 630
   THEN AMBDA=1,.                                                       FMFP 640
   ALFA =0,.                                                            FMFP 650
SAVE..                                 /*SAVE FUNCTION AND DERIVATIVE */FMFP 660
   FX    =FY,.                         /*VALUES FOR OLD ARGUMENT      */FMFP 670
   DX    =DY,.                                                          FMFP 680
         DO I = 1 TO NS,.              /*STEP ARGUMENT ALONG H        */FMFP 690
         X(I) =X(I)+AMBDA*H(I),.                                        FMFP 700
         END,.                                                          FMFP 710
   CALL FUNCT(X,FS,G),.                                                 FMFP 720
   FY    =FS,.                                                          FMFP 730
   DY    =0,.                          /*COMPUTE DIRECTIONAL DERIVA-  */FMFP 740
         DO I = 1 TO NS,.              /*TIVE DY FOR NEW ARGUMENT.    */FMFP 750
         DY    =DY+G(I)*H(I),.         /*TERMINATE SEARCH, IF DY GE 0 */FMFP 760
         END,.                         /*IF DY=0,THE MINIMUM IS FOUND */FMFP 770
   IF FY LT FX                         /*PROVIDED FUNCTION DECREASED  */FMFP 780
   THEN DO,.                                                            FMFP 790
         IF DY= 0                                                       FMFP 800
         THEN GO TO COMP,.                                              FMFP 810
         IF DY LT 0                    /*TERMINATE SEARCH IF          */FMFP 820
         THEN DO,.                     /*MINIMUM PASSED               */FMFP 830
               ALFA,AMBDA=AMBDA+ALFA,. /*DOUBLE STEPSIZE AND REPEAT   */FMFP 840
               IF HNRM*AMBDA LE 1E10                                    FMFP 850
               THEN GO TO SAVE,.                                        FMFP 860
               ERROR='2',.             /*ARGUMENT OUT OF RANGE        */FMFP 870
               GO TO RETURN,.                                           FMFP 880
               END,.                                                    FMFP 890
         END,.                                                          FMFP 900
   T     =0,.                                                           FMFP 910
LAB2..                                                                  FMFP 920
   IF AMBDA= 0                         /*INTERPOLATE IN NEW INTERVAL  */FMFP 930
   THEN GO TO COMP,.                   /*COMPUTE ARGUMENT X           */FMFP 940
   Z     =3*(FX-FY)/AMBDA+DX+DY,.                                       FMFP 950
   ALFA =MAX(ABS(Z),ABS(DX),ABS(DY)),.                                  FMFP 960
   DALFA=Z/ALFA,.                                                       FMFP 970
   DALFA=DALFA*DALFA-DX/ALFA*DY/ALFA,.                                  FMFP 980
   IF DALFA LT 0                                                        FMFP 990
   THEN GO TO REST,.                                                    FMFP1000
   W     =ALFA*SQRT(DALFA),.                                            FMFP1010
   ALFA =DY-DX+W+W,.                                                    FMFP1020
   IF ALFA=0                                                            FMFP1030
   THEN ALFA =(Z+DY-W)/(Z+DX+Z+DY),.                                    FMFP1040
   ELSE ALFA =(DY-Z+W)/ALFA,.                                           FMFP1050
   ALFA =ALFA*AMBDA,.                                                   FMFP1060
   DALFA=T-ALFA,.                                                       FMFP1070
         DO I = 1 TO NS,.                                               FMFP1080
         X(I) =X(I)+DALFA*H(I),.                                        FMFP1090
         END,.                                                          FMFP1100
   CALL FUNCT(X,FS,G),.                                                 FMFP1110
   IF FS LE FX                                                          FMFP1120
   THEN IF FS LE FY                                                     FMFP1130
   THEN GO TO COMP,.                   /*TERMINATE INTERPOLATION      */FMFP1140
   DALFA=0,.                                                            FMFP1150
         DO I = 1 TO NS,.                                               FMFP1160
         DALFA=DALFA+G(I)*H(I),.                                        FMFP1170
         END,.                                                          FMFP1180
   IF DALFA LT 0                                                        FMFP1190
   THEN IF FS LE FX                                                     FMFP1200
```

```
   THEN DO;.                                                        FMFP1210
        FX   =FS;.                                                  FMFP1220
        DX   =DALFA;.                                               FMFP1230
        T,AMBDA=ALFA;.                                              FMFP1240
        GO TO LAB2;.                    /*REPEAT INTERPOLATION      */FMFP1250
        END;.                                                       FMFP1260
   FY   =FS;.                                                       FMFP1270
   DY   =DALFA;.                                                    FMFP1280
   AMBDA=AMBDA-ALFA;.                                               FMFP1290
   T    =0;.                                                        FMFP1300
   GO TO LAB2;.                     /*REPEAT INTERPOLATION      */FMFP1310
COMP..                                                              FMFP1320
        DO J = 1 TO NS;.            /*COMPUTE DIFFERENCE VECTORS  */FMFP1330
        K    =NS+J;.                /*OF ARGUMENT AND GRADIENT    */FMFP1340
        H(K) =G(J)-H(K);.                                           FMFP1350
        K    =NS+K;.                                                FMFP1360
        H(K) =X(J)-H(K);.                                           FMFP1370
        END;.                                                       FMFP1380
   IF OLDF+EPS LT FS                                                FMFP1390
   THEN GO TO REST;.                /*TERMINATE ITERATION       */FMFP1400
   ERROR='0';.                                                      FMFP1410
   IF KOUNT GE NS                                                   FMFP1420
   THEN DO;.                                                        FMFP1430
        T,Z  =0;.                                                   FMFP1440
             DO J = 1 TO NS;.                                       FMFP1450
             W    =H(N2+J);.                                        FMFP1460
             T    =T+ABS(W);.                                       FMFP1470
             Z    =Z+H(NS+J)*W;.                                    FMFP1480
             END;.                                                  FMFP1490
        IF HNRM LE EPS                                              FMFP1500
        THEN IF T LE EPS            /*TERMINATE, IF ARGUMENT DIFF. */FMFP1510
        THEN GO TO RETURN;.         /*VECTOR AND DIRECTION VECTOR  */FMFP1520
        END;.                       /*ARE BOTH   LE EPS            */FMFP1530
   IF KOUNT GE LIMIT                                                FMFP1540
   THEN GO TO NCON;.                                                FMFP1550
   ALFA =0;.                                                        FMFP1560
        DO J = 1 TO NS;.                                            FMFP1570
        W    =0;.                                                   FMFP1580
        K    =N3+J;.                                                FMFP1590
             DO L = 1 TO NS;.                                       FMFP1600
             W    =W+H(NS+L)*H(K);.                                 FMFP1610
             IF L LT J                                              FMFP1620
             THEN K    =K+NS-L;.                                    FMFP1630
             ELSE K    =K+1;.                                       FMFP1640
             END;.                                                  FMFP1650
        ALFA =ALFA+W*H(NS+J);.                                      FMFP1660
        H(J) =W;.                                                   FMFP1670
        END;.                                                       FMFP1680
   IF Z*ALFA= 0                                                     FMFP1690
   THEN GO TO CONT;.                                                FMFP1700
   K    =N3+1;.                                                     FMFP1710
        DO L = 1 TO NS;.            /*UPDATE MATRIX H           */FMFP1720
        H1   =H(N2+L)/Z;.                                           FMFP1730
        H2   =H(L)/ALFA;.                                           FMFP1740
             DO J = L TO NS;.                                       FMFP1750
             H(K) =H(K)+H1*H(N2+J)                                  FMFP1760
                  -H2*H(J);.                                        FMFP1770
             K    =K+1;.                                            FMFP1780
             END;.                                                  FMFP1790
        END;.                                                       FMFP1800
   GO TO LOOP;.                     /*END OF ITERATION LOOP     */FMFP1810
NCON..                                                              FMFP1820
   ERROR='1';.                      /*NO CONVERGENCE            */FMFP1830
   GO TO RETURN;.                                                   FMFP1840
REST..                              /*RESTORE OLD VAL, ARG      */FMFP1850
        DO J = 1 TO NS;.                                            FMFP1860
        X(J) =H(N2+J);.                                             FMFP1870
        END;.                                                       FMFP1880
   CALL FUNCT(X,FS,G);.                                             FMFP1890
   IF GNRM GT EPS                                                   FMFP1900
   THEN IF ERROR= '3'                                               FMFP1910
   THEN GO TO RETURN;.                                              FMFP1920
   ELSE DO;.                                                        FMFP1930
        ERROR='3';.                 /*REPEAT, IF DERIVATIVE GT EPS */FMFP1940
        GO TO CONT;.                                                FMFP1950
        END;.                                                       FMFP1960
   ERROR='C';.                                                      FMFP1970
RETURN..                                                            FMFP1980
   F    =FS;.                                                       FMFP1990
   END;.                            /*END OF PROCEDURE FMFP     */FMFP2000
```

Purpose:

FMFP determines an unconstrained minimum of a function of several variables, given a starting value of argument vector.

Usage:

CALL FMFP (FUNCT, N, X, F, G, EST, EPS, LIMIT);

FUNCT - ENTRY
Given procedure computing function values and gradient vectors. This procedure must be supplied by the user.

Usage:
CALL FUNCT (X, FS, G);
X(N) - BINARY FLOAT [(53)]
Given n-dimensional argument vector.
FS - BINARY FLOAT [(53)]
Resultant function value.
G(N) - BINARY FLOAT [(53)]
Resultant gradient vector.

N - BINARY FIXED
Given number of variables (= dimension of argument vector).

X(N) - BINARY FLOAT [(53)]
Given starting value of argument vector. Resultant argument vector corresponding to the minimum.

F - BINARY FLOAT [(53)]
Resultant minimum function value.

G(N) - BINARY FLOAT [(53)]
Resultant gradient vector corresponding to the minimum.

EST - BINARY FLOAT [(53)]
Given estimate of minimum function value.

EPS - BINARY FLOAT [(53)]
Given test value representing the expected absolute error.

LIMIT - BINARY FIXED
Given maximum number of iterations to be performed.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR='1' means no convergence in LIMIT iterations.
ERROR='2' means no minimum is located by linear search technique.
ERROR='3' means error in gradient calculation.

Method:

FMFP uses a method of conjugate directions, proposed by Davidon. For a quadratic function of n variables the minimum is located within n iterations.

For reference see

R. Fletcher and M. J. Powell, "A Rapidly Convergent Descent Method for Minimization", Computer Journal, vol. 6, iss. 2, 1963, pp. 163-168.

Mathematical Background:

It is assumed that the function f of the n variables $x_1, \ldots, x_n$ (abbreviated as argument vector x) may be computed together with its gradient vector g(x) for any point x. The generalized Taylor expansion for functions of several variables is

$$f(x+u) = f(x) + g(x) \cdot u + \frac{1}{2} u^T G(x) u + \text{higher terms}$$

where g is the gradient vector and G the matrix of second order partial derivatives. Vectors are assumed to be column vectors; u^T means transpose of vector u. It is assumed that in the neighborhood of the required minimum x_{min} the function is approximated closely by the first three terms of its Taylor expansion, giving

$$f(x) = f(x_{min}) + \frac{1}{2} (x - x_{min})^T G(x_{min})(x - x_{min})$$

since $g(x_{min}) = 0$. Then the gradient is seen to be approximately $g(x) = G(x_{min})\ (x - x_{min})$.

Assume now that the symmetric matrix G is positive definite. Then the following equation holds true:

$$x - x_{min} = G^{-1}\ (x_{min}) \cdot g(x)$$

which would allow x_{min} to be calculated in one step if $G^{-1}\ (x_{min})$ were available.

To approach $G^{-1}\ (x_{min})$, a method of successive linear searches in G-conjugate directions is used. Starting with the identity matrix $G^{(0)} = I$, a sequence of symmetric matrices $G^{(i)}$ is generated that approximates G^{-1}. At the $(i+1)^{st}$ iteration step a linear search is made in direction $h^{(i)} = -G^{(i)} g^{(i)}$, where $g^{(i)}$ is an abbreviation for $g(x^{(i)})$. By means of the linear search the minimum of $y(t) = f(x^{(i)}) + t \cdot h^{(i)})$ is determined, giving argument $x^{(i+1)} = x^{(i)} + t_i \cdot h^{(i)}$.

The argument of the minimum $x^{(i+1)}$ on the line through $x^{(i)}$ in direction $h^{(i)}$ is determined by the relation that scalar product $(g^{(i+1)}, h^{(i)}) = 0$.

Now:

$$x^{(n)} = x^{(j)} + \sum_{i=j}^{n-1} t_i\, h^{(i)}$$

and:

$$g^{(n)} = g^{(j)} + \sum_{i=j}^{n-1} t_i\, Gh^{(i)}$$

Therefore:

scalar product

$$(g^{(n)}, h^{(j)}) = \sum_{i=j+1}^{n-1} t_i\, (Gh^{(i)}, h^{(j)})$$

Suppose now that the vectors $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ are G-conjugate, satisfying $(Gh^{(i)}, h^{(j)}) = 0$ for $i \neq j$. Then $(g^{(n)}, h^{(j)}) = 0$, and since $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ form a basis, $g^{(n)} = 0$ and $x^{(n)} = x_{min}$. This shows that the minimum is located at the nth iteration for a quadratic function when using successive linear searches for G-conjugate directions.

Programming Considerations:

For the generation of G-conjugate directions, start with $h^{(0)} = -g^{(0)}$ and calculate successive directions $h^{(i)}$ by means of $h^{(i)} = -G^{(i)} g^{(i)}$, where $G^{(i)}$ is modified to $G^{(i+1)}$ so that $h^{(i)}$ is an eigenvector of the matrix $G^{(i+1)}$ G with eigenvalue 1. This ensures that $G^{(i)}$ approaches G^{-1} as $x^{(i)}$ approaches x_{min}. An easy calculation shows:

$$G^{(i+1)} = G^{(i)} + \frac{dx \cdot dx^T}{dx^T \cdot dg} - \frac{G^{(i)} dg \cdot dg^T G^{(i)}}{dg^T\, G^{(i)} dg}$$

with $dg = g^{(i+1)} - g^{(i)}$

$$dx = x^{(i+1)} - x^{(i)}$$

where all vectors are regarded as column vectors, and superscript T means transpose of column vector--that is, row vector.

The strategy adopted for termination of the successive linear searches is as follows:

1. If the function value has not decreased in the last iteration step, the search for the minimum is terminated provided the gradient is already sufficiently small; otherwise, the next step is in the direction of steepest descent.
2. If the argument vector and the direction vector change by very small amounts, and at least n iterations are performed, the minimization is terminated again.
3. If the number of iterations exceeds an upper bound furnished by the user, further calculation is bypassed, and an error code is set to 1 indicating poor convergence.
4. If one of the successive linear searches indicates that no constrained minimum exists, further

calculation is bypassed again and the error code is set to 2, indicating that it is likely that no minimum exists.

The ith term $G^{(i)}$ is reset to the identity matrix if there is indication that the current $G^{(i)}$ is not positive definite, or if the formula for $G^{(i+1)}$ breaks down because of zero divisors.

The linear search technique used in procedure FMFP is as follows:
For a given argument vector x and a vector h defining a direction through x, a local minimum of the function $y(t) = f(x+t \cdot h)$ must be found. This means that a value t_m must be determined for which

$$y'(t_m) = \text{scalar product } (g(x+t_m \cdot h), h) = 0$$

From $y'(0) = (g(x),h) < 0$ it is evident that a minimum $y(t_m) < y(0)$ should be found for positive values of t.

The calculation of the minimum is in three stages:

1. Estimating the magnitude of t_m.
2. Determining an interval containing t_m.
3. Interpolating the value of t_m.

An estimate of the stepsize may be obtained, assuming that the true value of the constrained minimum is equal to the estimated value EST of the unconstrained minimum and that y(t) is closely represented by a quadratic polynomial passing through x, y(0) with derivative y' (0):

$$\text{step} = 2\,(\text{EST} - y(0))/y'(0)$$

This equation tends to overestimate the stepsize since the unconstrained minimum will normally not lie on the line through x with direction h. Therefore step is taken as stepsize s only if it is positive and less than one. Otherwise s = 1 is taken as stepsize.

At the second stage y(t) and y'(t) are examined at the points

$$t = s, 2s, 4s, \ldots, s_1, s_2$$

where successive values are obtained by doubling the stepsize.

This search is terminated at $t = s_2$ if:

$$y'(s_2) = 0$$

or $y'(s_2) > 0$

or $y(s_2) \geq y(s_1)$

or if $s_2 \cdot \left(\sum_{i=1}^{N} |h_i|\right) > 10^{10}$.

The last case (search argument runs out of range) is interpreted as an indication that no local minimum exists on the given line. Therefore, the error indicator is set to '2' and further calculation is bypassed; that is, FMFP returns the current minimal value with ERROR = '2'.

In case $y'(s_2) = 0$, t_m is set to s_2 and $x_m = x+s_2 \cdot h$ is used as argument of a constrained minimum on the line through x with direction h.

In the second and third case $y'(s_2) > 0$ and/or $y(s_2) \geq y(s_1)$, a minimum lies necessarily between s_1 and s_2. Its argument value gets approximated using cubic interpolation.

The extrema of the cubic interpolation passing through (s_1, $y_1 = y(s_1)$, $y'_1 = y'(s_1)$) and s_2, $y_2 = y(s_2)$, $y'_2 = y'(s_2)$) are the roots of the quadratic equation

$$y'_1 - 2(z+y'_1)\frac{t-s_1}{s_2-s_1} + (y'_1+y'_2+2z)\left(\frac{t-s_1}{s_2-s_1}\right)^2 = 0$$

$$\text{with } z = y'_1 + y'_2 - 3\frac{y_2-y_1}{s_2-s_1}$$

The substitution $\frac{t-s_1}{s_2-s_1} = 1-\alpha$ gives

$$y'_2 - 2\alpha(y'_2+z)+\alpha^2(y'_1+y'_2+2z) = 0$$

with the solutions

$$\alpha = \frac{y'_2+z \pm w}{y'_1+y'_2+2z}$$

where

$$w = +\sqrt{z^2 - y'_1 y'_2}$$

It is interesting to note that $y'_1 < 0$, $y'_2 \geq 0$, as well as $y'_1 < 0$, $y'_2 < 0$, $y_2 \geq y_1$, that is, $|z| < |y'_1 + y'_2|$, guarantee a real value of w. This means the cubic interpolation polynomial has real extrema.

The cubic interpolation polynomial may degenerate to a quadratic if $y'_1 + y'_2 + 2z = 0$

with minimum at

$$\alpha = \frac{y'_2}{y'_2 - y'_1}$$

The sign of w must be so chosen that α belongs to the minimum, which is necessarily between s_1 and s_2.

From

$$\alpha = \frac{y'_2 - z + w}{y'_2 - y'_1 + 2w}$$

$$= \frac{(y'_2 - z + w)(y'_2 - y'_1 - 2w)}{(y'_2 - y'_1 + 2w)(y'_2 - y'_1 - 2w)}$$

$$= \frac{(y'_2 + z - w)(y'_1 + y'_2 - 2z)}{(y'_1 + y'_2 + 2z)(y'_1 + y'_2 - 2z)} = \frac{y'_2 + z - w}{y'_1 + y'_2 + 2z}$$

It is easily seen that

$$\alpha = \frac{y'_2 - z + w}{y'_2 - y'_1 + 2w}$$

respectively, if $y'_2 - y'_1 + 2w = 0$

$$\alpha = \frac{y'_2 + z - w}{y'_1 + y'_2 + 2z}$$

give the argument of the minimum in all cases. The first formula gives extra numerical stability if y'_1 is close to $-y'_2$ and y_1 is close to y_2 and also contains the degenerate case as special. The second formula may be necessary if both extreme values lie between s_1 and s_2. Then the one closer to s_1 is the minimum. (This follows easily from geometrical considerations.)

The following analysis shows that $0 < \alpha < 1$:

$y'_2 > 0$, $y'_1 < 0$ implies $w > |z|$. Hence

$$0 < \frac{y'_2}{y'_2 + 2w - y'_1} < \alpha = \frac{y'_2 + w - z}{y'_2 - y'_1 + 2w}$$

$$< \frac{y'_2 + 2w}{y'_2 + 2w - y'_1} < 1 \qquad (1)$$

$y_2 \geq y'_1$, $y'_2 < 0$ implies $0 > z \leq y'_2 + y'_1$ and $w < |z|$.

Hence

$$0 < \frac{-y'_2 - z}{-y'_2 - 2z - y'_1} < \alpha = \frac{y'_2 + z - w}{y'_1 + y'_2 + 2z}$$

$$< \frac{-y'_2 - 2z}{-y'_2 - 2z - y'_1} < 1 . \qquad (2)$$

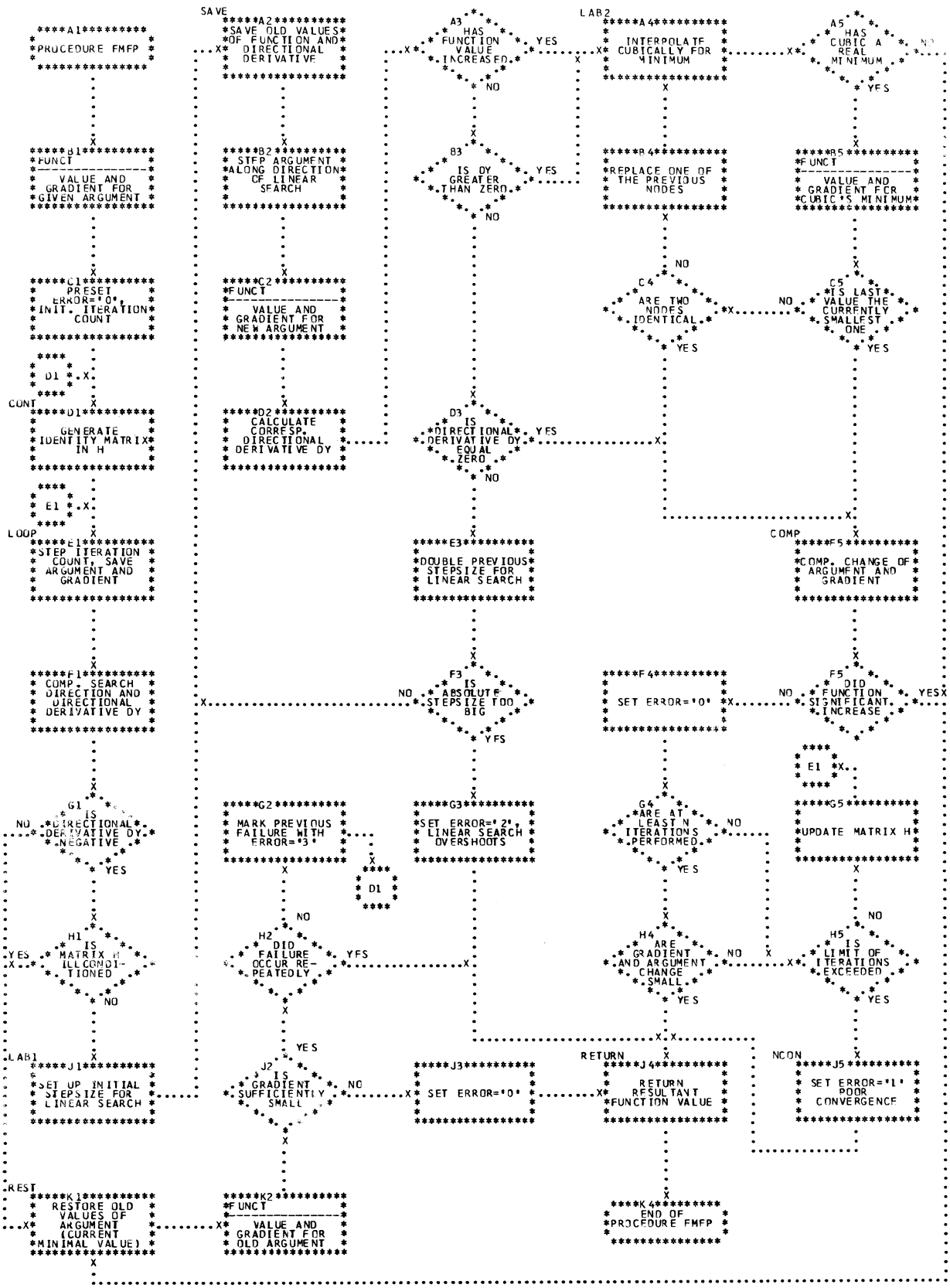
Note that for the other root

$$\frac{y'_2 + z + w}{y'_1 + y'_2 + 2z} < \frac{-y'_2 - z}{-y'_2 - 2z - y'_1} < \alpha .$$

The minimum of the cubic interpolation polynomial is located at

$$s_3 = s_1 + (1-\alpha)(s_2 - s_1) = s_2 - \alpha(s_2 - s_1)$$

If $y(s_3) \leq y(s_1)$ and $y(s_3) \leq y(s_2)$, then t_m is set equal to s_3 and $x_m = x + t_m \cdot h$ is used as argument of the wanted minimum along the given line. Otherwise, the interval (s_1, s_2) is reduced by replacing s_1 by s_3 if $y(s_3) \leq y(s_1)$ and $y'(s_3) < 0$ and by replacing s_2 by s_3 in all other cases. Then the interpolation process is repeated for this new reduced interval.


PROCEDURE FMFP DETERMINES AN UNCONSTRAINED MINIMUM OF A FUNCTION OF SEVERAL VARIABLES
PROCEDURE FMFP
A1
FUNCT
VALUE AND GRADIENT FOR GIVEN ARGUMENT
PRESET ERROR='0', INIT. ITERATION COUNT
CONT
GENERATE IDENTITY MATRIX IN H
LOOP
STEP ITERATION COUNT, SAVE ARGUMENT AND GRADIENT
COMP. SEARCH DIRECTION AND DIRECTIONAL DERIVATIVE DY
IS DIRECTIONAL DERIVATIVE DY NEGATIVE
YES
IS MATRIX H ILLCONDITIONED
NO
LAB1
SET UP INITIAL STEPSIZE FOR LINEAR SEARCH
REST
RESTORE OLD VALUES OF ARGUMENT (CURRENT MINIMAL VALUE)
SAVE
SAVE OLD VALUES OF FUNCTION AND DIRECTIONAL DERIVATIVE
STEP ARGUMENT ALONG DIRECTION OF LINEAR SEARCH
FUNCT
VALUE AND GRADIENT FOR NEW ARGUMENT
CALCULATE CORRESP. DIRECTIONAL DERIVATIVE DY
MARK PREVIOUS FAILURE WITH ERROR='3'
DID FAILURE OCCUR REPEATEDLY
YES
IS GRADIENT SUFFICIENTLY SMALL
NO
FUNCT
VALUE AND GRADIENT FOR OLD ARGUMENT
D1
A3
HAS FUNCTION VALUE INCREASED
NO
B3
IS DY GREATER THAN ZERO
NO
D3
IS DIRECTIONAL DERIVATIVE DY EQUAL ZERO
NO
DOUBLE PREVIOUS STEPSIZE FOR LINEAR SEARCH
F3
IS ABSOLUTE STEPSIZE TOO BIG
YES
SET ERROR='2', LINEAR SEARCH OVERSHOOTS
G1
D1
LAB2
INTERPOLATE CUBICALLY FOR MINIMUM
REPLACE ONE OF THE PREVIOUS NODES
C4
ARE TWO NODES IDENTICAL
YES
SET ERROR='0'
G4
ARE AT LEAST N ITERATIONS PERFORMED
YES
H4
ARE GRADIENT AND ARGUMENT CHANGE SMALL
YES
RETURN
RETURN RESULTANT FUNCTION VALUE
K4
END OF PROCEDURE FMFP
A5
HAS CUBIC A REAL MINIMUM
YES
FUNCT
VALUE AND GRADIENT FOR CUBIC'S MINIMUM
C5
IS LAST VALUE THE CURRENTLY SMALLEST ONE
YES
COMP
COMP. CHANGE OF ARGUMENT AND GRADIENT
F5
DID FUNCTION SIGNIFICANT INCREASE
YES
E1
UPDATE MATRIX H
H5
IS LIMIT OF ITERATIONS EXCEEDED
YES
NCON
SET ERROR='1' POOR CONVERGENCE

- Subroutine RTF

```
RTF..                                                                  RTF   10
/*********************************************************************/RTF   20
/*                                                                   */RTF   30
/*      CALCULATE ROOT OF GIVEN FUNCTION                             */RTF   40
/*      IF OPT = '0' BY LINEAR INTERPOLATION (SECANT METHOD)         */RTF   50
/*      IF OPT = '1' BY QUADRATIC INTERPOLATION (MULLER'S METHOD)    */RTF   60
/*      IF OPT = '2' BY HYPERBOLIC INTERPOLATION (HALLEY'S METHOD)   */RTF   70
/*                                                                   */RTF   80
/*********************************************************************/RTF   90
   PROCEDURE(X,F,FCT,LIMIT,OPT),.                                      RTF  100
   DECLARE                                                             RTF  110
        (ERROR EXTERNAL,INCL,LOPT,OPT)                                 RTF  120
        CHARACTER(1),                                                  RTF  130
        (STEP,CT,LIMIT)                                                RTF  140
        BINARY FIXED,                                                  RTF  150
        (X,F,T,Y,XX,DX,X1,X2,F1,F2,X10,X20,X21,                        RTF  160
        F10,F21,FF,XXX,TOL,MI,MA)                                      RTF  170
        BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/RTF  180
 /*     BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/RTF  190
        FCT ENTRY() RETURNS                                            RTF  200
        (BINARY FLOAT),.               /*SINGLE PRECISION VERSION  /*S*/RTF  210
 /*     (BINARY FLOAT(53)),.           /*DOUBLE PRECISION VERSION  /*D*/RTF  220
   STEP =1,.                           /*INIT. ITERATION COUNT       */RTF  230
   X2   =X,.                                                           RTF  240
   F,F2 =FCT(X2),.                     /*CALCULATE STARTING VALUE    */RTF  250
   INCL,ERROR='0',.                                                    RTF  260
   CT   =0,.                                                           RTF  270
SEEK..                                 /*LOCATE BETTER POINT         */RTF  280
   F1   =1,.                           /*BY SIMPLE SEARCH PROCESS    */RTF  290
   LOPT ='S',.                                                         RTF  300
   MI   =MIN(0.1,ABS(F)),.                                             RTF  310
   MA   =MAX(1,ABS(X)),.                                               RTF  320
SEEK2..                                                                RTF  330
   DX   =MI/F1,.                                                       RTF  340
   X1   =1,.                                                           RTF  350
SEEK1..                                                                RTF  360
   T    =X+DX,.                                                        RTF  370
   DX   =-DX,.                                                         RTF  380
TEST..                                                                 RTF  390
   Y    =FCT(T),.                      /*CALCULATE FUNCTION VALUE    */RTF  400
   STEP =STEP+1,.                      /*STEP ITERATION COUNT        */RTF  410
   IF STEP GE LIMIT                                                    RTF  420
   THEN GO TO EXIT,.                   /*TERMINATE WITH ERROR = 'C'  */RTF  430
   IF INCL='1'                         /*TEST FOR PREVIOUS SIGN-CHANGE*/RTF  440
   THEN DO,.                                                           RTF  450
        IF Y*FF LT 0                                                   RTF  460
        THEN XXX  =T,.                                                 RTF  470
        ELSE GO TO SIGN,.                                              RTF  480
        END,.                                                          RTF  490
   ELSE DO,.                                                           RTF  500
        IF Y*F LE 0                    /*TEST FOR SIGN-CHANGE        */RTF  510
        THEN DO,.                                                      RTF  520
             INCL ='1',.               /*MARK SIGN CHANGE            */RTF  530
             XXX  =X,.                                                 RTF  540
SIGN..                                                                 RTF  550
             XX   =T,.                                                 RTF  560
             FF   =Y,.                                                 RTF  570
             END,.                                                     RTF  580
        END,.                                                          RTF  590
   IF ABS(Y) LT ABS(F)                 /*TEST FOR IMPROVEMENT        */RTF  600
   THEN DO,.                                                           RTF  610
        X    =T,.                                                      RTF  620
        F    =Y,.                                                      RTF  630
        GO TO CHECK,.                                                  RTF  640
        END,.                                                          RTF  650
   IF INCL='1'                                                         RTF  660
   THEN GO TO CHECK,.                                                  RTF  670
   IF LOPT NE 'S'                                                      RTF  680
   THEN GO TO SEEK,.                                                   RTF  690
   IF DX LT 0                                                          RTF  700
   THEN GO TO SEEK1,.                  /*SEEK AT SYMMETRIC POINT     */RTF  710
   X1   =X1+1,.                                                        RTF  720
   DX   =DX+DX,.                       /*SEEK FARTHER AWAY           */RTF  730
   IF X1 LE F1                                                         RTF  740
   THEN GO TO SEEK1,.                                                  RTF  750
   F1   =F1+2,.                        /*STEP ODD INTEGER DENOMINATOR*/RTF  760
   GO TO SEEK2,.                                                       RTF  770
CHECK..                                                                RTF  780
   TOL  =1E-5*MA,.                     /*SINGLE PRECISION VERSION  /*S*/RTF  790
 /*TOL  =1E-12*MA,.                    /*DOUBLE PRECISION VERSION  /*D*/RTF  800
   IF ABS(DX) LE TOL                                                   RTF  810
   THEN DO,.                                                           RTF  820
        CT   =CT+1,.                                                   RTF  830
        IF ABS(Y) GT TOL               /*TERMINATE SUCCESSFULLY IF   */RTF  840
        THEN IF CT LE 5                /*BOTH ARGUMENT-CHANGE AND    */RTF  850
        THEN GO TO CONT,.              /*FUNCTION VALUE ARE SMALL    */RTF  860
        ELSE ERROR='W',.               /*WITH WARNING IF ARGUMENT-   */RTF  870
        GO TO RETURN,.                 /*CHANGE ONLY IS SMALL REPEAT.*/RTF  880
CONT..                                                                 RTF  890
        END,.                                                          RTF  900
   ELSE CT   =0,.                                                      RTF  910
   X20  =T-X1,.                                                        RTF  920
   X1   =X2,.                          /*SAVE OLD VALUES             */RTF  930
   F0   =F1,.                                                          RTF  940
   F1   =F2,.                                                          RTF  950
   X10  =X21,.                                                         RTF  960
   F10  =F21,.                                                         RTF  970
   X2   =T,.                           /*STORE NEW VALUES            */RTF  980
   F2   =Y,.                                                           RTF  990
   X21  =X2-X1,.                                                       RTF 1000
   IF X21= 0                                                           RTF 1010
   THEN GO TO EXIT,.                                                   RTF 1020
   F21  =(F2-F1)/X21,.                                                 RTF 1030
   IF LOPT='1'                                                         RTF 1040
   THEN DO,.                           /*QUADRATIC INTERPOLATION     */RTF 1050
        IF X20 NE 0                                                    RTF 1060
        THEN DO,.                                                      RTF 1070
             T    =(F21-F10)/X20,.                                     RTF 1080
             Y    =F21+X21*T,.                                         RTF 1090
             IF Y NE 0                                                 RTF 1100
             THEN DO,.                                                 RTF 1110
                  DX   =F2/Y,.                                         RTF 1120
                  T    =0.25-DX*T/Y,.                                  RTF 1130
                  IF T NL 0                                            RTF 1140
                  THEN DX   =DX/(0.5+SQRT(T)),.                        RTF 1150
                  GO TO COMP,.                                         RTF 1160
                  END,.                                                RTF 1170
             END,.                                                     RTF 1180
        END,.                                                          RTF 1190
   IF LOPT='2'                                                         RTF 1200
   THEN DO,.                           /*HYPERBOLIC INTERPOLATION    */RTF 1210
        T    =F2-F0*F21/F10,.                                          RTF 1220
        IF T NE 0                                                      RTF 1230
        THEN DX   =X20*F2/T,.                                          RTF 1240
        IF DX NE 0                                                     RTF 1250
        THEN GO TO COMP,.                                              RTF 1260
        END,.                                                          RTF 1270
   IF F21=0                                                            RTF 1280
   THEN IF INCL='1'                                                    RTF 1290
   THEN GO TO HALF,.                                                   RTF 1300
   ELSE GO TO SEEK,.                                                   RTF 1310
   DX   =F2/F21,.                                                      RTF 1320
COMP..                                                                 RTF 1330
   TOL  =MAX(MI,1E-3)*MA,.                                             RTF 1340
   IF INCL NE '1'                                                      RTF 1350
   THEN IF ABS(DX) GT TOL                                              RTF 1360
   THEN IF DX LT 0                                                     RTF 1370
   THEN DX   =-TOL,.                                                   RTF 1380
   ELSE DX   =TOL,.                                                    RTF 1390
   T    =X2-DX,.                                                       RTF 1400
   IF INCL='1'                                                         RTF 1410
   THEN IF (XX-T)*(XXX-T) GT 0         /*TEST IF INSIDE INTERVAL     */RTF 1420
   THEN                                                                RTF 1430
HALF..                                                                 RTF 1440
        T    =(XX+XXX)*0.5,.                                           RTF 1450
   LOPT =OPT,.                                                         RTF 1460
   GO TO TEST,.                                                        RTF 1470
EXIT..                                                                 RTF 1480
   ERROR='C',.                                                         RTF 1490
RETURN..                                                               RTF 1500
   END,.                               /*END OF PROCEDURE RTF        */RTF 1510
```

Purpose:

RTF refines a given initial guess for a root of the general (transcendental) equation f(x) = 0 using:

linear interpolation if OPT='0' (secant method)
quadratic interpolation if OPT='1'
hyperbolic interpolation if OPT='2'

Usage:

CALL RTF (X, F, FCT, LIMIT, OPT);

X - BINARY FLOAT [(53)]
Given initial guess for root of f(x) = 0.
Resultant refined approximation for root of f(x) = 0.

F - BINARY FLOAT [(53)]
Resultant function value for calculated value of x.

FCT - ENTRY (BINARY FLOAT [(53)]) RETURNS (BINARY FLOAT [(53)])
Given function procedure for calculation of the function values f(x). It must be supplied by the user.

Usage:
FCT(T)

FCT(T) - BINARY FLOAT [(53)]
Resultant function value f(t).

T - BINARY FLOAT [(53)]
Given argument of function.

LIMIT - BINARY FIXED
Given bound for the number of function evaluations to be performed at most.

OPT - CHARACTER(1)
Given option for selection of iteration method.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR='C' means no convergence obtained within LIMIT function evaluations, possibly because of poor initial guess or unrealistically small value of LIMIT.

ERROR='W' means small changes in successive refined approximations indicate covergence of method, while corresponding function values are not small enough. Possibly the function values cannot be obtained accurately enough by the user-supplied procedure FCT. The returned value of x has the absolutely smallest function value f(x) among all arguments used in the course of calculation.

Any value of OPT different from '1' and '2' is treated as if it were '0'.

Method:

A refined approximation of the root is calculated as root of the linear fit through two successive approximations if OPT='0' (secant method).

The root of a quadratic fit through three successive approximations is used if OPT='1' (Muller's method).

With OPT='2' the refined approximation is calculated as root of a hyperbolic fit through three successive approximations.

For reference see:

J. F. Traub, "The Solution of Transcendental Equations", edited by A. Ralston and H. S. Wilf, Mathematical Methods for Digital Computers, vol. 2, pp. 171-184.

Mathematical Background:

Secant iteration method

The linear interpolation polynomial through two successive approximants is given by (Newtonian formulation)

$$P(t) = f(x_i) + f\left[x_i, x_{i-1}\right](t-x_i),$$

where

$$f\left[x_i, x_{i-1}\right] = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \qquad (1)$$

A refined approximation is obtained setting $P(x_{i+1}) = 0$:

$$x_{i+1} = x_i - f(x_i)/f\left[x_i, x_{i-1}\right], \text{ for } i \geq 2$$

and

$$f(x_i) \neq f(x_{i-1}) \qquad (2)$$

The asymptotic order of convergence is p = 1.62.

Muller's iteration method

The quadratic interpolation polynomial through three successive approximants is given by

$$P(t) = f(x_i) + f\left[x_i, x_{i-1}\right](t-x_i) + f\left[x_i, x_{i-1}, x_{i-2}\right](t-x_i)(t-x_{i-1}) \qquad (3)$$

With the notation

$$2w = f\left[x_i, x_{i-1}\right] + f\left[x_i, x_{i-1}, x_{i-2}\right](x_i - x_{i-1}) \qquad (4)$$

this reads

$$P(t) = f(x_i) + 2w(t-x_i) + f\left[x_i, x_{i-1}, x_{i-2}\right](t-x_i)^2 \qquad (5)$$

A refined approximation is obtained setting $P(x_{i+1}) = 0$:

$$x_{i+1} = x_i - w\left(1 - \sqrt{1 - f(x_i) f\left[x_i, x_{i-1}, x_{i-2}\right]/w^2}\right) / f\left[x_i, x_{i-1}, x_{i-2}\right]$$

or preferably

$$x_{i+1} = x_i - \frac{f(x_i)}{w\left(1 + \sqrt{1 - f(x_i) f\left[x_i, x_{i-1}, x_{i-2}\right]/w^2}\right)} \qquad (6)$$

with $w \neq 0$ and $f(x_i) \cdot f\left[x_i, x_{i-1}, x_{i-2}\right] \leq w^2$

The asymptotic order of convergence is p = 1.84.

Hyperbolic interpolation iteration method

Hyperbolic interpolation is defined through

$$P(t) = (t-a) \; / \; (b+ct)$$

with

$$(b+c\,x_j)\,f(x_j) = x_j - a, \quad \text{for } j = i,\ i-1,\ i-2. \tag{7}$$

A refined approximation is obtained setting $P(x_{i+1}) = 0$, that is, $x_{i+1} = a$.

Symmetric formula:

$$x_{i+1} = \frac{\begin{array}{l} x_i \cdot (x_{i-2}-x_{i-1})/f(x_i) + x_{i-1} \cdot (x_i - x_{i-2})/f(x_{i-1}) \\ + x_{i-2}(x_{i-1}-x_i)/f(x_{i-2}) \end{array}}{\begin{array}{l} (x_{i-2}-x_{i-1})/f(x_i) + (x_i - x_{i-2})/f(x_{i-1}) \\ + (x_{i-1}-x_i)/f(x_{i-2}) \end{array}} \tag{8}$$

x_{i+1} is a weighted mean of x_i, x_{i-1}, x_{i-2}.

Preferable is the equivalent unsymmetric formula:

$$x_{i+1} = x_i - \frac{x_i - x_{i-2}}{1 - \dfrac{f(x_{i-2}) \cdot f[x_i, x_{i-1}]}{f(x_i) \cdot f[x_{i-1}, x_{i-2}]}} \tag{9}$$

with

$$f(x_{i-2}) \cdot f[x_i, x_{i-1}] \neq f(x_i) \cdot f[x_{i-1}, x_{i-2}] \neq 0$$

The asymptotic order of convergence is p = 1.84.

Programming Considerations:

1. The three above-defined iteration methods (1), (6), and (9) are combined with a search method that uses arguments

$$x \pm 2^k \cdot \Delta / (2i+1) \quad \text{for} \begin{cases} i = 0, 1, \ldots, k \\ k = 0, 1, \ldots \end{cases} \tag{10}$$

until an argument t is found for which either

$$|f(t)| < |f(x)| \quad \text{or} \quad f(t) \cdot f(x) \leq 0.$$

The value of Δ used internally is $\Delta = \min(0.1, |f(x)|)$.

2. If an interval (x_l, x_u) enclosing a root has been found, that is, $f(x_l) \cdot f(x_u) < 0$, then successive approximants from one of the iteration methods above must lie inside this interval. Otherwise, $(x_l+x_u)/2$ is used as next approximation. The interval bounds for this bisection method are updated in the course of calculation.

3. If no sign change has been located previously, the absolute argument change at a single iteration step is reduced to max (0.001, Δ) · max(1, |X|) if necessary, in order to avoid overshooting and overflow problems.

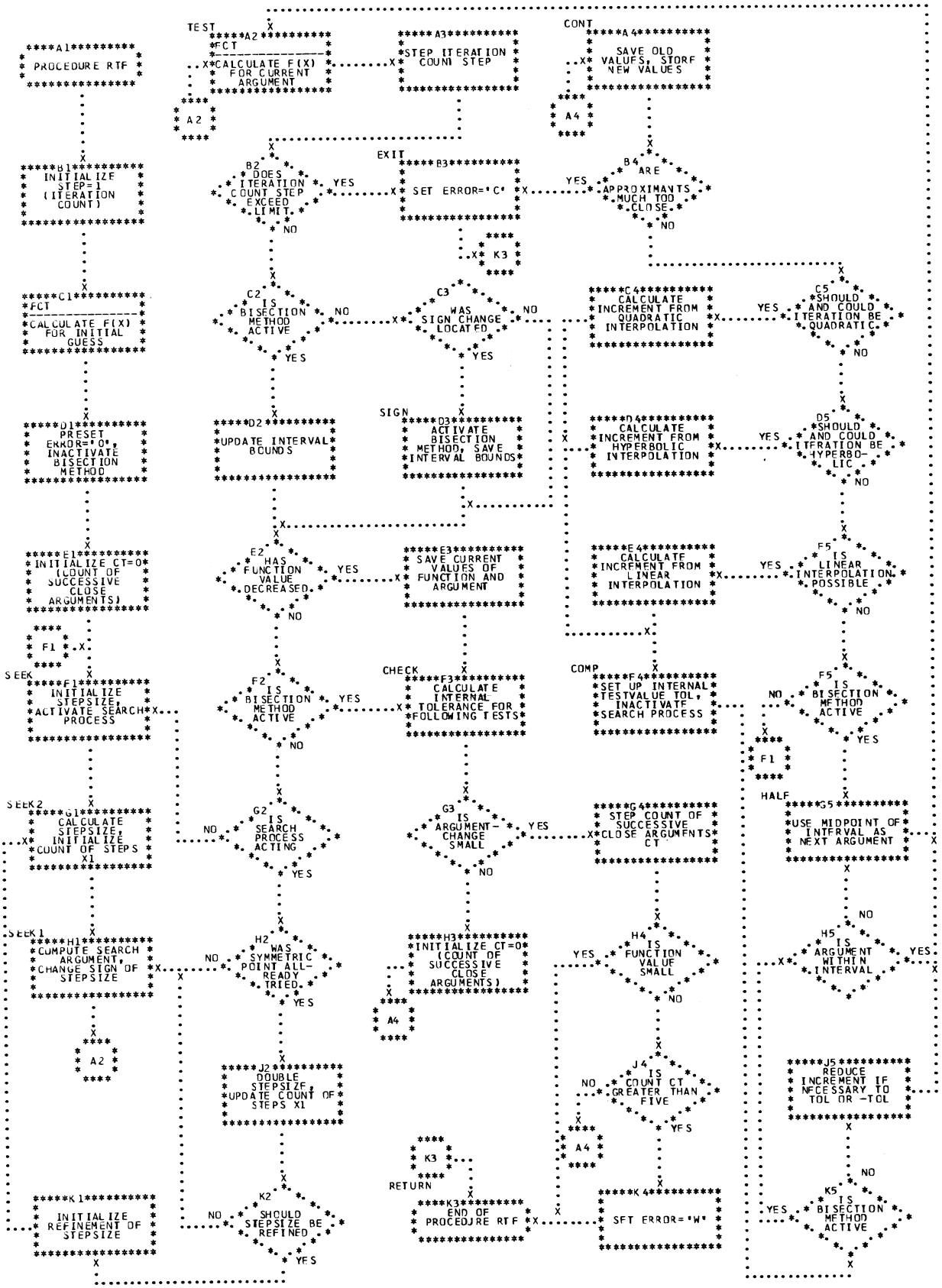
4. If, in case of no previous sign change, the iteration method fails to give an argument x_{i+1} for which either $f(x_{i+1}) \cdot f(x_i) \leq 0$ or $|f(x_{i+1})| < |f(x_i)|$, then the next approximant is calculated by the search method (1).

5. Calculation of the first approximant is based on the simple search method, while the second approximant is calculated with the secant method.

6. The convergence test used requires that both argument change and function value are absolutely less or equal to $10^{-5} \cdot \max(1, |X|)$ in single precision and $10^{-12} \cdot \max(1, |X|)$ in double precision. If the argument change is absolutely less than or equal to this internal tolerance five times in sequence, while the function values are not small enough, then the currently best values x, f(x) are returned with ERROW='W'.

7. The iteration process is terminated with ERROR='C' if the number of function evaluations exceeds the user-specified limit LIMIT.

PROCEDURE RTF REFINES AN INITIAL GUESS FOR A ROOT OF F(X)=0 USING LINEAR, QUADRATIC OR HYPERBOLIC INTERPOLATION



- Subroutine RTFD

```
RTFD..                                                                  RTFD  10
/*************************************************************************/RTFD  20
/*                                                                       */RTFD  30
/*      CALCULATE ROOT OF GIVEN FUNCTION USING DERIVATIVE VALUES         */RTFD  40
/*      IF OPT = 'C' BY LINEAR INTEPPOLATION (NEWTON METHOD)             */RTFD  50
/*      IF OPT = '1' BY INVERSE QUADRATIC INTERPOLATION                  */RTFD  60
/*      IF OPT = '2' BY HYPERBOLIC INTERPOLATION (HALLEY METHOD)         */RTFD  70
/*                                                                       */RTFD  80
/*************************************************************************/RTFD  90
   PROCEDURE(X,F,DF,FCT,LIMIT,OPT),.                                    RTFD 100
   DECLARE                                                              RTFD 110
        (ERROR EXTERNAL,INCL,LOPT,OPT)                                  RTFD 120
        CHARACTER(1),                                                   RTFD 130
        (STEP,CT,LIMIT)                                                 RTFD 140
        BINARY FIXED,                                                   RTFD 150
        (X,F,T,Y,XX,DX,X1,X2,F1,F2,DF1,DF2,DY,DF,TOL,MI,MA,FF,XXX)      RTFD 160
        BINARY FLOAT,                   /*SINGLE PRECISION VERSION  /*S*/RTFD 170
 /*     BINARY FLOAT(53),               /*DOUBLE PRECISION VERSION  /*D*/RTFD 180
        FCT ENTRY,.                                                     RTFD 190
   STEP =1,.                                                            RTFD 200
   X2   =X,.                                                            RTFD 210
   CALL FCT(X2,F2,DF2),.                /*CALCULATE STARTING VALUE     */RTFD 220
   F    =F2,.                                                           RTFD 230
   DF   =DF2,.                                                          RTFD 240
   INCL,ERROR='0',.                                                     RTFD 250
   CT   =0,.                                                            RTFD 260
   LOPT ='0',.                          /*NO PREVIOUS VALUE AVAILABLE  */RTFD 270
   GO TO COMP,.                         /*USE NEWTON METHOD            */RTFD 280
SEEK,.                                  /*LOCATE BETTER POINT          */RTFD 290
   F1   =1,.                            /*BY SIMPLE SEARCH PROCESS     */RTFD 300
   LOPT ='S',.                                                          RTFD 310
SEEK2,.                                                                 RTFD 320
   DX   =MI/F1,.                                                        RTFD 330
   X1   =1,.                                                            RTFD 340
SEEK1,.                                                                 RTFD 350
   T    =X+DX,.                                                         RTFD 360
   DX   =-DX,.                                                          RTFD 370
TEST,.                                                                  RTFD 380
   CALL FCT(T,Y,DY),.                   /*CALCULATE FUNCTION VALUE     */RTFD 390
   STEP =STEP+1,.                       /*STEP ITERATION COUNT         */RTFD 400
   IF STEP GE LIMIT                                                     RTFD 410
   THEN GO TO EXIT,.                    /*TERMINATE WITH ERROR ='C'    */RTFD 420
   IF INCL='1'                          /*TEST FOR PREVIOUS SIGN-CHANGE*/RTFD 430
   THEN DO,.                                                            RTFD 440
        IF Y*FF LT 0                                                    RTFD 450
        THEN XXX  =T,.                                                  RTFD 460
        ELSE GO TO SIGN,.                                               RTFD 470
        END,.                                                           RTFD 480
   ELSE DO,.                                                            RTFD 490
        IF Y*F LE 0                     /*TEST FOR SIGN-CHANGE         */RTFD 500
        THEN DO,.                                                       RTFD 510
             INCL ='1',.                /*MARK SIGN CHANGE             */RTFD 520
             XXX  =X,.                                                  RTFD 530
SIGN..                                                                  RTFD 540
             XX   =T,.                                                  RTFD 550
             FF   =Y,.                                                  RTFD 560
             END,.                                                      RTFD 570
        END,.                                                           RTFD 580
   IF ABS(Y) LT ABS(F)                  /*TEST FOR IMPROVEMENT         */RTFD 590
   THEN DO,.                                                            RTFD 600
        X    =T,.                                                       RTFD 610
        F    =Y,.                                                       RTFD 620
        DF   =DY,.                                                      RTFD 630
        GO TO CHECK,.                                                   RTFD 640
        END,.                                                           RTFD 650
   IF INCL='1'                                                          RTFD 660
   THEN GO TO CHECK,.                                                   RTFD 670
   IF LOPT NE 'S'                                                       RTFD 680
   THEN GO TO SEEK,.                                                    RTFD 690
   IF DX LT 0                                                           RTFD 700
   THEN GO TO SEEK1,.                   /*SEEK AT SYMMETRIC POINT      */RTFD 710
   X1   =X1+1,.                                                         RTFD 720
   DX   =DX+DX,.                        /*SEEK FARTHER AWAY            */RTFD 730
   IF X1 LE F1                                                          RTFD 740
   THEN GO TO SEEK1,.                                                   RTFD 750
   F1   =F1+2,.                         /*STEP ODD INTEGER DENOMINATOR */RTFD 760
   GO TO SEEK2,.                                                        RTFD 770
CHECK..                                                                 RTFD 780
   TOL  =1E-5*MA,.                      /*SINGLE PRECISION VERSION  /*S*/RTFD 790
 /*TOL  =1E-12*MA,.                    /*DOUBLE PRECISION VERSION  /*D*/RTFD 800
   IF ABS(DX) LE TOL                                                    RTFD 810
   THEN DO,.                                                            RTFD 820
        CT   =CT+1,.                                                    RTFD 830
        IF ABS(Y) GT TOL                /*TERMINATE SUCCESSFULLY IF    */RTFD 840
        THEN IF CT LE 5                 /*BOTH ARGUMENT-CHANGE AND     */RTFD 850
        THEN GO TO CONT,.               /*FUNCTION VALUE ARE SMALL     */RTFD 860
        ELSE ERROR='W',.                /*WITH WARNING IF ARGUMENT-    */RTFD 870
        GO TO RETURN,.                  /*CHANGE ONLY IS SMALL REPEAT. */RTFD 880
CONT..                                                                  RTFD 890
        END,.                                                           RTFD 900
   ELSE CT   =0,.                                                       RTFD 910
   X1   =X2,.                           /*SAVE OLD VALUES              */RTFD 920
   F1   =F2,.                                                           RTFD 930
   DF1  =DF2,.                                                          RTFD 940
   X2   =T,.                            /*STORE NEW VALUES             */RTFD 950
   F2   =Y,.                                                            RTFD 960
   DF2  =DY,.                                                           RTFD 970
   DY   =X2-X1,.                                                        RTFD 980
   IF DY= 0                                                             RTFD 990
   THEN GO TO EXIT,.                                                    RTFD1000
COMP,.                                                                  RTFD1010
   MA   =MAX(1,ABS(X)),.                                                RTFD1020
   MI   =MIN(0.1,ABS(F)),.                                              RTFD1030
   IF DF2 NE 0                                                          RTFD1040
   THEN DO,.                                                            RTFD1050
        DX   =F2/DF2,.                  /*NEWTON METHOD                */RTFD1060
        IF LOPT NE '0'                                                  RTFD1070
        THEN DO,.                                                       RTFD1080
             T    =(F2-F1)/DY,.                                         RTFD1090
             Y    =DF2-T,.                                              RTFD1100
             T    =DX*(DF1-T+Y+Y)/(DF2*DY),.                            RTFD1110
             IF LOPT='1'                /*MODIFICATION..               */RTFD1120
             THEN DX   =DX*(1+T),.      /*INVERSE QUADRATIC INTERPOLAT.*/RTFD1130
             IF LOPT='2'                /*MODIFICATION..               */RTFD1140
             THEN IF T NE 1             /*HYPERBOLIC INTERPOLATION     */RTFD1150
             THEN DX   =DX/(1-T),.                                      RTFD1160
             END,.                                                      RTFD1170
        LOPT =OPT,.                                                     RTFD1180
        TOL  =MAX(MI,1E-3)*MA,.                                         RTFD1190
        IF INCL NE '1'                                                  RTFD1200
        THEN DO,.                                                       RTFD121C
             IF ABS(DX) GT TOL                                          RTFD1220
             THEN IF DX LT 0                                            RTFD1230
             THEN DX   =-TOL,.                                          RTFD1240
             ELSE DX   = TOL,.                                          RTFD1250
             END,.                                                      RTFD1260
        T    =X2-DX,.                                                   RTFD1270
        IF INCL='1'                                                     RTFD1280
        THEN IF (XX-T)*(XXX-T) GT 0   /*TEST IF INSIDE INTERVAL       */RTFD1290
        THEN                                                            RTFD1300
HALF..                                                                  RTFD1310
             T    =(XX+XXX)*0.5,.                                       RTFD1320
        GO TO TEST,.                                                    RTFD1330
        END,.                                                           RTFD134C
   ELSE IF INCL='1'                                                     RTFD1350
   THEN GO TO HALF,.                                                    RTFD1360
   ELSE GO TO SEEK,.                                                    RTFD137C
EXIT..                                                                  RTFD138C
   ERROR='C',.                                                          RTFD1390
RETURN..                                                                RTFD1400
   END,.                                /*END OF PROCEDURE RTFD        */RTFD1410
```

Purpose:

RTFD refines a given initial guess for a root of the general (transcendental) equation f(x) = 0 using:
Linear interpolation if OPT='0'(Newton method)
Inverse quadratic interpolation if OPT='1'
Hyperbolic interpolation if OPT='2'

Usage:

CALL RTFD(X, F, DF, FCT, LIMIT, OPT);

X - BINARY FLOAT [(53)]
Given initial guess for root of f(x) = 0.
Resultant refined approximation for root of f(x) = 0.

F - BINARY FLOAT [(53)]
Resultant function value f(x) for returned X.

DF - BINARY FLOAT [(53)]
Resultant value of derivative f'(x) for returned X.

FCT - ENTRY (BINARY FLOAT [(53)], BINARY FLOAT [(53)], BINARY FLOAT [(53)])
Given procedure for calculation of values f(x), f'(x). It must be supplied by the user.

Usage:
CALL FCT(X, F, DF);

X - BINARY FLOAT [(53)]
Given argument value.

F - BINARY FLOAT [(53)]
Resultant function value f(x).

DF - BINARY FLOAT [(53)]
Resultant derivative value f'(x).

LIMIT - BINARY FIXED
Given bound for the number of function evaluations to be performed at most.

OPT - CHARACTER (1)
Given option for selection of iteration method.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute t possible error conditions that may be detected:

ERROR='C' - means no convergence is obtained within LIMIT function evaluations, possibly because of poor initial guess or unrealistic small value of LIMIT.

ERROR='W' - means that small changes in successive approximations indicate covergence of method, while corresponding function values are not small enough. Possibly the function values cannot be obtained accurately enough by the user-supplied procedure FCT.

The returned value of X has the absolutely smallest function value f(x) among all arguments tried during the iteration process.

Any value of OPT different from '1' and '2' is treated as if it were '0'.

Method:

A refined approximation of the root is calculated using Newton's method if OPT='0', higher-order methods doing inverse quadratic interpolation if OPT='1', and hperbolic interpolation if OPT='2'. With the higher-order methods the second derivative is estimated from a cubic interpolation polynomial through two successive approximations.

For reference see:

J. F. Traub, "The Solution of Transcendental Equations", edited by A. Ralston and H. S. Wilf, Mathematical Methods for Digital Computers, vol. 2, pp. 171 - 184.

Mathematical Background:

Newton's iteration method

The linear interpolation polynomial passing through x_i, $f(x_i)$ with derivative $f'(x_i)$ is given by

$$P(t) = f(x_i) + f'(x_i)\,(t-x_i) \qquad (1)$$

A refined approximation is obtained setting $P(x_{i+1}) = 0$:

$$x_{i+1} = x_i - f(x_i)/f'(x_i), \text{ for } i \geq 1 \text{ and } f'(x_i) \neq 0.$$

The asymptotic order of convergence is p = 2.

Inverse quadratic interpolation

Let x = F(y) denote the inverse function of y = f(x). The quadratic polynomial Q(y) passing through point y_i, x_i with derivatives $F'(y_i)$, $F''(y_i)$ is given by

$$Q(y) = F(y_i) + F'(y_i)\,(y-y_i) + \frac{F''}{2!}(y_i)\,(y-y_i)^2 \qquad (2)$$

A refined approximation is obtained setting $x_{i+1} = Q(0)$:

$$x_{i+1} = F(y_i) - F'(y_i)\,y_i + \frac{F''}{2!}(y_i)\,y_i^2 \qquad (3)$$

From the identity x = F(f(x)) follows easily:

$$F'(y) = \frac{dF}{dy} = 1 \Big/ \frac{df}{dx} = \frac{1}{f'(x)}$$

$$F''(y) = \frac{d^2F}{dy^2} = -\frac{f''(x)}{(f'(x))^3}$$

Hence

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}\left(1 + \frac{f(x_i)}{f'(x_i)}\,\frac{f''(x_i)}{2f'(x_i)}\right) \qquad (4)$$

The asymptotic order of convergence is p = 3.

Hyperbolic interpolation (Halley's iteration method)

Hyperbolic interpolation is defined by

$$P(t) = (t-a)/(b+ct) \qquad (5)$$

with

$$P(x_i) = f(x_i),\ P'(x_i) = f'(x_i),\ P''(x_i) = f''(x_i)$$

A refined approximation is obtained setting $P(x_{i+1}) = 0$, that is, $x_{i+1} = a$.

From

$$P(t)\,(b+ct) = t-a \text{ follows, by differentiation,} \qquad (6)$$

$$f(x_i)(b+cx_i) = x_i - a$$
$$f'(x_i)(b+cx_i) = 1 - f(x_i) \cdot c$$
$$f''(x_i)(b+cx_i) = -2f'(x_i) \cdot c$$

and from the last two equations

$$b+cx_i = -\frac{2f'(x_i)}{f(x_i)f''(x_i)-2(f'(x_i))^2}$$

and

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i) - \frac{f(x_i)\,f''(x_i)}{2f'(x_i)}} \tag{7}$$

The asymptotic order of convergence is p = 3.

Estimation of second derivative

A cubic interpolation polynomial passing through points x_i, $f(x_i)$ and x_{i-1}, $f(x_{i-1})$ is of the form

$$P(x) = f(x_i) + (x-x_i)f'(x_i) + \alpha(x-x_i)^2 + \beta(x-x_i)^2(x-x_{i-1}) \tag{8}$$

$P(x_i) = f(x_i)$ and $P'(x_i) = f'(x_i)$ are already satisfied. If we set

$P(x_{i-1}) = f(x_{i-1})$ and $P'(x_{i-1}) = f'(x_{i-1})$ then

$$\alpha = \frac{f[x_i, x_{i-1}] - f'(x_i)}{x_{i-1} - x_i}$$

and

$$\beta = \frac{f'(x_i) + f'(x_{i-1}) - 2f[x_i, x_{i-1}]}{(x_{i-1} - x_i)^2}$$

The second derivative $f''(x_i)$ is estimated by

$$P''(x_i) = 2(\alpha + \beta(x_i - x_{i-1})) = 2\left(2f'(x_i) + \frac{f'(x_{i-1}) - 3f[x_i, x_{i-1}]}{(x_i - x_{i-1})}\right) \tag{9}$$

Derivative estimated iteration methods

Replacing $f''(x_i)$ in (4) and (7) by $P''(x_i)$ gives

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \cdot \left(1 + \frac{f(x_i)}{f'(x_i)} \frac{2f'(x_i) + f'(x_{i-1}) - 3f[x_i, x_{i-1}]}{(x_i - x_{i-1})f'(x_i)}\right) \tag{4'}$$

and

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \cdot \frac{1}{1 - \frac{f(x_i)}{f'(x_i)} \cdot \frac{2f'(x_i) + f'(x_{i-1}) - 3f[x_i, x_{i-1}]}{(x_i - x_{i-1})f'(x_i)}} \tag{7'}$$

The asymptotic order of both these iteration methods is p = 2.73.

Programming Considerations:

1. The three above-defined iteration methods (1), (4'), and (7') are combined with a search method that uses arguments

$$x + 2^k \cdot \Delta/(2i+1) \quad \text{for} \begin{cases} i=0, 1, \ldots, k \\ k=0, 1, \ldots \end{cases} \tag{10}$$

until an argument t is found for which either

$$|f(t)| < |f(x)| \quad \text{or} \quad f(t) \cdot f(x) \le 0.$$

The value of Δ used internally is $\Delta = \min(0.1, |f(x)|)$.

2. If an interval (x_l, x_u) enclosing a root has been found, that is, $f(x_l) \cdot f(x_u) < 0$, then successive approximants from one of the iteration methods above must lie inside this interval. Otherwise, $(x_l + x_u)/2$ is used as the next guess. The interval bounds for this bisection method are updated in the course of calculation.

3. If no sign change has been located previously, the absolute argument change at a single iteration step is reduced to $\max(0.001, \Delta) \cdot \max(1, |x|)$ if necessary, in order to avoid overshooting and overflow problems.

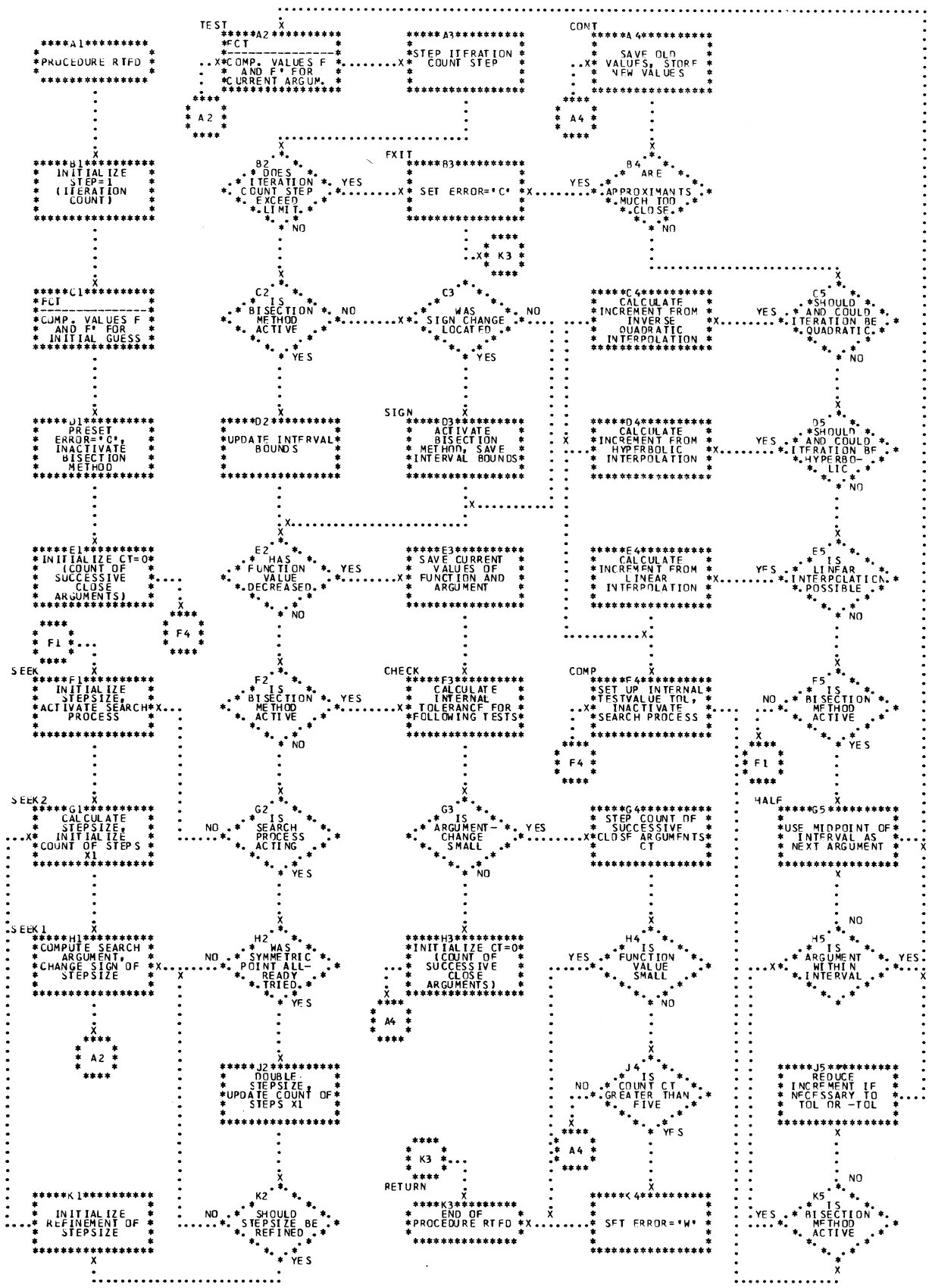
4. If, in case of no previous sign change, the iteration method fails to give an argument for which either $f(x_{i+1}) \cdot f(x_i) \le 0$ or $|f(x_{i+1})| < |f(x_i)|$ the next approximation is calculated by search method (1).

5. Calculation of the first approximant is based on Newton's method in all cases, while for those following, the higher-order iteration methods are used if specified.

6. The convergence test used requires that both argument change and function value are absolutely less than or equal to $10^{-5} \max(1, |x|)$ in single precision and $10^{-12} \max(1, |x|)$ in double precison. If the argument change is absolutely less than or equal to this tolerance five times in sequence, while the function values are not small enough, then the currently best values x, f(x) and f'(x) are returned with ERROR='W'.

7. The iteration process is terminated with ERROR='C' if the number of function evaluations exceeds the user-specified limit LIMIT.

PROCEDURE RTFD REFINES AN INITIAL GUESS FOR A ROOT OF F(X)=0 USING LINEAR, INVERSE QUADRATIC OR HYPERBOLIC INTERPOLATION



- Subroutine DERE

```
DERE..                                                                  DERE  10
/*************************************************************************/DERE  20
/*                                                                       */DERE  30
/*      PERFORM ONE INTEGRATION STEP FOR A SYSTEM OF ORDINARY DIF-       */DERE  40
/*      FERENTIAL EQUATIONS USING RATIONAL EXTRAPOLATION TECHNIQUE       */DERE  50
/*                                                                       */DERE  60
/*************************************************************************/DERE  70
   PROCEDURE(F,N,H,X,Y,EPS),.                                           DERE  80
   DECLARE                                                              DERE  90
         F ENTRY,                        /*Y' = F(X,Y) GIVEN ODE-SYSTEM */DERE 100
         (ERROR EXTERNAL,CONV) CHARACTER(1),                            DERE 110
         (EPS,YM(N),FMH,SQMH,FMM,SQMI,DSQMI)                            DERE 120
         BINARY FLOAT,                                                  DERE 130
         (H,X,Y(*),YI,DY(N),Z(N),DZ(N),LX,YC(N))                        DERE 140
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/DERE 150
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/DERE 160
         (LH,HA,CI,BI,V,FO(N),FE(N),ZI,CMI,DI,U,                        DERE 170
         DT(5*N))                      /*SINGLE PRECISION VERSION  /*S*/DERE 180
 /*      DT(10*N))                     /*DOUBLE PRECISION VERSION  /*D*/DERE 190
         BINARY FLOAT(53),                                              DERE 200
         (N,RR,CC,LN,DIAG,HSTEP,M,MM,I,J)                               DERE 210
         BINARY FIXED,.                                                 DERE 220
   LN   =N,.                                                            DERE 230
   ERROR='S',.                         /*MARK ILLEGAL SPECIFICATION   */DERE 240
   IF LN LE 0                          /*TEST SPECIFIED DIMENSION     */DERE 250
   THEN GO TO EXIT,.                                                    DERE 260
   LH   =H,.                           /*INIT. LOCAL STEPSIZE         */DERE 270
   HSTEP=0,.                           /*INIT. COUNT HALVING STEPSIZE */DERE 280
   IF LH= 0                            /*TEST SPECIFIED STEPSIZE      */DERE 290
   THEN GO TO EXIT,.                                                    DERE 300
   ERROR='0',.                         /*PRESET ERROR INDICATOR       */DERE 310
   CALL F(X,Y,DY),.                    /*DERIVATIVE FOR INITIAL VALUES*/DERE 320
   IF ERROR NE '0'                                                      DERE 330
   THEN GO TO EXIT,.                   /*TERMINATE IF ERROR IN F(X,Y) */DERE 340
                                       /*                            */DERE 350
HALF..                                 /*START OF ITERATION LOOP      */DERE 360
   CONV ='H',.                         /*MARK FIRST APPROXIMATION     */DERE 370
   DIAG =1,.                           /*INIT. DIAGONAL COUNT T-ARRAY */DERE 380
   FMH  =0,.                           /*INIT. FLOATING EXTRAPOL.COUNT*/DERE 390
                                       /*START OF EXTRAPOLATION LOOP  */DERE 400
         DO M = 2 TO 16 BY 2,.         /*SINGLE PRECISION VERSION  /*S*/DERE 410
 /*      DO M = 2 TO 28 BY 2,.         /*DOUBLE PRECISION VERSION  /*D*/DERE 420
         FMH  =FMH+1,.                 /*UPDATE EXTRAPOLATION COUNT   */DERE 430
         HA   =LH/FMH,.                /*CALCULATE INTERVAL SIZE      */DERE 440
         FMM  =1,.                                                      DERE 450
              DO MM = 1 TO M,.         /*COMP. DISCRETE APPROXIMATION */DERE 460
                   DO I = 1 TO LN,.                                     DERE 470
                   YI   =Y(I),.                                         DERE 480
                   IF MM= 1             /*MODIFY MID-POINT RULE FOR    */DERE 490
                   THEN DO,.            /*FIRST INTERVAL               */DERE 500
                        IF CONV='H'     /*FOR THE VERY FIRST INTERVAL  */DERE 510
                        THEN DO,.       /*INIT. VALUES FOR CONV. TEST  */DERE 520
                             YC(I)=YI,.                                 DERE 530
                             YM(I)=ABS(YI),.                            DERE 540
                             END,.                                      DERE 550
                        ZI,FE(I)=.50000000*DY(I),.                      DERE 560
                        FO(I)=0,.       /*INIT. SUM OF DERIVATIVES     */DERE 570
                        END,.                                           DERE 580
                   ELSE DO,.                                            DERE 590
                        ZI   =FO(I)+DZ(I),.                             DERE 600
                        FO(I)=FE(I),.   /*UPDATE AND INTERCHANGE SUM OF*/DERE 610
                        FE(J)=ZI,.      /*ODD/EVEN SPACED DERIVATIVES  */DERE 620
                        END,.                                           DERE 630
                   Z(I),YI=HA*ZI+YI,.   /*COMP. APPROXIMATE FUNCTION   */DERE 640
                   IF YM(I) LT ABS(YI) /*VALUE FOR LOCAL ARGUMENT LX    */DERE 650
                   THEN YM(I)=ABS(YI),./*STORE MAX ABSOLUTE VALUE       */DERE 660
                   END,.                                                DERE 670
              LX   =X+FMM*HA,.          /*COMP. LOCAL ARGUMENT         */DERE 680
              FMM  =FMM+1,.                                             DERE 690
              CALL F(LX,Z,DZ),.         /*CALCULATE DERIVATIVE         */DERE 700
              IF ERROR NE '0'                                           DERE 710
              THEN GO TO EXIT,.         /*TERMINATE IF ERROR IN F(X,Y) */DERE 720
              END,.                                                     DERE 730
         CONV ='C',.                    /*PRESET CONVERGENCE INDICATOR */DERE 740
         SQMH =FMH*FMH,.                /*SQUARE EXTRAPOLATION COUNT   */DERE 750
         HA   =HA*0.5,.                                                 DERE 760
              DO I =1 TO LN,.           /*EXTRAPOLATION ON COMPONENTS  */DERE 770
              V    =DT(I),.             /*SAVE OLD T-VALUE             */DERE 780
              ZI,CI,DT(I)=Y(I)+HA*      /*STORE NEW T-VALUE            */DERE 790
                   (.5000000*DZ(I)+FO(I)+FE(I)),.                       DERE 800
              SQMI =SQMH,.              /*INIT. VARYING SQUARE NUMBER  */DERE 810
              DSQMI=FMM,.               /*INIT. VARYING DECREMENT      */DERE 820
              MM   =1,.                                                 DERE 830
                   DO J = 2 TO DIAG,.                                   DERE 840
                   MM   =MM+LN,.                                        DERE 850
                   DSQMI=DSQMI-2,.      /*STEP ODD INTEGER DECREMENT   */DERE 860
                   SQMI =SQMI-DSQMI,.   /*COMPUTE NEXT LOWER SQUARE    */DERE 870
                   BI   =SQMH*V,.                                       DERE 880
                   CMI  =CI*SQMI,.                                      DERE 890
                   DI   =BI-CMI,.       /*DENOMINATOR OF CENTRAL ALGOR.*/DERE 900
                   U    =V,.                                            DERE 910
                   IF DI NE 0           /*TEST FOR ZERO DENOMINATOR    */DERE 920
                   THEN DO,.            /*PERFORM RHOMBUS ALGORITHM    */DERE 930
                        DI   =(CI-V)/DI,.                               DERE 940
                        U    =CMI*DI,.                                  DERE 950
                        CI   =BI*DI,.                                   DERE 960
                        END,.                                           DERE 970
                   V    =DT(MM),.       /*SAVE OLD T-VALUE-DIFFERENCE  */DERE 980
                   DT(MM)=U,.           /*STORE NEW T-VALUE-DIFFERENCE */DERE 990
                   ZI   =ZI+U,.         /*COMP. NEW T-VALUE            */DERE1000
                   END,.                                                DERE1010
              YI   =ABS(YC(I)-ZI),.                                     DERE1020
              IF YI LT ABS(U)           /*SET YI TO                    */DERE1030
              THEN YI   =ABS(U),.       /*MAX(ABS(U),ABS(YC(I)-ZI))    */DERE1040
              IF YI GT EPS*YM(I)        /*COMPONENTWISE CONVERGENCETEST*/DERE1050
              THEN CONV ='1',.          /*NEGATE CONVERGENCE INDICATOR */DERE1060
              YC(I)=ZI,.                /*STORE NEW COMPARISON VALUE   */DERE1070
              END,.  .                                                  DERE1080
         IF CONV='C'                    /*GLOBAL CONVERGENCE TEST      */DERE1090
         THEN GO TO END,.                                               DERE1100
         ELSE IF DIAG LT 5              /*SINGLE PRECISION VERSION  /*S*/DERE1110
 /*      ELSE IF DIAG LT 10             /*DOUBLE PRECISION VERSION  /*D*/DERE1120
         THEN DIAG =DIAG+1,.            /*UPDATE DIAGONAL COUNT        */DERE1130
```

```
         END,.                                                          DERE1140
                                       /*END OF EXTRAPOLATION LOOP    */DERE1150
   HSTEP=HSTEP+1,.                     /*UPDATE COUNT OF HALVING STEPS*/DERE1160
   LH   =LH*0.5,.                                                       DERE1170
   IF HSTEP LE 20                      /*MAXIMALLY 20 ITERATIONS WITH */DERE1180
   THEN GO TO HALF,.                   /*REDUCED STEPSIZE             */DERE1190
   ELSE GO TO EXIT,.                   /*TERMINATE IF NO CONVERGENCE  */DERE1200
                                       /*END OF ITERATION LOOP        */DERE1210
END..                                  /*SUCCESSFUL END OF OPERATION  */DERE1220
   X    =X+LH,.                        /*RETURN ARGUMENT              */DERE1230
   IF DIAG LE 4                        /*SINGLE PRECISION VERSION  /*S*/DERE1240
 /*IF DIAG LE 7                        /*DOUBLE PRECISION VERSION  /*D*/DERE1250
   THEN LH   =LH+LH,.                  /*DOUBLE STEPSIZE ESTIMATE     */DERE1260
   H    =LH,.                          /*RETURN ADJUSTED STEPSIZE     */DERE1270
        DO I = 1 TO LN,.                                                DERE1280
        Y(I) =YC(I),.                  /*RETURN EXTRAPOLATED FUNCTION-*/DERE1290
        END,.                          /*VALUES                       */DERE1300
                                                                        DERE1310
EXIT..                                 /*END OF PROCEDURE DERE        */DERE1320
   END,.
```

Purpose:

DERE performs one integration step for a system of first order ordinary differential equations Y' = F(X, Y) with given initial values Y. The stepsize H is adjusted for accuracy requirements and speed considerations.

Usage:

CALL DERE (F, N, H, X, Y, EPS);

F - ENTRY
Given procedure for calculation of the derivatives.
This procedure must be supplied by the user.

Usage:
CALL F (T, Z, DZ);

T - BINARY FLOAT [(53)]
Given independent variable.

Z - BINARY FLOAT [(53)]
Given vector of dependent variables.

DZ - BINARY FLOAT [(53)]
Resultant vector of derivatives.

N - BINARY FIXED
Given dimension of the ODE system.

H - BINARY FLOAT [(53)]
Given suggested stepsize for current integration step.

X - BINARY FLOAT [(53)]
Given independent variable for initial values.
Resultant dependent variable for calculated values.

Y(N) - BINARY FLOAT [(53)]
Given initial values of vector Y for given X.
Resultant calculated values of Y for resultant X.

EPS - BINARY FLOAT
Given relative tolerance for local error in calculated Y-values.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The

following constitute the possible error conditions that may be detected:

ERROR = 'S' means $N \le 0$ or $H = 0$
ERROR = '1' means no convergence was obtained with stepsizes $H/2^i$ for $i = 0, 1, \ldots, 20$

The last case may occur if stepsize $|H|$ is unrealistically large or if tolerance EPS is too small. Suggested values are $|H| = 1$ and EPS $\ge 10^{-5}$ in single precision and EPS $\ge 10^{-10}$ in double precision.

If ERROR is changed in the user-supplied procedure F(X, Y, DY) to a nonzero value, ERROR remains unchanged and DERE returns to the calling procedure immediately.

In all cases of a nonzero value of ERROR the parameters H, X, Y remain unchanged. The stepsize H of the integration step gets divided by a power of two if accuracy requirements are not met otherwise.

Method:

DERE uses a rational function for extrapolation and is based on the midpoint rule as the underlying discretization method.

For reference see:

R. Bulirsch and J. Stoer, "Numerical Treatment of Ordinary Differential Equations by Extrapolation Methods", Numerische Mathematik vol. 8, 1966, pp. 1-13.

Mathematical Background:

Notation

The problem is to solve the system of differential equations

$$y_1' = f_1(x, y_1, \ldots, y_n)$$
$$\vdots$$
$$y_n' = f_n(x, y_1, \ldots, y_n)$$

with given initial values

$$x_0,\ y_1(x_0) = y_{10}$$
$$\vdots$$
$$y_n(x_0) = y_{n0}$$

Using capital letters for vectors, this is written more compactly in vector form:

$$Y' = F(x, Y),\quad Y(x_0) = Y_0$$

Discretization method

The underlying discretization method proceeds as follows:

Set $h = H/2m$, $x_i = x_0 + ih$ and let $Z_i = Z(x_i, h)$

denote approximations to the exact value $Y(x_i)$ obtained with stepsize h by means of the midpoint rule:

$$Z_0 = Y_0,\quad Z_1 = Z_0 + hF(x_0, Z_0)$$

$$Z_{i+1} = Z_{i-1} + 2hF(x_i, Z_i) \quad \text{for } i = 1, 2, \ldots, 2m-1$$

Extrapolation is based on

$$T(h, x) = \frac{1}{2}(Z_{2m} + Z_{2m-1} + hF(x, Z_{2m}))$$

Under suitable differentiability assumptions the asymptotic expansion of T(h, x) proceeds with even powers of h:

$$T(h, x) = Y(x) + t_1(x)h^2 + t_2(x)h^4 + \ldots$$

Rational extrapolation method

Rational extrapolation is used to approximate

$$T(0, x) = Y(x)$$

Assume (h_k) to be a strictly decreasing sequence of stepsizes tending to zero and let

$$R_p^{(i)}(h) = \frac{p_0^{(i)} + p_1^{(i)} h^2 + \ldots + p_k^{(i)} h^{2k}}{q_0^{(i)} + q_1^{(i)} h^2 + \ldots + q_l^{(i)} h^{2l}},$$

$$k = \left[\frac{p}{2}\right],\quad l = p - k$$

be the rational function defined by p + 1 nodes:

$$R_p^{(i)}(h_j) = T(h_j, x),\quad j = i, i+1, \ldots, i+p$$

Then the extrapolated values $T_p^{(i)} = R_p^{(i)}(0)$ that approximate T(0, x) are obtained from the formulas

$$T_{-1}^{(i)} = 0$$

$$T_0^{(i)} = T(h_i, x)$$

$$T_k^{(i)} = T_{k-1}^{(i+1)} + \frac{T_{k-1}^{(i+1)} - T_{k-1}^{(i)}}{\left(\frac{h_i}{h_{i+k}}\right)^2 \left[1 - \frac{T_{k-1}^{(i+1)} - T_{k-1}^{(i)}}{T_{k-1}^{(i+1)} - T_{k-2}^{(i+1)}}\right] - 1}$$

for $k \geq 1$

The above formulas connect by a rhombus rule the elements

$T_{k-2}^{(i+1)}$, $T_{k-1}^{(i)}$, $T_{k-1}^{(i+1)}$, $T_k^{(i)}$ of the tableau

(T array):

$$\begin{array}{ccccc} T_{-1}^{(0)} & & & & \\ & T_0^{(0)} & & & \\ T_{-1}^{(1)} & & T_1^{(0)} & & \\ \vdots & T_0^{(1)} & \vdots & \cdots & T_p^{(0)} \\ \vdots & \vdots & \vdots & & \\ \vdots & \vdots & T_1^{(p-1)} & & \\ \vdots & \vdots & & & \\ & T_0^{(p)} & & & \\ T_{-1}^{(p+1)} & & & & \end{array}$$

Programming Considerations:

DERE uses the stepsize sequence

$$(h_1 = \frac{H}{2},\ h_2 = \frac{H}{4},\ \ldots,\ h_m = \frac{H}{2m},\ \ldots)$$

for extrapolation.
The square numbers

$$\left(\frac{H/2}{h_{m-k}}\right)^2 = (m-k)^2 \text{ are}$$

generated successively using the identity

$$(l-1)^2 = l^2 - (2l-1)$$

which means that the next lower squares are obtained by subtracting decreasing odd integers.

To avoid repeated calculation of differences, the rhombus rule is modified to

$$D_{k-1}^{(m-k+1)} = \frac{C_{k-1}^{(m-k+1)} - T_{k-1}^{(m-k)}}{\left(\frac{H/2}{h_m}\right)^2 \Delta T_{k-1}^{(m-k)} - \left(\frac{H/2}{h_{m-k}}\right)^2 C_{k-1}^{(m-k+1)}}$$

$$\Delta T_k^{(m-k)} = \left(\frac{H/2}{h_{m-k}}\right)^2 C_{k-1}^{(m-k+1)} D_{k-1}^{(m-k+1)}$$

$$C_k^{(m-k)} = \left(\frac{H/2}{h_m}\right)^2 \Delta T_{k-1}^{(m-k)} D_{k-1}^{(m-k+1)}$$

for $k = 1, 2, \ldots, m$

Starting values are

$$\Delta T_0^{(i)} = C_0^{(i)} = T(h_i, x)$$

and the notation

$$\Delta T_k^{(i)} = T_k^{(i)} - T_{k-1}^{(i+1)}, \quad C_k^{(i)} = T_k^{(i)} - T_{k-1}^{(i)}$$

implies

$$T_m^{(0)} = \sum_{k=0}^{m} \Delta T_k^{(m-k)}$$

The above formulas are evaluated successively for $m = 1, 2, \ldots$. Only one linear array is needed for storing the differences $\Delta T_k^{(m-k)}$.

Control of accuracy is done in a natural way: Comparing $T_{m-1}^{(0)}$ and $T_m^{(0)}$ one increases the subscript m until this difference and the difference $\Delta T_m^{(0)}$ are small enough, which means less than the user-specified tolerance EPS times absolute maximum of the approximate function values Z_i obtained in the current interval of length H. This convergence test is applied componentwise.

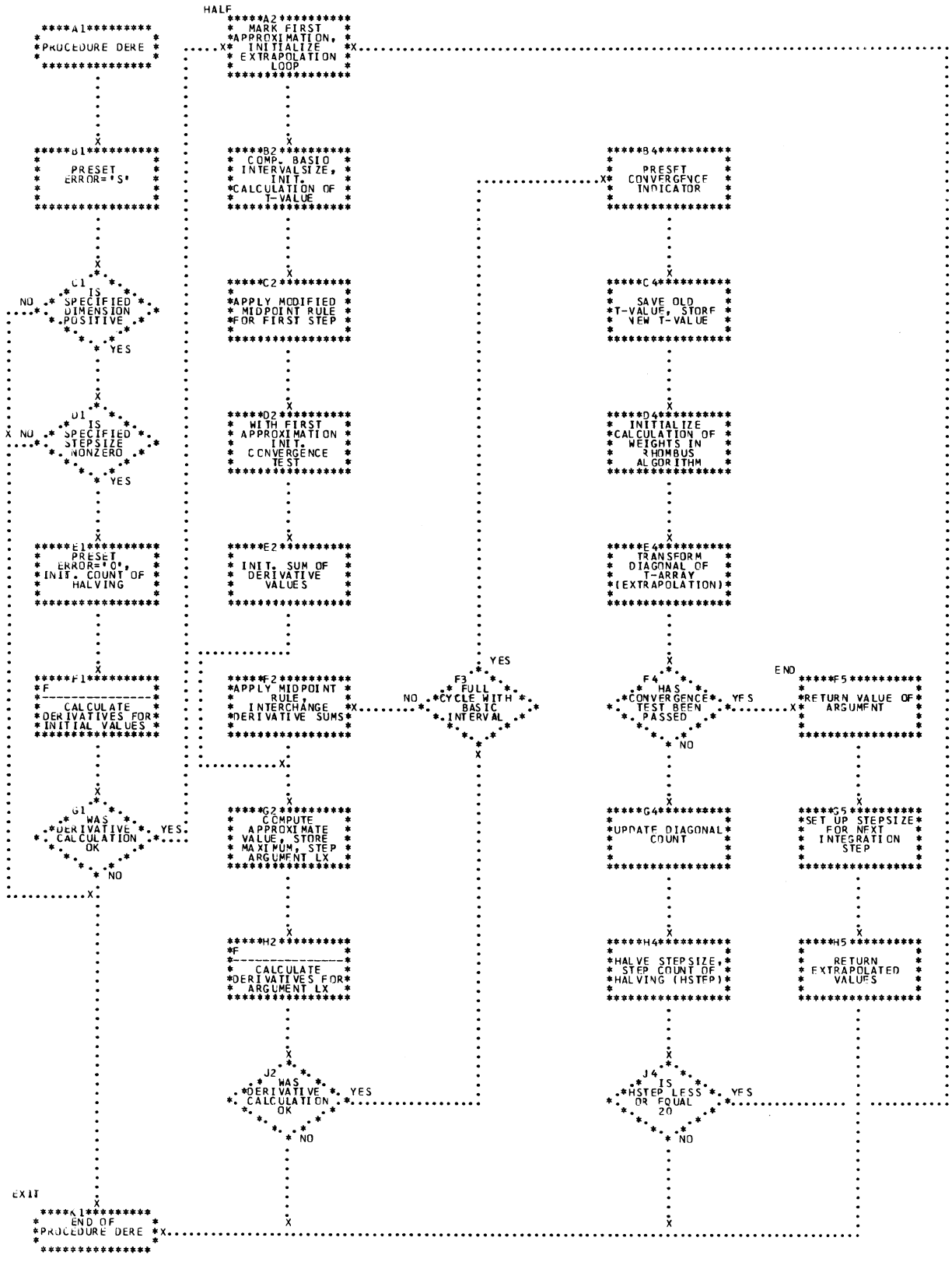
The sensitivity of the extrapolation process to roundoff increases with the order of extrapolation. Therefore, the number of columns of the T array is limited to c = 5 for the single-precision version and to c = 10 for the double-precision version. The number of rows is limited to r = 8 and r = 14 respectively.

If k is not less than the maximum number of columns, the values $T_{c-1}^{(k-c+1)}$ are taken as successive approximations to the resulting values of Y. This continues up to $T_{c-1}^{(r-c+1)}$. If no convergence is reached at that point, the whole procedure is repeated with H/2 instead of H. DERE provides at most 20 iterations, each with half the stepsize of the one before. When there is no convergence, DERE returns to the calling procedure with ERROR='1' and parameters H, X, Y remain unchanged.

Adjustment of the stepsize H is a by-product of the above iteration process on length of stepsize. If convergence was attained with stepsize $H/2^j$, then $H/2^j$ is returned as the adjusted stepsize if at least 4 (7) extrapolation steps have been performed in single (double) precision to obtain the result values $Y(X+H/2^j)$ from input values Y(X), X.

Otherwise, $H/2^{j-1}$ is returned as adjusted stepsize in order to speed up calculation time.

Since the extrapolation method does not necessarily work with a fixed order, adjustment of stepsize is uncritical. It does not critically affect accuracy, but only speed of computation.


A1
PROCEDURE DERE
B1
PRESET ERROR='S'
C1
IS SPECIFIED DIMENSION POSITIVE
NO
YES
D1
IS SPECIFIED STEPSIZE NONZERO
NO
YES
E1
PRESET ERROR='0', INIT. COUNT OF HALVING
F1
CALCULATE DERIVATIVES FOR INITIAL VALUES
G1
WAS DERIVATIVE CALCULATION OK
YES
NO
EXIT
X1
END OF PROCEDURE DERE
HALF
A2
MARK FIRST APPROXIMATION, INITIALIZE EXTRAPOLATION LOOP
B2
COMP. BASIC INTERVALSIZE, INIT. CALCULATION OF T-VALUE
C2
APPLY MODIFIED MIDPOINT RULE FOR FIRST STEP
D2
WITH FIRST APPROXIMATION INIT. CONVERGENCE TEST
E2
INIT. SUM OF DERIVATIVE VALUES
F2
APPLY MIDPOINT RULE, INTERCHANGE DERIVATIVE SUMS
G2
COMPUTE APPROXIMATE VALUE, STORE MAXIMUM STEP ARGUMENT LX
H2
CALCULATE DERIVATIVES FOR ARGUMENT LX
J2
WAS DERIVATIVE CALCULATION OK
YES
NO
F3
FULL CYCLE WITH BASIC INTERVAL
YES
NO
B4
PRESET CONVERGENCE INDICATOR
C4
SAVE OLD T-VALUE, STORE NEW T-VALUE
D4
INITIALIZE CALCULATION OF WEIGHTS IN RHOMBUS ALGORITHM
E4
TRANSFORM DIAGONAL OF T-ARRAY (EXTRAPOLATION)
F4
HAS CONVERGENCE TEST BEEN PASSED
YES
NO
G4
UPDATE DIAGONAL STEP COUNT OF
H4
HALVE STEPSIZE, STEP COUNT OF HALVING (HSTEP)
J4
IS HSTEP LESS OR EQUAL 20
YES
NO
END
F5
RETURN VALUE OF ARGUMENT
G5
SET UP STEPSIZE FOR NEXT INTEGRATION STEP
H5
RETURN EXTRAPOLATED VALUES

- Subroutine CEL1/CEL2

```
CEL1..                                                              CEL   10
/*******************************************************************/CEL   20
/*                                                                 */CEL   30
/*      COMPLETE ELLIPTIC INTEGRAL OF FIRST KIND                   */CEL   40
/*                                                                 */CEL   50
/*******************************************************************/CEL   60
   PROCEDURE(RES,K),.                                               CEL   70
   DECLARE                                                          CEL   80
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR    */CEL   90
        (RES,K,A,B,B1,ARI,AARI,GEO,AA,AN,W)                         CEL  100
        BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/CEL  110
 /*     BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/CEL  120
        SWITCH CHARACTER(1),.                                       CEL  130
   SWITCH='1',.                       /*INIT. CEL1 ENTRY          */CEL  140
   B1,AN=2,.                                                        CEL  150
   GO TO COM,.                                                      CEL  160
CEL2..                                                              CEL  170
/*******************************************************************/CEL  180
/*                                                                 */CEL  190
/*      GENERALIZED COMPLETE ELLIPTIC INTEGRAL OF SECOND KIND      */CEL  200
/*                                                                 */CEL  210
/*******************************************************************/CEL  220
   ENTRY(RES,K,A,B),.                                               CEL  230
   SWITCH='2',.                       /*INIT. CEL2 ENTRY          */CEL  240
   AA   =A,.                                                        CEL  250
   AN   =A+B,.                                                      CEL  260
   B1,W =B+B,.                                                      CEL  270
COM..                                 /*START COMMON CALCULATION  */CEL  280
   ERROR='0',.                        /*PRESET ERROR PARAMETER    */CEL  290
   GEO  =(0.5-K)+0.5,.                /*COMP. GEO = 1-K**K        */CEL  300
   GEO  =GEO+GEO*K,.                                                CEL  310
   IF GEO LE 0                        /*TEST FOR SPECIAL CASES OF K */CEL 320
   THEN DO,.                          /*ABS(K) NOT LESS THAN ONE  */CEL  330
        RES  =1.E75,.                 /*IS INTERPRETED AS IF EQUAL 1 */CEL 340
        IF B1 LT 0                                                  CEL  350
        THEN RES  =-RES,.             /*CEL2..NEGATIVE PARAMETER B */CEL  360
        IF B1=0                                                     CEL  370
        THEN RES  =AA,.               /*CEL2..ZERO PARAMETER B    */CEL  380
        IF GEO NE 0                                                 CEL  390
        THEN ERROR='1',.                                            CEL  400
        GO TO RETURN,.                                              CEL  410
        END,.                                                       CEL  420
   ARI  =2,.                          /*PROCESS OF THE ARITHMETIC- */CEL 430
ITER..                                /*GEOMETRIC MEAN            */CEL  440
   GEO  =SQRT(GEO),.                                                CEL  450
   GEO  =GEO+GEO,.                                                  CEL  460
   AARI =ARI,.                                                      CEL  470
   ARI  =ARI+GEO,.                                                  CEL  480
   IF SWITCH='2'                                                    CEL  490
   THEN DO,.                                                        CEL  500
        W    =W+AA*GEO,.                                           CEL  510
        W    =W+W,.                                                CEL  520
        B1   =W/ARI,.                                              CEL  530
        AA   =AN,.                                                 CEL  540
        END,.                                                      CEL  550
   B1,AN=AN+B1,.                                                    CEL  560
   IF GEO/AARI LT .9999               /*SINGLE PRECISION VERSION  /*S*/CEL 570
 /*IF GEO/AARI LT .999999995          /*DOUBLE PRECISION VERSION  /*D*/CEL 580
   THEN DO,.                                                        CEL  590
        GEO  =GEO*AARI,.                                           CEL  600
        GO TO ITER,.                                               CEL  610
        END,.                                                      CEL  620
   RES  =1.57079632679489 7E0*AN/ARI,.                             CEL  630
RETURN..                                                           CEL  640
   END,.                              /*END OF PROCEDURE CEL      */CEL  650
```

Purpose:

CEL1 computes the complete elliptic integral of the first kind:

$$\int_0^{\pi/2} dt/\sqrt{1 - k^2\sin^2 t}, \quad 0 \le k < 1$$

Usage:

CALL CEL1 (RES, K);

RES - BINARY FLOAT [(53)]
Resultant value of elliptic integral.

K - BINARY FLOAT [(53)]
Given modulus of elliptic integral.

Purpose:

CEL2 computes the generalized elliptic integral of the second kind:

$$\int_0^{\pi/2} \frac{[a + (b - a)\sin^2 t]\,dt}{\sqrt{1 - k^2\sin^2 t}} \qquad 0 \le k < 1$$

Usage:

CALL CEL2 (RES, K, A, B);

RES - BINARY FLOAT [(53)]
Resultant value of elliptic integral.

K - BINARY FLOAT [(53)]
Given modulus of elliptic integral.

A - BINARY FLOAT [(53)]
Given primary term in numerator.

B - BINARY FLOAT [(53)]
Given secondary term in numerator.

Remarks:

If no errors are detected in the processing of data the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR = '1' means $|k| > 1$.

An input value of k with $|k| > 1$ is treated as if it were equal to 1. The value of k, however, remains unchanged.

Instead of ± infinity, the procedure returns $\pm 10^{75}$ as result values.

Method:

Calculation is based on the process of the arithmetic-geometric mean, combined with Landen's transformation.

For reference see:

R. Bulirsch, "Numerical Calculation of Elliptic Integrals and Elliptic Functions", Handbook Series of Special Functions, Numerische Mathematik, vol. 7, 1965, pp. 78-90.
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Applied Mathematics Series 55, National Bureau of Standards, 1964, pp. 597-599.

Mathematical Background:

Notation and equivalent definitions

Let k_c denote the complementary modulus defined through $k^2 + k_c^2 = 1$, $0 < k_c \leq 1$.

$$\text{cel1}(k) = K(k) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-k^2\sin^2 t}}$$

$$= \int_0^{\infty} \frac{dx}{\sqrt{(1+x^2)(1+k_c^2 x^2)}}$$

$$\text{cel2}(k;a,b) = \int_0^{\pi/2} \frac{a+(b-a)\sin^2 t}{\sqrt{1-k^2\sin^2 t}}\, dt$$

$$= \int_0^{\infty} \frac{a+bx^2}{(1+x^2)\sqrt{(1+x^2)(1+k_c^2 x^2)}}\, dx$$

Important special cases of cel2 are the complete elliptic normal integrals:

$$K(k) = \text{cel2}(k;1,1) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-k^2\sin^2 t}}$$

$$= \int_0^{1} \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}$$

$$E(k) = \text{cel2}(k;1,k_c^2) = \int_0^{\pi/2} \sqrt{1-k^2\sin^2 t}\, dt$$

$$= \int_0^{1} \sqrt{\frac{1-k^2t^2}{1-t^2}}\, dt$$

$$D(k) = \text{cel2}(k;0,1) = \int_0^{\pi/2} \frac{\sin^2 t\, dt}{\sqrt{1-k^2\sin^2 t}}$$

$$= \int_0^{1} \frac{t^2\, dt}{\sqrt{(1-t^2)(1-k^2t^2)}}$$

$$B(k) = \text{cel2}(k;1,0) = \int_0^{\pi/2} \frac{\cos^2 t}{\sqrt{1-k^2\sin^2 t}}\, dt$$

$$= \int_0^{1} \sqrt{\frac{1-t^2}{1-k^2t^2}}\, dt$$

Process of the arithmetic-geometric mean

Starting with the pair of numbers:

$$a = 2,\ g = 2k_c$$

the sequences of numbers (a_n), (g_n) are generated using the definition:

$$a_n = (a_{n-1} + g_{n-1}),\ g_n = 2\sqrt{a_{n-1} \cdot g_{n-1}}$$

This iteration process is stopped at the Nth step when $a_N = g_N$ to the degree of accuracy of the finite arithmetic employed.

In case cel2 the sequences (A_i), (B_i) are also needed. They are defined by means of

$$A_0 = A, \quad B_0 = 2B$$

$$A_n = B_{n-1}/a_{n-1} + A_{n-1},$$

$$B_n = 2(B_{n-1} + g_{n-1} \cdot A_{n-1})$$

Result values obtained are

$$\text{cel1}(k) = \frac{\pi}{2} \cdot \frac{2^{N+1}}{a_N}$$

$$\text{cel2}(k,A,B) = \frac{\pi}{2} \cdot \frac{A_{N+1}}{a_N}$$

Programming Considerations:

The equality $a_N = g_N$ must be interpreted as $|a_N - g_N|$ is less than $a_N \cdot 10^{-D}$, where D is the number of decimal digits in the mantissa of floating-point numbers.

Since the sequences $(2^{-n} \cdot a_n)$, $(2^{-n} \cdot g_n)$ converge quadratically to the same limit (arithmetic-geometric mean), the above test may be replaced by comparing $|a_{N-1} - g_{N-1}|$ against $a_{N-1} \cdot 10^{-D/2}$, thus saving one calculation of the geometric mean.

- Subroutine ELI1/ELI2

```
ELI1..                                                          ELI   10
/*****************************************************************/ELI   20
/*                                                               */ELI   30
/*      ELLIPTIC INTEGRAL OF FIRST KIND                          */ELI   40
/*                                                               */ELI   50
/*****************************************************************/ELI   60
   PROCEDURE(RES,ARG,CMOD),.                                     ELI   70
   DECLARE                                                       ELI   80
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR  */ELI   90
         (RES,ARG,CMOD,A,B,AN,APIM,PIM,ARI,AARI,GEO,SGEO,ANG,     ELI  100
         AANG,C,D,P,X,R,AA,AMB)                                   ELI  110
         BINARY FLOAT,              /*SINGLE PRECISION VERSION  /*S*/ELI  120
 /*      BINARY FLOAT(53),          /*DOUBLE PRECISION VERSION  /*D*/ELI  130
         ISI BINARY FIXED,                                        ELI  140
         SWITCH CHARACTER(1),.                                    ELI  150
   SWITCH='1',.                     /*INIT. ELI1 ENTRY          */ELI  160
   P    =1,.                                                     ELI  170
   GO TO COM,.                                                   ELI  180
ELI2..                                                          ELI  190
/*****************************************************************/ELI  200
/*                                                               */ELI  210
/*      GENERALIZED ELLIPTIC INTEGRAL OF SECOND KIND             */ELI  220
/*                                                               */ELI  230
/*****************************************************************/ELI  240
   ENTRY(RES,ARG,CMOD,A,B),.                                     ELI  250
   SWITCH='2',.                     /*INIT. ELI2 ENTRY          */ELI  260
   D    =0.5,.                                                   ELI  270
   C    =0,.                                                     ELI  280
   AA   =A,.                                                     ELI  290
   R    =B,.                                                     ELI  300
   AMB  =AA-R,.                                                  ELI  310
   AN   =(AA+R)*.5,.                                             ELI  320
COM..                               /*START COMMON CALCULATION  */ELI  330
   ERROR='0',.                      /*SET ERROR PARAMETER       */ELI  340
   X    =ARG,.                                                   ELI  350
   IF X = 0                         /*TEST FOR ZERO ARGUMENT    */ELI  360
   THEN DO,.                                                     ELI  370
        GEO  =0,.                                                ELI  380
        GO TO RETURN,.                                           ELI  390
        END,.                                                    ELI  400
   GEO  =ABS(CMOD),.                /*SET UP GEO(0)             */ELI  410
   IF GEO= 0                        /*TEST FOR MODULUS EQUAL ONE*/ELI  420
   THEN DO,.                                                     ELI  430
        AN,ANG=1,.                                               ELI  440
        AANG,GEO=SQRT(1+X*X),.                                   ELI  450
        D    =ABS(X),.                                           ELI  460
        GEO  =R*LOG(D+GEO),.                                     ELI  470
        GO TO TWO,.                                              ELI  480
        END,.                                                    ELI  490
   ARI  =1,.                        /*SET UP ARI(0)             */ELI  500
   ANG  =ABS(1/X),.                 /*SET UP ANG(0)             */ELI  510
   PIM  =0,.                        /*INIT. MULTIPLE OF PI      */ELI  520
   ISI  =0,.                                                     ELI  530
LOOP..                              /*START CENTRAL LOOP        */ELI  540
   APIM =PIM,.                      /*COUNTER I STARTS WITH ONE */ELI  550
   AARI =ARI,.                      /*SAVE ARI(I-1)             */ELI  560
   ARI  =ARI+GEO,.                  /*CALCULATE ARI(I)          */ELI  570
   SGEO =AARI*GEO,.                                              ELI  580
   ANG  =ANG-SGEO/ANG,.             /*CALCULATE ANG(I)          */ELI  590
   SGEO =SQRT(SGEO),.                                            ELI  600
   IF ANG=0                         /*INCREASE ANG(I) IF ZERO   */ELI  610
   THEN ANG  =SGEO*1.E-8,.          /*SINGLE PRECISION VERSION  /*S*/ELI  620
 /*THEN ANG  =SGEO*1.E-16,.         /*DOUBLE PRECISION VERSION  /*D*/ELI  630
   IF ANG LT 0                                                   ELI  640
   THEN DO,.                                                     ELI  650
        PIM  =3.141592653589793E0+PIM,.                          ELI  660
        ISI  =ISI+1,.                                            ELI  670
        END,.                                                    ELI  680
   IF SWITCH='2'                                                 ELI  690
   THEN DO,.                                                     ELI  700
        R    =AA*GEO+R,.             /*CALCULATE B(I)            */ELI  710
        AA   =AN,.                   /*SAVE A(I)                 */ELI  720
        AN   =0.5*(AN+R/ARI),.       /*CALCULATE A(I+1)          */ELI  730
        AANG =ARI*ARI+ANG*ANG,.                                  ELI  740
        P    =D/SQRT(AANG),.         /*CALCULATE I-TH TERM OF SUM*/ELI  750
        IF ISI GE 4                                              ELI  760
        THEN ISI  =ISI-4,.                                       ELI  770
        IF ISI GE 2                 /*CHANGE SIGN IF ANGLE IS IN*/ELI  780
        THEN P    =-P,.             /*THIRD OR FOURTH QUADRANT  */ELI  790
        C    =C+P,.                                              ELI  800
        D    =D*(AARI-GEO)*0.5/ARI,.                             ELI  810
        END,.                                                    ELI  820
                                    /*TEST FOR CONVERGENCE      */ELI  830
   IF ABS(AARI-GEO) GT AARI*1E-4    /*SINGLE PRECISION VERSION  /*S*/ELI  840
 /*IF ABS(AARI-GEO) GT AARI*5E-9    /*DOUBLE PRECISION VERSION  /*D*/ELI  850
   THEN DO,.                                                     ELI  860
        GEO  =SGEO+SGEO,.                                        ELI  870
        PIM  =PIM+APIM,.                                         ELI  880
        ISI  =ISI+ISI,.                                          ELI  890
        GO TO LOOP,.                                             ELI  900
        END,.                       /*END OF CENTRAL LOOP       */ELI  910
   GEO  =(ATAN(ARI/ANG)+PIM)/ARI,.                               ELI  920
TWO..                                                           ELI  930
   IF SWITCH='2'                                                 ELI  940
   THEN DO,.                                                     ELI  950
        C    =C+D*ANG/AANG,.                                     ELI  960
        GEO  =GEO*AN+C*AMB,.                                     ELI  970
        END,.                                                    ELI  980
   IF X LT 0                                                     ELI  990
   THEN GEO  =-GEO,.                                             ELI 1000
RETURN..                                                        ELI 1010
   RES  =GEO,.                                                   ELI 1020
   END,.                            /*END OF PROCEDURE ELI      */ELI 1030
```

Purpose:

ELI1 computes the incomplete elliptic integral of first kind for given values of an argument x and complementary modulus ck.

$$\text{eli1}\ (x,\ ck) = \int_0^x \frac{dt}{\sqrt{(1+t^2)(1+ck^2 \cdot t^2)}}$$

Usage:

CALL ELI1 (RES, ARG, CMOD);

RES - BINARY FLOAT [(53)]
Resultant value of elliptic integral.

ARG - BINARY FLOAT [(53)]
Given argument of elliptic integral.

CMOD - BINARY FLOAT [(53)]
Given complementary modulus of elliptic integral.

Purpose:

ELI2 computes the generalized incomplete elliptic integral of second kind for given values of an argument x, complementary modulus ck, and constants a and b.

$$\text{eli2}\ (x,\ ck;\ a,\ b) = \int_0^x \frac{(a+bt^2)\quad dt}{(1+t^2)\sqrt{(1+t^2)(1+ck^2 \cdot t^2)}}$$

Usage:

CALL ELI2 (RES, ARG, CMOD, A, B);

RES - BINARY FLOAT [(53)]
Resultant value of elliptic integral.

ARG - BINARY FLOAT [(53)]
Given argument of elliptic integral.

CMOD - BINARY FLOAT [(53)]
Given complementary modulus of elliptic integral.

A - BINARY FLOAT [(53)]
Given primary term in numerator (see "Purpose").

B - BINARY FLOAT [(53)]
Given secondary term in numerator (see "Purpose").

Remarks:

Modulus k and complementary modulus ck satisfy the relation $k^2 + ck^2 = 1$. Internally, ck is needed for calculation rather than k. Therefore, ck is used as input parameter. This allows the modulus k to be any pure imaginary or real number such that $k^2 \leq 1$.

Method:

Calculation is based on the process of the arithmetic-geometric mean, combined with descending Landen's transformation.

For reference see:

R. Bulirsch, "Numerical Calculation of Elliptic Integrals and Elliptic Functions", Handbook Series of Special Functions, Numerische Mathematik vol. 7, 1965, pp. 78-90.

Mathematical Background:

Notation and equivalent definitions:

$$\text{eli1}(x, ck) = \int_0^x \frac{dt}{\sqrt{(1+t^2)(1+ck^2 \cdot t^2)}}$$

$$= \int_0^{\arctan x} \frac{dt}{\cos t \sqrt{1+ck^2 \cdot \tan^2 t}} = \int_0^{\arctan x} \frac{dt}{\sqrt{1-k^2 \sin^2 t}}$$

$$\text{eli2}(x, ck, a, b) = \int_0^x \frac{(a+bt^2)\, dt}{(1+t^2)\sqrt{(1+t^2)(1+ck^2 \cdot t^2)}}$$

$$= \int_0^{\arctan x} \frac{(a+b\tan^2 t)\, dt}{\sqrt{(1+\tan^2 t)(1+ck^2 \cdot \tan^2 t)}}$$

$$= \int_0^{\arctan x} \frac{(a+(b-a)\sin^2 t)\, dt}{\sqrt{1-k^2 \sin^2 t}}$$

Important special cases are:

$$F(\varphi, k) = \text{eli1}(\tan\varphi, ck) = \int_0^{\varphi} \frac{dt}{\sqrt{1-k^2 \sin^2 t}}$$

$$= \text{eli2}(\tan\varphi, ck; 1, 1)$$

$$E(\varphi, k) = \text{eli2}(\tan\varphi, ck; 1, ck^2) = \int_0^{\varphi} \sqrt{1-k^2 \sin^2 t}\, dt$$

$$D(\varphi, k) = \frac{F(\varphi, k) - E(\varphi, k)}{k^2} = \text{eli2}(\tan\varphi, ck; 0, 1)$$

$$= \int_0^{\varphi} \frac{\sin^2 t\, dt}{\sqrt{1-k^2 \sin^2 t}}$$

$$B(\varphi, k) = \frac{E(\varphi, k) - ck^2 F(\varphi, k)}{k^2} = \text{eli2}(\tan\varphi, ck; 1, 0)$$

$$= \int_0^{\varphi} \frac{\cos^2 t\, dt}{\sqrt{1-k^2 \sin^2 t}}$$

Process of the arithmetic-geometric mean

Starting with $ari_0 = 1$, $geo_0 = |ck|$, the sequences (ari_n), (geo_n) are generated using the recursion formulas

$$ari_{n+1} = ari_n + geo_n \tag{1}$$

$$geo_{n+1} = 2\sqrt{ari_n \cdot geo_n} \tag{2}$$

This iterative process is stopped at the Nth step, when $ari_N = geo_N$ to the degree of accuracy of the finite arithmetic employed.

Descending Landen's transformation

For the descending Landen transformation the modular angle α defined by $k = \sin\alpha$ decreases, while the amplitudinal angle φ defined by $x = \tan\varphi$ increases.

Successive values of α and φ are combined as follows:

$$(1+\sin\alpha_1)(1+\cos\alpha) = 2 \qquad \alpha_1 < \alpha \tag{3}$$

$$\tan(\varphi_1 - \varphi) = \cos\alpha \cdot \tan\varphi \qquad \varphi_1 > \varphi \tag{4}$$

Expressed in terms of argument x and complementary modulus ck, these equations read

$$ck_1 = \frac{2\sqrt{ck}}{1+ck} \tag{5}$$

$$x_1 = \frac{(1+ck)x}{1-ck \cdot x^2} \tag{6}$$

For values of argument and modulus that are connected by (5) and (6) we have

$$\text{eli1}\ (x, ck) = \frac{1}{1+ck}\ \text{eli1}\ (x_1, ck_1) \tag{7}$$

$$\text{eli2}\ (x, ck; a, b) = \frac{1}{1+ck}\ \text{eli2}(x_1, ck_1; a_1, b_1) + \frac{(a-b)}{2} \cdot \frac{x_1}{\sqrt{1+x_1^2}}\ ) \tag{8}$$

where

$$a_1 = (a+b)/2 \tag{9}$$

$$b_1 = \frac{1}{1+ck}\ (b+a \cdot ck) \tag{10}$$

The sign determination of $\frac{x_1}{\sqrt{1+x_1{}^2}} = \sin \varphi_1$ must be done such that $\varphi_1 = \arctan x_1$ is monotonically increasing ($\varphi_1 > \varphi$).

Final iteration process

We set: $x_0 = |x|$ and $ang_0 = 1/x_0$

$$x_i = \frac{ari_i}{ang_i} \tag{11}$$

$$ck_i = \frac{geo_i}{ari_i} \tag{12}$$

Furthermore, in case eli2 we use:

$$A_i = a_i,\ B_i = b_i \cdot ari_i$$

then:

$$A_0 = a,\ B_0 = b$$

$$A_{i+1} = 1/2\ (A_i + \frac{B_i}{ari_i}) \tag{13}$$

$$B_{i+1} = B_i + geo_i \cdot A_i \tag{14}$$

Successive application of the descending Landen transformation gives

$$\text{eli1}(x, ck) = \frac{ari_0}{ari_1}\ \text{eli1}(x_1, ck_1)$$

$$= \frac{ari_0}{ari_1} \cdot \frac{ari_1}{ari_2}\ \text{eli1}(x_2, ck_2) \ldots$$

$$= \frac{ari_0}{ari_N}\ \text{eli1}(x_N, ck_N)$$

$$\text{eli2}(x, ck; a, b) = \frac{ari_0}{ari_1}\ \text{eli2}(x_1, ck_1; a_1, b_1) + \frac{a-b}{2} \cdot \frac{\sin \varphi_1}{ari_1}$$

$$= \frac{ari_0}{ari_2}\ \text{eli2}\ (x_2, ck_2; a_2, b_2) + \frac{a-b}{2}\left(\frac{\sin \varphi_1}{ari_1} + \frac{ari_0 - geo_0}{ari_1} \frac{\sin \varphi_2}{2 \cdot ari_2}\right)$$

$$= \ldots$$

$$= \frac{ari_0}{ari_N}\ \text{eli2}\ (x_N,\ ck_N;\ a_N,\ b_N) + \text{SUM}$$

where:

$$\text{SUM} = \frac{a-b}{2}\left(\frac{1}{ari_1} \sin \varphi_1 + \frac{1}{ari_2} \cdot \frac{ari_0 - geo_0}{ari_1} \cdot \frac{\sin \varphi_2}{2} + \ldots + \frac{1}{ari_N} \cdot \frac{ari_0 - geo_0}{ari_1} \ldots \frac{ari_{N-2} - geo_{N-2}}{ari_{N-1}} \cdot \frac{\sin \varphi_N}{2^{N-1}}\right)$$

Since $ck_N = 1$ to working accuracy:

$\text{eli1}\ (x_N,\ ck_N) = \varphi_N$, where $\tan \varphi_N = \frac{ari_N}{ang_N}$

$$eli2\,(x_N,\ ck_N;\ a_N,\ b_N) = \frac{a_N+b_N}{2} \cdot \varphi_N + \frac{a_N-b_N}{2} \sin\varphi_N \cdot \cos\varphi_N$$

The final result is

$$eli1\,(x,\ ck) = \frac{\varphi_N}{ari_N}$$

$$eli2\,(x,\ ck;\ a,b) = \frac{A_{N+1}}{ari_N}\varphi_N + SUM + \frac{1}{ari_N}\left(\frac{a_N-b_N}{2}\right) \sin\varphi_N \cdot \cos\varphi_N$$

Degenerate cases of argument and modulus

x = 0 gives result eli2 = 0

ck = 0 gives result $eli2 = \left(b \cdot \ln\left(|x|+\sqrt{1+x^2}\right) + (a-b)\right) \frac{x \operatorname{sgn} x}{\sqrt{1+x^2}}$

Programming Considerations:

The equality $ari_N = geo_N$ must be interpreted as '$ari_N - geo_N|$ is less than $ari_N \cdot 10^{-D}$, where D is the number of decimal digits in the mantissa of floating-point numbers.

Since the sequences $(ari_n \cdot 2^{-n})$, $(geo_n \cdot 2^{-n})$ converge quadratically to the same limit (arithmetic-geometric mean), the above test may be replaced by comparing

$|ari_{N-1} - geo_{N-1}|$ against $ari_{N-1} \cdot 10^{-D/2}$, thus saving one calculation of the geometric mean.

- Subroutine JELF

```
JELF..                                                                  JELF  10
/*********************************************************************/JELF  20
/*                                                                   */JELF  30
/*      JACOBIAN ELLIPTIC FUNCTIONS SN, CN, DN                       */JELF  40
/*                                                                   */JELF  50
/*********************************************************************/JELF  60
   PROCEDURE(SN,CN,DN,X,SCK),.                                          JELF  70
   DECLARE                                                              JELF  80
         ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR     */JELF  90
         (SN,CN,DN,X,SCK,CM,Y,LSN,LCN,LDN,K,ARI(12),GEO(12),A,B,C,D)    JELF 100
         BINARY FLOAT,                 /*SINGLE PRECISION VERSION  /*S*/JELF 110
 /*      BINARY FLOAT(53),             /*DOUBLE PRECISION VERSION  /*D*/JELF 120
         (I,J) BINARY FIXED,.                                           JELF 130
   ERROR='0',.                                                          JELF 140
   CM   =SCK,.                                                          JELF 150
   Y    =X,.                                                            JELF 160
   IF CM= 0                      /*TEST VALUE OF MODULUS             /JELF 170
   THEN DO,.                     /*DEGENERATE CASE SCK = 0           */JELF 180
         LCN,LDN=1/COSH(Y),.                                            JELF 190
         LSN  =TANH(Y),.                                                JELF 200
         GO TO RETURN,.                                                 JELF 210
         END,.                                                          JELF 220
   IF CM LT 0                                                           JELF 230
   THEN DO,.                     /*MODULUS TRANSFORMATION            */JELF 240
         K    =(0.5-CM)+0.5,.                                           JELF 250
         CM   =-CM/K,.                                                  JELF 260
         K    =SQRT(K),.                                                JELF 270
         Y    =K*Y,.                                                    JELF 280
         END,.                                                          JELF 290
   C,LDN=1,.                     /*PROCESS OF THE ARITHMETIC-        */JELF 300
         DO I=1 TO 12,.          /*GEOMETRIC MEAN                    */JELF 310
         ARI(I),LCN=C,.                                                 JELF 320
         GEO(I),CM=SQRT(CM),.                                           JELF 330
         C    =.5*(LCN+CM),.                                            JELF 340
         IF ABS(LCN-CM) LE 1E-4*LCN  /*SINGLE PRECISION VERSION  /*S*/JELF 350
 /*      IF ABS(LCN-CM) LE 5E-9*LCN  /*DOUBLE PRECISION VERSION  /*D*/JELF 360
         THEN GO TO CONV,.                                              JELF 370
         CM   =CM*LCN,.                                                 JELF 380
         END,.                                                          JELF 390
CONV..                           /*INIT. INVERSE GAUSS-              */JELF 400
   Y    =Y*C,.                   /*TRANSFORMATION                    */JELF 410
   LSN,D=SIN(Y),.                                                       JELF 420
   LCN  =COS(Y),.                                                       JELF 430
   IF LSN= 0                                                            JELF 440
   THEN GO TO TEST,.                                                    JELF 450
   A    =LCN/LSN,.                                                      JELF 460
   C    =A*C,.                                                          JELF 470
         DO J =I TO 1 BY -1,.    /*INVERSE GAUSS-TRANSFORMATION      */JELF 480
         B    =ARI(J),.                                                 JELF 490
         A    =A*C,.                                                    JELF 500
         C    =LDN*C,.                                                  JELF 510
         LDN  =(GEO(J)+A)/(B+A),.                                       JELF 520
         A    =C/B,.                                                    JELF 530
         END,.                                                          JELF 540
   LSN  =SQRT(1/(1+C*C)),.                                              JELF 550
   IF D LT 0                                                            JELF 560
   THEN LSN  =-LSN,.                                                    JELF 570
   LCN  =C*LSN,.                                                        JELF 580
TEST..                           /*INVERSE MODULUS-TRANSFORMAT.      */JELF 590
   IF SCK LT 0                                                          JELF 600
   THEN DO,.                                                            JELF 610
         A    =LDN,.                                                    JELF 620
         LDN  =LCN,.                                                    JELF 630
         LCN  =A,.                                                      JELF 640
         LSN  =LSN/K,.                                                  JELF 650
         END,.                                                          JELF 660
RETURN..                         /*RETURN RESULT VALUES              */JELF 670
   SN   =LSN,.                                                          JELF 680
   CN   =LCN,.                                                          JELF 690
   DN   =LDN,.                                                          JELF 700
   END,.                         /*END OF PROCEDURE JELF             */JELF 710
```

Purpose:

JELF calculates the three Jacobian elliptic functions SN, CN, DN.

Usage:

CALL JELF (SN, CN, DN, X, SCK);

SN - BINARY FLOAT [(53)]
Resultant value of the sine of the amplitude.

CN - BINARY FLOAT [(53)]
Resultant value of the cosine of the amplitude.

DN - BINARY FLOAT [(53)]
Resultant value of the delta of the amplitude.

X - BINARY FLOAT [(53)]
Given argument of Jacobian elliptic functions.

SCK - BINARY FLOAT [(53)]
Given square of complementary modulus.

Remarks:

The values of SN, CN, DN are frequently needed together. Therefore, procedure JELF computes all three of them. This is no disadvantage, since computation of all three result values is no more complicated than computation of any one of them. The value SCK is chosen as an input parameter in order to allow for complex values of ck (k is not restricted to $k^2 \leq 1$).

Method:

The calculation is based on the process of the arithmetic-geometric mean together with Gauss' transformation.

For reference see:

R. Bulirsch, "Numerical Calculation of Elliptic Integrals and Elliptic Functions", Numerische Mathematik, vol. 7, 1965, pp. 78-90.

Mathematical Background:

Notation and definition

The value k is the modulus, ck is the complementary modulus, and sck is the square of the complementary modulus.

$$sck = ck^2 = 1-k^2 \qquad -\infty < sck < \infty$$

The three Jacobian elliptic functions arise as inverse functions of elliptic integrals.

Set:

$$x = F(\varphi,k) = \int_0^{\varphi} \frac{dt}{\sqrt{1-k^2 \sin^2 t}}$$

Then φ is called the amplitude of x.

$$\varphi = am\ (x,k) \tag{1}$$

Jacobi's functions are defined through

$$sn(x,k) = \sin\varphi = \sin am\ (x,k) \tag{2}$$

$$cn(x,k) = \cos\varphi = \cos am\ (x,k) \tag{3}$$

$$dn(x,k) = \sqrt{1-k^2\sin^2\varphi} \tag{4}$$

The degenerate case sck = 0 (that is, $|k| = 1$) must be treated separately:

$$sn(x,1) = \tanh x$$

$$cn(x,1) = dn\ (x,1) = 1/\cosh x$$

Jacobi's modulus transformation, applied to negative values of sck, gives

$$sn(x,k) = 1/k \cdot sn\ (kx, 1/k) \tag{5}$$

$$cn(x,k) = dn(kx, 1/k) \tag{6}$$

$$dn(x,k) = cn(kx, 1/k) \tag{7}$$

Process of the arithmetic-geometric mean

Starting with $ari_1 = 1$, $geo_1 = \sqrt{sck}$, the sequences (ari_n), (geo_n) are generated using the recursion formulas

$$ari_{n+1} = (ari_n + geo_n)/2 \tag{8}$$

$$geo_{n+1} = \sqrt{ari_n \cdot geo_n} \tag{9}$$

Numerical experience shows that eleven iterations are sufficient to obtain convergence, to full working accuracy, for all values of the squared complementary modulus that may be represented in floating point. The iteration process is stopped at the Nth step, as soon as ari_{N+1}-geo_{N+1} is negligibly small.

Gauss transformation

Gauss' transformation gives

$$F(\varphi_1, k_1) = (1 + k)\ F(\varphi, k) \tag{10}$$

for values of modulus and amplitudinal angle that are combined through

$$k_1 = \frac{2\sqrt{k}}{1+K} \tag{11}$$

and

$$\sin\varphi_1 = \frac{(1+k)\sin\varphi}{1+k\sin^2\varphi} \tag{12}$$

Inversion of this transformation results in

$$F(\varphi,k) = (1+k_1)\ F(\varphi_1, k_1) \tag{10'}$$

where:

$$\sin\varphi = \frac{(1+k_1)\sin\varphi_1}{1+k_1\sin^2\varphi_1} \qquad (11')$$

and

$$k = \frac{2\sqrt{k_1}}{1+k_1} \qquad (12')$$

Inversion of $F(\varphi, k)$

Successive application of transformation (10'), with

$$ck_i = \frac{geo_{i+1}}{ari_{i+1}} \qquad (13)$$

leads to $F(\varphi, k) = (1+k_1) \cdot \cdot \cdot (1+k_N)\, F(\varphi_N,\ k_N)$.

Equation (12') implies that $k_{i+1} = \frac{1-ck_i}{1+ck_i}$

and that

$$1 + k_{i+1} = \frac{ari_{i+1}}{ari_{i+2}}$$

If $k_N = 0$, it follows that

$$x = F(\varphi, k) = \frac{ari_1}{ari_{N+1}}$$

$$F(\varphi_N, k_N) = \frac{ari_1}{ari_{N+1}}\varphi_N \qquad (14)$$

or $\varphi_N = ari_{N+1} \cdot x$

Back transformation of φ_N

To obtain the Jacobian elliptic functions, the inverse transformation must be performed on φ_N. Equation (11') implies

$$\cot\varphi = \frac{1}{1+k_1}\cot\varphi_1\sqrt{1 - k_1^2\sin^2\varphi_1}$$

or generally

$$ari_n \cot\varphi_{n-1} = ari_{n+1}\cot\varphi_n\sqrt{1 - k_n^2\sin^2\varphi_n} \qquad (15)$$

From (11') and (12') it follows that

$$\sqrt{1-k_n^2\sin^2\varphi_n} = \frac{1-k_{n+1}\sin^2\varphi_{n+1}}{1+k_{n+1}\sin^2\varphi_{n+1}}$$

$$= \frac{\cot^2\varphi_{n+1} + 1-k_{n+1}}{\cot^2\varphi_{n+1} + 1+k_{n+1}} \qquad (16)$$

$$= \frac{geo_{n+1} + ari_{n+2}\cdot\cot^2\varphi_{n+1}}{ari_{n+1} + ari_{n+2}\cdot\cot^2\varphi_{n+1}}$$

since $\frac{1-k_{n+1}}{1+k_{n+1}} = ck_n = \frac{geo_{n+1}}{ari_{n+1}}$

and

$$1+k_{n+1} = \frac{ari_{n+1}}{ari_{n+2}}$$

Final iteration scheme

Setting $c_{N+1} = ari_{N+1} \cdot \cot\varphi_N$, with $d_{N+1} = 1$, the following iteration is performed for n = N, N-1, . . . , 1:

$$c_n = d_{n+1} \cdot c_{n+1}$$

$$d_n = \frac{c_{n+1}^2/ari_{n+2} + geo_{n+1}}{c_{n+1}^2/ari_{n+2} + ari_{n+1}}$$

The final result is

$$c_1 = \cot\varphi$$

$$d_1 = \sqrt{1-k^2\sin^2\varphi}$$

and therefore:

$$sn(x,k) = \frac{1}{\sqrt{1+c_1^2}} = \sin\varphi$$

$$cn(x,k) = sn \cdot c_1 = \cos\varphi$$

$$dn(x,k) = d_1 = \sqrt{1-k^2\sin^2\varphi}$$

- Subroutine LGAM

```
LGAM..                                                                  LGAM  10
/************************************************************************/LGAM  20
/*                                                                      */LGAM  30
/*      COMPUTES THE DOUBLE PRECISION NATURAL LOGARITHM OF THE GAMMA    */LGAM  40
/*      FUNCTION OF A GIVEN DOUBLE PRECISION ARGUMENT.                  */LGAM  50
/*                                                                      */LGAM  60
/************************************************************************/LGAM  70
   PROCEDURE (XX,DLNG),.                                                LGAM  80
   DECLARE                                                              LGAM  90
        (XX,ZZ,TERM,RZ2,DLNG) FLOAT BINARY (53),                        LGAM 100
        ERROR EXTERNAL CHARACTER (1),.                                  LGAM 110
   ERROR='0',.                                                          LGAM 120
   ZZ  =XX,.                                                            LGAM 130
   IF XX LE 1.E10                                                       LGAM 140
   THEN IF XX LE 1.E-09              /* XX IS NEAR 0 OR NEGATIVE      */LGAM 150
        THEN DO,.                    /* SET ERROR INDICATOR           */LGAM 160
             ERROR='2',.                                                LGAM 170
             DLNG =-1.E75,.                                             LGAM 180
             GO TO S20,.                                                LGAM 190
             END,.                                                      LGAM 200
        ELSE DO,.                    /* XX > 0 AND < OR = TO 1.E+10   */LGAM 210
             TERM =1.E0,.                                               LGAM 220
S10..                                                                   LGAM 230
             IF ZZ LE 18.E0          /* ZZ < OR = 18                  */LGAM 240
             THEN DO,.               /* TRANSLATE ARGUMENT            */LGAM 250
                  TERM =TERM*ZZ,.                                       LGAM 260
                  ZZ   =ZZ+1.E0,.                                       LGAM 270
                  GO TO S10,.                                           LGAM 280
                  END,.                                                 LGAM 290
             ELSE DO,.               /* CALC. EQUATION 1              */LGAM 300
                  RZ2  =1.E0/ZZ**2,.                                    LGAM 310
                  DLNG =(ZZ-C.5E0)*LOG(ZZ)-ZZ+0.918938533204672E0       LGAM 320
                       -LOG(TERM)+(1.E0/ZZ)*(.833333333333333E-01       LGAM 330
                       -(RZ2*(.2777777777777777E-02+(RZ2*               LGAM 340
                       (.793650793650793E-03-(RZ2*                      LGAM 350
                       (.595238095238095E-03))))))),.                   LGAM 360
                  GO TO S20,.                                           LGAM 370
                  END,.                                                 LGAM 380
             END,.                                                      LGAM 390
   ELSE IF XX LT 1.E70               /* XX > 1.E+10 AND < 1.E+70      */LGAM 400
        THEN DO,.                                                       LGAM 410
             DLNG =ZZ*(LOG(ZZ)-1.E0),./* CALC. EQUATION 2             */LGAM 420
             GO TO S20,.                                                LGAM 430
             END,.                                                      LGAM 440
        ELSE DO,.                    /* XX > OR = 1.E+70              */LGAM 450
             ERROR='1',.             /* SET ERROR INDICATOR           */LGAM 460
             DLNG =1.E75,.                                              LGAM 470
             END,.                                                      LGAM 480
S20..                                                                   LGAM 490
   RETURN,.                                                             LGAM 500
   END,.                             /* END OF PROCEDURE LGAM         */LGAM 510
```

Purpose:

LGAM computes the double-precision natural logarithm of the gamma function of a given double-precision argument.

Usage:

CALL LGAM (XX, DLNG);

XX - BINARY FLOAT (53)
Given double-precision argument for the log gamma function.

DLNG - BINARY FLOAT (53)
Resultant double-precision variable containing the log gamma function.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - If XX is greater than or equal to 10^{70}. If this condition exists, the value of DLNG is set to 1.E75.

ERROR=2 - If XX is less than or equal to 10^{-9}, DLNG is set to -1.E75.

Method:

For reference see:

M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, U. S. Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966, equation 6.1.4.

Mathematical Background:

This subroutine computes the double-precision natural logarithm of the gamma function of a given double-precision argument, xx, where $10^{-9} < xx < 10^{70}$. The Euler-McLaurin expansion, to the seventh derivative term, is used. For $xx > 0$:

$$\log \Gamma(xx) = (xx - 1/2) \log xx + 1/2 \log 2\pi - xx + 1/(12\,xx) - 1/360\,xx^3 + 1/1260\,xx^5 = 1/1680\,xx^7 \qquad (1)$$

This expression is very accurate for $xx > 18$. If $xx \leq 18$, xx is replaced by $z = k + xx$, where k is an integer such that $z > 18$. Log Γ (z) is then evaluated by (1), and log xx + log (xx + 1) + ... + log (xx + k - 1) is subtracted to obtain the desired result.

If xx is between 10^{10} and 10^{70}, terms of lowest order in (1) are neglected, and log Γ (xx) is computed as:

$$\log \Gamma(xx) = xx\,(\log(xx) - 1) \qquad (2)$$

Subroutine LGAM is available in a double-precision format only. If the single-precision value of the log gamma function of a given single-precision argument is desired, subroutine LGAM should be changed to single precision.

Data Screening and Analysis

- Subroutine TALY

```
TALY..                                                                  TALY  10
/*************************************************************************/TALY  20
/*                                                                       */TALY  30
/*      TO CALCULATE TOTAL, MEAN, STANDARD DEVIATION, MINIMUM,           */TALY  40
/*      MAXIMUM FOR EACH VARIABLE IN A SET (OR A SUBSET) OF OBSER-       */TALY  50
/*      VATIONS.                                                         */TALY  60
/*                                                                       */TALY  70
/*************************************************************************/TALY  80
   PROCEDURE (A,S,TOTAL,AVER,SD,VMIN,VMAX,NO,NV),.                      TALY  90
   DECLARE                                                              TALY 100
        ERROR EXTERNAL CHARACTER (1),                                   TALY 110
        (I,J,K,NO,NV)                                                   TALY 120
        FIXED BINARY,                                                   TALY 130
        (A(*,*),S(*),TOTAL(*),AVER(*),SD(*),VMIN(*),VMAX(*),SCNT,D)     TALY 140
        FLOAT BINARY,.                                                  TALY 150
/*                                                                      */TALY 160
/*      CLEAR OUTPUT VECTORS AND INITIALIZE VMIN,VMAX.                  */TALY 170
/*                                                                      */TALY 180
   ERROR='0',.                                                          TALY 190
        DO I=1 TO NV,.                                                  TALY 200
        TOTAL(I)  =0.,.                                                 TALY 210
        AVER(I)   =0.,.                                                 TALY 220
        SD(I)     =0.,.                                                 TALY 230
        VMIN(I)   =0.,.                                                 TALY 240
        VMAX(I)   =0.,.                                                 TALY 250
        END,.                                                           TALY 260
   IF NV LE 0 OR NO LE 0              /* NUMBER OF OBSERVATIONS OR     */TALY 270
   THEN DO,.                          /* THE NUMBER OF VARIABLES LESS  */TALY 280
        ERROR='1',.                   /* THAN OR EQUAL TO ZERO.        */TALY 290
        GO TO S50,.                                                     TALY 300
        END,.                                                           TALY 310
        DO J = 1 TO NV,.                                                TALY 320
        TOTAL(J)=0.0,.                                                  TALY 330
        AVER(J)=0.0,.                                                   TALY 340
        SD(J)=0.0,.                                                     TALY 350
        END,.                                                           TALY 360
        DO J = 1 TO NO,.                                                TALY 370
        IF S(J) NE 0.0                                                  TALY 380
        THEN DO,.                                                       TALY 390
             K    =J,.                                                  TALY 400
             GO TO S1C,.                                                TALY 410
             END,.                                                      TALY 420
        END,.                                                           TALY 430
/*                                                                      */TALY 440
/*      NO OBSERVATIONS ARE IN SUBSET                                   */TALY 450
/*                                                                      */TALY 460
   ERROR='2',.                                                          TALY 470
   GO TO S50,.                                                          TALY 480
S1C..                                                                   TALY 490
        DO J = 1 TO NV,.                                                TALY 500
        VMIN(J)=A(K,J),.                                                TALY 510
        VMAX(J)=VMIN(J),.                                               TALY 520
        END,.                                                           TALY 530
   SCNT =0.0,.                        /* TEST SUBSET VECTOR            */TALY 540
        DO I = K TO NO,.                                                TALY 550
        IF S(I) NE 0.0                                                  TALY 560
        THEN DO,.                                                       TALY 570
             SCNT =SCNT+1.0,.                                           TALY 580
                  DO J = 1 TO NV,.    /* CALCULATE TOTAL,MAX,MIN       */TALY 590
                  TOTAL(J)=TOTAL(J)+A(I,J),.                            TALY 600
                  IF A(I,J) LT VMIN(J)                                  TALY 610
                  THEN VMIN(J)=A(I,J),.                                 TALY 620
                  IF A(I,J) GT VMAX(J)                                  TALY 630
                  THEN VMAX(J)=A(I,J),.                                 TALY 640
                  SD(J)=SD(J)+A(I,J)*A(I,J),.                           TALY 650
                  END,.                                                 TALY 660
             END,.                                                      TALY 670
        END,.                                                           TALY 680
/*                                                                      */TALY 690
/*      CALCULATE MEANS AND STANDARD DEVIATIONS.                        */TALY 700
/*                                                                      */TALY 710
        DO J = 1 TO NV,.                                                TALY 720
        AVER(J)=TOTAL(J)/SCNT,.       /* COMPUTE MEAN                  */TALY 730
        IF SCNT= 1.0                                                    TALY 740
        THEN DO,.                                                       TALY 750
             ERROR='3',.              /* SAMPLE SIZE IN SUBSET = 1     */TALY 760
             SD(J)=0.0,.                                                TALY 770
             GO TO S2C,.                                                TALY 780
             END,.                                                      TALY 790
        ELSE DO,.                                                       TALY 800
             D    =SD(J)-TOTAL(J)*TOTAL(J)/SCNT,.                       TALY 810
             IF D LE 0.0                                                TALY 820
             THEN DO,.                                                  TALY 830
                  ERROR='4',.         /* VARIANCE = 0.0                */TALY 840
                  SD(J)=0.0,.                                           TALY 850
                  GO TO S20,.                                           TALY 860
                  END,.                                                 TALY 870
             ELSE SD(J)=SQRT(D/(SCNT-1.0)),.                            TALY 880
             END,.                                                      TALY 890
S2C..                                                                   TALY 900
        END,.                                                           TALY 910
S50..                                                                   TALY 920
   RETURN,.                                                             TALY 930
   END,.                              /*END OF PROCEDURE TALY         */TALY 940
```

Purpose:

TALY calculates total, mean, standard deviation, minimum, maximum for each variable in a set (or a subset) of observations.

Usage:

CALL TALY (A, S, TOTAL, AVER, SD, VMIN, VMAX, NO, NV);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given observation matrix.

S(NO) - BINARY FLOAT
Given vector indicating subset of A. Only those observations with a nonzero S(J) are considered.

TOTAL(NV) - BINARY FLOAT
Resultant vector of totals.

AVER(NV) - BINARY FLOAT
Resultant vector of means.

SD(NV) - BINARY FLOAT
Resultant vector of standard deviations.

VMIN(NV) - BINARY FLOAT
Resultant vector of minima.

VMAX(NV) - BINARY FLOAT
Resultant vector of maxima.

NO - BINARY FIXED
Given parameter equal to the number of observations.

NV - BINARY FIXED
Given parameter equal to the number of variables.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations or the number of variables less than or equal to zero.
ERROR=2 - no observations in subset vector.
ERROR=3 - sample size in subset equal to one.
ERROR=4 - variance equal to zero.

Method:

All observations corresponding to a nonzero element in the S vector are analyzed for each variable in matrix A. Totals are accumulated and minimum and maximum values are found. Following this, means and standard deviations are calculated. The divisor for standard deviations is one less than the number of observations used.

- Subroutine BOUN

```
BOUN..                                                                  BOUN  10
/*************************************************************************/BOUN  20
/*                                                                       */BOUN  30
/*      TO SELECT FROM A SET (OR A SUBSET) OF OBSERVATIONS THE           */BOUN  40
/*      NUMBER OF OBSERVATIONS UNDER, BETWEEN AND OVER TWO GIVEN         */BOUN  50
/*      BOUNDS FOR EACH VARIABLE.                                        */BOUN  60
/*                                                                       */BOUN  70
/*************************************************************************/BOUN  80
   PROCEDURE (A,S,BLO,BHI,UNDER,BETW,OVER,NO,NV),.                      BOUN  90
   DECLARE                                                              BOUN 100
        (I,J,NO,NV)                                                     BOUN 110
        FIXED BINARY,                                                   BOUN 120
        ERROR EXTERNAL CHARACTER(1),                                    BOUN 130
        (A(*,*),S(*),BLO(*),BHI(*),UNDER(*),BETW(*),OVER(*))            BOUN 140
        FLOAT BINARY,.                                                  BOUN 150
/*                                                                      */BOUN 160
   ERROR='0',.                                                          BOUN 170
   IF NV LE 0 OR NO LE 0              /* NUMBER OF OBSERVATIONS OR      */BOUN 180
   THEN DO,.                          /* THE NUMBER OF VARIABLES LESS   */BOUN 190
        ERROR='1',.                   /* THAN OR EQUAL TO ZERO.         */BOUN 200
        GO TO FIN,.                                                     BOUN 210
        END,.                                                           BOUN 220
        DO J = 1 TO NV,.              /* CLEAR OUTPUT VECTORS           */BOUN 230
        UNDER(J)=0.0,.                                                  BOUN 240
        BETW(J)=0.0,.                                                   BOUN 250
        OVER(J)=0.0,.                                                   BOUN 260
        END,.                                                           BOUN 270
        DO J = 1 TO NV,.                                                BOUN 280
        IF BHI(J) LE BLO(J)           /* LOWER BOUND GREATER THAN       */BOUN 290
        THEN DO,.                     /* UPPER BOUND.                   */BOUN 300
             ERROR='2',.                                                BOUN 310
             GO TO FIN,.                                                BOUN 320
             END,.                                                      BOUN 330
        END,.                                                           BOUN 340
        DO I = 1 TO NO,.                                                BOUN 350
        IF S(I) NE 0.0                /* TEST SUBSET VECTOR             */BOUN 360
        THEN DO,.                                                       BOUN 370
/*                                                                      */BOUN 380
/*      COMPARE OBSERVATIONS WITH BOUNDS                                */BOUN 390
/*                                                                      */BOUN 400
                DO J = 1 TO NV,.                                        BOUN 410
                IF A(I,J) GE BLO(J)                                     BOUN 420
                THEN DO,.                                               BOUN 430
                     IF A(I,J) LE BHI(J)                                BOUN 440
                     THEN BETW(J)=BETW(J)+1.0,.                         BOUN 450
                     ELSE OVER(J)=OVER(J)+1.0,.                         BOUN 460
                     END,.                                              BOUN 470
                ELSE UNDER(J)=UNDER(J)+1.0,.                            BOUN 480
                END,.                                                   BOUN 490
             END,.                                                      BOUN 500
        END,.                                                           BOUN 510
FIN..                                                                   BOUN 520
   RETURN,.                                                             BOUN 530
   END,.                           /*END OF PROCEDURE BOUN              */BOUN 540
```

Purpose:

BOUN selects from a set (or a subset) of observations the number of observations under, between, and over two given bounds for each variable.

Usage:

CALL BOUN (A, S, BLO, BHI, UNDER, BETW, OVER, NO, NV);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given observation matrix.

S(NO) - BINARY FLOAT
Given vector indicating subset of A. Only those observations with a nonzero S(J) are considered.

BLO(NV) - BINARY FLOAT
Given vector of lower bounds on all variables.

BHI(NV) - BINARY FLOAT
Given vector of upper bounds on all variables.

UNDER(NV) - BINARY FLOAT
Resultant vector indicating, for each variable, number of observations under lower bounds.

BETW(NV) - BINARY FLOAT
Resultant vector indicating, for each variable, number of observations equal to or between lower and upper bounds.

OVER(NV) - BINARY FLOAT
Resultant vector indicating, for each variable, number of observations over upper bounds.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables for each observation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations or number of variables less than or equal to zero.
ERROR=2 - lower bound greater than upper bound.

Method:

Each row (observation) of the matrix A with corresponding nonzero element in S vector is tested. Observations are compared with specified lower and upper variable bounds and counts are kept in vectors UNDER, BETW and OVER.

- Subroutine ABST

```
ABST..                                                                  ABST  10
/*************************************************************************/ABST  20
/*                                                                       */ABST  30
/*      TO TEST MISSING OR ZERO VALUES FOR OBSERVATION MATRIX A.         */ABST  40
/*                                                                       */ABST  50
/*************************************************************************/ABST  60
   PROCEDURE (A,S,NO,NV),.                                              ABST  70
   DECLARE                                                              ABST  80
        (I,J,NO,NV)                                                     ABST  90
        FIXED BINARY,                                                   ABST 100
        ERROR EXTERNAL CHARACTER(1),                                    ABST 110
        (A(*,*),S(*)) FLOAT BINARY,.                                    ABST 120
/*                                                                      */ABST 130
   ERROR='0',.                                                          ABST 140
   IF NV LE 0 OR NO LE 0            /* NUMBER OF OBSERVATIONS OR       */ABST 150
   THEN DO,.                        /* THE NUMBER OF VARIABLES LESS    */ABST 160
        ERROR='1',.                 /* THAN OR EQUAL TO ZERO.          */ABST 170
        GO TO FIN,.                                                     ABST 180
        END,.                                                           ABST 190
        DO I = 1 TO NO,.                                                ABST 200
             DO J = 1 TO NV,.                                           ABST 210
             IF A(I,J)= 0.0                                             ABST 220
             THEN DO,.                                                  ABST 230
                  S(I) =0.0,.                                           ABST 240
                  GO TO S10,.                                           ABST 250
                  END,.                                                 ABST 260
             END,.                                                      ABST 270
        S(I) =1.0,.                                                     ABST 280
S10..                                                                   ABST 290
        END,.                                                           ABST 300
FIN..                                                                   ABST 310
   RETURN,.                                                             ABST 320
   END,.                            /*END OF PROCEDURE ABST          */ABST 330
```

Purpose:

ABST tests for missing or zero elements in observation matrix A.

Usage:

CALL ABST (A, S, NO, NV);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given observation matrix.

S(NO) - BINARY FLOAT
Resultant vector indicating one of the following codes for each observation:
1 There is not a missing or zero value.
0 At least one variable has a value missing or zero.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables for each observation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR=1 - number of observations or number of variables less than or equal to zero.

Method:

A test is made on the I-th row (observation) of the matrix A, I = 1, ..., NO. If there is not a missing or zero value, 1 is placed in S(I). If at least one variable has a value missing or zero, 0 is placed in S(I).

- Subroutine SBST

```
SBST..                                                                  SBST  10
/*********************************************************************/SBST  20
/*                                                                   */SBST  30
/*      TO DERIVE A SUBSET VECTOR INDICATING WHICH OBSERVATIONS IN   */SBST  40
/*      A SET HAVE SATISFIED CERTAIN CONDITIONS.                     */SBST  50
/*                                                                   */SBST  60
/*********************************************************************/SBST  70
   PROCEDURE (A,C,R,B,S,NO,NV,NC),.                                     SBST  80
   DECLARE                                                              SBST  90
         B ENTRY,                                                       SBST 100
         ERROR EXTERNAL CHARACTER(1),                                   SBST 110
         (I,ICOL,IGO,J,NC,NO)                                           SBST 120
         FIXED BINARY,                                                  SBST 130
         (A(*,*),C(*,*),R(*),S(*),Q,TR)                                 SBST 140
         BINARY FLOAT,                                                  SBST 150
         T(6) LABEL,.                                                   SBST 160
/*                                                                    */SBST 170
   ERROR='0',.                                                          SBST 180
         DO I=1 TO NO,.                                                 SBST 190
         S(I) =0,.                                                      SBST 200
         END,.                                                          SBST 210
   IF NO LE 0 OR NV LE 0 OR NC LE 0   /* NUMBER OF OBSERVATIONS,      */SBST 220
   THEN DO,.                          /* VARIABLES, OR CONDITIONS IS */SBST 230
         ERROR='1',.                  /* LESS THAN OR EQUAL TO ZERO. */SBST 240
         GO TO FIN,.                                                    SBST 250
         END,.                                                          SBST 260
         DO I = 1 TO NO,.                                               SBST 270
               DO J = 1 TO NC,.                                         SBST 280
               R(J) =0.0,.              /* CLEAR R VECTOR           */SBST 290
/*                                                                    */SBST 300
/*      LOCATE ELEMENT IN OBSERVATION MATRIX AND RELATION CODE        */SBST 310
/*                                                                    */SBST 320
               ICOL =C(1,J),.                                           SBST 330
               IGO  =C(2,J),.                                           SBST 340
               IF IGO LT 1 OR IGO GT 6  /* CONDITION VALUE INVALID  */SBST 350
               THEN DO,.                                                SBST 360
                     ERROR='2',.                                        SBST 370
                     GO TO FIN,.                                        SBST 380
                     END,.                                              SBST 390
               IF ICOL LT 1 OR ICOL GT NV                               SBST 400
               THEN DO,.                                                SBST 410
                     ERROR ='3',.       /* INVALID VARIABLE NUMBER  */SBST 420
                     GO TO FIN,.                                        SBST 430
                     END,.                                              SBST 440
               Q     =A(I,ICOL)-C(3,J),. /* FORM R VECTOR            */SBST 450
               GO TO T(IGO),.                                           SBST 460
T(1)..                                                                  SBST 470
               IF Q LT 0.0                                              SBST 480
               THEN GO TO S10,.                                         SBST 490
               GO TO S20,.                                              SBST 500
T(2)..                                                                  SBST 510
               IF Q LE 0.0                                              SBST 520
               THEN GO TO S10,.                                         SBST 530
               GO TO S20,.                                              SBST 540
T(3)..                                                                  SBST 550
               IF Q = 0.0                                               SBST 560
               THEN GO TO S10,.                                         SBST 570
               GO TO S20,.                                              SBST 580
T(4)..                                                                  SBST 590
               IF Q NE 0.0                                              SBST 600
               THEN GO TO S10,.                                         SBST 610
               GO TO S20,.                                              SBST 620
T(5)..                                                                  SBST 630
               IF Q GE 0.0                                              SBST 640
               THEN GO TO S10,.                                         SBST 650
               GO TO S20,.                                              SBST 660
T(6)..                                                                  SBST 670
               IF Q LE 0.0                                              SBST 680
               THEN GO TO S20,.                                         SBST 690
S10..                                                                   SBST 700
               R(J) =1.0,.                                              SBST 710
S20..                                                                   SBST 720
               END,.                                                    SBST 730
         CALL B (F,TR),.              /* CALCULATE S VECTOR        */SBST 740
         S(I) =TR,.                                                     SBST 750
         END,.                                                          SBST 760
FIN..                                                                   SBST 770
   RETURN,.                                                             SBST 780
   END,.                              /*END OF PROCEDURE SBST      */SBST 790
```

Purpose:

SBST derives a subset vector indicating which observations in a set have satisfied certain conditions on the variables.

Usage:

CALL SBST (A, C, R, B, S, NO, NV, NC);
Parameter B must be declared as an entry attribute in the calling program.

A(NO, NV) - BINARY FLOAT
Given observation matrix.

C(3, NC) - BINARY FLOAT
Given matrix of conditions to be considered. The first element of each column of C represents the number of the variable (column of matrix A) to be tested. The second element of each column is a relation code as follows:

1 - less than
2 - less than or equal to
3 - equal to
4 - not equal to
5 - greater than or equal to
6 - greater than

The third element of each column is a quantity to be used for comparison with the observation values. For example, the following column in C:

2.
5.
92.5

causes the second variable to be tested for greater than or equal to 92.5.

R(NC) - BINARY FLOAT
Resultant working vector used to store intermediate results of above tests on a single observation. If condition is satisfied, R(I) is set to 1. If it is not, R(I) is set to 0.

B - ENTRY
Given name of subroutine to be supplied by the user. It consists of a Boolean expression linking the intermediate values stored in vector R. The Boolean operators are "*" for "and", "+" for "or".

Example

```
BOOL. .
   PROCEDURE (R, T), .
      DECLARE
      (R(*), T)
      FLOAT BINARY, .
   T=R(1)*R(2), .
   RETURN, .
   END, .
```

The above tests for R(1) and R(2).

S(NO) - BINARY FLOAT
Resultant vector indicating, for each observation, whether or not proposition B is satisfied. If it is, S(I) is nonzero. If it is not, S(I) is zero.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables.

NC - BINARY FIXED
Given number of basic conditions to be satisfied.

Remarks:

Subroutines and function subroutines required:

B - The name of the actual subroutine supplied by the user may be different from B (for example, BOOL), but subroutine SBST always calls B. In order for procedure SBST to do this, the name of the user-supplied procedure must be defined by an entry attribute in the calling program.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations, number of variables, or number of conditions is less than or equal to zero.
ERROR=2 - condition value invalid.
ERROR=3 - variable number is less than 1 or greater than the number of variables.

Method:

The following is done for each observation. Condition matrix is analyzed to determine which variables are to be examined. The intermediate vector R is formed. The Boolean expression (in subroutine B) is then evaluated to derive the element in subset vector S corresponding to the observation.

- Subroutine TAB1

```
TAB1..                                                                  TAB1  10
/*********************************************************************/TAB1  20
/*                                                                   */TAB1  30
/*      TO TABULATE FOR ONE VARIABLE IN AN OBSERVATION MATRIX (OR A  */TAB1  40
/*      SUBSET), THE FREQUENCY AND PERCENT FREQUENCY OVER GIVEN      */TAB1  50
/*      CLASS INTERVALS. IN ADDITION, CALCULATE FOR THE SAME VARIABLE*/TAB1  60
/*      THE TOTAL, MEAN, STANDARD DEVIATION, MINIMUM, AND            */TAB1  70
/*      MAXIMUM.                                                     */TAB1  80
/*                                                                   */TAB1  90
/*********************************************************************/TAB1 100
   PROCEDURE (A,S,NOVAR,UBO,FREQ,PCT,STATS,NO,NV),.                    TAB1 110
   DECLARE                                                             TAB1 120
        ERROR EXTERNAL CHARACTER (1),                                  TAB1 130
        (I,INN,INTX,J,K,NO,NOVAR,KK)                                   TAB1 140
        FIXED BINARY,                                                  TAB1 150
        (A(*,*),S(*),UBO(*),FREQ(*),PCT(*),STATS(*),SCNT,VMIN,VMAX,    TAB1 160
        SINT,TEMP)                                                     TAB1 170
        BINARY FLOAT,.                                                 TAB1 180
/*                                                                   */TAB1 190
   ERROR='0',.                                                         TAB1 200
        IF NOVAR LE 0 OR NOVAR GT NV  /* VALUE OF THE VARIABLE TO BE */TAB1 210
        THEN DO,.                     /* TABULATED IS INVALID        */TAB1 220
             ERROR='6',.                                               TAB1 230
             GO TO S50,.                                               TAB1 240
             END,.                                                     TAB1 250
   IF NV LE 0 OR NO LE 0                                               TAB1 260
   THEN DO,.                          /* NUMBER OF OBSERVATIONS OR   */TAB1 270
        ERROR='1',.                   /* THE NUMBER OF VARIABLES ARE */TAB1 280
        GO TO S50,.                   /* LESS THAN OR EQUAL TO ZERO. */TAB1 290
        END,.                                                          TAB1 300
   INN  =UBO(2),.                     /* CALCULATE INTERVAL SIZE     */TAB1 310
        DO J = 1 TO INN,.             /* CLEAR OUTPUT VECTORS        */TAB1 320
        FREQ(J)=0.0,.                                                  TAB1 330
        PCT(J)=0.0,.                                                   TAB1 340
        END,.                                                          TAB1 350
        DO J = 1 TO 5,.                                                TAB1 360
        STATS(J)=0.0,.                                                 TAB1 370
        END,.                                                          TAB1 380
   IF UBO(1) GT UBO(3) OR UBO(2) LE 2.0                                TAB1 390
   THEN DO,.                          /* INVALID BOUNDS OR THE NUMBER*/TAB1 400
        ERROR='2',.                   /* OF INTERVALS LESS THAN OR   */TAB1 410
        GO TO S50,.                   /* EQUAL TO TWO.               */TAB1 420
        END,.                                                          TAB1 430
        DO I = 1 TO NO,.              /* CALCULATE MAX AND MIN       */TAB1 440
        IF S(I) NE 0.0                                                 TAB1 450
        THEN DO,.                                                      TAB1 460
             KK   =I,.                                                 TAB1 470
             VMIN =A(I,NOVAR),.                                        TAB1 480
             VMAX =VMIN,.                                              TAB1 490
             GO TO S10,.                                               TAB1 500
             END,.                                                     TAB1 510
        END,.                                                          TAB1 520
   ERROR='3',.                        /* NO OBSERVATION IN SUBSET    */TAB1 530
   GO TO S50,.                                                         TAB1 540
S10..                                                                  TAB1 550
        DO I = KK TO NO,.                                              TAB1 560
        IF S(I) NE 0.0                                                 TAB1 570
        THEN DO,.                                                      TAB1 580
             IF A(I,NOVAR) LT VMIN                                     TAB1 590
             THEN VMIN =A(I,NOVAR),.                                   TAB1 600
             IF A(I,NOVAR) GT VMAX                                     TAB1 610
             THEN VMAX =A(I,NOVAR),.                                   TAB1 620
             END,.                                                     TAB1 630
        END,.                                                          TAB1 640
   STATS(4)=VMIN,.                                                     TAB1 650
   STATS(5)=VMAX,.                                                     TAB1 660
   IF UBO(1)= UBO(3)                                                   TAB1 670
   THEN DO,.                                                           TAB1 680
        UBO(1)=VMIN,.                                                  TAB1 690
        UBO(3)=VMAX,.                                                  TAB1 700
        END,.                                                          TAB1 710
   SINT =(UBO(3)-UBO(1))/(UBO(2)-2),.                                  TAB1 720
   SCNT =0.0,.                        /* TEST SUBSET VECTOR          */TAB1 730
        DO I = KK TO NO,.                                              TAB1 740
        IF S(I) NE 0.0                                                 TAB1 750
        THEN DO,.                                                      TAB1 760
             SCNT =SCNT+1.0,.                                          TAB1 770
/*                                                                   */TAB1 780
/*      DEVELOP TOTALS AND FREQUENCIES                               */TAB1 790
/*                                                                   */TAB1 800
             STATS(1)=STATS(1)+A(I,NOVAR),.                            TAB1 810
             STATS(3)=STATS(3)+A(I,NOVAR)**2,.                         TAB1 820
             TEMP =UBO(1)-SINT,.                                       TAB1 830
             INTX =INN-1,.                                             TAB1 840
                  DO J = 1 TO INTX,.                                   TAB1 850
                  TEMP =TEMP+SINT,.                                    TAB1 860
                  IF A(I,NOVAR) LT TEMP                                TAB1 870
                  THEN DO,.                                            TAB1 880
                       K    =J,.                                       TAB1 890
                       GO TO S20,.                                     TAB1 900
                       END,.                                           TAB1 910
                  END,.                                                TAB1 920
             IF A(I,NOVAR) GE TEMP                                     TAB1 930
             THEN DO,.                                                 TAB1 940
                  FREQ(INN)=FREQ(INN)+1.0,.                            TAB1 950
                  GO TO S30,.                                          TAB1 960
                  END,.                                                TAB1 970
S20..                                                                  TAB1 980
             FREQ(K)=FREQ(K)+1.0,.                                     TAB1 990
             END,.                                                     TAB11000
S30..                                                                  TAB11010
        END,.                                                          TAB11020
/*                                                                   */TAB11030
/*      CALCULATE RELATIVE FREQUENCIES                               */TAB11040
/*                                                                   */TAB11050
        DO J = 1 TO INN,.                                              TAB11060
        PCT(J)=FREQ(J)*100.0/SCNT,.                                    TAB11070
        END,.                                                          TAB11080
/*                                                                   */TAB11090
/*      CALCULATE MEAN AND STANDARD DEVIATION                        */TAB11100
/*                                                                   */TAB11110
   STATS(2)=STATS(1)/SCNT,.                                            TAB11120
   IF SCNT= 1.0                                                        TAB11130
   THEN DO,.                                                           TAB11140
        ERROR='4',.                   /* SAMPLE SIZE = 1             */TAB11150
        STATS(3)=0.0                                                   TAB11160
        GO TO S50,.                                                    TAB11170
        END,.                                                          TAB11180
   ELSE DO,.                                                           TAB11190
        TEMP =STATS(3)-STATS(1)*STATS(1)/SCNT,.                        TAB11200
        IF TEMP LE 0.0                                                 TAB11210
        THEN DO,.                                                      TAB11220
             ERROR='5',.              /* VARIANCE = 0.0              */TAB11230
```

```
            STATS(3)=0.0;.                                          TAB11240
            GO TO S50;.                                             TAB11250
            END;.                                                   TAB11260
         ELSE STATS(3)=SQRT(TEMP/(SCNT-1.0));.                      TAB11270
         END;.                                                      TAB11280
S50..                                                               TAB11290
   RETURN;.                                                         TAB11300
   END;.                          /*END OF PROCEDURE TAB1          */TAB11310
```

Purpose:

TAB1 tabulates for one variable in an observation matrix (or a matrix subset), the frequency and percent frequency over given class intervals. In addition, it calculates for the same variable the total, mean, standard deviation, minimum, and maximum.

Usage:

CALL TAB1 (A, S, NOVAR, UBO, FREQ, PCT, STATS, NO, NV);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given observation matrix A.

S(NO) - BINARY FLOAT
Given vector that indicates which of the observations enter the calculation. A zero element in S indicates that the corresponding observation of A is not to be included.

NOVAR - BINARY FIXED
Given variable to be tabulated.

UBO(3) - BINARY FLOAT
Given vector containing lower limit, number of intervals, and upper limit of variable to be tabulated in UBO(1), UBO(2), and UBO(3) respectively. If lower limit is equal to upper limit, the program replaces these with the minimum and maximum values of the variable. Number of intervals, UBO(2), must include two cells for values under and above limits.

FREQ (INN) - BINARY FLOAT
Resultant vector of frequencies. INN is given in UBO(2).

PCT(INN) - BINARY FLOAT
Resultant vector of relative frequencies. Vector length is UBO(2).

STATS(5) - BINARY FLOAT
Resultant vector of summary statistics, that is, total, mean, standard deviation, minimum, and maximum.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables for each observation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations or number of variables less than or equal to zero.
ERROR=2 - invalid bounds or number of intervals less than or equal to two.
ERROR=3 - no observations in subset.
ERROR=4 - sample size equal to one.
ERROR=5 - variance equal to zero.
ERROR=6 - value of the variable to be tabulated is invalid.

Method:

The interval size is calculated from the given information or optionally from the minimum and maximum values for variable NOVAR. The frequencies and percent frequencies are then calculated along with summary statistics. The divisor for standard deviation is one less than the number of observations used.

Mathematical Background:

This subroutine tabulates, for a selected variable in an observation matrix, the frequencies and percent frequencies over class intervals. Interval size is computed as follows:

$$k = \frac{UBO_3 - UBO_1}{UBO_2 - 2} \qquad (1)$$

where UBO_1 = given lower bound

UBO_2 = given number of intervals

UBO_3 = given upper bound

If $UBO_1 = UBO_3$, the subroutine finds and uses the minimum and maximum values of the variable.

A table lookup is used to obtain the frequency, F_i, of the ith class interval for the variable, where $i = 1, 2, \ldots, UBO_2$. Then each frequency is divided by the number of observations, n, to obtain the percent frequency:

$$P_i = \frac{100F_i}{n} \qquad (2)$$

In addition, the following statistics are calculated for the variable:

$$\text{Total: } T = \sum_{i=1}^{n} X_{ij} \tag{3}$$

where j = selected variable

$$\text{Mean: } \bar{X} = \frac{T}{n} \tag{4}$$

Standard deviation:

$$s = \sqrt{\frac{\left[\sum_{i=1}^{n} X_{ij}^2 - \left(\sum_{i=1}^{n} X_{ij}\right)^2\right] \Big/ n}{n-1}} \tag{5}$$

- Subroutine TAB2

```
TAB2..                                                                  TAB2  10
/*********************************************************************/TAB2  20
/*                                                                   */TAB2  30
/*      TO PERFORM A TWO-WAY CLASSIFICATION OF THE FREQUENCY,        */TAB2  40
/*      PERCENT FREQUENCY, AND OTHER STATISTICS, OVER GIVEN          */TAB2  50
/*      CLASS INTERVALS, FOR TWO SELECTED VARIABLES IN AN OBSERVATION*/TAB2  60
/*      MATRIX.                                                      */TAB2  70
/*                                                                   */TAB2  80
/*********************************************************************/TAB2  90
   PROCEDURE (A,S,NOV,UBO,FREQ,PCT,STAT1,STAT2,NO,NV),.                TAB2 100
   DECLARE                                                             TAB2 110
        ERROR EXTERNAL CHARACTER (1),                                  TAB2 120
        (A(*,*),UBO(*,*),FREQ(*,*),PCT(*,*),STAT1(*,*),STAT2(*,*),     TAB2 130
        S(*),SINT(2),VMIN,VMAX,SCNT,TEMP1,TEMP2)                       TAB2 140
        BINARY FLOAT,                                                  TAB2 150
        (I,INT1,INT2,J,K,KX,L,N,N1,N2,NO,NOV(*),KK)                    TAB2 160
        FIXED BINARY,.                                                 TAB2 170
/*                                                                     */TAB2 180
   ERROR='0',.                                                         TAB2 190
        DO I=1 TO 2,.                                                  TAB2 200
        IF NOV(I) LE 0 OR NOV(I) GT NV/* INVALID VALUE OF VARIABLE TO*/TAB2 210
        THEN DO,.                     /* BE CROSS TABULATED          */TAB2 220
             ERROR='6',.                                               TAB2 230
             GO TO S50,.                                               TAB2 240
             END,.                                                     TAB2 250
        END,.                                                          TAB2 260
   IF NV LE 0 OR NO LE 0              /* NUMBER OF OBSERVATIONS OR   */TAB2 270
   THEN DO,.                          /* THE NUMBER OF VARIABLES ARE */TAB2 280
        ERROR='1',.                   /* LESS THAN OR EQUAL TO ZERO. */TAB2 290
        GO TO S50,.                                                    TAB2 300
        END,.                                                          TAB2 310
   INT1 =UBO(2,1),.                                                    TAB2 320
   INT2 =UBO(2,2),.                                                    TAB2 330
   N1   =NOV(1),.                                                      TAB2 340
   N2   =NOV(2),.                                                      TAB2 350
        DO I = 1 TO 2,.                                                TAB2 360
        IF UBO(1,I) GT UBO(3,I) OR UBO(2,I) LE 2.0                     TAB2 370
        THEN DO,.                     /* INVALID BOUNDS OR THE NUMBER*/TAB2 380
             ERROR='2',.              /* OF INTERVALS LESS THAN OR   */TAB2 390
             GO TO S50,.              /* EQUAL TO TWO.               */TAB2 400
             END,.                                                     TAB2 410
        END,.                                                          TAB2 420
        DO I = 1 TO INT1,.           /* CLEAR OUTPUT VECTORS        */TAB2 430
             DO J = 1 TO INT2,.                                        TAB2 440
             PCT(I,J)=0.0,.                                            TAB2 450
             FREQ(I,J)=0.0,.                                           TAB2 460
             END,.                                                     TAB2 470
        END,.                                                          TAB2 480
        DO I = 1 TO 3,.                                                TAB2 490
             DO J = 1 TO INT1,.                                        TAB2 500
             STAT1(I,J)=0.0,.                                          TAB2 510
             END,.                                                     TAB2 520
             DO J = 1 TO INT2,.                                        TAB2 530
             STAT2(I,J)=0.0,.                                          TAB2 540
             END,.                                                     TAB2 550
        END,.                                                          TAB2 560
        DO I = 1 TO 2,.                                                TAB2 570
        IF UBO(1,I)= UBO(3,I)         /* DETERMINE LIMITS            */TAB2 580
        THEN DO,.                                                      TAB2 590
                  DO J = 1 TO NO,.                                     TAB2 600
                  IF S(J) NE 0.0                                       TAB2 610
                  THEN DO,.                                            TAB2 620
                       KK   =J,.                                       TAB2 630
                       N    =NOV(I),.                                  TAB2 640
                       VMAX =A(J,N),.                                  TAB2 650
                       VMIN =VMAX,.                                    TAB2 660
                       GO TO S10,.                                     TAB2 670
                       END,.                                           TAB2 680
                  END,.                                                TAB2 690
S10..                                                                  TAB2 700
                  DO J = KK TO NO,.                                    TAB2 710
                  IF S(J) NE 0.0                                       TAB2 720
                  THEN DO,.                                            TAB2 730
                       IF A(J,N) LT VMIN                               TAB2 740
                       THEN VMIN =A(J,N),.                             TAB2 750
                       IF A(J,N) GT VMAX                               TAB2 760
                       THEN VMAX =A(J,N),.                             TAB2 770
                       END,.                                           TAB2 780
                  END,.                                                TAB2 790
             UBO(1,I)=VMIN,.                                           TAB2 800
             UBO(3,I)=VMAX,.                                           TAB2 810
             END,.                                                     TAB2 820
        END,.                                                          TAB2 830
/*                                                                     */TAB2 840
/*      CALCULATE INTERVAL SIZE                                      */TAB2 850
/*                                                                     */TAB2 860
        DO J = 1 TO 2,.                                                TAB2 870
        SINT(J)   =(UBO(3,J)-UBO(1,J))/(UBO(2,J)-(2+1E-3)),.           TAB2 880
        END,.                                                          TAB2 890
   SCNT =0.0,.                                                         TAB2 900
        DO J = KK TO NO,.            /* TEST SUBSET VECTOR          */TAB2 910
        IF S(J) NE 0.0                                                 TAB2 920
        THEN DO,.                                                      TAB2 930
             SCNT =SCNT+1.0,.                                          TAB2 940
             TEMP1=UBO(1,1)-SINT(1),. /* CALCULATE FREQUENCIES      */TAB2 950
                  DO L = 1 TO INT1-1,.                                 TAB2 960
                  TEMP1=TEMP1+SINT(1),.                                TAB2 970
                  IF A(J,N1) LT TEMP1                                  TAB2 980
                  THEN DO,.                                            TAB2 990
                       K    =L,.                                       TAB21000
                       GO TO S20,.                                     TAB21010
                       END,.                                           TAB21020
                  END,.                                                TAB21030
             K    =INT1,.                                             TAB21040
S20..                                                                  TAB21050
             STAT1(1,K)=STAT1(1,K)+A(J,N1),.                           TAB21060
             STAT1(2,K)=STAT1(2,K)+1.0,.                               TAB21070
             STAT1(3,K)=STAT1(3,K)+A(J,N1)**2,.                        TAB21080
             TEMP2=UBO(1,2)-SINT(2),.                                  TAB21090
                  DO L = 1 TO INT2-1,.                                 TAB21100
                  TEMP2=TEMP2+SINT(2),.                                TAB21110
                  IF A(J,N2) LT TEMP2                                  TAB21120
                  THEN DO,.                                            TAB21130
                       KX   =L,.                                       TAB21140
                       GO TO S30,.                                     TAB21150
                       END,.                                           TAB21160
                  END,.                                                TAB21170
             KX   =INT2,.                                              TAB21180
S30..                                                                  TAB21190
             FREQ(K,KX)=FREQ(K,KX)+1.0,.                               TAB21200
             STAT2(1,KX)=STAT2(1,KX)+A(J,N2),.                         TAB21210
             STAT2(2,KX)=STAT2(2,KX)+1.0,.                             TAB21220
             STAT2(3,KX)=STAT2(3,KX)+A(J,N2)**2,.                      TAB21230
```

```
          END,.                                                    TAB21240
       END,.                                                       TAB21250
  IF SCNT= 0.0                                                     TAB21260
  THEN DO,.                                                        TAB21270
       ERROR='3',.                  /* NO OBSERVATIONS IN SUBSET  */TAB21280
       GO TO S50,.                                                 TAB21290
       END,.                                                       TAB21300
/*                                                                 */TAB21310
/*     CALCULATE PERCENT FREQUENCIES.                              */TAB21320
/*                                                                 */TAB21330
       DO I = 1 TO INT1,.                                          TAB21340
            DO J = 1 TO INT2,.                                     TAB21350
            PCT(I,J)=FREQ(I,J)*100.0/SCNT,.                        TAB21360
            END,.                                                  TAB21370
       END,.                                                       TAB21380
/*                                                                 */TAB21390
/*     CALCULATE TOTALS, MEANS, STANDARD DEVIATIONS                */TAB21400
/*                                                                 */TAB21410
       DO J = 1 TO INT1,.                                          TAB21420
       IF STAT1(2,J) LE 1.0                                        TAB21430
       THEN DO,.                                                   TAB21440
            ERROR='4',.             /* NUMBER OF OBSERVATIONS IS  */TAB21450
            STAT1(3,J)=0.0,.        /* LESS THAN OR EQUAL TO 1 IN */TAB21460
            STAT1(2,J)=STAT1(1,J),. /* SOME INTERVAL              */TAB21470
            END,.                                                  TAB21480
       ELSE DO,.                                                   TAB21490
            TEMP1=STAT1(3,J)-STAT1(1,J)**2/STAT1(2,J),.            TAB21500
            STAT1(2,J)=STAT1(1,J)/STAT1(2,J),.                     TAB21510
            IF TEMP1 LE 0.0                                        TAB21520
            THEN DO,.                                              TAB21530
                 ERROR='5',.        /* VARIANCE IS 0.0            */TAB21540
                 STAT1(3,J)=0.0,.                                  TAB21550
                 END,.                                             TAB21560
            ELSE STAT1(3,J)=SQRT(TEMP1/(STAT1(2,J)-1.0)),.         TAB21570
            END,.                                                  TAB21580
       END,.                                                       TAB21590
/*                                                                 */TAB21600
       DO J = 1 TO INT2,.                                          TAB21610
       IF STAT2(2,J) LE 1.0                                        TAB21620
       THEN DO,.                                                   TAB21630
            ERROR='4',.             /* NUMBER OF OBSERVATIONS IS  */TAB21640
            STAT2(3,J)=0.0,.        /* LESS THAN OR EQUAL TO 1 IN */TAB21650
            STAT2(2,J)=STAT2(1,J),. /* SOME INTERVAL              */TAB21660
            END,.                                                  TAB21670
       ELSE DO,.                                                   TAB21680
            STAT2(2,J)=STAT2(1,J)/STAT2(2,J),.                     TAB21690
            TEMP2=STAT2(3,J)-STAT2(1,J)**2/STAT2(2,J),.            TAB21700
            IF TEMP2 LE 0.0                                        TAB21710
            THEN DO,.                                              TAB21720
                 ERROR='5',.        /* VARIANCE = 0.0             */TAB21730
                 STAT2(3,J)=0.0,.                                  TAB21740
                 END,.                                             TAB21750
            ELSE STAT2(3,J)=SQRT(TEMP2/(STAT2(2,J)-1.0)),.         TAB21760
            END,.                                                  TAB21770
       END,.                                                       TAB21780
                                                                   TAB21790
S50.,                                                              TAB21800
   RETURN,.                                                        TAB21810
   END,.                        /*END OF PROCEDURE TAB2            */TAB21820
```

Purpose:

TAB2 performs a two-way classification for two variables in an observation matrix (or a matrix subset), of the frequency, percent frequency, and other statistics over given class intervals.

Usage:

CALL TAB2 (A, S, NOV, UBO, FREQ, PCT, STAT1, STAT2, NO, NV);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given observation matrix.

S(ND) - BINARY FLOAT
Given vector that indicates which of the observations enter the calculation. A zero element in S indicates that the corresponding observation of A is not to be included.

NOV(2) - BINARY FIXED
Given variables to be cross-tabulated. NOV(1) is variable 1; NOV(2) is variable 2.

UBO(3,2) - BINARY FLOAT
Given matrix giving lower limit, number of intervals, and upper limit of both variables to be tabulated (first column for variable 1, second column for variable 2). If lower limit is equal to upper limit for a variable, the program replaces these with the minimum and maximum values of that variable. Number of intervals must include two cells for under and above limits.

FREQ (INT1, INT2) - BINARY FLOAT
Resultant matrix of frequencies in the two-way classification. INT1 equals UBO(2,1) and INT2 equals UBO(2,2) where UBO(2,1) is the number of intervals of variable 1 and UBO(2, 2) is the number of intervals of variable 2. UBO(2, 1) and UBO(2, 2) must be specified in the second position of the respective column of UBO matrix.

PCT (INT1,INT2) - BINARY FLOAT
Resultant matrix of percent frequencies.

STAT1 (3, INT2) - BINARY FLOAT
Resultant matrix summarizing totals, means, and standard deviations for each class interval of variable 1.

STAT2 (3,INT2) -
Same as STAT1 but over variable 2.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables for each observation.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations or number of variables less than or equal to zero.
ERROR=2 - invalid bounds or number of intervals less than or equal to two.
ERROR=3 - no observations in subset.
ERROR=4 - number of observations one or less in some interval.

ERROR=5 - variance equal to zero. (If error conditions 4 and 5 exist, the last condition encountered overrides.)
ERROR=6 - invalid value of variable to be cross-tabulated.

Method:

Interval sizes for both variables are calculated from the given information or optionally from the minimum and maximum values. The frequency and percent frequency matrices are developed. Matrices STAT1 and STAT2 summarizing totals, means, and standard deviations are then calculated. The divisor for standard deviation is one less than the number of observations used in each class interval.

Mathematical Background:

This subroutine performs a two-way classification of the frequency, percent frequency, and other statistics over given class intervals, for two selected variables in an observation matrix.

Interval size for each variable is computed as follows:

$$k_j = \frac{UBO_{3j} - UBO_{1j}}{UBO_{2j} - 2} \qquad (1)$$

where UBO_{1j} = given lower bound

UBO_{2j} = given number of intervals

UBO_{3j} = given upper bound

$j = 1, 2$

if $UBO_{1j} = UBO_{3j}$, the subroutine finds and uses the minimum and maximum values of the jth variable.

A frequency tabulation is then made for each pair of observations in a two-way table as shown in Figure 10.

Symbols $\geq$ and $<$ in Figure 10 indicate that a count is classified into a particular interval if the data point is greater than or equal to the lower limit of that interval but less than the upper limit of the same interval.

Then, each entry in the frequency matrix, F_{ij}, is divided by the number of observations, N, to obtain the percent frequency:

$$P_{ij} = \frac{100F_{ij}}{N} \qquad (2)$$

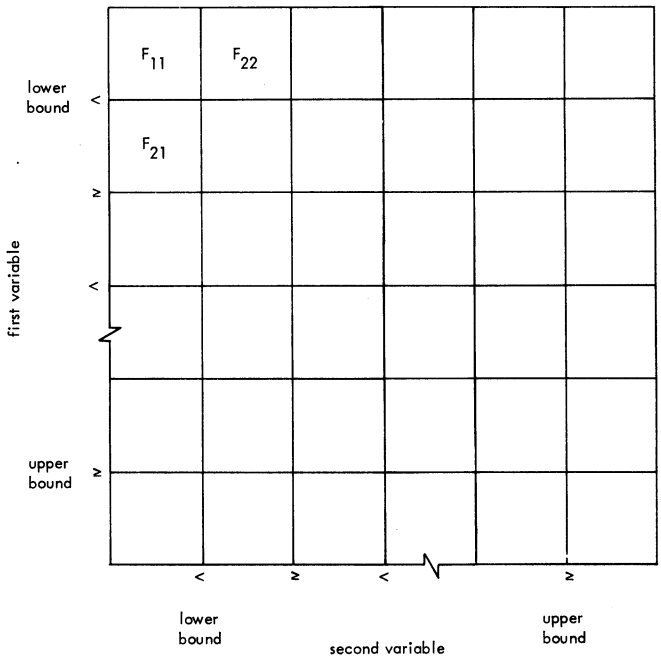


Figure 10. Frequency matrix

where $i = 1, 2, \ldots, UBO_{21}$

$j = 1, 2, \ldots, UBO_{22}$

As data are classified into the frequency matrix, the following intermediate results are accumulated for each class interval of both variables:

1. Number of data points, n
2. Sum of data points, $\sum_{i=1}^{n} X_i$
3. Sum of data points squared, $\sum_{i=1}^{n} X_i^2$

From these, the following statistics are calculated for each class interval:

Mean: $$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n} \qquad (3)$$

Standard deviation:

$$s = \sqrt{\frac{\sum_{i=1}^{n} X_i^2 - \left(\sum_{i=1}^{n} X_i\right)^2 \Big/ n}{n - 1}} \qquad (4)$$

- Subroutine SUBM

```
SUBM..                                                                  SUBM  10
/*********************************************************************/SUBM  20
/*                                                                   */SUBM  30
/*      BASED ON VECTOR S DERIVED FROM PROCEDURE SBST OR ABST, THIS  */SUBM  40
/*      PROCEDURE COPIES FROM A LARGER MATRIX OF OBSERVATION DATA A  */SUBM  50
/*      SUBSET MATRIX OF THOSE OBSERVATIONS WHICH HAVE SATISFIED     */SUBM  60
/*      CERTAIN CONDITIONS.                                          */SUBM  70
/*                                                                   */SUBM  80
/*********************************************************************/SUBM  90
   PROCEDURE (A,D,S,NO,NV,N),.                                         SUBM 100
   DECLARE                                                             SUBM 110
        (I,N,NO)                                                       SUBM 120
        FIXED BINARY,                                                  SUBM 130
        ERROR EXTERNAL CHARACTER(1),                                   SUBM 140
        (A(*,*),D(*,*),S(*)) FLOAT BINARY,.                            SUBM 150
/*                                                                   */SUBM 160
   ERROR='0',.                                                         SUBM 170
   D    =0,.                                                           SUBM 180
   N    =0,.                                                           SUBM 190
   IF NV LE 0 OR NO LE 0              /* NUMBER OF OBSERVATIONS OR   */SUBM 200
   THEN ERROR='1',.                   /* THE NUMBER OF VARIABLES ARE */SUBM 210
   ELSE DO,.                          /* LESS THAN OR EQUAL TO ZERO. */SUBM 220
             DO I = 1 TO NO,.                                          SUBM 230
             IF S(I) NE 0.0                                            SUBM 240
             THEN DO,.                                                 SUBM 250
                  N    =N+1,.                                          SUBM 260
                       DO J = 1 TO NV,.                                SUBM 270
                       D(N,J)=A(I,J),.                                 SUBM 280
                       END,.                                           SUBM 290
                  END,.                                                SUBM 300
             END,.                                                     SUBM 310
        END,.                                                          SUBM 320
   RETURN,.                                                            SUBM 330
   END,.                              /*END OF PROCEDURE SUBM       */SUBM 340
```

Purpose:

SUBM copies a submatrix from an observation matrix. The elements of this submatrix satisfy conditions specified by an input vector. This subroutine is used in preparing data for input to a statistical analysis such as multiple regression.

Usage:

CALL SUBM (A, D, S, NO, NV, N);

Description of parameters:

A(NO, NV) - BINARY FLOAT
Given matrix of observations.

D(N, NV) - BINARY FLOAT
Resultant matrix of observations.

S(NO) - BINARY FLOAT
Given vector containing the codes derived from procedures SBST or ABST.

NO - BINARY FIXED
Given number of observations.

NV - BINARY FIXED
Given number of variables for each observation.

N - BINARY FIXED
Resultant variable containing the number of nonzero codes in vector S.

Remarks:

Matrix D can be in the same location as matrix A.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero.

The following constitutes the possible error condition that may be detected:

ERROR=1 - number of observations or number of variables less than or equal to zero.

Method:

If S(I) contains a nonzero code, the I-th observation is copied from the input matrix to the output matrix.

Elementary Statistics

- Subroutine MOMN

```
MOMN..                                                              MOMN  10
/*******************************************************************/MOMN  20
/*                                                                 */MOMN  30
/*      TO FIND THE FIRST FOUR MOMENTS FOR GROUPED DATA ON EQUAL   */MOMN  40
/*      CLASS INTERVALS.                                           */MOMN  50
/*                                                                 */MOMN  60
/*******************************************************************/MOMN  70
   PROCEDURE (F,UBO,NOP,ANS),.                                      MOMN  80
   DECLARE                                                          MOMN  90
         (F(*),UBO(*),ANS(4),T,E,EE)                                MOMN 100
         BINARY FLOAT,                                              MOMN 110
         ERROR EXTERNAL CHARACTER (1),                              MOMN 120
         (I,JUMP,NOP)                                               MOMN 130
         FIXED BINARY,                                              MOMN 140
         S(5) LABEL,.                                               MOMN 150
/*                                                                  */MOMN 160
   T    =0,.                          /* INITIALIZE               */MOMN 170
   ANS  =0,.                                                        MOMN 180
   ERROR='0',.                                                      MOMN 190
   IF UBO(2) GT UBO(3) - UBO(1)                                     MOMN 200
   THEN DO,.                                                        MOMN 210
         ERROR='2',.                   /* INCORRECT NO. OF INTERVALS */MOMN 220
         GO TO S(1),.                  /* FOR THE SPECIFIED BOUNDS   */MOMN 230
         END,.                                                      MOMN 240
   IF UBO(1) GT UBO(3) OR UBO(2) LE 0 /* INVALID BOUNDS             */MOMN 250
   THEN DO,.                                                        MOMN 260
         ERROR='1',.                                                MOMN 270
         GO TO S(1),.                                               MOMN 280
         END,.                         /* CALC. NO. OF CLASS INTERVALS*/MOMN 290
   N    =FLOOR((UBO(3)-UBO(1))/UBO(2)+1.0E-3),.                     MOMN 300
         DO I = 1 TO N,.               /* CALCULATE TOTAL FREQUENCY  */MOMN 310
         T    =T+F(I),.                                             MOMN 320
         END,.                                                      MOMN 330
   JUMP =2,.                                                        MOMN 340
   IF NOP GE 5                                                      MOMN 350
   THEN DO,.                                                        MOMN 360
         NOP  =5,.                                                  MOMN 370
         JUMP =1,.                                                  MOMN 380
         END,.                                                      MOMN 390
   E    =UBO(1)-0.5*UBO(2),.                                        MOMN 400
         DO I = 1 TO N,.               /* FIRST MOMENT               */MOMN 410
         E    =E + UBO(2),.                                         MOMN 420
         ANS(1)=ANS(1)+F(I)*E,.                                     MOMN 430
         END,.                                                      MOMN 440
   ANS(1)=ANS(1)/T,.                                                MOMN 450
   E    =UBO(1)-0.5*UBO(2)-ANS(1),.                                 MOMN 460
   S(5) =S(2),.                                                     MOMN 470
   GO TO S(NOP),.                                                   MOMN 480
S(2),.                                                              MOMN 490
   EE   =E,.                                                        MOMN 500
         DO I = 1 TO N,.               /* SECOND MOMENT              */MOMN 510
         EE   =EE+UBO(2),.                                          MOMN 520
         ANS(2)=ANS(2)+F(I)*EE**2,.                                 MOMN 530
         END,.                                                      MOMN 540
   ANS(2)=ANS(2)/T,.                                                MOMN 550
   IF JUMP= 2                                                       MOMN 560
   THEN GO TO S(1),.                                                MOMN 570
S(3),.                                                              MOMN 580
   EE   =E,.                                                        MOMN 590
         DO I = 1 TO N,.               /* THIRD MOMENT               */MOMN 600
         EE   =EE+UBO(2),.                                          MOMN 610
         ANS(3)=ANS(3)+F(I)*EE**3,.                                 MOMN 620
         END,.                                                      MOMN 630
   ANS(3)=ANS(3)/T,.                                                MOMN 640
   IF JUMP = 2                                                      MOMN 650
   THEN GO TO S(1),.                                                MOMN 660
S(4),.                                                              MOMN 670
   EE   =E,.                                                        MOMN 680
         DO I = 1 TO N,.               /* FOURTH MOMENT              */MOMN 690
         EE   =EE+UBO(2),.                                          MOMN 700
         ANS(4)=ANS(4)+F(I)*EE**4,.                                 MOMN 710
         END,.                                                      MOMN 720
   ANS(4)=ANS(4)/T,.                                                MOMN 730
S(1),.                                                              MOMN 740
   RETURN,.                                                         MOMN 750
   END,.                         /* END PROCEDURE MOMN           */MOMN 760
```

Purpose:

MOMN finds the first four moments for grouped data on equal class intervals.

Usage:

CALL MOMN (F, UBO, NOP, ANS);

F(N) - BINARY FLOAT
Given vector containing grouped data, (frequencies), where N is the number of class intervals.

UBO(3) - BINARY FLOAT
Given vector containing the lower bound, UBO(1), the class interval, UBO(2), and the upper limit, UBO(3).

NOP - BINARY FIXED
Given option code with the following values:
NOP=1 calculate first moment
NOP=2 calculate second moment
NOP=3 calculate third moment
NOP=4 calculate fourth moment
NOP=5 calculate all four moments

ANS(4) - Resultant vector containing the moments calculated.

Remarks:

Note that the first moment is not central but the value of the mean itself. The mean is always calculated. Moments are biased and not corrected for grouping.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - lower bound greater than upper bound or number of intervals less than or equal to zero.

ERROR=2 - incorrect number of intervals for the specified bounds.

Method:

Refer to M. G. Kendall, The Advanced Theory of Statistics, vol. 1, Hafner Publishing Company, 1958, Chapter 3.

Mathematical Background:

This procedure computes four moments for grouped data $F_1, F_2, \ldots, F_N$ on equal class intervals. The number of class intervals is computed as follows:

where:

$N = (UBO_3 - UBO_1)/UBO_2$

UBO_1 = given lower bound

UBO_2 = given class interval

UBO_3 = given upper bound

and the total frequency

$$T = \sum_{i=1}^{N} F_i$$

where F_i = frequency in the i-th interval.
If we set

$$X_i = UBO_1 - 0.5UBO_2 + i\ UBO_2 \qquad i=1,\ldots,n$$

then the first moment (mean)

$$ANS_1 = 1/T \sum_{i=1}^{N} F_i X_i$$

and the jth moment (j=2,3,4) is

$$ANS_j = 1/T \sum_{i=1}^{N} F_i (X_i - ANS_1)^j$$

These moments are biased and not corrected for grouping.

- Subroutine TTST

```
TTST..                                                                  TTST  10
/*********************************************************************/TTST  20
/*                                                                   */TTST  30
/*      TO FIND CERTAIN T-STATISTICS ON THE MEANS OF POPULATIONS.    */TTST  40
/*                                                                   */TTST  50
/*********************************************************************/TTST  60
   PROCEDURE (A,NA,B,NB,NOP,NDF,ANS),.                                  TTST  70
   DECLARE                                                              TTST  80
         ERROR EXTERNAL CHARACTER (1),                                  TTST  90
         (A(*),B(*),ANS,AMEAN,BMEAN,FNA,FNB,SA2,SB2,S,A1,A2)            TTST 100
         FLOAT BINARY,                                                  TTST 110
         (T(6)) LABEL,.                                                 TTST 120
/*                                                                      */TTST 130
   NDF  ='0',.                          /* INITIALIZATION              */TTST 140
   ERROR='0',.                                                          TTST 150
   ANS  =0.0,.                                                          TTST 160
   IF NOP LT 1 OR NOP GT 4                                              TTST 170
   THEN DO,.                                                            TTST 180
         ERROR='1',.                    /* WRONG OPTION CODE           */TTST 190
         GO TO FIN,.                                                    TTST 200
         END,.                                                          TTST 210
   IF NOP=1 AND NA NE 1                                                 TTST 220
   THEN DO,.                            /* NA MUST BE 1 WHEN NOP=1     */TTST 230
         ERROR='5',.                                                    TTST 240
         GO TO FIN,.                                                    TTST 250
         END,.                                                          TTST 260
   IF NOP=4 AND NB NE NA                                                TTST 270
   THEN DO,.                            /* NA MUST EQUAL NB WHEN NOP=4 */TTST 280
         ERROR='6',.                                                    TTST 290
         GO TO FIN,.                                                    TTST 300
         END,.                                                          TTST 310
/*                                                                      */TTST 320
/*      TEST SAMPLE SIZE                                                */TTST 330
/*                                                                      */TTST 340
   IF NA LE 1                                                           TTST 350
   THEN DO,.                                                            TTST 360
         IF NOP GT 1                                                    TTST 370
         THEN DO,.                                                      TTST 380
               ERROR='2',.              /* FIRST SAMPLE FOR OPTIONS    */TTST 390
               GO TO FIN,.              /* 2-4 IS 1 OR LESS            */TTST 400
               END,.                                                    TTST 410
         END,.                                                          TTST 420
   IF NB LE 1                                                           TTST 430
   THEN DO,.                                                            TTST 440
         ERROR='2',.                    /* SECOND SAMPLE SIZE IS 1 OR  */TTST 450
         GO TO FIN,.                    /* LESS                        */TTST 460
         END,.                                                          TTST 470
   FNA  =NA,.                                                           TTST 480
   FNB  =NB,.                                                           TTST 490
   AMEAN=0.0,.                          /* CALCULATE MEAN OF A         */TTST 500
         DO I = 1 TO NA,.                                               TTST 510
         AMEAN=AMEAN+A(I),.                                             TTST 520
         END,.                                                          TTST 530
   AMEAN=AMEAN/FNA,.                                                    TTST 540
   BMEAN=0.0,.                          /* CALCULATE MEAN OF B         */TTST 550
         DO I = 1 TO NB,.                                               TTST 560
         BMEAN=BMEAN+B(I),.                                             TTST 570
         END,.                                                          TTST 580
   BMEAN=BMEAN/FNB,.                                                    TTST 590
/*                                                                      */TTST 600
/*      CALCULATE THE VARIANCE OF A                                     */TTST 610
/*                                                                      */TTST 620
   IF NOP LT 4 AND NOP GT 1                                             TTST 630
   THEN DO,.                                                            TTST 640
         SA2  =0.0,.                                                    TTST 650
               DO I = 1 TO NA,.                                         TTST 660
               SA2  =SA2+(A(I)-AMEAN)**2,.                              TTST 670
               END,.                                                    TTST 680
         SA2  =SA2/(FNA-1.0),.                                          TTST 690
         IF SA2 LE 0.0                                                  TTST 700
         THEN DO,.                                                      TTST 710
               ERROR='3',.              /* FIRST SAMPLE VARIANCE = 0.0 */TTST 720
               GO TO FIN,.                                              TTST 730
               END,.                                                    TTST 740
         END,.                                                          TTST 750
   IF NOP LT 4                                                          TTST 760
   THEN DO,.                                                            TTST 770
         SB2  =0.0,.                                                    TTST 780
               DO I = 1 TO NB,.                                         TTST 790
               SB2  =SB2+(B(I)-BMEAN)**2,.                              TTST 800
               END,.                                                    TTST 810
         SB2  =SB2/(FNB-1.0),.                                          TTST 820
         IF SB2 LE 0.0                                                  TTST 830
         THEN DO,.                                                      TTST 840
               ERROR='3',.              /* SECOND SAMPLE VARIANCE = 0.0*/TTST 850
               GO TO FIN,.                                              TTST 860
               END,.                                                    TTST 870
         END,.                                                          TTST 880
   GO TO T(NOP),.                                                       TTST 890
T(1),.                                  /* OPTION ONE                  */TTST 900
   ANS  =((BMEAN-AMEAN)/SQRT(SB2))*SQRT(FNB),.                          TTST 910
   NDF  =NB-1,.                                                         TTST 920
   GO TO FIN,.                                                          TTST 930
T(2),.                                  /* OPTION TWO                  */TTST 940
   NDF  =NA+NB-2,.                                                      TTST 950
   S    =SQRT(((FNA-1.0)*SA2+(FNB-1.0)*SB2)/NDF),.                      TTST 960
   ANS  =((BMEAN-AMEAN)/S)*(1.0/SQRT(1.0/FNA+1.0/FNB)),.                TTST 970
   GO TO FIN,.                                                          TTST 980
T(3),.                                  /* OPTION THREE                */TTST 990
   ANS  =(BMEAN-AMEAN)/SQRT(SA2/FNA+SB2/FNB),.                          TTST1000
   A1   =(SA2/FNA+SB2/FNB)**2,.                                         TTST1010
   A2   =(SA2/FNA)**2/(FNA+1.0)+(SB2/FNB)**2/(FNB+1.0),.                TTST1020
   NDF  =A1/A2-2.0+0.5,.                                                TTST1030
   GO TO FIN,.                                                          TTST1040
T(4),.                                  /* OPTION FOUR                 */TTST1050
   A1   =BMEAN-AMEAN,.                                                  TTST1060
   A2   =0.0,.                                                          TTST1070
         DO I = 1 TO NB,.                                               TTST1080
         A2   =A2+(B(I)-A(I)-A1)**2,.                                   TTST1090
         END,.                                                          TTST1100
   IF A2 LE 0.0                                                         TTST1110
   THEN DO,.                                                            TTST1120
         ERROR='4',.                    /* TWO SAMPLES ARE IDENTICAL   */TTST1130
         GO TO FIN,.                                                    TTST1140
         END,.                                                          TTST1150
   A2   =SQRT(A2/(FNB-1.0)),.                                           TTST1160
   ANS  =(A1/A2)*SQRT(FNB),.                                            TTST1170
   NDF  =NB-1,.                                                         TTST1180
FIN,.                                                                   TTST1190
   RETURN,.                                                             TTST1200
   END,.                                /*END OF PROCEDURE TTST        */TTST1210
```

Purpose:

TTST calculates certain t-statistics on the means of populations.

Usage:

CALL TTST (A, NA, B, NB, NOP, NDF, ANS);

A(NA) - BINARY FLOAT
Given vector containing data.

NA - BINARY FIXED
Given number of observations in A.

B(NB) - BINARY FLOAT
Given vector containing data.

NB - BINARY FIXED
Given number of observations in B.

NOP - BINARY FIXED
Given options for various hypotheses:
- NOP=1 - That population mean of B = given value of A (set NA=1).
- NOP=2 - That population mean of B = population mean of A, given that the variance of B = the variance of A.
- NOP=3 - That population mean of B = population mean of A, given the variance of B is not equal to the variance of A.
- NOP=4 - That population mean of A = population mean of B, given no information about variance of A and B (set NA = NB).

NDF - BINARY FIXED
Resultant variable containing degrees of freedom associated with t-statistic calculated.

ANS - BINARY FLOAT
Resultant variable containing t-statistic.

Remarks:

NA and NB must be greater than one, except that NA=1 in option 1. NA and NB must be the same in option 4. If NOP is other than 1, 2, 3, or 4, degrees of freedom and t-statistic will not be calculated. NDF and ANS will be set to zero.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - invalid option code.
ERROR=2 - sample size of one of the variables is less than or equal to 1 (except variable A in option 1).
ERROR=3 - variance of one of the variables is zero.
ERROR=4 - two samples identical.
ERROR=5 - NA must be 1 when NOP is 1.
ERROR=6 - NA must equal NB when NOP is 4.

Method:

Refer to Ostle, Bernard, "Statistics in Research", Iowa State College Press, 1954, Chapter 5.

Mathematical Background:

This subroutine computes certain t-statistics on the means of populations under various hypotheses.

The sample means of $A_1, A_2, \ldots, A_{NA}$, and $B_1, B_2, \ldots, B_{NB}$ are normally found by the following formulas:

$$\bar{A} = \frac{\sum_{i=1}^{NA} A_i}{NA}; \qquad \bar{B} = \frac{\sum_{i=1}^{NB} B_i}{NB} \tag{1}$$

and the corresponding sample variances by:

$$SA^2 = \frac{\sum_{i=1}^{NA} (A_i - \bar{A})^2}{NA - 1}; \qquad SB^2 = \frac{\sum_{i=1}^{NB} (B_i - \bar{B})^2}{NB - 1} \tag{2}$$

The quantities μ and σ^2 stand respectively for population mean and variance in the following hypotheses.

Hypothesis: $\mu_B = A$; A = a given value (option 1).

Let $\bar{B}$ = estimate of μ_B and set NA = 1 (A is stored in location A_1).

The subroutine computes:

$$ANS = \frac{\bar{B} - A}{SB} \cdot \sqrt{NB} \quad \text{(t-statistics)} \tag{3}$$

$$NDF = NB - 1 \quad \text{(degrees of freedom)} \tag{4}$$

Hypothesis: $\mu_A = \mu_B; \left(\sigma_A^2 = \sigma_B^2\right)$ (option 2)

The subroutine computes:

$$ANS = \frac{\bar{B} - \bar{A}}{S} \cdot \frac{1}{\sqrt{\frac{1}{NA} + \frac{1}{NB}}} \quad \text{(t-statistics)} \tag{5}$$

$$NDF = NA + NB - 2 \qquad \text{(degrees of freedom)} \qquad (6)$$

$$\text{where } S = \sqrt{\frac{(NA-1)SA^2 + (NB-1)SB^2}{NA + NB - 2}} \qquad (7)$$

Hypothesis: $\mu_A = \mu_B$; $\left(\sigma_A^2 \neq \sigma_B^2\right)$ (option 3)

The subroutine computes:

$$ANS = \frac{\overline{B} - \overline{A}}{\sqrt{\frac{SA^2}{NA} + \frac{SB^2}{NB}}} \qquad \text{(t-statistics)} \qquad (8)$$

$$NDF = \frac{\left(\frac{SA^2}{NA} + \frac{SB^2}{NB}\right)^2}{\left(\frac{SA^2}{NA}\right)^2 \Big/ (NA + 1) + \left(\frac{SB^2}{NB}\right)^2 \Big/ (NB + 1)} - 2 \qquad (9)$$

(degrees of freedom)

Note: The program returns a rounded NDF, not a truncated NDF.

Hypothesis: $\mu_A = \mu_B$; $\left(\text{no assumption on } \sigma^2\right)$ (option 4)

The subroutine computes:

$$ANS = \frac{\overline{D}}{SD} \cdot \sqrt{NB} \qquad \text{(t-statistics)} \qquad (10$$

NDF = NB - 1 (degrees of freed

where $\overline{D} = \overline{B} - \overline{A}$

$$SD = \sqrt{\frac{\sum_{i=1}^{NB} (B_i - A_i - \overline{D})^2}{NB}}$$

NA = NB

Correlation and Regression Analysis

- Subroutine CORR

```
CORR..                                                                  CORR  10
/*********************************************************************/CORR  20
/*                                                                   */CORR  30
/*      TO COMPUTE MEANS, STANDARD DEVIATIONS, SUMS OF CROSS-PRODUCTS*/CORR  40
/*      OF DEVIATIONS, AND CORRELATION COEFFICIENTS.                 */CORR  50
/*                                                                   */CORR  60
/*********************************************************************/CORR  70
   PROCEDURE (N,M,IO,X,XBAR,STD,RX,R,B),.                               CORR  80
   DECLARE                                                              CORR  90
        ERROR EXTERNAL CHARACTER (1),                                   CORR 100
        (I,IO,J,K,KK,M,N)                                               CORR 110
        FIXED BINARY,                                                   CORR 120
        (X(*,*),D(M),FN,FKK)                                            CORR 130
        FLOAT BINARY,                                                   CORR 140
        (R(*,*),RX(*,*),XBAR(*),STD(*),B(*),T(M))                       CORR 150
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/CORR 160
 /*     BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/CORR 170
/*                                                                   */CORR 180
   ERROR='0',.                                                          CORR 190
   IF N LE 0 OR M LE 0          /* THE NUMBER OF OBSERVATIONS  */CORR 200
   THEN DO,.                    /* OR THE NUMBER OF VARIABLES  */CORR 210
        ERROR='1',.             /* ARE LESS THAN OR EQUAL TO   */CORR 220
        GO TO FIN,.             /* ZERO.                       */CORR 230
        END,.                                                           CORR 240
   FN   =N,.                    /* INITIALIZATION              */CORR 250
   T    =0.0,.                                                          CORR 260
        DO I = 1 TO M,.                                                 CORR 270
        B(I) =0.0,.                                                     CORR 280
             DO J = 1 TO M,.                                            CORR 290
             R(I,J)=0.0,.                                               CORR 300
             END,.                                                      CORR 310
        END,.                                                           CORR 320
   IF IO NE 0                                                           CORR 330
   THEN DO,.                                                            CORR 340
             DO J = 1 TO M,.        /* DATA       IN CORE      */CORR 350
                  DO I = 1 TO N,.                                       CORR 360
                  T(J) =T(J)+X(I,J),.                                   CORR 370
                  END,.                                                 CORR 380
             XBAR(J)=T(J),.                                             CORR 390
             T(J) =T(J)/FN,.                                            CORR 400
             END,.                                                      CORR 410
             DO I = 1 TO N,.                                            CORR 420
                  DO J = 1 TO M,.                                       CORR 430
                  D(J) =X(I,J)-                                         CORR 440
                  B(J) =B(J)+D                                          CORR 450
                  END,.                                                 CORR 460
                  DO J = 1                                              CORR 470
                       DO                                               CORR 480
                                                                        CORR 490
                                                                        CORR 500
                  EN                                                    CORR 510
             END,.                                                      CORR 520
        GO TO CA                                                        CORR 530
        END,.                                                           CORR 540
/*                                                                   */CORR 550
/*      REA                                   EANS                   */CORR 560
/*                                                                   */CORR 570
   IF N                                                                 CORR 580
   THE                                                                  CORR 590
   EN                                                                   CORR 600
                                                                        CORR 610
                                                                        CORR 620
                                                                        CORR 630
                                                                        CORR 640
                                                                        CORR 650
                                                                        CORR 660
                                                                        CORR 670
                                                                        CORR 680
                                                                        CORR 690
                                                                        CORR 700
                                                                        CORR 710
                                                                        CORR 720
                                                                      */CORR 730
                                        ATIONS FROM                   */CORR 740
                                                                      */CORR 750
                                                                      */CORR 760
                                                                        CORR 770
                                                                        CORR 780
                                                                        CORR 790
                                                                        CORR 800
                                                                        CORR 810
                                                                        CORR 820
                                                                        CORR 830
                                                                        CORR 840
                                                                        CORR 850
                                                                        CORR 860
                                                                        CORR 870
                                                                        CORR 880
                                                                      */CORR 890
                                   TIME, SUM THE                      */CORR 900
                                   ODUCTS OF                          */CORR 910
                                                                      */CORR 920
                                                                      */CORR 930
                                                                        CORR 940
                                                                        CORR 950
                                                                        CORR 960
                                                                        CORR 970
                                                                        CORR 980
                                                                        CORR 990
                                                                        CORR1000
                                                                        CORR1010
                                                                        CORR1020
                                                                        CORR1030
                                   D(J)*D(K),.                          CORR1040
                                                                        CORR1050
                                                                        CORR1060
                                                                        CORR1070
                                                                        CORR1080
                                                                      */CORR1090
        JUST SUMS OF CROSS-PRODUCTS OF DEVIATIONS FROM TEMP. MEANS    */CORR1100
                                                                      */CORR1110
 LC..                                                                   CORR1120
        DO I = 1 TO M,.                                                 CORR1130
        XBAR(I)=XBAR(I)/FN,.        /* CALCULATE MEANS.            */CORR1140
             DO J = I TO M,.                                            CORR1150
             RX(I,J)=R(I,J)-B(I)*B(J)/FN,.                              CORR1160
             RX(J,I)=RX(I,J),.                                          CORR1170
             END,.                                                      CORR1180
```

```
        STD(I)=SQRT(ABS(RX(I,I))),.                                    CORR1190
/*                                                                     */CORR1200
/*    COPY THE DIAGONAL OF THE MATRIX OF SUMS OF CROSS PRODUCTS OF     */CORR1210
/*    DEVIATIONS FROM THE MEANS.                                       */CORR1220
/*                                                                     */CORR1230
        B(I) =RX(I,I),.                                                CORR1240
        END,.                                                          CORR1250
/*                                                                     */CORR1260
/*      COMPUTE CORRELATION COEFFICIENTS                               */CORR1270
/*                                                                     */CORR1280
        DO J = 1 TO M,.                                                CORR1290
             DO K = J TO M,.                                           CORR1300
             FKK  =STD(J)*STD(K),.                                     CORR1310
             IF FKK= 0.0                                               CORR1320
             THEN DO,.                                                 CORR1330
                  ERROR='2',.          /* SOME VARIANCES ARE ZERO     */CORR1340
                  R(J,K)=0.0,.                                         CORR1350
                  END,.                                                CORR1360
             ELSE R(J,K)=RX(J,K)/FKK,.                                 CORR1370
             R(K,J)=R(J,K),.                                           CORR1380
             END,.                                                     CORR1390
        END,.                                                          CORR1400
/*                                                                     */CORR1410
/*      COMPUTE STANDARD DEVIATIONS                                    */CORR1420
/*                                                                     */CORR1430
        IF N=1                                                         CORR1440
        THEN DO,.                                                      CORR1450
             DO I=1 TO N,.                                             CORR1460
             STD(1)    =0,.                                            CORR1470
             END,.                                                     CORR1480
             GO TO FIN,.                                               CORR1490
             END,.                                                     CORR1500
        FN   =SQRT(N-1),.                                              CORR1510
        DO I = 1 TO M,.                                                CORR1520
        STD(I)=STD(I)/FN,.                                             CORR1530
        END,.                                                          CORR1540
FIN..                                                                  CORR1550
   RETURN,.                                                            CORR1560
   END,.                              /*END OF PROCEDURE CORR         */CORR1570
```

Purpose:

CORR computes means, standard deviations, sums of cross-products of deviations, and correlation coefficients.

Usage:

CALL CORR (N, M, IO, X, XBAR, STD, RX, R, B);

Description of parameters:

N - BINARY FIXED
Given number of observations.

M - BINARY FIXED
Given number of variables for each observation.

IO - BINARY FIXED
Given option code for input data.

X(N, M) - BINARY FLOAT
IO=0 If data are to be read in from input device in the special procedure named DAT2 (see "Remarks").
IO≠0 If all data are already in core.
If IO=0, X is not used.
If IO≠0, X is the input matrix containing data already in core.

XBAR(M) - BINARY FLOAT [(53)]
Resultant vector of length M containing means.

STD - BINARY FLOAT [(53)]
Resultant vector of length M containing standard deviations.

RX(M, M) - BINARY FLOAT [(53)]
Resultant matrix (M by M) containing sums of cross-products of deviations from means.

R(M, M) - BINARY FLOAT [(53)]
Resultant matrix (M by M) containing correlation coefficients.

B(M) - BINARY FLOAT [(53)]
Resultant vector of length M containing the diagonal of the matrix of sums of cross-products of deviations from means.

Remarks:

Subroutines and function subroutines required:

DAT2(M, D). This subroutine may be provided by the user, but a suitable subroutine is used in several of the sample programs (for example, see REGR). Note that in using this procedure, the parameters NCARD and NV must be declared external and the proper values must be assigned to them.

1. If IO=0, this subroutine provides an observation in vector D from an input device.
2. If IO≠0, this procedure is not used by CORR but must be in the job deck. If the user has neither supplied a subroutine nor used the subroutine DAT2 from the Scientific Subroutine Package, the following is suggested:

```
DAT2..
   PROCEDURE,.
   RETURN,.
   END,.
```

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations less than or equal to zero.
ERROR=2 - at least one variance is zero.

Method:

Product-moment correlation coefficients are computed.

Mathematical Background:

This subroutine calculates means, standard deviations, sums of cross-products of deviations from means, and product moment correlation coefficients from input data X_{ij}, where i = 1, 2, ..., n implies observations and j = 1, 2, ..., m implies variables.

The following equations are used to calculate these statistics:

Sums of cross-products of deviations:

$$S_{jk} = \sum_{i=1}^{n} \left(X_{ij} - T_j\right)\left(X_{ik} - T_k\right) - \frac{\sum_{i=1}^{n} \left(X_{ij} - T_j\right) \sum_{i=1}^{n} \left(X_{ik} - T_k\right)}{n} \quad (1)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

$$T_j = \frac{\sum_{i=1}^{m} X_{ij}}{m} \quad (2)$$

(These temporary means T_j are subracted from the data in equation (1) to obtain computational accuracy.)

Means: $$\overline{X}_j = \frac{\sum_{i=1}^{n} X_{ij}}{n} \quad (3)$$

where j = 1, 2, ..., m

Correlation coefficients:

$$r_{jk} = \frac{S_{jk}}{\sqrt{S_{jj}}\ \sqrt{S_{kk}}} \quad (4)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

Standard deviations:

$$s_j = \frac{\sqrt{S_{jj}}}{\sqrt{n-1}} \quad (5)$$

where j = 1, 2, ..., m

- Subroutine ORDR

```
ORDR..                                                                  ORDR  10
/*********************************************************************/ORDR  20
/*                                                                    */ORDR  30
/*      TO CONSTRUCT FROM A LARGER MATRIX OF CORRELATION COEFFICIENTS*/ORDR  40
/*      A SUBSET MATRIX OF INTERCORRELATIONS AMONG INDEPENDENT VAR-   */ORDR  50
/*      IABLES AND A VECTOR OF INTERCORRELATIONS OF INDEPENDENT       */ORDR  60
/*      VARIABLES WITH DEPENDENT VARIABLE.                            */ORDR  70
/*                                                                    */ORDR  80
/*********************************************************************/ORDR  90
   PROCEDURE (M,R,NDEP,K,ISAVE,RX,RY),.                                 ORDR 100
   DECLARE                                                              ORDR 110
        (ISAVE(*),I,J,K,L,L1)                                           ORDR 120
        FIXED BINARY,                                                   ORDR 130
        ERROR EXTERNAL CHARACTER(1),                                    ORDR 140
        (R(*,*),RX(K,K),RY(K))                                          ORDR 150
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/ORDR 160
 /*     BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/ORDR 170
/*                                                                    */ORDR 180
/*      COPY INTERCORRELATIONS OF INDEPENDENT VARIABLES WITH          */ORDR 190
/*      DEPENDENT VARIABLE                                            */ORDR 200
/*                                                                    */ORDR 210
   ERROR='0',.                                                          ORDR 220
   IF M LE 0                    /* THE NUMBER OF VARIABLES IS        */ORDR 230
   THEN DO,.                    /* LESS THAN OR EQUAL TO ZERO.       */ORDR 240
        ERROR='1',.                                                     ORDR 250
        GO TO FIN,.                                                     ORDR 260
        END,.                                                           ORDR 270
        DO I=1 TO K,.                                                   ORDR 280
        IF ISAVE(K) = NDEP          /* INVALID K                       */ORDR 290
        OR ISAVE(K) LE 0                                                ORDR 300
        OR ISAVE(K) GT M                                                ORDR 310
        THEN DO,.                                                       ORDR 320
             ERROR='3',.                                                ORDR 330
             GO TO FIN,.                                                ORDR 340
             END,.                                                      ORDR 350
        END,.                                                           ORDR 360
   IF NDEP LE 0 OR NDEP GT M        /* INVALID DEPENDENT VARIABLE      */ORDR 370
   THEN DO,.                                                            ORDR 380
        ERROR='2',.                                                     ORDR 390
        GO TO FIN,.                                                     ORDR 400
        END,.                                                           ORDR 410
   IF K LE 0 OR K GE M              /*INVALID NUMBER OF INDEPENDENT*/ORDR 420
   THEN DO,.                        /*        VARIABLES           */ORDR 430
        ERROR='4',.                                                     ORDR 440
        GO TO FIN,.                                                     ORDR 450
        END,.                                                           ORDR 460
        DO I = 1 TO K,.                                                 ORDR 470
        L1   =ISAVE(I),.                                                ORDR 480
        RY(I)=R(NDEP,L1),.                                              ORDR 490
/*                                                                    */ORDR 500
/*      COPY A SUBSET MATRIX OF INTERCORRELATIONS AMONG INDEPENDENT   */ORDR 510
/*      VARIABLES                                                     */ORDR 520
/*                                                                    */ORDR 530
             DO J = 1 TO K,.                                            ORDR 540
             L2   =ISAVE(J),.                                           ORDR 550
             IF L2 LT L1                                                ORDR 560
             THEN RX(I,J)=RX(J,I),.                                     ORDR 570
             ELSE RX(I,J)=R(L1,L2),.                                    ORDR 580
             END,.                                                      ORDR 590
        END,.                                                           ORDR 600
/*                                                                    */ORDR 610
/*      PLACE THE SUBSCRIPT NUMBER OF THE DEPENDENT VARIABLE          */ORDR 620
/*      IN ISAVE(K+1)                                                 */ORDR 630
/*                                                                    */ORDR 640
   ISAVE(K+1)=NDEP,.                                                    ORDR 650
FIN..                                                                   ORDR 660
   RETURN,.                                                             ORDR 670
   END,.                            /*END OF PROCEDURE ORDR           */ORDR 680
```

Purpose:

ORDR is used to choose a dependent variable and a set of independent variables from a matrix of correlation coefficients, and form a submatrix of correlation coefficients to be used in performing a multiple linear regression analysis.

Usage:

CALL ORDR (M, R, NDEP, K, ISAVE, RX, RY);

Description of parameters:

M - BINARY FIXED
Given number of variables.

R(M, M) - BINARY FLOAT [(53)]
Given matrix containing correlation coefficients.

NDEP - BINARY FIXED
Given subscript number of the dependent variable.

K - BINARY FIXED
Given number of independent variables to be included in the forthcoming regression.

ISAVE - BINARY FIXED
(K+1) Given vector containing, in ascending order, the subscript numbers of K independent variables to be included in the forthcoming regression. Upon returning to the calling program, this vector contains, in addition, the subscript number of the dependent variable in K+1 position.

RX(K,K) - BINARY FLOAT [(53)]
Resultant matrix containing intercorrelations among independent variables to be used in forthcoming regression.

RY(K) - BINARY FLOAT [(53)]
Resultant vector containing intercorrelations of independent variables with dependent variables.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of variables less than or equal to zero.
ERROR=2 - invalid dependent variable subscript.
ERROR=3 - invalid independent variable subscript. If this condition exists, RX and RY will contain invalid values.
ERROR=4 - invalid number of independent variables.

Method:

From the subscript numbers of the variables to be included in the forthcoming regression, the procedure constructs the matrix RX and the vector RY.

• Subroutine MLTR

```
MLTR..                                                                  MLTR  10
/*********************************************************************/MLTR  20
/*                                                                   */MLTR  30
/*      TO PERFORM A MULTIPLE LINEAR REGRESSION ANALYSIS FOR A       */MLTR  40
/*      DEPENDENT VARIABLE AND A SET OF INDEPENDENT VARIABLES.       */MLTR  50
/*                                                                   */MLTR  60
/*********************************************************************/MLTR  70
   PROCEDURE (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,BETA,ANS),.             MLTR  80
   DECLARE                                                              MLTR  90
         ERROR EXTERNAL CHARACTER (1),                                  MLTR 100
         (I,IO,J,M,MM,MP,MQ,N,N1,ISAVE(*))                              MLTR 110
         FIXED BINARY,                                                  MLTR 120
         (XBAR(*),STD(*),D(*),RX(*,*),RY(*),B(*),SB(*),T(*),BETA(*),    MLTR 130
         ANS(10),RM,BO,SSAR,SSDR,FK,FNN,SY,SSARM,SSDRM,F)               MLTR 140
         BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/MLTR 150
/*       BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/MLTR 160
/*                                                                   */MLTR 170
   ERROR='0',.                                                          MLTR 180
   IF K LE 0 OR N LE K             /* THE NUMBER OF VARIABLES IS    */MLTR 190
   THEN DO,.                       /* LESS THAN OR EQUAL TO ZERO    */MLTR 200
         ERROR='1',.               /* OR THE NO. OF OBSERVATIONS    */MLTR 210
         GO TO S10,.               /* IS LESS THAN OR EQUAL TO THE  */MLTR 220
         END,.                     /* THE NUMBER OF VARIABLES       */MLTR 230
   MM   =K+1,.                                                          MLTR 240
   FK   =K,.                                                            MLTR 250
         DO J = 1 TO K,.                                                MLTR 260
         BETA(J)=0.0,.                                                  MLTR 270
         B(J) =0.0,.                                                    MLTR 280
               DO I = 1 TO K,.                                          MLTR 290
               BETA(J)=BETA(J)+RY(I)*RX(I,J),.                          MLTR 300
               END,.                                                    MLTR 310
         END,.                                                          MLTR 320
   RM   =0.0,.                                                          MLTR 330
   BO   =0.0,.                                                          MLTR 340
   L1   =ISAVE(MM),.                                                    MLTR 350
/*                                                                   */MLTR 360
/*       COEFFICIENT OF DETERMINATION                                */MLTR 370
/*                                                                   */MLTR 380
         DO I = 1 TO K,.                                                MLTR 390
         RM   =RM+BETA(I)*RY(I),.                                       MLTR 400
/*                                                                   */MLTR 410
/*       TEST ACCURACY OF THE RESULT                                 */MLTR 420
/*                                                                   */MLTR 430
         IF RM LT 0 OR RM GT 1                                          MLTR 440
         THEN DO,.                                                      MLTR 450
               ERROR='2',.           /* INVALID MULTIPLE R          */MLTR 460
               GO TO S10,.                                              MLTR 470
               END,.                                                    MLTR 480
         L    =ISAVE(I),.            /* REGRESSION COEFFICIENT      */MLTR 490
         B(I) =BETA(I)*(STD(L1)/STD(L)),.                               MLTR 500
         BO   =BO+B(I)*XBAR(L),.     /* INTERCEPT                   */MLTR 510
         END,.                                                          MLTR 520
   BO   =XBAR(L1)-BO,.                                                  MLTR 530
/*                                                                   */MLTR 540
/*       SUM OF SQUARES ATTRIBUTED TO REGRESSION                     */MLTR 550
/*                                                                   */MLTR 560
   SSAR =RM*D(L1),.                                                     MLTR 570
   IF SSAR GT D(L1)                /* TEST SUM OF SQUARES REDUCED */MLTR 580
   THEN DO,.                                                            MLTR 590
         ERROR='3',.               /* REDUCED SUM OF SQUARES      */MLTR 600
         GO TO S10,.               /* GREATER THAN THE TOTAL      */MLTR 610
         END,.                     /* SUM OF SQUARES              */MLTR 620
   RM   =SQRT(ABS(RM)),.           /* MULTIPLE CORRELATION COEFF. */MLTR 630
/*                                                                   */MLTR 640
/*       SUM OF SQUARES OF DEVIATIONS FROM REGRESSION                */MLTR 650
/*                                                                   */MLTR 660
   SSDR =D(L1)-SSAR,.                                                   MLTR 670
   FNN  =N-K-1,.                   /* DEGREES OF FREEDOM          */MLTR 680
   IF FNN LE 0.0                                                        MLTR 690
   THEN DO,.                                                            MLTR 700
         ERROR='1',.               /* SAMPLE SIZE TOO SMALL       */MLTR 710
         GO TO S10,.                                                    MLTR 720
         END,.                                                          MLTR 730
   SY   =SSDR/FNN,.                /* VARIANCE OF ESTIMATE        */MLTR 740
/*                                                                   */MLTR 750
/*       STANDARD DEVIATIONS OF REGRESSION COEFFICIENTS              */MLTR 760
/*                                                                   */MLTR 770
         DO J = 1 TO K,.                                                MLTR 780
         L    =ISAVE(J),.                                               MLTR 790
         SB(J)=SQRT(ABS((RX(J,J)/D(L))*SY)),.                           MLTR 800
         T(J) =B(J)/SB(J),.          /* COMPUTE T-VALUES            */MLTR 810
         END,.                                                          MLTR 820
   SY   =SQRT(ABS(SY)),.           /* STANDARD ERROR OF ESTIMATE  */MLTR 830
   SSARM=SSAR/FK,.                 /* F-VALUE                     */MLTR 840
   SSDRM=SSDR/FNN,.                                                     MLTR 850
   F    =SSARM/SSDRM,.                                                  MLTR 860
   ANS(1)=BO,.                                                          MLTR 870
   ANS(2)=RM,.                                                          MLTR 880
   ANS(3)=SY,.                                                          MLTR 890
   ANS(4)=SSAR,.                                                        MLTR 900
   ANS(5)=FK,.                                                          MLTR 910
   ANS(6)=SSARM,.                                                       MLTR 920
   ANS(7)=SSDR,.                                                        MLTR 930
   ANS(8)=FNN,.                                                         MLTR 940
   ANS(9)=SSDRM,.                                                       MLTR 950
   ANS(10)=F,.                                                          MLTR 960
S10..                                                                   MLTR 970
   RETURN,.                                                             MLTR 980
   END,.                           /*END OF PROCEDURE MLTR       */MLTR 990
```

Purpose:

MLTR performs a multiple linear regression analysis for a dependent variable and a set of independent variables.

Usage:

CALL MLTR (N, K, XBAR, STD, D, RX, RY, ISAVE, B, SB, T, BETA, ANS);

Description of parameters:

N - BINARY FIXED
Given number of observations (N must be greater than K).

K - BINARY FIXED
Given number of independent variables in this regression.

XBAR(M) - BINARY FLOAT [(53)]
Given vector containing means of all variables. M is the number of variables in an observation.

STD(M) - BINARY FLOAT [(53)]
Given vector containing standard deviations of all variables.

D(M) - BINARY FLOAT [(53)]
Given vector containing the diagonal of the matrix of sums of cross-products of deviations from means for all variables.

RX(K,K) - BINARY FLOAT [(53)]
Given matrix containing the inverse of intercorrelations among independent variables.

RY(K) - BINARY FLOAT [(53)]
Given vector containing intercorrelations of independent variables with dependent variable.

ISAVE - BINARY FIXED
(K+1) Given vector containing subscripts of independent variables in ascending order. The subscript of the dependent variable is stored in the last, K+1, position.

B(K) - BINARY FLOAT [(53)]
Resultant vector containing regression coefficients.

SB(K) - BINARY FLOAT [(53)]
Resultant vector containing standard deviations of regression coefficients.

T(K) - BINARY FLOAT [(53)]
Resultant vector containing T values.

BETA(K) - BINARY FLOAT [(53)]
Resultant vector containing beta coefficients.

ANS(10) - BINARY FLOAT [(53)]
Resultant vector containing the following information:

ANS(1) Intercept
ANS(2) Multiple correlation coefficient
ANS(3) Standard error of estimate
ANS(4) Sum of squares attributable to regression (SSAR)
ANS(5) Degrees of freedom associated with SSAR
ANS(6) Mean square of SSAR
ANS(7) Sum of squares of deviations from regression (SSDR)
ANS(8) Degrees of freedom associated with SSDR
ANS(9) Mean square of SSDR
ANS(10) F value

Remarks:

If there are no errors in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of independent variables K less than or equal to zero or the number of observations N is less than or equal to K.
ERROR=2 - coefficient of determination (RM) less than zero or greater than one.
ERROR=3 - reduced sum of squares (SSAR) greater than the total sum of squares.

Method:

The Gauss-Jordan method is used in the solution of the normal equations. Refer to W. W. Cooley and P. R. Lohnes, Multivariate Procedures for the Behavioral Sciences, John Wiley and Sons, 1962, Chapter 3, and B. Ostle, Statistics in Research, The Iowa State College Press, 1954 Chapter 8.

Mathematical Background:

This subroutine performs a multiple regression analysis for a dependent variable and a set of independent variables.

Beta weights are calculated using the following equation:

$$\beta_j = \sum_{i=1}^{k} r_{iy} \cdot r_{ij}^{-1} \qquad (1)$$

where:

r_{iy} = intercorrelation of i-th independent variable with dependent variable

r^{-1}_{ij} = the inverse of intercorrelation r_{ij}

i, j = 1, 2, ..., k imply independent variables

r_{iy} and r^{-1}_{ij} are input to this subroutine.

Then the regression coefficients are calculated as follows:

$$b_j = \beta_j \cdot \frac{s_y}{s_j} \tag{2}$$

where:

s_y = standard deviation of dependent variable

s_j = standard deviation of j-th independent variable

j = 1, 2, ..., k

s_y and s_j are input to this subroutine.

The intercept is found by the following equation:

$$b_0 = \overline{Y} - \sum_{j=1}^{k} b_j \cdot \overline{X}_j \tag{3}$$

where:

$\overline{Y}$ = mean of dependent variable

$\overline{X}_j$ = mean of jth independent variable

$\overline{Y}$ and $\overline{X}_j$ are input to this subroutine

Multiple correlation coefficient, R, is found first by calculating the coefficient of determination by the following equation:

$$R^2 = \sum_{i=1}^{k} \beta_i r_{iy} \tag{4}$$

and taking the square root of R^2:

$$R = \sqrt{R^2} \tag{5}$$

The sum of squares attributable to the regression is found by:

$$SSAR = R^2 \cdot D_{yy} \tag{6}$$

where:

D_{yy} = sum of squares of deviations from mean for dependent variable

D_{yy} is input to this subroutine.

The sum of squares of deviations from the regression is obtained by:

$$SSDR = D_{yy} - SSAR \tag{7}$$

Then, the F value for the analysis of variance is calculated as follows:

$$F = \frac{SSAR/k}{SSDR/(n-k-1)} = \frac{SSAR(n-k-1)}{SSDR(k)} \tag{8}$$

Certain other statistics are calculated as follows:

Variance and standard error of estimate:

$$S^2_{y.12...k} = \frac{SSDR}{n-k-1} \tag{9}$$

where n = number of observations

$$S_{y.12...k} = \sqrt{S^2_{y.12...k}} \tag{10}$$

Standard deviations of regression coefficients:

$$S_{b_j} = \sqrt{\frac{r^{-1}_{jj}}{D_{jj}} \cdot S^2_{y.12...k}} \tag{11}$$

where D_{jj} = sum of squares of deviations from mean for j^{th} independent variable. D_{jj} is input to this subroutine.

j = 1, 2, ..., k

Computed t:

$$t_j = \frac{b_j}{S_{b_j}} \tag{12}$$

j = 1, 2, ..., k

- Subroutine STRG

```
STRG..                                                              STRG  10
/*******************************************************************/STRG  20
/*                                                                 */STRG  30
/*      TO PERFORM A STEP-WISE MULTIPLE REGRESSION ANALYSIS FOR A  */STRG  40
/*      DEPENDENT VARIABLE AND A SET OF INDEPENDENT VARIABLES.     */STRG  50
/*                                                                 */STRG  60
/*******************************************************************/STRG  70
   PROCEDURE (M,N,D,XBAR,IDX,PCT,NSTEP,ANS,L,B,STD),.               STRG  80
   DECLARE                                                          STRG  90
         (I,ID,IJ,IK,J,K,KK,M,MK,MX,MY,N,NEW,NFO,NZ,NSTEP(*),IDX(*),STRG 100
         L(*),LL(M))                                              STRG 110
         FIXED BINARY,                                            STRG 120
         (D(*,*),XBAR(*),ANS(*),B(*),STD(*),T(M),S(M),BETA(M),RE) STRG 130
         BINARY FLOAT,              /*SINGLE PRECISION VERSION  /*S*/STRG 140
 /*      BINARY FLOAT (53),         /*DOUBLE PRECISION VERSION  /*D*/STRG 150
         (PCT,ONM,RD)                                             STRG 160
         FLOAT BINARY,                                            STRG 170
         (ERROR,NSTOP) EXTERNAL CHARACTER (1),.                   STRG 180
/*                                                                 */STRG 190
   ERROR='0',.                  /* INITIALIZATION                */STRG 200
   IF M LE 1 OR N LE M+1        /* THE NUMBER OF VARIABLES M IS*/STRG 210
   THEN DO,.                    /* NOT GREATER THAN 1 OR THE   */STRG 220
        ERROR='1',.             /* NUMBER OF OBSERVATIONS N IS */STRG 230
        GO TO S150,.            /* NOT GREATER THAN M+1        */STRG 240
        END,.                                                     STRG 250
   IF PCT GE 1.0                                                  STRG 260
   THEN DO,.                                                      STRG 270
        ERROR='4',.             /* SPECIFIED CONSTANT IS       */STRG 280
        GO TO S150,.            /* GREATER THAN OR = 1.0       */STRG 290
        END,.                                                     STRG 300
   ONM  =N-1,.                                                    STRG 310
   NFO  =0,.                                                      STRG 320
   NSTEP(3)=0,.                                                   STRG 330
   ANS(3)=0,.                                                     STRG 340
   ANS(4)=0,.                                                     STRG 350
   NSTOP='0',.                                                    STRG 360
/*                                                                 */STRG 370
/*      FIND DEPENDENT VARIABLE, NUMBER OF VARIABLES TO BE FORCED TO */STRG 380
/*      ENTER IN THE REGRESSION, AND THE NUMBER OF VARIABLES TO BE */STRG 390
/*      DELETED                                                    */STRG 400
/*                                                                 */STRG 410
        DO I = 1 TO M,.                                           STRG 420
        LL(I)=1,.                                                 STRG 430
        IF IDX(I) LE 0                                            STRG 440
        THEN GO TO S10,.                                          STRG 450
        IF IDX(I) LT 2                                            STRG 460
        THEN DO,.                                                 STRG 470
             NFO  =NFO+1,.                                        STRG 480
             IDX(NFO)=I,.                                         STRG 490
             GO TO S10,.                                          STRG 500
             END,.                                                STRG 510
        ELSE IF IDX(I)= 2                                         STRG 520
        THEN DO,.                                                 STRG 530
             NSTEP(3)=NSTEP(3)+1,.                                STRG 540
             LL(I)=-1,.                                           STRG 550
             GO TO S10,.                                          STRG 560
             END,.                                                STRG 570
        MY   =I,.                                                 STRG 580
        NSTEP(1)=MY,.                                             STRG 590
        ANS(5)=D(MY,MY),.                                         STRG 600
S10..                                                             STRG 610
        END,.                                                     STRG 620
   NSTEP(2)=NFO,.                                                 STRG 630
/*                                                                 */STRG 640
/*      FIND THE MAXIMUM NUMBER OF STEPS                           */STRG 650
/*                                                                 */STRG 660
   MX   =M-NSTEP(3)-1,.                                           STRG 670
/*                                                                 */STRG 680
/*      START SELECTION OF VARIABLES                               */STRG 690
/*                                                                 */STRG 700
        DO NZ = 1 TO MX,.                                         STRG 710
        IF N-NZ-1 LE 0                                            STRG 720
        THEN DO,.                                                 STRG 730
             ERROR='3',.            /* DEGREES OF FREEDOM IS 0   */STRG 740
             GO TO S150,.                                         STRG 750
             END,.                                                STRG 760
        RD   =0,.                                                 STRG 770
        IF NZ GT NFO                                              STRG 780
/*                                                                 */STRG 790
/*      SELECT NEXT VARIABLE TO ENTER AMONG FORCED VARIABLES       */STRG 800
/*                                                                 */STRG 810
        THEN GO TO S20,.                                          STRG 820
             DO I = 1 TO NFO,.                                    STRG 830
             K    =IDX(I),.                                       STRG 840
             IF LL(K) GT 0                                        STRG 850
             THEN DO,.                                            STRG 860
                  RE   =D(K,MY)**2/D(K,K),.                       STRG 870
                  IF RD LT RE                                     STRG 880
                  THEN DO,.                                       STRG 890
                       RD   =RE,.                                 STRG 900
                       NEW  =K,.                                  STRG 910
                       END,.                                      STRG 920
                  END,.                                           STRG 930
             END,.                                                STRG 940
        GO TO S25,.                                               STRG 950
/*                                                                 */STRG 960
/*      SELECT NEXT VARIABLE TO ENTER AMONG NON-FORCED VARIABLES   */STRG 970
/*                                                                 */STRG 980
S20..                                                             STRG 990
             DO I = 1 TO M,.                                      STRG1000
             IF I NE MY                                           STRG1010
             THEN DO,.                                            STRG1020
                  IF LL(I) GT 0                                   STRG1030
                  THEN DO,.                                       STRG1040
                       RE   =D(I,MY)**2/D(I,I),.                  STRG1050
                       IF RD LT RE                                STRG1060
                       THEN DO,.                                  STRG1070
                            RD   =RE,.                            STRG1080
                            NEW  =I,.                             STRG1090
                            END,.                                 STRG1100
                       END,.                                      STRG1110
                  END,.                                           STRG1120
             END,.                                                STRG1130
S25..                                                             STRG1140
        IF RD LE 0 OR  ANS(5) LE ANS(3)+RD                        STRG1150
        THEN DO,.                                                 STRG1160
             ERROR='2',.            /* NEGATIVE SUM OF SQUARES   */STRG1170
             GO TO S150,.                                         STRG1180
             END,.                                                STRG1190
        RE   =RD/ANS(5),.                                         STRG1200
/*                                                                 */STRG1210
/*      TEST WHETHER THE PROPORTION OF THE SUM OF SQUARES REDUCED BY */STRG1220
/*      THE LAST VARIABLE ENTERED IS GREATER THAN OR EQUAL TO THE  */STRG1230
/*      SPECIFIED PROPORTION                                       */STRG1240
/*                                                                 */STRG1250
        IF RE LT PCT                                              STRG1260
        THEN GO TO S150,.                                         STRG1270
        LL(NEW)=0,.                 /* IT IS GREATER THAN OR EQUAL */STRG1280
        L(NZ)=NEW,.                                               STRG1290
        ANS(1)=RD,.                                               STRG1300
        ANS(2)=RE,.                                               STRG1310
        ANS(3)=ANS(3)+RD,.                                        STRG1320
        ANS(4)=ANS(4)+RE,.                                        STRG1330
        NSTEP(4)=NZ,.                                             STRG1340
        NSTEP(5)=NEW,.                                            STRG1350
/*                                                                 */STRG1360
/*      COMPUTE MULTIPLE CORRELATION, F-VALUE FOR ANALYSIS OF      */STRG1370
/*      VARIANCE, AND STANDARD ERROR OF ESTIMATE                   */STRG1380
/*                                                                 */STRG1390
        ANS(6)=SQRT(ANS(4)),.                                     STRG1400
        RD   =NZ,.                                                STRG1410
        RE   =ONM-RD,.                                            STRG1420
        RE   =(ANS(5)-ANS(3))/RE,.                                STRG1430
        ANS(7)=(ANS(3)/RD)/RE,.                                   STRG1440
        ANS(8)=SQRT(RE),.                                         STRG1450
/*                                                                 */STRG1460
/*      DIVIDE BY THE PIVOTAL ELEMENT                              */STRG1470
/*                                                                 */STRG1480
        RD   =D(NEW,NEW),.                                        STRG1490
             DO J = 1 TO M,.                                      STRG1500
             IF LL(J) LT 0                                        STRG1510
             THEN GO TO S40,.                                     STRG1520
             ELSE IF LL(J) GT 0                                   STRG1530
             THEN GO TO S30,.                                     STRG1540
             IF J = NEW                                           STRG1550
             THEN DO,.                                            STRG1560
                  D(NEW,NEW)=1/RD,.                               STRG1570
                  GO TO S40,.                                     STRG1580
                  END,.                                           STRG1590
             D(J,J)=D(J,J)+D(NEW,J)**2/RD,.                       STRG1600
S30..                                                             STRG1610
             D(NEW,J)=D(NEW,J)/RD,.                               STRG1620
S40..                                                             STRG1630
             END,.                                                STRG1640
/*                                                                 */STRG1650
/*      COMPUTE REGRESSION COEFFICIENTS                            */STRG1660
/*                                                                 */STRG1670
        B(NZ)=D(NEW,MY),.                                         STRG1680
        IF NZ GT 1                                                STRG1690
        THEN DO,.                                                 STRG1700
             ID   =NZ-1,.                                         STRG1710
                  DO J = 1 TO ID,.                                STRG1720
                  IJ   =NZ-J,.                                    STRG1730
                  KK   =L(IJ),.                                   STRG1740
                  B(IJ)=D(KK,MY),.                                STRG1750
                       DO K = 1 TO J,.                            STRG1760
                       IK   =NZ-K+1,.                             STRG1770
                       MK   =L(IK),.                              STRG1780
                       B(IJ)=B(IJ)-D(KK,MK)*B(IK),.               STRG1790
                       END,.                                      STRG1800
                  END,.                                           STRG1810
             END,.                                                STRG1820
        ANS(9)=XBAR(MY),.           /* COMPUTE INTERCEPT          */STRG1830
             DO I = 1 TO NZ,.                                     STRG1840
             KK   =L(I),.                                         STRG1850
             ANS(9)=ANS(9)-B(I)*XBAR(KK),.                        STRG1860
             S(I) =ANS(8)*SQRT(D(KK,KK)),.                        STRG1870
             T(I) =B(I)/S(I),.                                    STRG1880
             BETA(I)=B(I)*STD(KK)/STD(MY),.                       STRG1890
             END,.                                                STRG1900
/*                                                                 */STRG1910
/*      PERFORM A REDUCTION TO ELIMINATE THE LAST VARIABLE ENTERED */STRG1920
/*                                                                 */STRG1930
             DO I = 1 TO M,.                                      STRG1940
             IF LL(I) GT 0                                        STRG1950
             THEN DO,.                                            STRG1960
                       DO J = 1 TO M,.                            STRG1970
                       IF LL(J) GE 0                              STRG1980
                       THEN DO,.                                  STRG1990
                            IF J NE NEW                           STRG2000
                            THEN D(I,J)=D(I,J)-D(I,NEW)*D(NEW,J),. STRG2010
                            END,.                                 STRG2020
                       END,.                                      STRG2030
                  D(I,NEW)=D(I,NEW)/(-RD),.                       STRG2040
                  END,.                                           STRG2050
             END,.                                                STRG2060
/*                                                                 */STRG2070
/*      ADJUST STANDARD ERROR OF THE ESTIMATE AND MULTIPLE         */STRG2080
/*      CORRELATION COEFFICIENT                                    */STRG2090
/*                                                                 */STRG2100
        RD   =N-NSTEP(4),.                                        STRG2110
        RD   =ONM/RD,.                                            STRG2120
        ANS(10)=SQRT(1-(1-ANS(6)**2)*RD),.                        STRG2130
        ANS(11)=ANS(8)*SQRT(RD),.                                 STRG2140
        CALL SOUT (NSTEP,ANS,L,B,S,T,BETA),.                      STRG2150
/*                                                                 */STRG2160
/*      TEST WHETHER THE STEP-WISE REGRESSION WAS TERMINATED       */STRG2170
/*      IN PROCEDURE SOUT.                                         */STRG2180
/*                                                                 */STRG2190
        IF NSTOP GT '0'                                           STRG2200
        THEN GO TO S150,.                                         STRG2210
        END,.                                                     STRG2220
S150..                                                            STRG2230
   RETURN,.                                                       STRG2240
   END,.                            /*END OF PROCEDURE STRG      */STRG2250
```

Purpose:

STRG performs a stepwise multiple linear regression analysis for a dependent variable and a set of independent variables.

Usage:

CALL STRG (M, N, D, XBAR, IDX, PCT, NSTEP, ANS, L, B, STD);

Description of parameters:

M - BINARY FIXED
Given total number of variables in data matrix.

N - BINARY FIXED
Given number of observations.

D(M, M) - BINARY FLOAT [(53)]
Given matrix of sums of cross-products of deviations from mean. This matrix will be destroyed.

XBAR(M) - BINARY FLOAT [(53)]
Given vector containing the means.

IDX(M) - BINARY FIXED
Given vector containing the following codes:
0 - independent variable available for selection.
1 - independent variable to be forced into the regression equation.
2 - variable not to be considered in the regression equation.
3 - dependent variable.
This input vector is destroyed.

PCT - BINARY FLOAT
Given constant value indicating the proportion of the total variance to be explained by any independent variable. Those independent variables that fall below this proportion will not enter the regression equation. To ensure that all variables enter the regression equation, set PCT=0.0.

NSTEP(5) - BINARY FIXED
Resultant vector containing the following information:

NSTEP(1) - number of the dependent variable.
NSTEP(2) - number of variables forced into the regression equation.
NSTEP(3) - number of variables deleted from the regression equation.
NSTEP(4) - the number of the last step.
NSTEP(5) - the number of the last variable entered.

ANS(11) - BINARY FLOAT [(53)]
Resultant vector containing the following information for the last step:

ANS(1) - Sum of squares reduced by this step
ANS(2) - Proportion of total sum of squares reduced
ANS(3) - Cumulative sum of squares reduced, up to this step
ANS(4) - Cumulative proportion of total sum of squares reduced
ANS(5) - Sum of squares of the dependent variable
ANS(6) - Multiple correlation coefficients
ANS(7) - F ratio for sum of squares due to regression
ANS(8) - Standard error of the estimate (residual mean square)
ANS(9) - Intercept constant
ANS(10) - Multiple correlation coefficient adjusted for degrees of freedom

L(K) - BINARY FIXED
Resultant vector containing the independent variables entered in the regression.
K is the number of independent variables in the regression equation.

B(K) - BINARY FLOAT [(53)]
Resultant vector containing the partial regression coefficients corresponding to the variables in vector L.

STD(M) - BINARY FLOAT [(53)]
Given vector containing the standard deviations.

Remarks:

There must be one, and only one, dependent variable and at least one independent variable.

The number of data points must be greater than the number of independent variables plus one. Forced variables are entered into the regression equation before all other independent variables. Within the set of forced variables, the one to be chosen first will be the one that explains the greater amount of variance.

Instead of using, as a stopping criterion, a proportion of the total variance, some other criterion may be added to the output routine.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of variables M not greater than 1, or N not greater than M+1.

ERROR=2 - reduced sum of squares exceeds total sum of squares.
ERROR=3 - degrees of freedom is zero, for the variable that is currently active.
ERROR=4 - specified constant, PCT, is greater than or equal to one.

Subroutines and function subroutines required: SOUT, a special output routine that must be provided by the user. The routine prints out the results of the stepwise regression. An example of such a routine may be found in the sample program STEP.

Method:

The abbreviated Doolittle method is used to (1) select variables entering the regression and (2) compute regression coefficients. Refer to C. A. Bennet and N. L. Franklin, Statistical Analysis in Chemistry and the Chemical Industry, John Wiley and Sons, 1954, Appendix 6A.

Mathematical Background:

This subroutine performs a stepwise multiple regression analysis for a dependent variable and a set of independent variables. In each step of the regression i=1,2,...,q, where q is the number of independent variables, the abbreviated Doolittle method is used to calculate the following statistics:

The independent variable entering in the regression is selected, first, by computing the amount of reduction of sum of squares for each variable:

$$C_j = \frac{a_{jy}^2}{a_{jj}} \qquad (1)$$

where:

a_{jj} is initially an element in the sums of cross-products of deviations matrix which will be modified in successive steps.
j = 1,2,..., q are independent variables ($j \neq$ variables deleted and variables entered before the i-th step)
y = dependent variable

and, second, by finding the largest value of C_j.

Set $S_i = C_j$ to indicate the sum of squares that will be reduced in the i-th step.

The proportion of S_i to the total is obtained by:

$$P = \frac{S_i}{D} \qquad (2)$$

where:

$$D = \sum_{j=1}^{n} (y_j - \bar{y})^2$$

(n = number of observations)

If p is less than the constant specified by the user to limit independent variables, the analysis will be terminated without entering the last variable selected; otherwise, the following calculations are continued:

The cumulative sum of squares reduced is obtained by

$$S_{cum} = S_{cum} + S_i \qquad (3)$$

and the cumulative proportion reduced by

$$P_{cum} = P_{cum} + p \qquad (4)$$

The multiple correlation coefficient is computed by

$$R = \sqrt{P_{cum}} \qquad (5)$$

and adjusted for degrees of freedom by

$$R_c = \sqrt{1-(1-R^2)\ (n-1)\ /\ (n-k)}$$

where there are k independent variables in the regression.

The F value for analysis of variance is given by

$$F = \frac{S_{cum} / k}{(D-S_{cum}) / (n-k-1)} \qquad (6)$$

The standard error of the estimated y is obtained by the use of the formula

$$s_{y.12...i} = \sqrt{\frac{D - S_{cum}}{n - k - 1}} \qquad (7)$$

and adjusted by

$$s_c = s\ \sqrt{(n-1)\ /\ (n-k)}$$

Then the following is computed:

$$a_{jj} = a_{jj} + \frac{a_{ij}^2}{a_{ii}} \qquad (8)$$

where:

i = variable entered in the i-th step

j = $v_1, v_2, \ldots, v_{i-1}$ are the variables entered in the regression before the i-th step, and

$$g_{ik} = \frac{a_{ik}}{a_{ii}} \tag{9}$$

where k = 1,2,...,m are variables including y ($k \neq$ variables deleted or the variable entered in the i-th step).

Regression coefficients are computed by

$$b_i = g_{iy}$$

$$b_{i-1} = g_{(i-1)y} - b_i\, g_{(i-1)\,i} \tag{10}$$

$$b_{i-2} = g_{(i-2)y} - b_i g_{(i-2)\,i} - b_{i-1} g_{(i-2)\,(i-1)}$$

etc.

and the value of the intercept as

$$b_0 = \bar{y} - \sum_{j=1}^{k} b_j \bar{x}_j \tag{11}$$

where k = number of independent variables in the regression.

Standardized regression coefficients, beta weights

$$B_j = b_j \cdot \frac{S_j}{S_y} \tag{12}$$

where S_j and S_y are standard deviations.

Standard errors of regression coefficients are given by

$$s_{b_j} = \sqrt{a_{jj}} \cdot s_{y.12\ldots i} \tag{13}$$

where $j = v_1, v_2, \ldots, v_i$ are variables in the regression and t-values as

$$t_j = \frac{b_j}{s_{b_j}} \tag{14}$$

Perform the reduction to eliminate the variable entered in i-th step:

$$a_{jk} = a_{jk} - a_{ji} g_{ik} \tag{15}$$

where:

i = variable entered in i-th step

j = 1, 2, ..., m ($j \neq$ variables deleted and variables in the regression)

k = 1, 2, ..., m ($k \neq$ variables deleted or the variable entered in i-th step)

$$a_{ji} = a_{ji} / -a_{ii} \tag{16}$$

$$a_{ii} = 1 / a_{ii} \tag{17}$$

Programming Considerations:

If the user provides the routine SOUT, the argument list must be consistent with the argument list of the call statement in subroutine STRG.

A description of the parameters follows:

NSTEP(5), ANS(11) - L(K), B(K)	These parameters are the same as in STRG. When used in SOUT, however, they appear as input.
S(M) -	BINARY FLOAT [(53)] Given vector containing standard error of regression.
T(M) -	BINARY FLOAT [(53)] Given computed T value.
BETA(M) -	BINARY FLOAT [(53)] Given beta coefficient.

- Subroutine CANC

```
CANC..                                                                  CANC  10
/*************************************************************************/CANC  20
/*                                                                       */CANC  30
/*      TO COMPUTE THE CANONICAL CORRELATIONS BETWEEN TWO SETS OF        */CANC  40
/*      VARIABLES.                                                       */CANC  50
/*                                                                       */CANC  60
/*************************************************************************/CANC  70
   PROCEDURE (N,MP,MQ,RR,ROOTS,WLAM,CANR,CHISQ,NDF,COEFR,COEFL),.       CANC  80
   DECLARE                                                              CANC  90
         ERROR EXTERNAL CHARACTER (1),                                  CANC 100
         (NDF(*),I,J,K,L,M,MP,MQ,N,N1,IERR)                             CANC 110
         FIXED BINARY,                                                  CANC 120
         (RR(*,*),ROOTS(*),WLAM(*),CANR(*),CHISQ(*),COEFR(*,*),         CANC 130
         COEFL(*,*),DET,BAT,CON)                                        CANC 140
         BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/CANC 150
 /*      BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/CANC 160
/*                                                                       */CANC 170
/*      CHECK WHETHER THE NUMBER OF LEFT-HAND VARIABLES IS EQUAL TO      */CANC 180
/*      OR GREATER THAN THAT OF RIGHT-HAND                               */CANC 190
/*                                                                       */CANC 200
   ERROR='0',.                                                          CANC 210
   IERR =0,.                                                            CANC 220
   IF MP LE 0 OR MQ LE 0       /* THERE ARE NO RIGHT OR LEFT            */CANC 230
   THEN DO,.                   /* HAND VARIABLES.                       */CANC 240
         ERROR='1',.                                                    CANC 250
         GO TO FIN,.                                                    CANC 260
         END,.                                                          CANC 270
   IF MP LT MQ                                                          CANC 280
   THEN DO,.                                                            CANC 290
         M    =MP,.                                                     CANC 300
         MP   =MQ,.                                                     CANC 310
         MQ   =M,.                                                      CANC 320
         ERROR='2',.                                                    CANC 330
         END,.                                                          CANC 340
COPY..                                                                  CANC 350
   BEGIN,.                                                              CANC 360
   DECLARE                                                              CANC 370
         (R(MP,MP),T(MP,MQ),A(MQ,MQ),X(MQ,MQ))                         CANC 380
         BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/CANC 390
 /*      BINARY FLOAT(53),.          /*DOUBLE PRECISION VERSION  /*D*/CANC 400
/*                                                                       */CANC 410
/*      PARTITION INTERCORRELATIONS AMONG LEFT HAND VARIABLES,BETWEEN*/CANC 420
/*      LEFT AND RIGHT HAND VARIABLES, AND AMONG RIGHT HAND VARIABLES*/CANC 430
/*                                                                       */CANC 440
   M    =MP+MQ,.                                                        CANC 450
   FM   =M+1,.                                                          CANC 460
   FN   =N,.                                                            CANC 470
   IF ERROR= '2'                                                        CANC 480
   THEN DO,.                                                            CANC 490
         IERR =1,.                                                      CANC 500
         K    =0,.                   /* CHANGE LEFT AND RIGHT HAND    */CANC 510
              DO I = MQ+1 TO M,.      /* VARIABLES                     */CANC 520
              K    =K+1,.                                               CANC 530
              L    =0,.                                                 CANC 540
                   DO J = MQ+1 TO M,.                                   CANC 550
                   L    =L+1,.                                          CANC 560
                                      /* RR 22 INTO R                  */CANC 570
              R(K,L)=RR(I,J),.                                          CANC 580
                   END,.                                                CANC 590
                                      /* RR 21 INTO COEFL              */CANC 600
                   DO J = 1 TO MQ,.                                     CANC 610
                   COEFL(K,J)=RR(I,J),.                                 CANC 620
                   END,.                                                CANC 630
              END,.                                                     CANC 640
              DO I = 1 TO MQ,.                                          CANC 650
                   DO J = 1 TO MQ,.                                     CANC 660
                                      /* RR 11 INTO COEFR              */CANC 670
                  COEFR(I,J)=RR(I,J),.                                  CANC 680
                   END,.                                                CANC 690
              END,.                                                     CANC 700
         END,.                                                          CANC 710
   ELSE DO,.                                                            CANC 720
              DO I = 1 TO M,.                                           CANC 730
                   DO J = 1 TO M,.                                      CANC 740
                   IF I LE MP AND J LE MP                               CANC 750
                   THEN DO,.                                            CANC 760
                                      /* RR 11 INTO R                  */CANC 770
                        R(I,J)=RR(I,J),.                                CANC 780
                        GO TO S10,.                                     CANC 790
                        END,.                                           CANC 800
                   IF I LE MP AND J GT MP                               CANC 810
                   THEN DO,.                                            CANC 820
                        K    =J-MP,.                                    CANC 830
                                      /* RR 12 INTO COEFL              */CANC 840
                        COEFL(I,K)=RR(I,J),.                            CANC 850
                        GO TO S10,.                                     CANC 860
                        END,.                                           CANC 870
                   IF I GT MP AND J GT MP                               CANC 880
                   THEN DO,.                                            CANC 890
                        L    =I-MP,.                                    CANC 900
                        K    =J-MP,.                                    CANC 910
                                      /* RR 22 INTO COEFR              */CANC 920
                        COEFR(L,K)=RR(I,J),.                            CANC 930
                        END,.                                           CANC 940
S10..                                                                   CANC 950
                   END,.                                                CANC 960
              END,.                                                     CANC 970
/*                                                                       */CANC 980
/*      SOLVE THE CANONICAL EQUATION                                     */CANC 990
/*                                                                       */CANC1000
         CON  =0,.                                                      CANC1010
         CALL MINV (R,MP,DET,CON),.                                     CANC1020
         IF ERROR NE '0'                                                CANC1030
         THEN DO,.                                                      CANC1040
              ERROR='3',.                                               CANC1050
              GO TO FIN,.                                               CANC1060
              END,.                                                     CANC1070
/*                                                                       */CANC1080
/*      CALCULATE T = INVERSE OF RR 11 * RR 12                           */CANC1090
/*                                                                       */CANC1100
              DO I = 1 TO MP,.                                          CANC1110
                   DO J = 1 TO MQ,.                                     CANC1120
                   T(I,J)=0.0,.                                         CANC1130
                        DO K = 1 TO MP,.                                CANC1140
                        T(I,J)=T(I,J)+R(I,K)*COEFL(K,J),.               CANC1150
                        END,.                                           CANC1160
                   END,.                                                CANC1170
              END,.                                                     CANC1180
/*                                                                       */CANC1190
/*      CALCULATE  A = RR 21 * T                                         */CANC1200
/*                                                                       */CANC1210
```

```
              DO I = 1 TO MQ,.                                          CANC1220
                   DO J = 1 TO MQ,.                                     CANC1230
                   A(I,J)=0.0,.                                         CANC1240
                        DO K = 1 TO MP,.                                CANC1250
                        A(I,J)=A(I,J)+COEFL(K,I)*T(K,J),.               CANC1260
                        END,.                                           CANC1270
                   END,.                                                CANC1280
              END,.                                                     CANC1290
/*                                                                       */CANC1300
/*      CALCULATE EIGENVALUES WITH ASSOCIATED EIGENVECTORS OF THE        */CANC1310
/*      INVERSE OF R 22 * A                                              */CANC1320
/*                                                                       */CANC1330
         CALL MSDU (MQ,A,COEFR,ROOTS,X),.                               CANC1340
         IF ERROR NE '0'                                                CANC1350
         THEN DO,.                                                      CANC1360
              ERROR='4',.               /* ERROR CONDITION IN ROUTINE  */CANC1370
              GO TO FIN,.               /* MSDU.                       */CANC1380
              END,.                                                     CANC1390
         IF IERR= '1'                                                   CANC1400
         THEN ERROR='2',.                                               CANC1410
/*                                                                       */CANC1420
/*      TEST WHETHER EIGENVALUES ARE GREATER THAN 0.0 BUT LESS THAN      */CANC1430
/*      1.0                                                              */CANC1440
/*                                                                       */CANC1450
              DO I = 1 TO MQ,.                                          CANC1460
              IF ROOTS(I) LE 0.0 OR ROOTS(I) GE 1.0                     CANC1470
              THEN DO,.                                                 CANC1480
                   ERROR='5',.          /* CANONICAL CORRELATION CANNOT*/CANC1490
                   GO TO FIN,.          /* BE COMPUTED                 */CANC1500
                   END,.                                                CANC1510
              END,.                                                     CANC1520
/*                                                                       */CANC1530
/*      FOR EACH VALUE OF I = 1,2,...,MQ CALCULATE THE STATISTICS        */CANC1540
/*      NOTED BELOW.                                                     */CANC1550
/*                                                                       */CANC1560
              DO I = 1 TO MQ,.                                          CANC1570
                                      /* CANONICAL CORRELATION         */CANC1580
              CANR(I)=SQRT(ROOTS(I)),.                                  CANC1590
              WLAM(I)=1.0,.                                             CANC1600
                   DO J = I TO MQ,.                                     CANC1610
                   WLAM(I)=WLAM(I)*(1.0-ROOTS(J)),.                     CANC1620
                   END,.                                                CANC1630
              BAT  =WLAM(I),.           /* CHI-SQUARE                  */CANC1640
              CHISQ(I)=-(FN-0.5*FM)*LOG(BAT),.                          CANC1650
/*                                                                       */CANC1660
/*      CALCULATE DEGREES OF FREEDOM FOR CHI-SQUARE                      */CANC1670
/*                                                                       */CANC1680
              N1  =I-1,.                                                CANC1690
              NDF(I)=(MP-N1)*(MQ-N1),.                                  CANC1700
/*                                                                       */CANC1710
/*      I-TH SET OF RIGHT HAND COEFICIENTS                               */CANC1720
/*                                                                       */CANC1730
                   DO J = 1 TO MQ,.                                     CANC1740
                   COEFR(J,I)=X(J,I),.                                  CANC1750
                   END,.                                                CANC1760
/*                                                                       */CANC1770
/*      I-TH SET OF LEFT HAND COEFFICIENTS                               */CANC1780
/*                                                                       */CANC1790
                   DO J = 1 TO MP,.                                     CANC1800
                   DET  =0.0,.                                          CANC1810
                        DO K = 1 TO MQ,.                                CANC1820
                        DET  =DET+T(J,K)*COEFR(K,I),.                   CANC1830
                        END,.                                           CANC1840
                   COEFL(J,I)=DET/CANR(I),.                             CANC1850
                   END,.                                                CANC1860
              END,.                                                     CANC1870
         END,.                                                          CANC1880
   END,.                                                                CANC1890
FIN..                                                                   CANC1900
   RETURN,.                                                             CANC1910
   END,.                            /*END OF PROCEDURE CANC            */CANC1920
```

Purpose:

CANC computes the canonical correlations between two sets of variables. It is normally preceded by a call to procedure CORR.

Usage:

CALL CANC (N, MP, MQ, RR, ROOTS, WLAM, CANR, CHISQ, NDF, COEFR, COEFL);

Description of parameters:

N - BINARY FIXED
Given number of observations.

MP - BINARY FIXED
Given number of left hand variables.

MQ - BINARY FIXED
Given number of right hand variables.

RR(M, M) - BINARY FLOAT [(53)]
Given matrix (where M=MP+MQ), containing correlation coefficients.

ROOTS(MQ) - BINARY FLOAT [(53)]
Resultant vector containing eigenvalues computed in the subroutine MGDU.

WLAM(MQ) - BINARY FLOAT [(53)]
Resultant vector of length MQ containing lambda.

CANR(MQ) - BINARY FLOAT [(53)]
Resultant vector containing canonical correlations.

CHISQ(MQ) - BINARY FLOAT [(53)]
Resultant vector containing the values of chi-squares.

NDF - BINARY FIXED
Resultant variable containing the number of degrees of freedom.

COEFR - (MQ, MQ) BINARY FLOAT [(53)]
Resultant matrix containing MQ sets of right-hand coefficients columnwise.

COEFL - (MP, MQ) BINARY FLOAT [(53)]
Resultant matrix containing MQ sets of left-hand coefficients columnwise.

Remarks:

The number of left-hand variables (MP) should be greater than or equal to the number of right-hand variables (MQ). If the value of MP is less than the value of MQ, the input matrix is rearranged to satisfy the above conditions. The right-hand variables become left-hand variables and left-hand variables become right-hand variables. If this condition exists, the error code indicator, ERROR, is set to 2.

Also, if the variables are changed, the values of MP and MQ are interchanged.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - no right-hand or left-hand variable -- returned values are meaningless.

ERROR=2 - number of left-hand variables smaller than the number of right-hand variables.

ERROR=3 - correlation coefficient matrix ill-conditioned (determined by MINV).

ERROR=4 - error condition in routine MGDU, from MSDU.

ERROR=5 - Eigenvalues less than or equal to zero or greater than or equal to one.

Subroutines and function subroutines required:

MINV
MGDU (which, in turn, calls the subroutine MSDU)

Method:

Refer to W.W. Cooley and P.R. Lohnes Multivariate Procedures for the Behavioral Sciences, John Wiley and Sons, 1962, Chapter 3.

Mathematical Background:

This subroutine performs a canonical correlation analysis between two sets of variables.

The matrix of intercorrelations, R, is partitioned into four submatrices:

$$R = \left[\begin{array}{c|c} R_{11} & R_{12} \\ \hline R_{21} & R_{22} \end{array}\right] \quad (1)$$

R_{11} = intercorrelations among p variables in the first set (that is, left-hand variables)

R_{12} = intercorrelations between the variables in the first and second sets

R_{21} = the transpose of R_{12}

R_{22} = intercorrelations among q variables in the second set (that is, right-hand variables)

The equation:

$$\left| R_{22}^{-1} R_{21} R_{11}^{-1} R_{12} - \lambda I \right| = 0 \quad (2)$$

is then solved for all values of λ, eigenvalues in the following matrix operation:

$$T = R_{11}^{-1} R_{12} \quad (3)$$

$$A = R_{21} T \quad (4)$$

The subroutine MGDU calculates eigenvalues (λ_i), with associated eigenvectors, of $R_{22}^{-1} A$, where i = 1, 2, ..., q.

For each subscript i = 1, 2, ..., q, the following statistics are calculated:

Canonical correlation:

$$CANR = \sqrt{\lambda_i} \quad (5)$$

where λ_i = i-th eigenvalue

Chi-square:

$$\chi^2 = -\left[n - 0.5\,(p + q + 1)\right] \log_e \Lambda \qquad (6)$$

where n = number of observations

$$\Lambda = \prod_{j=i}^{q} (1 - \lambda_j)$$

Degrees of freedom for χ^2:

$$DF = \left[p - (i - 1)\right] \left[q - (i - 1)\right] \qquad (7)$$

i-th set of right-hand coefficients:

$$b_k = v_{ki} \qquad (8)$$

where v_{ki} = eigenvector associated with λ_i

$k = 1, 2, \ldots, q$

i-th set of left-hand coefficients:

$$a_j = \frac{\sum_{k=1}^{q} t_{jk}\, b_k}{CANR} \qquad (9)$$

where $\left\{t_{jk}\right\} = T = R_{11}^{-1} R_{12}$

$j = 1, 2, \ldots, p$

Analysis of Variance

- Subroutine AVAR

```
AVAR..                                                                  AVAR  10
/*********************************************************************/AVAR  20
/*                                                                   */AVAR  30
/*      TO PERFORM AN ANALYSIS OF VARIANCE FOR A COMPLETE FACTORIAL  */AVAR  40
/*      DESIGN.                                                      */AVAR  50
/*                                                                   */AVAR  60
/*********************************************************************/AVAR  70
   PROCEDURE (K,LEVEL,N,X,GMEAN,SUMSQ,NDF,SMEAN),.                     AVAR  80
   DECLARE                                                           AVAR  90
        ERROR EXTERNAL CHARACTER(1),                                 AVAR 100
        (LEVEL(*),NDF(*),KOUNT(K),ISTEP(K),LASTS(K),I,INCRE,J,K,L,LAST,AVAR 110
        LL,N,N1,ND1,ND2,NN,NSIZ)                                     AVAR 120
        FIXED BINARY,                                                AVAR 130
        (X(*),SUMSQ(*),SMEAN(*),FSUM,GMEAN,FN,FN1,FN2)               AVAR 140
        BINARY FLOAT,.                  /*SINGLE PRECISION VERSION  /*S*/AVAR 150
/*      BINARY FLOAT (53),.             /*DOUBLE PRECISION VERSION  /*D*/AVAR 160
   ERROR='0',.                                                       AVAR 170
   NSIZ =(2**K)-1,.                                                  AVAR 180
   IF N LE 0                       /* THERE ARE NO DATA POINTS     */AVAR 190
   THEN DO,.                                                         AVAR 200
        ERROR='1',.                                                  AVAR 210
        GO TO FIN,.                                                  AVAR 220
        END,.                                                        AVAR 230
   FN   =N,.                                                         AVAR 240
   IF K LT 2                                                         AVAR 250
   THEN DO,.                                                         AVAR 260
        ERROR='2',.                 /* ONE OR LESS FACTORS          */AVAR 270
        GO TO FIN,.                                                  AVAR 280
        END,.                                                        AVAR 290
        DO I = 1 TO K,.                                              AVAR 300
        IF LEVEL(I) LT 2                                             AVAR 310
        THEN DO,.                                                    AVAR 320
             ERROR='3',.            /* 1 OR MORE LEVELS LESS THEN 2*/AVAR 330
             GO TO FIN,.                                             AVAR 340
             END,.                                                   AVAR 350
        END,.                                                        AVAR 360
/*                                                                   */AVAR 370
/*      CALCULATE MULTIPLIERS TO BE USED IN FINDING STORAGE LOCATIONS*/AVAR 380
/*      FOR INPUT DATA.                                              */AVAR 390
/*                                                                   */AVAR 400
   ISTEP(1)=1,.                                                      AVAR 410
        DO I = 2 TO K,.                                              AVAR 420
        ISTEP(I)=ISTEP(I-1)*(LEVEL(I-1)+1),.                         AVAR 430
        END,.                                                        AVAR 440
        DO I = 1 TO K,.             /* SET LEVEL COUNTER            */AVAR 450
        KOUNT(I)=LEVEL(I),.                                          AVAR 460
        END,.                                                        AVAR 470
   N1   =N,.                                                         AVAR 480
        DO I = 1 TO N,.             /* PLACE DATA IN PROPER PLACE   */AVAR 490
        L    =KOUNT(1),.                                             AVAR 500
             DO J = 2 TO K,.                                         AVAR 510
             L    =L+ISTEP(J)*(KOUNT(J)-1),.                         AVAR 520
             END,.                                                   AVAR 530
        X(L) =X(N1),.                                                AVAR 540
        N1   =N1-1,.                                                 AVAR 550
             DO J = 1 TO K,.                                         AVAR 560
             IF KOUNT(J) GT 1                                        AVAR 570
             THEN DO,.                                               AVAR 580
                  KOUNT(J)=KOUNT(J)-1,.                              AVAR 590
                  GO TO S10,.                                        AVAR 600
                  END,.                                              AVAR 610
             KOUNT(J)=LEVEL(J),.                                     AVAR 620
             END,.                                                   AVAR 630
S10..                                                                AVAR 640
        END,.                                                        AVAR 650
   L    =LEVEL(1),.                 /* CALCULATE LAST DATA POSITION*/AVAR 660
        DO J = 2 TO K,.                                              AVAR 670
        L    =L+ISTEP(J)*(LEVEL(J)-1),.                              AVAR 680
        END,.                                                        AVAR 690
/*                                                                   */AVAR 700
/*      CALCULATE THE LAST DATA POSITION OF EACH FACTOR              */AVAR 710
/*                                                                   */AVAR 720
   LASTS(1)=L+1,.                                                    AVAR 730
        DO I = 2 TO K,.                                              AVAR 740
        LASTS(I)=LASTS(I-1)+ISTEP(I),.                               AVAR 750
        END,.                                                        AVAR 760
        DO I = 1 TO K,.             /* PERFORM OPERATOR CALCULUS    */AVAR 770
        L    =1,.                                                    AVAR 780
        LL   =1,.                                                    AVAR 790
        FSUM =0.0,.                                                  AVAR 800
        NN   =LEVEL(I),.                                             AVAR 810
        INCRE=ISTEP(I),.                                             AVAR 820
        LAST =LASTS(I),.                                             AVAR 830
S20..                                                                AVAR 840
             DO J = 1 TO NN,.       /* SIGMA OPERATION              */AVAR 850
             FSUM =FSUM+X(L),.                                       AVAR 860
             L    =L+INCRE,.                                         AVAR 870
             END,.                                                   AVAR 880
        X(L) =FSUM,.                                                 AVAR 890
        FN1  =NN,.                                                   AVAR 900
             DO J = 1 TO NN,.       /* DELTA OPERATION              */AVAR 910
             X(LL)=FN1*X(LL)-FSUM,.                                  AVAR 920
             LL   =LL+INCRE,.                                        AVAR 930
             END,.                                                   AVAR 940
        FSUM =0.0,.                                                  AVAR 950
        IF L LT LAST                                                 AVAR 960
        THEN DO,.                                                    AVAR 970
             IF L LE LAST-INCRE                                      AVAR 980
             THEN DO,.                                               AVAR 990
                  L    =L+INCRE,.                                    AVAR1000
                  LL   =LL+INCRE,.                                   AVAR1010
                  GO TO S20,.                                        AVAR1020
                  END,.                                              AVAR1030
             L    =L+INCRE+1-LAST,.                                  AVAR1040
             LL   =LL+INCRE+1-LAST,.                                 AVAR1050
             GO TO S20,.                                             AVAR1060
             END,.                                                   AVAR1070
        END,.                                                        AVAR1080
        DO I = 1 TO NSIZ,.                                           AVAR1090
        SUMSQ=0.0,.                                                  AVAR1100
        END,.                                                        AVAR1110
/*                                                                   */AVAR1120
/*      SET UP CONTROL FOR MEAN SQUARE OPERATOR                      */AVAR1130
/*                                                                   */AVAR1140
   LASTS(1)=LEVEL(1),.                                               AVAR1150
   ISTEP(1)=1,.                                                      AVAR1160
        DO I = 2 TO K,.                                              AVAR1170
        LASTS(I)=LEVEL(I)+1,.                                        AVAR1180
```

```
      ISTEP(I)=ISTEP(I-1)*2,.                                    AVAR1190
      END,.                                                      AVAR1200
   NN =1,.                                                       AVAR1210
      DO I = 1 TO K,.                                            AVAR1220
      KOUNT(I)=0.0,.                                             AVAR1230
      END,.                                                      AVAR1240
S30..                                                            AVAR1250
   L  =0,.                                                       AVAR1260
      DO I = 1 TO K,.                                            AVAR1270
      IF KOUNT(I) NE LASTS(I)                                    AVAR1280
      THEN DO,.                                                  AVAR1290
           IF L LE 0                                             AVAR1300
           THEN DO,.                                             AVAR1310
                KOUNT(I)=KOUNT(I)+1,.                            AVAR1320
                IF KOUNT(I) LE LEVEL(I)                          AVAR1330
                THEN GO TO S40,.                                 AVAR1340
                GO TO S50,.                                      AVAR1350
                END,.                                            AVAR1360
           IF KOUNT(I)= LEVEL(I)                                 AVAR1370
           THEN GO TO S60,.                                      AVAR1380
S40..                                                            AVAR1390
           L    =L+ISTEP(I),.                                    AVAR1400
           GO TO S60,.                                           AVAR1410
           END,.                                                 AVAR1420
S50..                                                            AVAR1430
      KOUNT(I)=0,.                                               AVAR1440
S60..                                                            AVAR1450
      END,.                                                      AVAR1460
   IF L GT 0                                                     AVAR1470
   THEN DO,.                                                     AVAR1480
      SUMSQ(L)=SUMSQ(L)+X(NN)*X(NN),.                            AVAR1490
      NN   =NN+1,.                                               AVAR1500
      GO TO S30,.                                                AVAR1510
      END,.                                                      AVAR1520
   GMEAN=X(NN)/FN,.                  /* CALCULATE MEAN          */AVAR1530
/*                                                               */AVAR1540
/*    CALCULATE FIRST DIVISOR REQUIRED TO FORM SUM OF SQUARES AND */AVAR1550
/*    DIVISOR. WHICH IS EQUAL TO DEGREES OF FREEDOM, REQUIRED TO  */AVAR1560
/*    FORM MEAN SQUARES                                          */AVAR1570
/*                                                               */AVAR1580
   ISTEP=0,.                                                     AVAR1590
   ISTEP(1)=1,.                                                  AVAR1600
   NN   =0,.                                                     AVAR1610
S70..                                                            AVAR1620
   ND1  =1,.                                                     AVAR1630
   ND2  =1,.                                                     AVAR1640
      DO I = 1 TO K,.                                            AVAR1650
      IF ISTEP(I) NE 0                                           AVAR1660
      THEN DO,.                                                  AVAR1670
           ND1  =ND1*LEVEL(I),.                                  AVAR1680
           ND2  =ND2*(LEVEL(I)-1),.                              AVAR1690
           END,.                                                 AVAR1700
      END,.                                                      AVAR1710
   FN1  =N*ND1,.                                                 AVAR1720
   FN2  =ND2,.                                                   AVAR1730
   NN   =NN+1,.                                                  AVAR1740
   SUMSQ(NN)=SUMSQ(NN)/FN1,.                                     AVAR1750
   SMEAN(NN)=SUMSQ(NN)/FN2,.                                     AVAR1760
   NDF(NN)=ND2,.                                                 AVAR1770
   IF NN LT LL                                                   AVAR1780
   THEN DO,.                                                     AVAR1790
           DO I = 1 TO K,.                                       AVAR1800
           IF ISTEP(I) NE 0                                      AVAR1810
           THEN ISTEP(I)=0,.                                     AVAR1820
           ELSE DO,.                                             AVAR1830
                ISTEP(I)=1,.                                     AVAR1840
                GO TO S70,.                                      AVAR1850
                END,.                                            AVAR1860
           END,.                                                 AVAR1870
      END,.                                                      AVAR1880
FIN..                                                            AVAR1890
   RETURN,.                                                      AVAR1900
   END,.                             /*END OF PROCEDURE AVAR     */AVAR1910
```

Purpose:

AVAR performs an analysis of variance for a complete factorial design.

Usage:

CALL AVAR (K, LEVEL, N, X, GMEAN, SUMSQ, NDF, SMEAN);

Description of parameters:

K - BINARY FIXED
Given number of variables (factors).

LEVEL (K) - BINARY FIXED
Given vector, the i-th element being the number of levels for the i-th factor ($LEVEL_i$).

N - BINARY FIXED
Given total number of data points read in (N = [2 **K] -1).

X - BINARY FLOAT[(53)]
Given vector of length

$$\prod_{i=i}^{K} (LEVEL_i + 1)$$

with data positioned in locations one to N, where N is the total number of data points read in. The length of the vector must not exceed 32, 767.

GMEAN - BINARY FLOAT [(53)]
Resultant variable containing grand mean.

SUMSQ - BINARY FLOAT [(53)]
Resultant vector of length 2 to the Kth power minus one, ([2**K] - 1), containing the sums of squares.

NDF - BINARY FIXED
Resultant vector of length ([2**K] -1), containing degrees of freedom.

SMEAN - BINARY FLOAT [(53)]
Resultant vector of length ([2**K] - 1), containing mean squares.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - N, the number of data points, less than or equal to zero.
ERROR=2 - There is only one factor or less than one.
ERROR=3 - One or more factors have levels less than two.

Method:

The method is based on the technique discussed by H. O. Hartley in Mathematical Methods for Digital Computers, edited by A. Ralston and H. Wilf, John Wiley and Sons, 1962, Chapter 20.

Mathematical Background:

This procedure calculates an analysis of variance in three steps:

1. The data is placed in properly distributed positions of storage.

The size of the data array named X required for an analysis of variance problem is calculated as follows:

$$MM = \prod_{i=1}^{K} (L_i + 1) \qquad (1)$$

where:

L_i = number of levels of i-th factor
K = number of factors

The data is redistributed according to equation (4) below. Prior to that, multipliers, S_j, to be used in finding proper positions of storage, are calculated as follows:

$$S_1 = 1 \tag{2}$$

$$S_j = \prod_{i=1}^{j-1} (L_i + 1) \tag{3}$$

where j = 2, 3, ..., K.

Then the position to place each data point is calculated by the following equation:

$$S = KOUNT_1 + \sum_{j \equiv 2}^{K} S_j \cdot (KOUNT_j - 1) \tag{4}$$

where $KOUNT_j$ = value of the j-th subscript of the data to be stored. The procedure increments the value(s) of subscript(s) after each data point is stored.

2. The next step performs the calculus for the general K-factor experiment: operator Σ and operator Δ. An example is presented in terms of K = 3 to illustrate these operators.

Let X_{abc} denote the experimental reading from the a-th level of factor A, the b-th level of factor B, and the c-th level of factor C. The symbols A, B, C will also denote the number of levels for each factor so that a = 1, 2, ..., A; b = 1, 2, ..., B; c = 1, 2, ..., C.

With regard to the factor, A:

operator $\sum_a \equiv$ sum over all levels a = 1, 2, ..., A, holding the other subscripts at constant levels,

operator $\Delta_a \equiv$ multiply all items by A and subtract the result $\sum_a$ from all items

In mathematical notations, these operators are defined as follows:

$$\sum_a X_{abc} \equiv X_{.bc} \equiv \sum_{a=1}^{A} X_{abc} \tag{5}$$

$$\Delta_a X_{abc} \equiv AX_{abc} - X_{.bc} \tag{6}$$

The operators Σ and Δ will be applied sequentially with regard to all factors A, B, and C. Upon the completion of these operators, the storage array X contains deviates to be used for analysis of variance components.

3. In the next and final step the mean square operation for the general K-factor experiment is performed as follows:

a. Square each value of deviate for analysis of variance stored in array X, which is the result of the operators Σ and Δ applied in step 2.

b. Add the squared value into a proper summation storage. In a three-factor experiment, for example, the squared value is added into one of the seven storages ($7 = 2^3 - 1$) as shown in the first column of the following table. The symbols A, B, and C in the first column denote factors A, B, and C.

After the mean square operation is completed for all values in the storage array X, the procedure forms sums of squares of analysis of variance by dividing the totals of squared values by the proper divisors. These divisors for the three-factor experiment mentioned above are shown in the middle column of the Table. The symbols A, B, and C in the second column denote the number of levels for each factor.

The procedure then forms mean squares by dividing sums of squares by degrees of freedom. The third column of the table shows the degrees of freedom. The symbols A, B, and C denote the number of levels.

Designation of store and of quantity contained in it	Divisor required to form sum of squares of analysis of variance	Degrees of freedom required to form mean squares
$(A)^2$	ABC. A	(A-1)
$(B)^2$	ABC. B	(B-1)
$(AB)^2$	ABC. AB	(A-1) (B-1)
$(C)^2$	ABC. C	(C-1)
$(AC)^2$	ABC. AC	(A-1) (C-1)
$(BC)^2$	ABC. BC	(B-1) (C-1)
$(ABC)^2$	ABC. ABC	(A-1) (B-1) (C-1)

Programming Considerations:

Input data must be arranged in the following manner: Consider the three-variable analysis of variance design, where one variable has three levels and the other two variables have two levels. The data may be represented in the form X(I, J, K). The left subscript — namely, I — changes first. When I=3, the next left subscript, J, changes, and so on, until I=3, J=2, and K=2.

Discriminant Analysis

- Subroutine DMTX

```
DMTX..                                                                  DMTX  10
/*************************************************************************/DMTX  20
/*                                                                       */DMTX  30
/*      TO COMPUTE MEANS OF VARIABLES IN EACH GROUP AND A POOLED         */DMTX  40
/*      DISPERSION MATRIX FOR ALL THE GROUPS.                            */DMTX  50
/*                                                                       */DMTX  60
/*************************************************************************/DMTX  70
   PROCEDURE (K,M,N,X,XBAR,D),.                                         DMTX  80
   DECLARE                                                              DMTX  90
        ERROR EXTERNAL CHARACTER (1),                                   DMTX 100
        (N(*),I,J,K,K1,K2,KK,L,M,NN)                                    DMTX 110
        FIXED BINARY,                                                   DMTX 120
        (X(*,*),FSUM)                                                   DMTX 130
        FLOAT BINARY,                                                   DMTX 140
        (XBAR(*,*),D(*,*),CMEAN(M))                                     DMTX 150
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/DMTX 160
/*      BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/DMTX 170
/*                                                                      */DMTX 180
   ERROR='0',.                                                          DMTX 190
   IF M LE 1                    /* THE NUMBER OF VARIABLES IS  */DMTX 200
   THEN DO,.                    /* LESS THAN OR EQUAL TO ONE.  */DMTX 210
        ERROR='1',.                                                     DMTX 220
        GO TO FIN,.                                                     DMTX 230
        END,.                                                           DMTX 240
   IF K LE 1 OR K GT M          /* INVALID NUMBER OF GROUPS.   */DMTX 250
   THEN DO,.                                                            DMTX 260
        ERROR='2',.                                                     DMTX 270
        GO TO FIN,.                                                     DMTX 280
        END,.                                                           DMTX 290
        DO J = 1 TO K,.                                                 DMTX 300
        IF N(J) LE 0                /* NO OBSERVATIONS IN AT LEAST */DMTX 310
        THEN DO,.                   /* ONE OF THE GROUPS           */DMTX 320
             ERROR='3',.                                                DMTX 330
             GO TO FIN,.                                                DMTX 340
             END,.                                                      DMTX 350
        END,.                                                           DMTX 360
        DO I = 1 TO M,.                                                 DMTX 370
             DO J = 1 TO K,.                                            DMTX 380
             XBAR(I,J)=0.0,.                                            DMTX 390
             END,.                                                      DMTX 400
        END,.                                                           DMTX 410
        =0,.                                                            DMTX 420
        DO I = 1 TO K,.                                                 DMTX 430
        NN   =N(I),.                                                    DMTX 440
        FSUM =NN,.                                                      DMTX 450
             DO J = 1 TO NN,.                                           DMTX 460
             L    =L+1,.                                                DMTX 470
                  DO KK = 1 TO M,.                                      DMTX 480
                  XBAR(KK,I)=XBAR(KK,I)+X(L,KK),.                       DMTX 490
                  END,.                                                 DMTX 500
             END,.                                                      DMTX 510
             DO KK = 1 TO M,.                                           DMTX 520
             XBAR(KK,I)=XBAR(KK,I)/FSUM,.                               DMTX 530
             END,.                                                      DMTX 540
        END,.                                                           DMTX 550
/*                                                                      */DMTX 560
/*      COMPUTE THE DISPERSION MATRIX                                   */DMTX 570
/*                                                                      */DMTX 580
        DO I = 1 TO M,.                                                 DMTX 590
             DO J = 1 TO M,.                                            DMTX 600
             D(I,J)=0.0,.                                               DMTX 610
             END,.                                                      DMTX 620
        END,.                                                           DMTX 630
   L    =0,.                                                            DMTX 640
        DO I = 1 TO K,.                                                 DMTX 650
        NN   =N(I),.                                                    DMTX 660
             DO J = 1 TO NN,.                                           DMTX 670
             L    =L+1,.                                                DMTX 680
                  DO KK = 1 TO M,.                                      DMTX 690
                  CMEAN(KK)=X(L,KK)-XBAR(KK,I),.                        DMTX 700
                  END,.                                                 DMTX 710
                  DO K1 = 1 TO M,.                                      DMTX 720
                       DO K2 = K1 TO M,.                                DMTX 730
                       D(K1,K2)=D(K1,K2)+CMEAN(K1)*CMEAN(K2),.          DMTX 740
                       END,.                                            DMTX 750
                  END,.                                                 DMTX 760
             END,.                                                      DMTX 770
        END,.                                                           DMTX 780
   L    =0,.                                                            DMTX 790
        DO KK = 1 TO K,.                                                DMTX 800
        L    =L+N(KK),.                                                 DMTX 810
        END,.                                                           DMTX 820
   FSUM =L-K,.                                                          DMTX 830
        DO I = 1 TO M,.                                                 DMTX 840
             DO J = I TO M,.                                            DMTX 850
             D(I,J)=D(I,J)/FSUM,.                                       DMTX 860
             D(J,I)=D(I,J),.                                            DMTX 870
             END,.                                                      DMTX 880
        END,.                                                           DMTX 890
FIN..                                                                   DMTX 900
   RETURN,.                                                             DMTX 910
   END,.                            /*END OF PROCEDURE DMTX       */DMTX 920
```

Purpose:

DMTX computes means of variables in each group and a pooled dispersion matrix for all the groups. This subroutine is used in the performance of discriminant analysis.

Usage:

CALL DMTX (K, M, N, X, XBAR, D);

K - BINARY FIXED
Given number of groups. K must be greater than 1.

M - BINARY FIXED
Given number of variables (must be the same for all groups).

N(K) - BINARY FIXED
Given vector containing sample sizes of groups. N=(n_1, n_2, ..., n_k)

X(NN, M) BINARY FLOAT
Given matrix containing data in a manner equivalent to a three-dimensional array (X_{ijk}). The first subscript is case number; the second, variable number; the third, group number. NN=$n_1 + n_2 + \ldots + n_k$.

XBAR(M, K) - BINARY FLOAT [(53)]
Resultant matrix containing means of variables in K groups.

D(M, M) - BINARY FLOAT [(53)]
Resultant matrix containing pooled dispersion.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of variables less than or equal to one.
ERROR=2 - invalid number of groups (K ≤ 1 or K > M).
ERROR=3 - no observations in one or more groups.

The number of variables must be greater than or equal to the number of groups.

Method:

Refer to BMD Computer Programs Manual, edited by W. J. Dixon, UCLA, 1964, and T. W. Anderson, Introduction to Multivariate Statistical Analysis, John Wiley and Sons, 1958, Sections 6.6-6.8.

Mathematical Background:

This subroutine calculates means of variables in each group and a pooled dispersion matrix for the set of groups in a discriminant analysis.

For each group k = 1, 2, ..., K, the subroutine calculates means and sums of cross-products of deviations from means as shown below.

Means:

$$\bar{x}_{jk} = \frac{\sum_{i=1}^{n_k} x_{ijk}}{n_k} \qquad (1)$$

where n_k = sample size in the kth group

$j = 1, 2, \ldots, m$ are variables

Sum of cross-products of deviations from means:

$$S_k = \left\{ s_{j\,l}^{\,k} \right\} = \sum (x_{ijk} - \bar{x}_{jk})\ (x_{ilk} - \bar{x}_{lk}) \qquad (2)$$

where $j = 1, 2, \ldots, m$

$l = 1, 2, \ldots, m$

The pooled dispersion matrix is calculated as follows:

$$D = \frac{\sum_{k=1}^{K} S_k}{\sum_{k=1}^{K} n_k - K} \qquad (3)$$

where K = number of groups

- Subroutine DSCR

```
DSCR..                                                                  DSCR  10
/*********************************************************************/DSCR  20
/*                                                                   */DSCR  30
/*      TO COMPUTE A SET OF LINEAR FUNCTIONS WHICH SERVE AS INDICES  */DSCR  40
/*      FOR CLASSIFYING AN INDIVIDUAL INTO ONE OF SEVERAL GROUPS.    */DSCR  50
/*                                                                   */DSCR  60
/*********************************************************************/DSCR  70
   PROCEDURE (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG),.                          DSCR  80
   DECLARE                                                              DSCR  90
         (N(*),LG(*),I,J,K,K1,K2,L,LL,M,N1,NN)                          DSCR 100
         FIXED BINARY,                                                  DSCR 110
         ERROR EXTERNAL CHARACTER(1),                                   DSCR 120
         (X(*,*),FN(K))                                                 DSCR 130
         BINARY FLOAT,                                                  DSCR 140
         (XBAR(*,*),D(*,*),C(*,*),CMEAN(*),P(*),V,FSUM,PL)              DSCR 150
         BINARY FLOAT,.                 /*SINGLE PRECISION VERSION  /*S*/DSCR 160
/*       BINARY FLOAT (53),.            /*DOUBLE PRECISION VERSION  /*D*/DSCR 170
/*                                                                   */DSCR 180
   L    =0,.                                                           DSCR 190
   ERROR='0',.                                                        DSCR 200
   IF M LE 1                            /* NUMBER OF VARIABLES LESS  */DSCR 210
   THEN DO,.                            /* THAN OR EQUAL TO ONE.     */DSCR 220
         ERROR='1',.                                                  DSCR 230
         GO TO FIN,.                                                  DSCR 240
         END,.                                                        DSCR 250
   IF K LE 1 OR K GT M                  /* INVALID NUMBER OF GROUPS. */DSCR 260
   THEN DO,.                                                          DSCR 270
         ERROR='2',.                                                  DSCR 280
         GO TO FIN,.                                                  DSCR 290
         END,.                                                        DSCR 300
         DO I = 1 TO K,.                                              DSCR 310
         IF N(I) LE 0                   /* NO OBSERVATIONS IN ONE OR */DSCR 320
         THEN DO,.                      /* MORE GROUPS.              */DSCR 330
               ERROR='3',.                                            DSCR 340
               GO TO FIN,.                                            DSCR 350
               END,.                                                  DSCR 360
         END,.                                                        DSCR 370
         DO I = 1 TO K,.                                              DSCR 380
         L    =L+N(I),.                                               DSCR 390
         END,.                                                        DSCR 400
   FSUM =L,.                                                          DSCR 410
         DO I = 1 TO M,.                                              DSCR 420
         V    =0.0,.                                                  DSCR 430
               DO J = 1 TO K,.                                        DSCR 440
               V    =V+N(J)*XBAR(I,J),.                               DSCR 450
               END,.                                                  DSCR 460
         CMEAN(I)=V/FSUM,.                                            DSCR 470
         END,.                                                        DSCR 480
/*                                                                   */DSCR 490
/*       CALCULATE GENERALIZED MAHALANOBIS D SQUARE                  */DSCR 500
/*                                                                   */DSCR 510
   V    =0,.                                                         DSCR 520
         DO I = 1 TO M,.                                              DSCR 530
               DO J = 1 TO M,.                                        DSCR 540
               FSUM =0.0,.                                            DSCR 550
                     DO KK = 1 TO K,.                                 DSCR 560
                     FSUM =FSUM+N(KK)*(XBAR(I,KK)-CMEAN(I))          DSCR 570
                           *(XBAR(J,KK)-CMEAN(J)),.                  DSCR 580
                     END,.                                            DSCR 590
               V    =V+D(I,J)*FSUM,.                                  DSCR 600
               END,.                                                  DSCR 610
         END,.                                                        DSCR 620
/*                                                                   */DSCR 630
/*       CALCULATE THE COEFFICIENTS OF DISCRIMINANT FUNCTIONS        */DSCR 640
/*                                                                   */DSCR 650
         DO I = 1 TO K,.                                              DSCR 660
         FSUM =0,.                                                    DSCR 670
               DO J = 1 TO M,.                                        DSCR 680
                     DO KK = 1 TO M,.                                 DSCR 690
                     FSUM =FSUM+D(J,KK)*XBAR(J,I)*XBAR(KK,I),.        DSCR 700
                     END,.                                            DSCR 710
               END,.                                                  DSCR 720
         C(1,I)=-(FSUM/2),.                                           DSCR 730
               DO J = 1 TO M,.                                        DSCR 740
               C(J+1,I)=0.0,.                                         DSCR 750
                     DO KK = 1 TO M,.                                 DSCR 760
                     C(J+1,I)=C(J+1,I)+D(J,KK)*XBAR(KK,I),.           DSCR 770
                     END,.                                            DSCR 780
               END,.                                                  DSCR 790
         END,.                                                        DSCR 800
/*                                                                   */DSCR 810
/*       FOR EACH CASE IN EACH GROUP, CALCULATE.. DISCRIMINANT       */DSCR 820
/*       FUNCTIONS.                                                  */DSCR 830
/*                                                                   */DSCR 840
   N1   =0,.                                                          DSCR 850
   L    =0,.                                                          DSCR 860
         DO I = 1 TO K,.                                              DSCR 870
         NN   =N(I),.                                                 DSCR 880
               DO J = 1 TO NN,.                                       DSCR 890
               L    =L+1,.                                            DSCR 900
                     DO K1 = 1 TO K,.                                 DSCR 910
                     FN(K1)=C(1,K1),.                                 DSCR 920
                           DO K2 = 1 TO M,.                           DSCR 930
                           FN(K1)=FN(K1)+C(K2+1,K1)*X(L,K2),.         DSCR 940
                           END,.                                      DSCR 950
                     END,.                                            DSCR 960
/*                                                                   */DSCR 970
/*       THE LARGEST DISCRIMINANT FUNCTION                           */DSCR 980
/*                                                                   */DSCR 990
               LL   =1,.                                              DSCR1000
               FSUM =FN(1),.                                          DSCR1010
                     DO K1 = 2 TO K,.                                 DSCR1020
                     IF FSUM LT FN(K1)                                DSCR1030
                     THEN DO,.                                        DSCR1040
                           LL   =K1,.                                 DSCR1050
                           FSUM =FN(K1),.                             DSCR1060
                           END,.                                      DSCR1070
                     END,.                                            DSCR1080
/*                                                                   */DSCR1090
/*       PROBABILITY ASSOCIATED WITH THE LARGEST DISCRIMINANT        */DSCR1100
/*       FUNCTION.                                                   */DSCR1110
/*                                                                   */DSCR1120
               PL   =0,.                                              DSCR1130
                     DO KK = 1 TO K,.                                 DSCR1140
                     PL   =PL+EXP(FN(KK)-FSUM),.                      DSCR1150
                     END,.                                            DSCR1160
               N1   =N1+1,.                                           DSCR1170
               LG(N1)=LL,.                                            DSCR1180
               P(N1)=1/PL,.                                           DSCR1190
               END,.                                                  DSCR1200
         END,.                                                        DSCR1210
FIN..                                                                 DSCR1220
   RETURN,.                                                           DSCR1230
   END,.                                /*END OF PROCEDURE DSCR      */DSCR1240
```

Purpose:

DSCR performs a discriminant analysis by calculating a set of linear functions that serve as indices for classifying an individual into one of K groups.

Usage:

CALL DSCR (K, M, N, X, XBAR, D, CMEAN, V, C, P, LG);

K - BINARY FIXED
Given number of groups. K must be greater than 1.

M - BINARY FIXED
Given number of variables.

N(K) - BINARY FIXED
Given vector containing sample sizes of groups.
$N = (n_1, n_2, \ldots, n_K)$

X(NN, M) - BINARY FLOAT
Given matrix containing data in the manner equivalent to a three-dimensional array $\{X_{ijk}\}$. The first subscript is case number; the second, variable number; the third, group number. $NN = n_1 + n_2 + \ldots + n_k$.

XBAR(M, K) - BINARY FLOAT [(53)]
Given matrix containing means of M variables in K groups.

D(M, M) - BINARY FLOAT [(53)]
Given matrix containing the inverse of pooled dispersion matrix.

CMEAN(M) - BINARY FLOAT [(53)]
Resultant vector containing common means.

V - BINARY FLOAT [(53)]
Resultant variable containing generalized Mahalanobis D-square.

C(M+1, K) - BINARY FLOAT [(53)]
Resultant matrix containing the coefficients of discriminant functions. The first position of each column (function) contains the value of the constant for that function.

P(NN) - BINARY FLOAT [(53)]
Resultant vector containing the probability associated with the largest discriminant functions of all cases in all groups. Calculated results are stored in the manner equivalent to a two-dimensional array (the first subscript is case number, and the second subscript is group number).
$NN = n_1 + n_2 + \ldots + n_K$

LG(NN) - BINARY FIXED
Resultant vector containing the subscripts of the largest discriminant functions stored in vector P.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of variables less than or equal to one.
ERROR=2 - invalid number of groups ($K \leq 1$ or $K > M$).
ERROR=3 - no observations in one or more groups.

The number of variables must be greater than or equal to the number of groups.

Method:

Refer to BMD Computer Programs Manual, edited by W.J. Dixon, UCLA, 1964, and T.W. Anderson, Introduction to Multivariate Statistical Analysis, John Wiley and Sons, 1958.

Mathematical Background:

This subroutine performs a discriminant analysis by calculating a set of linear functions that serve as indices for classifying an individual into one of K groups.

For all groups combined, the following are obtained.

Common means:

$$\bar{X}_j = \frac{\sum_{k=1}^{K} n_k \bar{x}_{jk}}{\sum_{k=1}^{K} n_k} \qquad (1)$$

where:

K = number of groups

j = 1, 2, ..., m are variables

n_k = sample size in the k-th group

$\bar{x}_{jk}$ = mean of j-th variable in k-th group

Generalized Mahalanobis D^2 statistics, V:

$$V = \sum_{i=1}^{m} \sum_{j=1}^{m} d_{ij} \sum_{k=1}^{K} a_{ijk}$$

$$a_{ijk} = n_k (\bar{x}_{ik} - \bar{X}_i)(\bar{x}_{jk} - \bar{X}_j) \quad (2)$$

where:

d_{ij} = the inverse element of the pooled dispersion matrix D

V can be used as chi-square (under assumption of normality) with m (K-1) degrees of freedom to test the hypothesis that the mean values are the same in all the K groups for these m variables. For each discriminant function $k_* = 1, 2, \ldots, K$, the following statistics are calculated.

Coefficients:

$$C_{ik_*} = \sum_{j=1}^{m} d_{ij} \bar{x}_{jk} \quad (3)$$

where:

$i = 1, 2, \ldots, m$

$k = k_*$

Constant:

$$C_{0k_*} = -1/2 \sum_{j=1}^{m} \sum_{l=1}^{m} d_{jl} \bar{x}_{jk} \bar{x}_{lk} \quad (4)$$

For each i-th case in each k-th group, the following calculations are performed.

Discriminant functions:

$$f_{k_*} = \sum_{j=1}^{m} C_{jk} x_{ijk} + C_{0k_*} \quad (5)$$

where:

$k_* = 1, 2, \ldots, K$

Probability associated with largest discriminant function:

$$P_L = \frac{1}{\sum_{k^*=1}^{K} e^{(f_{k^*} - f_L)}} \quad (6)$$

where:

f_L = the value of the largest discriminant function

L = the subscript of the largest discriminant function

Principal Components Analysis

- Subroutine TRAC

```
TRAC..                                                              TRAC  10
/*******************************************************************/TRAC  20
/*                                                                 */TRAC  30
/*      TO COMPUTE CUMULATIVE PERCENTAGE OF EIGENVALUES GREATER    */TRAC  40
/*      THAN OR EQUAL TO A CONSTANT SPECIFIED BY THE USER.         */TRAC  50
/*                                                                 */TRAC  60
/*******************************************************************/TRAC  70
   PROCEDURE (M,R,CON,K,D),.                                        TRAC  80
   DECLARE                                                          TRAC  90
        ERROR EXTERNAL CHARACTER (1),                               TRAC 100
        (I,J,K,M)                                                   TRAC 110
        FIXED BINARY,                                               TRAC 120
        (R(*,*),D(*),CON)                                           TRAC 130
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/TRAC 140
 /*     BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/TRAC 150
/*                                                                 */TRAC 160
   ERROR='0',.                                                      TRAC 170
   IF M LE 0                    /* ORDER OF MATRIX IS ZERO.    */TRAC 180
   THEN DO,.                                                        TRAC 190
        ERROR='1',.                                                 TRAC 200
        GO TO S2C,.                                                 TRAC 210
        END,.                                                       TRAC 220
        DO I = 1 TO M,.                                             TRAC 230
        END,.                                                       TRAC 250
   K    =C,.                                                        TRAC 260
/*                                                                 */TRAC 270
/*      TEST WHETHER I-TH EIGENVALUE IS GREATER THAN OR EQUAL TO   */TRAC 280
/*      THE CONSTANT.                                              */TRAC 290
/*                                                                 */TRAC 300
        DO I = 1 TO M,.                                             TRAC 310
        IF D(I) LT CON                                              TRAC 320
        THEN GO TO S1C,.                                            TRAC 330
        K    =K+1,.                                                 TRAC 340
        D(I) =D(I)/M,.                                              TRAC 350
        END,.                                                       TRAC 360
S1O..                                                               TRAC 370
   IF K LE 1                                                        TRAC 380
   THEN DO,.                                                        TRAC 390
        ERROR='2',.                 /* NOT ENOUGH EIGENVALUES  */TRAC 400
        GO TO S2C,.                 /* ARE RETAINED            */TRAC 410
        END,.                                                       TRAC 420
        DO I = 2 TO K,.                                             TRAC 430
        D(I) =D(I)+D(I-1),.                                         TRAC 440
        END,.                                                       TRAC 450
S2C..                                                               TRAC 460
   RETURN,.                                                         TRAC 470
   END,.                            /*END OF PROCEDURE TRAC    */TRAC 480
```

Purpose:

TRAC computes cumulative percentage of eigenvalues greater than or equal to a constant specified by the user.

Usage:

CALL TRAC (M, R, CON, K, D);

Description of parameters:

M - BINARY FIXED
Given number of variables.

R(M, M) - BINARY FLOAT [(53)]
Given matrix containing eigenvalues in diagonal. Eigenvalues are assumed to be arranged in descending order.

CON - BINARY FLOAT [(53)]
Given constant used to decide how many eigenvalues to retain. Cumulative percentage of eigenvalues greater than or equal to this value is calculated.

K - BINARY FIXED
Resultant variable containing the number of eigenvalues greater than or equal to CON. (K is the number of factors.)

D(M) - BINARY FLOAT [(53)]
Resultant vector containing cumulative percentage of eigenvalues greater than or equal to CON.

Remark:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - order of matrix equal to zero.
ERROR=2 - number of eigenvalues retained less than or equal to one.

Method:

Each eigenvalue greater than or equal to CON is divided by M, and the result is added to the previous total to obtain the cumulative percentage for each eigenvalue.

Mathematical Background:

This procedure finds K, the number of eigenvalues greater than or equal to the value of a special constant. The given eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_M$ must be arranged in descending order.

Cumulative percentages for those K eigenvalues are:

$$d_j = \sum_{i=1}^{j} \frac{\lambda_i}{M} \qquad (1)$$

where:

$j = 1, 2, \ldots, K$

M = number of eigenvalues (or variables)

$K \leq M$

- Subroutine LOAD

```
LOAD..                                                                  LOAD  10
/*************************************************************************/LOAD  20
/*                                                                       */LOAD  30
/*      TO COMPUTE A FACTOR MATRIX (LOADING) FROM EIGENVALUES AND        */LOAD  40
/*      ASSOCIATED EIGENVECTORS.                                         */LOAD  50
/*                                                                       */LOAD  60
/*************************************************************************/LOAD  70
   PROCEDURE (M,K,R,V),.                                                LOAD  80
   DECLARE                                                              LOAD  90
        (I,J,K)                                                         LOAD 100
        FIXED BINARY,                                                   LOAD 110
        ERROR EXTERNAL CHARACTER(1),                                    LOAD 120
        (R(*,*),V(*,*),SQ)                                              LOAD 130
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/LOAD 140
 /*     BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/LOAD 150
/*                                                                       */LOAD 160
   ERROR='0',.                                                          LOAD 170
   IF K LE 1 OR K GT M              /* INVALID VALUE OF K           */LOAD 180
   THEN DO,.                                                            LOAD 190
        ERROR='2',.                                                     LOAD 200
        GO TO FIN,.                                                     LOAD 210
        END,.                                                           LOAD 220
   IF M LE 0                        /* ORDER OF MATRIX IS ZERO      */LOAD 230
   THEN ERROR='1',.                                                     LOAD 240
   ELSE DO,.                                                            LOAD 250
            DO J = 1 TO K,.                                             LOAD 260
            SQ   =SQRT(R(J,J)),.                                        LOAD 270
                 DO I = 1 TO M,.                                        LOAD 280
                 V(I,J)=SQ*V(I,J),.                                     LOAD 290
                 END,.                                                  LOAD 300
            END,.                                                       LOAD 310
        END,.                                                           LOAD 320
FIN..                                                                   LOAD 330
   RETURN,.                                                             LOAD 340
   END,.                            /*END OF PROCEDURE LOAD        */LOAD 350
```

Purpose:

LOAD computes a factor matrix (loading) from eigenvalues and associated eigenvectors.

Usage:

CALL LOAD (M, K, R, V);

Description of parameters:

M - BINARY FIXED
Given number of variables.

K - BINARY FIXED
Given number of factors.

R(M, M) - BINARY FLOAT [(53)]
Given matrix containing eigenvalues in the diagonal. Eigenvalues are assumed to be arranged in descending order. The first K eigenvalues are used by this procedure.

V(M, M) - BINARY FLOAT [(53)]
Given matrix V contains eigenvectors columnwise.
Resultant matrix V contains a factor matrix (M by K).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - the order of the matrix is zero.
ERROR=2 - invalid number of factors ($K \leq 1$ or $K > M$).

Method:

Normalized eigenvectors are converted to the factor pattern by multiplying the elements of each vector by the square root of the corresponding eigenvalue.

Mathematical Background:

This procedure calculates the coefficients of each factor by multiplying the elements of each normalized eigenvector by the square root of the corresponding eigenvalue.

$$a_{ij} = V_{ij} \cdot \sqrt{\lambda_j}$$

where:

$i = 1, 2, \ldots, M$ are indices of variables

$j = 1, 2, \ldots, K$ are indices of eigenvalues retained (see the subroutine TRAC)

$K \leq M$

- Subroutine VRMX

```
VRMX..                                                                  VRMX  10
/*********************************************************************/VRMX  20
/*                                                                   */VRMX  30
/*      TO PERFORM ORTHOGONAL ROTATION OF A FACTOR MATRIX.           */VRMX  40
/*                                                                   */VRMX  50
/*********************************************************************/VRMX  60
   PROCEDURE (M,K,A,NC,TV,H,F,D);..                                     VRMX  70
   DECLARE                                                              VRMX  80
        (I,II,J,K,K1,LL,M,NC,NV)                                        VRMX  90
        FIXED BINARY,                                                   VRMX 100
        ERROR EXTERNAL CHARACTER(1),                                    VRMX 110
        (A(*,*),TV(*),H(*),F(*),D(*),EPS,TVLT,FN,AA,BB,CC,DD,G,B,U,T,   VRMX 120
        COS4T,SIN4T,TAN4T,SINP,COSP,CTN4T,COS2T,SIN2T,COST,SINT,CONS)   VRMX 130
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/VRMX 140
 /*     BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/VRMX 150
/*                                                                   */VRMX 160
   EPS  =.00116,.                   /* INITIALIZATION              */VRMX 170
   TVLT =0,.                                                          VRMX 180
   LL   =K-1,.                                                        VRMX 190
   NV   =1,.                                                          VRMX 200
   NC   =0,.                                                          VRMX 210
   FN   =M*M,.                                                        VRMX 220
   CONS =.7071066,.                                                   VRMX 230
   ERROR='0',.                                                        VRMX 240
   IF M LE 1                        /* NUMBER OF VARIABLES LESS    */VRMX 250
   THEN DO,.                        /* THAN OR EQUAL TO ONE        */VRMX 260
        ERROR='1',.                                                   VRMX 270
        GO TO FIN,.                                                   VRMX 280
        END,.                                                         VRMX 290
   IF K LE 1 OR K GT M              /* INVALID VALUE OF K          */VRMX 300
   THEN DO,.                                                          VRMX 310
        ERROR='2',.                                                   VRMX 320
        GO TO FIN,.                                                   VRMX 330
        END,.                                                         VRMX 340
/*                                                                   */VRMX 350
/*      CALCULATE ORIGINAL COMMUNALITIES                             */VRMX 360
/*                                                                   */VRMX 370
        DO I = 1 TO M,.                                               VRMX 380
        H(I) =0,.                                                     VRMX 390
             DO J = 1 TO K,.                                          VRMX 400
             H(I) =H(I)+A(I,J)*A(I,J),.                               VRMX 410
             END,.                                                    VRMX 420
        END,.                                                         VRMX 430
/*                                                                   */VRMX 440
/*      CALCULATE NORMALIZED FACTOR MATRIX                           */VRMX 450
/*                                                                   */VRMX 460
        DO I = 1 TO M,.                                               VRMX 470
        H(I) =SQRT(H(I)),.                                            VRMX 480
             DO J = 1 TO K,.                                          VRMX 490
             A(I,J)=A(I,J)/H(I),.                                     VRMX 500
             END,.                                                    VRMX 510
        END,.                                                         VRMX 520
   GO TO S20,.                                                        VRMX 530
/*                                                                   */VRMX 540
/*      CALCULATE VARIANCE FOR FACTOR MATRIX                         */VRMX 550
/*                                                                   */VRMX 560
S10..                                                                 VRMX 570
   NV   =NV+1,.                                                       VRMX 580
   TVLT =TV(NV-1),.                                                   VRMX 590
S20..                                                                 VRMX 600
   TV(NV)=0,.                                                         VRMX 610
        DO J = 1 TO K,.                                               VRMX 620
        AA   =0,.                                                     VRMX 630
        BB   =0,.                                                     VRMX 640
             DO I = 1 TO M,.                                          VRMX 650
             CC   =A(I,J)*A(I,J),.                                    VRMX 660
             AA   =AA+CC,.                                            VRMX 670
             BB   =BB+CC*CC,.                                         VRMX 680
             END,.                                                    VRMX 690
        TV(NV)=TV(NV)+(M*BB-AA*AA)/FN,.                               VRMX 700
        END,.                                                         VRMX 710
   IF NV GE 51                                                        VRMX 720
   THEN DO,.                        /* NUMBER OF ITERATIONS = 50   */VRMX 730
        ERROR='3',.                                                   VRMX 740
        GO TO S80,.                                                   VRMX 750
        END,.                                                         VRMX 760
   IF TV(NV)-TVLT LE 1.CE-7         /* PERFORM CONVERGENCE TEST    */VRMX 770
   THEN DO,.                                                          VRMX 780
        NC   =NC+1,.                                                  VRMX 790
        IF NC GT 3                                                    VRMX 800
        THEN GO TO S80,.                                              VRMX 810
        END,.                                                         VRMX 820
/*                                                                   */VRMX 830
/*      ROTATION OF TWO FACTORS BEGINS                               */VRMX 840
/*                                                                   */VRMX 850
        DO J = 1 TO LL,.                                              VRMX 860
        II   =J+1,.                                                   VRMX 870
             DO K1 = II TO K,.                                        VRMX 880
             AA   =0,.                  /* CALCULATE NUM AND DEN    */VRMX 890
             BB   =0,.                                                VRMX 900
             CC   =0,.                                                VRMX 910
             DD   =0,.                                                VRMX 920
                  DO I = 1 TO M,.                                     VRMX 930
                  U    =(A(I,J)+A(I,K1))*(A(I,J)-A(I,K1)),.           VRMX 940
                  T    =A(I,J)*A(I,K1)*2,.                            VRMX 950
                  CC   =CC+(U+T)*(U-T),.                              VRMX 960
                  DD   =DD+2*U*T,.                                    VRMX 970
                  AA   =AA+U,.                                        VRMX 980
                  BB   =BB+T,.                                        VRMX 990
                  END,.                                               VRMX1000
             T    =DD-2*AA*BB/M,.                                     VRMX1010
             B    =CC-(AA*AA-BB*BB)/M,.                               VRMX1020
             IF T = B                                                 VRMX1030
             THEN DO,.                                                VRMX1040
                  IF T+B LT EPS                                       VRMX1050
                  THEN GO TO S70,.                                    VRMX1060
/*                                                                   */VRMX1070
/*      NUM + DEN IS GREATER THAN OR EQUAL TO THE TOLERANCE FACTOR   */VRMX1080
/*                                                                   */VRMX1090
             COS4T=CONS,.                                             VRMX1100
                  SIN4T=CONS,.                                        VRMX1110
                  GO TO S40,.                                         VRMX1120
                  END,.                                               VRMX1130
             IF T GT B                                                VRMX1140
             THEN GO TO S30,.                                         VRMX1150
             TAN4T=ABS(T)/ABS(B),.      /* NUM IS LESS THAN DEN     */VRMX1160
             IF TAN4T GE EPS                                          VRMX1170
             THEN DO,.                                                VRMX1180
                  COS4T=1/SQRT(1+TAN4T*TAN4T),.                       VRMX1190
                  SIN4T=TAN4T*COS4T,.                                 VRMX1200
                  GO TO S40,.                                         VRMX1210
                  END,.                                               VRMX1220
             IF B GE 0                                                VRMX1230
             THEN GO TO S70,.                                         VRMX1240
             SINP =CONS,.                                             VRMX1250
             COSP =CONS,.                                             VRMX1260
             GO TO S60,.                                              VRMX1270
S30..                                                                 VRMX1280
             CTN4T=ABS(T/B),.           /* NUM IS GREATER THAN DEN  */VRMX1290
             IF CTN4T GE EPS                                          VRMX1300
             THEN DO,.                                                VRMX1310
                  SIN4T=1/SQRT(1+CTN4T*CTN4T),.                       VRMX1320
                  COS4T=CTN4T*SIN4T,.                                 VRMX1330
                  GO TO S40,.                                         VRMX1340
                  END,.                                               VRMX1350
             COS4T=0,.                                                VRMX1360
             SIN4T=1,.                                                VRMX1370
/*                                                                   */VRMX1380
/*      DETERMINE COS THEAT AND SIN THETA                            */VRMX1390
/*                                                                   */VRMX1400
S40..                                                                 VRMX1410
             COS2T=SQRT((1+COS4T)/2),.                                VRMX1420
             SIN2T=SIN4T/(2*COS2T),.                                  VRMX1430
             COST =SQRT((1+COS2T)/2),.                                VRMX1440
             SINT =SIN2T/(2*COST),.                                   VRMX1450
/*                                                                   */VRMX1460
/*      DETERMINE COS PHI AND SIN PHI                                */VRMX1470
/*                                                                   */VRMX1480
             IF B GT 0                                                VRMX1490
             THEN DO,.                                                VRMX1500
                  COSP =COST,.                                        VRMX1510
                  SINP =SINT,.                                        VRMX1520
                  GO TO S50,.                                         VRMX1530
                  END,.                                               VRMX1540
             COSP =CONS*(COST+SINT),.                                 VRMX1550
             SINP =ABS(CONS*(COST-SINT)),.                            VRMX1560
S50..                                                                 VRMX1570
             IF T LE 0                                                VRMX1580
             THEN SINP =-SINP,.                                       VRMX1590
S60..                                                                 VRMX1600
                  DO I = 1 TO M,.     /* PERFORM ROTATION            */VRMX1610
                  AA   =A(I,J)*COSP+A(I,K1)*SINP,.                    VRMX1620
                  A(I,K1)=-A(I,J)*SINP+A(I,K1)*COSP,.                 VRMX1630
                  A(I,J)=AA,.                                         VRMX1640
                  END,.                                               VRMX1650
S70..                                                                 VRMX1660
             END,.                                                    VRMX1670
        END,.                                                         VRMX1680
   GO TO S10,.                                                        VRMX1690
/*                                                                   */VRMX1700
/*      DENORMALIZE VARIMAX LOADINGS                                 */VRMX1710
/*                                                                   */VRMX1720
S80..                                                                 VRMX1730
        DO I = 1 TO M,.                                               VRMX1740
             DO J = 1 TO K,.                                          VRMX1750
             A(I,J)=A(I,J)*H(I),.                                     VRMX1760
             END,.                                                    VRMX1770
        END,.                                                         VRMX1780
   NC   =NV-1,.                     /* CHECK ON COMMUNALITIES      */VRMX1790
   H    =H*H,.                                                        VRMX1800
        DO I = 1 TO M,.                                               VRMX1810
        F(I) =0,.                                                     VRMX1820
             DO J = 1 TO K,.                                          VRMX1830
             F(I) =F(I)+A(I,J)*A(I,J),.                               VRMX1840
             END,.                                                    VRMX1850
        D(I) =H(I)-F(I),.                                             VRMX1860
        END,.                                                         VRMX1870
FIN..                                                                 VRMX1880
   RETURN,.                                                           VRMX1890
   END,.                            /*END OF PROCEDURE VRMX       */VRMX1900
```

Purpose:

VRMX performs an orthogonal rotation of a factor matrix.

Usage:

CALL VRMX (M, K, A, NC, TV, H, F, D);

M - BINARY FIXED
Given number of variables.

K - BINARY FIXED
Given number of factors.

A(M,K) - BINARY FLOAT [(53)]
Given factor matrix.
Resultant rotated M x K factor matrix.

NC - BINARY FIXED
Resultant variable containing the number of iteration cycles performed.

TV(51) - BINARY FLOAT [(53)]
Resultant vector containing the variance of the factor matrix for each iteration cycle. The variance prior to

the first iteration cycle is also calculated. This means that NC+1 variances are stored in vector TV. Maximum number of iteration cycles allowed in this procedure is 50.

H(M) - BINARY FLOAT [(53)]
Resultant vector containing the original communalities.

F(M) - BINARY FLOAT [(53)]
Resultant vector containing the final communalities.

D(M) - BINARY FLOAT [(53)]
Resultant vector containing the difference between the original and final communalities.

Remarks:

If the variance computed after each iteration cycle does not increase for four successive times, the procedure stops rotation.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of variables less than or equal to one.
ERROR=2 - invalid number of factors (K ≤ 1 or K > M).
ERROR=3 - 50 iterations executed without convergence.

Method:

Kaiser's varimax rotation as described in "Computer Program for Varimax Rotation in Factor Analysis" by the same author, Educational and Psychological Measurement, vol. XIX, no. 3, 1959.

Mathematical Background:

This subroutine performs orthogonal rotations on an m by k factor matrix such that

$$\sum_j \left\{ m \sum_i \left(a_{ij}^2 / h_i^2 \right)^2 - \left[\sum_i \left(a_{ij}^2 / h_i^2 \right) \right]^2 \right\} \quad (1)$$

is a maximum, where i = 1, 2, . . . , m are variables, j = 1, 2, . . . , k are factors, a_{ij} is the loading for the i-th variable on the j-th factor, and h_i^2 is the communality of the i-th variable defined below.

Communalities:

$$h_i^2 = \sum_{j=1}^{k} a_{ij}^2 \quad (2)$$

where i = 1, 2, . . . , m

Normalized factor matrix:

$$b_{ij} = a_{ij} \Big/ \sqrt{h_i^2} \quad (3)$$

where:

i = 1, 2, . . . , m

j = 1, 2, . . . , k

Variance for factor matrix:

$$V_c = \sum_j \left\{ \left[m \sum_i \left(b_{ij}^2 \right)^2 - \left(\sum_i b_{ij}^2 \right)^2 \right] \Big/ m^2 \right\} \quad (4)$$

where c = 1, 2, . . . (iteration cycle)

Convergence test:

$$\text{If } V_c - V_{c-1} \leq 10^{-7} \quad (5)$$

four successive times, the program stops rotation and performs equation (28). Otherwise, the program repeats rotation of factors until the convergence test is satisfied.

Rotation of two factors:

The subroutine rotates two normalized factors (b_{ij}) at a time -- 1 with 2, 1 with 3, . . . , 1 with k, 2 with 3, . . . , 2 with k, . . . , k - 1 with k. This constitutes one iteration cycle.

Assuming that x and y are factors to be rotated, where x is the lower-numbered or left-hand factor, the following notation for rotating these two factors is used:

$$\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ x_m & y_m \end{bmatrix} \cdot \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} = \begin{bmatrix} X_1 & Y_1 \\ X_2 & Y_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ X_m & Y_m \end{bmatrix} \quad (6)$$

where x_i and y_i are presently available normalized loadings, and X_i and Y_i, the desired normalized loadings, are functions of ϕ, the angle of rotation. The computational steps are 1 through 5 below:

1. Calculation of NUM and DEN:

$$A = \sum_i (x_i + y_i)(x_i - y_i)$$

$$B = 2 \sum_i x_i y_i$$

$$C = \sum_i \left[(x_i + y_i)(x_i - y_i) + 2x_i y_i\right] \left[(x_i + y_i)(x_i - y_i) - 2x_i y_i\right]$$

$$D = 4 \sum_i (x_i + y_i)(x_i - y_i) x_i y_i \qquad (7)$$

$$NUM = D - 2AB/m$$

$$DEN = C - [(A+B)(A-B)]/m$$

2. Comparison of NUM and DEN:

The following four cases may arise.

NUM < DEN, go to (2a) below

NUM > DEN, go to (2b) below

(NUM + DEN) $\geq \epsilon$*, go to (2c) below

(NUM + DEN) $< \epsilon$, skip to the next rotation

* ϵ is a small tolerance factor.

a. $\tan 4\theta = |NUM|/|DEN|$ (8)

If $\tan 4\theta < \epsilon$ and

DEN is positive, skip to the next rotation.

DEN is negative, set $\cos\phi = \sin\phi = (\sqrt{2})/2$ and go to step 5.

If $\tan 4\theta \geq \epsilon$, calculate:

$$\cos 4\theta = 1/\sqrt{1 + \tan^2 4\theta} \qquad (9)$$

$$\sin 4\theta = \tan 4\theta \cdot \cos 4\theta \qquad (10)$$

and go to step 3.

b. $\text{ctn}\, 4\theta = |NUM|/|DEN|$ (11)

If $\text{ctn}\, 4\theta < \epsilon$, set $\cos 4\theta = 0$ and $\sin 4\theta = 1$. Go to step 3.

If $\text{ctn}\, 4\theta \geq \epsilon$, calculate:

$$\sin 4\theta = 1/\sqrt{1 + \text{ctn}^2 4\theta} \qquad (12)$$

$$\cos 4\theta = \text{ctn}\, 4\theta \cdot \sin 4\theta \qquad (13)$$

and go to step 3.

c. Set $\cos 4\theta = \sin 4\theta = (\sqrt{2})/2$ and go to step 3.

3. Determining $\cos\theta$ and $\sin\theta$:

$$\cos 2\theta = \sqrt{(1 + \cos 4\theta)/2} \qquad (14)$$

$$\sin 2\theta = \sin 4\theta/2 \cos 2\theta \qquad (15)$$

$$\cos\theta = \sqrt{(1 + \cos 2\theta)/2} \qquad (16)$$

$$\sin\theta = \sin 2\theta / 2\cos\theta \qquad (17)$$

4. Determining $\cos\phi$ and $\sin\phi$:

a. If DEN is positive, set

$$\cos\phi = \cos\theta \qquad (18)$$

$$\sin\phi = \sin\theta \qquad (19)$$

and go to (4b).

If DEN is negative, calculate

$$\cos\phi = \frac{\sqrt{2}}{2}\cos\theta + \frac{\sqrt{2}}{2}\sin\theta \qquad (20)$$

$$\sin\phi = \left|\frac{\sqrt{2}}{2}\cos\theta - \frac{\sqrt{2}}{2}\sin\theta\right| \qquad (21)$$

and go to (4b).

b. If NUM is positive, set

$$\cos\phi = |\cos\phi| \qquad (22)$$

$$\sin\phi = |\sin\phi| \qquad (23)$$

and go to step 5.

If NUM is negative, set

$$\cos\phi = \left|\cos\phi\right| \tag{24}$$

$$\sin\phi = -\left|\sin\phi\right| \tag{25}$$

5. Rotation:

$$X_i = x_i \cos\phi + y_i \sin\phi \tag{26}$$

$$Y_i = x_i \sin\phi + y_i \cos\phi \tag{27}$$

where

$$i = 1, 2, \ldots, m$$

After one cycle of k(k - 1)/2 rotations is completed, the subroutine goes back to calculate the variance for the factor matrix by equation (4).

Denormalization:

$$a_{ij} = b_{ij} \cdot h_i \tag{28}$$

where:

$$i = 1, 2, \ldots, m$$

$$j = 1, 2, \ldots, k$$

Check on communalities:

Final communalities

$$f_i^2 = \sum_{j=1}^{k} a_{ij}^2 \tag{29}$$

Difference

$$d_i = h_i^2 - f_i^2 \tag{30}$$

where i = 1, 2, ..., m.

- Subroutine KLMO

```
KLMO..                                                                  KLMO  10
/*********************************************************************/KLMO  20
/*                                                                   */KLMO  30
/*      TESTS THE DIFFERENCE BETWEEN EMPIRICAL AND THEORETICAL       */KLMO  40
/*      DISTRIBUTIONS USING THE KOLMOGOROV-SMIRNOV TEST.             */KLMO  50
/*                                                                   */KLMO  60
/*********************************************************************/KLMO  70
   PROCEDURE(X,N,Z,PROB,IFCOD,U,S),.                                    KLMO  80
   DECLARE                                                              KLMO  90
        (X(*),Y,TEMP,PROB,S,U,Z,D,DN,EI,ES,FI,FS) FLOAT BINARY,         KLMO 100
        (I,J,IL,N,IFCOD) FIXED BINARY,                                  KLMO 110
        ERROR EXTERNAL CHARACTER (1),.                                  KLMO 120
   ERROR='0',.                                                          KLMO 130
   IF N LT 100                                                          KLMO 140
   THEN IF N=0                          /* N < 100--SET ERROR IND.     */KLMO 150
        THEN DO,.                                                       KLMO 160
             ERROR='4',.                                                KLMO 170
             GO TO S80,.                                                KLMO 180
             END,.                                                      KLMO 190
        ELSE ERROR='3',.                                                KLMO 200
        DO I=1 TO N-1,.                 /* SORT X INTO                 */KLMO 210
             DO J=I+1 TO N,.            /* ASCENDING SEQUENCE          */KLMO 220
             IF X(I) GT X(J)                                            KLMO 230
             THEN DO,.                                                  KLMO 240
                  TEMP =X(I),.                                          KLMO 250
                  X(I) =X(J),.                                          KLMO 260
                  X(J) =TEMP,.                                          KLMO 270
                  END,.                                                 KLMO 280
             END,.                                                      KLMO 290
        END,.                                                           KLMO 300
                                        /* COMPUTES MAX. DEV. DN IN    */KLMO 310
                                        /* ABS. VAL. BETWEEN EMP. AND  */KLMO 320
                                        /* THEO. FUNCTIONS OVER ALL X  */KLMO 330
   DN,FS=0.0,.                                                          KLMO 340
   IL   =1,.                                                            KLMO 350
S10..                                                                   KLMO 360
        DO I=IL TO N-1,.                                                KLMO 370
        J    =I,.                                                       KLMO 380
        IF X(J)=X(J+1)                                                  KLMO 390
        THEN GO TO S20,.                                                KLMO 400
        ELSE GO TO S40,.                                                KLMO 410
S20..                                                                   KLMO 420
   END,.                                                                KLMO 430
S30..                                                                   KLMO 440
   J    =N,.                                                            KLMO 450
S40..                                                                   KLMO 460
   IL   =J+1,.                                                          KLMO 470
   FI   =FS,.                                                           KLMO 480
   FS   =FLOAT(J)/N,.                   /* EMP. DIST. FUNCT. CALCULATED*/KLMO 490
   IF IFCOD=2                                                           KLMO 500
   THEN DO,.                                                            KLMO 510
        IF S LE 0                                                       KLMO 520
        THEN                                                            KLMO 530
S50..                                                                   KLMO 540
             DO,.                       /* INVALID VALUE OF S          */KLMO 550
             ERROR='1',.                                                KLMO 560
             GO TO S80,.                                                KLMO 570
             END,.                                                      KLMO 580
        ELSE DO,.                       /* EXPONENTIAL PDF             */KLMO 590
             Z    =(X(J)-U)/S+1.0,.                                     KLMO 600
             IF Z LE 0                                                  KLMO 610
             THEN                       /* Z < OR = 0                  */KLMO 620
S60..                                                                   KLMO 630
                  DO,.                                                  KLMO 640
                  Y    =0.0,.                                           KLMO 650
S70..                                                                   KLMO 660
                  EI   =ABS(Y-FI),.                                     KLMO 670
                  ES   =ABS(Y-FS),.                                     KLMO 680
                                        /* COMPUTE MAX. DEV. DN BETWEEN*/KLMO 690
                                        /* EMP. AND THEO. FUNCTIONS    */KLMO 700
                  DN   =MAX(DN,EI,ES),.                                 KLMO 710
                  IF IL=N                                               KLMO 720
                  THEN GO TO S30,.                                      KLMO 730
                  ELSE IF IL LT N                                       KLMO 740
                       THEN GO TO S10,.                                 KLMO 750
                       ELSE DO,.                                        KLMO 760
                                        /* CALC. ASYMPTOTIC VALUES     */KLMO 770
                                        /* USING SMIR                  */KLMO 780
                            Z    =DN*SQRT(N),.                          KLMO 790
                            CALL SMIR (Z,PROB),.                        KLMO 800
                            PROB=1.0E0-PROB,.                           KLMO 810
                            GO TO S80,.                                 KLMO 820
                            END,.                                       KLMO 830
                  END,.                                                 KLMO 840
             ELSE DO,.                  /* EXPONENTIAL PDF             */KLMO 850
                  Y=1.-EXP(-Z),.                                        KLMO 860
                  GO TO S70,.                                           KLMO 870
                  END,.                                                 KLMO 880
             END,.                                                      KLMO 890
        END,.                                                           KLMO 900
   ELSE IF IFCOD LT 2                                                   KLMO 910
        THEN IF S LE 0                                                  KLMO 920
             THEN GO TO S50,.           /* INVALID VALUE OF S          */KLMO 930
             ELSE DO,.                  /* NORMAL PDF                  */KLMO 940
                  Z    =(X(J)-U)/S,.                                   KLMO 950
                  CALL NDTR(Z,Y,D),.                                    KLMO 960
                  GO TO S70,.                                           KLMO 970
                  END,.                                                 KLMO 980
        ELSE IF IFCOD=4                                                 KLMO 990
             THEN IF S LE U                                             KLM01000
                  THEN GO TO S50,.      /* INVALID VAL. OF S OR U      */KLM01010
                  ELSE IF X(J) LE U     /* UNIFORM PDF                 */KLM01020
                       THEN GO TO S60,.                                 KLM01030
                       ELSE IF X(J) LE S                                KLM01040
                            THEN DO,.                                   KLM01050
                                 Y    =(X(J)-U)/(S-U),.                 KLM01060
                                 GO TO S70,.                            KLM01070
                                 END,.                                  KLM01080
                            ELSE DO,.                                   KLM01090
                                 Y    =1.0,.                            KLM01100
                                 GO TO S70,.                            KLM01110
                                 END,.                                  KLM01120
             ELSE IF IFCOD LT 4                                         KLM01130
                  THEN IF S=0           /* INVALID VALUE OF S          */KLM01140
                       THEN GO TO S50,.                                 KLM01150
                       ELSE DO,.        /* CAUCHY PDF                  */KLM01160
                            Y    =ATAN((X(J)-U)/S)*0.3183099+0.5,.      KLM01170
                            GO TO S70,.                                 KLM01180
                            END,.                                       KLM01190
```

```
                ELSE ERROR='2',.    /* USER'S PDF                  */KLM01200
S80..                                                                KLM01210
  RETURN,.                                                           KLM01220
  END,.                             /*END OF PROCEDURE KLMO        */KLM01230
```

Purpose:

KLMO tests the difference between empirical and theoretical distributions using the Kolmogorov-Smirnov test.

Usage:

CALL KLMO (X, N, Z, PROB, IFCOD, U, S);

X(N) - BINARY FLOAT
Given vector of independent observations.

N - BINARY FIXED
Given number of observations in X.

Z - BINARY FLOAT
Resultant variable containing the greatest value with respect to X of $\sqrt{N}$ ($|F_N(x) - F(x)|$), where F(x) is a theoretical distribution function and $F_N(x)$ is an empirical distribution function.

PROB - BINARY FLOAT
Resultant variable containing the probability of the statistic being greater than or equal to Z if the hypothesis that X is from the density under consideration is true. For example, PROB=0.05 implies that X can be considered to be from the density under consideration with 5% probability of being incorrect.
PROB=1. - SMIR (Z).

IFCOD - BINARY FIXED
Given code denoting the particular theoretical probability distribution function being considered. When IFCOD
=1, F(x) is the normal PDF
=2, F(x) is the exponential PDF
=3, F(x) is the Cauchy PDF
=4, F(x) is the uniform PDF
=5, F(x) is user-supplied.

U - BINARY FLOAT
When IFCOD is 1 or 2, U is the given mean of the density given above.
When IFCOD is 3, U is the given median of the Cauchy density.
When IFCOD is 4, U is the given left endpoint of the uniform density.
When IFCOD is 5, U is user-specified.

S - BINARY FLOAT
When IFCOD is 1 or 2, S is the given standard deviation of density given above, and should be positive.
When IFCOD is 3, (U-S) specifies the first quartile of the Cauchy density.
S given should be nonzero.
If IFCOD is 4, S is the given right endpoint of the uniform density. S should be greater than U.
If IFCOD is 5, S is user-specified.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - invalid value of S (if IFCOD = 4, S or U is invalid).
ERROR=2 - requested user's PDF has not been supplied.
ERROR=3 - number of observations less than 100.
ERROR=4 - number of observations equal to zero.

N should be greater than or equal to 100 (see the mathematical background for subroutine SMIR, for the asymptotic formulae). Also, probability levels determined by this program will not be correct if the same samples used in this test are used to estimate parameters for the continuous distribution.

Any user-supplied cumulative probability distribution function should be coded beginning with program comments "USER'S PDF" and should return to S70.

Subroutines and function subroutines required:

SMIR
NDTR

Method:

For references see:

W. Feller, "On the Kolmogorov-Smirnov limit theorems for empirical distributions", Annals of Math. Stat., 19, pp. 177-189.

N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat., 19, pp. 279-281.

R. Von Mises, Mathematical Theory of Probability and Statistics. Academic Press, New York, 1964, pp. 490-493.

B. V. Gnedenko, The Theory of Probability. Chelsea Publishing Co., New York, 1962, pp. 384-401.

H.W. Lilliefors, "On the Kolmogorov-Smirnov test for normality with mean and variance unknown", J.A.S.A., 62 (1967), pp. 399-402.

Mathematical Background:

Given a sample of n independent and identically distributed random variables $X_1, X_2, \ldots, X_n$ with continuous cumulative distribution function F(x), this subroutine tests the difference in absolute value between the empirical distribution $F_n(x)$ and theoretical distribution F(x), using Kolmogorov-Smirnov's limiting distribution.

For this purpose:

1. The order statistics $\{x(i)\}$ are determined from the set $\{x_i\}$ by sorting $\{x_i\}$ into a nondecreasing sequence.

2. The empirical cumulative distribution function $F_n(x)$ is computed. This is the following step-function:

$$F_n(x) = \begin{cases} 0 & x < x_{(1)} \\ k/n & x_{(k)} \le x < x_{(k+1)};\ k=1,\ldots,n-1 \\ 1 & x_{(n)} \le x \end{cases}$$

3. The maximum deviation D_n in absolute value between the empirical and theoretical distribution is computed:

$$D_n = \max_{-\infty<x<\infty} \left| F_n(x) - F(x) \right|$$

Since $F_n(x)$ and F(x) are nondecreasing functions, the result is:

$$D_n = \max_{1\le k\le n} \left| F_n\left[x_{(k)}\right] - F\left[x_{(k)}\right] \right|$$

D_n is a random variable, and L(z) is the limiting cumulative distribution function of $n^{1/2} D_n$:

$$\lim_{n\to\infty} \text{Prob}\left\{n^{1/2} D_n < z\right\} = L(z)$$

4. Finally, the values are computed for:

$$z = n^{1/2} D_n$$

and the probability of being greater than or equal to the computed value of $n^{1/2} D_n$ is computed:

$$P = 1 - L(z)$$

Generally, theoretical distribution functions are to be included by the user, as specified in the program. However, four functions are evaluated in KLMO, as follows:

$$\int_{-\infty}^{x} dF(t) = F(x) \qquad (1)$$

is evaluated at the points of the set $\{X_{(i)}\}$, where F(x) is one of the following:

- The normal pdf with mean u and variance s^2
- The exponential pdf with mean u and variance s^2
- The Cauchy pdf with median u, and first quartile s - u
- The uniform pdf with endpoints u and s

Any user-written pdf should evaluate equation (1) above, using the parameters u and s at his convenience. Instructions given in the program KLMO should be followed.

Lilliefors (1967) notes that critical values determined by this test are not correct when one or more parameters are estimated from the sample. The user should refer to his article for notes on approximations that may be considered if such estimates are used.

Programming Considerations:

It is doubtful that the user will wish to perform this test using double-precision accuracy. However, if one wishes to communicate with KLMO in a double-precision program, he might declare

```
XX FLOAT BINARY (53)
X  FLOAT BINARY
```

Before calling KLMO, the user might do the following:

```
DO I = 1 TO N, .
X(I)  = XX(I), .
END,.
```

After exiting from KLMO, the user might do the the following:

```
DO I = 1 TO N, .
XX(I) = X(I), .
END,.
```

(Note that subroutine SMIR has the double-precision option.)

- Subroutine KLM2

```
KLM2..                                                                  KLM2  10
/*************************************************************************/KLM2  20
/*                                                                       */KLM2  30
/*      TESTS THE DIFFERENCE BETWEEN TWO SAMPLE DISTRIBUTION             */KLM2  40
/*      FUNCTIONS USING THE KOLMOGORCV-SMIRNOV TEST.                     */KLM2  50
/*                                                                       */KLM2  60
/*************************************************************************/KLM2  70
   PROCEDURE(X,Y,N,M,Z,PROB),.                                          KLM2  80
   DECLARE                                                              KLM2  90
        (X(*),Y(*),TEMP,XM1,XN1,Z,PROB,D) FLOAT BINARY,                 KLM2 100
        (I,J,K,L,M,N) FIXED BINARY,                                     KLM2 110
        ERROR EXTERNAL CHARACTER (1),.                                  KLM2 120
   ERROR='0',.                                                          KLM2 130
   IF N LT 100 OR M LT 100              /* M OR N IS LESS THAN 100     */KLM2 140
   THEN IF N=0 OR M=0                   /* SET ERROR INDICATOR         */KLM2 150
        THEN DO,.                                                       KLM2 160
             ERROR='4',.                                                KLM2 170
             GO TO S60,.                                                KLM2 180
             END,.                                                      KLM2 190
        ELSE ERROR='3',.                                                KLM2 200
        DO I=1 TO N-1,.                 /* SORT X INTO                 */KLM2 210
             DO J=I+1 TO N,.            /* ASCENDING SEQUENCE          */KLM2 220
             IF X(I) GT X(J)                                            KLM2 230
             THEN DO,.                                                  KLM2 240
                  TEMP =X(I),.                                          KLM2 250
                  X(I) =X(J),.                                          KLM2 260
                  X(J) =TEMP,.                                          KLM2 270
                  END,.                                                 KLM2 280
             END,.                                                      KLM2 290
        END,.                                                           KLM2 300
        DO I=1 TO M-1,.                 /* SORT Y INTO                 */KLM2 310
             DO J=I+1 TO M,.            /* ASCENDING SEQUENCE          */KLM2 320
             IF Y(I) GT Y(J)                                            KLM2 330
             THEN DO,.                                                  KLM2 340
                  TEMP =Y(I),.                                          KLM2 350
                  Y(I) =Y(J),.                                          KLM2 360
                  Y(J) =TEMP,.                                          KLM2 370
                  END,.                                                 KLM2 380
             END,.                                                      KLM2 390
        END,.                                                           KLM2 400
   XN1  =1/FLOAT(N),.               /* CALC. D=ABS(FN-GM)             */KLM2 410
   XM1  =1/FLOAT(M),.               /* OVER THE SPECTRUM OF X & Y     */KLM2 420
   D,I,J,K,L =0,.                                                       KLM2 430
S10..                                                                   KLM2 440
   IF Y(J+1) GT X(I+1)                                                  KLM2 450
   THEN DO,.                                                            KLM2 460
        K=1,.                                                           KLM2 470
S20..                                                                   KLM2 480
        I=I+1,.                                                         KLM2 490
        IF N LE I                                                       KLM2 500
        THEN DO,.                                                       KLM2 510
             L=1,.                                                      KLM2 520
             GO TO S30,.                                                KLM2 530
             END,.                                                      KLM2 540
        ELSE IF X(I) GE X(I+1)                                          KLM2 550
             THEN GO TO S20,.                                           KLM2 560
             ELSE                                                       KLM2 570
S30..                                                                   KLM2 580
                  IF K = 0                                              KLM2 590
                  THEN                                                  KLM2 600
S40..                                                                   KLM2 610
                       DO,.                                             KLM2 620
                       J=J+1,.                                          KLM2 630
                       IF J LT M                                        KLM2 640
                       THEN IF Y(J+1) LE Y(J)                           KLM2 650
                            THEN GO TO S40,.                            KLM2 660
                            ELSE GO TO S50,.                            KLM2 670
                       ELSE DO,.                                        KLM2 680
                            L=1,.                                       KLM2 690
                            GO TO S50,.                                 KLM2 700
                            END,.                                       KLM2 710
                       END,.                                            KLM2 720
                  ELSE GO TO S50,.                                      KLM2 730
        END,.                                                           KLM2 740
   ELSE IF X(I+1) = Y(J+1)                                              KLM2 750
        THEN DO,.                                                       KLM2 760
             K=0,.                                                      KLM2 770
             GO TO S20,.                                                KLM2 780
             END,.                                                      KLM2 790
        ELSE GO TO S40,.                                                KLM2 800
                                    /* CHOOSE THE MAXIMUM              */KLM2 810
                                    /* DIFFERENCE, D                   */KLM2 820
S50..                                                                   KLM2 830
   D    =MAX(D,ABS(FLOAT(I)*XN1-FLOAT(J)*XM1)),.                        KLM2 840
   IF L=0                                                               KLM2 850
   THEN GO TO S10,.                                                     KLM2 860
   ELSE DO,.                                                            KLM2 870
                                    /* CALCULATE THE STATISTIC Z       */KLM2 880
                                    /* AND Z'S PROBABILITY             */KLM2 890
        Z    =D*SQRT((FLOAT(N)*FLOAT(M))/(FLOAT(N)+FLOAT(M))),.         KLM2 900
        CALL SMIR (Z,PROB),.                                            KLM2 910
        END,.                                                           KLM2 930
S60..                                                                   KLM2 940
   RETURN,.                                                             KLM2 950
   END,.                            /* END OF PROCEDURE KLM2          */KLM2 960
```

Purpose:

KLM2 tests the difference between two sample distribution functions using the Kolmogorov-Smirnov test.

Usage:

CALL KLM2 (X, Y, N, M, Z, PROB);

X(N) - BINARY FLOAT
Given vector containing N independent observations.

Y(M) - BINARY FLOAT
Given vector containing M independent observations.

N - BINARY FIXED
Given number of observations in X.

M - BINARY FIXED
Given number of observations in Y.

Z - BINARY FLOAT
Resultant variable containing the greatest value with respect to the spectrum of X and Y of

$$\sqrt{\frac{MN}{M+N}}\left(\left|F_N(x)-G_M(y)\right|\right)$$

where F_N is the empirical distribution function of the set (x) and $G_M(y)$ is the empirical distribution function of the set (y).

PROB - BINARY FLOAT
Resultant variable containing the probability of the statistic being greater than or equal to Z if the hypothesis that X and Y are from the same PDF is true. For example, PROB=0.05 implies that one can reject the null hypothesis that the sets X and Y are from the same density with 5% probability of being incorrect. PROB=1-SMIR (Z).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=3 - number of observations N, or number of observations M, less than 100.
ERROR=4 - number of observations N, or number of observations M, equal to zero.

See the mathematical background for this subroutine and for subroutine SMIR, concerning asymptotic formulae.

Subroutines and function subroutines required:
SMIR

Method:

For references see:

W. Feller, "On the Kolmogorov-Smirnov limit theorems for empirical distributions", Annals of Math. Stat., 19, pp. 177-189.

N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat., 19, pp. 279-281.

B. V. Gnedenko, The Theory of Probability. Chelsea Publishing Co. New York, 1962, pp. 384-401.

Mathematical Background:

Given a sample of n i.i.d. (independent and indentically distributed) random variables X, and a sample of m i.i.d. random variables Y, this subroutine tests the difference between the two empirical distribution functions $F_n(x)$ and $G_m(y)$ using Kolmogorov-Smirnov's limiting distribution. For this purpose:

1. The sets X and Y are sorted into the ordered sets $\{X_{(i)}\}$ and $\{Y_{(i)}\}$, which are nondecreasing sequences.

2. The empirical cumulative distribution functions $F_n(x)$ for the set X, and $G_m(y)$ for the set Y, are computed. For example,

$$F_n(x) = \begin{cases} 0 & x < x_{(1)} \\ k/n & x_{(k)} \leq x < x_{(k+1)};\ k=1,\ldots,n-1 \\ 1 & x_{(n)} \leq x \end{cases}$$

3. The maximum difference in absolute value between the two sample distribution functions is computed:

$$D_{m,n} = \max_{x,\,y} \left| F_n(x) - G_m(y) \right|$$

The statistic $\sqrt{\frac{mn}{m+n}}\, D_{m,n}$ is a random variable with limiting cumulative distribution function L(z), which is described under subroutine SMIR in this manual. That is,

$$\lim_{m,n\to\infty,\,\infty} \text{Prob}\left\{ \sqrt{\frac{mn}{m+n}}\, D_{m,n} < z \right\} = L(z)$$

4. Finally, the probability (asymptotic) of the statistic $\sqrt{\frac{mn}{m+n}}\, D_{m,n}$ being not less than its computed value, under the assumption of equality of the two theoretical distribution functions from which X and Y were taken, is computed:

$$P = 1 - L(z)$$

Programming Considerations:

It is doubtful that the user will wish to perform this test using double-precision accuracy. However, if one wishes to communicate with KLM2 in a double-precision program, he might declare

```
(XX, YY)   FLOAT BINARY (53)
(Y, X)     FLOAT BINARY
```

giving X and XX, Y and YY the same dimensions.

Before calling KLM2, he might do the following:

```
DO I=1 TO N,.        DO J=1 TO M,.
X(I) =XX(I),.        Y(J) =YY(J),.
END,.                END,.
```

Immediately after exiting from KLM2, he might do the following:

```
DO I=1 TO N,.        DO J=1 TO M,.
XX(I)=X(I),.         YY(J)=Y(J),.
END,.                END,.
```

- Subroutine SMIR

```
SMIR..                                                              SMIR  10
/*******************************************************************/SMIR  20
/*                                                                 */SMIR  30
/*      COMPUTES VALUES OF THE LIMITING DISTRIBUTION FUNCTION FOR THE*/SMIR  40
/*      KOLMOGOROV-SMIRNOV STATISTIC.                              */SMIR  50
/*                                                                 */SMIR  60
/*******************************************************************/SMIR  70
   PROCEDURE (X,Y),.                                                SMIR  80
   DECLARE                                                          SMIR  90
         (X,Y,Q1,Q2,Q4,Q8) FLOAT BINARY,./*SINGLE PRECISION       /*S*/SMIR 100
 /*      (X,Y,Q1,Q2,Q4,Q8) FLOAT BINARY (53),./*DOUBLE PRECISION  /*D*/SMIR 110
   IF X LT 1.0                                                      SMIR 120
   THEN IF X LE .27                  /* X LESS THAN .27-SET Y      */SMIR 130
        THEN Y    =0.0,.                                            SMIR 140
                                     /* CALCULATE L(X)             */SMIR 150
                                     /* IN RANGE (.27,1)           */SMIR 160
        ELSE DO,.                                                   SMIR 170
             Q1   =EXP(-1.233701E0/X**2),.      /* SINGLE PREC.   /*S*/SMIR 180
 /*          Q1   =EXP(-1.2337005013617OE0/X**2),.                 SMIR 190
                                     /* DOUBLE PREC.   /*D*/SMIR 200
             Q2   =Q1*Q1,.                                          SMIR 210
             Q4   =Q2*Q2,.                                          SMIR 220
             Q8   =Q4*Q4,.                                          SMIR 230
             IF Q8-1.0E-25 GE 0                                     SMIR 240
             THEN Y    =(2.506628E0/X)*Q1*(1.0E0+Q8*(1.0E0+Q8*Q8)),. SMIR 250
                                     /* SINGLE PREC.   /*S*/SMIR 260
 /*          THEN Y    =(2.5066282746310O1E0/X)*Q1*(1.0E0+Q8*     SMIR 270
                        (1.0E0+Q8*Q8)),.     /* DOUBLE PREC.   /*D*/SMIR 280
             ELSE Y    =(2.506628E0/X)*Q1,.   /* SINGLE PREC.   /*S*/SMIR 290
 /*          ELSE Y    =(2.5066282746310O1E0/X)*Q1,.               SMIR 300
                                     /* DOUBLE PREC.   /*D*/SMIR 310
             END,.                                                  SMIR 320
   ELSE IF X LT 3.1                                                 SMIR 330
                                     /* CALCULATE L(X)             */SMIR 340
        THEN DO,.                    /* IN RANGE (1,3.1)           */SMIR 350
             Q1   =EXP(-2.0E0*X*X),.                                SMIR 360
             Q2   =Q1*Q1,.                                          SMIR 370
             Q4   =Q2*Q2,.                                          SMIR 380
             Q8   =Q4*Q4,.                                          SMIR 390
             Y    =1.0EC-2.0E0*(Q1-Q4+Q8*(Q1-Q8)),.                 SMIR 400
             END,.                                                  SMIR 410
        ELSE Y    =1.0,.             /* X > OR = 3.1--SET Y        */SMIR 420
   RETURN,.                                                         SMIR 430
   END,.                             /* END OF PROCEDURE SMIR      */SMIR 440
```

Purpose:

SMIR computes values of the limiting distribution function for the Kolmogorov-Smirnov statistic.

Usage:

CALL SMIR (X, Y);

X - BINARY FLOAT [(53)]
Given variable containing the argument of the Smirnov function.

Y - BINARY FLOAT [(53)]
Resultant variable containing the Smirnov function value.

Remarks:

Accuracy tests were made referring to the table given in the reference below.

Two arguments, X=.62, and X=1.87, gave results that differ from the Smirnov tables by 2.9 and 1.9 in the 5th decimal place. All other results showed smaller errors, and error specifications are given in the accuracy tables in this manual. In double-precision mode, these same arguments resulted in differences from tabled values by 3 and 2 in the 5th decimal place. It is noted in Lindgren (reference below) that for high-significance levels (say, .01 and .05) asymptotic formulas give values that are too high (by 1.5% when N=80). That is, at high-significance levels, the hypothesis of no difference will be rejected too seldom using asymptotic formulas.

Method:

For references see:

E. T. Whittaker and G. N. Watson, A Course of Modern Analysis, Cambridge University Press, Cambridge, England, 1952, 462-476.

W. Feller, "On the Kolmogorov-Smirnov limit theorems for empiral distributions", Annals of Math. Stat. 19, pp. 177-189.

N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat. 19, pp. 279-281.

V. W. Lindgren, Statistical Theory, The Macmillan Company, New York, 1962.

Mathematical Background:

This subroutine computes the values of Kolmogorov-Smirnov's limiting distribution for a given argument x.

$$L(x) = \begin{cases} 0 & x \le 0 \\ 1 - 2\sum_{k=1}^{\infty} (-1)^{k-1} \exp(-2k^2x^2) & x > 0 \end{cases} \quad (1)$$

L(x) is the limit (Kolmogorov) of the cumulative distribution function of $\sqrt{n}\, D_n$, and of (Smirnov) $[mn/(m+n)]^{1/2} D_{m,n}$ where:

D_n is the maximum, over all x, of the difference $|F_n(x) - F(x)|$ between the sample distribution function $F_n(x)$ and the continuous theoretical distribution function F(x), and

$D_{m,n}$ is the maximum, over all x, of the difference between the two sample distribution functions $F_m(x)$ and $G_n(x)$, from two independent samples of sizes m and n.

When x is very small, the series (1) converges slowly, but, using Jacobi's theta-functions $\theta_2(u,t)$ and $\theta_4(u,t)$:

$$\theta_2(u,t) = 2\sum_{k=0}^{\infty} \exp\left[i\pi(k+1/2)^2 t\right] \cos\left[(2k+1)u\right]$$

$$\theta_4(u,t) = 1 - 2\sum_{k=0}^{\infty} (-1)^{k-1} \exp(i\pi k^2 t) \cos(2ku)$$

and using the Jacobi imaginary transformation

$$\theta_4(0,t) = (-it)^{-1/2}\,\theta_2(0,\ -1/t)$$

it follows that:

$$L(x) = \theta_4(0,\ 2ix^2/\pi)$$

$$= (\sqrt{2\pi}/x)\sum_{k=1}^{\infty} \exp\left[-(2k-1)^2\pi^2/8x^2\right]$$

which converges quickly when x is small. The computation here uses, with errors $E_i(x)$, i=1,2:

$$L(x) = \begin{cases} 0 & x \le 0.27 \\ (\sqrt{2\pi}/x)\sum_{k=1}^{3} \exp\left[-(2k-1)^2\pi^2/8x^2\right] + E_1(x); & 0.27 < x < 1.0 \\ 1 - 2\sum_{k=1}^{4} (-1)^{k-1} \exp(-2k^2x^2) + E_2(x) & 1.0 \le x < 3.1 \\ 1 & 3.1 \le x < \infty \end{cases}$$

where:

$$E_1(x) \le 6\ (10^{-15}) \text{ when } x < 1$$

$$E_2(x) < 10^{-20} \quad \text{when } x \ge 1$$

- Subroutine CHSQ

```
CHSQ..                                                                  CHSQ  10
/**********************************************************************/CHSQ  20
/*                                                                    */CHSQ  30
/*      TO COMPUTE CHI-SQUARE FROM A CONTINGENCY TABLE.               */CHSQ  40
/*                                                                    */CHSQ  50
/**********************************************************************/CHSQ  60
   PROCEDURE (A,N,M,CS,NDF,P,TP),.                                      CHSQ  70
   DECLARE                                                              CHSQ  80
         ERROR EXTERNAL CHARACTER (1),                                  CHSQ  90
         (A(*,*),CS,GS,TR(N),TC(M),P,TP,E)                              CHSQ 100
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/CHSQ 110
 /*      BINARY FLOAT(53),              /*DOUBLE PRECISION VERSION  /*D*/CHSQ 120
         (I,ICOUNT,J,M,N,NDF,NA,NB,NC,ND,NAB,NCD,NAC,NBD,NZ)            CHSQ 130
         FIXED BINARY,                                                  CHSQ 140
         (WN,F,W,W1,W2,W3,W4) FLOAT BINARY(53),.                        CHSQ 150
/*                                                                    */CHSQ 160
   ERROR='0',.                                                          CHSQ 170
   CS   =0.0,.                                                          CHSQ 180
   P    =0.0,.                                                          CHSQ 190
   TP   =0.0,.                                                          CHSQ 200
   NDF  =(N-1)*(M-1),.              /* FIND DEGREES OF FREEDOM      */CHSQ 210
   IF N LE 1 OR M LE 1                                                  CHSQ 220
   THEN DO,.                                                            CHSQ 230
         ERROR='2',.                /* DEGREES OF FREEDOM = 0       */CHSQ 240
         GO TO FIN,.                                                    CHSQ 250
         END,.                                                          CHSQ 260
/*                                                                    */CHSQ 270
         DO I = 1 TO N,.            /* CALCULATE ROW TOTALS         */CHSQ 280
         TR(I)=0.0,.                                                    CHSQ 290
               DO J = 1 TO M,.                                          CHSQ 300
               TR(I)=TR(I)+A(I,J),.                                     CHSQ 310
               END,.                                                    CHSQ 320
         IF TR(I) LE 0                                                  CHSQ 330
         THEN DO,.                  /* SOME ROW TOTAL = ZERO        */CHSQ 340
               ERROR='3',.                                              CHSQ 350
               GO TO FIN,.                                              CHSQ 360
               END,.                                                    CHSQ 370
         END,.                                                          CHSQ 380
         DO J = 1 TO M,.            /* CALCULATE COLUMN TOTALS      */CHSQ 390
         TC(J)=0.0,.                                                    CHSQ 400
               DO I = 1 TO N,.                                          CHSQ 410
               TC(J)=TC(J)+A(I,J),.                                     CHSQ 420
               END,.                                                    CHSQ 430
         IF TC(J) LE 0                                                  CHSQ 440
         THEN DO,.                                                      CHSQ 450
               ERROR='3',.          /* SOME COLUMN TOTAL = ZERO     */CHSQ 460
               GO TO FIN,.                                              CHSQ 470
               END,.                                                    CHSQ 480
         END,.                                                          CHSQ 490
   GS   =0.0,.                      /* COMPUTE GRAND SUM            */CHSQ 500
         DO I = 1 TO N,.                                                CHSQ 510
         GS   =GS+TR(I),.                                               CHSQ 520
         END,.                                                          CHSQ 530
/*                                                                    */CHSQ 540
/*      COMPUTE CHI-SQUARE FOR 2 BY 2 TABLE (SPECIAL CASE)            */CHSQ 550
/*                                                                    */CHSQ 560
   IF N = 2 AND M = 2                                                   CHSQ 570
   THEN DO,.                                                            CHSQ 580
               CS   =GS*(ABS(A(1,1)*A(2,2)-A(2,1)*A(1,2))               CHSQ 590
                     -GS/2.0)**2/(TC(1)*TC(2)*TR(1)*TR(2)),.            CHSQ 600
         IF GS GT 40.0                                                  CHSQ 610
         THEN GO TO FIN,.                                               CHSQ 620
         ELSE DO,.                                                      CHSQ 630
               IF (TR(1)*TC(1))/GS GE 5.0 AND                           CHSQ 640
                  (TR(2)*TC(1))/GS GE 5.0 AND                           CHSQ 650
                  (TR(1)*TC(2))/GS GE 5.0 AND                           CHSQ 660
                  (TR(2)*TC(2))/GS GE 5.0                               CHSQ 670
               THEN GO TO FIN,.                                         CHSQ 680
               ELSE DO,.                                                CHSQ 690
                     NA   =A(1,1),.                                     CHSQ 700
                     NB   =A(1,2),.                                     CHSQ 710
                     NC   =A(2,1),.                                     CHSQ 720
                     ND   =A(2,2),.                                     CHSQ 730
                     K    =1,.                                          CHSQ 740
/*                                                                    */CHSQ 750
/*      OBTAIN THE MARGINAL TOTALS AND GRAND TOTAL                    */CHSQ 760
/*                                                                    */CHSQ 770
                  NAB  =NA+NB,.                                         CHSQ 780
                   NCD  =NC+ND,.                                        CHSQ 790
                   NAC  =NA+NC,.                                        CHSQ 800
                   NBD  =NB+ND,.                                        CHSQ 810
                   NZ   =NA+NB+NC+ND,.                                  CHSQ 820
/*                                                                    */CHSQ 830
/*      COMPUTE N FACTORIAL                                           */CHSQ 840
/*                                                                    */CHSQ 850
                  WN    =1,.                                            CHSQ 860
                   IF NZ GT 1                                           CHSQ 870
                   THEN DO,.                                            CHSQ 880
                              DO I = 2 TO NZ,.                          CHSQ 890
                              FI   =I,.                                 CHSQ 900
                              WN   =WN*FI,.                             CHSQ 910
                              END,.                                     CHSQ 920
                        END,.                                           CHSQ 930
/*                                                                    */CHSQ 940
/*      COMPUTE EXACT PROBABILITY                                     */CHSQ 950
/*                                                                    */CHSQ 960
S10..                                                                   CHSQ 970
                  W1    =1,.                                            CHSQ 980
                   IF NB GT 0                                           CHSQ 990
                   THEN DO,.                                            CHSQ1000
                        J    =NA+1,.                                    CHSQ1010
                              DO I = J TO NAB,.                         CHSQ1020
                              FI   =I,.                                 CHSQ1030
                              W1   =W1*FI,.                             CHSQ1040
                              END,.                                     CHSQ1050
                        END,.                                           CHSQ1060
                   W2   =1.0,.                                          CHSQ1070
                   IF NC GT 0                                           CHSQ1080
                   THEN DO,.                                            CHSQ1090
                        J    =ND+1,.                                    CHSQ1100
                              DO I = J TO NCD,.                         CHSQ1110
                              FI   =I,.                                 CHSQ1120
                              W2   =W2*FI,.                             CHSQ1130
                              END,.                                     CHSQ1140
                        END,.                                           CHSQ1150
                   W3   =1.0,.                                          CHSQ1160
                   IF NA GT 0                                           CHSQ1170
                   THEN DO,.                                            CHSQ1180
                        J    =NC+1,.                                    CHSQ1190
                              DO I = J TO NAC,.                         CHSQ1200
                              FI   =I,.                                 CHSQ1210
                              W3   =W3*FI,.                             CHSQ1220
                              END,.                                     CHSQ1230
```

```
                    END,.                                                CHSQ1240
                W4  =1.0,.                                               CHSQ1250
                IF ND GT 0                                               CHSQ1260
                THEN DO,.                                                CHSQ1270
                     J    =NB+1,.                                        CHSQ1280
                          DO I = J TO NBD,.                              CHSQ1290
                          FI   =I,.                                      CHSQ1300
                          W4   =W4*FI,.                                  CHSQ1310
                          END,.                                          CHSQ1320
                     END,.                                               CHSQ1330
                W1  =W1*W2*W3*W4,.                                       CHSQ1340
                W   =W1/WN,.                                             CHSQ1350
                P   =P+W,.                                               CHSQ1360
                IF K GT 1                                                CHSQ1370
                THEN TP  =TP+W,.                                         CHSQ1380
                K   =K+1,.                                               CHSQ1390
/*                                                                      */CHSQ1400
/*      TEST WHETHER FREQUENCY IS ZERO (0)                              */CHSQ1410
/*                                                                      */CHSQ1420
              IF NA LE 0 OR NB LE 0 OR NC LE 0 OR ND LE 0                CHSQ1430
               THEN GO TO FIN,.                                          CHSQ1440
/*                                                                      */CHSQ1450
/*      ADJUST DATA IN ORDER TO COMPUTE THE PROBABILITY ASSOCIATED      */CHSQ1460
/*      WITH MORE EXTREME FREQUENCIES (BUT WITH SAME MARGINAL TOTALS)   */CHSQ1470
/*                                                                      */CHSQ1480
              IF NA LE NB                                                CHSQ1490
               THEN DO,.                                                 CHSQ1500
                    IF NC LE ND                                          CHSQ1510
                    THEN DO,.                                            CHSQ1520
                         IF NA GT NC                                     CHSQ1530
                         THEN GO TO S20,.                                CHSQ1540
                         END,.                                           CHSQ1550
                    GO TO S25,.                                          CHSQ1560
                    END,.                                                CHSQ1570
               IF NC GT ND                                               CHSQ1580
               THEN DO,.                                                 CHSQ1590
                    IF NB GT ND                                          CHSQ1600
                    THEN GO TO S25,.                                     CHSQ1610
                    END,.                                                CHSQ1620
/*                                                                      */CHSQ1630
/*      MOVE B TO A AND C TO D                                          */CHSQ1640
/*                                                                      */CHSQ1650
S20..                                                                    CHSQ1660
              NA    =NA+1,.                                              CHSQ1670
               NB   =NB-1,.                                              CHSQ1680
               NC   =NC-1,.                                              CHSQ1690
               ND   =ND+1,.                                              CHSQ1700
               GO TO S10,.                                               CHSQ1710
/*                                                                      */CHSQ1720
/*      MOVE A TO B AND D TO C                                          */CHSQ1730
/*                                                                      */CHSQ1740
S25..                                                                    CHSQ1750
              NA    =NA-1,.                                              CHSQ1760
               NB   =NB+1,.                                              CHSQ1770
               NC   =NC+1,.                                              CHSQ1780
               ND   =ND-1,.                                              CHSQ1790
               GO TO S10,.                                               CHSQ1800
               END,.                                                     CHSQ1810
          END,.                                                          CHSQ1820
        END,.                          /* END OF TWO BY TWO CASE       */CHSQ1830
/*                                                                      */CHSQ1840
/*      COMPUTE CHI SQUARE FOR OTHER CONTINGENCY TABLES                 */CHSQ1850
/*                                                                      */CHSQ1860
        ICOUNT=0,.                                                       CHSQ1870
        DO J = 1 TO M,.                                                  CHSQ1880
             DO I = 1 TO N,.                                             CHSQ1890
             E    =TR(I)*TC(J)/GS,.                                      CHSQ1900
             IF E LE 5.0                                                 CHSQ1910
             THEN ICOUNT=ICOUNT+1,.                                      CHSQ1920
             CS   =CS+(A(I,J)-E)*(A(I,J)-E)/E,.                          CHSQ1930
             END,.                                                       CHSQ1940
        END,.                                                            CHSQ1950
   IF ICOUNT GT 0                                                        CHSQ1960
   THEN ERROR='1',.                    /* SOME EXPECTED VALUES ARE     */CHSQ1970
/*                                     /* LESS THAN 5.0                */CHSQ1980
FIN..                                                                    CHSQ1990
   RETURN,.                                                              CHSQ2000
   END,.                               /* END OF PROCEDURE CHSQ        */CHSQ2010
```

Purpose:

CHSQ computes chi-square from a contingency table.

Usage:

CALL CHSQ (A, N, M, CS, NDF, P, TP);

A(N,M) - BINARY FLOAT [(53)]
Given matrix containing contingency table of integer values.

N - BINARY FIXED
Given number of rows in matrix A.

M - BINARY FIXED
Given number of columns in matrix A.

CS - BINARY FLOAT [(53)]
Resultant chi-square.

NDF - BINARY FIXED
Resultant number of degrees of freedom.

P - BINARY FLOAT [(53)]
Resultant exact probability for a 2x2 contingency table. If the contingency table is not 2x2, the value of P will be zero (P=0).

TP - BINARY FLOAT [(53)]
Resultant variable containing the probability by the Tocher-modification method for a 2x2 contingency table. If the contingency table is not 2x2, the value of TP will be set to zero (TP=0).

Remarks:

P, CS, and TP above are computed only when the contingency table is 2x2, the total of the frequencies is less than or equal to 40, and the expected frequency in any cell is less than five.

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - some expected values less than 5.0.
ERROR=2 - degrees of freedom equal to zero.
ERROR=3 - some row total or column total less than or equal to zero.

Method:

Described in S. Siegel Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapters 6 and 8.

Mathematical Background:

When the observations are classified by two characteristics (two-way classification), the chi-square test may be used to test the hypothesis that the two characteristics are independent--namely, that the distribution of one characteristic is the same regardless of the other characteristic. Two-way-classification tables of this type are frequently called contingency tables, and different formulas are used to compute chi-square for the following two types of contingency tables:

1. For 2 x 2 table:

$$a.\ \chi^2 = \frac{N\left(\left|AD-BC\right| - \frac{N}{2}\right)^2}{(A+B)\ (C+D)\ (A+C)\ (B+D)} \qquad (1)$$

where A, B, C, and D stand for frequencies in a 2 x 2 table as shown below, and N = A + B + C + D.

	Yes	No
Male	A	B
Female	C	D

b. If $N \leq 40$ and the expected frequency in any cell is 5, the Fisher exact probability is computed.

The exact probability of observing a particular set of frequencies in a 2 x 2 table, when the marginal totals are regarded as fixed, is given by the formula:

$$p = \frac{(A+B)!\ (C+D)!\ (A+C)!\ (B+D)!}{N!\ A!\ B!\ C!\ D!} \qquad (2)$$

However, more extreme distributions of frequencies could occur with the same marginal totals.

To find the Fisher exact probability, we add the probability of obtaining the existing distribution of frequencies to the probabilities of obtaining all the more extreme distributions of frequencies.

The more extreme distributions of frequencies are determined by systematically subtracting one from the smallest frequency in the table, while keeping the marginal totals fixed. This iterative process continues until the smallest cell has a zero value. This is the most extreme case.

$$p_F = p_a + p_b + p_c + \ldots .$$

For example:

Observed data

table a

2	6	8
4	2	6
6	8	14

More extreme outcomes with same marginal totals

table b

1	7	8
5	1	6
6	8	14

table c

0	8	8
6	0	6
6	8	14

$$p_a = \frac{8!\ 6!\ 6!\ 8!}{14!\ 2!\ 6!\ 4!\ 2!} = 20/143 = .13986$$

$$p_b = \frac{8!\ 6!\ 6!\ 8!}{14!\ 1!\ 7!\ 5!\ 1!} = 16/1001 = .01598$$

$$p_c = \frac{8!\ 6!\ 6!\ 8!}{14!\ 0!\ 8!\ 6!\ 0!} = 1/3003 = .00033$$

The probability associated with the occurrence of values as extreme or more extreme than those observed (table a) is given by adding the three probabilities

$.13986 + .01598 + .00033 = .15617$

Thus, $p_F = .15617$ is the Fisher exact probability.

Tocher's modification determines the probability of all cases more extreme than the observed one, and not including the observed one.

$$p_T = p_b + p_c + \ldots . \qquad (3)$$

That is,

$$p_T = p_F - p_a \qquad (4)$$

For the example in tables a, b, and c:

$p_T = .01598 + .00033 = .01631$ using equation (3)

$p_T = .15617 - .13986 = .01631$ using equation (4)

The probability (p_T) provided by Tocher's modification to the Fisher exact test is for a one-tailed test of H_0. For a two-tailed test, the p_T yielded must be doubled.

2. For other contingency tables:

$$\chi^2 = \sum_{i=1}^{n} \sum_{j=1}^{m} \frac{(A_{ij} - E_{ij})^2}{E_{ij}} \qquad (5)$$

where:

A_{ij} = frequency in the cell i, j

$$E_{ij} = \frac{T_i\ T_j}{N} \qquad (6)$$

$$T_i = \sum_{j=1}^{n} A_{ij} \qquad i = 1, 2, \ldots, n \text{ (row totals)} \qquad (7)$$

$$T_j = \sum_{i=1}^{n} A_{ij} \quad j = 1, 2, \ldots, m \text{ (column totals)} \tag{8}$$

$$N = \sum_{i=1}^{n} T_i \quad \text{(grand total)} \tag{9}$$

The degrees of freedom:

$$\text{d. f.} = (n - 1)\ (m - 1) \tag{10}$$

- Subroutine KRNK

```
KRNK..                                                                  KRNK  10
/*********************************************************************/KRNK  20
/*                                                                   */KRNK  30
/*      TO TEST CORRELATION BETWEEN TWO VARIABLES BY MEANS OF THE    */KRNK  40
/*      KENDALL RANK CORRELATION COEFFICIENT.                        */KRNK  50
/*                                                                   */KRNK  60
/*********************************************************************/KRNK  70
   PROCEDURE (A,B,R1,R2,N,TAU,SD,Z,NR),.                                KRNK  80
   DECLARE                                                              KRNK  90
        (A(*),B(*),R1(*),R2(*),TAU,SD,Z,RSAVE,SAVER,S,TA,TB,FN1,FN)     KRNK 100
        FLOAT BINARY,                                                   KRNK 110
        (I,ISORT,J,KT,N,NR)                                             KRNK 120
        BINARY FIXED,                                                   KRNK 130
        ERROR EXTERNAL CHARACTER (1),.                                  KRNK 140
/*                                                                   */KRNK 150
   ERROR='0',.                          /* INITIALIZATION            */KRNK 160
        DO I=1 TO N,.                                                   KRNK 170
        R1(I)     =0,.                                                  KRNK 180
        R2(I)     =0,.                                                  KRNK 190
        END,.                                                           KRNK 200
   TAU  =0.0,.                                                          KRNK 210
   SD   =0.0,.                                                          KRNK 220
   Z    =0.0,.                                                          KRNK 230
   IF N LE 1                            /* NUMBER OF OBSERVATIONS LESS */KRNK 240
   THEN DO,.                            /* THAN OR EQUAL TO ONE.     */KRNK 250
        ERROR='1',.                                                     KRNK 260
        GO TO FIN,.                                                     KRNK 270
        END,.                                                           KRNK 280
   FN   =N,.                                                            KRNK 290
   FN1  =N*(N-1),.                                                      KRNK 300
   IF NR= 1                             /* DETERMINE IF DATA IS RANKED */KRNK 310
   THEN DO,.                                                            KRNK 320
             DO I = 1 TO N,.                                            KRNK 330
             R1(I)=A(I),.               /* MOVE RANKED DATA TO R1 R2   */KRNK 340
             R2(I)=B(I),.                                               KRNK 350
             END,.                                                      KRNK 360
        END,.                                                           KRNK 370
   ELSE DO,.                                                            KRNK 380
/*                                                                   */KRNK 390
/*      RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS     */KRNK 400
/*      AVERAGE OF TIED RANKS.                                       */KRNK 410
/*                                                                   */KRNK 420
        CALL RANK (A,R1,N),.                                            KRNK 430
        CALL RANK (B,R2,N),.                                            KRNK 440
        END,.                                                           KRNK 450
S10..                                                                   KRNK 460
   ISORT=0,.                                                            KRNK 470
/*                                                                   */KRNK 480
/*      SORT RANK VECTORS R1 AND R2 IN SEQUENCE OF VARIABLE A        */KRNK 490
/*                                                                   */KRNK 500
        DO I = 2 TO N,.                                                 KRNK 510
        IF R1(I) LT R1(I-1)                                             KRNK 520
        THEN DO,.                                                       KRNK 530
             ISORT=ISORT+1,.                                            KRNK 540
             RSAVE=R1(I),.                                              KRNK 550
             R1(I)=R1(I-1),.                                            KRNK 560
             R1(I-1)=RSAVE,.                                            KRNK 570
             SAVER=R2(I),.                                              KRNK 580
             R2(I)=R2(I-1),.                                            KRNK 590
             R2(I-1)=SAVER,.                                            KRNK 600
             END,.                                                      KRNK 610
        END,.                                                           KRNK 620
   IF ISORT NE 0                                                        KRNK 630
   THEN GO TO S1C,.                                                     KRNK 640
/*                                                                   */KRNK 650
/*      COMPUTE S ON VARIABLE B. STARTING WITH THE FIRST RANK, ADD 1 */KRNK 660
/*      TO S FOR EACH LARGER RANK TO ITS RIGHT AND SUBTRACT 1 FOR    */KRNK 670
/*      EACH SMALLER RANK. REPEAT FOR ALL RANKS.                     */KRNK 680
/*                                                                   */KRNK 690
   S    =0,.                                                            KRNK 700
        DO I = 1 TO N-1,.                                               KRNK 710
             DO J = I+1 TO N,.                                          KRNK 720
             IF R2(J) GT R2(I)                                          KRNK 730
             THEN S    =S+1.0,.                                         KRNK 740
             ELSE IF R2(J) LT R2(I)                                     KRNK 750
             THEN S    =S-1.0,.                                         KRNK 760
             END,.                                                      KRNK 770
        END,.                                                           KRNK 780
/*                                                                   */KRNK 790
/*      COMPUTE TIED SCORE INDEX FOR BOTH VARIABLES                  */KRNK 800
/*                                                                   */KRNK 810
   KT   =2,.                                                            KRNK 820
   CALL TIE (R1,N,KT,TA),.                                              KRNK 830
   IF ERROR='2'                                                         KRNK 840
   THEN                                                                 KRNK 850
S20..                                                                   KRNK 860
        DO,.                            /* ALL RANKS FOR ONE VARIABLE */KRNK 870
        ERROR='3',.                     /* ARE EQUAL                  */KRNK 880
        GO TO FIN,.                                                     KRNK 890
        END,.                                                           KRNK 900
   CALL TIE (R2,N,KT,TB),.                                              KRNK 910
   IF ERROR='2'                                                         KRNK 920
   THEN GO TO S20,.                                                     KRNK 930
   IF TA= 0.0 AND TB = 0.0              /* COMPUTE TAU                */KRNK 940
   THEN TAU  =S/(0.5*FN1),.                                             KRNK 950
   ELSE TAU  =S/((SQRT(C.5*FN1-TA))*(SQRT(0.5*FN1-TB))),.               KRNK 960
/*                                                                   */KRNK 970
/*      COMPUTE STANDARD DEVIATION AND Z VALUE IF N IS 10 OR GREATER */KRNK 980
/*                                                                   */KRNK 990
   IF N GE 10                                                           KRNK1000
   THEN DO,.                                                            KRNK1010
        SD   =(SQRT((2.0*(FN+FN+5))/(9.0*FN1))),.                       KRNK1020
        Z    =TAU/SD,.                                                  KRNK1030
        END,.                                                           KRNK1040
   ELSE ERROR='2',.                     /* SAMPLE SIZE LESS THAN 10   */KRNK1050
FIN..                                                                   KRNK1060
   RETURN,.                                                             KRNK1070
   END,.                                /*END OF PROCEDURE KRNK       */KRNK1080
```

Purpose:

KRNK measures the correlation between two variables by means of the Kendall rank correlation coefficient.

Usage:

CALL KRNK (A, B, R1, R2, N, TAU, SD, Z, NR);

A(N) - BINARY FLOAT
Given vector containing observations for the first variable.

B(N) - BINARY FLOAT
Given vector containing observations for the second variable.

R1(N) - BINARY FLOAT
Resultant vector containing rank of the data in vector A.

R2(N) - BINARY FLOAT
Resultant vector containing rank of the data in vector B.

N - BINARY FIXED
Given number of observations.

TAU - BINARY FLOAT
Resultant variable containing the Kendall rank correlation coefficient.

SD - BINARY FLOAT
Resultant variable containing standard deviation.

Z - BINARY FLOAT
Resultant variable containing statistic to be used to measure the significance of TAU in terms of normal distribution.

NR - BINARY FIXED
Given code containing the following:
0 - for raw data in vectors A and B.
1 - for the rank of data in vectors A and B.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations less than or equal to one.

ERROR=2 - sample size less then 10. If this condition exists, R1 and R2 will contain invalid values; SD and Z will be set to zero.

ERROR=3 - all ranks for one variable are equal.

Subroutines and function subroutines required:
RANK
TIE

Method:

Described in S. Siegel, Nonparameteric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 9.

Mathematical Background:

The subroutine computes the Kendall rank correlation coefficient, given two vectors of n observations for two variables, A and B. The observations on each variable are ranked from 1 to n. Tied observations are assigned the average of the tied ranks. Ranks are sorted in sequence of variable A.

A correction factor for ties is obtained:

$$T_a = \sum \frac{t(t-1)}{2} \quad \text{for variable A}$$

$$T_b = \sum \frac{t(t-1)}{2} \quad \text{for variable B} \qquad (1)$$

where t = number of observations tied for a given rank.

The Kendall rank correlation coefficient is then computed for the following two cases:

(1) if T_a and T_b are zero,

$$\tau = \frac{S}{\frac{1}{2} n (n-1)} \qquad (2)$$

where:

n = number of ranks
S = total score calculated for ranks in variable B by selecting each rank in turn, adding 1 for each larger rank to its right, subtracting 1 for each smaller rank to its right.

(2) if T_a and/or T_b are not zero,

$$\tau = \frac{S}{\sqrt{\frac{1}{2} n (n-1) - T_a}\sqrt{\frac{1}{2} n (n-1) - T_b}} \qquad (3)$$

The standard deviation is calculated:

$$s = \sqrt{\frac{2(2n+5)}{9n(n-1)}} \qquad (4)$$

The statistic used to measure the significance of τ is:

$$z = \frac{\tau}{s}$$

- Subroutine QTST

```
QTST..                                                          QTST  10
/*****************************************************************/QTST  20
/*                                                               */QTST  30
/*      TO TEST WHETHER THREE OR MORE MATCHED GROUPS OF DICHOTOMOUS */QTST  40
/*      DATA DIFFER SIGNIFICANTLY BY THE COCHRAN Q-TEST.         */QTST  50
/*                                                               */QTST  60
/*****************************************************************/QTST  70
   PROCEDURE (A,N,M,Q,NDF),.                                    QTST  80
   DECLARE                                                      QTST  90
         ERROR EXTERNAL CHARACTER (1),                          QTST 100
         (A(*,*),TR(N),TC(M),Q,RSQ,CSQ,GD,FM)                   QTST 110
         BINARY FLOAT,                                          QTST 120
         (I,J,M,N,NDF)                                          QTST 130
         BINARY FIXED,.                                         QTST 140
/*                                                             */QTST 150
                                                                QTST 160
   ERROR='0',.                                                  QTST 170
   IF M LT 3 OR N LE 1                  /* NUMBER OF CASES IN EACH  */QTST 180
   THEN DO,.                            /* GROUP IS LESS THAN 3 OR  */QTST 190
         ERROR='1',.                    /* THE NUMBER OF OBSERVATIONS */QTST 200
         GO TO FIN,.                    /* IS LESS THAN OR EQUAL TO */QTST 210
         END,.                          /* ONE.                     */QTST 220
   FM   =M,.                                                    QTST 230
/*                                                             */QTST 240
/*      COMPUTE SUM OF SQUARES OF ROW AND COLUMN TOTALS RSQ AND CSQ, */QTST 250
/*      AND GRAND TOTAL OF ALL ELEMENTS.                         */QTST 260
/*                                                               QTST 270
         DO I = 1 TO N,.                                        QTST 280
         TR(I)=0.0,.                                            QTST 290
               DO J = 1 TO M,.                                  QTST 300
               TR(I)=TR(I)+A(I,J),.                             QTST 310
               END,.                                            QTST 320
         END,.                                                  QTST 330
         DO J = 1 TO M,.                /* CALCULATE COLUMN SUMS    */QTST 340
         TC(J)=0.0,.                                            QTST 350
               DO I = 1 TO N,.                                  QTST 360
               TC(J)=TC(J)+A(I,J),.                             QTST 370
               END,.                                            QTST 380
         END,.                                                  QTST 390
   Q     =0.0,.                                                 QTST 400
   NDF   =0.0,.                                                 QTST 410
   GD    =0.0,.                                                 QTST 420
   RSQ   =0.0,.                                                 QTST 430
   CSQ   =0.0,.                                                 QTST 440
         DO I = 1 TO N,.                                        QTST 450
         GD    =GD+TR(I),.              /* GRAND TOTAL              */QTST 460
         RSQ   =RSQ+TR(I)*TR(I),.       /* SUM OF ROW TOTAL SQUARED */QTST 470
         END,.                                                  QTST 480
         DO J = 1 TO M,.                                        QTST 490
         CSQ   =CSQ+TC(J)*TC(J),.       /* SUM OF COLUMN TOTAL SQUARED */QTST 500
         END,.                                                  QTST 510
   Q     =FM*GD-RSQ,.                                           QTST 520
   IF Q LT 1                            /* TEST FOR Q NEAR ZERO     */QTST 530
   THEN DO,.                                                    QTST 540
         ERROR='2',.                                            QTST 550
         GO TO FIN,.                                            QTST 560
         END,.                                                  QTST 570
/*                                                             */QTST 580
/*    COMPUTE COCHRAN Q TEST VALUE.                            */QTST 590
/*                                                             */QTST 600
   Q     =(FM-1.0)*(FM*CSQ-GD*GD)/(FM*GD-RSQ),.                 QTST 610
   NDF   =M-1,.                         /* FIND DEGREES OF FREEDOM  */QTST 620
FIN..                                                           QTST 630
   RETURN,.                                                     QTST 640
   END,.                                /*END OF PROCEDURE QTST     */QTST 650
```

Purpose:

QTST uses the Cochran Q-test to determine whether three or more matched groups of dichotomous data differ significantly.

Usage:

CALL QTST (A, N, M, Q, NDF);

A(N,M) - BINARY FLOAT
Given matrix of dichotomous data. Data elements must be either 0 or 1.

N - BINARY FIXED
Given number of sets in each group.

M - BINARY FIXED
Given number of groups.

Q - BINARY FLOAT
Resultant Cochran Q statistic.

NDF - BINARY FIXED
Resultant number of degrees of freedom.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of groups, M, is less than three and/or the number of sets, N, is less than or equal to one.

ERROR=2 - all values of matrix A are equal.

Method:

Described in S. Siegel, Nonparameteric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 7.

Mathematical Background:

This subroutine determines the Cochran Q-test statistic, given a matrix A of dichotomous data with n rows (sets) and m columns (groups).

Row and column totals are calculated:

$$L_i = \sum_{j=1}^{m} A_{ij} \qquad \text{(row totals)} \tag{1}$$

where i = 1, 2, . . . , n

$$G_j = \sum_{i=1}^{n} A_{ij} \qquad \text{(column totals)} \tag{2}$$

where j = 1, 2, . . . , m

The Cochran Q statistic is computed:

$$Q = \frac{(m-1)\left[m\sum_{j=1}^{m} G_j^2 - \left(\sum_{j=1}^{m} G_j\right)^2\right]}{m\sum_{i=1}^{n} L_i - \sum_{i=1}^{n} L_i^2} \tag{3}$$

The degrees of freedom are:

$$\text{d.f.} = m - 1 \tag{4}$$

- Subroutine RANK

```
RANK..
/*********************************************************************/
/*                                                                   */
/*      TO RANK A VECTOR OF VALUES.                                  */
/*                                                                   */
/*********************************************************************/
   PROCEDURE (A,R,N),.
   DECLARE
        ERROR EXTERNAL CHARACTER(1),
        (A(*),R(*),EQUAL,P,SMALL,X)
        BINARY FLOAT,
        (I,J,N)
        BINARY FIXED,.
/*                                                                   */
   ERROR='0',.
        DO I = 1 TO N,.
        R(I) =0.0,.
        END,.
   IF N LE 1
   THEN DO,.                          /* VECTOR LENGTH IS ONE OR LESS*/
        ERROR='1',.
        GO TO FIN,.
        END,.
/*                                                                   */
/*      FIND RANK OF DATA                                            */
/*                                                                   */
        DO I = 1 TO N,.
/*                                                                   */
/*      TEST WHETHER DATA POINT IS ALREADY RANKED                    */
/*                                                                   */
        IF R(I) LE 0
        THEN DO,.
             SMALL=0.0,.
             EQUAL=0.0,.
             X    =A(I),.              /* DATA POINT TO BE RANKED    */
                  DO J = 1 TO N,.
                  IF A(J) LT X
/*                                                                   */
/*      COUNT NUMBER OF DATA POINTS WHICH ARE SMALLER                */
/*                                                                   */
                  THEN SMALL=SMALL+1.0,.
                  ELSE IF A(J)= X
                  THEN DO,.
/*                                                                   */
/*      COUNT NUMBER OF DATA POINTS WHICH ARE EQUAL                  */
/*                                                                   */
                       EQUAL=EQUAL+1,.
                       R(J) =-1.0,.
                       END,.
                  END,.
             IF EQUAL LE 1.0            /* TEST FOR TIE              */
/*                                                                   */
/*      STORE RANK OF DATA POINT WHERE NO TIE                        */
/*                                                                   */
             THEN R(I) =SMALL+1.0,.
/*                                                                   */
/*      CALCULATE RANK OF TIED DATA POINTS                           */
/*                                                                   */
             ELSE P    =SMALL+(EQUAL+1.0)/2.0,.
                  DO J = 1 TO N,.
                  IF R(J)= -1.0
                  THEN R(J) =P,.
                  END,.
             END,.
        END,.
FIN..
   RETURN,.
   END,.                              /*END OF PROCEDURE RANK       */
```

Purpose:

RANK ranks a vector of data.

Usage:

CALL RANK (A, R, N);

A(N) - BINARY FLOAT
Given vector containing data to be ranked.

R(N) - BINARY FLOAT
Resultant vector containing the ranks of the data in A. Smallest value is ranked 1; largest is ranked N. Ties are assigned the average of the tied ranks.

N - BINARY FIXED
Given number of values.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR=1 - vector length one or less.

Method:

Vector is searched for successively larger elements. If ties occur, they are located and their rank value is computed. For example, if two values are tied for sixth rank, they are assigned a rank of 6.5 (=(6+7) /2).

- Subroutine SRNK

```
SRNK..                                                              SRNK  10
/*******************************************************************/SRNK  20
/*                                                                 */SRNK  30
/*      TO TEST CORRELATION BETWEEN TWO VARIABLES BY MEANS OF      */SRNK  40
/*      SPEARMAN RANK CORRELATION COEFFICIENT.                     */SRNK  50
/*                                                                 */SRNK  60
/*******************************************************************/SRNK  70
   PROCEDURE (A,B,R1,R2,N,RS,T,NDF,NR),.                            SRNK  80
   DECLARE                                                          SRNK  90
         (A(*),B(*),R1(*),R2(*),RS,T,D,X,Y,TSA,TSB,FNN)             SRNK 100
         BINARY FLOAT,                                              SRNK 110
         (KT,N,NDF,NR)                                              SRNK 120
         BINARY FIXED,                                              SRNK 130
         ERROR EXTERNAL CHARACTER (1),.                             SRNK 140
/*                                                                 */SRNK 150
   FNN  =N*N*N-N,.                                                  SRNK 160
   NDF  =0,.                                                        SRNK 170
   T    =0.0,.                                                      SRNK 180
   RS   =0.0,.                                                      SRNK 190
   ERROR='0',.                                                      SRNK 200
         DO I=1 TO N,.                                              SRNK 210
         R1(I)      =0,.                                            SRNK 220
         R2(I)      =0,.                                            SRNK 230
         END,.                                                      SRNK 240
   IF N LE 1                          /* NUMBER OF OBSERVATIONS IS  */SRNK 250
   THEN DO,.                          /*LESS THAN OR EQUAL TO ONE.  */SRNK 260
         ERROR='1',.                                                SRNK 270
         GO TO FIN,.                                                SRNK 280
         END,.                                                      SRNK 290
/*                                                                 */SRNK 300
/*      DETERMINE WHETHER DATA IS RANKED.                          */SRNK 310
/*                                                                 */SRNK 320
   IF NR NE 1                                                       SRNK 330
/*                                                                 */SRNK 340
/*      RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS   */SRNK 350
/*      AVERAGE OF TIED RANKS.                                     */SRNK 360
/*                                                                 */SRNK 370
   THEN DO,.                                                        SRNK 380
         CALL RANK (A,R1,N),.                                       SRNK 390
         CALL RANK (B,R2,N),.                                       SRNK 400
         END,.                                                      SRNK 410
   ELSE DO,.                                                        SRNK 420
              DO I = 1 TO N,.       /* MOVE RANKED DATA             */SRNK 430
              R1(I)=A(I),.                                          SRNK 440
              R2(I)=B(I),.                                          SRNK 450
              END,.                                                 SRNK 460
         END,.                                                      SRNK 470
/*                                                                 */SRNK 480
/*      COMPUTE SUM OF SQUARES OF RANK DIFFERENCES.                */SRNK 490
/*                                                                 */SRNK 500
   D    =0,.                                                        SRNK 510
         DO I = 1 TO N,.                                            SRNK 520
         D    =D+(R1(I)-R2(I))**2,.                                 SRNK 530
         END,.                                                      SRNK 540
   KT   =1,.                                                        SRNK 550
   CALL TIE (R1,N,KT,TSA),.           /* COMPUTE TIED SCORE INDEX  */SRNK 560
   IF ERROR='2'                       /* ALL RANKS FOR ONE VARIABLE*/SRNK 570
   THEN                               /* ARE EQUAL                 */SRNK 580
S10..                                                               SRNK 590
         DO,.                       /* ALL RANKS FOR ONE VARIABLE  */SRNK 600
         ERROR='3',.                /* ARE EQUAL                   */SRNK 610
         GO TO FIN,.                                                SRNK 620
         END,.                                                      SRNK 630
   CALL TIE (R2,N,KT,TSB),.                                         SRNK 640
   IF ERROR='2'                                                     SRNK 650
   THEN GO TO S10,.                                                 SRNK 660
/*                                                                 */SRNK 670
/*      COMPUTE SPEARMAN RANK CORRELATION COEFFICIENT              */SRNK 680
/*                                                                 */SRNK 690
   IF TSA NE 0 AND TSB NE 0                                         SRNK 700
   THEN DO,.                                                        SRNK 710
         X    =FNN/12.0-TSA,.                                       SRNK 720
         Y    =X+TSA-TSB,.                                          SRNK 730
         RS   =(X+Y-D)/(2.0*(SQRT(X*Y))),.                          SRNK 740
         END,.                                                      SRNK 750
   ELSE RS   =1.0-6.0*D/FNN,.                                       SRNK 760
/*                                                                 */SRNK 770
/*      COMPUTE T AND DEGREES OF FREEDOM IF N IS 10 OR LARGER      */SRNK 780
/*                                                                 */SRNK 790
   IF N GE 10                                                       SRNK 800
   THEN DO,.                                                        SRNK 810
         T    =RS*SQRT((N-2.0)/(1.0-RS*RS)),.                       SRNK 820
         NDF  =N-2,.                                                SRNK 830
         END,.                                                      SRNK 840
   ELSE ERROR='2',.                   /* SAMPLE SIZE LESS THAN 10  */SRNK 850
FIN..                                                               SRNK 860
   RETURN..                                                         SRNK 870
   END,.                              /*END OF PROCEDURE SRNK      */SRNK 880
```

Purpose:

SRNK tests the correlation between two variables by means of the Spearman rank correlation coefficient.

Usage:

CALL SRNK (A, B, R1, R2, N, RS, T, NDF, NR);

A(N) - BINARY FLOAT
Given vector containing the observations for the first variable.

B(N) - BINARY FLOAT
Given vector containing the observations for the second variable.

R1(N) - BINARY FLOAT
Resultant vector containing rank of the data in vector A.

R2(N) - BINARY FLOAT
Resultant vector containing rank of the data in vector B.

N - BINARY FIXED
Given number of observations.

RS - BINARY FLOAT
Resultant variable containing the Spearman rank correlation coefficients.

T - BINARY FLOAT
Resultant variable containing the measure to be used to test the significance of RS.

NDF - BINARY FIXED
Resultant variable containing the number of degrees of freedom.

NR - BINARY FIXED
Given code containing the following:
0 - for raw data in vectors A and B.
1 - for the rank of data in vectors A and B.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of observations less than or equal to one. If this condition exists, R1 and R2 will contain invalid values.

ERROR=2 - sample size less than 10. (T and NDF are not computed if this condition is detected.)

ERROR=3 - All ranks for one variable are equal.

Procedures and function procedures required:
RANK
TIE

Method:

Described in S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 9.

Mathematical Background:

This subroutine measures the correlation between two variables by means of the Spearman rank correlation coefficient, given two vectors of n observations for the variables.

The observations on each variable are ranked from 1 to n. Tied observations are assigned the average of the tied ranks.

The sum of squares of rank differences is calculated:

$$D = \sum_{i=1}^{n} (A_i - B_i)^2 \qquad (1)$$

where:

A_i = first ranked vector

B_i = second ranked vector

n = number of ranks

A correction factor for ties is obtained:

$$T_a = \sum \frac{t^3 - t}{12} \quad \text{over variable A}$$

$$T_b = \sum \frac{t^3 - t}{12} \quad \text{over variable B} \qquad (2)$$

where t = number of observations tied for a given rank.

The Spearman rank correlation coefficient is then computed for the following two cases:

(1) if T_a and T_b are zero

$$r_s = 1 - \frac{6D}{n^3 - n} \qquad (3)$$

(2) if T_a and/or T_b are not zero

$$r_s = \frac{X + Y - D}{2\sqrt{XY}} \qquad (4)$$

where:

$$X = \frac{N^3 - N}{12} - T_a \qquad (5)$$

$$Y = \frac{N^3 - N}{12} - T_b \qquad (6)$$

The significance of r_s can be measured by the statistic:

$$t = r_s \sqrt{\frac{N-2}{1-r_s^2}} \qquad (7)$$

The degrees of freedom are:

$$\text{d. f.} = N-2 \qquad (8)$$

- Subroutine TIE

```
TIE..                                                                  TIE   10
/*********************************************************************/TIE   20
/*                                                                   */TIE   30
/*      TO CALCULATE CORRELATION FACTOR DUE TO TIES.                 */TIE   40
/*                                                                   */TIE   50
/*********************************************************************/TIE   60
   PROCEDURE (R,N,KT,T),.                                              TIE   70
   DECLARE                                                             TIE   80
        (R(*),T,X,Y,CT)                                                TIE   90
        BINARY FLOAT,  .                                               TIE  100
        ERROR EXTERNAL CHARACTER(1),                                   TIE  110
        (I,IND,KT,N)                                                   TIE  120
        BINARY FIXED,.                                                 TIE  130
/*                                                                    */TIE  140
   ERROR='0',.                                                         TIE  150
   IF N LE 1                                                           TIE  160
   THEN DO,.                          /* VECTOR LENGTH IS ONE OR LESS*/TIE  170
        ERROR='1',.                                                    TIE  180
        GO TO FIN,.                                                    TIE  190
        END,.                                                          TIE  200
   T    =0.0,.                        /* INITIALIZATION             */TIE  210
   Y    =0.0,.                                                         TIE  220
S10..                                                                  TIE  230
   X    =N+1,.                                                         TIE  240
   IND  =0,.                                                           TIE  250
        DO I = 1 TO N,.               /* FIND NEXT LARGEST RANK     */TIE  260
        IF R(I) GT Y AND R(I) LT X                                     TIE  270
        THEN DO,.                                                      TIE  280
             X    =R(I),.                                              TIE  290
             IND  =IND+1,.                                             TIE  300
             END,.                                                     TIE  310
        END,.                                                          TIE  320
/*                                                                    */TIE  330
/*      IF ALL RANKS HAVE BEEN TESTED RETURN                         */TIE  340
/*                                                                    */TIE  350
   IF IND NE 0                                                         TIE  360
   THEN DO,.                                                           TIE  370
        Y    =X,.                                                      TIE  380
        CT   =0.0,.                                                    TIE  390
             DO I = 1 TO N,.          /* COUNT TIES                 */TIE  400
             IF R(I)= X                                                TIE  410
             THEN CT   =CT+1.0,.                                       TIE  420
             END,.                                                     TIE  430
        IF CT NE 0.0                                                   TIE  440
        THEN DO,.                                                      TIE  450
             IF KT= 1                                                  TIE  460
             THEN T    =T+(CT*CT*CT-CT)/12.0,.                         TIE  470
             ELSE T    =T+CT*(CT-1.0)/2.0,.                            TIE  480
             END,.                                                     TIE  490
        GO TO S10,.                                                    TIE  500
        END,.                                                          TIE  510
FIN..                                                                  TIE  520
   IF CT=N                            /* ALL RANKS FOR ONE VARIABLE */TIE  530
   THEN ERROR='2',.                   /* ARE EQUAL                  */TIE  540
   RETURN,.                                                            TIE  550
   END,.                              /*END OF PROCEDURE TIE        */TIE  560
```

Purpose:

TIE calculates correction factor due to ties.

Usage:

CALL TIE (R, N, KT, T);

R(N) - BINARY FLOAT
Given vector of ranks containing values from 1 to N.

N - BINARY FIXED
Given number of ranked values.

KT - BINARY FIXED
Given code for calculation of correction factor
1 - solve equation 1
2 - solve equation 2

T - BINARY FLOAT
Resultant variable containing correction factor
Equation 1 T=SUM(CT**3-CT)/12
Equation 2 T=SUM(CT*(CT-1)/2)
where CT is the number of observations tied for a given rank.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - vector length one or less.
ERROR=2 - all ranks of one variable are equal.

Method:

Vector is searched for successively larger ranks. Ties are counted and correction factor 1 or 2 summed.

• Subroutine TWAV

```
TWAV..                                                              TWAV  10
/*******************************************************************/TWAV  20
/*                                                                 */TWAV  30
/*      TO TEST WHETHER A NUMBER OF SAMPLES ARE FROM THE SAME      */TWAV  40
/*      POPULATION BY THE FRIEDMAN TWO-WAY ANALYSIS OF VARIANCE    */TWAV  50
/*      TEST.                                                      */TWAV  60
/*                                                                 */TWAV  70
/*******************************************************************/TWAV  80
   PROCEDURE (A,R,N,M,XR,NDF,NR),.                                  TWAV  90
   DECLARE                                                          TWAV 100
         ERROR EXTERNAL CHARACTER (1),                              TWAV 110
         (A(*,*),R(*,*),WA(M),WB(M),XR,FM,FNM,RTSQ)                 TWAV 120
         BINARY FLOAT,                                              TWAV 130
         (I,NR,N,M,NDF)                                             TWAV 140
         BINARY FIXED,.                                             TWAV 150
/*                                                                 */TWAV 160
   ERROR='0',.                                                      TWAV 170
   XR   =0.0,.                                                      TWAV 180
   NDF  =0,.                                                        TWAV 190
   IF M LT 3 OR N LE 1              /* THE NUMBER OF CASES IS LESS */TWAV 200
   THEN DO,.                        /* THAN 3 OR THE NUMBER OF     */TWAV 210
         ERROR='1',.                /* GROUPS IS LESS THAN OR EQUAL*/TWAV 220
         GO TO FIN,.                /* TO ONE                      */TWAV 230
         END,.                                                      TWAV 240
   FM   =M,.                                                        TWAV 250
   FNM  =N*(M+1),.                                                  TWAV 260
   IF NR NE 1                                                       TWAV 270
   THEN DO,.                                                        TWAV 280
/*                                                                 */TWAV 290
/*      RANK DATA IN EACH GROUP AND ASSIGN TIED OBSERVATIONS       */TWAV 300
/*      AVERAGE OF TIED RANK.                                      */TWAV 310
/*                                                                 */TWAV 320
            DO I = 1 TO N,.                                         TWAV 330
               DO J = 1 TO M,.                                      TWAV 340
               WA(J)=A(I,J),.                                       TWAV 350
               END,.                                                TWAV 360
            CALL RANK (WA,WB,M),.                                   TWAV 370
               DO J = 1 TO M,.                                      TWAV 380
               R(I,J)=WB(J),.                                       TWAV 390
               END,.                                                TWAV 400
            END,.                                                   TWAV 410
         END,.                                                      TWAV 420
   ELSE DO,.                                                        TWAV 430
            DO I = 1 TO N,.                                         TWAV 440
               DO J = 1 TO M,.                                      TWAV 450
               R(I,J)=A(I,J),.                                      TWAV 460
               END,.                                                TWAV 470
            END,.                                                   TWAV 480
         END,.                                                      TWAV 490
/*                                                                 */TWAV 500
/*      CALCULATE SUM OF SQUARES OF SUMS OF RANKS                  */TWAV 510
/*                                                                 */TWAV 520
   RTSQ =0.0,.                                                      TWAV 530
         DO I = 1 TO M,.                                            TWAV 540
         WA(I)=0.0,.                                                TWAV 550
               DO J = 1 TO N,.                                      TWAV 560
               WA(I)=WA(I)+R(J,I),.                                 TWAV 570
               END,.                                                TWAV 580
         RTSQ =RTSQ+WA(I)*WA(I),.                                   TWAV 590
         END,.                                                      TWAV 600
/*                                                                 */TWAV 610
/*      CALCULATE FRIEDMAN TEST VALUE, XR, AND DEGREES OF FREEDOM  */TWAV 620
/*                                                                 */TWAV 630
   XR   =(12.0/(FM*FNM))*RTSQ-3.0*FNM,.                             TWAV 640
   NDF  =M-1,.                                                      TWAV 650
FIN..                                                               TWAV 660
   RETURN,.                                                         TWAV 670
   END,.                            /*END OF PROCEDURE TWAV        */TWAV 680
```

Purpose:

TWAV tests whether a number of samples are from the same population, by the Friedman two-way analysis of variance test.

Usage:

CALL TWAV (A, R, N, M, XR, NDF, NR);

A(N,M) - BINARY FLOAT
Given matrix of original data.

R(N,M) - BINARY FLOAT
Resultant matrix of the ranks of the data.

N - BINARY FIXED
Given number of groups.

M - BINARY FIXED
Given number of cases in each group.

XR - BINARY FLOAT
Resultant Friedman statistic.

NDF - BINARY FIXED
Resultant number of degrees of freedom.

NR - BINARY FIXED
Given code:
0 for raw data in A;
1 for ranks of the data in A.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitutes the possible error condition that may be detected:

ERROR=1 - number of groups less than or equal to one, or number of cases less than three.

Subroutines and function subroutines required:

RANK

Method:

Described in S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 7.

Mathematical Background:

This subroutine determines the Friedman two-way analysis of variance statistic, given a matrix A with n rows (groups) and m columns (cases). Data in each group is ranked from 1 to m. Tied observations are assigned the average of the tied ranks.

The sum of ranks is calculated:

$$R_j = \sum_{i=1}^{n} A_{ij} \qquad (1)$$

Friedman's statistic is then computed:

$$\chi_r^2 = \frac{12}{nm(m+1)} \sum_{j=1}^{m} (R_j)^2 - 3n(m+1) \qquad (2)$$

The degrees of freedom are:

$$d.f. = m - 1 \qquad (3)$$

- Subroutine UTST

```
UTST..                                                                  UTST  10
/*********************************************************************/UTST  20
/*                                                                   */UTST  30
/*      TO TEST WHETHER TWO INDEPENDENT GROUPS ARE FROM THE SAME     */UTST  40
/*      POPULATION BY MEANS OF A MANN-WHITNEY U-TEST.                */UTST  50
/*                                                                   */UTST  60
/*********************************************************************/UTST  70
   PROCEDURE (A,R,N1,N2,U,Z),.                                          UTST  80
   DECLARE                                                              UTST  90
        ERROR EXTERNAL CHARACTER (1),                                   UTST 100
        (A(*),R(*),U,Z,R2,UP,TS,S,FN,FN2,FNX)                           UTST 110
        BINARY FLOAT,                                                   UTST 120
        (I,KT,N,N1,N2)                                                  UTST 130
        BINARY FIXED,.                                                  UTST 140
/*                                                                     */UTST 150
   ERROR='0',.                                                          UTST 160
/*                                                                     */UTST 170
/*      RANK SCORES FROM BOTH GROUPS TOGETHER IN ASCENDING ORDER,      */UTST 180
/*      AND ASSIGN TIED OBSERVATIONS AVERAGE OF TIED RANKS             */UTST 190
/*                                                                     */UTST 200
   N    =N1+N2,.                                                        UTST 210
        DO I=1 TO N,.                                                   UTST 220
        R(I) =0,.                                                       UTST 230
        END,.                                                           UTST 240
   U    =0.0,.                                                          UTST 250
   Z    =0.0,.                                                          UTST 260
   IF N1 GT N2                                                          UTST 270
   THEN DO,.                                                            UTST 280
        ERROR='1',.                    /* N1 IS GREATER THAN N2       */UTST 290
        GO TO FIN,.                                                     UTST 300
        END,.                                                           UTST 310
   IF N LE 2                                                            UTST 320
   THEN DO,.                           /* COMBINED SAMPLE LESS THAN OR*/UTST 330
        ERROR='2',.                    /* EQUAL TO TWO.               */UTST 340
        GO TO FIN,.                                                     UTST 350
        END,.                                                           UTST 360
   CALL RANK (A,R,N),.                                                  UTST 370
   IF N1 LE 1 OR N2 LE 1                                                UTST 380
   THEN DO,.                                                            UTST 390
        ERROR='2',.                                                     UTST 400
        GO TO FIN,.                                                     UTST 410
        END,.                                                           UTST 420
   R2   =0.0,.                         /* SUM RANKS IN LARGE GROUP    */UTST 430
        DO I = N1+1 TO N,.                                              UTST 440
        R2   =R2+R(I),.                                                 UTST 450
        END,.                                                           UTST 460
   FNX  =N1*N2,.                                                        UTST 470
   FN   =N,.                                                            UTST 480
   FN2  =N2,.                                                           UTST 490
   UP   =FNX+FN2*((FN2+1.0)/2.0)-R2,. /* CALCULATE U                  */UTST 500
   U    =FNX-UP,.                                                       UTST 510
   IF UP LT U                                                           UTST 520
   THEN U    =UP,.                                                      UTST 530
   IF N1 GE 10                         /* TEST FOR N1 LESS THAN 10    */UTST 540
   THEN DO,.                                                            UTST 550
        KT   =1,.                                                       UTST 560
        CALL TIE (R,N,KT,TS),.         /* COMPUTE STANDARD DEVIATION  */UTST 570
        IF ERROR='2'                                                    UTST 580
        THEN DO,.                      /* ALL RANKS FOR ONE VARIABLE  */UTST 590
             ERROR='4',.               /* ARE EQUAL                   */UTST 600
             GO TO FIN,.                                                UTST 610
             END,.                                                      UTST 620
        IF TS NE 0                                                      UTST 630
        THEN S    =SQRT((FNX/(FN*(FN-1.0)))*(((FN*FN*FN-FN)/12.)-TS)),.UTST 640
        ELSE S    =SQRT(FNX*(FN+1.0)/12.0),.                            UTST 650
        Z    =(U-FNX*0.5)/S,.                                           UTST 660
        END,.                                                           UTST 670
   ELSE ERROR='3',.                    /* NUMBER OF CASES IN THE      */UTST 680
FIN..                                  /* SMALLER GROUP IS LESS THAN  */UTST 690
   RETURN,.                            /* TEN                         */UTST 700
   END,.                               /*END OF PROCEDURE UTST        */UTST 710
```

Purpose:

UTST tests whether two independent groups are from the same population, by means of Mann-Whitney U-test.

Usage:

CALL UTST (A, R, N1, N2, U, Z);

A(N) - BINARY FLOAT
Given vector of cases consisting of two independent groups. Smaller group precedes larger group. N = N1 + N2.

R(N) - BINARY FLOAT
Resultant vector of ranks. Smallest value is ranked 1; largest is ranked N. Ties are assigned average of tied ranks.

N1 - BINARY FIXED
Given number of cases in smaller group.

N2 - BINARY FIXED
Given number of cases in larger group.

U - BINARY FLOAT
Resultant statistic used to test homogeneity of the two groups.

Z - BINARY FLOAT
Resultant measure for determining the significance of U in terms of normal distribution (if N1 is less than 10, Z is set to zero).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - N1 greater than N2.
ERROR=2 - Combined samples less than or equal to two.
ERROR=3 - number of cases in the smaller group is less than 10 (in this case Z is set to zero).
ERROR=4 - all ranks for one variable are equal.

Subroutines and function subroutines required:

RANK
TIE

Method:

Described in S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 6.

Mathematical Background:

This subroutine tests whether two independent groups are from the same population, by means of the Mann-Whitney U-test, given an input vector A with the smaller group preceding the larger group. The scores for both groups are ranked together in ascending order. Tied observations are assigned the average of the tied ranks.

The sum of ranks in the larger group, R2, is calculated. The U statistic is then computed as follows:

$$U' = n_1 n_2 + \frac{n_2 (n_2 + 1)}{2} - R_2 \qquad (1)$$

where:

n_1 = number of cases in smaller group

n_2 = number of cases in larger group

$U = n_1 n_2 - U'$

if $U' < U$, set $U = U'$ (2)

A correction factor for ties is obtained:

$$T = \sum \frac{t^3 - t}{12} \quad (3)$$

where t = number of observations tied for a given rank.

The standard deviation is computed for two cases:

(1) if T = 0

$$s = \sqrt{\frac{n_1 n_2 (n_1 + n_2 + 1)}{12}} \quad (4)$$

(2) if T > 0

$$s = \sqrt{\left(\frac{n_1 n_2}{N(N-1)}\right)\left(\frac{N^3 - N}{12} - T\right)} \quad (5)$$

where N = total number of cases $(n_1 + n_2)$

The measure used to determine the significance of U is then calculated:

$$Z = \frac{U - \overline{X}}{S} \quad (6)$$

where $\overline{X}$ = mean = $\frac{N1\ N2}{2}$

Z is set to zero if N1 is less than 10.

- Subroutine WTST

```
WTST..                                                                  WTST  10
/*********************************************************************/WTST  20
/*                                                                   */WTST  30
/*      TO TEST DEGREE OF ASSOCIATION AMONG A NUMBER OF VARIABLES    */WTST  40
/*      BY THE KENDALL COEFFICIENT OF CONCORDANCE.                   */WTST  50
/*                                                                   */WTST  60
/*********************************************************************/WTST  70
   PROCEDURE (A,R,N,M,W,CS,NDF,NR),.                                    WTST  80
   DECLARE                                                              WTST  90
        ERROR EXTERNAL CHARACTER (1),                                   WTST 100
        (A(*,*),R(*,*),WA(M),WB(M),W,CS,SM,S,TI,T,FN,FM)                WTST 110
        BINARY FLOAT,                                                   WTST 120
        (I,J,KT,M,N,NDF,NR)                                             WTST 130
        BINARY FIXED,.                                                  WTST 140
/*                                                                   */WTST 150
   ERROR='0',.                                                          WTST 160
        DO I=1 TO N,.                                                   WTST 170
             DO J=1 TO M,.                                              WTST 180
             R(I,J)    =0,.                                             WTST 190
             END,.                                                      WTST 200
        END,.                                                           WTST 210
   W    =0.0,.                                                          WTST 220
   CS   =0.0,.                                                          WTST 230
   NDF  =0,.                                                            WTST 240
   IF N LT 3 OR M LT 3                                                  WTST 250
   THEN DO,.                                                            WTST 260
        ERROR='1',.                  /* NUMBER OF VARIABLES (N) OR   */WTST 270
        GO TO FIN,.                  /* NUMBER OF CASES (M) IS LESS  */WTST 280
        END,.                        /* THAN 3                       */WTST 290
/*                                                                   */WTST 300
/*      DETERMINE WHETHER DATA IS RANKED. IF IT HAS NOT BEEN DONE    */WTST 310
/*      RANK DATA FOR ALL VARIABLES ASSIGNING TIED OBSERVATIONS      */WTST 320
/*      AVERAGE OF TIED RANKS AND COMPUTE CORRECTION FOR TIED SCORES */WTST 330
/*                                                                   */WTST 340
   T    =0,.                                                            WTST 350
   KT   =1,.                                                            WTST 360
        DO I = 1 TO N,.                                                 WTST 370
        IF NR NE 1                                                      WTST 380
        THEN DO,.                                                       WTST 390
                  DO J = 1 TO M,.                                       WTST 400
                  WA(J)=A(I,J),.                                        WTST 410
                  END,.                                                 WTST 420
             CALL RANK (WA,WB,M),.                                      WTST 430
             END,.                                                      WTST 440
        ELSE DO,.                                                       WTST 450
                  DO J = 1 TO M,.                                       WTST 460
                  WB(J)=A(I,J),.                                        WTST 470
                  END,.                                                 WTST 480
             END,.                                                      WTST 490
        CALL TIE (WB,M,KT,TI),.                                         WTST 500
        IF ERROR='2'                                                    WTST 510
        THEN DO,.                                                       WTST 520
             ERROR='3',.             /* ALL RANKS FOR ONE VARIABLE   */WTST 530
             GO TO FIN,.             /* ARE EQUAL                    */WTST 540
             END,.                                                      WTST 550
        T    =T+TI,.                                                    WTST 560
             DO J = 1 TO M,.                                            WTST 570
             R(I,J)=WB(J),.                                             WTST 580
             END,.                                                      WTST 590
        END,.                                                           WTST 600
   FN   =N,.                                                            WTST 610
   FM   =M,.                                                            WTST 620
   SM   =0.0,.                                                          WTST 630
/*                                                                   */WTST 640
/*      CALCULATE VECTOR SUMS AND COMPUTE MEANS OF SUMS              */WTST 650
/*                                                                   */WTST 660
        DO J = 1 TO M,.                                                 WTST 670
        WA(J)=0.0,.                                                     WTST 680
             DO I = 1 TO N,.                                            WTST 690
             WA(J)=WA(J)+R(I,J),.                                       WTST 700
             END,.                                                      WTST 710
        SM   =SM+WA(J),.                                                WTST 720
        END,.                                                           WTST 730
   SM   =SM/FM,.                                                        WTST 740
/*                                                                   */WTST 750
/*      COMPUTE THE SUM OF SQUARES OF DEVIATION                      */WTST 760
/*                                                                   */WTST 770
   S    =0,.                                                            WTST 780
        DO J = 1 TO M,.                                                 WTST 790
        S    =S+(WA(J)-SM)**2,.                                         WTST 800
        END,.                                                           WTST 810
   W    =S/(((FN*FN)*(FM*FM*FM-FM)/12.0)-FN*T),.                        WTST 820
/*                                                                   */WTST 830
/*      COMPUTE DEGREES OF FREEDOM AND CHI-SQUARE IF M IS OVER 7     */WTST 840
/*                                                                   */WTST 850
   IF M GT 7                                                            WTST 860
   THEN DO,.                                                            WTST 870
        CS   =FN*(FM-1.0)*W,.                                           WTST 880
        NDF  =M-1,.                                                     WTST 890
        END,.                                                           WTST 900
   ELSE ERROR='2',.                  /* NUMBER OF CASES (M) IS LESS */WTST 910
/*                                   /* THAN OR EQUAL TO 7          */WTST 920
FIN..                                                                   WTST 930
   RETURN,.                                                             WTST 940
   END,.                             /*END OF PROCEDURE WTST        */WTST 950
```

Purpose:

WTST measures the degree of association among a number of variables by the Kendall coefficient of concordance.

Usage:

CALL WTST (A, R, N, M, W, CS, NDF, NR);

A(N, M) - BINARY FLOAT
Given matrix of original data.

R(N, M) - BINARY FLOAT
Resultant matrix, N by M, of the ranks of the data. Smallest value is ranked 1; largest is ranked M. Ties are assigned average of tied ranks. The data is ranked by rows.

N - BINARY FIXED
Given number of variables.

M - BINARY FIXED
Given number of cases.

W - BINARY FLOAT
Resultant variable containing Kendall coefficient of concordance.

CS - BINARY FLOAT
Resultant variable containing the value of chi-square.

NDF - BINARY FIXED
Resultant variable containing number of degrees of freedom.

NR - BINARY FIXED
Given code containing the following:
0 for raw data in A.
1 for the rank of data in A.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR = 1 - number of variables, N, or number of cases, M, less than three.
ERROR = 2 - number of cases, M, less than or equal to seven (CS and NDF are set to zero.)
ERROR = 3 - all ranks for one variable are equal.

Subroutines and function subroutines are required:

RANK
TIE

Method:

Described in S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 6.

Mathematical Background:

This subroutine computes the Kendall coefficient of concordance, given a matrix A of n rows (variables) and m columns (cases). The observations on all variables are ranked from 1 to m. Tied observations are assigned the average of the tied ranks.

A correction factor for ties is obtained:

$$T = \sum_{i=1}^{n} \frac{t^3 - t}{12} \tag{1}$$

where t = number of observations tied for a given rank.

Sums of ranks are calculated:

$$Y_j = \sum_{i=1}^{n} R_{ij} \tag{2}$$

where j = 1, 2, ..., m.

From these, the mean of sums of ranks is found:

$$\bar{R} = \frac{\sum_{j=1}^{m} Y_j}{m} \tag{3}$$

The sum of squares of deviations is derived:

$$S = \sum_{j=1}^{m} (Y_j - \bar{R})^2 \tag{4}$$

The Kendall coefficient of concordance is then computed:

$$W = \frac{S}{\frac{1}{12} n^2 (m^3 - m) - n T} \tag{5}$$

For m larger than 7, chi-square is:

$$\chi^2 = n (m - 1) W \tag{6}$$

The degrees of freedom are:

$$d.f. = n - 1 \tag{7}$$

- Subroutine HTES

```
HTES..
/*********************************************************************/
/*                                                                   */
/*      TO CALCULATE THE KRUSKAL-WALLIS H-STATISTIC FROM THE RANKS   */
/*      OF OBSERVATIONS WHICH ARE OBTAINED FROM THREE OR MORE INDE-  */
/*      PENDENT SAMPLES.                                             */
/*                                                                   */
/*********************************************************************/
   PROCEDURE (A,R,M,NS,H),.
   DECLARE
        (A(*),R(*),H,S,SUMR,T,XK,XN)
        BINARY FLOAT,
        (M(*),I,J,K,L,N,NS)
        BINARY FIXED,
        ERROR EXTERNAL CHARACTER (1),.
/*
        ERROR='0',.                    /* INITIALIZATION
   H    =0.0,.
   IF NS LT 3
   THEN ERROR='1',.                    /* SET ERROR INDICATOR
   ELSE DO,.
        N    =0,.
             DO I = 1 TO NS,.          /* CALCULATE TOTAL NUMBER OF
             IF M(I) LE 0              /* CASES IN ALL SAMPLES
             THEN DO,.
                  ERROR='3',.
                  GO TO S10,.
                  END,.
             N    =N+M(I),.
             END,.
        XN   =N,.
/*
/*      RANK DATA FROM ALL SAMPLES IN ASCENDING ORDER AND ASSIGN
/*      TIED OBSERVATIONS AVERAGE OF TIED RANKS
/*
        CALL RANK (A,R,N),.
/*
        S    =0,.
        J    =0,.
             DO I = 1 TO NS,.
             K    =M(I),.
             XK   =K,.
             SUMR =0.0,.
                  DO L = 1 TO K,.      /* SUM RANKS FOR EACH SAMPLE
                  J    =J+1,.
                  SUMR =SUMR+R(J),.
                  END,.
             S    =S+SUMR*SUMR/XK,.
             END,.
/*
/*      CALCULATE H, UNCORRECTED FOR TIES
/*
        H    =((12.0*S)/(XN*XN+XN))-3.0*(XN+1),.
/*
/*      COMPUTE CORRECTION FACTOR FOR TIES
/*
        K    =1,.
        CALL TIE (R,N,K,T),.
        IF T = 0.0 OR ERROR='2'
        THEN GO TO S10,.
        ELSE DO,.
             S    =1.0-((12.0*T)/(XN**3-XN)),.
/*
/*      CORRECT H FOR TIES
/*
             H    =H/S,.
             END,.
        END,.
S10..
   RETURN,.
   END,.                              /*END OF PROCEDURE HTES
```

Purpose:

HTES calculates the Kruskal-Wallis H-statistic from the ranks of observations obtained from three or more independent samples.

Usage:

CALL HTES (A, R, M, NS, H);

A(N) - BINARY FLOAT
Given vector of observed data stored columnwise. In other words, the data from the first sample, second, third, etc., are stored in consecutive locations of vector A. N=M(1)+M(2)+...+M(NS) (that is, the total number of cases)

R(N) - BINARY FLOAT
Resultant vector containing the ranks of data of vector A. The smallest value is ranked one, and the largest is ranked N. Ties are assigned the average of the tied ranks.

M - BINARY FIXED
Given vector of length NS containing the number of cases in each sample.

NS - BINARY FIXED
Given variable containing the number of samples.

H - BINARY FLOAT
Resultant variable containing the value of H-statistic.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - number of samples, NS, less than three. If this condition exists, R will contain invalid values.

ERROR=2 - all ranks for one variable are equal.

ERROR=3 - the number of cases in one of the samples is less than or equal to zero. If this condition exists, R will contain invalid values.

Subroutines and function subroutines required:

TIE
RANK

Method:

Refer to:

The computational procedures are described in S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw Hill, New York, 1956, chapter 8.

Mathematical Background:

From the data in vector A, the ranks are computed by the subroutine RANK and stored in vector R according to ascending values of the cases, with ties assigned the average of the tied ranks. The ranks are summed for each sample, and the H-statistic is calculated from the formula:

$$H = \left[\frac{12}{N(N+1)} \sum_{i=1}^{NS} \frac{SUMR_i^2}{M_i} \right] -3(N+1) \qquad (1)$$

where:

N = total number of cases

$SUMR_i$ = sum of ranks for the i-th sample
M_i = number of cases in the i-th sample
NS = the number of samples

H is corrected for ties, if present, using the value of T obtained from procedure TIE. The correction formula is:

$$H_{corrected} = \frac{H_{uncorrected}}{1 - \frac{12T}{N^3 - N}} \qquad (2)$$

where:

$$T = \sum \frac{(t^3 - t)}{12}, \text{ summed over all samples}$$

t = number of tied observations in a group

H is approximately distributed as χ^2 with (NS-1) degrees of freedom, if the number of cases in each group is not too small (not less than five).

Distribution Functions

- Subroutine NDTR

```
NDTR:.                                                              NDTR  10
/*******************************************************************NDTR  20
/*                                                                  */NDTR  30
/*      COMPUTES Y=P(X)=THE PROBABILITY THAT THE RANDOM VARIABLE U,  */NDTR  40
/*      DISTRIBUTED NORMALLY (0,1) IS LESS THAN OR EQUAL TO X.  F(X),*/NDTR  50
/*      THE ORDINATE OF THE NORMAL DENSITY AT X, IS ALSO COMPUTED.   */NDTR  60
/*                                                                  */NDTR  70
/*******************************************************************NDTR  80
   PROCEDURE (X,P,D),.                                              NDTR  90
   DECLARE                                                          NDTR 100
      (D,T,P,X,AX) FLOAT BINARY,.                                   NDTR 110
   AX   =ABS(X),.                    /* CALC. PROB. P & DENSITY D   */NDTR 120
   T    =1.0E0/(1.0E0+.2316419E0*AX),.                             NDTR 130
   D    =0.3989423E0*EXP(-X*X/2.0E0),.                             NDTR 140
   P    =1.0E0-D*T*(((((1.330274E0*T-1.821256E0)*T+1.781478E0)*T-   NDTR 150
         0.3565638)*T+0.3193815E0),.                                NDTR 160
   IF X LT 0                         /* X < 0                       */NDTR 170
   THEN P=1.0E0-P,.                  /* COMPLEMENT PROB. P          */NDTR 180
   RETURN,.                                                         NDTR 190
   END,.                             /* END OF PROCEDURE NDTR       */NDTR 200
```

Purpose:

NDTR computes Y=P(x), the probability that the random available X, distributed normally (0, 1), is less than or equal to x. f(x), the ordinate of the normal density at x, is also computed.

Usage:

CALL NDTR (X, P, D);

X - BINARY FLOAT
Given variable containing the scalar for which P(x) is computed.
P - BINARY FLOAT
Resultant variable containing probability.
D - BINARY FLOAT
Resultant variable containing density.

Method:

Refer to:

C. Hastings, Approximations for Digital Computers. Princeton University Press, Princeton, N.J., 1955.
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. Dover Publications, Inc., N.Y., equation 26.2.17.

Mathematical Background:

This subroutine computes y = P(x) = Prob ($X \leq x$), where X is a random variable distributed normally with mean zero and variance one.

$$P(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-u^2/2)du$$

The following approximation is used:

$$P(x) = 1 - f(x) \sum_{i=1}^{5} a_i w^i; \quad x \geq 0$$

where:

$w = 1/(1 + px)$

$f(x) = \exp(-x^2/2) / \sqrt{2\pi}$

$P = 0.2316419$

$a_1 = 0.3193815$

$a_2 = -0.3565638$

$a_3 = 1.781478$

$a_4 = -1.821256$

$a_5 = 1.330274$

The maximum error is $7(10^{-7})$; f(x) is also presented in output.

- Subroutine BDTR

```
BDTR..                                                                  BDTR  10
/*********************************************************************/BDTR  20
/*                                                                   */BDTR  30
/*      BDTR COMPUTES P(X) = PROBABILITY THAT THE RANDOM VARIABLE    */BDTR  40
/*      DISTRIBUTED ACCORDING TO THE BETA DISTRIBUTION WITH PARA-    */BDTR  50
/*      METERS A AND B, IS LESS THAN OR EQUAL TO X. F(A,B,X), THE    */BDTR  60
/*      ORDINATE OF THE BETA DENSITY AT X, IS ALSO COMPUTED.         */BDTR  70
/*                                                                   */BDTR  80
/*********************************************************************/BDTR  90
   PROCEDURE (X,A,B,P,D),.                                              BDTR 100
   DECLARE                                                              BDTR 110
        (XX,DLXX,DL1X,AA,BB,G1,G2,G3,G4,DD,PP,XO,FF,FN,XI,SS,CC,        BDTR 120
        RR,DLBETA) BINARY(53),                                          BDTR 130
        (X,A,B,P,D,XS,OF,DUMMY) BINARY,                                 BDTR 140
        ID BINARY FIXED,                                                BDTR 150
        ERROR EXTERNAL CHARACTER(1),.                                   BDTR 160
   IF X LT 0  OR X GT 1                 /* TEST THE VALUE OF X         */BDTR 170
   THEN DO,.                                                            BDTR 180
        ERROR='1',.                                                     BDTR 190
        GO TO S10,.                                                     BDTR 200
        END,.                                                           BDTR 210
   IF A LT .49999  OR B LT .49999       /* TEST THE VALUES OF A AND B  */BDTR 220
   OR A GT 1E+5    OR B GT 1E+5                                         BDTR 230
   THEN DO,.                                                            BDTR 240
        ERROR='2',.                                                     BDTR 250
S10..                                                                   BDTR 260
        D,P  =-1E+75,.                                                  BDTR 270
        GO TO S14C,.                                                    BDTR 280
        END,.                                                           BDTR 290
   AA   =A,.                            /* COMPUTE LOG(BETA(A,B))      */BDTR 300
   BB   =B,.                                                            BDTR 310
   CALL LGAM(AA,G1),.                                                   BDTR 320
   CALL LGAM(BB,G2),.                                                   BDTR 330
   CALL LGAM(AA+BB,G3),.                                                BDTR 340
   DLBETA=G1+G2-G3,.                                                    BDTR 350
   IF X LE 1E-8                         /* TEST FOR X NEAR 0.0         */BDTR 360
   THEN DO,.                                                            BDTR 370
        P    =0,.                                                       BDTR 380
        IF A LT 1                                                       BDTR 390
        THEN                                                            BDTR 400
S20..                                                                   BDTR 410
             DO,.                                                       BDTR 420
             D    =1E+75,.                                              BDTR 430
             GO TO S13C,.                                               BDTR 440
             END,.                                                      BDTR 450
        ELSE IF A = 1                                                   BDTR 460
             THEN                                                       BDTR 470
S30..                                                                   BDTR 480
                  DO,.                                                  BDTR 490
                  DD   =-DLBETA,.                                       BDTR 500
                  IF DD GT -1.68E+2                                     BDTR 510
                  THEN DO,.                                             BDTR 520
                       D    =EXP(DD),.                                  BDTR 530
                       GO TO S13C,.                                     BDTR 540
                       END,.                                            BDTR 550
                  ELSE GO TO S40,.                                      BDTR 560
                  END,.                                                 BDTR 570
             ELSE                                                       BDTR 580
S40..                                                                   BDTR 590
                  DO,.                                                  BDTR 600
                  D    =0,.                                             BDTR 610
                  GO TO S13O,.                                          BDTR 620
                  END,.                                                 BDTR 630
        END,.                                                           BDTR 640
   IF 1-X LE 1E-8                       /* TEST FOR X NEAR 1.0         */BDTR 650
   THEN DO,.                                                            BDTR 660
        P    =1,.                                                       BDTR 670
        IF B LT 1                                                       BDTR 680
        THEN GO TO S20,.                                                BDTR 690
        ELSE IF B=1                                                     BDTR 700
             THEN GO TO S30,.                                           BDTR 710
             ELSE GO TO S4C,.                                           BDTR 720
        END,.                                                           BDTR 730
   XX   =X,.                            /* SET PROGRAM PARAMETERS      */BDTR 740
   DLXX =LOG(XX),.                                                      BDTR 750
   DL1X =LOG(1-XX),.                                                    BDTR 760
   XO   =XX/(1-XX),.                                                    BDTR 770
   ID   =0,.                                                            BDTR 780
   DD   =(AA-1)*DLXX+(BB-1)*DL1X-DLBETA,.  /* COMPUTE ORDINATE         */BDTR 790
   IF DD GT 1.68E+2                                                     BDTR 800
   THEN DO,.                                                            BDTR 810
        D    =1E+75,.                                                   BDTR 820
        GO TO S50,.                                                     BDTR 830
        END,.                                                           BDTR 840
   ELSE IF DD LE -1.68E+2                                               BDTR 850
        THEN DO,.                                                       BDTR 860
             D    =C,.                                                  BDTR 870
             GO TO S5C,.                                               BDTR 880
             END,.                                                      BDTR 890
   D    =EXP(DD),.                                                      BDTR 900
S50..                                                                   BDTR 910
   IF ABS(A-1) LE 1E-8                  /* A OR B BOTH WITHIN 1E-8 OF 1*/BDTR 920
   THEN IF ABS(B-1) LE 1E-8                                             BDTR 930
        THEN DO,.                                                       BDTR 940
             P    =X,.                                                  BDTR 950
             GO TO S13C,.                                               BDTR 960
             END,.                                                      BDTR 970
        ELSE DO,.                                                       BDTR 980
             PP   =BB*DL1X,.                                            BDTR 990
             IF PP LE 1.68E+2                                           BDTR1000
             THEN DO,.                                                  BDTR1010
                  P    =1,.                                             BDTR1020
                  GO TO S13O,.                                          BDTR1030
                  END,.                                                 BDTR1040
             ELSE DO,.                                                  BDTR1050
                  P    =1-EXP(PP),.                                     BDTR1060
                  GO TO S12O,.                                          BDTR1070
                  END,.                                                 BDTR1080
             END,.                                                      BDTR1090
   IF ABS(B-1) LE 1E-8                                                  BDTR1100
   THEN DO,.                                                            BDTR1110
        PP   =AA*DLXX,.                                                 BDTR1120
        IF PP LE -1.68E+2                                               BDTR1130
        THEN DO,.                                                       BDTR1140
             P    =C,.                                                  BDTR1150
             GO TO S13O,.                                               BDTR1160
             END,.                                                      BDTR1170
        ELSE DO,.                                                       BDTR1180
             P    =EXP(PP),.                                           BDTR1190
             GO TO S12O,.                                               BDTR1200
             END,.                                                      BDTR1210
        END,.                                                           BDTR1220
```

```
   IF A GT 1000                          /* TEST FOR A OR B GREATER      */BDTR1230
   THEN DO,.                             /*         THAN 1000            */BDTR1240
        XS   =2*AA/XO,.                                                   BDTR1250
        DF   =2*BB,.                                                      BDTR1260
        CALL CDTR(XS,DF,P,DUMMY),.                                        BDTR1270
        P    =1-P,.                                                       BDTR1280
        GO TO S140,.                                                      BDTR1290
        END,.                                                             BDTR1300
   IF B GT 1000                                                           BDTR1310
   THEN DO,.                                                              BDTR1320
        XS   =2*BB*XO,.                                                   BDTR1330
        DF   =2*AA,.                                                      BDTR1340
        CALL CDTR(XS,DF,P,DUMMY),.                                        BDTR1350
        GO TO S140,.                                                      BDTR1360
        END,.                                                             BDTR1370
   IF X LE .5                            /* SELECT PARAMETERS FOR CON-   */BDTR1380
   THEN IF AA LE 1                       /* TINUED FRACTION COMPUTATION  */BDTR1390
        THEN DO,.                                                         BDTR1400
             RR   =AA+1,.                                                 BDTR1410
             GO TO S60,.                                                  BDTR1420
             END,.                                                        BDTR1430
        ELSE DO,.                                                         BDTR1440
             RR   =AA,.                                                   BDTR1450
S60..                                                                     BDTR1460
             DD   =(RR-1)-(RR+BB-1)*XX*EXP(DLXX/5)+2,.                    BDTR1470
             IF DD LE 0                                                   BDTR1480
             THEN GO TO S80,.                                             BDTR1490
             ELSE GO TO S90,.                                             BDTR1500
             END,.                                                        BDTR1510
   IF BB LE 1                                                             BDTR1520
   THEN DO,.                                                              BDTR1530
        RR   =BB+1,.                                                      BDTR1540
        GO TO S70,.                                                       BDTR1550
        END,.                                                             BDTR1560
   RR   =BB,.                                                             BDTR1570
S70..                                                                     BDTR1580
   DD   =(RR-1)-(AA+RR-1)*(1-XX)*EXP(DL1X/5)+2,.                          BDTR1590
   IF DD LE 0                                                             BDTR1600
   THEN GO TO S90,.                                                       BDTR1610
S80..                                                                     BDTR1620
   ID   =1,.                                                              BDTR1630
   FF   =DL1X,.                                                           BDTR1640
   DL1X =DLXX,.                                                           BDTR1650
   DLXX =FF,.                                                             BDTR1660
   XO   =1/XO,.                                                           BDTR1670
   FF   =AA,.                                                             BDTR1680
   AA   =BB,.                                                             BDTR1690
   BB   =FF,.                                                             BDTR1700
   G2   =G1,.                                                             BDTR1710
S90..                                                                     BDTR1720
   FF   =0,.                                                              BDTR1730
   IF AA LE 1                            /* TEST FOR A LESS THAN 1       */BDTR1740
   THEN DO,.                                                              BDTR1750
        CALL LGAM(AA+1,G4),.                                              BDTR1760
        DD   =AA*DLXX+BB*DL1X+G3-G2-G4,.                                  BDTR1770
        IF DD GT -1.68E+2                                                 BDTR1780
        THEN FF=FF+EXP(DD),.                                              BDTR1790
        AA   =AA+1,.                                                      BDTR1800
        END,.                                                             BDTR1810
   FN   =AA+BB-1,.                       /* COMPUTE P USING CONTINUED    */BDTR1820
   RR   =AA-1,.                          /* FRACTION EXPANSION           */BDTR1830
   SS   =(((BB-80)*(RR+80))/((RR+2*80-1)*(RR+2*80)))*XO,.                 BDTR1840
        DO XI=79 TO 1 BY -1,.                                             BDTR1850
        DD   =((XI*(FN+XI))/((RR+2*XI+1)*(RR+2*XI)))*XO,.                 BDTR1860
        CC   =(((BB-XI)*(RR+XI))/((RR+2*XI-1)*(RR+2*XI)))*XO,.            BDTR1870
        SS   =CC/(1+DD/(1-SS)),.                                          BDTR1880
        END,.                                                             BDTR1890
   SS   =1/(1-SS),.                                                       BDTR1900
   IF SS LE 0                                                             BDTR1910
   THEN GO TO S110,.                                                      BDTR1920
   CALL LGAM(AA+BB,G1),.                                                  BDTR1930
   CALL LGAM(AA+1,G4),.                                                   BDTR1940
   PP   =G1-G2-G4+AA*DLXX+(BB-1)*DL1X+LOG(SS),.                           BDTR1950
   IF PP LE -1.68E+2                                                      BDTR1960
   THEN DO,.                                                              BDTR1970
        PP   =FF,.                                                        BDTR1980
        GO TO S100,.                                                      BDTR1990
        END,.                                                             BDTR2000
   PP   =EXP(PP)+FF,.                                                     BDTR2010
S100..                                                                    BDTR2020
   IF ID GT 0                                                             BDTR203C
   THEN PP=1-PP,.                                                         BDTR2040
   P    =PP,.                                                             BDTR2050
   IF P LT 0                             /* SET ERROR INDICATOR          */BDTR2060
   THEN IF ABS(P) GT 1E-7                                                 BDTR2070
        THEN GO TO S110,.                                                 BDTR2080
        ELSE DO,.                                                         BDTR2090
             P    =0,.                                                    BDTR2100
             GO TO S130,.                                                 BDTR2110
             END,.                                                        BDTR2120
   ELSE IF P GT 1                                                         BDTR2130
        THEN IF ABS(1-P) GT 1E-7                                          BDTR2140
             THEN                                                         BDTR2150
S110..                                                                    BDTR2160
                  DO,.                                                    BDTR2170
                  ERROR='3',.                                             BDTR2180
                  P    =+1E+75,.                                          BDTR2190
                  GO TO S140,.                                            BDTR2200
                  END,.                                                   BDTR2210
             ELSE DO,.                                                    BDTR2220
                  P    =1,.                                               BDTR2230
                  GO TO S130,.                                            BDTR2240
                  END,.                                                   BDTR2250
        ELSE                                                              BDTR2260
S120..                                                                    BDTR2270
             IF P LE 1E-8                                                 BDTR2280
             THEN DO,.                                                    BDTR2290
                  P    =0,.                                               BDTR2300
                  GO TO S130,.                                            BDTR2310
                  END,.                                                   BDTR2320
             ELSE IF 1-P LE 1E-8                                          BDTR2330
                  THEN P=1,.                                              BDTR2340
S130..                                                                    BDTR2350
        ERROR='0',.                                                       BDTR2360
S140..                                                                    BDTR2370
   RETURN,.                                                               BDTR2380
   END,.                                 /* END OF PROCEDURE BDTR        */BDTR2390
```

Purpose:

BDTR computes P(x) = probability that the random variable X, distributed according to the beta distribution with parameters A and B, is less than or equal to x. f (A, B, X), the ordinate of the beta density of X, is also computed.

Usage:

CALL BDTR (X, A, B, P, D);

X - BINARY FLOAT
Given variable containing the scalar for which P(x) is computed.

A - BINARY FLOAT
Given variable containing the beta distribution parameter.

B - BINARY FLOAT
Given variable containing the beta distribution parameter.

P - BINARY FLOAT
Resultant variable containing the probability.

D - BINARY FLOAT
Resultant variable containing the density.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following constitute the possible error conditions that may be detected:

ERROR=1 - invalid value of X. (X<0 or X>1)

ERROR=2 - invalid value of A or B (A or B <.5, or A or B > 10^5).
If either of the above conditions exists, the values of P and D are set to -1.E75.

ERROR=3 - Invalid output (P<0 or P>1). If this condition exists, the value of P is set to 1.E75.

Subroutines and function subroutines required:

CDTR
LGAM
NDTR

Method:

Refer to:

R. E. Bargmann and S. P. Ghosh, "Statistical Description Programs for a Computer Language", IBM Research Report RC-1094, 1963.
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. U. S. Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966.

Mathematical Background:

This subroutine computes $P=I_x(m,n)=\text{Prob}(X \leq x)$, where X is a random variable following the beta

distribution with degrees of freedom (continuous parameters) m and n. For computation to take place, $0 \le x \le 1$, $0.5 \le m \le 10^{+5}$, and $0.5 \le n \le 10^{+5}$. D, the ordinate of the beta density at x, is also presented in the output.

For $0 \le x \le 1$, $I_x(m, n)$ may be written as:

$$I_x(m, n) = \int_0^x f(m, n, y)\, dy$$

where:

$$f(m, n, y) = \frac{1}{B(m,n)} y^{m-1}(1-y)^{n-1}$$

$$B(m,n) = \frac{\Gamma(m)\,\Gamma(n)}{\Gamma(m+n)}; \quad D = f(m,n,x) \tag{1}$$

$I_x(m,n)$ can be reduced to a binominal partial sum that can be evaluated by means of a continued fraction expansion.

Let $N = m+n-1$ and $r = m-1$. Then:

$$I_x(m,n) = I_x(r+1, N-r)$$

$$I_x(r+1, N-r) = \sum_{s=r+1}^{N} \binom{N}{s} x^s (1-x)^{N-s}$$

$$= \binom{N}{r+1} x^{r+1} (1-x)^{N-r-1} S \tag{2}$$

where $0 \le s \le N$

S is a continued fraction, with 80 terms being sufficient for the desired accuracy.

$$S = \frac{1}{1-}\,\frac{c_1}{1+}\,\frac{d_1}{1-}\,\frac{c_2}{1+}\,\frac{d_2}{1-}\,\cdots\,\frac{c_{80}}{1+}\,\frac{d_{80}}{1} \tag{3}$$

$$c_i = \frac{(N-i-r)(r+i)}{(r+2i-1)(r+2i)}\,\frac{x}{1-x} \tag{4}$$

$$d_i = \frac{i(N+i)}{(r+2i+1)(r+2i)}\,\frac{x}{1-x} \tag{5}$$

The above continued fraction expansion of $I_x(m,n)$ holds for positive m and n (integers or nonintegers), $N \ge 0$ $(m+n \ge 1)$, and $r \ge 0$ $(m \ge 1)$. In order to fulfill these last two conditions, if $m < 1$, the following transformation must be made before computation of $I_x(m,n)$ can take place:

$$I_x(m,n) = \frac{\Gamma(m+n)}{\Gamma(m+1)\Gamma(n)} x^m (1-x)^n + I_x(m+1,n) \tag{6}$$

The quantities on the right-hand side of equation (6) are those that are computed.

It is known that $I_x(m,n) = I_{1-x}(n,m)$. Thus, either of the two parameter sets indicated by this equation may be used in computing the beta integral. The parameter set selection is made by applying the following empirically derived rule:

> Let p and q be the degrees of freedom corresponding to z, where $z = x$ if $x \le .5$ or $(1-x)$ otherwise. If the quantity $[(p-1) - (p+q-1)\, z^{6/5} + 2]$ is positive, use the parameter set corresponding to z. Otherwise, use the parameter set corresponding to (1-z).

If $0 \le x \le 10^{-8}$ or $0 \le 1-x \le 10^{-8}$, the approximation is made that x = 0 or 1 respectively. P and D are then set according to the following table:

$0 \le x \le 10^{-8}$		$0 \le 1-x \le 10^{-8}$	
P = 0		P = 1	
If:	Then:	If:	Then:
A < 1	$D = 10^{75}$	B < 1	$D = 10^{75}$
A = 1	D = 1/B(m,n)	B = 1	D = 1/B(m,n)
A > 1	D = 0	B > 1	D = 0

If either m or n, or both are within 10^{-8} of 1, the beta integral is solved explicitly for m = 1, n = 1, or m = n = 1:

If:	Then:
A = 1, B = 1	P = x
A = 1, $B \neq 1$	$P = 1 - (1-x)^n$
$A \neq 1$, B = 1	$P = x^m$

If m or n is greater than 1000, the chi-square approximation is used:

$z_1 = 2m\,(1-x)/x$ is distributed as χ^2 with 2n degrees of freedom and $P = 1 - P_{\chi^2}(z_1)$ for m > 1000.

$z_2 = 2nx/(1-x)$ is distributed as χ^2 with 2 m degrees of freedom and $P = P_{\chi^2}(z_2)$ for n > 1000. If both m and n are greater than 1000, the approximation corresponding to z_1 is used.

The values of P very near zero or one may be somewhat imprecise. To eliminate possible misinterpretation of results, if $0 \le P \le 10^{-8}$ or $0 \le 1-P \le 10^{-8}$, P is set to 0 or 1 respectively.

- Subroutine CDTR

```
CDTR..                                                                  CDTR  10
/*********************************************************************/CDTR  20
/*                                                                   */CDTR  30
/*      COMPUTES P(X) = PROBABILITY THAT THE RANDOM VARIABLE U,      */CDTR  40
/*      DISTRIBUTED ACCORDING TO THE CHI-SQUARE DISTRIBUTION WITH G  */CDTR  50
/*      DEGREES OF FREEDOM, IS LESS THAN OR EQUAL TO X.  F(G,X), THE */CDTR  60
/*      ORDINATE OF THE CHI-SQUARE DENSITY AT X, IS ALSO COMPUTED.   */CDTR  70
/*                                                                   */CDTR  80
/*********************************************************************/CDTR  90
   PROCEDURE (X,G,P,D),.                                                CDTR 100
   DECLARE                                                              CDTR 110
        (XX,DLXX,DLX2,GG,G2,DLT3,THETA,THP1,GLG2,DD,T11,SER,CC,X2,      CDTR 120
        XI,FAC,TLOG,TERM,GTH,A2,A,B,C,DT2,DT3,THPI)                     CDTR 130
        FLOAT BINARY (53),                                              CDTR 140
        (I,J,K,I3) FIXED BINARY,                                        CDTR 150
        ERROR EXTERNAL CHARACTER (1),                                   CDTR 160
        (X,G,D,SC,P,T1,T2,T3,DUMMY) FLOAT BINARY,.                      CDTR 170
                                  /* TEST INPUT VALIDITY              */CDTR 180
   IF G LT .49999 OR G GT 2.E+05 OR X LT 0                              CDTR 190
   THEN DO,.                      /* SET ERROR INDICATOR              */CDTR 200
        D,P  =-1.E75,.                                                  CDTR 210
        ERROR='1',.                                                     CDTR 220
        GO TO S150,.                                                    CDTR 230
        END,.                                                           CDTR 240
   ELSE IF X LE 1.E-08            /* TEST FOR X NEAR ZERO             */CDTR 250
        THEN DO,.                 /* SET P AND D DEPENDING            */CDTR 260
             P    =0.0,.          /* ON THE PARAMETER G               */CDTR 270
             IF G LT 2.0                                                CDTR 280
             THEN DO,.                                                  CDTR 290
                  D    =1.E75,.                                         CDTR 300
                  GO TO S30,.                                           CDTR 310
                  END,.                                                 CDTR 320
             ELSE IF G = 2.0                                            CDTR 330
                  THEN DO,.                                             CDTR 340
                       D    =0.5,.                                      CDTR 350
                       GO TO S30,.                                      CDTR 360
                       END,.                                            CDTR 370
                  ELSE DO,.                                             CDTR 380
                       D    =0.0,.                                      CDTR 390
                       GO TO S30,.                                      CDTR 400
                       END,.                                            CDTR 410
             END,.                                                      CDTR 420
        ELSE IF X GT 1.E+06         /* TEST FOR X > 1.E+06             */CDTR 430
             THEN DO,.              /* SET P AND D                     */CDTR 440
                  D    =0.0,.                                           CDTR 450
                  P    =1.0,.                                           CDTR 460
                  GO TO S30,.                                           CDTR 470
                  END,.                                                 CDTR 480
             ELSE DO,.              /* SET PROGRAM PARAMETERS          */CDTR 490
                  XX   =PRECISION(X,53),.                               CDTR 500
                  DLXX =LOG(XX),.                                       CDTR 510
                  X2   =XX/2.E0,.                                       CDTR 520
                  DLX2 =LOG(X2),.                                       CDTR 530
                  GG   =PRECISION(G,53),.                               CDTR 540
                  G2   =GG/2.E0,.                                       CDTR 550
                                  /* COMPUTE THE ORDINATE             */CDTR 560
                  CALL LGAM(G2,GLG2),.                                  CDTR 570
                  DD   =(G2-1.E0)*DLXX-X2-G2*.693147180559945E0-GLG2,.  CDTR 580
                  IF DD LE 1.68E02                                      CDTR 590
                  THEN IF (DD+1.68E02) LE 0                             CDTR 600
                       THEN DO,.                                        CDTR 610
                            D    =0.0,.                                CDTR 620
S10..                                                                   CDTR 630
                                  /* TEST FOR G > 1000 & X > 2000     */CDTR 640
                            IF G LE 1000                                CDTR 650
                            THEN IF X GT 2000                           CDTR 660
                                 THEN                                   CDTR 670
S20..                                                                   CDTR 680
                                      DO,.                              CDTR 690
                                      P    =1.0,.                       CDTR 700
S30..                                                                   CDTR 710
                                      ERROR='0',.                       CDTR 720
                                      GO TO S150,.                      CDTR 730
                                      END,.                             CDTR 740
                                 ELSE DO,.                              CDTR 750
                                      /* COMPUTE THETA                */CDTR 760
                                      K    =FLOOR(G2),.                 CDTR 770
                                      THETA=G2-FLOAT(K,53),.            CDTR 780
                                      GO TO S40,.                       CDTR 790
                                      END,.                             CDTR 800
                            ELSE DO,. /* WILSON HILFERTY APPROX.      */CDTR 810
                                 A    =LOG(XX/GG)/3.E0,.                CDTR 820
                                 A    =EXP(A),.                         CDTR 830
                                 B    =2.E0/(9.E0*GG),.                 CDTR 840
                                 C,SC =(A-1.E0+B)/SQRT(B),.             CDTR 850
                                 CALL NDTR(SC,P,DUMMY),.                CDTR 860
                                 GO TO S60,.                            CDTR 870
                                 END,.                                  CDTR 880
                            END,.                                       CDTR 890
                       ELSE DO,.                                        CDTR 900
                            DD,D =EXP(DD),.                             CDTR 910
                            GO TO S10,.                                 CDTR 920
                            END,.                                       CDTR 930
                  ELSE DO,.                                             CDTR 940
                       D    =1.E75,.                                    CDTR 950
                       GO TO S10,.                                      CDTR 960
                       END,.                                            CDTR 970
                  END,.                                                 CDTR 980
S40..                                                                   CDTR 990
   IF THETA LE 1.E-8                                                    CDTR1000
   THEN THETA=0.E0,.                                                    CDTR1010
   THP1 =THETA+1.E0,.                                                   CDTR1020
                                  /* SELECT METHOD FOR                */CDTR1030
                                  /* COMPUTING T1                     */CDTR1040
   IF THETA GT 0                                                        CDTR1050
                                  /* COMPUTE T1 FO                    */CDTR1060
                                  /* THETA > 0 & X < OR = 10          */CDTR1070
   THEN IF XX LE 10.E0                                                  CDTR1080
        THEN DO,.                                                       CDTR1090
             SER  =X2*(1.E0/THP1-X2/(THP1+1.E0)),.                      CDTR1100
             J    =1,.                                                  CDTR1110
             CC   =FLOAT(J,53),.                                        CDTR1120
             DO IT1=3 TO 30,.                                           CDTR1130
             XI   =FLOAT(IT1,53),.                                      CDTR1140
             CALL LGAM(XI,FAC),.                                        CDTR1150
             TLOG =XI*DLX2-FAC-LOG(XI+THETA),.                          CDTR1160
             TERM =EXP(TLOG),.                                          CDTR1170
             TERM =SIGN(CC)*ABS(TERM),.                                 CDTR1180
             SER  =SER+TERM,.                                           CDTR1190
             CC   =-CC,.                                                CDTR1200
             IF ABS(TERM) LT 1.E-9                                      CDTR1210
             THEN GO TO S80,.                                           CDTR1220
             END,.                                                      CDTR1230
```

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            GO TO S90,.                                                  CDTR1240
            END,.                                                        CDTR1250
       ELSE DO,.                        /* T1 FOR THETA>0 AND 10<X<2000*/CDTR1260
            A2   =0.E0,.                                                 CDTR1270
            DO I=1 TO 25,.                                               CDTR1280
            XI   =FLOAT(I,53),.                                          CDTR1290
            CALL LGAM(THPI,GTH),.                                        CDTR1300
            T11  =-(13.E0*XX)/XI+THPI*LOG(13.E0*XX/XI)-GTH-LOG(XI),.     CDTR1310
            IF (T11+1.68E02) GT 0                                        CDTR1320
            THEN DO,.                                                    CDTR1330
                 T11  =EXP(T11),.                                        CDTR1340
                 A2   =A2+T11,.                                          CDTR1350
                 END,.                                                   CDTR1360
            END,.                                                        CDTR1370
            GO TO S130,.                                                 CDTR1380
            END,.                                                        CDTR1390
   ELSE IF X2 GE 1.68E02                                                 CDTR1400
       THEN DO,.                        /* COMPUTE T1 FOR THETA = 0    */CDTR1410
            T1   =1.0,.                                                  CDTR1420
S50..                                                                    CDTR1430
            IF G GE 2                   /* SELECT APPRO. EXP. FOR P    */CDTR1440
            THEN IF G GE 4                                               CDTR1450
                 THEN DO,.                                               CDTR1460
                                        /* CALC. FOR G > OR = 4        */CDTR1470
                                        /* AND < OR = 100              */CDTR1480
                      DT3  =0.E0,.                                       CDTR1490
                      DO I3=2 TO K,.                                     CDTR1500
                      THPI =FLOAT(I3,53)+THETA,.                         CDTR1510
                      CALL LGAM (THPI,GTH),.                             CDTR1520
                      DLT3 =THPI*DLX2-DLXX-X2-GTH,.                      CDTR1530
                      IF (DLT3+1.68E02) GT 0                             CDTR1540
                      THEN DT3  =DT3+EXP(DLT3),.                         CDTR1550
                      END,.                                              CDTR1560
                      T3   =DT3,.                                        CDTR1570
                      P    =T1-T3-T3,.                                   CDTR1580
                      GO TO S60,.                                        CDTR1590
                      END,.                                              CDTR1600
                 ELSE DO,.                                               CDTR1610
                      P    =T1,.                                         CDTR1620
S60..                                                                    CDTR1630
                      IF P LT 0                                          CDTR1640
                      THEN IF ABS(P) LE 1.E-7                            CDTR1650
                           THEN                                          CDTR1660
S70..                                                                    CDTR1670
                                DO,.                                     CDTR1680
                                P    =0.0,.                              CDTR1690
                                GO TO S30,.                              CDTR1700
                                END,.                                    CDTR1710
                           ELSE GO TO S90,.                              CDTR1720
                      ELSE IF P GT 1.0                                   CDTR1730
                           THEN IF ABS(1.-P) GT 1.E-7                    CDTR1740
                                THEN GO TO S90,.                         CDTR1750
                                ELSE GO TO S20,.                         CDTR1760
                           ELSE GO TO S100,.                             CDTR1770
                      END,.                                              CDTR1780
            ELSE GO TO S145,.                                            CDTR1790
            END,.                                                        CDTR1800
       ELSE DO,.                                                         CDTR1810
            T11,T1    =1.E0-EXP(-X2),.                                   CDTR1820
            GO TO S50,.                                                  CDTR1830
            END,.                                                        CDTR1840
S80..                                                                    CDTR1850
   IF (SER) LE 0                                                         CDTR1860
   THEN GO TO S90,.                                                      CDTR1870
   ELSE DO,.                                                             CDTR1880
        CALL LGAM (THP1,GTH),.                                           CDTR1890
        TLOG =THETA*DLX2+LOG(SER)-GTH,.                                  CDTR1900
        IF (TLOG+1.68E02) LE 0                                           CDTR1910
        THEN GO TO S110,.                                                CDTR1920
        ELSE GO TO S120,.                                                CDTR1930
        END,.                                                            CDTR1940
S90..                                                                    CDTR1950
   ERROR='2',.                          /* SET ERROR INDICATOR         */CDTR1960
   P    =1.E75,.                                                         CDTR1970
   GO TO S150,.                                                          CDTR1980
S100..                                                                   CDTR1990
   IF P LE 1.E-8                                                         CDTR2000
   THEN GO TO S70,.                                                      CDTR2010
   ELSE IF (1.0-P) LE 1.E-8                                              CDTR2020
        THEN GO TO S20,.                                                 CDTR2030
        ELSE GO TO S30,.                                                 CDTR2040
S110..                                                                   CDTR2050
   T1   =0.0,.                                                           CDTR2060
   GO TO S50,.                                                           CDTR2070
S120..                                                                   CDTR2080
   T11,T1    =EXP(TLOG),.                                               CDTR2090
   GO TO S50,.                                                           CDTR2100
S130..                                                                   CDTR2110
   A    =1.01282051+THETA/156.E0-XX/312.E0,.                             CDTR2120
   B    =ABS(A),.                                                        CDTR2130
   C    =-X2+THP1*DLX2+LOG(B)-GTH-3.95124371858142E0,.                   CDTR2140
   IF (C+1.68E02) LE 0                                                   CDTR2150
   THEN DO,.                                                             CDTR2160
        C    =0.E0,.                                                     CDTR2170
S140..                                                                   CDTR2180
        C    =A2+C,.                                                     CDTR2190
        T11,T1    =1.E0-C,.                                              CDTR2200
        GO TO S50,.                                                      CDTR2210
        END,.                                                            CDTR2220
   ELSE IF A LT 0                                                        CDTR2230
        THEN DO,.                                                        CDTR2240
             C    =-EXP(C),.                                             CDTR2250
             GO TO S140,.                                                CDTR2260
             END,.                                                       CDTR2270
        ELSE IF A =0                                                     CDTR2280
             THEN DO,.                                                   CDTR2290
                  C    =0.E0,.                                           CDTR2300
                  GO TO S140,.                                           CDTR2310
                  END,.                                                  CDTR2320
             ELSE DO,.                                                   CDTR2330
                  C    =EXP(C),.                                         CDTR2340
                  GO TO S140,.                                           CDTR2350
                  END,.                                                  CDTR2360
S145..                                                                   CDTR2370
   CALL LGAM (THP1,GTH),.               /*CCMPUTE P FOR 0<G<2         */CDTR2380
   DT2  =THETA*DLXX-X2-THP1*.693147180559945E0-GTH,.                     CDTR2390
   IF (DT2+1.68E02) LE 0                                                 CDTR2400
   THEN DO,.                            /*COMPUTE P FOR G > OR = 2    */CDTR2410
        P    =T1,.                                                       CDTR2420
        GO TO S60,.                                                      CDTR2430
        END,.                                                            CDTR2440
   ELSE DO,.                                                             CDTR2450
        DT2,T2    =EXP(DT2),.                                            CDTR2460
        P    =T1+T2+T2,.                                                 CDTR2470
        GO TO S60,.                                                      CDTR2480
        END,.                                                            CDTR2490
S150..                                                                   CDTR2500
   RETURN,.                                                              CDTR2510
   END,.                                /* END OF PROCEDURE CDTR       */CDTR2520
```

Purpose:

CDTR computes P(x) = the probability that the random variable X, distributed according to the chi-square distribution with G degrees of freedom, is less than or equal to x. f (G x), the ordinate of the chi-square density at x, is also computed.

Usage:

CALL CDTR (X, G, P, D);

X - BINARY FLOAT
Given random variable following the chi-square distribution.

G - BINARY FLOAT
Given variable containing the number of degrees of freedom of the chi-square distribution. G is a continuous parameter such that $.5 \leq G \leq 2\ (10^5)$.

P - BINARY FLOAT
Resultant variable containing the probability.

D - BINARY FLOAT
Resultant variable containing the density.

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. The following consitute the possible error conditions that may be detected:

ERROR=1 - invalid value of X.
($X < 0$) or invalid value of G.
($G < .5$ or $G > 200,000$)
If this condition exists, the values of P and D are set to -1.E75.

ERROR=2 - invalid output ($P < 0$ or $P > 1$) or the series T1 has failed to converge. If this condition exists, the values of P and D are set to -1.E75.

Subroutines and function subroutines required:

LGAM
NDTR

Method:

For reference see:

1. R. E. Bargmann and S. P. Ghosh, "Statistical Distribution Programs for a Computer Language", IBM Research Report RC-1094, 1963.
2. M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions U. S.

Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966.

Mathematical Background:

This subroutine computes P=P(x)=Prob. ($X \le x$), where X is a random variable following the χ^2 distribution with continuous parameter g. X must be greater than or equal to zero and $.5 \le g \le 2\ (10^5)$ for computation to take place. D, the ordinate of the χ^2 density at x, is also presented in the output.

For $x \ge 0$, P(x) may be written as:

$$P(x) = \int_0^x f(g, y)\, dy \qquad (1)$$

where:

$$f(g,y) = y^{(g-2)/2} e^{-y/2} \Big/ \left(2^{g/2}\, \Gamma\left(\frac{g}{2}\right)\right)$$

$$D = f(g,x)$$

To evaluate the integral, we first define

$$\theta = \frac{g}{2} - \left[\frac{g}{2}\right],$$

where $\frac{g}{2}$ denotes the largest integer less than or equal to $\frac{g}{2}$. θ is thus the fractional part of $\frac{g}{2}$.

Substituting this expression into the integral and performing the proper reductions, we find:

If:	Then:
$0 < g < 2$	$P(x) = T1 + T2$
$2 \le g < 4$	$P(x) = T1$
$g \ge 4$	$P(x) = T1 - 2T3$

where:

$$T1 = \int_0^x \frac{y^{\theta} e^{-y/2}\, dy}{2^{1+\theta}\, \Gamma(1+\theta)}$$

$$T2 = f(2+2\theta, x)$$

$$T3 = \sum_{i=2}^{\left[\frac{g}{2}\right]} f(2i+2\theta, x)$$

T2 and T3 may be evaluated directly using logs and antilogs.

If $\theta = 0$ ($\frac{g}{2}$ is an integer), T1 is easily evaluated as:

$$T1 = 1 - e^{-x/2}$$

If $\theta > 0$, T1 can be expanded in the following infinite series:

$$T1 = \frac{Z^{\theta}}{\Gamma(1+\theta)} \left\{ \frac{Z}{1+\theta} - \frac{Z^2}{2+\theta} + \frac{Z^3}{2!(3+\theta)} - \frac{Z^4}{3!(4+\theta)} \cdots \right\} \qquad (2)$$

where $Z = \frac{x}{2}$.

This series is used in the range $10^{-8} < x \le 10$, and not more than 30 terms are necessary to ensure convergence within error bounds of 10^{-9}.

For $x > 10$, 1-T1 is evaluated by the Euler-McLaurin formula up to third derivative terms (see Reference 2, equation 23.1.30). One finds:

$$1 - T1 = \int_0^N h(u)\, du \qquad (3)$$

where:

$$h(u) = \frac{1}{\Gamma(1+\theta)} \left(\frac{2u}{Nx}\right)^{-(1+\theta)} u^{-1} e^{-Nx/2u}$$

$$\int_0^N h(u)\, du = \sum_{u=0}^{N-1} h(u) + \frac{1}{2} h(N) - \frac{1}{12} h'(N) + \frac{1}{720} h'''(N)$$

(Note: $h' = h''' = 0$ at 0.)

In order to achieve accuracy consistent with that obtained by the method of equation (2), N=26 is used in equation (3).

If $0 \le x \le 10^{-8}$, the approximation is made that x=0. P is set to 0, and D is set to 1.E75, .5, or 0, corresponding to g less than 2, equal to 2, or greater than 2 respectively.

If $g > 1000$, Wilson and Hilferty's approximation is used. $\left(\frac{x^2}{g}\right)^{1/3}$ is approximately normally distributed with mean $1 - \frac{2}{9g}$ and variance $\frac{2}{9g}$ (see reference 2, equation 26.4.14). If $g \le 1000$ and $x > 2000$, or $g > 1000$ and $x > 10^6$, P is set to 1.

Since T1 may have an error of about 10^{-9}, values of P(x) very near zero or one may be somewhat imprecise. To eliminate possible misinterpretation

of results, if $0 \leq P(x) \leq 10^{-8}$ or $0 \leq 1 - P(x) \leq 10^{-8}$, P(x) is set to 0 or 1 respectively.

The χ^2 distribution is a member of the gamma family of probability distributions. The general form for distributions of this class is:

$$P_G(x) = \int_0^x G(n, A, \Psi; u)\, du$$

where

$$G(n, a, \Psi; u) = (u-a)^{n-1} e^{-(u-a)/\Psi} / (\Psi^n \Gamma(n)).$$

This subroutine may, therefore, also be used to compute the probability integral from zero to x and the corresponding ordinate at x for any member of this gamma family by setting:

$x = 2(u-a) / \Psi$ and $g = 2n$

Then P(x) will be the desired probability, and $\frac{2f(g,x)}{\Psi}$ will be the desired ordinate.

- Subroutine NDTI

```
NDTI..                                                                  NDTI  10
/*************************************************************************/NDTI  20
/*                                                                       */NDTI  30
/*      COMPUTES X=P**X(-1)(Y), THE ARGUMENT X SUCH THAT Y=P(X)=THE      */NDTI  40
/*      PROBABILITY THAT THE RANDOM VARIABLE U, DISTRIBUTED NORMALLY     */NDTI  50
/*      (0,1), IS LESS THAN OR EQUAL TO X.  F(X) THE ORDINATE OF THE     */NDTI  60
/*      NORMAL DENSITY, AT X, IS ALSO COMPUTED.                          */NDTI  70
/*                                                                       */NDTI  80
/*************************************************************************/NDTI  90
   PROCEDURE(P,X,D),.                                                   NDTI 100
   DECLARE                                                              NDTI 110
        (P,X,D,T2,T) FLOAT BINARY,                                      NDTI 120
        ERROR EXTERNAL CHARACTER (1),.                                  NDTI 130
   ERROR='0',.                                                          NDTI 140
   X,D  =0,.                                                            NDTI 150
   IF P LT 0.0                                                          NDTI 160
   THEN                                                                 NDTI 170
S10..                                                                   NDTI 180
        DO,.                          /* P < 0--SET ERROR INDICATOR    */NDTI 190
        ERROR='1',.                                                     NDTI 200
        GO TO S30,.                                                     NDTI 210
        END,.                                                           NDTI 220
   ELSE IF P = 0.0                                                      NDTI 230
        THEN DO,.                     /* P = 0--SET X AND D            */NDTI 240
             X    =-.999999E+74,.                                       NDTI 250
S20..                                                                   NDTI 260
             D    =0.0,.                                               NDTI 270
             GO TO S30,.                                                NDTI 280
             END,.                                                      NDTI 290
        ELSE IF P GT 1.0                                                NDTI 300
             THEN GO TO S10,.         /* P > 1--SET ERROR INDICATOR    */NDTI 310
             ELSE IF P = 1.0                                            NDTI 320
                  THEN DO,.           /* P = 1--SET X AND D            */NDTI 330
                       X    =.999999E+74,.                             NDTI 340
                       GO TO S20,.                                     NDTI 350
                       END,.                                           NDTI 360
                  ELSE DO,.           /* P > 0 AND P < 1               */NDTI 370
                       D    =P,.                                       NDTI 380
                       IF D GT 0.5                                     NDTI 390
                                      /* COMPLEMENT P                  */NDTI 400
                       THEN D    =1.0-D,.                              NDTI 410
                                      /* CALC. EQUATION 2 IN WRITE UP  */NDTI 420
                       T2   =LOG(1.0/(D*D)),.                          NDTI 430
                       T    =SQRT(T2),.                                NDTI 440
                                      /* CALC. EQUATION 1 IN WRITE UP  */NDTI 450
                       X    =T-(2.515517+0.802853*T+0.010328*T2)/      NDTI 460
                        (1.0+1.432788*T+0.189269*T2+0.001308*T         NDTI 470
                        *T2),.                                         NDTI 480
                       IF P LE 0.5    /* P < OR = .5                   */NDTI 490
                       THEN X    =-X,./* NEGATE X                     */NDTI 500
                                      /* CALCULATE DENSITY             */NDTI 510
                       D    =0.3989423*EXP(-X*X/2.0),.                 NDTI 520
                       END,.                                           NDTI 530
S30..                                                                   NDTI 540
   RETURN,.                                                             NDTI 550
   END,.                              /* END OF PROCEDURE NDTI         */NDTI 560
```

Purpose:

NDTI computes $x = P^{-1}(y)$ such that $y = P(x)$, the probability that the random variable X, distributed normally (0, 1) is less than or equal to x. f(x), the ordinate of the normal density at x, is also computed.

Usage:

CALL NDTI (P, X, D);

P - BINARY FLOAT
Given variable containing the probability.

X - BINARY FLOAT
Resultant variable such that P=Y= the probability that u, the random variable, is less than or equal to X.

D - BINARY FLOAT
Resultant variable containing the density f (X).

Remarks:

If no errors are detected in the processing of data, the error indicator, ERROR, is set to zero. However, if P=0, X is set to $-(10)^{74}$, and D is set to zero. If P=1, X is set to $(10)^{74}$ and D is set to

zero. The following constitutes the possible error condition that may be detected:

ERROR=1 - Invalid value of P. P is either less than zero or greater than one.

Method:

Refer to:

C. Hastings, Approximations for Digital Computers, Princeton University Press, Princeton, N. J., 1955.

M. Abramowitz and Stegun, I. A. Handbook of Mathematical Functions, Dover Publications, Inc., N. Y., equation 26.2.23.

Mathematical Background:

This subroutine computes $x = P^{-1}(y)$ such that $y = P(x) = \text{Prob}(X \leq x)$, where X is a random variable distributed normally with mean zero and variance one. That is, given P(x), the following is solved for x:

$$P(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-u^2/2)\, du$$

The following approximation is used:

$$x = w - \sum_{i=0}^{2} a_i w^i / \sum_{i=0}^{3} b_i w^i \qquad (1)$$

where:

$$w = \sqrt{\ln(1/p^2)} \quad (0 < p \leq .5) \qquad (2)$$

$a_0 = 2.515517$

$a_1 = 0.802853$

$a_2 = 0.010328$

$b_1 = 1.432788$

$b_2 = 0.189269$

$b_3 = 0.001308$

If P(x) is greater than 0.5, 1-P(x) is used as p in (2) above, and the result of (1), x, is negated. The maximum error is 0.00045; f(x) is also calculated.

APPENDIX A: ACCURACY OF SUBROUTINES

The subroutines in SSP can be broken down into three major categories from the standpoint of accuracy:

(1) those having little or no effect on accuracy,

(2) those whose accuracy depends on the characteristics of the input data, and

(3) those in which definite statements on accuracy can be made.

SUBROUTINES WITH LITTLE OR NO EFFECT ON ACCURACY

The following subroutines do not materially affect the accuracy of the results, either because of the simple nature of the computation or because they do not modify the data.

ABST	RANK
BUND	SRNK
CHSQ	SUBM
HTES	SBST
KLM2	TAB1
KRNK	TAB2
MOMN	TALY
MPIT	TIE
MPRM	TRAC
MTPI	TTST
MSCG	TWAV
MSCS	UTST
ORDR	WTST
QTST	

SUBROUTINES WITH DATA-DEPENDENT ACCURACY

The accuracy of the following subroutines cannot be predicted because it depends on the characteristics of the input data and on the size of the problem. The programmer using these subroutines must be aware of the limitations dictated by numerical analysis considerations. It cannot be assumed that the results are accurate simply because subroutine execution is completed.

ACFM/ACFE	DFEC	MATE
AHIM/AHIE	DFEO	MATU
ALIM/ALIE	DGT3	MDLG
APCI/APC2	DMTX	MDLS/MDRS
APLL	DSCR	MDSB
ASN	EXSM	MEAT
AVAR	FFT	MEBS
CANC	FFTM	MEST
CORR	FMFP	MFG
DERE	KLMO	MFGR
DET3	LOAD	MFS
DET5	MAGS	MFSB
MGB1/MGB2	POSV	QH24
MGDU	PRTC	QH32
MIG	PRTR	QH48
MINV	QA2	QHFG/QHFE/
MIS	QA4	QHSQ/QHSE
MLSQ	QA8	QL2
MLTR	QA12	QL4
MMGG	QA16	QL8
MMGS	QA24	QL12
MMGT	QATR	QL16
MMSS	QG2	QL24
MSDU	QG4	QSF
MSTU	QG8	QTFG/QTFE
MVAT	QG16	RTF
MVEB	QG24	RTFD
MVST	QG32	SE15
MVSU	GH2	SE35
MVUB	QH4	SG13/SE13
PEC/PTC	QH8	STRG
POST	QH16	VRMX

SUBROUTINES WITH DEFINITE ACCURACY CHARACTERISTICS

The subroutines in this section have accuracy characteristics that can be specified on an individual basis. The mathematical descriptions for many of these subroutines contain information on truncation error of a strictly theoretical nature. The actual implementation of these subroutines on System/360 results in the accuracy noted in the following table. The standard reference for comparing the accuracy of these subroutines is M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, National Bureau of Standards, Washington, D.C., March 1965. However, in certain cases, other tables were used, as noted below. It should be remembered that in System/360 single-precision floating point, there are just over six significant figures.

Maximum differences below are given in terms of number of decimal places (DP) and/or number of significant digits (SD) that agree. The number of digits tabled should be considered when accuracy statements are viewed; that is, certain tables are given to only five places, whereas the algorithms used may be more accurate. In compiling maximum differences, the maximum was taken over the set of

points indicated in the table. The average difference was normally much smaller.

The notation x = a (b) c implies that a, a + b, a + 2b, . . . , c were the arguments (x) used.

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
BDTR	$p = I_x(a,b)$	$I_x^{-1}(a,b)$ Tables by Leon H. Harter: New Tables of the Incomplete Gamma Function Ratio and of Percentage Points of the χ^2 and Beta Distribution, 1964	p=.0001, .0005 a=1(1)40 b=5(5)40 p=.0100, .0500 a=2(2)10 b=5(5)30	correct to 5 DP
CDTR	$y = P_g(x)$ where P is the χ^2 distribution function with parameter g.	$y = P_g(x)$	x=.001(.001).01; .01(.01)1.0; 1.0(.1)2.0; 2.0(.2)10.0; 10.0(.5)20.0; 20 (1) 40 40 (2) 76 for g=1(1)30	1 in the 5th DP
CELI Complete elliptic 1st integral	K(k) (single precision)	$K(m);\ k = \sqrt{m}$	m=.01 (.01).99	2 in 7th SD
		$K(\alpha);\ k = \sin\alpha$	α = 1(1)73	2 in 7th SD
		(α in degrees)	α = 74(1)86	3 in 7th SD
	K(k) (double precision)	$K(m);\ k = \sqrt{m}$	m = .01(.01).86	1 in 16th SD
			m = .87(.01).96	4 in 16th SD
			m = .97(.01).99	11 in 16th SD
		$K(\alpha);\ k = \sin\alpha$	α = 1(1)75	1 in 16th SD
		(α in degrees)	α = 76(1)80	2 in 16th SD
			α = 81(1)86	11 in 16th SD

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
CEL2 Generalized complete elliptic 2nd integral	K(k) with A = B = 1 E(k) with A = 1 $B = 1 - k^2$ (single precision)	K(m); $k = \sqrt{m}$ K(α); k = sin α (α in degrees) E(m); $k = \sqrt{m}$ E(α); k = sin α K'E + E'K - KK' (Legendre's relation)	m = .01(.01) .99 α = 1(1) 73 α = 74(1)86 m = .01(01) α = 1(1) 86 m = .01(.01) .99 α = 1(1) 89	2 in 7th SD 2 in 7th SD 3 in 7th SD 2 in 7th SD 2 in 7th SD 7 in 7th SD 1 in 6th SD
	K(k) with A = B = 1 E(k) with A = 1 $B = 1 - k^2$ (double precision)	K(m); $k = \sqrt{m}$ K(α); k = sin α (α in degrees) E(α); k = sin α K'E + E'K - KK' (Legendre's relation)	m = .01(.01).99 α = 1(1)80 α = 81(1)86 α = 1(1)89 m = .01(.01).99 α = 1(1)89	2 in 16th SD 2 in 16th SD 11 in 16th SD 2 in 16th SD 9 in 16th SD 9 in 16th SD
ELI1 Incomplete elliptic 1st integral	F(ζ /α) with x = tan ζ k = sin α $ck = \sqrt{1-k^2}$ (single precision)	F(ζ/α) (ζ, α in degrees)	ζ = 0(5)10 α = 0(2)90 ζ = 15(5)35 α = 0(2)90 ζ = 40(5)50 α = 0(2)90 ζ = 55(5)85 α = 0(2)90	2 in 7th DP 7 in 7th SD 11 in 7th DP 3 in 7th SD
	F(φ /α) with x = tan φ k = sin α $ck = \sqrt{1 - k^2}$ (double precision)	F(φ /α) (φ , α in degrees) F(φ /α) + F(ψ/α). $= F\left(\frac{\pi}{2} /\alpha\right)$ (φ, α, ψ in degrees)	φ = 0(5)85 α = 0(2)90 φ = 0(5)85 α = 0(2)80 ψ = arctan f f = 1/(cos α ·tan φ)	1 in 9th DP (probably due to rounding errors in table) 2 in 15th DP

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
ELI2 Generalized incomplete elliptic 2nd integral	$F(\zeta/\alpha)$ with A = B = 1	$F(\zeta/\alpha)$ (ζ, α in degrees)	ζ = 0(5)10 α = 0(2)90	2 in 7th DP
	$E(\zeta/\alpha)$ with A = 1 and $B = 1 - k^2$		ζ = 15(5)35 α = 0(2)90	7 in 7th SD
	$x = \tan \zeta$ $k = \sin \alpha$ $ck = \sqrt{1 - k^2}$		ζ = 40(5)50 α = 0(2)90	11 in 7th DP
			ζ = 55(5)85 α = 0(2)90	3 in 7th SD
	(single precision)	$E(\zeta/\alpha)$ (ζ, α in degrees)	ζ = 0, 5 α = 0(2)90	2 in 7th DP
			ζ = 10(5)35 α = 0(2)90	7 in 7th SD
			ζ = 40(5)55 α = 0(2)90	12 in 7th DP
			ζ = 60(5)85 α = 0(2)90	36 in 7th DP
	$F(\varphi/\alpha)$ with A = B = 1 $E(\varphi/\alpha)$ with A = 1 $B = 1-k^2$ and $x = \tan \varphi$ $k = \sin \alpha$ $ck = \sqrt{1-k^2}$	$F(\varphi/\alpha)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90	1 in 9th DP (probably due to rounding errors in table)
		$E(\varphi/\alpha)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90	1 in 9th DP (probably due to rounding errors in table)
	(double precision)	$E(\varphi/\alpha) + E(\psi/\alpha)$ $= E\left(\frac{\pi}{2}/\alpha\right) + \sin^2\alpha \sin\phi \sin\psi$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90 ψ = arctan f f = 1/(cos α · tan φ)	2 in 15th DP
		$F(\varphi/\alpha) + F(\psi/\alpha)$ $= F\left(\frac{\pi}{2}/\alpha\right)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)82 ψ = arctan f f = 1/(cos α · tan φ)	3 in 15th DP

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
JELF Jacobian elliptic functions	sn u = sin φ cn u = cos φ dn u = $\sqrt{1-k^2 \sin^2\varphi}$ with φ = am u or u = F(φ/α), k = sin α sck = $1-k^2$ (single precision)	sn u = sin φ (φ, α in degrees)	φ = 0(1)89 α = 0(5)85	1 in 6th DP +
		cn u = cos φ (φ, α in degrees)	φ = 0(1)89 α = 0(5)85	2 in 6th DP +
		dn u = $\sqrt{1-k^2\sin^2\varphi}$ (φ, α in degrees)	φ = 0(1)89 α = 0(5)85	1 in 6th DP +
		sn u	k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25	1 in 6th DP ++
		cn u	k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25	2 in 6th DP ++
		dn u	k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25	1 in 6th DP ++
		sn u - sn(2K-u)	k^2 = .00(.05).90 t = 0(1)25 u = t.K(k)/25	6 in 6th DP
		sn u + sn(2K + u)		6 in 6th DP
		sn u + sn(4K - u)		10 in 6th DP
		cn u + cn(2K - u)	k^2 = .00(.05).90 t = 0(1)25 u = t.K(k)/25	4 in 6th DP
		cn u + cn(2K + u)		4 in 6th DP
		cn u - cn(4K - u)		6 in 6th DP
		dn u - dn(2K - u)	k^2 = .00(.05).90 t = 0(1)25 u = t.K(k)/25	3 in 6th DP
		dn u - dn(2K + u)		3 in 6th DP
		dn u - dn(4K - u)		5 in 6th DP

+ Calculation of u = F(φ/α) with double-precision subroutine
++ Difference between result of single- and double-precision routines

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
Jacobian elliptic functions	sn u = sin φ	sn u = sin φ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	2 in 15th DP +
	cn u = cos φ	cn u = cos φ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	3 in 15th DP +
	dn u = $\sqrt{1 - k^2\alpha}$ ($\alpha = \sin^2\varphi$)	dn u = $\sqrt{1-k^2\sin^2\varphi}$ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	2 in 15th DP +
	with φ = am u u = F(φ/α) k = sin α sck = 1 - k^2 (double precision)	sn u - sn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	5 in 15th DP
		sn u + sn(2K + u)	u = t.K(k)/25	5 in 15th DP
		sn u + sn(4K - u)		12 in 15th DP
		cn u + cn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	3 in 15th DP
		cn u + cn(2K + u)	u = t.K(k)/25	3 in 15th DP
		cn u - cn(4K - u)		7 in 15th DP
		dn u - dn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	3 in 15th DP
		dn u - dn(2K + u)	u = t.K(k)/25	2 in 15th DP
		dn u - dn(4K - u)		6 in 15th DP
LGAM (log of the gamma function)	ln Γ (x)	ln Γ (x)	x=1	6 in 9th DP
			x=1.005(.005) 1.025	9 in 8th DP
			x=1.980(.005) 1.995	9 in 8th SD
			x=1.03(.01)1.31	8 in 9th SD
			x=1.32(.01)1.67	8 in 10th SD
			x=1.68(.01)1.97	7 in 9th SD
			x=2	6 in 9th SD
		$\log_{10}\Gamma$ (x)	x=3.0(1.0)100.0	No error in 8 place tables
NDTR	y = P (x) P = normal pdf	y = P (x)	x = -6 (.01)6	7 in 7th DP
NDTI	x = P^{-1} (y) p = normal pdf	x = P^{-1}(y)	y =.01(.01).99	5 in 4th DP

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
SMIR Kolmogorov-Smirnov limiting distribution	L(x)	L (x); Tables by N. Smirnov, reprinted in Annals of Math. Stat. 19, pp. 280-281 (6- and 7- place tables). Double-precision version differences are given in parentheses in the right-hand column.	x = 0(.01) .61	1 in 6th DP (1 in 6th DP)
			x = .62	3 in 5th DP (see program comments) (3 in 5th DP)
			x = .63 (.01) 1.04	3 in 6th DP (2 in 6th DP)
			x = 1.05(.01)1.15	6 in 6th DP (2 in 6th DP)
			x = 1.16(.01) 1.20	9 in 6th DP (2 in 6th DP)
			x = 1.21 (.01) 1.45	8 in 6th DP (3 in 6th DP)
			x = 1.46(.01) 1.65	6 in 6th DP (1 in 6th DP)
			x = 1.66(.01) 1.86	2 in 6th DP (0 in 6th DP)
			x = 1.87	2 in 5th DP (2 in 5th DP)
			x = 1.88 (.01) 2.04	2 in 6th DP (1 in 6th DP)
			x = 2.05 (.01) 2.50	1 in 6th DP (1 in 6th DP)
			x = 2.51 (.01) 3.5	2 in 7th DP (1 in 7th DP)

APPENDIX B: SAMPLE PROGRAM DESCRIPTIONS

The following programs are intended to exemplify linkage of subroutines within SSP/PL/I. These programs are only examples and are not meant to be representative of the state of the art.

When supplying data for the sample programs, the user is reminded that all fixed point numbers must be right-adjusted and that all floating point numbers may appear anywhere in the field, provided the decimal point is included.

The necessary job control and process cards are included in the sample programs but are not separately shown in the deck setup illustrations.

Note that arrays are limited, for each dimension, to an upper bound of 32,767.

DATA SCREENING DACR

Problem Description

A set of observations is read along with information on propositions to be satisfied and limits on a selected variable. From this input a subset is obtained and a histogram of frequency over given class intervals is plotted for the selected variable. Total, average, standard deviation, minimum, and maximum are calculated for the selected variable. This procedure is repeated until all sets of input data have been processed.

Program

Description

The data screening sample program consists of a main routine, DACR, a special input routine DAT1, and three subroutines from the Scientific Subroutine Package: SBST, TAB1, and BOOL. There is also one special plotting routine, HIST. For a description of subroutine BOOL see subroutine SBST.

Capacity

1. Up to 4999 observations
2. Up to 70 variables
3. Up to 99 conditions (with the existing subroutine BOOL only two conditions are considered).
4. Up to 10 data cards per observation

Input

Control Cards

A parameter card with the following format must precede each matrix of observations.

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	0100
12-16	Number of variables	0004
17-21	Number of conditions	02
22-26	Number of selections	00003
27-31	Number of data cards per observation	01

Data Cards

1. For the observation matrix, data cards have seven fields of ten columns each. The decimal point may appear anywhere in a field. If no decimal point is included, it is assumed that the decimal point is to the right of the last digit. The number in each field may be preceded by blanks. All values for an observation are punched consecutively and may continue from card to card. However, a new observation must start in the first field of a new card.
2. For the condition matrix three ten-column fields are used. The first contains the variable number (right-justified); the next, the relations code; and the last, a floating point number that relates to the condition.

Selection Card

For each selection there will be a new selection card. The card is prepared as follows:

Columns	Contents	For Sample Problem
1-5	Number of the variable to be tabulated	00003
6-15	Lower bound	120.
16-25	Number of intervals*	20.
26-35	Upper bound	210.

The number of selection cards must agree with the value of the selection indicator, which appears in columns 22-26 of the control card.

*In the number of intervals, it should be noted that two extra intervals must be specified for those elements that fall below the lower bound and those that fall above the upper bound.

Deck Setup

The deck setup is shown in Figure 11.

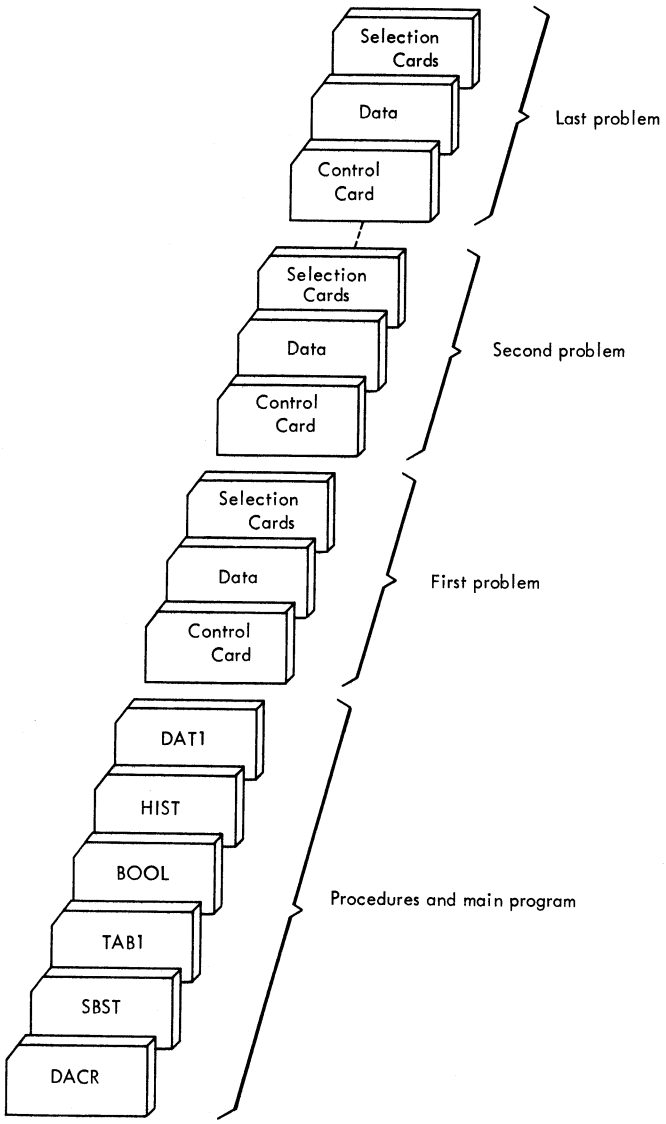


Figure 11.

Sample

A listing of input cards for the sample problem is shown in Figure 12.

```
SAMPLE  10C    4    2    3    1                                    10
46.       64.       173.      12.                                  20
24.       72.       17C.       8.                                  30
32.       71.       154.      16.                                  40
41.       68.       129.      10.                                  50
50.       65.       192.       9.                                  60
63.       75.       203.      12.                                  70
29.       70.       122.      14.                                  80
28.       64.       136.      13.                                  90
52.       77.       147.      11.                                 100
36.       67.       153.      18.                                 110
31.       68.       165.       9.                                 120
72.       7C.       178.      10.                                 130
53.       71.       2C5.      14.                                 140
21.       65.       219.      12.                                 150
49.       63.       150.       6.                                 160
28.       62.       16C.      16.                                 170
53.       72.       161.      13.                                 180
47.       73.       142.      15.                                 190
37.       67.       193.      18.                                 200
64.       68.       156.      14.                                 210
65.       6C.       114.      10.                                 220
62.       64.       153.      12.                                 230
19.       68.       225.       9.                                 240
46.       67.       158.      11.                                 250
33.       72.       121.       4.                                 260
37.       65.       132.      13.                                 270
41.       76.       148.      16.                                 280
52.       71.       123.      16.                                 290
29.       68.       128.      14.                                 300
32.       65.       155.      17.                                 310
24.       72.       172.      16.                                 320
56.       73.       163.      10.                                 330
63.       65.       158.      11.                                 340
67.       69.       146.       2.                                 350
58.       66.       171.       9.                                 360
41.       65.       153.      12.                                 370
49.       66.       165.      14.                                 380
52.       72.       172.      16.                                 390
23.       78.       183.      15.                                 400
56.       71.       195.      16.                                 410
52.       68.       118.       7.                                 420
40.       66.       165.      14.                                 430
39.       68.       215.      16.                                 440
23.       71.       154.      12.                                 450
56.       65.       149.      10.                                 460
25.       65.       162.      16.                                 470
37.       68.       152.      16.                                 480
46.       7C.       159.      15.                                 490
41.       69.       137.      14.                                 500
62.       71.       163.      12.                                 510
29.       72.       191.       4.                                 520
19.       68.       168.      10.                                 530
46.       63.       158.      16.                                 540
37.       64.       139.      18.                                 550
34.       68.       156.      10.                                 560
64.       67.       153.      12.                                 570
57.       67.       141.      13.                                 580
32.       68.       157.      17.                                 590
29.       7C.       183.      15.                                 600
53.       72.       164.      18.                                 610
47.       72.       156.      18.                                 620
56.       73.       16C.      16.                                 630
61.       74.       169.      12.                                 640
21.       68.       161.      10.                                 650
25.       76.       178.      11.                                 660
23.       72.       157.      16.                                 670
29.       68.       186.      16.                                 680
39.       7C.       159.      14.                                 690
42.       7C.       154.      1C.                                 700
56.       62.       159.      12.                                 710
63.       7C.       177.      12.                                 720
51.       71.       161.       9.                                 730
41.       66.       158.      10.                                 740
33.       69.       158.      16.                                 750
37.       68.       157.      16.                                 760
25.       7C.       163.      15.                                 770
63.       68.       159.      12.                                 780
53.       71.       202.       6.                                 790
51.       72.       167.      14.                                 800
47.       73.       164.      14.                                 810
39.       75.       151.      12.                                 820
28.       68.       166.      10.                                 830
64.       69.       156.      16.                                 840
55.       67.       144.      16.                                 850
51.       66.       177.      10.                                 860
46.       65.       157.      12.                                 870
72.       66.       125.      10.                                 880
66.       65.       131.      12.                                 890
28.       74.       149.      18.                                 900
27.       71.       168.      11.                                 910
23.       72.       158.      12.                                 920
23.       72.       163.      12.                                 930
6C.       68.       157.       9.                                 940
3C.       66.       142.      10.                                 950
39.       67.       162.      16.                                 960
46.       74.       154.      16.                                 970
5C.       68.       158.      10.                                 980
61.       66.       161.      14.                                 990
36.       64.       157.      15.                                1000
32.       71.       156.      16.                                1010
          1         2         65                                 1020
          4         6         8                                  1030
    3    12C.      2C.       21C.                                1040
    1    2C.       7.        7C.                                 1050
    4    1C.       12.       2C.                                 1060
```

Figure 12.

Output

Description

The output consists of the subset vector whose element values indicate which corresponding observations are rejected (element = zero) and accepted

(element ≠ nonzero), summary statistics for each selected variable, and a histogram of frequencies versus intervals for that variable.

Sample

The output listing for the sample problem is shown in Figure 13.

```
DATA SCREENING PROBLEM    SAMPLE

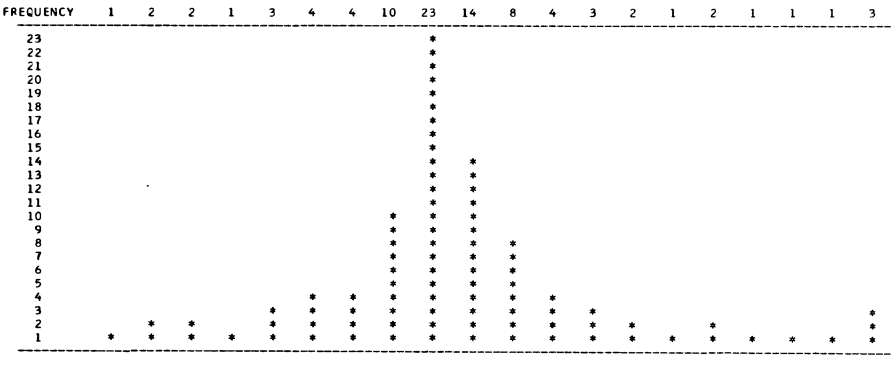
SUBSET VECTOR
     1  1.0    51  0.0
     2  0.0    52  1.0
     3  1.0    53  1.0
     4  1.0    54  1.0
     5  1.0    55  1.0
     6  1.0    56  1.0
     7  1.0    57  1.0
     8  1.0    58  1.0
     9  1.0    59  1.0
    10  1.0    60  1.0
    11  1.0    61  1.0
    12  0.0    62  1.0
    13  1.0    63  1.0
    14  1.0    64  1.0
    15  0.0    65  1.0
    16  1.0    66  1.0
    17  1.0    67  1.0
    18  1.0    68  1.0
    19  1.0    69  1.0
    20  1.0    70  1.0
    21  1.0    71  1.0
    22  1.0    72  1.0
    23  1.0    73  1.0
    24  1.0    74  1.0
    25  0.0    75  1.0
    26  1.0    76  1.0
    27  1.0    77  1.0
    28  1.0    78  0.0
    29  1.0    79  1.0
    30  1.0    80  1.0
    31  1.0    81  1.0
    32  1.0    82  1.0
    33  1.0    83  1.0
    34  0.0    84  1.0
    35  1.0    85  1.0
    36  1.0    86  1.0
    37  1.0    87  0.0
    38  1.0    88  0.0
    39  1.0    89  1.0
    40  1.0    90  1.0
    41  0.0    91  1.0
    42  1.0    92  1.0
    43  1.0    93  1.0
    44  1.0    94  1.0
    45  1.0    95  1.0
    46  1.0    96  1.0
    47  1.0    97  1.0
    48  1.0    98  1.0
    49  1.0    99  1.0
    50  1.0   100  1.0

SUMMARY STATISTICS FOR VARIABLE    3

TOTAL =14492.000  AVERAGE =  161.022  STANDARD DEVIATION =   19.329  MINIMUM =  114.000  MAXIMUM =  225.000

                                        HISTOGRAM   1

FREQUENCY    1   2   2   1   3   4   4  10  23  14   8   4   3   2   1   2   1   1   1   3
```




```
INTERVAL     1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
CLASS
```

Figure 13.

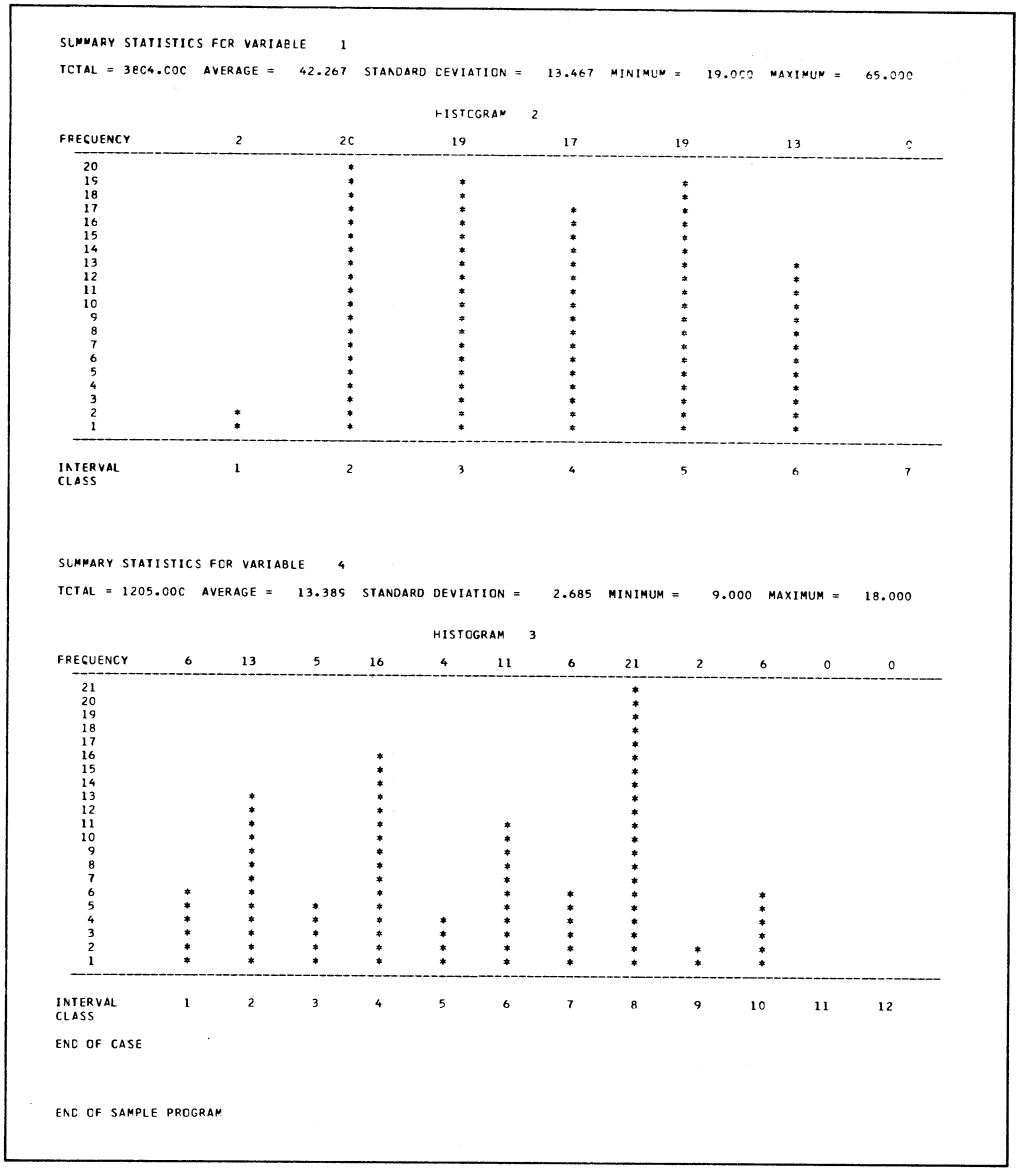


Figure 13. (Continued)

Program Modifications

1. Changes in the input format statement of the special input routine, DAT1:

Only the format statement for input data may be changed. Since sample data are either two- or three-digit numbers, rather than using ten-column fields, as in the sample problem, each row of data might have been keypunched in three-column fields; if so, the format is changed to (7F(3,0)). This format assumes seven 3-column fields per card.

2. If there are more than seven variables in a problem, each row of data is continued on the second card until the last data point is keypunched. However, each row must begin on a new card. If there is more than one data card per observation, the value of the data card count indicator (NCARD), which appears in columns 27-31 of the control card, must be changed to agree with the number of data cards.

3. Subroutine BOOL can be replaced if the user wishes to use a different boolean expression (see description in subroutine SBST). The boolean expression provided in the sample program is for both conditions to be satisfied:

$$T = R(1) * R(2)$$

Operating Instructions

The sample program for data screening is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT is used for output.

Timing

The execution time of this sample program on System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 40 seconds.

```
DACR..                                                                  DACR  10
/*********************************************************************/DACR  20
/*                                                                   */DACR  30
/*      TO PERFORM DATA SCREENING CALCULATIONS ON A SET OF           */DACR  40
/*      OBSERVATIONS.                                                */DACR  50
/*                                                                   */DACR  60
/*********************************************************************/DACR  70
   PROCEDURE OPTIONS (MAIN),.                                           DACR  80
   DECLARE                                                              DACR  90
         (NO,NS,NN,NNN,NC,I,J,NOVAR,NX,NCOL,L1,L2)                      DACR 100
         FIXED BINARY,                                                  DACR 110
         PR1  CHARACTER (6),                                            DACR 120
         ERROR EXTERNAL CHARACTER(1),                                   DACR 130
         CH CHARACTER (80),                                             DACR 140
         (NV,NCARD) EXTERNAL,                                           DACR 150
         BOOL ENTRY,.                                                   DACR 160
/*                                                                    */DACR 170
         ON ENDFILE (SYSIN) GO TO EXIT,.                                DACR 180
STRT..                                                                  DACR 190
   GET EDIT (CH) (A(80)),.                                              DACR 200
   GET STRING (CH) EDIT (PR1,NO,NX,NC,NS,NCARD) (A(6),5 F(5)),.         DACR 210
/*                                                                    */DACR 220
/*      PR1.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                  */DACR 230
/*      NO........NUMBER OF OBSERVATIONS                              */DACR 240
/*      NX........NUMBER OF VARIABLES                                 */DACR 250
/*      NC........NUMBER OF CONDITIONS                                */DACR 260
/*      NS........NUMBER OF SELECTIONS                                */DACR 270
/*      NCARD.....NUMBER OF DATA CARDS PER OBSERVATION                */DACR 280
/*                                                                    */DACR 290
         NCARD=NCARD*80,.                                               DACR 300
ONE..                                                                   DACR 310
   BEGIN,.                                                              DACR 320
   DECLARE                                                              DACR 330
         (A(NO,NX),C(3,NC),UBO(3),S(NO),R(NC),STATS(5),D(NX),DD(3))     DACR 340
         FLOAT BINARY,.                                                 DACR 350
/*                                                                    */DACR 360
/*      IF INPUT DATA IS TO BE SAVED ON A DATA SET, INITIALIZE        */DACR 370
/*      NV=1. OTHERWISE NV=0.                                         */DACR 380
/*                                                                    */DACR 390
   NV    =0,.                                                           DACR 400
         DO  I = 1 TO NO,.              /* READ IN DATA               */DACR 410
         CALL DAT1(NX,D),.                                              DACR 420
              DO J = 1 TO NX,.                                          DACR 430
              A(I,J)=D(J),.                                             DACR 440
              END,.                                                     DACR 450
         END,.                                                          DACR 460
   NCARD=80,.                                                           DACR 470
         DO  I = 1 TO NC,.              /* READ IN CONDITIONS         */DACR 480
         NNN  =3,.                                                      DACR 490
         CALL DAT1 (NNN,DD),.                                           DACR 500
              DO J = 1 TO 3,.                                           DACR 510
              C(J,I)=DD(J),.                                            DACR 520
              END,.                                                     DACR 530
         END,.                                                          DACR 540
   CALL SBST (A,C,R,BOOL,S,NO,NX,NC),.                                  DACR 550
   PUT EDIT ('DATA SCREENING PROBLEM',PR1) (PAGE,COLUMN(10),A,X(4),A),. DACR 560
   IF ERROR NE '0'                                                      DACR 570
   THEN DO,.                                                            DACR 580
         PUT EDIT ('IN ROUTINE SBST ERROR CODE = ',ERROR)               DACR 590
              (SKIP(2),COLUMN(10),A,A(1)),.                             DACR 600
         GO TO FIN,.                                                    DACR 610
         END,.                                                          DACR 620
   PUT EDIT ('SUBSET VECTOR') (SKIP(3),COLUMN(10),A,SKIP(3)),.          DACR 630
   NCOL =CEIL(NO/50),.                                                  DACR 640
   IF NCOL LE 1                                                         DACR 650
   THEN PUT EDIT ((I,S(I) DO I= 1 TO NO)) (COLUMN(10),F(6),F(5,1)),.    DACR 660
   ELSE DO,.                                                            DACR 670
         L1    =0,.                                                     DACR 680
              DO I = 1 TO 50,.                                          DACR 690
              L1   =L1+1,.                                              DACR 700
              L2   =50*(NCOL-1)+L1,.                                    DACR 710
              IF L2= NO                                                 DACR 720
              THEN NCOL =NCOL-1,.                                       DACR 730
              PUT EDIT ((J,S(J) DO J= L1 TO L2 BY 50)) (SKIP,COLUMN(10) DACR 740
                   ,(9)(F(6),F(5,1))),.                                 DACR 750
              END,.                                                     DACR 760
         END,.                                                          DACR 770
         DO J = 1 TO NS,.                                               DACR 780
         GET EDIT (CH) (A(80)),.                                        DACR 790
         GET STRING (CH) EDIT (NOVAR,(UBO(I) DO I= 1 TO 3))             DACR 800
              (F(5),3 F(10,0)),.                                        DACR 810
/*                                                                    */DACR 820
/*      NOVAR.....NUMBER OF THE VARIABLE TO BE TABULATED              */DACR 830
/*      UBO(1)....LOWER BOUND                                         */DACR 840
/*      UBO(2)....NUMBER OF INTERVALS                                 */DACR 850
/*      UBO(3)....UPPER BOUND                                         */DACR 860
/*                                                                    */DACR 870
   NN    =UBO(2),.                                                      DACR 880
TWO..                                                                   DACR 890
   BEGIN,.                                                              DACR 900
         DECLARE                                                        DACR 910
              (FREQ(NN),PCT(NN)) FLOAT BINARY,.                         DACR 920
         CALL TAB1 (A,S,NOVAR,UBO,FREQ,PCT,STATS,NO,NX),.               DACR 930
         IF ERROR NE '0'                                                DACR 940
         THEN PUT EDIT ('IN ROUTINE TAB1 ERROR CODE = ',ERROR)          DACR 950
              (SKIP(1),COLUMN(10),A,A(1)),.                             DACR 960
         ELSE DO,.                                                      DACR 970
              PUT EDIT ('SUMMARY STATISTICS FOR VARIABLE  ',NOVAR)      DACR 980
              (PAGE,SKIP(4),COLUMN(10),A,F(3)),.                        DACR 990
              PUT EDIT ('TOTAL =',STATS(1),'AVERAGE =',STATS(2),        DACR1000
                   'STANDARD DEVIATION =',STATS(3),'MINIMUM =',STATS(4),DACR1010
                   'MAXIMUM =',STATS(5))                                DACR1020
                   (SKIP(2),COLUMN(10),5(A,F(9,3),X(2))),.              DACR1030
              CALL HIST (J,FREQ,NN),.                                   DACR1040
```

```
            END,.                                                       DACR1050
      END,.                                                             DACR1060
   END,.                                                                DACR1070
   PUT EDIT ('END OF CASE') (SKIP(2),COLUMN(10),A),.                    DACR1080
   END,.                                                                DACR1090
   GO TO STRT,.                                                         DACR1100
EXIT..                                                                  DACR1110
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                   DACR1120
        (SKIP(5),COLUMN(10),A),.                                        DACR1130
FIN..                                                                   DACR1140
   END,.                              /*END OF PROCEDURE DACR         */DACR1150
```

```
BOOL..                                                                  BOOL  10
/*********************************************************************/BOOL  20
/*                                                                   */BOOL  30
/*      TO PERFORM A BOOLEAN OPERATION FOR THE PROCEDURE SBST, WHICH */BOOL  40
/*      IS USED BY THE DATA SCREENING SAMPLE PROGRAM.                */BOOL  50
/*                                                                   */BOOL  60
/*********************************************************************/BOOL  70
   PROCEDURE (R,T),.                                                    BOOL  80
   DECLARE (R(*),T) FLOAT BINARY,.                                      BOOL  90
/*    BOOL CHECKS ONLY THE FIRST TWO CONDITIONS OF PROCEDURE SBST    */BOOL 100
   T     =R(1)*R(2),.                                                   BOOL 110
   RETURN,.                                                             BOOL 120
   END,.                              /*END OF PROCEDURE BOOL         */BOOL 130
```

```
HIST..                                                                  HIST  10
/*********************************************************************/HIST  20
/*                                                                   */HIST  30
/*      TO PLOT A HISTOGRAM OF FREQUENCIES FOR THE DATA SCREENING    */HIST  40
/*      SAMPLE PROGRAM.                                              */HIST  50
/*                                                                   */HIST  60
/*********************************************************************/HIST  70
   PROCEDURE (NZ,FREQ,IN),.                                             HIST  80
   DECLARE                                                              HIST  90
         (I,IN,IX,J,JSCAL,L,MAX,NU,NZ)                                  HIST 100
         FIXED BINARY,                                                  HIST 110
         (K,JOUT(IN)) CHARACTER (1),                                    HIST 120
         (FREQ(*),FMAX,X) FLOAT BINARY,.                                HIST 130
/*                                                                    */HIST 140
/*      PRINT TITLE AND FREQUENCY VECTOR                              */HIST 150
/*                                                                    */HIST 160
   PUT EDIT ('HISTOGRAM ',NZ) (SKIP(3),COLUMN(57),A,F(3)),.             HIST 170
   NU   =FLOOR(100/IN),.                                                HIST 180
   PUT EDIT ('FREQUENCY',(FREQ(I) DO I = 1 TO IN))                      HIST 190
        (SKIP(2),COLUMN(10),A,(IN)F(NU)),.                              HIST 200
   PUT EDIT ('-------------------------------------------------',       HIST 210
        '-------------------------------------------------')           HIST 220
        (R(FM1)),.                                                      HIST 230
                                                                        HIST 240
FM1..                                                                   HIST 250
   FORMAT (SKIP,COLUMN(12),A,A),.                                       HIST 260
   FMAX =0,.                          /* FIND LARGEST FREQUENCY     */HIST 270
        DO I = 1 TO IN,.                                                HIST 280
        IF FREQ(I) GT FMAX                                              HIST 290
        THEN FMAX =FREQ(I),.                                            HIST 300
        END,.                                                           HIST 310
   JSCAL=1,.                          /* SCALE IF NECESSARY         */HIST 320
   IF FMAX GT 50                                                        HIST 330
   THEN DO,.                                                            HIST 340
        JSCAL=FLOOR((FMAX+49)/50),.                                     HIST 350
        PUT EDIT ('EACH','*',' EQUAL ',JSCAL,' POINTS')                 HIST 360
             (SKIP,COLUMN(10),A,A(1),A,F(2),A,SKIP),.                   HIST 370
        END,.                                                           HIST 380
   JOUT =' ',.                        /* CLEAR OUTPUT AREA TO BLANKS*/HIST 390
/*                                                                    */HIST 400
/*      LOCATE FREQUENCIES IN EACH INTERVAL                           */HIST 410
/*                                                                    */HIST 420
   MAX  =FLOOR(FMAX/JSCAL),.                                            HIST 430
        DO I = 1 TO MAX,.                                               HIST 440
        X    =MAX-(I-1),.                                               HIST 450
             DO J = 1 TO IN,.                                           HIST 460
             IF FREQ(J)/JSCAL GE X                                      HIST 470
             THEN JOUT(J)='*',.                                         HIST 480
             END,.                                                      HIST 490
        IX   =X*JSCAL,.                                                 HIST 500
/*                                                                    */HIST 510
/*      PRINT LINE OF FREQUENCIES                                     */HIST 520
/*                                                                    */HIST 530
        PUT EDIT (IX,(JOUT(L) DO L = 1 TO IN)) (SKIP,COLUMN(10),F(5),   HIST 540
             X(4),(IN)(X(NU-1),A(1))),.                                 HIST 550
        END,.                                                           HIST 560
        DO I = 1 TO IN,.              /* GENERATE CONSTANTS          */HIST 570
        FREQ(I)=I,.                                                     HIST 580
        END,.                                                           HIST 590
   PUT EDIT ('-------------------------------------------------',       HIST 600
        '-------------------------------------------------')           HIST 610
        (R(FM1)),.                                                      HIST 620
   PUT EDIT ('INTERVAL ',(FREQ(I) DO I = 1 TO IN))                      HIST 630
        (SKIP(2),COLUMN(10),A,(IN)F(NU)),.                              HIST 640
   PUT EDIT ('CLASS') (SKIP,COLUMN(10),A),.                             HIST 650
   RETURN,.                                                             HIST 660
   END,.                              /*END OF PROCEDURE HIST         */HIST 660
```

```
DAT1..                                                                  DAT1  10
/*********************************************************************/DAT1  20
/*                                                                   */DAT1  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.      */DAT1  40
/*      DATA MAY BE SAVED ON A DATA SET.                             */DAT1  50
/*                                                                   */DAT1  60
/*********************************************************************/DAT1  70
   PROCEDURE (M,D),.                                                    DAT1  80
   DECLARE                                                              DAT1  90
         XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),       DAT1 100
         (NCARD,NV) EXTERNAL,                                           DAT1 110
         CH CHARACTER(NCARD),                                           DAT1 120
         (I,M,MM) BINARY FIXED,                                         DAT1 130
         D(*) FLOAT BINARY,.                                            DAT1 140
/*                                                                    */DAT1 150
   ON ENDFILE (SYSIN)                                                   DAT1 160
   GO TO EXIT,.                                                         DAT1 170
   GET EDIT (CH) (A(NCARD)),.                                           DAT1 180
   MM   =CEIL(M/7),.                                                    DAT1 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                           DAT1 200
        ((MM)(7)F(10,0),X(10))),.                                       DAT1 210
```

```
   IF NV= 1                                                          DAT1 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,0)),.    DAT1 230
   REVERT ENDFILE (SYSIN),.                                          DAT1 240
   RETURN,.                                                          DAT1 250
EXIT.,                                                               DAT1 260
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')             DAT1 270
        (SKIP(1),COLUMN(10),A),.                                     DAT1 280
   STOP,.                                                            DAT1 290
   END,.                          /*END OF PROCEDURE DAT1          */DAT1 300
```

MULTIPLE LINEAR REGRESSION REGR

Problem Description

Multiple linear regression analysis is performed for a set of independent variables and a dependent variable. Selection of different sets of independent variables and designation of a dependent variable can be made as many times as desired.

The sample problem for multiple linear regression consists of 30 observations with six variables, as presented in Table 1. The first five variables are independent variables (predictors), and the last is the dependent variable (criteria). All five independent variables are used to predict the dependent variable in the first analysis, and only the second, third, and fifth variables are used to predict the dependent variable in the second analysis.

Table 1. Sample Data for Multiple Linear Regression

	Variables					
Observation	X_1	X_2	X_3	X_4	X_5	X_6
1	29	289	216	85	14	1
2	30	391	244	92	16	2
3	30	424	246	90	18	2
4	30	313	239	91	10	0
5	35	243	275	95	30	2
6	35	365	219	95	21	2
7	43	396	267	100	39	3
8	43	356	274	79	19	2
9	44	346	255	126	56	3
10	44	156	258	95	28	0
11	44	278	249	110	42	4
12	44	349	252	88	21	1
13	44	141	236	129	56	1
14	44	245	236	97	24	1
15	45	297	256	111	45	3
16	45	310	262	94	20	2
17	45	151	339	96	35	3
18	45	370	357	88	15	4
19	45	379	198	147	64	4
20	45	463	206	105	31	3
21	45	316	245	132	60	4
22	45	280	225	108	36	4
23	44	395	215	101	27	1
24	49	139	220	136	59	0
25	49	245	205	113	37	4
26	49	373	215	88	25	1
27	51	224	215	118	54	3
28	51	677	210	116	33	4
29	51	424	210	140	59	4
30	51	150	210	105	30	0

Program

Description

The multiple linear regression program consists of the main program named REGR, two special input routines named DAT2 and IDT1, and four subroutines from the Scientific Subroutine Package: CORR, ORDR, MINV, and MLTR.

Capacity

1. Up to 99,999 observations can be read if observations are read into the computer one at a time by the special input subroutine named DAT2. If all data are to be stored in core before the calculation of correlation coefficients, the limitation on the number of observations depends on the size of core storage available for input data.
2. Up to 96 variables can be handled.
3. Up to 99 selections can be handled.
4. Up to eight cards per observation can be read.
5. (12 F (6, 0)) format for input data cards.

Therefore, if a problem satisfies the above conditions, the sample program need not be modified. If the input data cards are prepared using a different format, the input format in the subroutine DAT2 must be modified. The general rules for program modifications are described later.

6. Up to 40 independent variables for one selection can be read.

Input

Control Cards

One control card is required for each problem and is read by the main program, REGR. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	00030
12-13	Number of variables	06
14-15	Number of selections (see below)	02
16-17	Number of data cards per observation	01

Leading zeros do not have to be keypunched.

Data Cards

Since input data is read into the computer one observation at a time, each row of data in Table 1 is keypunched on a separate card using the format (12 F (6, 0)). This format assumes twelve 6-column fields per card.

Selection Cards

For each selection there must be at least two cards, as described below. If the number of selections specified is zero, the program will terminate. An error message is printed out.

The first card is used to specify a single dependent variable in a multiple linear regression analysis. Any one variable in the set of original variables can be designated as a dependent variable, and any positive number of variables can be specified as independent variables. Selection of a single dependent variable and a set of independent variables can be performed over and over again using the same set of original variables.

The first card is prepared as follows:

Columns	Contents	For Sample Problem Selection 1	Selection 2
1-2	Option code for table of residuals 0 if table is not desired; 1 if table is desired.	01	01
3-4	Dependent variable designated for the forthcoming regression.	06	06
5-6	Number of independent variables included in the forthcoming regression (the subscript numbers of individual variables are specified below).	05	03

The second card is prepared as follows:

Columns	Contents	For Sample Problem Selection 1	Selection 2
1-2	1st independent variable included	01	02
3-4	2nd independent variable included	02	03
5-6	3rd independent variable included	03	05
7-8	4th independent variable included	04	
9-10	5th independent variable included	05	
etc.			

The input format of (40 F (2)) is used for the second card.

Deck Setup

Deck setup is shown in Figure 14.

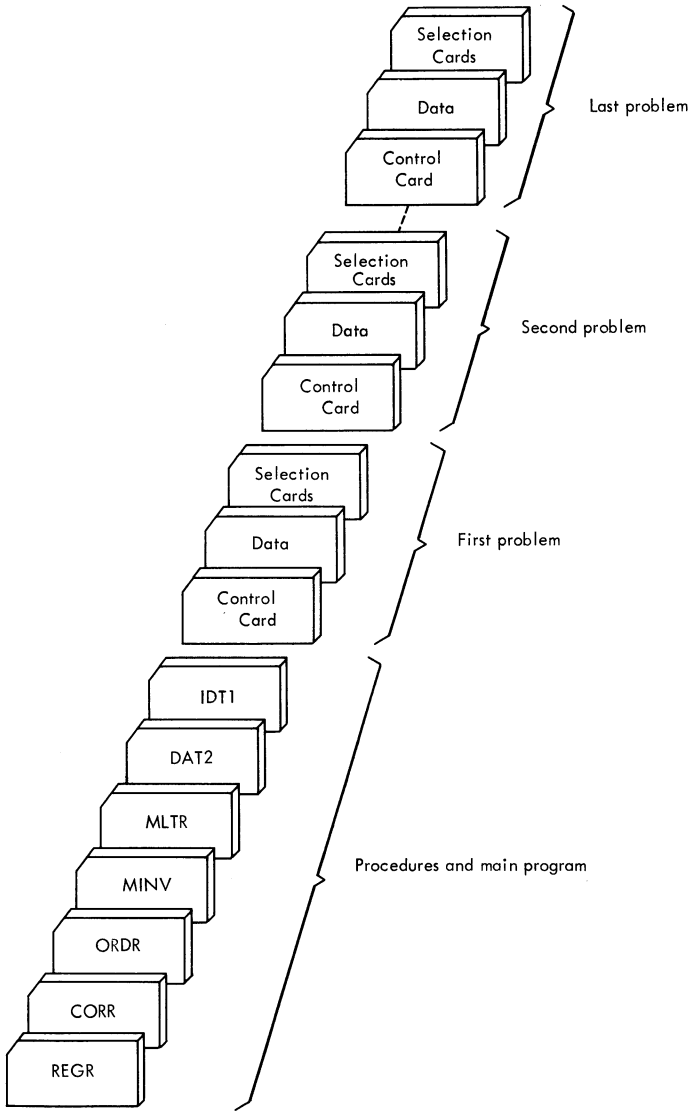


Figure 14.

Sample

The listing of input cards for the sample problem is shown in Figure 15.

```
SAMPLECCC3CC602 1                                                    10
    29   289   216    85    14     1                                 20
    3C   391   244    92    16     2                                 30
    3C   424   246    9C    18     2                                 40
    3C   313   239    91    1C     C                                 50
    35   243   275    95    3C     2                                 60
    35   365   219    95    21     2                                 70
    43   396   267   1CC    39     3                                 80
    43   356   274    79    19     2                                 90
    44   346   255   126    56     3                                100
    44   156   258    95    28     0                                110
    44   278   249   11C    42     4                                120
    44   349   252    88    21     1                                130
    44   141   236   129    56     1                                140
    44   245   236    97    24     1                                150
    45   297   256   111    45     3                                160
    45   31C   262    94    2C     2                                170
    45   151   339    96    35     3                                180
    45   37C   357    88    15     4                                190
    45   379   198   147    64     4                                200
    45   463   206   1C5    31     3                                210
    45   316   245   132    6C     4                                220
    45   28C   225   1C8    36     4                                230
    44   395   215   1C1    27     1                                240
    49   139   22C   136    59     0                                250
    49   245   205   113    37     4                                260
    49   373   215    88    25     1                                270
    51   224   215   118    54     3                                280
    51   677   210   116    33     4                                290
    51   424   210   14C    59     4                                300
    51   15C   210   1C5    3C     C                                310
C106C5                                                              320
C1C2C3C4C5                                                          330
C1C6C3                                                              340
C2C3C5                                                              350
```

Figure 15.

Output

Description

The output based on the selection card of the sample program for multiple linear regression includes:

1. Means
2. Standard deviations
3. Correlation coefficients between independent variables and dependent variables
4. Regression coefficients
5. Standard errors of regression coefficients
6. Computed T values
7. Intercept
8. Multiple correlation coefficients
9. Standard error of estimate
10. Beta coefficients
11. Analysis of variance for the multiple regression
12. Table of residuals (optional)

Sample

The output listing for the sample problem is shown in Figure 16.

```
MULTIPLE REGRESSION.....SAMPLE

NUMBER OF OBSERVATIONS...   30

NUMBER OF VARIABLES......    6

SELECTION..... 1

VARIABLE      MEAN        STANDARD      CORRELATION    REGRESSION    STD. ERROR     COMPUTED       BETA
  NO.                     DEVIATION       X VS Y       COEFFICIENT   OF REG.COEFF.   T VALUE       COEFF.
   1       43.13333        6.52176       0.28422       0.01242       0.03635       0.34171       0.05735
   2      316.16650      114.42990       0.42189       0.00739       0.00186       3.96545       0.59826
   3      241.79999       36.43074       0.11900       0.01504       0.00635       2.36881       0.38790
   4      105.66666       17.85640       0.37822       0.00151       0.03679       0.04100       0.01907
   5       34.13333       15.97571       0.39412       0.04919       0.04141       1.18782       0.55631

DEPENDENT
   6        2.26667        1.41259


INTERCEPT                   -6.07928

MULTIPLE CORRELATION         0.73575

STD. ERROR OF ESTIMATE       1.05162

                    ANALYSIS OF VARIANCE FOR THE REGRESSION

     SOURCE OF VARIATION        DEGREES       SUM OF          MEAN           F VALUE
                                OF FREEDOM    SQUARES         SQUARES
ATRRIBUTABLE TO REGRESSION          5        31.32506        6.26501         5.66508
DEVIATION FROM REGRESSION          24        26.54161        1.10590
     TOTAL                         29        57.86667
```

Figure 16

```
MULTIPLE REGRESSION.....SAMPLE

SELECTION..... 1
                TABLE OF RESIDUALS

CASE NO.      Y VALUE      Y ESTIMATE      RESIDUAL
    1         1.00000        0.48091        0.51909
    2         2.00000        1.77670        0.22330
    3         2.00000        2.14586       -0.14586
    4         0.00000        0.82880       -0.82880
    5         2.00000        1.90522        0.09478
    6         2.00000        1.52125        0.47875
    7         3.00000        3.46447       -0.46447
    8         2.00000        2.25887       -0.25887
    9         3.00000        3.80259       -0.80259
   10         0.00000        1.02042       -1.02042
   11         4.00000        2.49735        1.50265
   12         1.00000        2.00066       -1.00066
   13         1.00000        2.00735       -1.00735
   14         1.00000        1.15308       -0.15308
   15         3.00000        2.90446        0.09554
   16         2.00000        1.83532        0.16468
   17         3.00000        2.56004        0.43996
   18         4.00000        3.45229        0.54771
   19         4.00000        3.62661        0.37339
   20         3.00000        2.68068        0.31932
   21         4.00000        3.64885        0.35115
   22         4.00000        1.86542        2.13458
   23         1.00000        2.09863       -1.09863
   24         0.00000        1.97217       -1.97217
   25         4.00000        1.41253        2.58747
   26         1.00000        1.88027       -0.88027
   27         3.00000        2.27646        0.72354
   28         4.00000        4.51080       -0.51080
   29         4.00000        3.95745        0.04255
   30         0.00000        0.45458       -0.45458



MULTIPLE REGRESSION.....SAMPLE

NUMBER OF OBSERVATIONS...   30

NUMBER OF VARIABLES......    6

SELECTION..... 2

VARIABLE      MEAN        STANDARD       CORRELATION     REGRESSION     STD. ERROR      COMPUTED        BETA
  NO.                     DEVIATION        X VS Y        COEFFICIENT    OF REG.COEFF.    T VALUE        COEFF.
   2      316.16650      114.42990        0.42189        0.00744        0.00172        4.31763        0.60233
   3      241.79999       36.43074        0.11900        0.01497        0.00551        2.71693        0.38618
   5       34.13333       15.97571        0.39412        0.05363        0.01258        4.26262        0.60648

DEPENDENT
   6        2.26667        1.41259

INTERCEPT                   -5.53528

MULTIPLE CORRELATION         0.73423

STD. ERROR OF ESTIMATE       1.01282

                    ANALYSIS OF VARIANCE FOR THE REGRESSION

     SOURCE OF VARIATION        DEGREES       SUM OF          MEAN            F VALUE
                              OF FREEDOM     SQUARES         SQUARES
ATRRIBUTABLE TO REGRESSION         3         31.19594        10.39865         10.13714
DEVIATION FROM REGRESSION         26         26.67073         1.02580
     TOTAL                        29         57.86667



MULTIPLE REGRESSION.....SAMPLE

SELECTION..... 2
                TABLE OF RESIDUALS

CASE NO.      Y VALUE      Y ESTIMATE      RESIDUAL
    1         1.00000        0.59869        0.40131
    2         2.00000        1.88363        0.11637
    3         2.00000        2.26619       -0.26619
    4         0.00000        0.90704       -0.90704
    5         2.00000        1.99812        0.00188
    6         2.00000        1.58408        0.41592
    7         3.00000        3.49858       -0.49858
    8         2.00000        2.23348       -0.23348
    9         3.00000        3.85875       -0.85875
   10         0.00000        0.98943       -0.98943
   11         4.00000        2.51254        1.48746
   12         1.00000        1.95925       -0.95925
   13         1.00000        2.04998       -1.04998
   14         1.00000        1.10726       -0.10726
   15         3.00000        2.91951        0.08049
   16         2.00000        1.76539        0.23461
   17         3.00000        2.54052        0.45948
   18         4.00000        3.36591        0.63409
   19         4.00000        3.67961        0.32039
   20         3.00000        2.65435        0.34565
   21         4.00000        3.70045        0.29955
   22         4.00000        1.84629        2.15371
   23         1.00000        2.06900       -1.06900
   24         0.00000        1.95640       -1.95640
   25         4.00000        1.34019        2.65981
   26         1.00000        1.79817       -0.79817
   27         3.00000        2.24542        0.75458
   28         4.00000        4.41268       -0.41268
   29         4.00000        3.92577        0.07423
   30         0.00000        0.33332       -0.33332


END OF SAMPLE PROGRAM
```

Figure 16. (Continued)

Program Modifications

Input data in a different format can also be handled by providing a special format statement.

1. Changes in the input format statement of the special input routine DAT2:

Only the format statement for input data may be changed. Since sample data are either one-, two-, or three-digit numbers, rather than using six-column fields, as in the sample problem, each row of data might have been keypunched in six 3-column fields; if so, the format is changed to (6 F (3, 0)).

The special input subroutine, DAT2, is normally written by the user to handle different formats for different problems. The user may modify this routine to perform listing of input data, transformation of data, and so on. When doing so, attention should be paid to the format statement in DAT2 (DAT2 230) which writes on the intermediate data set. The format in this statement must be the same as the format in statement REGR 1860.

2. If there are more than twelve variables in a problem, each row of data is continued on the next cards, until the last data point is keypunched. However, each row of data must begin on a new card.

In the sample problem there is one data card per row, so the value of the card count indicator (NCARD), which appears in columns 16 and 17 of the control card, is set to one. If there is more than one data card per row, the value of the card count indicator (NCARD) must agree with the number of data cards per row.

3. Although the program will allow 96 variables, the maximum number of independent variables that may be specified on one selection is 40.

Error Messages

The following error conditions will result in messages:

1. The number of selections is not specified on the control card: NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED.

Operating Instructions

The sample program for multiple linear regression is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output. A scratch tape (data set XDATA) is used as intermediate storage.

Timing

The execution time of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 40 seconds.

```
REGR..                                                                  REGR  10
/*********************************************************************/REGR  20
/*                                                                   */REGR  30
/*      TO READ THE PROBLEM PARAMETER CARD FOR A MULTIPLE REGRESSION,*/REGR  40
/*      READ SUBSET SELECTION CARDS, CALL THE PROCEDURES TO CALCULATE*/REGR  50
/*      MEANS, STANDARD DEVIATIONS, SIMPLE AND MULTIPLE CORRELATION  */REGR  60
/*      COEFFICIENTS, REGRESSION COEFFICIENTS, T-VALUES, BETA COEFF- */REGR  70
/*      ICIENTS, AND ANALYSIS OF VARIANCE FOR MULTIPLE REGRESSION,   */REGR  80
/*      AND PRINT THE RESULTS.                                       */REGR  90
/*                                                                   */REGR 100
/*********************************************************************/REGR 110
   PROCEDURE OPTIONS (MAIN),.                                           REGR 120
   DECLARE                                                              REGR 130
        (I,II,IO,J,K,L,M,MM,N,NDEP,NRESI,NS,L1,L2) FIXED BINARY,        REGR 140
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),        REGR 150
        (NCARD,NV) EXTERNAL,                                            REGR 160
        ERROR EXTERNAL CHARACTER (1),                                   REGR 170
        CH  CHARACTER (80),                                             REGR 180
        PR1 CHARACTER (6),.                                             REGR 190
/*                                                                     */REGR 200
FM1..                                                                   REGR 210
        FORMAT (A(6),F(5),3 F(2)),.                                     REGR 220
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      REGR 230
/*                                                                     */REGR 240
/*      INPUT DATA IS SAVED IF NV IS SET TO 1                          */REGR 250
/*                                                                     */REGR 260
   NV   =1,.                                                            REGR 270
/*                                                                     */REGR 280
S100..                                                                  REGR 290
   GET EDIT (CH) (A(80)),.                                              REGR 300
   GET STRING (CH) EDIT (PR1,N,M,NS,NCARD) (R(FM1)),.                   REGR 310
/*                                                                     */REGR 320
/*      NAME - PROBLEM NUMBER (MAY BE ALPHAMERIC)                      */REGR 330
/*      N    - NUMBER OF OBSERVATIONS                                  */REGR 340
/*      M    - NUMBER OF VARIABLES                                     */REGR 350
/*      NS   - NUMBER OF SELECTIONS                                    */REGR 360
/*      NCARD- NUMBER OF DATA CARDS PER OBSERVATION                    */REGR 370
/*                                                                     */REGR 380
   NCARD=NCARD*80,.                                                     REGR 390
/*                                                                     */REGR 400
STRT..                                                                  REGR 410
   BEGIN,.                                                              REGR 420
FM2..                                                                   REGR 430
   FORMAT (PAGE,SKIP(4),COLUMN(10),A,A(6),SKIP(2),COLUMN(10),A,A,       REGR 440
        F(5),SKIP(2),COLUMN(10),A,F(5),SKIP(2),COLUMN(10),A,F(2)),.     REGR 450
   DECLARE                                                              REGR 460
        (X(1,1),W(M),RESI)                                              REGR 470
        FLOAT BINARY,                                                   REGR 480
        (R(M,M),RX(M,M),XBAR(M),RY(M),D(M),STD(M),ANS(10),FSUM,DET,CON)REGR 490
        BINARY FLOAT,.              /*SINGLE PRECISION VERSION  /*S*/REGR 500
/*      BINARY FLOAT (53),.         /*DOUBLE PRECISION VERSION  /*D*/REGR 510
/*                                                                     */REGR 520
   IO   =0,.                                                            REGR 530
   X    =0,.                                                            REGR 540
   OPEN FILE (XDATA) OUTPUT,.                                           REGR 550
   CALL CORR (N,M,IO,X,XBAR,STD,RX,R,D),.                               REGR 560
   CLOSE FILE (XDATA),.                                                 REGR 570
   IF ERROR NE '0'                                                      REGR 580
   THEN PUT EDIT ('IN ROUTINE CORR ERROR CODE = ',ERROR)                REGR 590
        (SKIP(2),COLUMN(10),A,A(1)),.                                   REGR 600
/*                                                                     */REGR 610
/*      TEST NUMBER OF SELECTIONS                                      */REGR 620
/*                                                                     */REGR 630
   IF NS LE 0                                                           REGR 640
   THEN DO,.                                                            REGR 650
        PUT EDIT ('NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED')REGR 660
             (SKIP(4),COLUMN(10),A),.                                   REGR 670
        GO TO S300,.                                                    REGR 680
        END,.                                                           REGR 690
        DO I = 1 TO NS,.                                                REGR 700
        PUT EDIT ('MULTIPLE REGRESSION.....',PR1,'NUMBER OF OBSERVA',   REGR 710
             'TIONS...',N,'NUMBER OF VARIABLES.....',M,                 REGR 720
             'SELECTION.....',I) (R(FM2)),.                             REGR 730
/*                                                                     */REGR 740
/*      READ SUBSET SELECTION CARD                                     */REGR 750
/*                                                                     */REGR 760
   GET EDIT (CH) (A(80)),.                                              REGR 770
        GET STRING (CH) EDIT (NRESI,NDEP,K) (3 F(2)),.                  REGR 780
KRED..                                                                  REGR 790
   BEGIN,.                                                              REGR 800
FM3..                                                                   REGR 810
        FORMAT (SKIP,COLUMN(10),F(4),7 F(14,5)),.                       REGR 820
FM4..                                                                   REGR 830
        FORMAT (PAGE,SKIP(4),COLUMN(10),A,A(6),SKIP(2),COLUMN(10),      REGR 840
             A,F(2)),.                                                  REGR 850
        DECLARE                                                         REGR 860
             (RZ(K,K),B(K),SB(K),T(K),BETA(K),RT(K))                    REGR 870
             BINARY FLOAT,          /*SINGLE PRECISION VERSION  /*S*/REGR 880
/*           BINARY FLOAT (53),     /*DOUBLE PRECISION VERSION  /*D*/REGR 890
             (ISAVE(K+1))                                               REGR 900
             FIXED BINARY,.                                             REGR 910
/*                                                                     */REGR 920
        CALL IDT1 (K,ISAVE),.                                           REGR 930
/*                                                                     */REGR 940
/*      NRESI - OPTION CODE FOR TABLE OF RESIDUALS                     */REGR 950
/*              0 IF IT IS NOT DESIRED.                                */REGR 960
/*              1 IF IT IS DESIRED.                                    */REGR 970
/*      NDEP  - DEPENDENT VARIABLE.                                    */REGR 980
/*      K     - NUMBER OF INDEPENDENT VARIABLES INCLUDED               */REGR 990
/*      ISAVE - A VECTOR CONTAINING THE INDEPENDENT VARIABLES          */REGR1000
/*              INCLUDED                                               */REGR1010
/*                                                                     */REGR1020
        CALL ORDR (M,R,NDEP,K,ISAVE,RZ,RT),.                            REGR1030
        IF ERROR NE '0'                                                 REGR1040
        THEN DO,.                                                       REGR1050
             PUT EDIT ('IN ROUTINE ORDR ERROR CODE = ',ERROR)           REGR1060
                  (SKIP(2),COLUMN(10),A,A(1)),.                         REGR1070
             GO TO S200,.                                               REGR1080
             END,.                                                      REGR1090
        CON  =0.0,.                                                     REGR1100
        CALL MINV(RZ,K,DET,CON),.                                       REGR1110
/*                                                                     */REGR1120
/*      TEST SINGULARITY OF THE MATRIX INVERTED                        */REGR1130
/*                                                                     */REGR1140
        IF ERROR NE '0'                                                 REGR1150
        THEN DO,.                                                       REGR1160
             PUT EDIT('IN ROUTINE MINV ERROR = ',ERROR) (SKIP(2),       REGR1170
                  COLUMN(10),A,A(1)),.                                  REGR1180
             GO TO S200,.                                               REGR1190
             END,.                                                      REGR1200
/*                                                                     */REGR1210
```

```
      CALL MLTR (N,K,XBAR,STD,D,RZ,RT,ISAVE,B,SB,T,BETA,ANS),.      REGR1220
      IF ERROR NE '0'                                               REGR1230
      THEN DO,.                                                     REGR1240
           PUT EDIT ('IN ROUTINE MLTR ERROR CODE = ',ERROR)         REGR1250
                (SKIP(2),COLUMN(10),A,A(1)),.                       REGR1260
           GO TO S200,.                                             REGR1270
           END,.                                                    REGR1280
/*                                                                 */REGR1290
/*      PRINT MEANS, STANDARD DEVIATIONS, INTERCORRELATIONS BETWEEN */REGR1300
/*      X AND Y, REGRESSION COEFFICIENTS, STANDARD DEVIATIONS OF   */REGR1310
/*      REGRESSION COEFFICIENTS, COMPUTED T VALUES, AND BETA       */REGR1320
/*      COEFFICIENTS.                                              */REGR1330
/*                                                                 */REGR1340
      MM   =K+1,.                                                   REGR1350
      PUT EDIT ('VARIABLE','MEAN','STANDARD','CORRELATION',         REGR1360
           'REGRESSION','STD. ERROR','COMPUTED','BETA','NO.',       REGR1370
           'DEVIATION','X VS Y','COEFFICIENT','OF REG.COEFF.',      REGR1380
           'T VALUE','COEFF.') (SKIP(2),COLUMN(10),A,X(5),A,        REGR1390
           X(6),A,X(6),A,X(4),A,X(4),A,X(5),A,X(7),A,SKIP,          REGR1400
           COLUMN(12),A,X(18),A,X(7),A,X(7),A,X(3),A,X(3),A,        REGR1410
           X(7),A),.                                                REGR1420
           DO J = 1 TO K,.                                          REGR1430
           L    =ISAVE(J),.                                         REGR1440
           PUT EDIT (L,XBAR(L),STD(L),RT(J),B(J),SB(J),T(J),BETA(J)) REGR1450
                (R(FM3)),.                                          REGR1460
           END,.                                                    REGR1470
      PUT EDIT ('DEPENDENT') (SKIP(2),COLUMN(10),A),.               REGR1480
      L    =ISAVE(MM),.                                            REGR1490
      PUT EDIT (L,XBAR(L),STD(L)) (R(FM3)),.                        REGR1500
/*                                                                 */REGR1510
/*      PRINT INTERCEPT, MULTIPLE CORRELATION COEFFICIENT, AND     */REGR1520
/*      STANDARD ERROR OF ESTIMATE                                 */REGR1530
/*                                                                 */REGR1540
      PUT EDIT ('INTERCEPT',ANS(1),'MULTIPLE CORRELATION  ',ANS(2), REGR1550
           'STD. ERROR OF ESTIMATE',ANS(3)) (SKIP(3),COLUMN(10),    REGR1560
           A,X(10),F(16,5),(2)(SKIP(2),COLUMN(10),A,F(13,5))),.     REGR1570
/*                                                                 */REGR1580
/*           PRINT ANALYSIS OF VARIANCE FOR THE REGRESSION         */REGR1590
/*                                                                 */REGR1600
      PUT EDIT ('ANALYSIS OF VARIANCE FOR THE REGRESSION ',         REGR1610
           'SOURCE OF VARIATION','DEGREES','SUM OF','MEAN',         REGR1620
           '  F VALUE','OF FREEDOM','SQUARES','SQUARES')            REGR1630
           (SKIP(2),COLUMN(31),A,SKIP(2),COLUMN(15),A,X(7),A,       REGR1640
           X(7),A,X(10),A,X(09),A,SKIP,COLUMN(40),A,X(4),A,         REGR1650
           X(9),A),.                                                REGR1660
      L    =ANS(8),.                                               REGR1670
      PUT EDIT ('ATRRIBUTABLE TO REGRESSION   ',K,ANS(4),ANS(6),    REGR1680
           ANS(10),'DEVIATION FROM REGRESSION    ',L,ANS(7),        REGR1690
           ANS(9)) (SKIP,COLUMN(10),A,F(6),3 F(16,5),SKIP,          REGR1700
           COLUMN(10),A,F(6),2 F(16,5)),.                           REGR1710
      L    =N-1,.                                                  REGR1720
      FSUM =ANS(4)+ANS(7),.                                         REGR1730
      PUT EDIT('TOTAL',L,FSUM) (COLUMN(15),A,X(19),F(6),F(16,5)),.  REGR1740
      IF NRESI LE 0                                                 REGR1750
      THEN GO TO S200,.                                             REGR1760
      PUT EDIT ('MULTIPLE REGRESSION.....',PR1,'SELECTION.....',I)  REGR1770
           (R(FM4)),.                                               REGR1780
      PUT EDIT ('TABLE OF RESIDUALS','CASE NO.','Y VALUE',          REGR1790
           'Y ESTIMATE','RESIDUAL') (SKIP,COLUMN(25),A,SKIP(2),     REGR1800
           COLUMN(10),A,X(5),A,X(5),A,X(6),A),.                     REGR1810
      MM   =ISAVE(K+1),.                                            REGR1820
      OPEN FILE (XDATA) INPUT,.                                     REGR1830
           DO II = 1 TO N,.                                         REGR1840
           GET FILE (XDATA) EDIT ((W(J) DO J= 1 TO M))              REGR1850
                ((M)F(6,0)),.                                       REGR1860
           FSUM =ANS(1),.                                           REGR1870
                DO J = 1 TO K,.                                     REGR1880
                L    =ISAVE(J),.                                    REGR1890
                FSUM =FSUM+W(L)*B(J),.                              REGR1900
                END,.                                               REGR1910
           RESI =W(MM)-FSUM,.                                       REGR1920
           PUT EDIT (II,W(MM),FSUM,RESI) (COLUMN(10),F(5),F(15,5),  REGR1930
                2 F(14,5)),.                                        REGR1940
           END,.                                                    REGR1950
      CLOSE FILE (XDATA),.                                          REGR1960
   GO TO S100,.                                                     REGR2010
EXIT..                                                              REGR2020
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')               REGR2030
        (SKIP(5),COLUMN(10),A),.                                    REGR2040
S300..                                                              REGR2050
   END,.                              /*END OF PROCEDURE REGR      */REGR2060
```

```
DAT2..                                                              DAT2  10
/*******************************************************************/DAT2  20
/*                                                                 */DAT2  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.    */DAT2  40
/*      DATA MAY BE SAVED ON A DATA SET.                           */DAT2  50
/*                                                                 */DAT2  60
/*******************************************************************/DAT2  70
   PROCEDURE (M,D),.                                                DAT2  80
   DECLARE                                                          DAT2  90
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),    DAT2 100
        (NCARD,NV) EXTERNAL,                                        DAT2 110
        CH CHARACTER(NCARD),                                        DAT2 120
        (I,M,MM) FIXED BINARY,                                      DAT2 130
        D(*) FLOAT BINARY,.                                         DAT2 140
/*                                                                 */DAT2 150
   ON ENDFILE (SYSIN)                                               DAT2 160
   GO TO EXIT,.                                                     DAT2 170
   GET EDIT (CH) (A(NCARD)),.                                       DAT2 180
   MM   =CEIL(M/12),.                                               DAT2 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                       DAT2 200
        ((MM)((12)F(6,0),X(8))),.                                   DAT2 210
   IF NV= 1                                                         DAT2 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,0)),.   DAT2 230
   REVERT ENDFILE (SYSIN),.                                         DAT2 240
   RETURN,.                                                         DAT2 250
EXIT..                                                              DAT2 260
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')            DAT2 270
        (SKIP(1),COLUMN(10),A),.                                    DAT2 280
   STOP,.                                                           DAT2 290
   END,.                              /*END OF PROCEDURE DAT2      */DAT2 300
```

```
IDT1..                                                              IDT1  10
/*******************************************************************/IDT1  20
/*                                                                 */IDT1  30
/*      TO READ FIXED POINT DATA.                                  */IDT1  40
/*                                                                 */IDT1  50
/*******************************************************************/IDT1  60
   PROCEDURE (M,IX),.                                               IDT1  70
   DECLARE                                                          IDT1  80
        CH CHARACTER (80),                                          IDT1  90
        (IX(*),NF,N1,N2,M,I)                                        IDT1 100
        FIXED BINARY,.                                              IDT1 110
   NF   =40,.                                                       IDT1 120
   N1   =1,.                                                        IDT1 130
   N2   =NF,.                                                       IDT1 140
S10..                                                               IDT1 150
   IF M LE N2                                                       IDT1 160
   THEN N2   =M,.                                                   IDT1 170
   GET EDIT (CH) (A(80)),.                                          IDT1 180
   GET STRING (CH) EDIT ((IX(I) DO I= N1 TO N2)) ((NF)F(2)),.       IDT1 190
   N1   =N2+1,.                                                     IDT1 200
   IF N1 LE M                                                       IDT1 210
   THEN DO,.                                                        IDT1 220
        N2   =N2+NF,.                                               IDT1 230
        GO TO S10,.                                                 IDT1 240
        END,.                                                       IDT1 250
   RETURN,.                                                         IDT1 260
   END,.                              /*END OF PROCEDURE IDT1      */IDT1 270
```

STEPWISE MULTIPLE REGRESSION STEP

Problem Description

Stepwise multiple regression analysis is performed for a set of independent variables and a dependent variable. Selection of different sets of independent variables and designation of a dependent variable can be made as many times as desired.

1. The sample problem for stepwise multiple regression consists of 30 observations with six variables, as presented in Table 1 earlier in this Appendix.

2. The first five variables are independent variables, and the last variable is the dependent variable. All five independent variables are used to predict the dependent variable in the first analysis, and only the second, third, and fifth variables are used to predict the dependent variable in the second analysis.

Program

Description

The stepwise multiple regression program consists of the main routine named STEP, two special input subroutines named DAT2 and IDT2, an output subroutine named SOUT, and two routines from the Scientific Subroutine Package: CORR and STRG.

Capacity

1. Up to 99,999 observations if observations are read into the computer one at a time by the special input routine. If all data are to be stored in core before the calculation of correlation coefficients, the limitation on the number of observations depends on the size of core storage available for input data.

2. Up to 72 variables

3. Up to 99 selections (must be greater than zero)

4. (12 F(6, 0)) format for input data cards. Therefore if a problem satisfies the above conditions, the sample program need not be modified. If the input

data cards are prepared using a different format, the input format in the special input routine, DAT2, must be modified. The general rules for program modifications are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, STEP. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	00030
12-13	Number of variables	06
14-15	Number of selections	02
16-20	A constant value of proportion of sum of squares that will be used to limit variables entering in the regression	0.0
21	Option code for table of residuals 0 - if it is not desired 1 - if it is desired	1
22-23	Number of cards per observation	1

Leading zeros do not have to be keypunched.

Data Cards

Since input data is read into the computer one observation at a time, each row of data in table is keypunched on a separate card using the format (12 F (6, 0)). This format assumes twelve 6-column fields per card. If there are more than twelve variables in a problem, each row of data is continued on the next card until the last data point is keypunched. However, each row of data must begin on a new card.

Selection Card

The selection card is used to specify a single dependent variable and a non-null set of independent variables in a stepwise multiple regression analysis. Any variable in the set of original variables can be designated as a dependent variable, and any number of variables can be specified as independent variables. Selection of a dependent variable and a set of independent variables can be performed over and over again using the same set of original variables.

There must be a selection card in order for the program to continue. In the selection card each variable is specified using one of the following codes:

0 or blank - Independent variable available for selection
1 - Independent variable forced in regression
2 - Variable to be deleted
3 - Dependent variable

Columns	Contents	For Sample Problem Selection 1	Selection 2
1	First variable	0	2
2	Second variable	0	0
3	Third variable	0	0
4	Fourth variable	0	2
5	Fifth variable	0	0
6	Sixth variable	3	3
	.		
	.		
	.		
72	72nd variable		

Leading zeros do not have to be keypunched. If more than 72 selections are made, continue selection specification codes beginning in column 1 of a second card.

Deck Setup

Deck setup is shown in Figure 17.

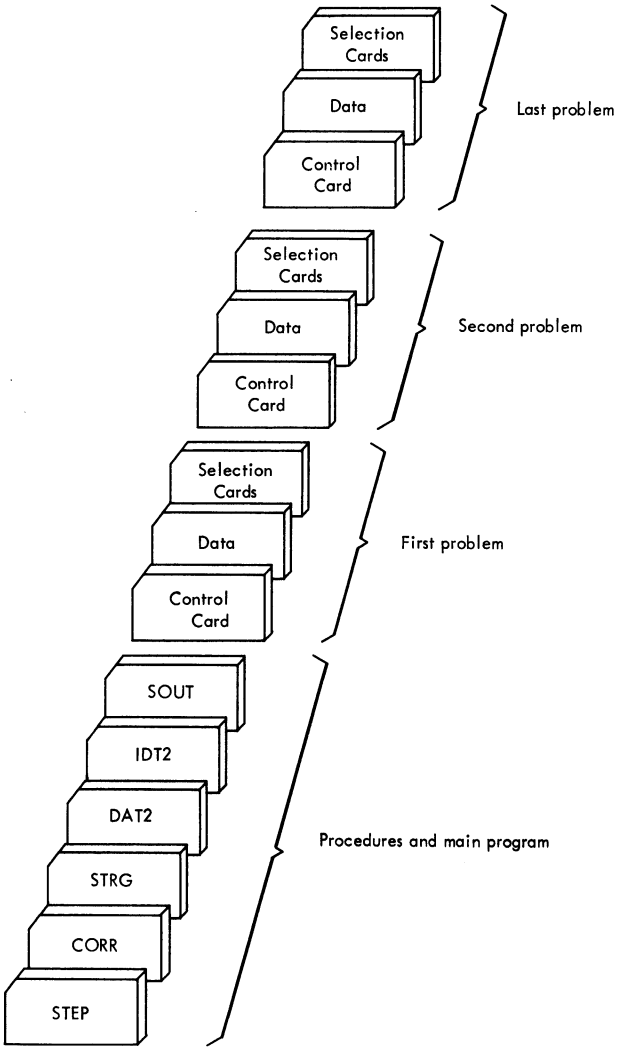


Figure 17.

Sample

The listing of the input cards for the sample problem is shown in Figure 18.

```
SAMPLECCC3C0602   C.01 1                                                10
    29   289   216    85    14     1                                    20
    3C   391   244    92    16     2                                    30
    3C   424   246    90    18     2                                    40
    3C   313   239    91    10     0                                    50
    35   243   275    95    3C     2                                    60
    35   365   219    95    21     2                                    70
    43   396   267   100    39     3                                    80
    43   356   274    79    19     2                                    90
    44   346   255   126    56     3                                   100
    44   156   258    95    28     0                                   110
    44   278   249   11C    42     4                                   120
    44   349   252    88    21     1                                   130
    44   141   236   129    56     1                                   140
    44   245   236    97    24     1                                   150
    45   297   256   111    45     3                                   160
    45   31C   262    94    2C     2                                   170
    45   151   339    96    35     3                                   180
    45   37C   357    88    15     4                                   190
    45   379   198   147    64     4                                   200
    45   463   206   1C5    31     3                                   210
    45   316   245   132    6C     4                                   220
    45   28C   225   1C8    36     4                                   230
    44   395   215   1C1    27     1                                   240
    49   139   220   136    59     0                                   250
    49   245   205   113    37     4                                   260
    49   373   215    88    25     1                                   270
    51   224   215   118    54     3                                   280
    51   677   210   116    33     4                                   290
    51   424   210   140    59     4                                   300
    51   15C   210   1C5    3C     0                                   310
C00003                                                                 320
2CC2C3                                                                 330
```

Figure 18.

Output

Description

The output of the sample program for stepwise multiple regression includes:

1. Means
2. Standard deviations
3. Correlation coefficients between independent variables and dependent variables
4. Sum of squares reduced in the step
5. Proportion reduced in the step
6. Multiple correlation coefficient
7. F value for analysis of variance
8. Standard error of estimate
9. Computed T value
10. Beta coefficients
11. Table of residuals (optional)

Sample

The output listing for the sample problem is shown in Figure 19.

```
STEP-WISE MULTIPLE REGRESSION.....SAMPLE

NUMBER OF OBSERVATIONS   30
NUMBER OF VARIABLES       6
NUMBER OF SELECTIONS      2

CONSTANT TO LIMIT VARIABLE  0.00000

VARIABLE      MEAN      STANDARD
   NO.                  DEVIATION
    1       43.13333     6.52176
    2      316.16650   114.42990
    3      241.79999    36.43074
    4      105.66666    17.85640
    5       34.13333    15.97571
    6        2.26667     1.41259

CORRELATION MATRIX

ROW  1
     1.00000    -0.06721    -0.13689     0.49755     0.55849     0.28422

ROW  2
    -0.06721     1.00000    -0.17857    -0.05227    -0.18381     0.42189

ROW  3
    -0.13689    -0.17857     1.00000    -0.40874    -0.26319     0.11900

ROW  4
     0.49755    -0.05227    -0.40874     1.00000     0.93552     0.37822

ROW  5
     0.55849    -0.18381    -0.26319     0.93552     1.00000     0.39412

ROW  6
     0.28422     0.42189     0.11900     0.37822     0.39412     1.00000

SELECTION..... 1

DEPENDENT VARIABLE............ 6
NUMBER OF VARIABLES FORCED.... 0
NUMBER OF VARIABLES DELETED... 0

STEP  1

VARIABLE ENTERED..... 2

SUM OF SQUARES REDUCED IN THIS STEP....        10.300
PROPORTION REDUCED IN THIS STEP........         0.178

CUMULATIVE SUM OF SQUARES REDUCED......        10.300
CUMULATIVE PROPORTION REDUCED..........         0.178  OF        57.867

FOR  1 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.422
       (ADJUSTED FOR D.F.)...........     0.422
  F-VALUE FOR ANALYSIS OF VARIANCE...     6.063
  STANDARD ERROR OF ESTIMATE.........     1.303
       (ADJUSTED FOR D.F.)...........     1.303

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
     2            0.00521          0.00212          2.462        0.42189
  INTERCEPT       0.62005
```

Figure 19.

```
STEP  2

VARIABLE ENTERED..... 5


SUM OF SQUARES REDUCED IN THIS STEP....        13.324
PROPORTION REDUCED IN THIS STEP........         0.230


CUMULATIVE SUM OF SQUARES REDUCED......        23.624
CUMULATIVE PROPORTION REDUCED.........         0.408  OF       57.867

FOR  2 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.639
       (ADJUSTED FOR D.F.)...........     0.622
  F-VALUE FOR ANALYSIS OF VARIANCE...     9.314
  STANDARD ERROR OF ESTIMATE.........     1.126
       (ADJUSTED FOR D.F.)...........     1.146

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00632          0.00186          3.397        0.51162
      5           0.04316          0.01332          3.241        0.48817
  INTERCEPT      -1.20349


STEP  3

VARIABLE ENTERED..... 3


SUM OF SQUARES REDUCED IN THIS STEP....         7.572
PROPORTION REDUCED IN THIS STEP........         0.131


CUMULATIVE SUM OF SQUARES REDUCED......        31.196
CUMULATIVE PROPORTION REDUCED.........         0.539  OF       57.867

FOR  3 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.734
       (ADJUSTED FOR D.F.)...........     0.711
  F-VALUE FOR ANALYSIS OF VARIANCE...    10.137
  STANDARD ERROR OF ESTIMATE.........     1.013
       (ADJUSTED FOR D.F.)...........     1.050

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00744          0.00172          4.318        0.60233
      5           0.05363          0.01258          4.263        0.60648
      3           0.01497          0.00551          2.717        0.38618
  INTERCEPT      -5.53529


STEP  4

VARIABLE ENTERED..... 1


SUM OF SQUARES REDUCED IN THIS STEP....         0.127
PROPORTION REDUCED IN THIS STEP........         0.002


CUMULATIVE SUM OF SQUARES REDUCED......        31.323
CUMULATIVE PROPORTION REDUCED.........         0.541  OF       57.867

FOR  4 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.736
       (ADJUSTED FOR D.F.)...........     0.699
  F-VALUE FOR ANALYSIS OF VARIANCE...     7.375
  STANDARD ERROR OF ESTIMATE.........     1.030
       (ADJUSTED FOR D.F.)...........     1.088

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00741          0.00175          4.222        0.59997
      5           0.05076          0.01524          3.332        0.57411
      3           0.01493          0.00561          2.662        0.38499
      1           0.01226          0.03541          0.346        0.05661
  INTERCEPT      -5.94617


STEP  5

VARIABLE ENTERED..... 4


SUM OF SQUARES REDUCED IN THIS STEP....         0.002
PROPORTION REDUCED IN THIS STEP........         0.000


CUMULATIVE SUM OF SQUARES REDUCED......        31.325
CUMULATIVE PROPORTION REDUCED.........         0.541  OF       57.867

FOR  5 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.736
       (ADJUSTED FOR D.F.)...........     0.684
  F-VALUE FOR ANALYSIS OF VARIANCE...     5.665
  STANDARD ERROR OF ESTIMATE.........     1.052
       (ADJUSTED FOR D.F.)...........     1.133

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00739          0.00186          3.965        0.59826
      5           0.04919          0.04141          1.188        0.55632
      3           0.01504          0.00635          2.369        0.38790
      1           0.01242          0.03635          0.342        0.05735
      4           0.00151          0.03679          0.041        0.01907
  INTERCEPT      -6.07929
```

Figure 19. (Continued)

```
STEP-WISE MULTIPLE REGRESSION.....SAMPLE

SELECTION..... 1

                TABLE OF RESIDUALS

CASE NO.      Y VALUE       Y ESTIMATE       RESIDUAL
    1         1.00000         0.48090         0.51910
    2         2.00000         1.77670         0.22330
    3         2.00000         2.14586        -0.14586
    4         0.00000         0.82880        -0.82880
    5         2.00000         1.90522         0.09478
    6         2.00000         1.52125         0.47875
    7         3.00000         3.46447        -0.46447
    8         2.00000         2.25887        -0.25887
    9         3.00000         3.80259        -0.80259
   10         0.00000         1.02042        -1.02042
   11         4.00000         2.49735         1.50265
   12         1.00000         2.00065        -1.00065
   13         1.00000         2.00736        -1.00736
   14         1.00000         1.15308        -0.15308
   15         3.00000         2.90446         0.09554
   16         2.00000         1.83531         0.16469
   17         3.00000         2.56004         0.43996
   18         4.00000         3.45228         0.54772
   19         4.00000         3.62661         0.37339
   20         3.00000         2.68068         0.31932
   21         4.00000         3.64886         0.35114
   22         4.00000         1.86541         2.13459
   23         1.00000         2.09863        -1.09863
   24         0.00000         1.97217        -1.97217
   25         4.00000         1.41254         2.58746
   26         1.00000         1.88027        -0.88027
   27         3.00000         2.27646         0.72354
   28         4.00000         4.51080        -0.51080
   29         4.00000         3.95746         0.04254
   30         0.00000         0.45458        -0.45458

STEP-WISE MULTIPLE REGRESSION.....SAMPLE

SELECTION..... 2

DEPENDENT VARIABLE..... 6
NUMBER OF VARIABLES FORCED.... 0
NUMBER OF VARIABLES DELETED... 2


STEP  1

VARIABLE ENTERED..... 2


SUM OF SQUARES REDUCED IN THIS STEP....        10.300
PROPORTION REDUCED IN THIS STEP........         0.178


CUMULATIVE SUM OF SQUARES REDUCED......        10.300
CUMULATIVE PROPORTION REDUCED.........         0.178  OF       57.867

FOR  1 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.422
       (ADJUSTED FOR D.F.)...........     0.422
  F-VALUE FOR ANALYSIS OF VARIANCE...     6.063
  STANDARD ERROR OF ESTIMATE.........     1.303
       (ADJUSTED FOR D.F.)...........     1.303

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00521          0.00212          2.462        0.42189
  INTERCEPT       0.62005


STEP  2

VARIABLE ENTERED..... 5


SUM OF SQUARES REDUCED IN THIS STEP....        13.324
PROPORTION REDUCED IN THIS STEP........         0.230


CUMULATIVE SUM OF SQUARES REDUCED......        23.624
CUMULATIVE PROPORTION REDUCED.........         0.408  OF       57.867

FOR  2 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.639
       (ADJUSTED FOR D.F.)...........     0.622
  F-VALUE FOR ANALYSIS OF VARIANCE...     9.314
  STANDARD ERROR OF ESTIMATE.........     1.126
       (ADJUSTED FOR D.F.)...........     1.146

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00632          0.00186          3.397        0.51162
      5           0.04316          0.01332          3.241        0.48817
  INTERCEPT      -1.20349


STEP  3

VARIABLE ENTERED..... 3


SUM OF SQUARES REDUCED IN THIS STEP....         7.572
PROPORTION REDUCED IN THIS STEP........         0.131


CUMULATIVE SUM OF SQUARES REDUCED......        31.196
CUMULATIVE PROPORTION REDUCED.........         0.539  OF       57.867

FOR  3 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...     0.734
       (ADJUSTED FOR D.F.)...........     0.711
  F-VALUE FOR ANALYSIS OF VARIANCE...    10.137
  STANDARD ERROR OF ESTIMATE.........     1.013
       (ADJUSTED FOR D.F.)...........     1.050

  VARIABLE      REGRESSION      STD. ERROR OF      COMPUTED      BETA
   NUMBER       COEFFICIENT     REG. COEFF.        T-VALUE       COEFFICIENT
      2           0.00744          0.00172          4.318        0.60233
      5           0.05363          0.01258          4.263        0.60648
      3           0.01497          0.00551          2.717        0.38618
  INTERCEPT      -5.53529
```

Figure 19. (Continued)

```
STEP-WISE MULTIPLE REGRESSION.....SAMPLE

SELECTION..... 2

                TABLE OF RESIDUALS

CASE NO.      Y VALUE      Y ESTIMATE       RESIDUAL
    1         1.00000        0.59869         0.40131
    2         2.00000        1.88363         0.11637
    3         2.00000        2.26620        -0.26620
    4         0.00000        0.90704        -0.90704
    5         2.00000        1.99813         0.00187
    6         2.00000        1.58408         0.41592
    7         3.00000        3.49859        -0.49859
    8         2.00000        2.23348        -0.23348
    9         3.00000        3.85876        -0.85876
   10         0.00000        0.98943        -0.98943
   11         4.00000        2.51255         1.48745
   12         1.00000        1.95926        -0.95926
   13         1.00000        2.04998        -1.04998
   14         1.00000        1.10726        -0.10726
   15         3.00000        2.91951         0.08049
   16         2.00000        1.76539         0.23461
   17         3.00000        2.54052         0.45948
   18         4.00000        3.36591         0.63409
   19         4.00000        3.67961         0.32039
   20         3.00000        2.65435         0.34565
   21         4.00000        3.70045         0.29955
   22         4.00000        1.84629         2.15371
   23         1.00000        2.06900        -1.06900
   24         0.00000        1.95640        -1.95640
   25         4.00000        1.34020         2.65980
   26         1.00000        1.79817        -0.79817
   27         3.00000        2.24542         0.75458
   28         4.00000        4.41268        -0.41268
   29         4.00000        3.92577         0.07423
   30         0.00000        0.33332        -0.33332


 END OF SAMPLE PROGRAM
```

Figure 19. (Continued)

Program Modifications

Input data in a different format can be handled by providing a special format statement. The special input routine, DAT2 is normally written by the user to handle different formats for different problems. The user may modify this routine to perform testing of input data, transformation of data and so on. When doing so, attention should be paid to the format statement in DAT2 (DAT2 230), which writes on the intermediate data set. The format in this statement must be the same as the format in statement STEP 1390.

Operating Instructions

The sample program for stepwise multiple regression is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output. A scratch tape (data set XDATA) is used as intermediate storage.

Error Messages

The following error condition will result in a message:

1. The number of selections not specified on the control card: NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED.

Timing

The execution of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 41 seconds.

```
STEP..                                                                  STEP  10
/*********************************************************************/STEP  20
/*                                                                   */STEP  30
/*      TO READ THE PROBLEM PARAMETER CARD FOR A STEP-WISE REGRESSION*/STEP  40
/*      READ SUBSET SELECTION CARD, CALL THE PROCEDURES TO CALCULATE */STEP  50
/*      MEANS, STANDARD DEVIATIONS, AND THE PROCEDURE THAT PERFORMS  */STEP  60
/*      STEP-WISE REGRESSION.                                        */STEP  70
/*                                                                   */STEP  80
/*********************************************************************/STEP  90
   PROCEDURE OPTIONS (MAIN),.                                           STEP 100
   DECLARE                                                              STEP 110
         XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),       STEP 120
         (I,IO,J,K,KK,M,MM,N,NR,NS,NSEL) FIXED BINARY,                  STEP 130
         PR1  CHARACTER (6),                                            STEP 140
         (NCARD,NV) EXTERNAL,                                           STEP 150
         ERROR EXTERNAL CHARACTER (1),                                  STEP 160
         CH   CHARACTER (80),.                                          STEP 170
/*                                                                    */STEP 180
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      STEP 190
S100..                                                                  STEP 200
   GET EDIT (CH) (A(80)),.                                              STEP 210
   GET STRING (CH) EDIT  (PR1,N,M,NS,PCT,NR,NCARD) (A(6),F(5),2 F(2),   STEP 220
         F(6,0),F(1),F(2)),.                                            STEP 230
/*                                                                    */STEP 240
/*      READ PROBLEM PARAMETER CARD                                   */STEP 250
/*                                                                    */STEP 260
/*      PR1 - PROBLEM CODE (MAY BE ALPHAMERIC)                        */STEP 270
/*      N   - NUMBER OF OBSERVATIONS                                  */STEP 280
/*      M   - NUMBER OF VARIABLES                                     */STEP 290
/*      NS  - NUMBER OF SELECTIONS                                    */STEP 300
/*      PCT - A CONSTANT VALUE OF PROPORTION OF SUM OF SQUARES THAT   */STEP 310
/*            WILL BE USED TO LIMIT VARIABLES ENTERING IN THE REGRES-*/STEP 320
/*            SION                                                    */STEP 330
/*      NR  - OPTION CODE FOR TABLE OF RESIDUALS                      */STEP 340
/*             0 - IF IT IS NOT DESIRED                               */STEP 350
/*             1 - IF IT IS DESIRED                                   */STEP 360
/*      NCARD - NUMBER OF DATA CARDS PER OBSERVATION                  */STEP 370
/*                                                                    */STEP 380
   NV   =NR,.                                                           STEP 390
   NCARD=NCARD*80,.                                                     STEP 400
/*                                                                    */STEP 410
   PUT EDIT ('STEP-WISE MULTIPLE REGRESSION.....',PR1)                  STEP 420
         (PAGE,COLUMN(10),A,A),.                                        STEP 430
   PUT SKIP(2),.                                                        STEP 440
   PUT EDIT ('NUMBER OF OBSERVATIONS',N) (R(FM1)),.                     STEP 450
   PUT EDIT ('NUMBER OF VARIABLES   ',M) (R(FM1)),.                     STEP 460
   PUT EDIT ('NUMBER OF SELECTIONS  ',NS) (R(FM1)),.                    STEP 470
FM1..                                                                   STEP 480
   FORMAT (SKIP(1),COLUMN(10),A,F(5)),.                                 STEP 490
   PUT EDIT ('CONSTANT TO LIMIT VARIABLE',PCT)                          STEP 500
         (SKIP(2),COLUMN(10),A,F(9,5)),.                                STEP 510
ONE..                                                                   STEP 520
   BEGIN,.                                                              STEP 530
   DECLARE                                                              STEP 540
         (XBAR(M),STD(M),D(M),B(M),RX(M,M),R(M,M),ANS(11),X(1,1),       STEP 550
         RESI,YEST)                                                     STEP 560
         BINARY FLOAT,                  /*SINGLE PRECISION VERSION  /*S*/STEP 570
/*       BINARY FLOAT (53),             /*DOUBLE PRECISION VERSION  /*D*/STEP 580
         (IDX(M),L(M),NSTEP(5)) FIXED BINARY,.                          STEP 590
   IO   =0,.                                                            STEP 600
   X    =0,.                                                            STEP 610
   OPEN FILE (XDATA) OUTPUT,.                                           STEP 620
   CALL CORR (N,M,IO,X,XBAR,STD,RX,R,B),.                               STEP 630
   CLOSE FILE (XDATA),.                                                 STEP 640
   IF ERROR NE '0'                                                      STEP 650
   THEN PUT EDIT ('IN ROUTINE CORR ERROR CODE = ',ERROR)                STEP 660
         (SKIP(2),COLUMN(10),A,A(1)),.                                  STEP 670
/*                                                                    */STEP 680
/*      PRINT MEANS AND STANDARD DEVIATION                            */STEP 690
/*                                                                    */STEP 700
   PUT EDIT ('VARIABLE','MEAN','STANDARD','NO.','DEVIATION')            STEP 710
         (SKIP(2),COLUMN(10),A,X(5),A,X(5),A,SKIP,COLUMN(13),A,X(16)    STEP 720
         ,A),.                                                          STEP 730
         DO I = 1 TO M,.                                                STEP 740
         PUT EDIT (I,XBAR(I),STD(I)) (SKIP,COLUMN(13),F(2),F(14,5),     STEP 750
               F(12,5)),.                                               STEP 760
         END,.                                                          STEP 770
/*                                                                    */STEP 780
/*      PRINT CORRELATION MATRIX                                      */STEP 790
/*                                                                    */STEP 800
   PUT EDIT ('CORRELATION MATRIX') (SKIP(2),COLUMN(10),A),.             STEP 810
         DO I = 1 TO M,.                                                STEP 820
         PUT EDIT ('ROW',I) (SKIP(2),COLUMN(10),A,F(3)),.               STEP 830
         PUT EDIT ((R(I,J) DO J= 1 TO M)) (SKIP,COLUMN(10),9 F(12,5)),. STEP 840
         END,.                                                          STEP 850
   IF NS LE 0                          /* TEST NUMBER OF SELECTIONS   */STEP 860
   THEN DO,.                                                            STEP 870
         PUT EDIT ('NUMBER OF SELECTIONS NOT SPECIFIED')                STEP 880
               (SKIP(2),COLUMN(10),A),.                                 STEP 890
         GO TO S200,.                                                   STEP 900
         END,.                                                          STEP 910
/*                                                                    */STEP 920
/*      SAVE THE MATRIX OF SUMS OF CROSS-PRODUCTS OF DEVIATION        */STEP 930
/*                                                                    */STEP 940
   R    =RX,.                                                           STEP 950
   NSEL =1,.                                                            STEP 960
   GO TO S150,.                                                         STEP 970
/*                                                                    */STEP 980
/*      COPY THE MATRIX OF SUMS OF CROSS-PRODUCTS OF DEVIATIONS       */STEP 990
/*                                                                    */STEP1000
S145..                                                                  STEP1010
         RX   =R,.                                                      STEP1020
S150..                                  /* READ A SELECTION CARD      */STEP1030
   PUT EDIT ('SELECTION.....',NSEL) (SKIP(3),COLUMN(10),A,F(2)),.       STEP1040
   CALL IDT2 (M,IDX),.                                                  STEP1050
/*                                                                    */STEP1060
/*      IN EACH POSITION OF IDX, ONE OF THE FOLLOWING CODES MUST BE   */STEP1070
/*      SPECIFIED.                                                    */STEP1080
/*        0 OR BLANK - INDEPENDENT VARIABLE AVAILABLE FOR SELECTION   */STEP1090
/*        1          - INDEPENDENT VARIABLE TO BE FORCED IN REGRES-   */STEP1100
/*                     SION                                           */STEP1110
/*        2          - VARIABLE TO BE DELETED                        */STEP1120
/*        3          - DEPENDENT VARIABLE                            */STEP1130
```

```
/*                                                                    */STEP1140
/*      CALL THE PROCEDURE TO PERFORM A STEP-WISE REGRESSION ANALYSIS*/STEP1150
/*                                                                    */STEP1160
   CALL STRG (M,N,RX,XBAR,IDX,PCT,NSTEP,ANS,L,B,STD),.                  STEP1170
   IF ERROR NE '0'                                                      STEP1180
   THEN PUT EDIT ('IN ROUTINE STRG ERROR CODE = ',ERROR)                STEP1190
        (SKIP(2),COLUMN(10),A,A(1)),.                                   STEP1200
/*                                                                    */STEP1210
/*      FIND WHETHER TO PRINT THE TABLE OF RESIDUALS                  */STEP1220
/*                                                                    */STEP1230
   IF NR LE 0                                                           STEP1240
   THEN GO TO S185,.                                                    STEP1250
/*                                                                    */STEP1260
/*      PRINT TABLE OF RESIDUALS                                      */STEP1270
/*                                                                    */STEP1280
   PUT EDIT ('STEP-WISE MULTIPLE REGRESSION.....',PR1)                  STEP1290
        (PAGE,COLUMN(10),A,A),.                                         STEP1300
   PUT EDIT ('SELECTION.....',NSEL) (SKIP(3),COLUMN(10),A,F(2)),.       STEP1310
   PUT EDIT ('TABLE OF RESIDUALS','CASE NO.','Y VALUE','Y ESTIMATE',    STEP1320
        'RESIDUAL')                                                     STEP1330
        (SKIP(2),COLUMN(26),A,SKIP(2),COLUMN(10),A,X(5),A,X(5),A,       STEP1340
        X(6),A),.                                                       STEP1350
   MM   =NSTEP(1),.                                                     STEP1360
   OPEN FILE (XDATA) INPUT,.                                            STEP1370
        DO I = 1 TO N,.                                                 STEP1380
        GET FILE (XDATA) EDIT ((D(J) DO J= 1 TO M)) ((M)F(6,0)),.       STEP1390
        YEST =ANS(9),.                                                  STEP1400
        K    =NSTEP(4),.                                                STEP1410
             DO J = 1 TO K,.                                            STEP1420
             KK   =L(J),.                                               STEP1430
             YEST =YEST+B(J)*D(KK),.                                    STEP1440
             END,.                                                      STEP1450
        RESI =D(MM)-YEST,.                                              STEP1460
        PUT EDIT (I,D(MM) ,YEST,RESI) (COLUMN(10),F(5),F(15,5),         STEP1470
             2 F(14,5)),.                                               STEP1480
        END,.                                                           STEP1490
   CLOSE FILE (XDATA),.                                                 STEP1500
/*                                                                    */STEP1510
/*      TEST WHETHER ALL SELECTIONS ARE COMPLETED                     */STEP1520
/*                                                                    */STEP1530
S185.,                                                                  STEP1540
   IF NSEL LT NS                                                        STEP1550
   THEN DO,.                                                            STEP1560
        NSEL =NSEL+1,.                                                  STEP1570
        PUT EDIT ('STEP-WISE MULTIPLE REGRESSION.....',PR1)             STEP1580
             (PAGE,COLUMN(10),A,A),.                                    STEP1590
        GO TO S145,.                                                    STEP1600
        END,.                                                           STEP1610
   END,.                                                                STEP1620
   GO TO S100,.                                                         STEP1630
EXIT.,                                                                  STEP1640
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                   STEP1650
        (SKIP(5),COLUMN(10),A),.                                        STEP1660
S200.,                                                                  STEP1670
   END,.                              /*END OF PROCEDURE STEP         */STEP1680
```

```
DAT2.,                                                                  DAT2  10
/*********************************************************************/DAT2  20
/*                                                                   */DAT2  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.      */DAT2  40
/*      DATA MAY BE SAVED ON A DATA SET.                             */DAT2  50
/*                                                                   */DAT2  60
/*********************************************************************/DAT2  70
   PROCEDURE (M,D),.                                                    DAT2  80
   DECLARE                                                              DAT2  90
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),        DAT2 100
        (NCARD,NV) EXTERNAL,                                            DAT2 110
        CH CHARACTER(NCARD),                                            DAT2 120
        (I,M,MM) FIXED BINARY,                                          DAT2 130
        D(*) FLOAT BINARY,.                                             DAT2 140
/*                                                                    */DAT2 150
   ON ENDFILE (SYSIN)                                                   DAT2 160
   GO TO EXIT,.                                                         DAT2 170
   GET EDIT (CH) (A(NCARD)),.                                           DAT2 180
   MM   =CEIL(M/12),.                                                   DAT2 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                           DAT2 200
        ((MM)((12)F(6,0),A(8))),.                                       DAT2 210
   IF NV= 1                                                             DAT2 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,0)),.       DAT2 230
   REVERT ENDFILE (SYSIN),.                                             DAT2 240
   RETURN,.                                                             DAT2 250
EXIT.,                                                                  DAT2 260
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')                DAT2 270
        (SKIP(1),COLUMN(10),A),.                                        DAT2 280
   STOP,.                                                               DAT2 290
   END,.                              /*END OF PROCEDURE DAT2         */DAT2 300
```

```
IDT2.,                                                                  IDT2  10
/*********************************************************************/IDT2  20
/*                                                                   */IDT2  30
/*      TO READ FIXED POINT DATA.                                    */IDT2  40
/*                                                                   */IDT2  50
/*********************************************************************/IDT2  60
   PROCEDURE (M,IX),.                                                   IDT2  70
   DECLARE                                                              IDT2  80
        CH CHARACTER (80),                                              IDT2  90
        (IX(*),NF,N1,N2,M,I)                                            IDT2 100
        FIXED BINARY,.                                                  IDT2 110
   NF   =72,.                                                           IDT2 120
   N1   =1,.                                                            IDT2 130
   N2   =NF,.                                                           IDT2 140
S10.,                                                                   IDT2 150
   IF M LE N2                                                           IDT2 160
   THEN N2   =M,.                                                       IDT2 170
   GET EDIT (CH) (A(80)),.                                              IDT2 180
   GET STRING (CH) EDIT ((IX(I) DO I= N1 TO N2)) ((NF)F(1)),.           IDT2 190
   N1   =N2+1,.                                                         IDT2 200
   IF N1 LE M                                                           IDT2 210
   THEN DO,.                                                            IDT2 220
        N2   =N2+NF,.                                                   IDT2 230
        GO TO S10,.                                                     IDT2 240
        END,.                                                           IDT2 250
   RETURN,.                                                             IDT2 260
   END,.                              /*END OF PROCEDURE IDT2         */IDT2 270
```

```
SOUT.,                                                                  SOUT  10
/*********************************************************************/SOUT  20
/*                                                                   */SOUT  30
/*      TO PRINT THE RESULTS OF A STEP-WISE MULTIPLE REGRESSION.     */SOUT  40
/*                                                                   */SOUT  50
/*********************************************************************/SOUT  60
   PROCEDURE (NSTEP,ANS,L,B,S,T,BETA),.                                 SOUT  70
   DECLARE                                                              SOUT  80
        NSTOP EXTERNAL CHARACTER (1),                                   SOUT  90
        (ANS(*),B(*),S(*),T(*),BETA(*))                                 SOUT 100
        BINARY FLOAT,              /*SINGLE PRECISION VERSION  /*S*/   SOUT 110
 /*     BINARY FLOAT (53),         /*DOUBLE PRECISION VERSION  /*D*/   SOUT 120
        (NSTEP(*),L(*),I,N)                                             SOUT 130
        FIXED BINARY,.                                                  SOUT 140
/*                                                                    */SOUT 150
/*      TEST WHETHER THIS IS THE FIRST STEP                           */SOUT 160
/*                                                                    */SOUT 170
   IF NSTEP(4) LE 1                                                     SOUT 180
   THEN DO,.                                                            SOUT 190
        PUT EDIT ('DEPENDENT VARIABLE.....',NSTEP(1))                   SOUT 200
             (SKIP(2),COLUMN(10),A,F(2)),.                              SOUT 210
        PUT EDIT ('NUMBER OF VARIABLES FORCED....',NSTEP(2))            SOUT 220
             (SKIP,COLUMN(10),A,F(2)),.                                 SOUT 230
        PUT EDIT ('NUMBER OF VARIABLES DELETED...',NSTEP(3))            SOUT 240
             (SKIP,COLUMN(10),A,F(2)),.                                 SOUT 250
        END,.                                                           SOUT 260
/*                                                                    */SOUT 270
/*      PRINT THE RESULTS OF A STEP                                   */SOUT 280
/*                                                                    */SOUT 290
   PUT EDIT ('STEP',NSTEP(4)) (SKIP(3),COLUMN(10),A,F(3)),.             SOUT 300
   PUT EDIT ('VARIABLE ENTERED....',NSTEP(5))                           SOUT 310
        (SKIP(2),COLUMN(10),A,F(2)),.                                   SOUT 320
   PUT SKIP(2),.                                                        SOUT 330
   IF NSTEP(4) LE NSTEP(2)                                              SOUT 340
   THEN PUT EDIT ('  (FORCED VARIABLE)') (SKIP,COLUMN(10),A),.          SOUT 350
   PUT EDIT ('SUM OF SQUARES REDUCED IN THIS STEP....',ANS(1))          SOUT 360
        (R(FM1)),.                                                      SOUT 370
FM1.,                                                                   SOUT 380
   FORMAT (SKIP(1),COLUMN(10),A,F(13,3)),.                              SOUT 390
   PUT EDIT ('PROPORTION REDUCED IN THIS STEP.......',ANS(2))           SOUT 400
        (R(FM1)),.                                                      SOUT 410
   PUT SKIP(2),.                                                        SOUT 420
   PUT EDIT ('CUMULATIVE SUM OF SQUARES REDUCED.....',ANS(3))           SOUT 430
        (R(FM1)),.                                                      SOUT 440
   PUT EDIT ('CUMULATIVE PROPORTION REDUCED.....',ANS(4),' OF',         SOUT 450
        ANS(5)) (SKIP,COLUMN(10),A,F(13,3),A,F(13,3)),.                 SOUT 460
   PUT EDIT ('FOR',NSTEP(4),' VARIABLES ENTERED')                       SOUT 470
        (SKIP(2),COLUMN(10),A,F(3),A),.                                 SOUT 480
   PUT EDIT ('MULTIPLE CORRELATION COEFFICIENT...',ANS(6))              SOUT 490
        (SKIP(1),COLUMN(12),A,F(9,3)),.                                 SOUT 500
   PUT EDIT ('(ADJUSTED FOR D.F.).....',ANS(10))                        SOUT 510
        (SKIP(1),COLUMN(17),A,F(9,3)),.                                 SOUT 520
   PUT EDIT ('F-VALUE FOR ANALYSIS OF VARIANCE...',ANS(7))              SOUT 530
        (SKIP(1),COLUMN(12),A,F(9,3)),.                                 SOUT 540
   PUT EDIT ('STANDARD ERROR OF ESTIMATE.....',ANS(8))                  SOUT 550
        (SKIP(1),COLUMN(12),A,F(9,3)),.                                 SOUT 560
   PUT EDIT ('(ADJUSTED FOR D.F.).....',ANS(11))                        SOUT 570
        (SKIP(1),COLUMN(17),A,F(9,3)),.                                 SOUT 580
   PUT EDIT ('VARIABLE','REGRESSION','STD. ERROR OF ','COMPUTED',       SOUT 590
        'BETA','NUMBER','COEFFICIENT','REG. COEFF.','T-VALUE',          SOUT 600
        'COEFFICIENT')                                                  SOUT 610
        (SKIP(2),COLUMN(12),5(A,X(5)),SKIP(1),COLUMN(13),A,X(6),A,      SOUT 620
        X(4),A,X(8),A,X(6),A),.                                         SOUT 630
   N    =NSTEP(4),.                                                     SOUT 640
        DO I = 1 TO N,.                                                 SOUT 650
        PUT EDIT (L(I),B(I),S(I),T(I),BETA(I)) (SKIP(1),COLUMN(14),     SOUT 660
             F(3),F(18,5),F(16,5),F(14,3),F(14,5)),.                    SOUT 670
        END,.                                                           SOUT 680
   PUT EDIT ('INTERCEPT',ANS(9)) (SKIP,COLUMN(12),A,F(14,5)),.          SOUT 690
   NSTOP='0',.                                                          SOUT 700
   RETURN,.                                                             SOUT 710
   END,.                              /*END OF PROCEDURE SOUT         */SOUT 720
```

CANONICAL CORRELATION CANO

Problem Description

This program analyzes the interrelations between two sets of variables measured on the same subjects. These variables are predictors in one set and criteria in the other set, but it is irrelevant whether the variables in the first set or in the second set are considered as the prediction variables. The canonical correlation, which gives the maximum correlation between linear functions of the two sets of variables, is calculated. χ^2 is also computed to test the significance of canonical correlation.

The sample problem for canonical correlation consists of four variables in the first set (left-hand side) and three variables in the second set (right-hand side) as presented in Table 2. These two sets of measurements have been made on 23 subjects.

Table 2. Sample Data for Canonical Correlation

	First set				Second set		
Observation	X_1	X_2	X_3	X_4	Y_1	Y_2	Y_3
1	191	155	65	19	179	145	70
2	195	149	70	20	201	152	69
3	181	148	71	19	185	149	75
4	183	153	82	18	188	149	86
5	176	144	67	18	171	142	71
6	208	157	81	22	192	152	77
7	189	150	75	21	190	149	72
8	197	159	90	20	189	152	82
9	188	152	76	19	197	159	84
10	192	150	78	20	187	151	72
11	179	158	99	18	186	148	89
12	183	147	65	18	174	147	70
13	174	150	71	19	185	152	65
14	190	159	91	19	195	157	99
15	188	151	98	20	187	158	87
16	163	137	59	18	161	130	63
17	195	155	85	20	183	158	81
18	196	153	80	21	173	148	74
19	181	145	77	20	182	146	70
20	175	140	70	19	165	137	81
21	192	154	69	20	185	152	63
22	174	143	79	20	178	147	73
23	176	139	70	20	176	143	69

Program

Description

The canonical correlation program consists of the main routine named CANO, a special input routine, DAT2, and five subroutines from the Scientific Subroutine Package: CORR, CANC, MINV, MGDU, and MSDU.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. The number of variables in the first set (that is, left-hand variables) must be greater than or equal to the number of variables in the second set (that is, right-hand variables).
2. Up to 99,999 observations
3. Up to ten data cards per observation
4. (12 F (6,0)) format for input data cards.

Therefore, if a problem satisfies the above conditions, it is not necessary to modify the sample program. However, if the input data cards are prepared using a different format, the input format in the special input subroutine, DAT2, must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, CANO. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	00023
12-13	Number of variables in the first set (that is, left-hand variables)*	04
14-15	Number of variables in the second set (that is, right-hand variables)	03
16-17	Number of data cards per observation	01

Leading zeros do not have to be keypunched, but must be right-justified within the field.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 2 is keypunched on a separate card using the format (12 F (6, 0)). This format assumes twelve 6-column fields per card.

Deck Setup

Deck setup is shown in Figure 20.

*The number of variables in the first set must be greater than or equal to the number of variables in the second set.

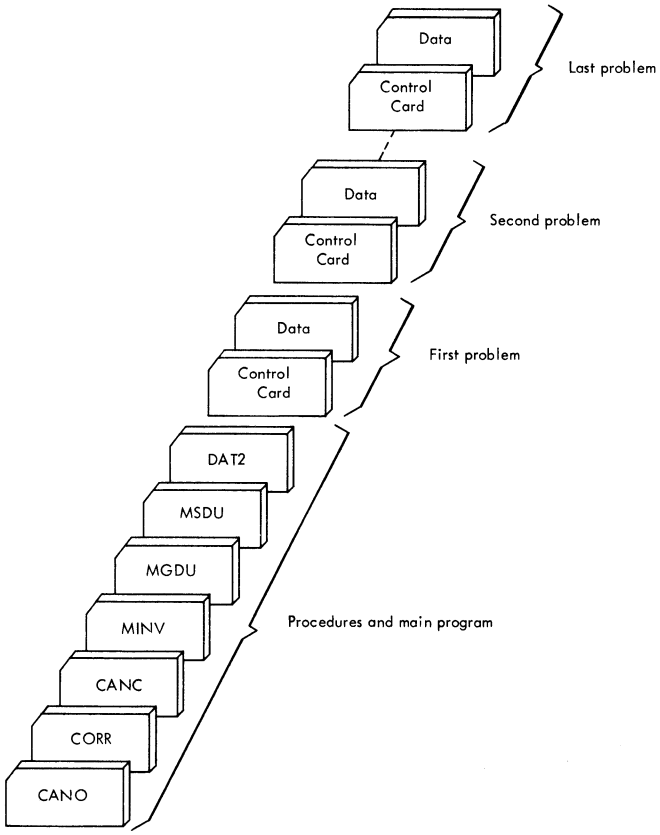


Figure 20.

Sample

The listing of input cards for the sample problem is shown in Figure 21.

```
SAMPLECCC23C40301
  191   155    65    19   179   145    7C
  195   145    70    20   201   152    65
  181   148    71    19   185   149    75
  183   153    82    18   188   149    86
  176   144    67    18   171   142    71
  208   157    81    22   192   152    77
  189   150    75    21   19C   149    72
  197   155    90    20   189   152    82
  188   152    76    19   197   159    84
  192   15C    78    20   187   151    72
  179   158    95    18   186   148    89
  183   147    65    18   174   147    7C
  174   15C    71    19   185   152    65
  19C   155    91    19   195   157    95
  188   151    98    20   187   158    87
  163   137    55    18   161   130    63
  195   155    85    20   183   158    81
  196   153    80    21   173   148    74
  181   145    77    20   182   146    7C
  175   14C    7C    19   165   137    81
  192   154    69    20   185   152    63
  174   143    75    20   178   147    73
  176   135    70    20   176   143    65
```

Figure 21.

Output

Description

The output of the sample program for canonical correlation includes:

1. Means
2. Standard deviations
3. Correlation coefficients
4. Eigenvalues and corresponding canonical correlation
5. Lambda
6. Chi-square for left- and right-hand variables.

Sample

The output listing for the sample problem is shown in Figure 22.

```
CANONICAL CORRELATION.....SAMPLE
  NO. OF OBSERVATIONS          23
  NO. OF LEFT HAND VARIABLES    4
  NO. OF RIGHT HAND VARIABLES   3

MEANS
      185.47826      149.91304       76.86955       19.47826      183.00000      148.82608       75.73912

STANDARD DEVIATIONS
       10.10342       6.31673       10.46338        1.08165        9.84424        6.73965        9.05647

CORRELATION COEFFICIENTS

ROW   1
     1.00000     0.74852     0.37082     0.66441     0.62291     0.66080     0.24683

ROW   2
     0.74852     1.00000     0.63252     0.22590     0.66811     0.72780     0.53194

ROW   3
     0.37082     0.63252     1.00000     0.20657     0.47394     0.60169     0.79684

ROW   4
     0.66441     0.22590     0.20657     1.00000     0.32870     0.34863    -0.10733

ROW   5
     0.62291     0.66811     0.47394     0.32870     1.00000     0.82555     0.39258

ROW   6
     0.66080     0.72780     0.60169     0.34863     0.82555     1.00000     0.47657

ROW   7
     0.24683     0.53194     0.79684    -0.10733     0.39258     0.47657     1.00000
```

Figure 22.

```
   NUMBER OF      LARGEST        CORRESPONDING                                    DEGREES
  EIGENVALUES    EIGENVALUE       CANONICAL                                        OF
    REMOVED      REMAINING       CORRELATION        LAMBDA      CHI-SQUARE      FREEDOM
       0           0.79880          0.89376         0.11598       40.93277         12
       1           0.41910          0.64738         0.57644       10.46676          6
       2           0.00767          0.08760         0.99233        0.14636          2


CANONICAL CORRELATION      0.89376

COEFFICIENTS FOR LEFT HAND VARIABLES
        0.56310        -0.16059         1.05822        -0.56651

COEFFICIENTS FOR RIGHT HAND VARIABLES
       -0.02133         0.44090         0.89730


CANONICAL CORRELATION      0.64738

COEFFICIENTS FOR LEFT HAND VARIABLES
        0.09454        -0.83915         0.66309        -0.64892

COEFFICIENTS FOR RIGHT HAND VARIABLES
       -0.43841        -0.55503         0.70692


CANONICAL CORRELATION      0.08760

COEFFICIENTS FOR LEFT HAND VARIABLES
        0.02681         0.36055        -0.28827        -0.32496

COEFFICIENTS FOR RIGHT HAND VARIABLES
        0.70325        -0.70384         0.10028


END OF SAMPLE PROGRAM
```

Figure 22. (Continued)

Program Modifications

Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with program modifications, the following general rule is supplied in terms of the sample problem:

1. Changes in the input format statement of the special input routine, DAT2.

Since sample data are either two- or three-digit numbers, rather than using six-column fields as in the sample problem, each row of data might have been keypunched in seven 3-column fields; if so, the format would be changed to (7 F (3, 0)). Note that the current input format statement will allow a maximum of twelve variables per card.

The special input routine is normally written by the user to handle different formats for different problems. The user may modify this subroutine to perform testing of input data, transformation of data, and so on.

2. If there is more than one card per row of data, the value of the card count indicator (NCARD), which appears in columns 16-17 of the control card, must be changed to agree with the number of data cards per row.

Operating Instructions

The sample program for canonical correlation is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output.

Timing

The execution of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 17 seconds.

```
CANO..                                                                  CANO  10
/*********************************************************************/CANO  20
/*                                                                   */CANO  30
/*      TO READ THE PROBLEM PARAMETER CARD FOR A CANONICAL CORRE-    */CANO  40
/*      LATION, CALL TWO PROCEDURES TO CALCULATE SIMPLE CORRELATIONS,*/CANO  50
/*      CANONICAL CORRELATIONS, CHI-SQUARES, DEGREES OF FREEDOM FOR  */CANO  60
/*      CHI-SQUARES, AND COEFFICIENTS FOR LEFT AND RIGHT HAND        */CANO  70
/*      VARIABLES, NAMELY CANONICAL VARIATES, AND PRINT THE RESULTS. */CANO  80
/*                                                                   */CANO  90
/*********************************************************************/CANO 100
   PROCEDURE OPTIONS (MAIN),.                                           CANO 110
   DECLARE                                                              CANO 120
         (I,IO,J,M,MM,MP,MQ,N,N1)                                       CANO 130
         FIXED BINARY,                                                  CANO 140
         CH  CHARACTER (80),                                            CANO 150
         ERROR EXTERNAL CHARACTER (1),                                  CANO 160
         (NCARD,NV) EXTERNAL,                                           CANO 170
         PR  CHARACTER (6),.                                            CANO 180
/*                                                                     */CANO 190
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      CANO 200
S100..                                                                  CANO 210
   GET EDIT (CH) (A(80)),.                                              CANO 220
   GET STRING (CH) EDIT (PR,N,MP,MQ,NCARD) (A(6),F(5),3 F(2)),.         CANO 230
/*                                                                     */CANO 240
/*      PR.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                    */CANO 250
/*      N........NUMBER OF OBSERVATIONS                                */CANO 260
/*      MP.......NUMBER OF LEFT HAND VARIABLES                         */CANO 270
/*      MQ.......NUMBER OF RIGHT HAND VARIABLES                        */CANO 280
/*      NCARD....NUMBER OF CARDS PER OBSERVATION                       */CANO 290
/*                                                                     */CANO 300
   PUT EDIT ('CANONICAL CORRELATION.....',PR,'NO. OF OBSERVATIONS',N,    CANO 310
         'NO. OF LEFT HAND VARIABLES',MP,                               CANO 320
         'NO. OF RIGHT HAND VARIABLES',MQ) (PAGE,COLUMN(10),A,A(6),     CANO 330
         SKIP(1),COLUMN(12),A,X(8),F(4),SKIP(1),COLUMN(12),A,F(5),      CANO 340
         SKIP(1),COLUMN(12),A,F(4)),.                                   CANO 350
   M    =MP+MQ,.                                                        CANO 360
   NCARD=NCARD*80,.                                                     CANO 370
   NV   =0,.                                                            CANO 380
STRT..                                                                  CANO 390
   BEGIN,.                                                              CANO 400
   DECLARE                                                              CANO 410
         (COEFL(MP,MQ),COEFR(MQ,MQ),R(M,M),RX(M,M),CHISQ(MQ),CANR(MQ),  CANO 420
         STD(M),XBAR(M),X(1,1),B(M),ROOTS(MQ),WLAM(MQ))                 CANO 430
         BINARY FLOAT,              /*SINGLE PRECISION VERSION  /*S*/CANO 440
 /*      BINARY FLOAT (53),         /*DOUBLE PRECISION VERSION  /*D*/CANO 450
         NDF(MQ)  FIXED BINARY,.                                        CANO 460
   IO   =0,.                                                            CANO 470
   X    =0.0,.                                                          CANO 480
   CALL CORR (N,M,IO,X,XBAR,STD,RX,R,B),.                               CANO 490
   IF ERROR NE '0'                                                      CANO 500
   THEN DO,.                                                            CANO 510
         PUT EDIT ('IN ROUTINE CORR ERROR CODE = ',ERROR)               CANO 520
              (SKIP(2),COLUMN(10),A,A(1)),.                             CANO 530
         GO TO S100,.                                                   CANO 540
         END,.                                                          CANO 550
/*                                                                     */CANO 560
/*      PRINT MEANS, STANDARD DEVIATIONS, AND CORRELATION              */CANO 570
/*      COEFFICIENTS OF ALL VARIABLES                                  */CANO 580
```

```
/*                                                                    */CANO 590
   PUT EDIT ('MEANS') (R(FM1)),.                                       CANO 600
FM1..                                                                  CANO 610
   FORMAT (SKIP(2),COLUMN(10),A),.                                     CANO 620
   PUT EDIT ((XBAR(I) DO I= 1 TO M)) (R(FM2)),.                        CANO 630
FM2..                                                                  CANO 640
   FORMAT (SKIP,COLUMN(10),7 F(15,5)),.                                CANO 650
   PUT EDIT ('STANDARD DEVIATIONS') (R(FM1)),.                         CANO 660
   PUT EDIT ((STD(I) DO I= 1 TO M)) (R(FM2)),.                         CANO 670
   PUT EDIT ('CORRELATION COEFFICIENTS') (SKIP(2),COLUMN(10),A),.      CANO 680
        DO I = 1 TO M,.                                                CANO 690
        PUT EDIT ('ROW',I) (SKIP(2),COLUMN(10),A,F(4)),.               CANO 700
        PUT EDIT ((R(I,J) DO J= 1 TO M)) (SKIP,COLUMN(10),9 F(12,5)),. CANO 710
        END,.                                                          CANO 720
   CALL CANC (N,MP,MQ,R,ROOTS,WLAM,CANR,CHISQ,NDF,COEFR,COEFL),.       CANO 730
   IF ERROR NE '0'                                                     CANO 740
   THEN DO,.                                                           CANO 750
        PUT EDIT ('IN ROUTINE CANC ERROR CODE = ',ERROR)               CANO 760
             (SKIP(2),COLUMN(10),A,A(1)),.                             CANO 770
        IF ERROR = '1'                                                 CANO 780
        THEN GO TO S100,.                                              CANO 790
        END,.                                                          CANO 800
/*                                                                     */CANO 810
/*      PRINT EIGENVALUES, CANONICAL CORRELATIONS, LAMBDA,             */CANO 820
/*      CHI-SQUARES DEGREES OF FREEDOM                                 */CANO 830
/*                                                                     */CANO 840
   PUT EDIT ('NUMBER OF ','LARGEST','CORRESPONDING','DEGREES',         CANO 850
        'EIGENVALUES','EIGENVALUE','CANONICAL','LAMBDA',               CANO 860
        'CHI-SQUARE','DF','REMOVED','REMAINING','CORRELATION',         CANO 870
        'FREEDOM') (SKIP(4),COLUMN(13),A,X(5),A,X(7),A,X(31),A,        CANO 880
        SKIP,COLUMN(11),A,X(5),A,X(7),A,X(7),A,X(5),A,X(7),A,          CANO 890
        SKIP,COLUMN(13),A,X(7),A,X(7),A,X(32),A),.                     CANO 900
        DO I = 1 TO MQ,.                                               CANO 910
        N1   =I-1,.                                                    CANO 920
/*                                                                     */CANO 930
/*      TEST WHETHER EIGENVALUE IS GREATER THAN ZERO                   */CANO 940
/*                                                                     */CANO 950
        MM   =N1,.                                                     CANO 960
        IF ROOTS(I) GT 0.0                                             CANO 970
        THEN DO,.                                                      CANO 980
             PUT EDIT (N1,ROOTS(I),CANR(I),WLAM(I),CHISQ(I),NDF(I))    CANO 990
                  (SKIP(1),COLUMN(10),F(7),F(19,5),F(16,5),            CAN01000
                  2 F(14,5),X(5),F(5)),.                               CAN01010
             MM   =MQ,.                                                CAN01020
             END,.                                                     CAN01030
        END,.                                                          CAN01040
/*                                                                     */CAN01050
/*      PRINT CANONICAL CORRELATION                                    */CAN01060
/*                                                                     */CAN01070
        DO I = 1 TO MM,.                                               CAN01080
        PUT EDIT ('CANONICAL CORRELATION',CANR(I)) (SKIP(5),COLUMN(10),CAN01090
             A,F(12,5)),.                                              CAN01100
        PUT EDIT ('COEFFICIENTS FOR LEFT HAND VARIABLES') (R(FM1)),.   CAN01110
        PUT EDIT ((COEFL(J,I) DO J= 1 TO MP)) (R(FM2)),.               CAN01120
        PUT EDIT ('COEFFICIENTS FOR RIGHT HAND VARIABLES') (R(FM1)),.  CAN01130
        PUT EDIT ((COEFR(J,I) DO J= 1 TO MQ)) (R(FM2)),.               CAN01140
        END,.                                                          CAN01150
   END,.                                                               CAN01160
   GO TO S100,.                                                        CAN01170
EXIT..                                                                 CAN01180
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                  CAN01190
        (SKIP(5),COLUMN(10),A),.                                       CAN01200
   END,.                              /*END OF PROCEDURE CANO         */CAN01210
```

```
DAT2..                                                                 DAT2  10
/**********************************************************************/DAT2  20
/*                                                                    */DAT2  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.       */DAT2  40
/*      DATA MAY BE SAVED ON A DATA SET.                              */DAT2  50
/*                                                                    */DAT2  60
/**********************************************************************/DAT2  70
   PROCEDURE (*,D),.                                                   DAT2  80
   DECLARE                                                             DAT2  90
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),       DAT2 100
        (NCARD,NV) EXTERNAL,                                           DAT2 110
        CH CHARACTER(NCARD),                                           DAT2 120
        (I,M,MM) FIXED BINARY,                                         DAT2 130
        D(*) FLOAT BINARY,.                                            DAT2 140
/*                                                                     */DAT2 150
   ON ENDFILE (SYSIN)                                                  DAT2 160
   GO TO EXIT,.                                                        DAT2 170
   GET EDIT (CH) (A(NCARD)),.                                          DAT2 180
   MM   =CEIL(M/12),.                                                  DAT2 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                          DAT2 200
        ((MM)(12)F(6,0),X(8))),.                                       DAT2 210
   IF NV= 1                                                            DAT2 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,C)),.      DAT2 230
   REVERT ENDFILE (SYSIN),.                                            DAT2 240
   RETURN,.                                                            DAT2 250
EXIT..                                                                 DAT2 260
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')               DAT2 270
        (SKIP(1),COLUMN(10),A),.                                       DAT2 280
   STOP,.                                                              DAT2 290
   END,.                              /*END OF PROCEDURE DAT2         */DAT2 300
```

ANALYSIS OF VARIANCE ANOV

Problem Description

An analysis of variance is performed for a factorial design by use of three special operators suggested by H. O. Hartley.* The analysis of many other designs can be derived by first reducing them to factorial designs, and then pooling certain components of the analysis-of-variance table.

Consider a three-factor factorial experiment in a randomized complete block design, as presented in Table 3. In this experiment factor A has four levels, factors B and C have three levels, and the entire experiment is replicated twice. The replicates are completely unrelated and do not constitute a factor.

Table 3. Sample Data for Analysis of Variance

Replicate (Block)		b_1				b_2				b_3			
		a_1	a_2	a_3	a_4	a_1	a_2	a_3	a_4	a_1	a_2	a_3	a_4
r_1	c_1	3	10	9	8	24	8	9	3	2	8	9	8
	c_2	4	12	3	9	22	7	16	2	2	2	7	2
	c_3	5	10	5	8	23	9	17	3	2	8	6	3
r_2	c_1	2	14	9	13	29	16	11	3	2	7	5	3
	c_2	7	11	5	8	28	18	10	6	6	6	5	9
	c_3	9	10	27	8	28	16	11	7	8	9	8	15

Nevertheless, for the purpose of this program, a four-factor experiment (with factors A, B, C, and R) is assumed. Thus, each element of the data in Table 3 may be represented in the form:

x_{abcr} where $a = 1,2,3,4$

$b = 1,2,3$

$c = 1,2,3$

$r = 1,2$

The general principle of the analysis-of-variance procedure used in the program is first to perform a formal factorial analysis and then to pool certain components in accordance with summary instructions that specifically apply to the particular design. The summary instructions for four different designs are presented in the output section.

Program

Description

The analysis of variance program consists of the main routine, named ANOV, a special input routine DAT3, and one subroutine from the Scientific Subroutine Package: AVAR.

*H. O. Hartley, "Analysis of Variance" in Mathematical Methods for Digital Computers, edited by A. Ralston and H. Wilf, John Wiley and Sons, 1962, Chapter 20.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 14 factors
2. The total number of data points is limited only by the size of available core storage used for input.
3. (12 F(6,0)) format for input data cards. Therefore, if a problem satisfies the above conditions, it is not necessary to modify the sample program. However, if the input data cards are prepared using a different format, the input format statement must be modified. The general rules for program modifications are described later.

Input

Control Cards

Two control cards are required for each problem and are read by the main program, ANOV.

The first card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-8	Number of factors	04

The second card is prepared as follows:

Columns	Contents	For Sample Problem
1	Label for the first factor	A
2-5	Number of levels for the first factor	0004
6	Label for the second factor	B
7-10	Number of levels for the second factor	0003
11	Label for the third factor	C
12-15	Number of levels for the third factor	0003
16	Label for the fourth factor	R
17-20	Number of levels for the fourth factor	0002
	•	
	•	
	•	
66	Label of the fourteenth factor	
67-70	Number of levels of the fourteenth factor	

Leading zeros do not have to be keypunched.

Data Cards

Data is keypunched in the following order: X_{1111}, X_{2111}, X_{3111}, X_{1211}, X_{2211}, X_{3211}, ···, X_{4332}. In other words, the leftmost subscript (namely, the first factor) is changed first; then the second, third, and fourth subscripts. In the sample problem, the first subscript corresponds to factor A; the second, third, and fourth subscripts, to factors B, C, and R. Since the number of data fields per card is twelve, implied by the format (12 F(6,0)), each row in Table 3 is keypunched on a separate card.

Deck Setup

Deck setup is shown in Figure 23.

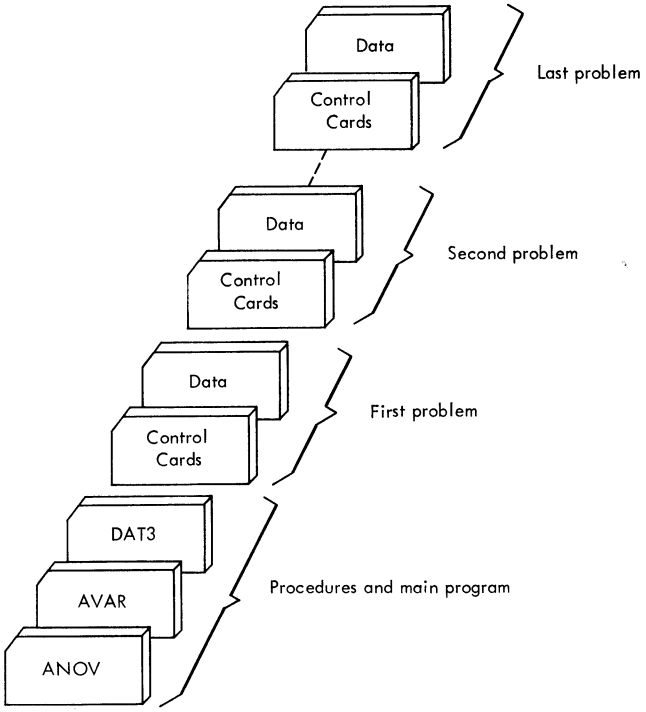


Figure 23.

Sample

The listing of input cards for the sample problem is shown in Figure 24.

```
SAMPLE 4                                                        10
A  4B  3C  3R  2                                                20
   3  10   9   8  24   8   9   3   2   8   9   8                30
   4  12   3   9  22   7  16   2   2   2   7   2                40
   5  10   5   8  23   9  17   3   2   8   6   3                50
   2  14   9  13  29  16  11   3   2   7   5   3                60
   7  11   5   8  28  18  10   6   6   6   5   9                70
   9  10  27   8  28  16  11   7   8   9   8  15                80
```

Figure 24.

Output

Description

The output of the sample analysis-of-variance program includes the numbers of levels of factors as input, the mean of all data, and the table of analysis of variance. In order to complete the analysis of variance properly, however, certain components in the table may need to be pooled. This is accomplished by means of summary instructions that specifically apply to the particular experiment. Some of these are presented in Table 4.

As mentioned earlier, the sample problem is a randomized complete block design with three factors replicated twice. Therefore, it is necessary to pool certain components in the table of analysis of variance shown in Figure 25. Specifically, the components AR, BR, ABR, CR, ACR, BCR, and ABCR are combined into one value, called the error term. The result is indicated in Figure 25. Since these data are purely hypothetical, interpretations of the various effects are not made.

Table 4. Instructions to Summarize Components of Analysis of Variance

	Single Classification with Replicates	Two-way Classification with Cell Replicates	Randomized Complete Block with Two Factors	Split Plot
(Input) Factor No. 1 2 3	Groups = A Replicates = R	Rows = A Columns = B Replicates = R	Factor 1 = A Factor 2 = B Blocks = R	Main treatment = A Subtreatment = B Blocks = R
(Output) Sums of squares	A R AR	A B AB R AR BR ABR	A B AB R AR BR ABR	A B AB R AR BR ABR
Summary instruction	Error = R + (AR)	Error = R + (AR) +(BR)+(ABR)	Error = (AR)+(BR) +(ABR)	Error = (BR)+(ABR) (b)
Analysis of variance	Groups A Error	Rows A Columns B Interaction AB Error	Factor 1 A Factor 2 B Interaction AB Blocks R Error	Main treatment A Blocks R Error (a) AR Subtreatment B Interaction AB Error (b)

Sample

The output listing for the sample problem is shown in Figure 25.

```
ANALYSIS OF VARIANCE.....SAMPLE

LEVELS OF FACTORS
   A          4
   B          3
   C          3
   R          2

GRAND MEAN              9.40278

SOURCE OF                  SUMS OF        DEGREES OF        MEAN
VARIATION                  SQUARES         FREEDOM          SQUARES

A                        229.04166            3            76.34721
B                        722.69434            2           361.34717
AB                      1382.08325            6           230.34720
C                         55.11110            2            27.55554
AC                        42.00000            6             7.00000
BC                        13.13889            4             3.28472
ABC                      140.75000           12            11.72917
R                        141.68054            1           141.68054
AR                        18.81944            3             6.27315
BR                         6.02778            2             3.01389
ABR                      176.97221            6            29.49536
CR                        40.77777            2            20.38889
ACR                       50.55554            6             8.42592
BCR                       62.63889            4            15.65972
ABCR                     151.02777           12            12.58565

TOTAL                   3233.31763           71

END OF SAMPLE PROGRAM
```

Figure 25.

Program Modifications

Input data in a different format can also be handled by providing a different format statement. In order to familiarize the user with the program modifications, the following general rule is supplied in terms of the sample problem:

Only the format statement and the variable per card count indicator for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using a six-column field, as in the sample problem, each row of data might have been keypunched in a two-column field; if so, the format is changed to (12 F(2, 0)). This format assumes twelve 2-column fields per card, beginning in column 1.

Operating Instructions

The sample analysis of variance program is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output.

Timing

The execution of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 11 seconds.

```
ANOV..                                                                  ANOV  10
/*************************************************************************/ANOV  20
/*                                                                       */ANOV  30
/*      TO READ THE PROBLEM PARAMETER CARD FOR ANALYSIS OF VARIANCE,     */ANOV  40
/*      CALL THE PROCEDURES FOR THE CALCULATION OF SUMS OF SQUARES,      */ANOV  50
/*      DEGREES OF FREEDOM AND MEAN SQUARE, AND PRINT FACTOR LEVELS,     */ANOV  60
/*      GRAND MEAN AND ANALYSIS OF VARIANCE TABLE.                       */ANOV  70
/*                                                                       */ANOV  80
/*************************************************************************/ANOV  90
   PROCEDURE OPTIONS (MAIN),.                                           ANOV 100
   DECLARE                                                              ANOV 110
         (I,J,K,L,M,MM,N)                                               ANOV 120
         FIXED BINARY,                                                  ANOV 130
         ERROR EXTERNAL CHARACTER(1),                                   ANOV 140
         PR1 CHARACTER (6),                                             ANOV 150
         CH  CHARACTER (80),.                                           ANOV 160
/*                                                                      */ANOV 170
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      ANOV 180
S100..                                                                  ANOV 190
   GET EDIT (CH) (A(80)),.                                              ANOV 200
   GET STRING (CH) EDIT (PR1,K) (A(6),F(2)),.                           ANOV 210
/*                                                                      */ANOV 220
/*      PR1....PROBLEM NUMBER (MAY BE ALPHAMERIC)                       */ANOV 230
/*      K......NUMBER OF FACTORS                                        */ANOV 240
/*                                                                      */ANOV 250
   N    =(2**K)-1,.                                                     ANOV 260
ONE..                                                                   ANOV 270
   BEGIN,.                                                              ANOV 280
   DECLARE                                                              ANOV 290
         (SUMSQ(N),SMEAN(N),GMEAN,SUM)                                  ANOV 300
         FLOAT BINARY,                 /*SINGLE PRECISION VERSION  /*S*/ANOV 310
 /*      FLOAT BINARY (53),.           /*DOUBLE PRECISION VERSION  /*D*/ANOV 320
         (LEVEL(K),NDF(N),ISTEP(K)) BINARY FIXED,                       ANOV 330
         (HEAD(K),FMT(K)) CHARACTER (1),.                               ANOV 340
   GET EDIT (CH) (A(80)),.                                              ANOV 350
   GET STRING (CH) EDIT ((HEAD(I),LEVEL(I) DO I= 1 TO K))               ANOV 360
         (14(A(1),F(4))),.                                              ANOV 370
/*                                                                      */ANOV 380
/*      HEAD...FACTOR LEVELS                                            */ANOV 390
/*      LEVEL..LEVELS OF FACTORS                                        */ANOV 400
/*                                                                      */ANOV 410
   PUT EDIT ('ANALYSIS OF VARIANCE.....',PR1,'LEVELS OF FACTORS')       ANOV 420
         (PAGE,SKIP(4),COLUMN(10),A,A(6),SKIP(4),COLUMN(10),A),.        ANOV 430
   PUT EDIT ((HEAD(I),LEVEL(I) DO I= 1 TO K))                           ANOV 440
         (SKIP,COLUMN(13),A(1),X(7),F(4)),.                             ANOV 450
   M    = PROD (LEVEL),.                                                ANOV 460
   MM   = PROD (LEVEL+1),.                                              ANOV 470
TWO..                                                                   ANOV 480
   BEGIN,.                                                              ANOV 490
   DECLARE                                                              ANOV 500
         X(MM)                                                          ANOV 510
         FLOAT BINARY..                /*SINGLE PRECISION VERSION  /*S*/ANOV 520
 /*      FLOAT BINARY (53),.           /*DOUBLE PRECISION VERSION  /*D*/ANOV 530
   X    =0,.                                                            ANOV 540
/*                                                                      */ANOV 550
/*      READ IN ALL INPUT DATA                                          */ANOV 560
/*                                                                      */ANOV 570
   CALL DAT3 (M,X),.                                                    ANOV 580
   CALL AVAR (K,LEVEL,M,X,GMEAN,SUMSQ,NDF,SMEAN),.                      ANOV 590
   IF ERROR NE '0'                                                      ANOV 600
   THEN DO,.                                                            ANOV 610
         PUT EDIT ('IN ROUTINE AVAR ERROR CODE = ',ERROR) (SKIP(2),     ANOV 620
               COLUMN(10),A,A(1)),.                                     ANOV 630
         GO TO S100,.                                                   ANOV 640
         END,.                                                          ANOV 650
/*                                                                      */ANOV 660
/*      PRINT THE GRAND MEAN                                            */ANOV 670
/*                                                                      */ANOV 680
   PUT EDIT ('GRAND MEAN',GMEAN) (SKIP(6),COLUMN(10),A,F(20,5)),.       ANOV 690
/*                                                                      */ANOV 700
/*      PRINT ANALYSIS OF VARIANCE TABLE                                */ANOV 710
/*                                                                      */ANOV 720
   PUT EDIT ('SOURCE OF' ,'SUMS OF','DEGREES OF','MEAN',                ANOV 730
         'VARIATION','SQUARES','FREEDOM','SQUARES')                     ANOV 740
         (SKIP(6),COLUMN(10),A,X(18),A,X(10),A,X(9),A,SKIP,             ANOV 750
         COLUMN(10),A,X(18),A,X(11),A,X(10),A),.                        ANOV 760
   PUT SKIP(2),.                                                        ANOV 770
   ISTEP= 0,.                          /* INITIALIZE FOR PRINT OUT    */ANOV 780
   ISTEP(1)= 1,.                                                        ANOV 790
         DO I = 1 TO N,.                                                ANOV 800
         L    = 0,.                                                     ANOV 810
               DO J = 1 TO K,.                                          ANOV 820
               FMT(J)=' ',.                                             ANOV 830
               IF ISTEP(J) NE 0                                         ANOV 840
               THEN DO,.                                                ANOV 850
                     L    =L+1,.                                        ANOV 860
                     FMT(L)=HEAD(J),.                                   ANOV 870
                     END,.                                              ANOV 880
               END,.                                                    ANOV 890
         PUT EDIT ((FMT(L) DO L= 1 TO K),SUMSQ(I),NDF(I),SMEAN(I))      ANOV 900
               (SKIP,COLUMN(10),(K)A(1),COLUMN(23),F(20,5),X(10),       ANOV 910
               F(6),F(20,5)),.                                          ANOV 920
         IF I LT N                                                      ANOV 930
         THEN DO,.                                                      ANOV 940
                     DO J = 1 TO K,.                                    ANOV 950
                     IF ISTEP(J)= 0                                     ANOV 960
                     THEN DO,.                                          ANOV 970
                           ISTEP(J)=1,.                                 ANOV 980
                           GO TO S160,.                                 ANOV 990
                           END,.                                        ANOV1000
                     ISTEP(J)=0,.                                       ANOV1010
                     END,.                                              ANOV1020
               END,.                                                    ANOV1030
S160..                                                                  ANOV1040
         END,.                                                          ANOV1050
   M    =M-1,.                                                          ANOV1060
   SUM  =SUM(SUMSQ),.                                                   ANOV1070
   PUT EDIT ('TOTAL',SUM,M) (SKIP(2),COLUMN(10),A,X(10),F(18,5),        ANOV1080
         X(10),F(6)),.                                                  ANOV1090
   END,.                                                                ANOV1100
   END,.                                                                ANOV1110
   GO TO S100,.                                                         ANOV1120
EXIT..                                                                  ANOV1130
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                   ANOV1140
         (SKIP(5),COLUMN(10),A),.                                       ANOV1150
   END,.                               /*END OF PROCEDURE ANOV       */ANOV1160
```

```
DAT3..                                                                  DAT3  10
/*************************************************************************/DAT3  20
/*                                                                       */DAT3  30
/*      TO READ A VECTOR OF FLOATING POINT DATA.                         */DAT3  40
/*                                                                       */DAT3  50
/*************************************************************************/DAT3  60
   PROCEDURE (M,D),.                                                    DAT3  70
   DECLARE                                                              DAT3  80
         CH CHARACTER(80),                                              DAT3  90
         (I,M,N,N1,N2)                                                  DAT3 100
         FIXED BINARY,                                                  DAT3 110
         D(M) FLOAT BINARY,.                                            DAT3 120
/*                                                                      */DAT3 130
/*      N EQUAL THE NUMBER OF DATA POINTS PER 80 COLUMNS OF A DATA      */DAT3 140
/*      CARD.                                                           */DAT3 150
/*                                                                      */DAT3 160
   ON ENDFILE (SYSIN)                                                   DAT3 170
   GO TO EXIT,.                                                         DAT3 180
   N    =12,.                                                           DAT3 190
   N1   =1,.                                                            DAT3 200
   N2   =N,.                                                            DAT3 210
S10..                                                                   DAT3 220
   IF M LE N2                                                           DAT3 230
   THEN N2   =M,.                                                       DAT3 240
   GET EDIT (CH) (A(80)),.                                              DAT3 250
   GET STRING (CH) EDIT ((D(I) DO I= N1 TO N2)) ((N)F(6,0)),.           DAT3 260
   N1   =N2+1,.                                                         DAT3 270
   IF N1 LE M                                                           DAT3 280
   THEN DO,.                                                            DAT3 290
         N2   =N2+N,.                                                   DAT3 300
         GO TO S10,.                                                    DAT3 310
         END,.                                                          DAT3 320
   REVERT ENDFILE (SYSIN),.                                             DAT3 330
   RETURN,.                                                             DAT3 340
EXIT..                                                                  DAT3 350
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')                DAT3 360
         (SKIP(1),COLUMN(10),A),.                                       DAT3 370
   STOP,.                                                               DAT3 380
   END,.                               /*END OF PROCEDURE DAT3       */DAT3 390
```

DISCRIMINANT ANALYSIS MDSC

Problem Description

A set of linear functions is calculated from data on many groups for the purpose of classifying new individuals into one of several groups. The classification of an individual into a group is performed by evaluating each of the calculated linear functions, then finding the group for which the associated probability is largest.

The sample problem for discriminant analysis consists of four groups of observations, as presented in Table 5. The number of observations in the first group is eight, the second group seven, the third group seven, and the fourth group eight. The number of variables in all groups is six.

Program

Description

The discriminant analysis consists of the main program MDSC, a special input routine DAT2, and three subroutines from the Scientific Subroutine Package: DMTX, MINV, DSCR.

Table 5. Sample Data for Discriminant Analysis

	Observation	X_1	X_2	X_3	X_4	X_5	X_6
Group 1	1	3	10	9	8	24	8
	2	4	12	3	8	22	7
	3	9	3	2	8	9	8
	4	16	2	2	2	7	2
	5	5	10	5	8	23	9
	6	17	3	2	8	6	3
	7	2	10	9	8	29	16
	8	7	10	5	8	28	18
Group 2	1	9	10	27	8	28	16
	2	11	7	8	9	8	15
	3	8	10	2	8	27	16
	4	1	6	8	14	14	13
	5	7	8	9	6	18	2
	6	7	9	8	2	19	9
	7	7	10	5	8	27	17
Group 3	1	3	11	9	15	20	10
	2	9	4	10	7	9	9
	3	4	13	10	7	21	15
	4	8	5	16	16	16	7
	5	6	9	10	5	23	11
	6	8	10	5	8	27	16
	7	17	3	2	7	6	3
Group 4	1	3	10	8	8	23	8
	2	4	12	3	8	23	7
	3	9	3	2	8	21	7
	4	15	2	2	2	7	2
	5	9	10	26	8	27	16
	6	8	9	2	8	26	16
	7	7	8	6	9	18	2
	8	7	10	5	8	26	16

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 25 groups
2. The number of variables and the number of observations depend on the size of core available for input.
3. (12 F(6,0)) format for input data. Therefore, if a problem satisfies the above conditions, it is not necessary to modify the sample program. However, if input data cards are prepared using a different format, the input format statement in the special input routine may be modified. The general rules for program modification are described later.

Input

Control Cards

Two control cards are required for each problem and are read by the main program, MDSC.

The first card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-8	Number of groups (greater than 1)	04
9-10	Number of variables	06
11-12	Number of cards per observation	01

The second card is prepared as follows:

Columns	Contents	For Sample Problem
1-3	Number of observations in the first group	08
4-6	Number of observations in the second group	07
7-9	Number of observations in the third group	08
10-12	Number of observations in the fourth group	
	.	
	.	
	.	
73-75	Number of observations in the 25th group	

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 5 is keypunched on a separate card, using the format (12 F(6,0)). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

If there is more than one data card per observation, the data card count indicator (NCARD), which appears in columns 11-12 of the first control card, must be changed to agree with the number of data cards per observation.

Deck Setup

The deck setup is shown in Figure 26.

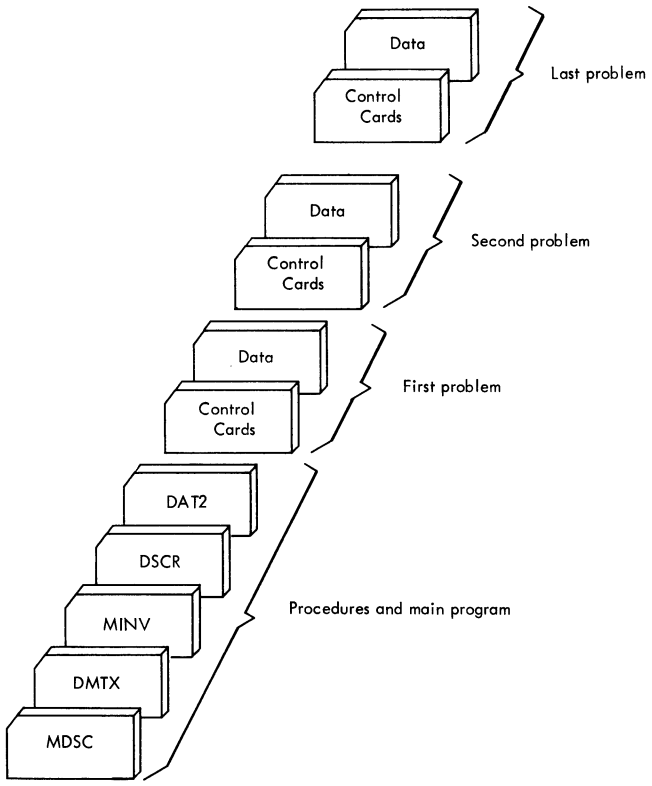


Figure 26.

Sample

The listing of input cards for the sample is shown in Figure 27.

```
SAMPLE 4 6 1                                                          10
  8  7  7  8                                                         20
     3   10    9    8   24    8                                      30
     4   12    3    8   22    7                                      40
     9    3    2    8    9    8                                      50
    16    2    2    2    7    2                                      60
     5   10    5    8   23    9                                      70
    17    3    2    8    6    3                                      80
     2   10    9    8   29   16                                      90
     7   10    5    8   28   18                                     100
     9   10   27    8   28   16                                     110
    11    7    8    9    8   15                                     120
     8   10    2    8   27   16                                     130
     1    6    8   14   14   13                                     140
     7    8    9    6   18    2                                     150
     7    9    8    2   19    9                                     160
     7   10    5    8   27   17                                     170
     3   11    9   15   20   10                                     180
     9    4   10    7    9    9                                     190
     4   13   10    7   21   15                                     200
     8    5   16   16   16    7                                     210
     6    9   10    5   23   11                                     220
     8   10    5    8   27   16                                     230
    17    3    2    7    6    3                                     240
     3   10    8    8   23    8                                     250
     4   12    3    8   23    7                                     260
     9    3    2    8   21    7                                     270
    15    2    2    2    7    2                                     280
     9   10   26    8   27   16                                     290
     8    9    2    8   26   16                                     300
     7    8    6    9   18    2                                     310
     7   10    5    8   26   16                                     320
```

Figure 27.

Output

Description

The output of the sample program for discriminant analysis includes:

1. Means of variables in each group
2. Pooled dispersion matrix
3. Common means
4. General Mahalanobis D-square
5. Constant and coefficient of each discriminant function
6. Probability associated with the largest discriminant function evaluated for each observation

Sample

The output listing for the sample problem is shown as Figure 28.

```
DISCRIMINANT ANALYSIS.....SAMPLE

  NUMBER OF GROUPS          4
  NUMBER OF VARIABLES       6
  SAMPLE SIZES..
          GROUP
            1           8
            2           7
            3           7
            4           8


 GROUP  1  MEANS
       7.87500        7.50000        4.62500        7.25000       18.50000        8.87500

 GROUP  2  MEANS
       7.14286        8.57143        9.57143        7.85714       20.14285       12.57143

 GROUP  3  MEANS
       7.85714        7.85714        8.85714        9.28571       17.42856       10.14286

 GROUP  4  MEANS
       7.75000        8.00000        6.75000        7.37500       21.37500        9.25000

POOLED DISPERSION MATRIX

ROW  1
      19.61876      -11.16208       -5.21497       -6.09890      -22.74855       -9.54052

ROW  2
     -11.16208       11.94505        5.61813        1.91758       22.60982       10.66757

ROW  3
      -5.21497        5.61813       39.45938        3.93681       16.23486        9.34546

ROW  4
      -6.09890        1.91758        3.93681        9.83310        4.62156        3.83791

ROW  5
     -22.74855       22.60982       16.23486        4.62156       62.78633       30.18262

ROW  6
      -9.54052       10.66757        9.34546        3.83791       30.18262       29.57480
```

Figure 28.

```
COMMON MEANS
      7.66667        7.96667        7.33333        7.90000       19.39998       10.13332


GENERALIZED MAHALANOBIS D-SQUARE       12.78063
DISCRIMINANT FUNCTION  1

     CONSTANT    *   COEFFICIENTS

    -28.49431    *
                        2.63870        2.12205       -0.17167        1.91198        0.58476       -0.40477
DISCRIMINANT FUNCTION  2

     CONSTANT    *   COEFFICIENTS

    -29.21017    *
                        2.61930        2.25230       -0.04816        1.88319        0.43732       -0.21784
DISCRIMINANT FUNCTION  3

     CONSTANT    *   COEFFICIENTS

    -31.86435    *
                        2.74450        2.39588       -0.06457        2.13260        0.42619       -0.32718
DISCRIMINANT FUNCTION  4

     CONSTANT    *   COEFFICIENTS

    -30.82028    *
                        2.71860        2.03937       -0.13352        1.94539        0.71677       -0.48760


EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH OBSERVATION

GROUP  1
                  PROBABILITY ASSOCIATED WITH          LARGEST
 OBSERVATION      LARGEST DISCRIMINANT FUNCTION        FUNCTION NO.
      1                    0.38065                        4
      2                    0.37045                        1
      3                    0.36261                        1
      4                    0.44190                        1
      5                    0.34454                        1
      6                    0.44215                        3
      7                    0.31787                        2
      8                    0.29274                        2

GROUP  2
                  PROBABILITY ASSOCIATED WITH          LARGEST
 OBSERVATION      LARGEST DISCRIMINANT FUNCTION        FUNCTION NO.
      1                    0.51029                        2
      2                    0.50060                        3
      3                    0.34760                        4
      4                    0.43130                        3
      5                    0.44282                        4
      6                    0.36407                        2
      7                    0.28515                        2

GROUP  3
                  PROBABILITY ASSOCIATED WITH          LARGEST
 OBSERVATION      LARGEST DISCRIMINANT FUNCTION        FUNCTION NO.
      1                    0.67611                        3
      2                    0.46629                        2
      3                    0.54636                        2
      4                    0.66688                        3
      5                    0.30600                        2
      6                    0.33043                        4
      7                    0.39005                        3

GROUP  4
                  PROBABILITY ASSOCIATED WITH          LARGEST
 OBSERVATION      LARGEST DISCRIMINANT FUNCTION        FUNCTION NO.
      1                    0.33727                        4
      2                    0.37475                        1
      3                    0.62340                        4
      4                    0.45697                        1
      5                    0.52175                        2
      6                    0.34061                        4
      7                    0.43135                        4
      8                    0.27849                        1


END OF SAMPLE PROGRAM
```

Figure 28. (Continued)

Program Modification

1. Changes in the input format statement of the special input routine, DAT2:
Only the format statement for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using six-column fields, as in the sample problem, each row of data might have been keypunched in two-column fields; if so, the format is changed to (6 F(2,0)). This format assumes six 2-column fields per card, beginning in column 1.

2. If there are more than twelve variables in a problem, each row of data is continued on the second card until the last data point is keypunched. However, each row of data must begin in a new card. If there is more than one data card per observation, the value of the data card count indicator (NCARD), which appears in columns 11-12 of the first control card, must be changed to agree with the number of data cards.

Operating Instructions

The sample program for discriminant analysis is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output.

Timing

The execution of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 28 seconds.

```
MDSC..                                                                  MDSC  10
/*********************************************************************/MDSC  20
/*                                                                   */MDSC  30
/*      TO READ THE PROBLEM PARAMETER CARD AND DATA FOR DISCRIMINANT */MDSC  40
/*      ANALYSIS, CALL THE PROCEDURES TO CALCULATE VARIABLE MEANS IN */MDSC  50
/*      EACH GROUP, POOLED DISPERSION MATRIX, COMMON COEFFICIENTS OF */MDSC  60
/*      DISCRIMINANT FUNCTIONS AND PROBABILITY ASSOCIATED WITH LARG- */MDSC  70
/*      EST DISCRIMINANT FUNCTION OF EACH CASE IN EACH GROUP, AND    */MDSC  80
/*      PRINT THE RESULTS.                                           */MDSC  90
/*                                                                   */MDSC 100
/*********************************************************************/MDSC 110
   PROCEDURE OPTIONS (MAIN),.                                           MDSC 120
   DECLARE                                                              MDSC 130
        (I,J,K,L,M,N1,N2,NN)                                            MDSC 140
        FIXED BINARY,                                                   MDSC 150
        PR1 CHARACTER (6),                                              MDSC 160
        ERROR EXTERNAL CHARACTER (1),                                   MDSC 170
        (NCARD,NV) EXTERNAL,                                            MDSC 180
        CH  CHARACTER (80),.                                            MDSC 190
/*                                                                   */MDSC 200
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      MDSC 210
S100..                                                                  MDSC 220
   GET EDIT (CH) (A(80)),.                                              MDSC 230
   GET STRING (CH) EDIT (PR1,K,M,NCARD) (A(6),3 F(2)),.                 MDSC 240
/*                                                                   */MDSC 250
/*      PR1......PROBLEM NUMBER (MAY BE ALPHAMERIC)                  */MDSC 260
/*      K........NUMBER OF GROUPS                                    */MDSC 270
/*      M........NUMBER OF VARIABLES                                 */MDSC 280
/*      NCARD....NUMBER OF CARDS PER OBSERVATION                     */MDSC 290
/*                                                                   */MDSC 300
   NCARD=NCARD*80,.                                                     MDSC 310
   NV   =0,.                                                            MDSC 320
ONE..                                                                   MDSC 330
   BEGIN,.                                                              MDSC 340
   DECLARE                                                              MDSC 350
        N(K)  FIXED BINARY,                                             MDSC 360
        (XBAR(M,K),C(M+1,K),D(M,M),CMEAN(M),DET,V,CON)                  MDSC 370
        BINARY FLOAT,.                 /*SINGLE PRECISION VERSION  /*S*/MDSC 380
 /*     BINARY FLOAT (53),.            /*DOUBLE PRECISION VERSION  /*D*/MDSC 390
/*                                                                   */MDSC 400
/*      READ SAMPLE SIZE OF EACH GROUP                               */MDSC 410
/*                                                                   */MDSC 420
   GET EDIT (CH) (A(80)),.                                              MDSC 430
   GET STRING (CH) EDIT ((N(I) DO I= 1 TO K))                           MDSC 440
        (25 F(3)),.                                                     MDSC 450
   NN   =SUM (N),.                                                      MDSC 460
TWO..                                                                   MDSC 470
   BEGIN,.                                                              MDSC 480
   DECLARE                                                              MDSC 490
        LG(NN)  FIXED BINARY,                                           MDSC 500
        X(NN,M) FLOAT BINARY,                                           MDSC 510
        P(NN)                                                           MDSC 520
        BINARY FLOAT,.                 /*SINGLE PRECISION VERSION  /*S*/MDSC 530
 /*     BINARY FLOAT (53),.            /*DOUBLE PRECISION VERSION  /*D*/MDSC 540
   PUT EDIT ('DISCRIMINANT ANALYSIS.....',PR1, '  NUMBER OF GROUPS',K, MDSC 550
        '  NUMBER OF VARIABLES',M,'  SAMPLE SIZES..','GROUP')           MDSC 560
        (PAGE,SKIP(4),COLUMN(10),A,A,SKIP(2),COLUMN(10),A,X(7),F(3),    MDSC 570
        SKIP(1),COLUMN(10),A,F(7),SKIP(1),COLUMN(10),A,SKIP(1),         MDSC 580
        COLUMN(22),A),.                                                 MDSC 590
   PUT EDIT ((I,N(I) DO I= 1 TO K)) (SKIP(1),COLUMN(22),F(3),X(8),      MDSC 600
        F(4)),.                                                         MDSC 610
   PUT EDIT (' ') (SKIP(2),A),.                                         MDSC 620
/*                                                                   */MDSC 630
/*      READ IN DATA. IN THE MANNER EQUIVALENT TO A 3-DIMENSIONAL    */MDSC 640
/*      ARRAY X(1,1,1),X(2,1,1),X(3,1,1),ETC. THE FIRST SUBSCRIPT    */MDSC 650
/*      IS THE CASE NUMBER,THE SECOND SUBSCRIPT IS THE VARIABLE      */MDSC 660
/*      NUMBER AND THE THIRD SUBSCRIPT IS THE GROUP NUMBER           */MDSC 670
/*                                                                   */MDSC 680
        DO I = 1 TO NN,.                                                MDSC 690
        CALL DAT2 (M,CMEAN),.                                           MDSC 700
             DO J = 1 TO M,.                                            MDSC 710
             X(I,J)=CMEAN(J),.                                          MDSC 720
             END,.                                                      MDSC 730
        END,.                                                           MDSC 740
   CALL DMTX (K,M,N,X,XBAR,D),.                                         MDSC 750
   IF ERROR NE '0'                                                      MDSC 760
   THEN DO,.                                                            MDSC 770
        PUT EDIT ('IN ROUTINE DMTX ERROR CODE = ',ERROR)                MDSC 780
             (SKIP(2),COLUMN(10),A,A(1)),.                              MDSC 790
        GO TO FIN,.                                                     MDSC 800
        END,.                                                           MDSC 810
/*                                                                   */MDSC 820
/*      PRINT MEANS AND POOLED DISPERSION MATRIX                     */MDSC 830
/*                                                                   */MDSC 840
        DO I = 1 TO K,.                                                 MDSC 850
        PUT EDIT ('GROUP',I,'MEANS') (SKIP(2),COLUMN(11),A,F(3),X(2),   MDSC 860
             A),.                                                       MDSC 870
        PUT EDIT ((XBAR(J,I) DO J= 1 TO M)) (SKIP(1),COLUMN(10),        MDSC 880
             (6)F(15,5)),.                                              MDSC 890
        END,.                                                           MDSC 900
   PUT EDIT ('POOLED DISPERSION MATRIX') (SKIP(3),COLUMN(10),A),.       MDSC 910
        DO I = 1 TO M,.                                                 MDSC 920
        PUT EDIT ('ROW',I) (SKIP(2),COLUMN(10),A,F(3)),.                MDSC 930
        PUT EDIT ((D(I,J) DO J= 1 TO M)) (SKIP,COLUMN(10),6 F(15,5)),.  MDSC 940
        END,.                                                           MDSC 950
   CON  =0,.                                                            MDSC 960
```

```
   CALL MINV (D,M,DET,CON),.                                            MDSC 970
   IF ERROR NE '0'                                                      MDSC 980
   THEN DO,.                                                            MDSC 990
        PUT EDIT ('IN ROUTINE MINV ERROR CODE = ',ERROR) (SKIP(2),      MDSC1000
             COLUMN(10),A,A(1)),.                                       MDSC1010
        GO TO CONT,.                                                    MDSC1020
        END,.                                                           MDSC1030
   CALL DSCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG),.                          MDSC1040
   IF ERROR NE '0'                                                      MDSC1050
   THEN DO,.                                                            MDSC1060
        PUT EDIT ('IN ROUTINE DSCR ERROR CODE = ',ERROR)                MDSC1070
             (SKIP(2),COLUMN(10),A,A(1)),.                              MDSC1080
        GO TO S100,.                                                    MDSC1090
        END,.                                                           MDSC1100
/*                                                                   */MDSC1110
/*      PRINT THE COMMON MEANS.                                      */MDSC1120
/*                                                                   */MDSC1130
   PUT EDIT ('COMMON MEANS') (SKIP(4),COLUMN(10),A),.                   MDSC1140
   PUT EDIT ((CMEAN(I) DO I= 1 TO M)) (SKIP,COLUMN(10),(6)F(15,5)),.    MDSC1150
/*                                                                   */MDSC1160
/*      PRINT GENERALIZED MAHALANOBIS D-SQUARE                       */MDSC1170
/*                                                                   */MDSC1180
   PUT EDIT ('GENERALIZED MAHALANOBIS D-SQUARE',V)                      MDSC1190
        (SKIP(4),COLUMN(10),A,F(15,5),SKIP(2)),.                        MDSC1200
/*                                                                   */MDSC1210
/*      PRINT CONSTANTS AND COEFFICIENTS OF DISCRIMINANT FUNCTIONS   */MDSC1220
/*                                                                   */MDSC1230
        DO I = 1 TO K,.                                                 MDSC1240
        PUT EDIT ('DISCRIMINANT FUNCTION',I,'CONSTANT   *',             MDSC1250
             'COEFFICIENTS') (SKIP(2),COLUMN(10),A,F(3),SKIP(2),        MDSC1260
             COLUMN(16),A,X(3),A),.                                     MDSC1270
        PUT EDIT (C(1,I),'   *   ') (SKIP(2),COLUMN(10),F(14,5),A),.    MDSC1280
        PUT EDIT ((C(J,I) DO J= 2 TO M+1)) (SKIP,COLUMN(32),            MDSC1290
             (6)F(14,5)),.                                              MDSC1300
        END,.                                                           MDSC1310
/*                                                                   */MDSC1320
/*      PRINT EVALUATION OF CLASSIFICATION FUNCTIONS OF EACH         */MDSC1330
/*      OBSERVATION.                                                 */MDSC1340
/*                                                                   */MDSC1350
   PUT EDIT ('EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH',         MDSC1360
        ' OBSERVATION') (SKIP(4),COLUMN(10),A,A),.                      MDSC1370
   N1   =1,.                                                            MDSC1380
   N2   =N(1),.                                                         MDSC1390
        DO I = 1 TO K,.                                                 MDSC1400
        PUT EDIT ('GROUP',I,'PROBABILITY ASSOCIATED WITH','LARGEST',    MDSC1410
             ' OBSERVATION','LARGEST DISCRIMINANT FUNCTION',            MDSC1420
             'FUNCTION NO.')                                            MDSC1430
             (SKIP(2),COLUMN(10),A,F(3),SKIP,COLUMN(28),A,X(11),A,      MDSC1440
             SKIP,COLUMN(10),A,X(5),A,X(8),A),.                         MDSC1450
        L    =0,.                                                       MDSC1460
             DO J = N1 TO N2,.                                          MDSC1470
             L    =L+1,.                                                MDSC1480
             PUT EDIT (L,P(J),LG(J)) (SKIP,COLUMN(10),F(6),X(20),F(8,5)MDSC1490
                  ,X(20),F(6)),.                                        MDSC1500
             END,.                                                      MDSC1510
        IF I = K                                                        MDSC1520
        THEN GO TO CONT,.                                               MDSC1530
        N1   =N1+N(I),.                                                 MDSC1540
        N2   =N2+N(I+1),.                                               MDSC1550
        END,.                                                           MDSC1560
CONT..                                                                  MDSC1570
   END,.                                                                MDSC1580
   END,.                                                                MDSC1590
   GO TO S100,.                                                         MDSC1600
EXIT..                                                                  MDSC1610
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                   MDSC1620
        (SKIP(5),COLUMN(10),A),.                                        MDSC1630
FIN..                                                                   MDSC1640
   END,.                              /*END OF PROCEDURE MDSC        */MDSC1650
```

```
DAT2..                                                                  DAT2  10
/*********************************************************************/*DAT2  20
/*                                                                   */DAT2  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.      */DAT2  40
/*      DATA MAY BE SAVED ON A DATA SET.                             */DAT2  50
/*                                                                   */DAT2  60
/*********************************************************************/DAT2  70
   PROCEDURE (M,D),.                                                    DAT2  80
   DECLARE                                                              DAT2  90
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),        DAT2 100
        (NCARD,NV) EXTERNAL,                                            DAT2 110
        CH CHARACTER(NCARD),                                            DAT2 120
        (I,M,MM) FIXED BINARY,                                          DAT2 130
        D(*) FLOAT BINARY,.                                             DAT2 140
/*                                                                   */DAT2 150
   ON ENDFILE (SYSIN)                                                   DAT2 160
   GO TO EXIT,.                                                         DAT2 170
   GET EDIT (CH) (A(NCARD)),.                                           DAT2 180
   MM   =CEIL(M/12),.                                                   DAT2 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                           DAT2 200
        ((MM)(12)F(6,0),X(8)),.                                         DAT2 210
   IF NV= 1                                                             DAT2 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,0)),.       DAT2 230
   REVERT ENDFILE (SYSIN),.                                             DAT2 240
   RETURN,.                                                             DAT2 250
EXIT..                                                                  DAT2 260
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')                DAT2 270
        (SKIP(1),COLUMN(10),A),.                                        DAT2 280
   STOP,.                                                               DAT2 290
   END,.                              /*END OF PROCEDURE DAT2        */DAT2 300
```

PRINCIPAL COMPONENTS ANALYSIS FACT

Problem Description

A principal component solution and the varimax rotation of the factor matrix are performed. Principal components analysis is used to determine the minimum number of independent dimensions needed

to account for most of the variance in the original set of variables. The varimax rotation is used to simplify columns (factors) rather than rows (variables) of the factor matrix.

The sample problem for principal components analysis consists of 23 observations with nine variables, as presented in Table 6. In order to keep the number of independent dimensions as small as possible, only those eigenvalues (of correlation coefficients) greater than or equal to 1.0 are retained in the analysis.

Table 6. Sample Data for Principal Components Analysis

Observation	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9
1	7	7	9	7	15	36	60	15	24
2	13	18	25	15	13	35	61	18	30
3	9	18	24	23	12	43	62	14	31
4	7	13	25	36	11	12	63	26	32
5	6	8	20	7	15	46	18	28	15
6	10	12	30	11	10	42	27	12	17
7	7	6	11	7	15	35	60	20	25
8	16	19	25	16	13	30	64	20	30
9	9	22	26	24	13	40	66	15	32
10	8	15	26	30	13	10	66	25	34
11	8	10	20	8	17	40	20	30	18
12	9	12	28	11	8	45	30	15	19
13	11	17	21	30	10	45	60	17	30
14	9	16	26	27	14	31	59	19	17
15	10	15	24	18	12	29	48	18	26
16	11	11	30	19	19	26	57	20	30
17	16	9	16	20	18	31	60	21	17
18	9	8	19	14	16	33	67	9	19
19	7	18	22	9	15	37	62	11	20
20	8	11	23	18	9	36	61	22	24
21	6	6	27	23	7	40	55	24	31
22	10	9	26	26	10	37	57	27	29
23	8	10	26	15	11	42	59	20	28

Program

Description

The principal components analysis sample program consists of a main routine, FACT, a special input routine named DAT2, and five subroutines from the Scientific Subroutine Package: CORR, MSDU, TRAC, LOAD, and VRMX.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 96 variables can be read.
2. Up to 99999 observations can be read.
3. Up to eight data cards per observation can be read.
4. (12 F(6,0)) format for input data cards.

Therefore, if a problem satisfies the above conditions, it is not necessary to modify the sample program. However, if input data cards are prepared using a different format, the input format statement in the input procedure, DAT2, must be modified. The general rules for program modification are described later.

Input

Control Card

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	00023
12-13	Number of variables	09
14-19	Value used to limit the number of eigenvalues of correlation coefficients. Only those eigenvalues greater than or equal to this value are retained in the analysis. (A decimal point must be specified.)	0001.0
20-21	Number of data cards per observation.	01

Leading zeros do not have to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 6 is keypunched on a separate card, using the format (12 F(6,0)). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

Deck Setup

The deck setup is shown in Figure 29.

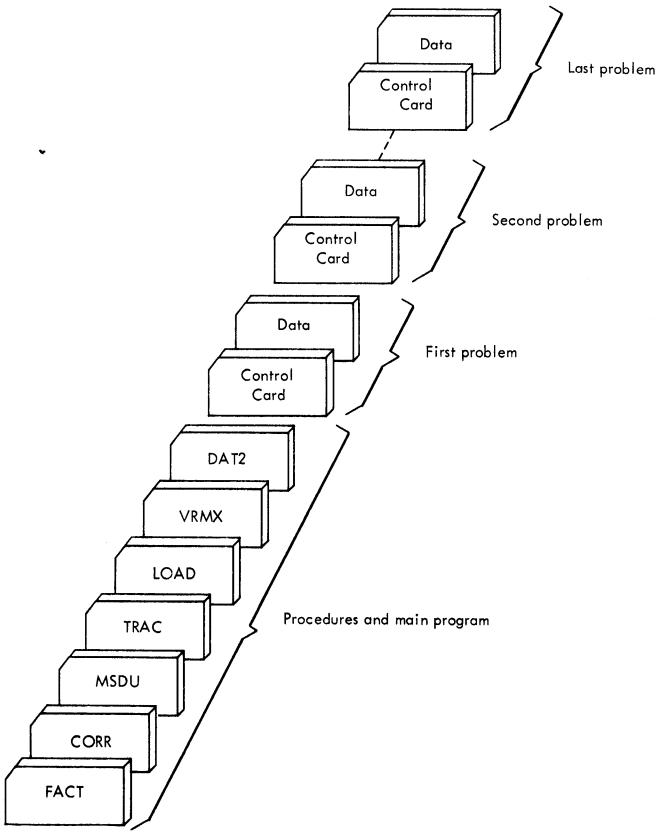


Figure 29.

Sample

The listing of input cards for the sample problem is shown in Figure 30.

```
SAMPLEC0C23090C01.C 1                                                    10
    7    7    9    7   15   36   60   15   24                            20
   13   18   25   15   13   35   61   18   30                            30
    9   18   24   23   12   43   62   14   31                            40
    7   13   25   36   11   12   63   26   32                            50
    6    8   20    7   15   46   18   28   15                            60
   10   12   30   11   1C   42   27   12   17                            70
    7    6   11    7   15   35   6C   20   25                            80
   16   19   25   16   13   30   64   20   30                            90
    9   22   26   24   13   40   66   15   32                           100
    8   15   26   30   13   10   66   25   34                           110
    8   10   20    8   17   40   2C   30   18                           120
    9   12   28   11    8   45   3C   15   19                           130
   11   17   21   3C   1C   45   6C   17   30                           140
    9   16   26   27   14   31   59   19   17                           150
   1C   15   24   18   12   29   48   18   26                           160
   11   11   30   19   19   26   57   20   30                           170
   16    9   16   20   18   31   6C   21   17                           180
    9    8   19   14   16   33   67    9   19                           190
    7   18   22    9   15   37   62   11   20                           200
    8   11   23   18    9   36   61   22   24                           210
    6    6   27   23    7   40   55   24   31                           220
   10    9   26   26   1C   37   57   27   29                           230
    8   1C   26   15   11   42   59   20   28                           240
```

Figure 30.

Output

Description

The output of the sample program for principal components analysis includes:

1. Means
2. Standard deviations
3. Correlation coefficients
4. Eigenvalues
5. Cumulative percentage of eigenvalues
6. Eigenvectors
7. Factor matrix
8. Variance of factor matrix for each iteration cycle
9. Rotated factor matrix
10. Check on communalities

Sample

The output listing for the sample problem is shown in Figure 31.

```
PRINCIPAL COMPONENT ANALYSIS.....SAMPLE

   NO. OF CASES        23
   NO. OF VARIABLES     9

MEANS
        9.30435      12.60870      23.00000      18.00000      12.86957      34.82608      54.00000
       19.39130      25.13043

STANDARD DEVIATIONS
        2.70412       4.59978       5.33427       8.33393       3.13781       9.29149      14.87826
        5.56563       6.09249

CORRELATION COEFFICIENTS

ROW  1
     1.00000     0.34987     0.11975     0.12102     0.21917    -0.09549     0.20901    -0.12908     0.05818

ROW  2
     0.34987     1.00000     0.41311     0.35572    -0.08243    -0.09100     0.29622    -0.32044     0.35387

ROW  3
     0.11975     0.41311     1.00000     0.41512    -0.43179    -0.08346    -0.10252     0.03215     0.27833

ROW  4
     0.12102     0.35572     0.41512     1.00000    -0.31288    -0.50365     0.49856     0.22539     0.59890

ROW  5
     0.21917    -0.08243    -0.43179    -0.31288     1.00000    -0.23000     0.03310    -0.00475    -0.30341

ROW  6
    -0.09549    -0.09100    -0.08346    -0.50365    -0.23000     1.00000    -0.44520    -0.25441    -0.37456

ROW  7
     0.20901     0.29622    -0.10252     0.49856     0.03310    -0.44520     1.00000    -0.28050     0.60124

ROW  8
    -0.12908    -0.32044     0.03215     0.22539    -0.00475    -0.25441    -0.28050     1.00000     0.13516

ROW  9
     0.05818     0.35387     0.27833     0.59890    -0.30341    -0.37456     0.60124     0.13516     1.00000
```

Figure 31.

```
EIGENVALUES
     2.94988      1.64368      1.55514      1.06579

CUMULATIVE PERCENTAGE OF EIGENVALUES
     0.32776      0.51040      0.68319      0.80161


EIGENVECTORS

VECTOR  1
     0.16437      0.34836      0.28797      0.49661     -0.16806     -0.32922      0.39935      0.01287      0.47518

VECTOR  2

     0.34837      0.06552     -0.44647     -0.11893      0.61210     -0.26428      0.38860     -0.24845     -0.06014

VECTOR  3
    -0.29899     -0.46825     -0.23534      0.17377      0.14468     -0.43545      0.01881      0.61587      0.12470

VECTOR  4
     0.54441      0.16909      0.38288      0.04163      0.30537     -0.16163     -0.43410      0.40283     -0.23789

FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
     0.28232      0.44663     -0.37286      0.56203

VARIABLE  2
     0.59831      0.08400     -0.58394      0.17457

VARIABLE  3
     0.49460     -0.57240     -0.29348      0.39528

VARIABLE  4
     0.85293     -0.15248      0.21671      0.04297

VARIABLE  5
    -0.28865      0.78475      0.18043      0.31525

VARIABLE  6
    -0.56544     -0.33882     -0.54303     -0.16686

VARIABLE  7
     0.68590      0.49621      0.02345     -0.44816

VARIABLE  8
     0.02211     -0.31853      0.76802      0.41587

VARIABLE  9
     0.81614     -0.07710      0.15551     -0.24559


ITERATION       VARIANCES
  CYCLE
    0            0.211288
    1            0.336136
    2            0.397020
    3            0.403004
    4            0.405175
    5            0.405527
    6            0.405579
    7            0.405586
    8            0.405586
    9            0.405586
   10            0.405586
   11            0.405586
   12            0.405586


ROTATED FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
     0.05498      0.07183     -0.05578      0.85017

VARIABLE  2
     0.29329     -0.39653     -0.35581      0.60549

VARIABLE  3
     0.05114     -0.82493      0.15068      0.32984

VARIABLE  4
     0.74040     -0.41401      0.24579      0.13972

VARIABLE  5
    -0.09091      0.80662      0.13525      0.39228

VARIABLE  6
    -0.68236     -0.21579     -0.44983     -0.20503

VARIABLE  7
     0.86997      0.18299     -0.34918      0.08830

VARIABLE  8
     0.03602     -0.05500      0.91375     -0.15962

VARIABLE  9
     0.80531     -0.32759      0.00994     -0.02380


CHECK ON COMMUNALITIES

VARIABLE       ORIGINAL            FINAL          DIFFERENCE
    1           0.73409           0.73408           0.00001
    2           0.73649           0.73647           0.00001
    3           0.81464           0.81463           0.00001
    4           0.79955           0.79954           0.00001
    5           0.83109           0.83107           0.00001
    6           0.75725           0.75724           0.00001
    7           0.92006           0.92005           0.00001
    8           0.86476           0.86474           0.00001
    9           0.75652           0.75651           0.00001



END OF SAMPLE PROGRAM
```

Figure 31. (Continued)

Program Modifications

Input data in a different format can also be handled by providing a different format statement. In order to familiarize the user with the program modifications, the following general rules are supplied in terms of the sample problem:

1. Changes in the input format statement of the special input subroutine, DAT2:

Only the format statement for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using six-column fields as in the sample problem, each row of data might have been keypunched in two-column fields; if so, the format is changed to 9F(2,0). This format assumes nine 2-column fields per card, beginning in column 1.

The special input subroutine, DAT2, is normally written by the user to handle different formats for different problems. The user may modify this procedure to perform testing of input data, transformation of data, and so on.

2. If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card. If this condition exists, the value of the data card count indicator (NCARD), which appears in columns 20-21 of the control card, must be changed to agree with the number of data cards per row.

Operating Instructions

The sample program for principal components analysis is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output.

Timing

The execution of this sample program on a System/360 Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model N1, as output, is 45 seconds.

```
FACT..                                                                  FACT  10
/*********************************************************************/FACT  20
/*                                                                   */FACT  30
/*      TO READ THE PROBLEM PARAMETER CARD, CALL FIVE PROCEDURES TO  */FACT  40
/*      PERFORM A PRINCIPAL COMPONENT SOLUTION AND THE VARIMAX ROTA- */FACT  50
/*      TION OF A FACTOR MATRIX, AND PRINT THE RESULTS.              */FACT  60
/*                                                                   */FACT  70
/*********************************************************************/FACT  80
   PROCEDURE OPTIONS (MAIN),.                                           FACT  90
   DECLARE                                                              FACT 100
         (I,IO,J,K,M,MV,N,NC,NW)                                        FACT 110
         FIXED BINARY,                                                  FACT 120
         ERROR EXTERNAL CHARACTER(1),                                   FACT 130
         (NV,NCARD) EXTERNAL,                                           FACT 140
         CON                                                            FACT 150
         FLOAT BINARY,                                                  FACT 160
         PR1 CHARACTER (6),                                             FACT 170
         CH  CHARACTER (80),.                                           FACT 180
/*                                                                   */FACT 190
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      FACT 200
```

```
S10C..                                                                  FACT 210
   GET EDIT (CH) (A(80)),.                                              FACT 220
   GET STRING (CH) EDIT (PR1,N,M,CON,NCARD) (A(6),F(5),F(2),F(6,0),     FACT 230
         F(2)),.                                                        FACT 240
/*                                                                   */FACT 250
/*      PR1........PROBLEM NUMBER (MAY BE ALPHAMERIC )               */FACT 260
/*      N..........NUMBER OF CASES                                   */FACT 270
/*      M..........NUMBER OF VARIABLES                               */FACT 280
/*      CON........CONSTANT USED TO DECIDE HOW MANY EIGENVALUES      */FACT 290
/*                 TO RETAIN                                         */FACT 300
/*      NCARD......NUMBER OF DATA CARDS PER OBSERVATION              */FACT 310
/*                                                                   */FACT 320
   NCARD=NCARD*80,.                                                     FACT 330
ONE..                                                                   FACT 340
   BEGIN,.                                                              FACT 350
   DECLARE                                                              FACT 360
         (R(M,M),V(M,M),B(M),D(M),S(M),T(M),XBAR(M),TV(51),X(1,1))      FACT 370
         BINARY FLOAT,.                 /*SINGLE PRECISION VERSION  /*S*/FACT 380
/*       BINARY FLOAT (53),.            /*DOUBLE PRECISION VERSION  /*D*/FACT 390
   PUT EDIT ('PRINCIPAL COMPONENT ANALYSIS.....',PR1, 'NO. OF CASES',   FACT 400
         N,'NO. OF VARIABLES',M)                                        FACT 410
         (PAGE,SKIP(4),COLUMN(10),A,A,SKIP(2),COLUMN(13),A,X(4),F(6)    FACT 420
         ,SKIP(1),COLUMN(13),A,F(6),SKIP),.                             FACT 430
   IO   =0,.                                                            FACT 440
   X    =0,.                                                            FACT 450
   NV   =0,.                                                            FACT 460
   CALL CORR (N,M,IO,X,XBAR,S,V,R,D),.                                  FACT 470
   IF ERROR NE '0'                                                      FACT 480
   THEN DO,.                                                            FACT 490
         PUT EDIT ('IN ROUTINE CORR ERROR CODE = ',ERROR)               FACT 500
               (SKIP(2),COLUMN(10),A,A(1)),.                            FACT 510
         GO TO S10C,.                                                   FACT 520
         END,.                                                          FACT 530
   PUT EDIT ('MEANS') (SKIP(2),COLUMN(10),A),.                          FACT 540
   PUT EDIT ((XBAR(J) DO J= 1 TO M)) (SKIP,COLUMN(10),(7)F(15,5)),.     FACT 550
/*                                                                   */FACT 560
/*       PRINT MEANS AND STANDARD DEVIATIONS                         */FACT 570
/*                                                                   */FACT 580
   PUT EDIT ('STANDARD DEVIATIONS') (SKIP(2),COLUMN(10),A),.            FACT 590
   PUT EDIT ((S(J) DO J= 1 TO M)) (SKIP,COLUMN(10),(7)F(15,5)),.        FACT 600
/*                                                                   */FACT 610
/*       PRINT CORRELATION COEFFICIENTS                              */FACT 620
/*                                                                   */FACT 630
   PUT EDIT ('CORRELATION COEFFICIENTS') (SKIP(2),COLUMN(10),A),.       FACT 640
         DO I = 1 TO M,.                                                FACT 650
         PUT EDIT ('ROW',I) (SKIP(2),COLUMN(10),A,F(3)),.               FACT 660
         PUT EDIT ((R(I,J) DO J= 1 TO M)) (SKIP,COLUMN(10),9 F(12,5)),. FACT 670
         END,.                                                          FACT 680
   MV   =0,.                                                            FACT 690
   CALL MSDU (R,V,M,MV),.                                               FACT 700
   IF ERROR NE '0'                                                      FACT 710
   THEN DO,.                                                            FACT 720
         PUT EDIT ('IN ROUTINE MSDU ERROR CODE ',ERROR)                 FACT 730
               (SKIP(2),COLUMN(10),A,A(1)),.                            FACT 740
         GO TO S10C,.                                                   FACT 750
         END,.                                                          FACT 760
   CALL TRAC (M,R,CON,K,D),.                                            FACT 770
   IF ERROR NE '0'                                                      FACT 780
   THEN DO,.                                                            FACT 790
         PUT EDIT ('IN ROUTINE TRAC ERROR CODE = ',ERROR)               FACT 800
               (SKIP(2),COLUMN(10),A,A(1)),.                            FACT 810
         GO TO S10C,.                                                   FACT 820
         END,.                                                          FACT 830
         DO I = 1 TO K,.                /* PRINT EIGENVALUES        */FACT 840
         S(I) =R(I,I),.                                                 FACT 850
         END,.                                                          FACT 860
   PUT EDIT ('EIGENVALUES') (SKIP(3),COLUMN(10),A),.                    FACT 870
   PUT EDIT ((S(J) DO J= 1 TO K)) (SKIP,COLUMN(10),9 F(12,5)),.         FACT 880
/*                                                                   */FACT 890
/*       PRINT CUMULATIVE PERCENTAGE OF EIGENVALUES                  */FACT 900
/*                                                                   */FACT 910
   PUT EDIT ('CUMULATIVE PERCENTAGE OF EIGENVALUES')                    FACT 920
         (SKIP(2),COLUMN(10),A),.                                       FACT 930
   PUT EDIT ((D(J) DO J= 1 TO K)) (SKIP,COLUMN(10),9 F(12,5)),.         FACT 940
/*                                                                   */FACT 950
/*       PRINT EIGENVECTORS AND FACTOR MATRIX                        */FACT 960
/*                                                                   */FACT 970
   PUT EDIT ('EIGENVECTORS') (SKIP(3),COLUMN(10),A),.                   FACT 980
         DO J = 1 TO K,.                                                FACT 990
         PUT EDIT ('VECTOR',J) (SKIP(2),COLUMN(10),A,F(3)),.            FACT1000
         PUT EDIT ((V(I,J) DO I= 1 TO M)) (SKIP,COLUMN(10),9 F(12,5)),. FACT1010
         END,.                                                          FACT1020
   PUT EDIT ('FACTOR MATRIX (',K,' FACTORS)')                           FACT1030
         (SKIP(3),COLUMN(10),A,F(3),A),.                                FACT1040
   CALL LOAD (M,K,F,V),.                                                FACT1050
   IF ERROR NE '0'                                                      FACT1060
   THEN DO,.                                                            FACT1070
         PUT EDIT ('IN ROUTINE LOAD ERROR CODE = ',ERROR)               FACT1080
               (SKIP(2),COLUMN(10),A,A(1)),.                            FACT1090
         GO TO S10C,.                                                   FACT1100
         END,.                                                          FACT1110
         DO I = 1 TO M,.                                                FACT1120
         PUT EDIT ('VARIABLE',I) (SKIP(2),COLUMN(10),A,F(3)),.          FACT1130
         PUT EDIT ((V(I,J) DO J= 1 TO K)) (SKIP,COLUMN(10),9 F(12,5)),. FACT1140
         END,.                                                          FACT1150
   CALL VRMX (M,K,V,NC,TV,B,T,D),.                                      FACT1160
   IF ERROR NE '0'                                                      FACT1170
   THEN DO,.                                                            FACT1180
         PUT EDIT ('IN ROUTINE VRMX ERROR CODE = ',ERROR)               FACT1190
               (SKIP(2),COLUMN(10),A,A(1)),.                            FACT1200
         GO TO S10C,.                                                   FACT1210
         END,.                                                          FACT1220
   NW   =NC+1,.                         /* PRINT VARIANCES          */FACT1230
   PUT EDIT ('ITERATION','VARIANCES',' CYCLE') (SKIP(3),COLUMN(10),A,   FACT1240
         X(7),A,SKIP,COLUMN(10),A),.                                    FACT1250
         DO I = 1 TO NW,.                                               FACT1260
         NC   =I-1,.                                                    FACT1270
         PUT EDIT (NC,TV(I)) (SKIP,COLUMN(10),F(5),F(20,6)),.           FACT1280
         END,.                                                          FACT1290
/*                                                                   */FACT1300
/*       PRINT ROTATED FACTOR MATRIX                                 */FACT1310
/*                                                                   */FACT1320
   PUT EDIT ('ROTATED FACTOR MATRIX (',K,' FACTORS)')                   FACT1330
         (SKIP(3),COLUMN(10),A,F(3),A),.                                FACT1340
         DO I = 1 TO M,.                                                FACT1350
         PUT EDIT ('VARIABLE',I) (SKIP(2),COLUMN(10),A,F(3)),.          FACT1360
         PUT EDIT ((V(I,J) DO J= 1 TO K)) (SKIP,COLUMN(10),9 F(12,5)),. FACT1370
         END,.                                                          FACT1380
/*                                                                   */FACT1390
/*       PRINT COMMUNALITIES                                         */FACT1400
/*                                                                   */FACT1410
   PUT EDIT ('CHECK ON COMMUNALITIES','VARIABLE','ORIGINAL','FINAL',    FACT1420
         'DIFFERENCE') (SKIP(3),COLUMN(10),A,SKIP(2),COLUMN(10),A,      FACT1430
         X(7),A,X(12),A,X(10),A),.                                      FACT1440
         DO I = 1 TO M,.                                                FACT1450
```

```
      PUT EDIT (I,B(I),T(I),D(I)) (SKIP,COLUMN(10),F(5),3 F(18,5)),. FACT1460
      END,.                                                         FACT1470
S200..                                                              FACT1480
   END,.                                                            FACT1490
   GO TO S100,.                                                     FACT1500
EXIT..                                                              FACT1510
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')               FACT1520
        (SKIP(5),COLUMN(10),A),.                                    FACT1530
   END,.                          /*END OF PROCEDURE FACT         */FACT1540
```

```
DAT2..                                                              DAT2  10
/*******************************************************************/DAT2  20
/*                                                                 */DAT2  30
/*      TO READ FLOATING POINT DATA, ONE OBSERVATION AT A TIME.    */DAT2  40
/*      DATA MAY BE SAVED ON A DATA SET.                           */DAT2  50
/*                                                                 */DAT2  60
/*******************************************************************/DAT2  70
   PROCEDURE (M,D),.                                                DAT2  80
   DECLARE                                                          DAT2  90
        XDATA FILE STREAM ENVIRONMENT (CONSECUTIVE V(2000,200)),    DAT2 100
        (NCARD,NV) EXTERNAL,                                        DAT2 110
        CH CHARACTER(NCARD),                                        DAT2 120
        (I,M,MM) FIXED BINARY,                                      DAT2 130
        D(*) FLOAT BINARY,.                                         DAT2 140
/*                                                                 */DAT2 150
   ON ENDFILE (SYSIN)                                               DAT2 160
   GO TO EXIT,.                                                     DAT2 170
   GET EDIT (CH) (A(NCARD)),.                                       DAT2 180
   MM   =CEIL(M/12),.                                               DAT2 190
   GET STRING (CH) EDIT ((D(I) DO I= 1 TO M))                       DAT2 200
        ((MM)((12)F(6,0),X(8))),.                                   DAT2 210
   IF NV= 1                                                         DAT2 220
   THEN PUT FILE (XDATA) EDIT ((D(I) DO I= 1 TO M)) ((M)F(6,0)),.   DAT2 230
   REVERT ENDFILE (SYSIN),.                                         DAT2 240
   RETURN,.                                                         DAT2 250
EXIT..                                                              DAT2 260
  PUT FILE (SYSPRINT) EDIT ('ERROR   INSUFFICIENT DATA')            DAT2 270
        (SKIP(1),COLUMN(10),A),.                                    DAT2 280
   STOP,.                                                           DAT2 290
   END,.                          /*END OF PROCEDURE DAT2         */DAT2 300
```

KOLMOGOROV-SMIRNOV TEST KOLM

Problem Description

This program is concerned with the problem of determining from what probability density function a particular sample is drawn, or whether two different samples were drawn from the same population. In other words, in the one-sample case, the actual distribution function of the sample is compared with one or more theoretical distribution functions, which may be normal, and/or exponential, and/or Cauchy, and/or uniform, and/or a user-specified distribution. In the two-sample case, the two sample (actual) distribution functions making up the pair are compared with one another.

From the above comparisons, a statistic is derived. In the one-sample case, this statistic evaluates the probability that the statistic will be as great as or greater than its current value, if the hypothesis that the actual (sample) and the theoretical distribution functions are equal is correct. In other words, if the probability is determined to be 0.40, for example, rejecting the hypothesis of equality of the distribution functions will be an incorrect action 40 times out of 100. Similarly, in the two-sample case, the hypothesis being tested is the equality of the two actual (sample) distribution functions.

This probability is calculated using asymptotic formulae. This means that the sample sizes involved should be large. Sizes greater than 100 are suggested by the literature. In this connection, the remarks given under subroutine SMIR should be considered.

Note also that added problems arise when, in the one-sample case, the parameters of the continuous distribution in question are estimated from the sample. Lilliefors discusses these problems (see reference given in KLMO description).

Program

Description

This program consists of the main routine KOLM, and four subroutines from the Scientific Subroutine Package: KLMO, KLM2, SMIR, and NDTR.

Capacity

This program allows up to two samples, each with 500 or fewer observations to be examined. If the user desires to modify this program to handle more observations, the instructions given below under "Program Modification" should be followed.

Input

Each job consists of two control cards and the data cards (1-3 below).

1. Job control card (minus signs in cc 1-4)
2. Program control card. Each job requires one program control card, defined below:

Columns	Contents	For Sample Problems
1 - 20	Title (alphameric)	Uniform test (Job 1) Uniform-Gauss Test (job 2)
21	1 -- one-sample test 2 -- two-sample test	1 (job 1) 2 (job 2)
22	Leave blank for one-sample test. 0 -- Read both samples (two-sample tests). 1 -- Read only one sample and compare it with the first sample read on preceding job.	0 (job 1) 1 (job 2)
23	0 -- Do not print the sample(s). 1 -- Print the sorted sample(s).	0 (job 1) 1 (job 2)

(F10.3, ten per line)

(The rest of this control card pertains to a one-sample test.)

Columns	Contents	For Sample Problems
24	0 -- Do not compare with normal pdf. 1 -- Compare with normal pdf.	1 (job 1)
25 - 29	u -- mean of the normal pdf	0.5 (job 1)
30 - 34	s -- standard deviation of the normal pdf	0.5 (job 1)
35	0 -- Do not compare with exponential pdf. 1 -- Compare with exponential pdf.	1 (job 1)
36 - 40	u -- mean of the exponential pdf	0.5 (job 1)
41 - 45	s -- standard deviation of the exponential pdf	1.0 (job 1)
46	0 -- Do not compare with Cauchy pdf. 1 -- Compare with Cauchy pdf.	1 (job 1)
47 - 51	u -- median of the Cauchy pdf	0.5 (job 1)
52 - 56	s -- u-s is the first quartile of the Cauchy pdf	1.0 (job 1)
57	0 -- Do not compare with uniform pdf. 1 -- Compare with uniform pdf.	1 (job 1)
58 - 62	u -- left endpoint of the uniform pdf	0 (job 1)
63 - 67	s -- right endpoint of uniform pdf	1.0 (job 1)
68	0 -- Do not compare with user's pdf. 1 -- Compare with user-specified pdf.	0 (job 1)
69 - 73 74 - 78	u, s -- Parameters for user-specified pdf	0 (job 1) 0 (job 1)

u and s are described fully in "Description of Parameters" under subroutine KLMO, and are read using Format F(5,0); decimal points will override the format specification.

3. Data is read into the computer one sample at a time. The reading of a sample is terminated by a data element of 999999. New samples must begin on a new card. Data elements are punched on cards using format F(6,0), which assumes twelve 6-column fields per card; decimal points on the card override the format specification. Since the routines KLMO and KLM2 sort the samples, no particular order within a sample is necessary.

Deck Setup

The deck setup is shown in Figure 32.

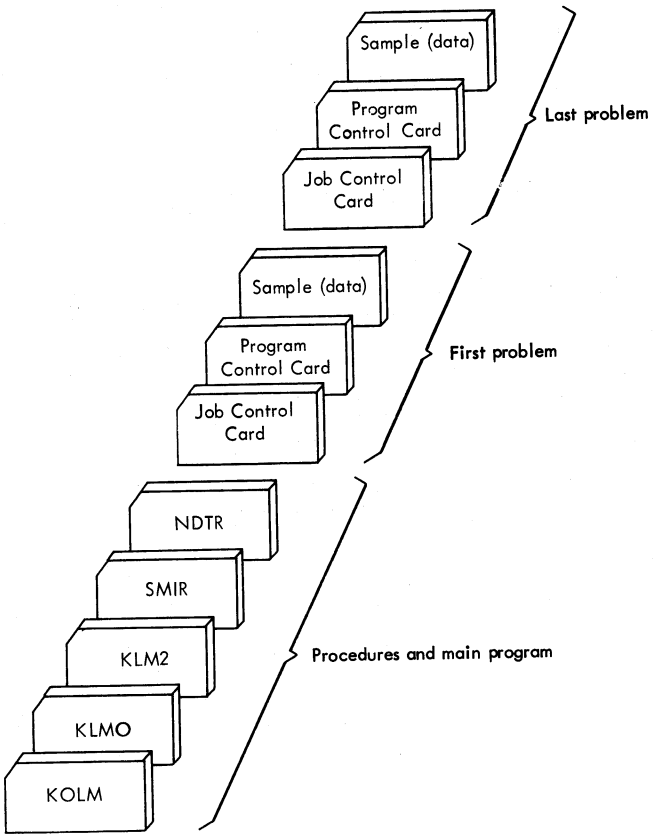


Figure 32.

Sample

The listing of input cards for the sample problems is shown in Figure 33.

```
----
UNIFORM TEST          1CC100C.5C00.510CC0.5CCCC1100C.50CCC110C0C00000C1
 0.377 C.26C 0.172 0.668 0.581 C.290 0.514 C.472 0.204 0.976 0.018 0.326
 0.795 0.827 0.870 C.686 C.288 0.555 0.737 C.427 0.931 0.745 0.092 C.843
 0.231 C.8C6 0.753 0.263 C.6C4 C.458 0.508 C.528 0.964 C.608 0.702 0.743
 0.005 C.551 0.664 0.425 C.57C C.596 0.444 0.3C2 C.817 0.183 0.746 0.833
 0.282 C.2C1 C.662 0.167 C.C43 C.750 0.117 0.953 0.665 0.411 0.477 0.164
 0.692 0.6E3 C.667 C.C54 0.51E C.624 0.083 0.882 C.540 0.301 0.953 0.006
 0.458 0.6S4 0.041 C.555 0.6C4 0.666 0.561 0.367 0.156 0.630 0.377 0.589
 0.139 C.536 0.963 C.556 C.C68 0.801 0.199 0.S65 0.113 0.816 0.880 0.931
 0.67C 0.64C 0.805 0.C73 0.19E C.516 0.336 0.371 0.157 0.843 0.288 0.139
 0.242 0.2CC 0.C25 0.349 C.87C C.C80 0.652 0.190 C.275 0.939 0.161 0.514
 0.636 C.19C 0.416 C.786 C.573 0.767 0.845 C.16E 0.40C 0.888 0.726 0.365
 0.652 C.632 0.923 C.E44 C.761 0.S69 0.965 0.C73 C.751 C.851 0.340 0.383
 0.243 C.CC8 C.86C 0.C53 C.816 C.C58 0.006 0.515 0.033 0.565 0.093 0.470
 0.982 0.666 0.154 C.933 0.215 C.E9C 0.40S 0.441 0.963 C.810 0.195 0.876
 0.501 C.123 0.228 0.264 0.531 0.810 C.C83 0.202 0.46S 0.996 0.752 0.545
 0.503 0.117 C.17C 0.S72 0.298 0.C42 0.574 0.C65 0.225 0.766 0.57C 0.520
 0.996 C.292 0.79C 0.111 0.556 0.337 0.C12 0.C42 0.143 0.482 0.607 0.302
 0.353 0.357 0.206 0.662 0.119 0.754 0.45C 0.518 0.453 0.463 0.699 0.022
 0.842 C.E59 0.577 0.725 0.163 0.450 0.232 0.345 0.0C0 0.864 0.181 0.311
 0.236 0.622 0.607 0.C42 0.787 0.348 0.C06 0.9C4 0.365 0.C53 0.037 0.745
 0.136 0.113 0.455 0.7C8 0.15E 0.572 0.012 0.928 0.455 0.381 0.193 0.728
 0.629 0.220 0.657 0.962 0.86C 0.501 0.268 0.C98 0.181 0.203 0.588 0.701
 0.905 0.14E 0.7C8 0.9C9 0.C88 0.345 0.277 0.556 0.840 0.033 0.639 0.539
 0.482 0.041 0.907 0.077 0.295 0.097 0.892 0.47E 0.835 0.7C7 0.733 0.029
 0.581 0.224 0.112 0.655 0.945 0.741 0.94C 0.96S 0.360 0.434 0.365 0.285
 0.422 0.567 0.005 0.328 0.924 0.595 0.253 0.157 0.668 0.594 0.554 0.984
 0.913 0.622 0.516 0.502 0.364 0.667 0.724 0.344 0.546 0.178 0.151 0.302
 0.457 0.021 0.019 0.923 0.365 0.882 0.01C C.121 0.637 0.734 0.671 0.416
 0.455 0.CC5 0.919 0.434 0.331 0.C79 0.50C 0.284 0.209 0.694 0.283 0.454
 0.178 0.978 0.272 0.827 0.512 0.634 0.195 0.462 0.01S 0.956 0.560 0.761
 0.524 0.254 0.047 0.634 0.382 0.591 0.103 0.3C3 0.889 0.607 0.638 0.367
 0.463 0.471 0.664 0.742 0.476 0.178 0.785 0.113 0.610 0.646 0.390 0.520
 0.611 0.588 0.431 0.699 0.312 0.580 0.672 0.810 0.814 0.597 0.256 0.164
 0.675 0.6C3 0.504 0.595 0.C33 0.846 0.783 0.C79 0.430 0.868 0.343 0.244
 0.376 0.C62 0.59C 0.381 0.371 0.801 0.467 0.592 0.348 0.759 0.422 0.697
 0.388 0.055 0.836 0.518 0.585 0.842 0.793 0.177 0.926 0.964 0.450 0.022
 0.C85 0.311 0.102 0.816 0.573 0.494 0.20E 0.8C3 0.948 0.462 0.242 0.287
 0.546 0.658 0.269 0.339 0.6C7 0.594 0.102 0.266 0.677 0.668 0.913 0.462
 0.562 0.2C7 0.188 0.264 0.895 0.991 0.853 0.442 0.615 0.7C9 0.722 0.950
 0.208 0.656 0.304 0.557 0.605 0.617 0.256 0.584 0.595 0.715 0.936 0.178
 0.141 0.153 0.654 0.544 0.376 0.363 0.793 0.492 0.812 0.447 0.376 0.231
 0.644 0.263 0.785 0.341 0.982 0.829999999
----
UNIFORM-GALSS TEST  211
-0.283 0.S16 0.776 0.65C 0.91C 0.506 0.816 0.348 0.659-0.301 0.630-0.397
 0.515 0.227 1.253 0.421 0.495 0.288 1.189-0.264 0.099 0.051 0.411 0.951
 0.273 0.154 0.861 0.537 0.446 0.702 1.451 0.035 0.515 0.770 0.559 1.053
-1.157 0.9C2 0.533 1.270 0.761 1.110 1.19C 0.433 0.573 0.374 1.317 1.255
 0.547 1.145 0.667-0.077 0.422-0.159-0.037 0.C88 0.406 0.849 0.898 0.372
-0.324 0.025 0.632 0.365 0.375 0.694-0.206 0.126-0.381 1.149 0.983 1.184
-0.011 0.653 0.266 1.C35 0.53E 0.936 1.177 1.644 0.782 0.198 0.222 0.445
 0.714 0.6C7 0.374 0.341 0.79C 0.302 1.075 0.2C4 0.436 0.887 0.234 0.874
 0.048 0.938 0.733-0.340-0.C12 0.497 0.41E 0.840 0.091 0.578 0.606-0.340
 0.656 0.66C 0.584 0.837 0.454 0.695 0.606 0.053-0.276 1.600 1.394-0.038
 1.173 0.762 0.642 0.185-0.C23 0.037 0.508 0.313-0.718-0.249 0.124-0.096
-0.299 0.196 1.086 0.487 0.317 0.635 0.462 0.559 0.181 1.799 0.287 0.583
 0.313 0.387 1.C67 0.956 0.7C2 0.068-0.227 0.158 0.305-0.021 0.849 1.063
 1.049 0.226-0.297 0.930 0.82E 0.884 1.217-0.391 0.007-0.004 1.238 0.376
 0.418 1.075 0.C83-0.020 0.362 0.601 0.037 0.634 0.109 0.524 1.356 1.024
-0.602 0.763 1.261 0.3C2-0.C63 0.704 0.446-0.410 0.401 0.704 1.070-0.023
-0.064 1.C87-0.737-0.476 1.156 0.648 0.624 0.257 0.643 0.147 0.719 0.174
-0.552-0.183 0.583 0.740 0.592-0.144 0.222 0.388 0.563 0.933 1.108 1.022
 0.818 0.66E 0.683 0.514 0.284-0.280 0.35E 1.2C3-0.643 0.110 0.012 0.399
 0.895 0.4CC 0.994 0.880 0.743 0.1C2 1.12C 0.391 0.191 0.196 1.176 0.149
 0.512 1.132 0.916 0.838 0.445 1.330 0.563 0.610 0.659 0.675 0.310 0.586
 0.44E-0.475 0.317 0.858 0.835-0.297 0.214 0.585 0.484 1.004 1.598 0.494
 0.467 1.188 0.536 0.381 1.339-0.011 0.064 0.113 0.619 0.604 0.687 0.622
 0.297 0.2C3 0.378 1.313 0.825 0.422 0.C78 0.C57 0.143 0.868-0.302 0.693
 0.633 1.116 0.118-0.469 0.663 0.7C8 0.685 0.850 0.566 0.657 1.217 0.394
 0.643-0.055-0.C00 0.881 1.163 0.520 0.787 1.493 1.366 0.801 0.301 1.384
-0.541 1.176 0.236 0.675 1.115 1.C00 0.250 0.457-0.01C 0.098 0.975 0.288
 0.68E 0.764 0.007 0.697 0.789 0.259 0.414 0.68C 0.852 0.315 0.231 0.203
 1.394 0.131 0.963 0.659 0.404-0.124 0.583 0.071 1.838-0.313-0.467 0.191
 0.125 1.67C 0.224 0.4C0 0.65E 0.900 1.034 0.0C5 0.801 0.920-0.188 0.786
 0.387 1.243 0.875 0.989 0.718-0.152 0.00S 1.329 0.562 0.687 0.968 0.490
 0.16C 0.177-0.025 1.125 0.217 1.206 1.221-0.145-0.088 0.629-0.131 0.272
 0.388 0.772 1.046-0.067 0.76C 0.428 0.852 0.667 0.610 0.359 1.352 0.571
-0.01I-0.2C5 1.084 0.00S 0.517 0.438 1.C50 0.616 0.884 0.954-0.275 1.295
 0.346-1.018 1.049 0.417 1.23C 1.127 1.435 0.823-0.069 0.464 1.261-0.179
 0.812 0.537 0.875 0.190 0.707 0.857 0.C94 0.176 0.916 0.406 0.204 0.494
 1.709 0.133 0.460 0.828-0.174 0.457 0.584 0.832-0.026 1.265-0.232-0.373
-0.172 0.913 0.673 0.303 0.035 1.226-0.072 0.920 1.207-0.003 0.632 0.004
 0.951 0.3C7 0.798 1.479 0.196 1.058 0.873 0.C60 0.524 0.501 0.373 0.954
-0.C72 0.988 0.351 0.C53 0.24E 0.430-0.379 0.533 0.688 0.524 0.447 1.376
-0.263-0.064 0.301 1.486 0.351 0.806-0.374 0.735 0.958-0.262 0.332 0.963
559999
```

Figure 33.

Output

Description

The output from the program KOLM gives the statistics and probability statements described below, and in addition identifies the distribution functions being considered. Sorted samples are printed on option.

The following items are produced as output:

1. Z score, where

   $z = \sqrt{n}\, D_n$ for the one-sample test; n is the sample size, and D_n is the maximum difference between the empirical distribution function and the theoretical distribution function.

   $z = \sqrt{\frac{mn}{m+n}}\, D_{m,n}$ for the two-sample test;

   m is the size of the second sample; n is the size of the first sample; $D_{m,n}$ is the maximum difference between the two empirical distribution functions.

2. The probability of incorrectly rejecting the hypothesis of equality of distribution functions.

Sample

Sample output is shown in Figure 34.

```
UNIFORM TEST

 A 1 SAMPLE TEST WAS REQUESTED.


 THE SIZE OF SAMPLE 1 IS 498.


 THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)          NORMAL       DISTRIBUTION
 WITH MEAN       0.5000 AND VARIANCE        0.2500
 CAN BE REJECTED WITH PROBABILITY 0.000 OF BEING INCORRECT.  THE STATISTIC Z
 IS  3.5839E+00 FOR THIS SAMPLE.


 THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)      EXPONENTIAL     DISTRIBUTION
 WITH MEAN       0.5000 AND VARIANCE        1.0000
 CAN BE REJECTED WITH PROBABILITY 0.000 OF BEING INCORRECT.  THE STATISTIC Z
 IS  8.8033E+00 FOR THIS SAMPLE.


 THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)          CAUCHY       DISTRIBUTION
 WITH MEAN       0.5000 AND FIRST QUARTILE       -0.5000
 CAN BE REJECTED WITH PROBABILITY 0.000 OF BEING INCORRECT.  THE STATISTIC Z
 IS  7.8873E+00 FOR THIS SAMPLE.


 THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)         UNIFORM       DISTRIBUTION
 IN THE INTERVAL       0.0000 TO         1.0000 INCLUSIVE
 CAN BE REJECTED WITH PROBABILITY 0.989 OF BEING INCORRECT.  THE STATISTIC Z
 IS  4.4444E-01 FOR THIS SAMPLE.


   THE JOB WITH TITLE UNIFORM TEST        WAS COMPLETED.
```

Figure 34.

```
UNIFORM-GAUSS TEST

 A 2 SAMPLE TEST WAS REQUESTED.

 THE SIZE OF SAMPLE 2 IS 492.

 SORTED SAMPLE ONE AS FOLLOWS
    0.000    0.005    0.005    0.006    0.006    0.006    0.008    0.009    0.010    0.012
    0.012    0.018    0.019    0.019    0.021    0.022    0.022    0.025    0.029    0.033
    0.033    0.033    0.037    0.041    0.041    0.042    0.042    0.042    0.043    0.047
    0.053    0.054    0.055    0.058    0.062    0.065    0.068    0.073    0.073    0.077
    0.079    0.079    0.080    0.083    0.083    0.085    0.088    0.092    0.093    0.093
    0.097    0.098    0.102    0.102    0.103    0.111    0.112    0.113    0.113    0.113
    0.117    0.117    0.119    0.121    0.123    0.136    0.139    0.139    0.141    0.143
    0.148    0.151    0.153    0.154    0.156    0.157    0.158    0.161    0.163    0.164
    0.164    0.167    0.168    0.170    0.172    0.177    0.178    0.178    0.178    0.178
    0.181    0.181    0.183    0.188    0.190    0.190    0.193    0.195    0.195    0.196
    0.197    0.199    0.200    0.201    0.202    0.203    0.204    0.206    0.207    0.208
    0.208    0.209    0.215    0.220    0.224    0.225    0.228    0.231    0.231    0.232
    0.236    0.242    0.242    0.243    0.244    0.253    0.256    0.256    0.260    0.263
    0.263    0.264    0.264    0.266    0.268    0.269    0.272    0.275    0.277    0.282
    0.283    0.284    0.285    0.287    0.288    0.288    0.290    0.292    0.294    0.298
    0.299    0.301    0.302    0.302    0.302    0.303    0.304    0.311    0.311    0.312
    0.326    0.328    0.331    0.336    0.337    0.339    0.340    0.341    0.343    0.344
    0.345    0.348    0.348    0.349    0.349    0.353    0.360    0.363    0.364    0.365
    0.365    0.365    0.365    0.367    0.367    0.371    0.371    0.376    0.376    0.376
    0.377    0.377    0.381    0.381    0.382    0.383    0.388    0.390    0.397    0.400
    0.409    0.411    0.416    0.416    0.422    0.422    0.425    0.427    0.430    0.431
    0.434    0.434    0.441    0.442    0.444    0.447    0.450    0.450    0.450    0.453
    0.454    0.455    0.455    0.457    0.458    0.458    0.459    0.462    0.462    0.462
    0.463    0.463    0.467    0.469    0.470    0.471    0.472    0.476    0.477    0.478
    0.482    0.482    0.492    0.494    0.500    0.501    0.501    0.502    0.503    0.504
    0.508    0.512    0.514    0.514    0.515    0.516    0.516    0.518    0.518    0.520
    0.520    0.524    0.531    0.536    0.539    0.540    0.544    0.545    0.546    0.546
    0.554    0.555    0.556    0.556    0.557    0.560    0.561    0.562    0.565    0.570
    0.570    0.572    0.574    0.577    0.580    0.581    0.581    0.585    0.588    0.589
    0.591    0.592    0.594    0.594    0.595    0.595    0.595    0.596    0.597    0.603
    0.604    0.605    0.607    0.607    0.607    0.607    0.608    0.610    0.611    0.615
    0.617    0.622    0.622    0.624    0.629    0.630    0.632    0.634    0.634    0.636
    0.637    0.638    0.639    0.640    0.644    0.646    0.652    0.652    0.654    0.657
    0.659    0.662    0.662    0.664    0.664    0.665    0.666    0.666    0.667    0.668
    0.668    0.670    0.671    0.672    0.677    0.679    0.683    0.686    0.688    0.692
    0.694    0.694    0.696    0.697    0.698    0.699    0.699    0.701    0.702    0.707
    0.708    0.708    0.709    0.715    0.722    0.724    0.725    0.726    0.728    0.733
    0.734    0.737    0.741    0.742    0.743    0.745    0.745    0.746    0.750    0.751
    0.752    0.753    0.754    0.759    0.761    0.761    0.766    0.767    0.783    0.785
    0.785    0.786    0.787    0.790    0.793    0.793    0.795    0.801    0.801    0.803
    0.804    0.805    0.806    0.810    0.810    0.810    0.812    0.814    0.816    0.816
    0.816    0.817    0.827    0.829    0.833    0.835    0.836    0.837    0.840    0.842
    0.842    0.843    0.843    0.844    0.845    0.846    0.851    0.859    0.860    0.860
    0.864    0.867    0.868    0.870    0.870    0.876    0.880    0.882    0.882    0.888
    0.889    0.890    0.892    0.893    0.895    0.904    0.907    0.909    0.909    0.913
    0.913    0.918    0.919    0.923    0.923    0.924    0.926    0.928    0.928    0.931
    0.931    0.933    0.936    0.939    0.940    0.945    0.948    0.950    0.951    0.953
    0.953    0.955    0.956    0.962    0.963    0.963    0.964    0.965    0.967    0.969
    0.969    0.972    0.973    0.973    0.976    0.978    0.982    0.982    0.984    0.984
    0.985    0.988    0.990    0.991    0.994    0.995    0.996    0.996
 SORTED SAMPLE TWO AS FOLLOWS
   -1.157   -1.018   -0.737   -0.718   -0.643   -0.602   -0.552   -0.541   -0.476   -0.475
   -0.469   -0.467   -0.410   -0.357   -0.391   -0.381   -0.379   -0.374   -0.373   -0.340
   -0.340   -0.324   -0.313   -0.302   -0.301   -0.299   -0.297   -0.297   -0.283   -0.280
   -0.276   -0.275   -0.264   -0.263   -0.262   -0.249   -0.232   -0.227   -0.206   -0.205
   -0.188   -0.183   -0.179   -0.174   -0.172   -0.159   -0.152   -0.145   -0.144   -0.131
   -0.124   -0.096   -0.088   -0.077   -0.072   -0.072   -0.069   -0.067   -0.064   -0.064
   -0.063   -0.055   -0.038   -0.037   -0.026   -0.025   -0.023   -0.023   -0.021   -0.020
   -0.012   -0.011   -0.011   -0.011   -0.010   -0.004   -0.003    0.000    0.004    0.005
    0.007    0.007    0.009    0.009    0.012    0.025    0.035    0.035    0.037    0.037
    0.048    0.051    0.053    0.053    0.057    0.060    0.064    0.068    0.071    0.078
    0.083    0.088    0.091    0.094    0.098    0.099    0.102    0.109    0.110    0.113
    0.118    0.124    0.125    0.126    0.131    0.133    0.143    0.147    0.149    0.154
    0.160    0.174    0.176    0.177    0.181    0.185    0.190    0.191    0.191    0.196
    0.196    0.196    0.198    0.198    0.203    0.203    0.204    0.204    0.214    0.217
    0.222    0.222    0.224    0.226    0.227    0.231    0.234    0.236    0.248    0.250
    0.257    0.259    0.266    0.272    0.273    0.284    0.287    0.288    0.288    0.297
    0.301    0.301    0.302    0.302    0.303    0.305    0.307    0.310    0.313    0.313
    0.315    0.317    0.317    0.332    0.341    0.346    0.348    0.351    0.351    0.358
    0.359    0.362    0.365    0.372    0.373    0.374    0.374    0.375    0.376    0.378
    0.381    0.387    0.387    0.388    0.388    0.391    0.394    0.399    0.400    0.400
    0.401    0.404    0.406    0.406    0.411    0.414    0.417    0.418    0.418    0.421
    0.422    0.422    0.428    0.430    0.433    0.436    0.438    0.445    0.445    0.446
    0.446    0.447    0.448    0.454    0.457    0.457    0.460    0.462    0.464    0.467
    0.484    0.487    0.490    0.494    0.494    0.497    0.499    0.501    0.506    0.508
    0.512    0.514    0.515    0.515    0.520    0.524    0.524    0.524    0.533    0.533
    0.536    0.536    0.537    0.547    0.559    0.559    0.562    0.563    0.563    0.566
    0.571    0.573    0.576    0.583    0.583    0.583    0.584    0.584    0.586    0.592
    0.601    0.604    0.606    0.606    0.607    0.610    0.610    0.616    0.619    0.622
    0.624    0.629    0.630    0.632    0.632    0.633    0.634    0.635    0.642    0.643
    0.643    0.648    0.653    0.656    0.657    0.658    0.659    0.660    0.663    0.667
    0.673    0.675    0.675    0.680    0.683    0.685    0.686    0.686    0.687    0.687
    0.688    0.690    0.693    0.694    0.695    0.697    0.699    0.699    0.702    0.702
    0.704    0.704    0.707    0.708    0.714    0.718    0.719    0.733    0.735    0.740
    0.743    0.760    0.761    0.762    0.763    0.764    0.770    0.772    0.776    0.782
    0.786    0.787    0.789    0.790    0.798    0.801    0.801    0.806    0.812    0.816
    0.818    0.823    0.828    0.828    0.829    0.832    0.837    0.838    0.839    0.840
    0.849    0.849    0.850    0.852    0.852    0.857    0.858    0.861    0.867    0.868
    0.873    0.874    0.875    0.875    0.880    0.881    0.884    0.884    0.887    0.898
    0.899    0.900    0.902    0.910    0.913    0.916    0.916    0.916    0.917    0.920
    0.920    0.930    0.933    0.936    0.937    0.938    0.951    0.951    0.954    0.954
    0.958    0.963    0.963    0.968    0.975    0.983    0.985    0.988    0.989    0.994
    0.996    1.000    1.004    1.022    1.024    1.034    1.035    1.046    1.049    1.049
    1.050    1.053    1.058    1.063    1.067    1.070    1.075    1.075    1.084    1.086
    1.087    1.108    1.110    1.116    1.119    1.120    1.125    1.127    1.132    1.145
    1.149    1.156    1.163    1.173    1.176    1.176    1.177    1.184    1.188    1.189
    1.190    1.203    1.206    1.207    1.217    1.217    1.221    1.226    1.230    1.238
    1.243    1.253    1.255    1.261    1.261    1.265    1.270    1.295    1.313    1.317
    1.329    1.330    1.339    1.352    1.356    1.366    1.376    1.384    1.394    1.394
    1.435    1.451    1.479    1.486    1.493    1.598    1.600    1.644    1.670    1.709
    1.799    1.838

 THE HYPOTHESIS THAT THE TWO SAMPLES ARE FROM THE  SAME POPULATION CAN BE REJECTED WITH (ASYMPTOTIC)
 PROBABILITY OF BEING INCORRECT OF 0.000. THE STATISTIC Z IS   2.590OE+00 FOR THESE SAMPLES.

   THE JOB WITH TITLE UNIFORM-GAUSS TEST WAS COMPLETED.

         END OF SAMPLE PROGRAM
```

Figure 34. (Continued)

Program Modifications

1. Program capacity may be increased or decreased by making changes in the allocation statements. If this is done, the limits on the DO statements may require modification, as will be the case if data formats require changing. It is also possible that output formats may require changes.
2. Any modifications to the subroutine KLMO in terms of added continuous pdf's should be reflected in the program KOLM. It may be necessary to:
   a. Modify the declaration of DIST (5, 3), which contains the switches calling on pdf's and also contains the parameters u and s used by KLMO.
   b. Modify the pdf titling cards numbered KOLM 230 through 270.
   c. Modify the section of the program from S70 through S100 to reflect changes a and b above. These statements call KLMO to perform tests and output results.
3. List of variables in KOLM, and their usage:

D -	Temporary vector used in reading samples
DAS2 -	Job Control Card name (----)
DIST -	5 by 3 matrix. The five elements in column 1 are switches that allow the 5 pdf's to be used in one-sample tests. Columns 2 and 3 contain the parameters u and s for the associated test.
ERROR -	Error (in using KLMO, used for skipping the test concerned)
I -	Counter used to print correct pdf name for pdf used in the test
IFL -	Error indicator (job deck error)
IES -	Error (in using KLMO, used for error message)
IO -	Switch (used for printing samples)
IR -	Number of samples to be read in current job
IS -	Number of samples to be used in current job (1 or 2)
M -	Size of the second sample
N -	Size of first sample
P -	Probability of being incorrect if hypothesis is rejected
S2 -	Temporary storage for u and s output
TIT1 -	Current pdf names
TITLE -	Job title
X -	Sample 1
Y -	Sample 2
Z -	Z statistic from KLMO or KLM2

Operating Instructions

This sample program is a standard PL/I program and needs no special operating instructions. Data set SYSIN is used for input; data set SYSPRINT, for output.

Error Messages

The following error conditions will result in messages, followed by the action specified:

1. Neither a one-nor two-sample test is requested, or the size of either sample is larger than 500 -- CC.21, CONTROL CARD, INCORRECT, OR SAMPLE SIZE TOO LARGE. JOB IGNORED. Action: Cards are read until a new job control card is found, or until the hopper is empty.
2. Sample size is less than 100 (not an error) -- NOTE THE REMARKS CONCERNING ASYMPTOTIC RESULTS AND SAMPLE SIZE IN SUBROUTINE SMIR. Action: none. Job continues.
3. The requirement of subroutine KLMO that certain parameters be nonzero or positive is violated -- AT LEAST ONE (S) ENTRY PARAMETER FOR THE SUBROUTINE KLMO WAS INCORRECT. THE TEST FOR THE ASSOCIATED CONTINUOUS PDF WAS IGNORED. Action: All tests are made for cases where the parameter s was correct.
4. A case in which an error requires aborting the job, and the succeeding job in the job stack requests a two-sample test where the second sample is to be compared with a (first) sample, which was read on the previous job -- THIS JOB CALLS FOR THE USE OF A PREVIOUSLY READ SAMPLE, AND THE PREVIOUS JOB WAS IGNORED BECAUSE OF ERRORS. JOB IGNORED. Action: Cards are read until a new job control card is found, or until the hopper is empty.
5. The job control card preceding a job is not there or is incorrect -- FIRST CARD IN JOB DECK (JOB CONTROL CARD) IS INCORRECT. Action: Cards are read until a new job control card is found, or until the hopper is empty.

Timing

The execution time of this program on a System /360 Model 40, using a 2540 Card Reader as input and a 1403 Printer, Model N1, as output, is 35 seconds for job 1 and 55 seconds for job 2.

```
KOLM..                                                                KOLM  10
/*********************************************************************/KOLM  20
/*                                                                   */KOLM  30
/* THE PURPOSE OF THIS ROUTINE IS TO:                                */KOLM  40
/*      (1) READ THE CONTROL CARD FOR A ONE OR TWO SAMPLE TEST.      */KOLM  50
/*      (2) READ THE SAMPLE DATA AND DETERMINE THE SAMPLE SIZES.     */KOLM  60
/*      (3) CALL SMIR, KLM0, AND KLM2 FOR CALCULATION OF             */KOLM  70
/*          PROBABILITIES.                                           */KOLM  80
/*      (4) PRINT RESULTS.                                           */KOLM  90
/*                                                                   */KOLM 100
/*********************************************************************/KOLM 110
   PROCEDURE OPTIONS (MAIN),.                                         KOLM 120
   DECLARE                                                            KOLM 130
        (DASH,DAS2) CHARACTER (4),                                    KOLM 140
        (I,J,K,L,M,N,IS,IR,IO,IFL,E) FIXED BINARY,                    KOLM 150
        (DIST(5,3),D(12),X(501),Y(501),P,Z,S2) FLOAT BINARY,          KOLM 160
        TITLE CHARACTER (20),                                         KOLM 170
        TIT1(5) CHARACTER (16),                                       KOLM 180
        IES CHARACTER (1),                                            KOLM 190
        ERROR EXTERNAL CHARACTER (1),.                                KOLM 200
   ON ENDFILE(SYSIN) GO TO S200,.                                     KOLM 210
   SW   =0,.                                                          KOLM 220
   IFL  =0,.                                                          KOLM 230
   DASH ='----',.                       /* INITIALIZE NAMES         */KOLM 240
   TIT1(1)   ='     NORMAL     ',.      /* AND JOB CONTROL CARD     */KOLM 250
   TIT1(2)   =' EXPONENTIAL    ',.                                    KOLM 260
   TIT1(3)   ='     CAUCHY     ',.                                    KOLM 270
   TIT1(4)   ='    UNIFORM     ',.                                    KOLM 280
   TIT1(5)   =' USER-SPECIFIED ',.                                    KOLM 290
                                                                      KOLM 300
S10..                                                                 KOLM 310
   GET EDIT(DAS2,E)(A(4),X(75),F(1)),.                                KOLM 320
   IF DASH=DAS2                                                       KOLM 330
   THEN                                 /* READ TITLE AND           */KOLM 340
                                        /* PROGRAM PARAMETERS       */KOLM 350
S20..                                                                 KOLM 360
        DO,.                                                          KOLM 370
        GET EDIT(TITLE,IS,IR,IO,DIST(*,*),E)(A(20),3 F(1),5(F(1),2 F(5)KOLM 380
            ),X(1),F(1)),.                                            KOLM 390
        IES  ='0',.                                                   KOLM 400
        PUT EDIT (TITLE)(A(20)) PAGE,.                                KOLM 410
        PUT EDIT (' A',IS,' SAMPLE TEST WAS REQUESTED.')(SKIP(3),A(2), KOLM 420
            F(2),A(27)),.                                             KOLM 430
        IF SW=0 AND IS=2 AND IR=1                                     KOLM 440
        THEN DO,.                                                     KOLM 450
             PUT EDIT(' FIRST JOB REQUIRES PREVIOUS DATA FOR A TWO SAM'KOLM 460
                 ,'PLE TEST.')(SKIP(3),A(47),A(9)),.                  KOLM 470
             SW   =1,.                                                KOLM 480
             GO TO S40,.                                              KOLM 490
             END,.                                                    KOLM 500
        SW   =1,.                                                     KOLM 510
        IF IR=0                         /* NO. OF SAMPLES DECISION  */KOLM 520
        THEN IF IS GE 1                                               KOLM 530
             THEN GO TO S140,.                                        KOLM 540
             ELSE                       /* NO. OF SAMPLES WRONG     */KOLM 550
S30..                                                                 KOLM 560
                  DO,.                                                KOLM 570
                  PUT EDIT(' CC.21 OF THE PROGRAM CONTROL CARD IS INCO'KOLM 580
                      ,'RRECT.  JOB IGNORED.')(SKIP(3),A(42),A(20)),. KOLM 590
S40..                                                                 KOLM 600
                  GET EDIT(DAS2,E)(A(4),X(75),F(1)),.                 KOLM 610
                  IF DASH=DAS2                                        KOLM 620
                  THEN DO,.                                           KOLM 630
                       IFL  =1,.                                      KOLM 640
                       GO TO S20,.                                    KOLM 650
                       END,.                                          KOLM 660
                  ELSE GO TO S40,.                                    KOLM 670
                  END,.                                               KOLM 680
        ELSE IF IFL NE 0                                              KOLM 690
             THEN DO,.                  /* ERROR IN PREVIOUS JOB    */KOLM 700
                  PUT EDIT(' THIS JOB CALLS FOR THE USE OF A PREVIOUSL'KOLM 710
                      ,'Y READ SAMPLE, AND THE PREVIOUS JOB WAS IGNORE'KOLM 720
                      ,'D BECAUSE OF ERRORS.','JOB IGNORED.')(SKIP(3), KOLM 730
                      A(42),A(46),A(20),SKIP,A(13)),.                 KOLM 740
                  GO TO S40,.                                         KOLM 750
                  END,.                                               KOLM 760
             ELSE GO TO S180,.                                        KOLM 770
        END,.                                                         KOLM 780
   ELSE DO,.                                                          KOLM 790
        PUT EDIT(' FIRST CARD IN JOB DECK (JOB CONTROL CARD) IS INCORR'KOLM 800
            ,'ECT.')(SKIP(3),A(52),A(4)),.                            KOLM 810
        GO TO S40,.                                                   KOLM 820
        END,.                                                         KOLM 830
S50..                                                                 KOLM 840
   IF IS=2                                                            KOLM 850
   THEN GO TO S180,.                                                  KOLM 860
   ELSE IF IS GT 2                                                    KOLM 870
        THEN GO TO S30,.                                              KOLM 880
        ELSE GO TO S65,.                                              KOLM 890
S60..                                                                 KOLM 900
   IF IS LE 1                           /* ONE SAMPLE TEST USING ALL*/KOLM 910
   THEN DO,.                            /* DISTRIBUTIONS REQUESTED  */KOLM 920
S65..                                                                 KOLM 930
        DO I=1 TO 5,.                                                 KOLM 940
        IF DIST(I,1) NE 0                                             KOLM 950
        THEN GO TO S70,.                                              KOLM 960
        END,.                                                         KOLM 970
        PUT EDIT(' NO PDF COMPARISON IS ASKED FOR.')(SKIP(3),A(32)),. KOLM 980
S70..                                                                 KOLM 990
        DO I=1 TO 5 ,.                                                KOLM1000
        IF DIST(I,1) = 1                                              KOLM1010
        THEN CALL KLM0(X,N,Z,P,I,DIST(I,2),DIST(I,3)),.               KOLM1020
        IF ERROR='0' OR ERROR='3'                                     KOLM1030
        THEN                                                          KOLM1040
             DO,.                       /* OUTPUT RESULTS           */KOLM1050
             PUT EDIT(' THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)   'KOLM1060
                ,TIT1(I),' DISTRIBUTION' )(SKIP(3),A(47),A(16),A(13)) KOLM1070
                ,.                                                    KOLM1080
             IF I LT 3                  /* PREPARE OUTPUT           */KOLM1090
             THEN DO,.                                                KOLM1100
                  S2   =DIST(I,3)**2,.                                KOLM1110
                  PUT EDIT(' WITH MEAN',DIST(I,2),' AND VARIANCE',S2) KOLM1120
                      (SKIP,A(10),F(13,4),A(13),F(13,4)),.            KOLM1130
                  GO TO S80,.                                         KOLM1140
                  END,.                                               KOLM1150
             ELSE IF I=3                                              KOLM1160
                  THEN DO,.                                           KOLM1170
                       S2   =DIST(I,2)-DIST(I,3),.                    KOLM1180
                       PUT EDIT(' WITH MEAN',DIST(I,2),' AND FIRST ', KOLM1190
                           'QUARTILE',S2)(SKIP,A(10),F(13,4),A(11),   KOLM1200
                           A(8),F(13,4)),.                            KOLM1210
                       GO TO S80,.                                    KOLM1220
                       END,.                                          KOLM1230
                  ELSE IF I LE 4                                      KOLM1240
                       THEN DO,.                                      KOLM1250
                            PUT EDIT(' IN THE INTERVAL',DIST(I,2),' TO'KOLM1260
                                ,DIST(I,3),' INCLUSIVE')(SKIP,A(16),  KOLM1270
                                F(13,4),A(3),F(13,4),A(10)),.         KOLM1280
S80..                                                                 KOLM1290
                                PUT EDIT(' CAN BE REJECTED WITH PROBABILIT'KOLM1300
                                    ,'Y',P,' OF BEING INCORRECT.  THE STAT'KOLM1310
                                    ,'ISTIC Z',' IS',Z,' FOR THIS SAMPLE.')KOLM1320
                                    (SKIP,A(32),A(1),F(6,3),A(30),A(7),SKIPKOLM1330
                                    ,A(3),E(12,4),A(17)),.                KOLM1340
                            END,.                                     KOLM1350
                       GO TO S90,.                                    KOLM1360
                  END,.                                               KOLM1370
             ELSE IES  =ERROR,.                                       KOLM1380
S90..                                                                 KOLM1390
        END,.                                                         KOLM1400
        END,.                                                         KOLM1410
   ELSE GO TO S110,.                                                  KOLM1420
   IF IO NE 0                           /* OUTPUT SAMPLE ONE DECISION*/KOLM1430
   THEN DO,.                                                          KOLM1440
        PUT EDIT (' SORTED SAMPLE ONE FOLLOWS')(SKIP(3),A(26)),.      KOLM1450
        PUT EDIT ((X(J) DO J=1 TO N))(SKIP,10 (F(10,3))),.            KOLM1460
        END,.                                                         KOLM1470
   IF IES    ='0'                                                     KOLM1480
   THEN                                                               KOLM1490
S100..                                                               KOLM1500
        DO,.                                                          KOLM1510
        IFL  =0,.                                                     KOLM1520
        PUT EDIT ('   THE JOB WITH TITLE',TITLE,' WAS COMPLETED.')    KOLM1530
            (SKIP(3),A(22),A(18),A(15)),.                             KOLM1540
        IF ERROR='3'                                                  KOLM1550
        THEN PUT EDIT ('NOTE THE REMARKS CONCERNING ASYMPTOTIC RESULTS'KOLM1560
             ,' AND SAMPLE SIZE IN SUBROUTINE SMIR.')(SKIP(3),A(46),  KOLM1570
             A(36)),.                                                 KOLM1580
        GO TO S10,.                                                   KOLM1590
        END,.                                                         KOLM1600
   ELSE DO,.                                                          KOLM1610
        PUT EDIT(' AT LEAST ONE (S) ENTRY PARAMETER FOR THE SUBROUTINE'KOLM1620
            ,' KLM0 WAS INCORRECT. ',' TEST FOR THE ASSOCIATED CONTINU'KOLM1630
            ,'OUS PDF WAS IGNORED.')(SKIP(3),A(52),A(21),SKIP,A(32),  KOLM1640
            A(20)),.                                                  KOLM1650
        GO TO S100,.                                                  KOLM1660
        END,.                                                         KOLM1670
S110..                                                               KOLM1680
   CALL KLM2(X,Y,N,M,Z,P),.             /* TWO SAMPLE TEST          */KOLM1690
   IF IO=0                              /* OUTPUT SAMPLES DECISION  */KOLM1700
   THEN                                                               KOLM1710
S120..                                                               KOLM1720
        DO,.                                                          KOLM1730
        PUT EDIT(' THE HYPOTHESIS THAT THE TWO SAMPLES ARE FROM THE ', KOLM1740
            ' SAME POPULATION CAN BE REJECTED WITH (ASYMPTOTIC)',     KOLM1750
            ' PROBABILITY OF BEING INCORRECT OF',P,'. THE STATISTIC Z '
            ,'IS ',Z,' FOR THESE SAMPLES.')(SKIP(3),A(50),A(50),SKIP, KOLM1760
            A(34),F(6,3),A(18),A(3),E(12,4),A(19)),.                  KOLM1770
        GO TO S100,.                                                  KOLM1780
        END,.                                                         KOLM1790
   ELSE                                                               KOLM1800
S130..                                                               KOLM1810
        DO,.                                                          KOLM1820
        PUT EDIT (' SORTED SAMPLE ONE AS FOLLOWS')(SKIP(3),A(29)),.   KOLM1830
        PUT EDIT ((X(J) DO J=1 TO N))(SKIP,10 F(10,3)),.              KOLM1840
        PUT EDIT (' SORTED SAMPLE TWO AS FOLLOWS')(SKIP(3),A(29)),.   KOLM1850
        PUT EDIT ((Y(J) DO J=1 TO M))(SKIP,10 F(10,3)),.              KOLM1860
        GO TO S120,.                                                  KOLM1870
        END,.                                                         KOLM1880
S140..                                                               KOLM1890
   N    =0,.                            /* READ FIRST SAMPLE        */KOLM1900
        DO I=1 TO 50,.                                                KOLM1910
        GET EDIT((D(K) DO K=1 TO 12),E)(12 F(6),X(7),F(1)),.          KOLM1920
             DO J=1 TO 12,.                                           KOLM1930
             IF D(J) = 999999.0         /* CHECK FOR END OF SAMPLE  */KOLM1940
             THEN GO TO S170,.                                        KOLM1950
             N    =N+1,.                                              KOLM1960
             IF N GE 501                /* MAXIMUM SAMPLE SIZE      */KOLM1970
             THEN                                                     KOLM1980
S150..                                                               KOLM1990
                  DO,.                                                KOLM2000
                  PUT EDIT (' SAMPLE SIZE IS TOO LARGE.  JOB IGNORED.')KOLM2010
                      (SKIP(3),A(43)),.                               KOLM2020
                  GO TO S40,.                                         KOLM2030
                  END,.                                               KOLM2040
             X(N) =D(J),.               /* PLACE SAMPLE IN X        */KOLM2050
             END,.                                                    KOLM2060
        END,.                                                         KOLM2070
S170..                                                               KOLM2080
   PUT EDIT(' THE SIZE OF SAMPLE 1 IS',N,'.')(SKIP(3),A(24),F(4),A(1)) KOLM2090
      ,.                                                              KOLM2100
   GO TO S50,.                                                        KOLM2110
S180..                                                               KOLM2120
   M    =0,.                            /* READ SECOND SAMPLE       */KOLM2130
        DO I=1 TO 50,.                                                KOLM2140
        GET EDIT((D(K) DO K=1 TO 12),E)(12 F(6),X(7),F(1)),.          KOLM2150
             DO J=1 TO 12,.                                           KOLM2160
             IF D(J)=999999.0           /* CHECK FOR END OF SAMPLE  */KOLM2170
             THEN GO TO S190,.                                        KOLM2180
             M    =M+1,.                                              KOLM2190
             IF M GE 501                /* MAX SIZE OF SAMPLE       */KOLM2200
             THEN DO,.                                                KOLM2210
                  PUT EDIT(' SAMPLE SIZE IS TOO LARGE.  JOB IGNORED.') KOLM2220
                      (SKIP(3),A(43)),.                               KOLM2230
                  GO TO S40,.                                         KOLM2240
                  END,.                                               KOLM2250
             Y(M) =D(J),.               /* PLACE SAMPLE IN Y        */KOLM2260
             END,.                                                    KOLM2270
        END,.                                                         KOLM2280
S190..                                                               KOLM2290
   PUT EDIT(' THE SIZE OF SAMPLE 2 IS',M,'.')(SKIP(3),A(24),F(4),A(1)) KOLM2300
      ,.                                                              KOLM2310
   GO TO S60,.                                                        KOLM2320
S200..                                                               KOLM2330
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                 KOLM2340
       (SKIP(2),COLUMN(10),A),.                                       KOLM2350
   END,.                                /* END OF PROCEDURE KOLM    */KOLM2360
```

TRIPLE EXPONENTIAL SMOOTHING EXPN

Problem Description

Given a time series X, a smoothing constant, and three coefficients of the prediction equation, this sample program finds the triple exponentially smoothed series S of the time series X.

Program

Description

The sample program for triple exponential smoothing consists of the main program, named EXPN, a special input routine, named DAT3, and one subroutine from the Scientific Subroutine Package: EXSM.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

(12F(6,0)) format for input data cards. Therefore, if a problem satisfies the above conditions, the sample program need not be modified. However, if input data cards are prepared using a different format, the input format in the input routine DAT3 must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, EXPN. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem number (may be alphameric)	SAMPLE
7-10	Number of data points in a given time series	0038
11-15	Smoothing constant, α ($0.0 < \alpha < 1.0$)	0.1
16-25	First coefficient (A) of the prediction equation	0.0
26-35	Second coefficient (B) of the prediction equation	0.0
36-45	Third coefficient (C) of the prediction equation	0.0

Smoothing constant and three coefficients must be keypunched with decimal points.

Leading zeros do not have to be keypunched.

Data Cards

Time series data are keypunched using the format (12 F(6,0)). This format assumes that each data point is keypunched in a six-column field, with twelve fields per card.

Data Setup

The deck setup is shown in Figure 35.

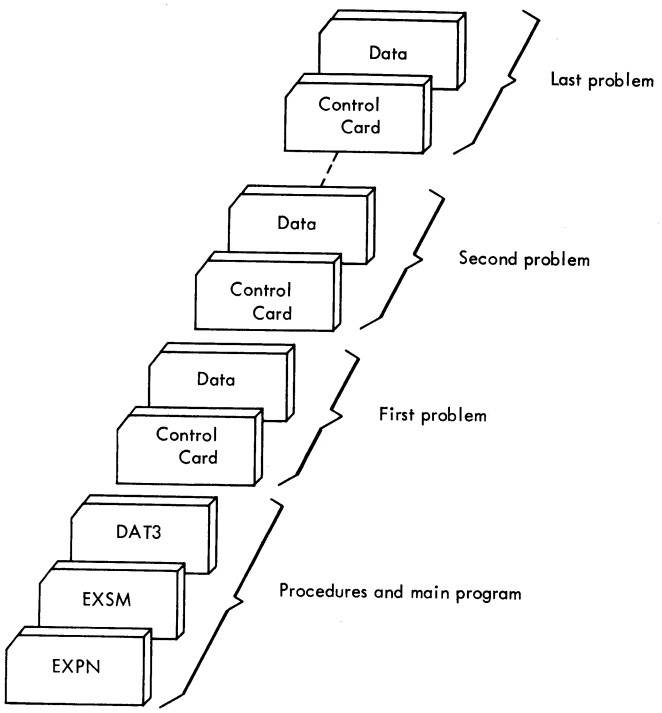


Figure 35.

Sample

The listing of input cards for the sample problem is shown in Figure 36.

```
SAMPLE  38   .1        0.C       0.C       C.C
   430  426  422  419  414  413  412  409  411  417  422  430        10
   438  441  447  455  461  453  448  449  454  463  470  472        20
   476  481  483  487  491  492  485  486  482  479  479  476        30
   472  470                                                         40
                                                                    50
```

Figure 36.

Output

Description

The output of the sample program for triple exponential smoothing includes:

1. Original and updated coefficients
2. Time series as input and triple exponentially smoothed time series

Sample

The output listing for the sample problem is shown in Figure 37.

```
TRIPLE EXPONENTIAL SMOOTHING.....SAMPLE

NUMBER OF DATA POINTS     38
SMOOTHING CONSTANT     C.1CC

COEFFICIENTS          A              B              C

ORIGINAL           C.CCCCC        C.CCCCC        C.CCCCC

UPDATE          484.8C17E         1.71309        C.C4166


                              SMOOTHED DATA
        INPUT DATA             (FORECAST)
          43C.CCCCC              430.CCCCC
          426.CCCCC              426.CCCCC
          422.CCCCC              422.CCCCC
          419.CCCCC              418.CCCCC
          414.CCCCC              414.29980
          413.CCCCC              41C.23950
          412.CCCCC              407.08960
          4C9.CCCCC              4C4.66797
          411.CCCCC              4C2.22363
          417.CCCCC              4C1.25049
          422.CCCCC              402.64575
          43C.CCCCC              4C5.61621
          438.CCCCC              41C.71338
          441.CCCCC              417.46948
          447.CCCCC              423.99829
          455.CCCCC              431.18286
          461.CCCCC              439.43359
          4F3.CCCCC              447.87866
          448.CCCCC              452.21558
          449.CCCCC              454.1C522
          454.CCCCC              455.8C713
          463.CCCCC              458.54614
          47C.CCCCC              463.3C518
          472.CCCCC              469.C6445
          476.CCCCC              474.C9521
          481.CCCCC              479.11C35
          483.CCCCC              484.38623
          487.CCCCC              486.94629
          491.CCCCC              493.5C854
          492.CCCCC              498.C5444
          485.CCCCC              501.66992
          486.CCCCC              5C2.12549
          482.CCCCC              5C2.44434
          479.CCCCC              501.16724
          475.CCCCC              498.92749
          476.CCCCC              496.84155
          472.CCCCC              494.CC8C6
          47C.CCCCC              49C.3C42C
```

Figure 37.

Program Modifications

Input data in a different format can also be handled by providing a different format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

Changes in the input format statement of the input routine DAT3.

Only the format statement and the variables per card count indicator (NF), which appears in subroutine DAT3, can be changed. Since sample data are three-digit numbers, rather than using six-column fields, as in the sample problem, each data point might have been keypunched in a three-column field, with 24 fields per card. If so, the format is changed to (24 F(3,0)) and the variables per card count indicator (NF) is changed to agree with the number of variables per data card.

Operating Instructions

The sample program for triple exponential smoothing is a standard PL/I program. Special operating instructions are not required. Data set SYSIN is used for input; data set SYSPRINT, for output.

Timing

The execution of this sample program on a System/360 Model 40, using a 2540 Card Reader as input and a 1403 Printer, Model N1, as output, is 33 seconds.

```
EXPN..                                                                  EXPN  10
/*************************************************************************/EXPN  20
/*                                                                       */EXPN  30
/*      TO READ THE PROBLEM PARAMETER CARD AND A TIME SERIES, CALL       */EXPN  40
/*      THE PROCEDURE EXSM TO SMOOTH THE TIME SERIES, AND PRINT THE      */EXPN  50
/*      RESULT.                                                          */EXPN  60
/*                                                                       */EXPN  70
/*************************************************************************/EXPN  80
   PROCEDURE OPTIONS (MAIN),.                                           EXPN  90
   DECLARE                                                              EXPN 100
         (A,B,C,AL) FLOAT BINARY,                                       EXPN 110
         (I,NX)                                                         EXPN 120
         FIXED BINARY,                                                  EXPN 130
         ERROR EXTERNAL CHARACTER(1),                                   EXPN 140
         CH  CHARACTER (80),                                            EXPN 150
         PR1 CHARACTER (6),.                                            EXPN 160
/*                                                                      */EXPN 170
   ON ENDFILE (SYSIN) GO TO EXIT,.                                      EXPN 180
                                                                        EXPN 190
S100..                                                                  EXPN 200
   GET EDIT (CH) (A(80)),.          /* READ PROBLEM PARAMETER CARD     */EXPN 210
   GET STRING (CH) EDIT (PR1,NX,AL,A,B,C)                               EXPN 220
         (A(6),F(4),F(5,0),3 F(10,0)),.                                 EXPN 230
/*                                                                      */EXPN 240
/*      PR1.....PROBLEM NUMBER (MAY BE ALPHAMERIC)                      */EXPN 250
/*      NX......NUMBER OF DATA POINTS IN TIME SERIES                    */EXPN 260
/*      AL......SMOOTHING CONSTANT                                      */EXPN 270
/*      A,B,C...COEFFICIENTS OF THE PREDICTION EQUATION                 */EXPN 280
/*                                                                      */EXPN 290
   PUT EDIT ('TRIPLE EXPONENTIAL SMOOTHING.....',PR1) (PAGE,SKIP(4),    EXPN 300
         COLUMN(1C),A,A),.                                              EXPN 310
   PUT EDIT ('NUMBER OF DATA POINTS',NX) (SKIP(2),COLUMN(1C),A,F(6)),.  EXPN 320
   PUT EDIT ('SMOOTHING CONSTANT',AL) (SKIP,COLUMN(10),A,F(9,3)),.      EXPN 330
/*                                                                      */EXPN 340
/*      PRINT ORIGINAL COEFFICIENTS                                     */EXPN 350
/*                                                                      */EXPN 360
   PUT EDIT ('CCEFFICIENTS','A','B','C') (SKIP(2),COLUMN(10),A,X(9),A,  EXPN 370
         X(14),A,X(14),A),.                                             EXPN 380
   PUT EDIT ('ORIGINAL',A,B,C) (SKIP(2),COLUMN(10),A,F(19,5),           EXPN 390
         2 F(15,5)),.                                                   EXPN 400
ONE..                                                                   EXPN 410
   BEGIN,.                                                              EXPN 420
   DECLARE                                                              EXPN 430
         (X(NX),S(NX)) FLOAT BINARY,.                                   EXPN 440
   CALL DAT3 (NX,X),.               /* READ TIME SERIES DATA          */EXPN 450
   CALL EXSM (X,NX,AL,A,B,C,S),.                                        EXPN 460
   IF ERROR NE '0'                                                      EXPN 470
   THEN DO,.                                                            EXPN 480
         PUT EDIT ('IN ROUTINE EXSM ERROR CODE = ',ERROR)               EXPN 490
               (SKIP(2),COLUMN(1C),A,A(1)),.                            EXPN 500
         GO TO S10C,.                                                   EXPN 510
         END,.                                                          EXPN 520
/*                                                                      */EXPN 530
/*      PRINT UPDATED COEFFICIENTS                                      */EXPN 540
/*                                                                      */EXPN 550
   PUT EDIT ('UPDATE',A,B,C) (SKIP(2),COLUMN(10),A,F(20,5),             EXPN 560
         2 F(15,5)),.                                                   EXPN 570
/*                                                                      */EXPN 580
/*      PRINT INPUT AND SMOOTHED DATA                                   */EXPN 590
/*                                                                      */EXPN 600
   PUT EDIT ('SMOOTHED DATA','INPUT DATA','(FORECAST)')                 EXPN 610
         (SKIP(3),COLUMN(39),A,SKIP,COLUMN(17),A,X(13),A),.             EXPN 620
   PUT EDIT ((X(I),S(I) DO I= 1 TO NX)) (SKIP,COLUMN(10),F(17,5),       EXPN 630
         X(8),F(15,5)),.                                                EXPN 640
   END,.                                                                EXPN 650
   GO TO S100,.                                                         EXPN 660
EXIT,.                                                                  EXPN 670
   PUT FILE (SYSPRINT) EDIT ('END OF SAMPLE PROGRAM')                   EXPN 680
         (SKIP(5),COLUMN(10),A),.                                       EXPN 690
   END,.                            /*END OF PROCEDURE EXPN           */EXPN 700
```

```
DAT3..                                                                  DAT3  10
/*************************************************************************/DAT3  20
/*                                                                       */DAT3  30
/*      TO READ A VECTOR OF FLOATING POINT DATA.                         */DAT3  40
/*                                                                       */DAT3  50
/*************************************************************************/DAT3  60
   PROCEDURE (M,D),.                                                    DAT3  70
   DECLARE                                                              DAT3  80
         CH CHARACTER(80),                                              DAT3  90
         (I,M,N,N1,N2)                                                  DAT3 100
         FIXED BINARY,                                                  DAT3 110
         D(M) FLOAT BINARY,.                                            DAT3 120
/*                                                                      */DAT3 130
/*      N EQUAL THE NUMBER OF DATA POINTS PER 80 COLUMNS OF A DATA      */DAT3 140
/*      CARD.                                                           */DAT3 150
/*                                                                      */DAT3 160
   ON ENDFILE (SYSIN)                                                   DAT3 170
   GO TO EXIT,.                                                         DAT3 180
   N    =12,.                                                           DAT3 190
   N1   =1,.                                                            DAT3 200
   N2   =N,.                                                            DAT3 210
S1C..                                                                   DAT3 220
   IF M LE N2                                                           DAT3 230
   THEN N2   =M,.                                                       DAT3 240
   GET EDIT (CH) (A(8C)),.                                              DAT3 250
   GET STRING (CH) EDIT ((D(I) DO I= N1 TO N2)) ((N)F(6,0)),.           DAT3 260
   N1   =N2+1,.                                                         DAT3 270
   IF N1 LE M                                                           DAT3 280
   THEN DO,.                                                            DAT3 290
         N2   =N2+N,.                                                   DAT3 300
         GO TO S10,.                                                    DAT3 310
         END,.                                                          DAT3 320
   REVERT ENDFILE (SYSIN),.                                             DAT3 330
   RETURN,.                                                             DAT3 340
EXIT..                                                                  DAT3 350
   PUT FILE (SYSPRINT) EDIT ('ERROR  INSUFFICIENT DATA')                DAT3 360
         (SKIP(1),COLUMN(10),A),.                                       DAT3 370
   STOP,.                                                               DAT3 380
   END,.                            /*END OF PROCEDURE DAT3           */DAT3 390
```

ALLOCATION OF OVERHEAD COSTS (COST)

Problem Description

A standard problem in finance is the allocation of overhead costs (for example, electricity, transportation, . . .) to productive (charge) departments.

Overhead costs are initially charged to auxiliary departments. The costs of the auxiliary departments must be distributed among the productive departments using a given allocation key. For any auxiliary department the allocation key gives the distribution of unit costs among all departments (productive and auxiliary).

The problem is to calculate a transition matrix that can be used to obtain the final cost allocation to productive departments (by multiplying it with the given cost vector).

Mathematical Background

The calculation procedure is best described using matrix notation.

Let n be the number of auxiliary departments and m the number of productive departments.

The given allocation keys form a matrix K of dimension n+m by n, where the i-th column gives the distribution of unit costs of the i-th auxiliary department among all m+n departments.

$$K = \begin{matrix} \text{n-columns} \\ \begin{pmatrix} R \\ S \end{pmatrix} \begin{matrix} \} \text{ n-rows} \\ \} \text{ m-rows} \end{matrix} \end{matrix} \qquad (1)$$

K (given) is segmented into two parts, R and S.

R is of dimension n by n and S of dimension m by n. R contains the allocation keys for charging auxiliary departments by an auxiliary department, while S contains the allocation keys for charging productive departments by an auxiliary department.

If R is null, S is already the required transition matrix.

Note that all elements of K are nonnegative and that the sum of all elements in any column is one.

Let C be the vector of dimension n+m containing the costs of auxiliary departments (first n elements) and the costs of productive departments (last m elements):

$$C = \begin{pmatrix} CA \\ CP \end{pmatrix} \begin{matrix} \} \text{ n} \\ \} \text{ m} \end{matrix} \qquad (2)$$

Distributing overhead costs CA according to allocation key K gives a new vector

$$C_1 = \begin{pmatrix} CA_1 \\ CP_1 \end{pmatrix} \text{ with } \begin{matrix} CA_1 = R.\,CA \\ CP_1 = S.\,CA + CP \end{matrix} \qquad (3)$$

and by iteration

$$C_k = \begin{pmatrix} CA_k \\ CP_k \end{pmatrix} \text{ with } \begin{matrix} CA_k = R.\,CA_{k-1} = R^k.\,CA \\ CP_k = S.\,CA_{k-1} + CP_{k-1} \end{matrix} \qquad (3)$$

A realistic allocation key requires each auxiliary department to allot part of its costs to productive departments.

Under this assumption for the elements r_{ik} of R.

$$0 \le r_{ik} \le \alpha < 1 \text{ for all } \begin{matrix} i = 1,2, \ldots, n \\ k = 1,2, \ldots, n \end{matrix} \qquad (4)$$

and

$$\sum_{i=1}^{n} r_{ik} \le \alpha < 1 \text{ for all } k = 1,2, \ldots, n \qquad (5)$$

This means $R^k \to 0$ for $k \to \infty$ and I-R is nonsingular.

Therefore, iteration (3) will give the allocation of costs C to productive departments.

One step is sufficient if R = 0 (when no auxiliary department is charging an auxiliary department again).

The process (3) is easily described in matrix notation:

$$C_0 = C, \quad C_k = \begin{pmatrix} R & 0 \\ S & I \end{pmatrix} \cdot C_{k-1} = \begin{pmatrix} R & 0 \\ S & I \end{pmatrix}^k \cdot C_0 \qquad (6)$$

Therefore:

$$\lim_{k \to \infty} \begin{pmatrix} R & 0 \\ S & I \end{pmatrix}^k =$$

$$\lim_{k \to \infty} \begin{pmatrix} R^k & 0 \\ S(I+R+\ldots+R^{k-1}) & I \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ T & I \end{pmatrix}$$

defines the desired transition matrix T, which will give the final cost allocation with a single matrix multiplication:

$$T = \lim_{k \to \infty} S \cdot (I+R+\ldots+R^{k-1}) = S \cdot (I-R)^{-1}$$

The rows of T may be calculated one at a time from

$$T^T = (I-R)^{-T} \cdot S^T \qquad (7)$$

Programming Considerations

Calculation of T is done in two major steps:

1. The matrix $(I-R)^T$ is factored into a product of two triangular matrices $L \cdot U = (I-R)^T$.

2. The column vectors of S^T (that is, row vectors of S) are divided by the triangular factors L and U.

Doing the second step sequentially, one column at a time, saves considerable storage space, since the only data needed in core simultaneously is an n by n matrix, containing $(I-R)^T$, the triangular factors L and U, and a vector of dimension n. This allows calculation of the transition matrix T, which allocates overhead costs, for a very large number of charge departments, as long as the number of auxiliary departments is of moderate size.

Program

The program for allocation of overhead costs consists of the main program, COST, and two procedures from the Scientific Subroutine Package:

MFG -- triangular factorization of a general matrix

MDLG-- division by triangular factors from left-hand side

Capacity

The limitation on the number of auxiliary departments depends on the size of storage available for data. The number of productive departments is not limited by core size.

Dynamic storage allocation is used for data arrays with extent n+1 by n.

Input

One control card is required for each data set. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-10	Problem number (may be alphameric)	HILBERT
11-15	Number of auxiliary departments	6
16-20	Number of productive departments	4

Leading zeros do not have to be keypunched.

Data Cards

The rows of matrix $K = \begin{pmatrix} R \\ S \end{pmatrix}$ are read into the computer one at a time.

The elements are keypunched in successive cards, assuming six 10-column fields per card. These fields are 11-20, 21-30, 31-40, 41-50, 51-60, 61-70. Columns 1-4 are used for identification of the row. Each row must start with a new card. An input format of F(10,8) is used for the ten-column fields.

Deck setup is shown in Figure 38.

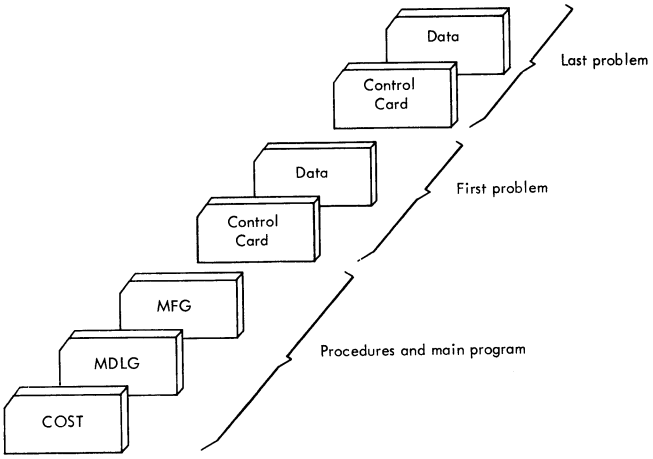


Figure 38.

Sample

A listing of input cards for the sample problem is shown in Figure 39.

```
HILBERT      6    4                                                          10


AA01     0.341417430.247540110.207916310.185625310.171199560.16104686       20
AA02     0.170708710.165026720.155937250.148500200.142666220.13804018       30
AA03     0.113805770.123770050.124749770.123750150.122285360.12078517       40
AA04     0.085354320.099016010.103958120.106071590.106999690.10736459       50
AA05     0.068283430.082513330.089106970.092812650.095110830.09662812       60
AA06     0.056902890.070725730.077968590.082500100.085599720.08784371       70


AA01     0.048773910.061885020.069305410.074250100.077817910.08052343       80
AA02     0.042677180.055008910.062374890.067500050.071333110.07432931       90
AA03     0.037935260.049508000.056704450.061875090.065845960.06902003      100
AA04     0.034141730.045007280.051979080.057115480.061142670.06441873      110
```

Figure 39.

Output

As output, the resulting transition matrix T is listed rowwise.

Sample

The output listing for the sample problem is shown in Figure 40.

```
                    ******************************************
                    *                                        *
                    *       ALLOCATION OF OVERHEAD COSTS     *
                    *                                        *
                    ******************************************

                    PROBLEM = HILBERT

                    NUMBER OF AUXILIARY  DEPARTMENTS =    6

                    NUMBER OF PRODUCTIVE DEPARTMENTS =    4

      RESULTANT ERROR INDICATOR WITHIN PROCEDURE MFG          ERROR =O

AAC1          2.90817678E-01  2.89823174E-01  2.88753211E-01  2.87737966E-01  2.86809385E-01  2.85970271E-01

AAC2          2.59813845E-01  2.59676158E-01  2.59507656E-01  2.59332657E-01  2.59161770E-01  2.58998632E-01

AAC3          2.34915495E-01  2.35311449E-01  2.3573333CE-01  2.3613C297E-01  2.364909C5E-01  2.36814141E-01

AAC4          2.14453995E-01  2.15190649E-01  2.16006935E-01  2.16799796E-01  2.17539072E-01  2.18217134E-01
```

Figure 40.

Program Modifications

Input data in a different format can be handled by providing different formats in corresponding GET EDIT statements.

Error Messages

The value of the error indicator as set by procedure MFG is included in the listing:

ERROR = 'O' means successful factorization.
ERROR = 'P' means incorrect value N.
ERROR = 'S' means incorrect data matrix R. (I-R) is singular.
ERROR = 'C' means (I-R) is nearly singular. To avoid a breakdown of the method, input data has been slightly modified.
ERROR = 'W' means (I-R) is nearly singular. Results may have poor accuracy.

In the case ERROR = 'S', calculation is bypassed.

Operating Instructions

The sample program for overhead cost allocation is a standard PL/I procedure. Special operating instructions are not required. Data set SYSIN is used for input; and data set SYSPRINT, for output.

Timing

The execution time of this sample program on a System/360 Model 40, using a 2540 Card Reader and a 1403 Printer, Model N2, as output, is 19 seconds.

```
COST..                                                                  COST  10
/*************************************************************************/COST  20
/*                                                                       */COST  30
/*                    ALLOCATION OF OVERHEAD COSTS                       */COST  40
/*                                                                       */COST  50
/*************************************************************************/COST  60
   PROCEDURE OPTIONS(MAIN),.                                            COST  70
   DECLARE                                                              COST  80
        ERROR EXTERNAL CHARACTER(1),  /*EXTERNAL ERROR INDICATOR        */COST  90
        (CNR,CHNR) CHARACTER(10),                                       COST 100
        CH CHARACTER(1),                                                COST 110
        EPS BINARY FLOAT,                                               COST 120
        (I,IND,K,L,M,N)                                                 COST 130
        BINARY FIXED,.                                                  COST 140
   ON ENDFILE (SYSIN) GO TO BACK,.                                      COST 150
START..                                                                 COST 160
   EPS  =1E-6,.                  /*SET EPS FOR INTERNAL TEST FOR       */COST 170
   GET EDIT                      /*LOSS OF SIGNIFICANT DIGITS          */COST 180
        (CNR,N,M,CH)             /*READ NUMBER OF COLUMNS, ROWS        */COST 190
        (A(10),F(5),F(5),X(59),A(1)),.                                  COST 200
   PUT EDIT                      /*WRITE HEADING                       */COST 210
        ('*****************************************',                   COST 220
        '*                                       *',                    COST 230
        '*       ALLOCATION OF OVERHEAD COSTS    *',                    COST 240
        '*                                       *',                    COST 250
        '*****************************************')                   COST 260
        (PAGE,SKIP(2),(5)(X(30),A,SKIP)),.                              COST 270
   PUT EDIT                                                             COST 280
        ('PROBLEM =',CNR,'NUMBER OF AUXILIARY  DEPARTMENTS =',N,        COST 290
        'NUMBER OF PRODUCTIVE DEPARTMENTS =',M)                         COST 300
        (SKIP(2),X(30),A,A,(2)(SKIP(2),X(30),A,F(5))),.                 COST 310
        BEGIN,.                                                         COST 320
        DECLARE                                                         COST 330
             R(N,N),S(N,1),                                             COST 340
             W(N) DEFINED S(1SUB,1))                                    COST 350
             BINARY FLOAT,            /*SINGLE PRECISION VERSION  /*S*/COST 360
/*           BINARY FLOAT(53),        /*DOUBLE PRECISION VERSION  /*D*/COST 370
             IPER(N)                                                    COST 380
             BINARY FIXED,.                                             COST 390
        IND  =1,.                                                       COST 400
        L    =N,.                     /*CALCULATE VALUES FOR INPUT    */COST 410
             DO WHILE (L GT 6),.      /*FORMAT LIST                   */COST 420
             L    =L-6,.                                                COST 430
             IND  =IND+1,.            /*IND MEANS THE NUMBER OF CARDS */COST 440
             END,.                    /*FOR ONE ROW OF R              */COST 450
        L    =(6-L)*10,.              /*L SPECIFIES HORIZONT. SPACING */COST 460
             DO I =1 TO N,.           /*EXECUTE LOOP OVER ROWS OF R   */COST 470
             GET EDIT                 /*READ I-TH ROW OF MATRIX R     */COST 480
                  (CHNR,W)                                              COST 490
                  (A(10),(IND)((6)F(10,8),X(20))),.                     COST 500
             GET EDIT                 /*HORIZONTAL SPACING            */COST 510
                  (CNR)                                                 COST 520
                  (X(L),A(10)),.                                        COST 530
             W(I) =W(I)-1,.           /*COMPUTE  TRANSPOSED (U-R)     */COST 540
             R(*,I)=-W,.              /*WHERE U MEANS UNIT MATRIX     */COST 550
             END,.                                                      COST 560
        CALL MFG(R,IPER,N,EPS),.      /*CALL FACTORIZATION PROCEDURE  */COST 570
        PUT EDIT                      /*WRITE ERROR INDICATOR OF MFG  */COST 580
             ('RESULTANT ERROR INDICATOR WITHIN PROCEDURE MFG',         COST 590
             'ERROR =',ERROR)(SKIP(3),X(10),A,X(10),A,A),.              COST 600
             DO I =1 TO M,.           /*EXECUTE LOOP OVER ROWS OF S   */COST 610
             GET EDIT                 /*READ ANY ROW OF MATRIX S      */COST 620
                  (CHNR,W)                                              COST 630
                  (A(10),(IND)((6)F(10,8),X(20))),.                     COST 640
             GET EDIT                                                   COST 650
                  (CNR)                                                 COST 660
                  (X(L),A(10)),.                                        COST 670
             IF ERROR NE 'S'                                            COST 680
             THEN DO,.                /*PERFORM MATRIX DIVISION       */COST 690
                  CALL MDLG(R,S,IPER,N,18,'O'),.                        COST 700
                  PUT EDIT            /*WRITE ALLOCATION ROW          */COST 710
                       (CHNR,W)                                         COST 720
                       (SKIP(2),X(3),A,X(5),(IND)((6)E(17,8),X(18))),.  COST 730
                  END,.                                                 COST 740
             END,.                                                      COST 750
        END,.                                                           COST 760
   GO TO START,.                                                        COST 770
BACK..                                                                  COST 780
   END,.                          /*END OF PROCEDURE COST             */COST 790
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International Business Machines Corporation
Data Processing Division
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IBM World Trade Corporation
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(International)