IBM Application Program GH20-0252-4

1130 Scientific Subroutine Package Programmer's Manual

Program Number 1130-CM-02X

The Scientific Subroutine Package (SSP) is a collection of 121 FORTRAN subroutines divided, for the sake of presentation, into three groups: statistics, matrix manipulation, and other mathematics. It is a collection of input/output-free computational building blocks that can be combined with a user's input, output, or computational routines to meet his needs. The package can be applied to the solution of many problems in industry, science, and engineering.

Fifth Edition (June 1970)

This edition, GH20-0252-4, is a reprint of H20-0252-3 incorporating TNL N20-1962 and changing the order number prefix from H20 to GH20. It does not obsolete H20-0252-3 as updated by N20-1962.

This edition applies to Version 1, Modification 2 of the 1130 Scientific Subroutine Package (1130-CM-02X) and to all subsequent versions and modifications until otherwise indicated in new editions or Technical Newsletters.

Changes are continually made to the specifications herein. Before using this publication in connection with the operation of IBM systems, consult the latest 1130 SRL Newsletter, N20-1130, for the editions that are applicable and current.

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CONTENTS

INTRODUCTION

The IBM 1130 Scientific Subroutine Package makes available a mathematical and statistical subroutine library. The user may supplement or modify the collection to meet his needs. This library 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.

AREAS OF APPLICATION

Individual subroutines, or a combination of them, can be used to carry out the listed functions in the following areas:

Statistics

- Analysis of variance (factorial design)
- Correlation analysis
- Multiple linear regression
- Polynomial regression
- Canonical correlation
- Factor analysis (principal components, varimax)
- Discriminant analysis (many groups)
- Time series analysis
- Data screening and analysis
- Nonparametric tests
- Random number generation (uniform, normal)

Matrix Manipulation

- Inversion
- Eigenvalues and eigenvectors (real symmetric case)
- Simultaneous linear algebraic equations
- Transpositions
- Matrix arithmetic (addition, product, etc.)
- Partitioning
- Tabulation and sorting of rows or columns
- Elementary operations on rows or columns

Other Mathematical Areas

- Integration of given or tabulated functions
- Integration of first-order differential equations
- Fourier analysis of given or tabulated functions
- Bessel and modified Bessel function evaluation
- Gamma function evaluation
- Legendre function evaluation
- Elliptic, exponential, sine, cosine, Fresnel integrals
- Finding real roots of a given function
- Finding real and complex roots of a real polynomial
- Polynomial arithmetic (addition, division, etc.)
- Polynomial evaluation, integration, differentiation

CHARACTERISTICS

Some of the characteristics of the Scientific Subroutine Package are:

- All subroutines are free of input/output statements.
- Subroutines do not contain fixed maximum dimensions for the data arrays named in their calling sequences.
- All subroutines are written in 1130 FORTRAN.
- Many matrix manipulation subroutines handle symmetric and diagonal matrices (stored in economical, compressed formats) as well as general matrices. This can result in considerable saving in data storage for large arrays.
- The use of the more complex subroutines (or groups of them) is illustrated in the program documentation by sample main programs with input/output.
- All subroutines are documented uniformly.

DESIGN PHILOSOPHY

CHOICE OF ALGORITHMS

The algorithms in SSP have been chosen after considering questions of storage, accuracy, and past experience with the algorithm. Conservation of storage has been the primary criterion except in those situations where other considerations outweighed that of storage. As a result, many compromises have been made both with respect to level of sophistication and execution time. One such compromise is the use of the Runge-Kutta integration technique rather than predictor-corrector methods. A departure from the primary criterion of storage is illustrated by the algorithm for matrix inversion. If only row pivoting had been used, the subroutine would not have required working storage and would have needed fewer FORTRAN statements for implementation. However, pivoting on both rows and columns was chosen because of the accuracy requirement for matrix inversion in statistical operations.

PROGRAMMING

The subroutines in SSP have been programmed in 1130 FORTRAN. Many of the larger functions such as those in statistics have been programmed as a series or sequence of subroutines.

An example of the use of sequences of subroutines is the statistical function called factor analysis. Factor analysis is a method of analyzing the intercorrelations within a set of variables. It determines whether the variance in the original set of variables can be accounted for adequately by a smaller number of basic categories; namely, factors. In the Scientific Subroutine Package, factor analysis is normally performed by calling the following five subroutines in sequence:

1. CORRE - to find means, standard deviations, and correlation matrix
2. EIGEN - to compute eigenvalues and associated eigenvectors of the correlation matrix
3. TRACE - to select the eigenvalues that are greater than or equal to the control value specified by the user
4. LOAD - to compute a factor matrix
5. VARMX - to perform varimax rotation of the factor matrix

The multiple use of subroutines is illustrated by the fact that subroutine CORRE is also utilized in the multiple linear regression and canonical correlation. Subroutine EIGEN is used in canonical correlation as a third level subroutine.

OVERALL RULES OF USAGE

GENERAL RULES

All subroutines in the Scientific Subroutine Package (SSP) are entered by means of the standard FORTRAN CALL statement. These 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, whatever input/output and other operations are necessary for the total solution of his problem. In addition, the user must define by DIMENSION 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 no different from any user-supplied subroutine. All of the normal rules of FORTRAN concerning subroutines must, therefore, be adhered to with the exception that the dimensioned areas in the SSP subroutine are not required to be the same as those in the calling 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 if the argument is a constant or a variable. When the argument is an array or function subprogram name, the address of the array or subprogram is transmitted to the called subroutine.

The arguments in a CALL statement must agree in order, number, and type with the corresponding arguments in the subroutine. A number may be passed to a subroutine either as a variable name in the argument list or as a constant in the argument list. For example, if the programmer wishes to add matrix AR1 to matrix AR2 in order to form matrix AR3 using the SSP subroutine GMADD and if AR1 and AR2 are both matrices with ten rows and twenty columns, either of the two following methods could be used:

```
Method 1      .
        CALL GMADD(AR1,AR2,AR3,10,20)
              .

Method 2      .

        N = 10

        M = 20

        CALL GMADD(AR1,AR2,AR3,N,M)
              .
```

Many of the subroutines in SSP require the name of a user function subprogram or a FORTRAN-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 also appear in an EXTERNAL statement at the beginning of that program.

For example, the SSP subroutine RK2 integrates a function furnished by the user. It is therefore necessary for the user to program the function and give the name of the function to RK2 as a parameter in the CALL statement. If the user wished to integrate the function $\frac{dy}{dx} = 3.0x + 2.0Y$, his main program might look like:

```
        EXTERNAL DERY
              .
              .
        CALL RK2(DERY, .....)
              .
              .
        RETURN
        END
```

His function subprogram could be:

```
        FUNCTION DERY (X,Y)
        DERY=3.0*X+2.0*Y
        RETURN
        END
```

The user's main program gives the name of the programmed function to RK2 by including that name in the CALL statement and in an EXTERNAL statement. RK2, in turn, goes to the function DERY each time it requires a value for the derivative. The subroutine RK2 is not modified by the programmer. The dummy function name FUN in subroutine RK2 is, in effect, replaced by the name appearing in the user's CALL statement during execution of the subroutine.

MATRIX OPERATIONS

Special consideration must be given to the subroutines that perform matrix operations. These subroutines have two characteristics that affect the 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 a vector storage approach. Under this approach, each column of a matrix is immediately followed in storage by the next column. Vector storage and two-dimensional storage result in the same layout of data in core, so long as the number of rows and columns in the matrix are the same as those in the user's dimension statement. If, however, the matrix is smaller than the dimensioned area, the two forms of storage are not compatible.

Consider the layout of data storage when operating on a 5 by 5 array of numbers in an area dimensioned as 10 by 10. If the programmer has been using double subscripted variables in the normal FORTRAN sense, the 25 elements of data will appear as shown in Figure 1. FORTRAN stores double subscripted data by column based on the column length specified in the DIMENSION statement. Thus, in the example, sequential core locations would contain data elements 1 to 5, five blank locations, data elements 6 to 10, five blank locations, etc. The matrix subroutines take a vector approach in storing arrays by column, which means that they assume the data is stored as shown in Figure 2.

		Column									
		1	2	3	4	5	6	7	8	9	10
	1	(1)	(6)	(11)	(16)	(21)					
	2	(2)	(7)	(12)	(17)	(22)					
	3	(3)	(8)	(13)	(18)	(23)					
	4	(4)	(9)	(14)	(19)	(24)					
Row	5	(5)	(10)	(15)	(20)	(25)					
	6										
	7										
	8										
	9										
	10										

Figure 1. Double subscripted data storage

(1)	(11)	(21)
(2)	(12)	(22)
(3)	(13)	(23)
(4)	(14)	(24)
(5)	(15)	(25)
(6)	(16)	
(7)	(17)	
(8)	(18)	
(9)	(19)	
(10)	(20)	

Figure 2. Vector storage

As has been stated previously, for the case where the dimensioned area is the same as the matrix size, the two approaches will have the same data storage layout and the user can proceed in a regular double subscripted fashion. If, however, he is operating in a mode where the dimensioned area is larger than the arrays and if he wishes to use the SSP subroutines, he must be certain that his data is stored in the vector fashion illustrated by Figure 2. A subroutine called ARRAY is available in SSP to change from one form of storage to the other. In addition, a subroutine called LOC is available to assist in referencing elements in an array stored in the vector fashion.

Storage Compression

Many subroutines in SSP can operate on compressed forms of matrices, as well as the normal form. Using this capability, which is called "storage mode", considerable savings in data storage can be obtained for special forms of large arrays. The three modes of storage are termed general, symmetric, and diagonal. In this context, general mode is one in which all elements of the matrix are in storage. Symmetric mode is one in which only the upper triangular portion of the matrix is retained columnwise in sequential locations in storage. (The assumption is made that the corresponding elements in the lower triangle have the same value.) Diagonal mode is one in which only the diagonal elements of the matrix are retained in sequential locations in storage. (The off-diagonal elements are assumed to be zero.) This capability has been implemented using the vector storage approach. To illustrate the effect of the storage mode capability, refer to Figure 3. A symmetric matrix is shown in Figure 3A. If this array is to be manipulated using the SSP matrix subroutines with storage mode capability, then the array may be stored as shown in Figure 3B. This is the upper triangular portion of the array and corresponds to a storage mode code of 1. Symmetric matrices of order N may be stored in a vector only N*(N+1)/2 locations rather than N*N locations. For larger matrices, this will be a saving of almost one half.

The effect of storage mode when dealing with diagonal matrices is even more pronounced. Diagonal matrices of order N may be stored in a vector only N locations long. Figure 3C shows a 3 by 3 diagonal matrix. If this array is to be manipulated using the SSP matrix subroutines with storage mode capability, then only the diagonal elements of the array need be stored. This is shown in Figure 3D and corresponds to a storage mode code of 2.

General matrices of order N by M require a vector N*M long and use a storage mode code of 0.

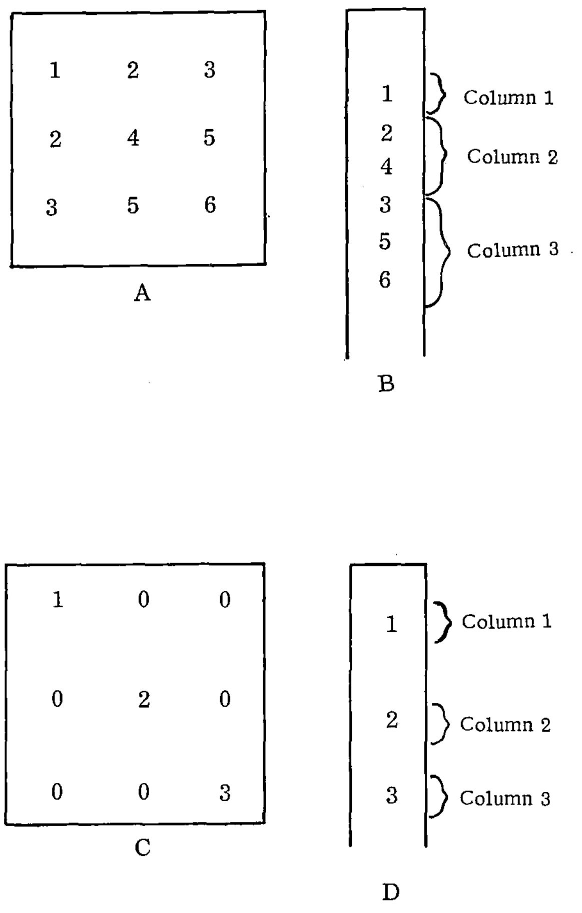


Figure 3. Storage mode

Thus, if the programmer wishes to use SSP subroutines on matrix A, which is general, matrix B, which is symmetric, and matrix C, which is diagonal, and all matrices are 10 by 10 or smaller, the dimension statement in his program could be:

```
DIMENSION A(100), B(55), C(10)
```

<u>Matrix Element References</u>

Subroutine LOC in the Scientific Subroutine Package may be used to reference elements within a matrix that is stored in a vector fashion and may involve storage mode compression. The calling sequence for LOC is:

```
CALL LOC (I, J, IJ, N, M, MS)
```

The capabilities of subroutine LOC are as follows: If reference is required to the element at row I and column J of matrix A whose dimensions are N by M and if the storage mode code is MS, then a CALL to the LOC subroutine as shown above will result in the computation of the subscript IJ such that A(IJ) is the desired element. The parameters represented by I, J, N, M, MS can either be integer variables or integer constants. The parameter represented by IJ is an integer variable. Note that the user must dimension the array A as a single subscripted variable to meet the restrictions of some FORTRAN systems. To illustrate the use of LOC: If reference is required to the element at row 2, column 2 of the 3 by 3 symmetric matrix illustrated in Figure 3A and stored as shown in Figure 3B (storage mode code 1), the sequence might be:

```
CALL LOC (2, 2, IJ, 3, 3, 1)
```

The value of IJ computed by LOC would be 3; meaning that the proper element is the third element in the specially stored symmetric matrix (Figure 3B). If the storage mode code is for a symmetric matrix where only the upper triangular portion is retained in storage and if I and J refer to an element in the lower triangular portion, IJ will contain the subscript for the corresponding element in the retained upper triangle. Thus if the user wanted the element in row 3, column 1 of the matrix shown in Figure 3A and the array was stored as in Figure 3B, the statement:

```
CALL LOC (3, 1, IJ, 3, 3, 1)
```

would result in IJ having the value of 4; that is, the fourth element in Figure 3B. If a matrix is stored as shown in Figure 3D (storage mode 2) and LOC is used to compute the subscript for an off-diagonal element (I not equal to J), the result in IJ will be zero. This is due to the fact that the element does not exist in storage. In this situation, the user must not utilize IJ as a subscript. Following is an illustration of how to take care of this condition and also handle the case where the current storage mode is unknown.

If the user wishes to set a variable X equal to the element in the third row and fourth column of a 10 by 10 array named A for either a symmetric, diagonal, or general matrix, the required program can be implemented for any storage mode MS as follows:

```
    CALL LOC (3, 4, IJ, 10, 10, MS)

    X = 0.0

    IF(IJ)20, 30, 20

 20 X = A(IJ)

 30 --------
```

MS is assumed to have been set at 0, 1, or 2 at some earlier point in the program. This sequence would then set the proper value for X given any storage mode that might be encountered. The second and third statements take care of the off-diagonal condition for a matrix with a storage mode of 2.

As a special case, LOC can be used to compute the total length of an array in storage with a statement such as:

```
CALL LOC (N, M, IJ, N, M, MS)
```

For example, if the user has a 3 by 3 matrix whose storage mode is 1 (Figure 3B), the statement:

```
CALL LOC (3, 3, IJ, 3, 3, 1)
```

will result in IJ being set to 6. This is not only the proper subscript to reference element 3, 3 but is also the actual length of the vector in storage.

The information contained in the fifth parameter (number of columns) in the calling sequence for LOC is not actually used in the calculations performed by LOC. It has been included in the calling sequence in case the user wishes to expand LOC to cover other forms of data storage.

OPTIMIZATION OF TIME

The subroutines in SSP are designed to conserve storage. If the user wishes to exchange space for time, there are several ways in which SSP may be modified to effect this end. For example, many of the subroutines in SSP make use of LOC subroutine to handle vector storage and storage mode referencing. The execution time of these subroutines can be substantially reduced by implementing LOC in Assembler Language. (The distributed version of LOC is implemented in FORTRAN.) Another approach is to incorporate the function of LOC within each subroutine and thus avoid the "setup" costs of repeated calls to LOC. This has the effect of reducing execution time but at some cost in subroutine storage and in the ease with which other modes of storage such as triangular matrix storage or storage by row rather than by column can be implemented. Figure 4 shows how matrix addition and the LOC capabilities can be implemented within the same subroutine.

In the mathematical area, the user may find it desirable to implement entirely different algorithms for integration. The use of techniques that automatically adjust the integration interval depending on the rate of change of the function will often have the effect of reducing total execution time.

EXTENDED 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. All of the subroutines will compile correctly for extended precision by placing the *EXTENDED PRECISION control card at the appropriate place in the deck. Note that 1130 FORTRAN does not allow the intermixing of regular and extended precision in the same program.

```
      SUBROUTINE MADX(A,B,R,N,M,MSA,MSB)
      DIMENSION A(1),B(1),R(1)
C
C        TEST FOR SAME STORAGE MODE
C
      IF(MSA-MSB) 30,1C,30
C
C        COMPUTE VECTOR LENGTH
C
   10 ND=N*M
      IF(MSA-1) 24,22,23
   22 ND=(ND+N)/2
      GO TO 24
   23 ND=N
C
C        ADD MATRICES CF SAME STORAGE MODE
C
   24 CO 25 I=1,NC
   25 R(I)=A(I)+B(I)
      RETURN
C
C        GET STORAGE MCDE CF OUTPUT MATRIX
C
   30 MTEST=MSA*MSB
      MSR=0
      IF(MTEST) 35,35,32
   32 MSR=1
   35 DO 60 J=1,M
      CO 60 I=1,N
C
C        LOCATE ELEMENT IN OUTPUT MATRIX
C
      KX=-1
      MS=MSR
      GO TO 65
   40 IJR=IR
C
C        LOCATE ELEMENT IN MATRIX A
C
      KX=0
      MS=MSA
      GO TO 65
   45 IJA=IR
      AEL=0.0
      IF(IJA) 46,48,46
   46 AEL=A(IJA)
C
C        LOCATE ELEMENT IN MATRIX B
C
   48 KX=1
      MS=MSB
      GO TC 65
   50 IJB=IR
      BEL=0.0
      IF(IJB) 55,60,55
   55 BEL=B(IJB)
C
C        ADD MATRICES CF CIFFERENT STCRAGE MODES
C
   60 R(IJR)=AEL+BEL
      RETURN
C
C        IN LINE LOC
C
   65 IF(MS-1) 70,75,9C
   70 IR=N*(J-1)+I
      GC TC 95
   75 IF(I-J) 80,85,85
   80 IR=I+(J*J-J)/2
      GO TO 95
   85 IR=J+(I*I-1)/2
      GO TC 95
   90 IR=0
      IF(I-J) 95,92,95
   92 IR=I
   95 IF(KX) 40,45,50
      ENC
```

Figure 4. Inline LOC

FORMAT OF THE DOCUMENTATION

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

SUBROUTINE DESCRIPTIONS

A guide to the subroutines, designed to aid in locating any particular subroutine, is given in the pages that follow. Each of the subroutine descriptions contains a program listing and, in some cases, a mathematical description. If there are restrictions on the ranges of values that the parameters may take, these are included under the remarks section of each subroutine description. References to books and periodicals will be found under the method section of the description. The mathematical description pages do not, in most cases, indicate the derivation of the mathematics. They are intended to indicate what mathematical operations are actually being performed in the subroutines. Some of the major statistical functions are performed by a sequence of SSP subroutines. An abstract describing this sequence will be found just before the description of the first subroutine that is specific to this function.

SAMPLE PROGRAM DESCRIPTIONS

The sample program listings are given in Appendix D. They are immediately preceded by a guide to aid in locating the sample program calling a particular SSP subroutine or (where applicable) typical user-written subroutine. Each sample program consists of a detailed description including information on the problem, the program, input, output, program modification, operating instructions, error messages, and machine listings of the programs, input data and output results. Timings for these programs is given in Appendix C. The sample programs have been chosen to (1) illustrate a sequence of SSP subroutines, (2) illustrate the use of a complex subroutine, or (3) show the way in which one member of a large set of related subroutines might be used.

As part of the development of the sample programs, some special sample subroutines have been implemented that may prove useful to the programmer. These include:

HIST	- Print a histogram of frequencies
MATIN	- Read an input matrix into storage in vector form for use by SSP matrix subroutines
PLOT	- Plot several variables versus a base variable
MXOUT	- Print a matrix stored in the SSP vector format

Listings of the above subroutines are included in the sample program documentation in this manual.

The sample programs all require 8K words of core for execution and several of them require (in addition) the overlay capabilities of the Disk Monitor.

MACHINE CONFIGURATION

The machine configuration necessary to run SSP/1130 is dependent upon the use that is to be made of the package. All of the subroutines are I/O free, compile to less than 1500 words of core, and are, therefore, configuration independent. However, many of the routines are intended to be used in conjunction with other subroutines or to solve problems using large arrays of data. For this reason, many of the subroutines are not useful with less than 8K words of core.

The following items should be taken into consideration when deciding upon the applicability of this package to a particular machine configuration:

1. The size of problem which may be executed on a given 1130 depends upon 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.
2. SSP/1130 programs will be distributed in card form only.
3. Several of the sample problems require 8K words of core and the use of the Disk Monitor, and the remaining sample problems require 8K words of core.

It is possible to estimate program sizes by using the manual Core Requirements for 1130 FORTRAN (C20-1641) in conjunction with the core size listing found in Appendix A.

GUIDE TO SUBROUTINES

SUBROUTINE LISTINGS AND WRITEUPS

The following pages give the subroutine listings. Wherever necessary, additional explanatory matter on the routine, or a discussion of the underlying mathematics has been included.

Statistics - Data Screening

TALLY

Purpose:
Calculate total, mean, standard deviation, minimum, maximum for each variable in a set (or a subset) of observations.

Usage:
CALL TALLY(A, S, TOTAL, AVER, SD, VMIN, VMAX, NO, NV)

Description of parameters:

A	-	Observation matrix, NO by NV
S	-	Input vector indicating subset of A. Only those observations with a non-zero S(J) are considered. Vector length is NO.
TOTAL	-	Output vector of totals of each variable. Vector length is NV.
AVER	-	Output vector of averages of each variable. Vector length is NV.
SD	-	Output vector of standard deviations of each variable. Vector length is NV.
VMIN	-	Output vector of minima of each variable. Vector length is NV.
VMAX	-	Output vector of maxima of each variable. Vector length is NV.
NO	-	Number of observations.
NV	-	Number of variables for each observation.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
All observations corresponding to a non-zero element in 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 deviation is one less than the number of observations used.

```
      SUBROUTINE TALLY(A,S,TOTAL,AVER,SD,VMIN,VMAX,NO,NV)
      DIMENSION A(1),S(1),TOTAL(1),AVER(1),SD(1),VMIN(1),VMAX(1)
C        CLEAR OUTPUT VECTORS AND INITIALIZE VMIN,VMAX
      DO 1 K=1,NV
      TOTAL(K)=0.0
      AVER(K)=0.0
      SD(K)=0.0
      VMIN(K)=1.0E38
    1 VMAX(K)=-1.0E38
C        TEST SUBSET VECTOR
      SCNT=0.0
      DO 7 J=1,NO
      IJ=J-NO
      IF(S(J)) 2,7,2
    2 SCNT=SCNT+1.0
C        CALCULATE TOTAL, MINIMA, MAXIMA
      DO 6 I=1,NV
      IJ=IJ+NO
      TOTAL(I)=TOTAL(I)+A(IJ)
      IF(A(IJ)-VMIN(I)) 3,4,4
    3 VMIN(I)=A(IJ)
    4 IF(A(IJ)-VMAX(I)) 6,6,5
    5 VMAX(I)=A(IJ)
    6 SD(I)=SD(I)+A(IJ)*A(IJ)
    7 CONTINUE
C        CALCULATE MEANS AND STANDARD DEVIATIONS
      DO 8 I=1,NV
      AVER(I)=TOTAL(I)/SCNT
    8 SD(I)=SQRT(ABS((SD(I)-TOTAL(I)*TOTAL(I)/SCNT)/(SCNT-1.0)))
      RETURN
      END
```

BOUND

Purpose:
Select from a set (or a subset) of observations the number of observations under, between and over two given bounds for each variable.

Usage:
CALL BOUND (A, S, BLO, BHI, UNDER, BETW, OVER, NO, NV)

Description of parameters:

A	- Observation matrix, NO by NV
S	- Vector indicating subset of A. Only those observations with a non-zero S(J) are considered. Vector length is NO.
BLO	- Input vector of lower bounds on all variables. Vector length is NV.
BHI	- Input vector of upper bounds on all variables. Vector length is NV.
UNDER	- Output vector indicating, for each variable, number of observations under lower bounds. Vector length is NV.
BETW	- Output vector indicating, for each variable, number of observations equal to or between lower and upper bounds. Vector length is NV.
OVER	- Output vector indicating, for each variable, number of observations over upper bounds. Vector length is NV.
NO	- Number of observations
NV	- Number of variables for each observation

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Each row (observation) of matrix A with corresponding non-zero element in S vector is tested. Observations are compared with specified lower and upper variable bounds and a count is kept in vectors under, between, and over.

```
      SUBROUTINE BOUND(A,S,BLO,BHI,UNDER,BETW,OVER,NO,NV)
      DIMENSION A(1),S(1),BLO(1),BHI(1),UNDER(1),BETW(1),OVER(1)
C        CLEAR OUTPUT VECTORS.
      DO 1 K=1,NV
      UNDER(K)=0.0
      BETW(K)=0.0
    1 OVER(K)=0.0
C        TEST SUBSET VECTOR
      DO 8 J=1,NO
      IJ=J-NO
      IF(S(J)) 2,8,2
C        COMPARE OBSERVATIONS WITH BOUNDS
    2 DO 7 I=1,NV
      IJ=IJ+NO
      IF(A(IJ)-BLO(I)) 5,3,3
    3 IF(A(IJ)-BHI(I)) 4,4,6
C       COUNT
    4 BETW(I)=BETW(I)+1.0
      GO TO 7
    5 UNDER(I)=UNDER(I)+1.0
      GO TO 7
    6 OVER(I)=OVER(I)+1.0
    7 CONTINUE
    8 CONTINUE
      RETURN
      END
```

SUBST

Purpose:
Derive a subset vector indicating which observations in a set have satisfied certain conditions on the variables.

Usage:
CALL SUBST (A, C, R, B, S, NO, NV, NC)
Parameter B must be defined by an external statement in the calling program.

Description of parameters:

A - Observation matrix, NO by NV

C - Input matrix, 3 by NC, of conditions to be considered. The first element of each column of C represents the number of the variable (column of the matrix A) to be tested, the second element of each column is a relational code as follows:

1. for less than
2. for less than or equal to
3. for equal to
4. for not equal to
5. for greater than or equal to
6. for 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 - 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. Vector length is NC.

B - 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:

```
SUBROUTINE BOOL(R,T)
DIMENSION R(3)
T=R(1)*(R(2)+R(3))
RETURN
END
```

The above expression is tested for

R(1).AND.(R(2).OR.R(3))

S - Output vector indicating, for each observation, whether or not proposition B is satisfied. If it is, S(I) is non-zero. If it is not, S(I) is zero. Vector length is NO.

NO - Number of observations.

NV - Number of variables.

NC - Number of basic conditions to be satisfied.

Subroutines and function subprograms required:

B The name of actual subroutine supplied by the user may be different (e.g., BOOL), but subroutine SUBST always calls it as B. In order for subroutine SUBST to do this, the name of the user-supplied subroutine must be defined by an EXTERNAL statement in the calling program. The name must also be listed in the "CALL SUBST" statement. (See usage above.)

Method:
The following is done for each observation. Condition matrix is analyzed to determine which variables are to be examined. 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 SUBST(A,C,R,B,S,NO,NV,NC)
      DIMENSION A(1),C(1),R(1),S(1)
      DO 9 I=1,NO
      IQ=I-NO
      K=-2
      DO 8 J=1,NC
C        CLEAR R VECTOR
      R(J)=0.0
C        LOCATE ELEMENT IN OBSERVATION MATRIX AND RELATIONAL CODE
      K=K+3
      IZ=C(K)
      IA=IQ+IZ*NO
      IGO=C(K+1)
C        FORM R VECTOR
      Q=A(IA)-C(K+2)
      GO TO(1,2,3,4,5,6),IGO
    1 IF(Q) 7,8,8
    2 IF(Q) 7,7,8
    3 IF(Q) 8,7,8
    4 IF(Q) 7,8,7
    5 IF(Q) 8,7,7
    6 IF(Q) 8,8,7
    7 R(J)=1.0
    8 CONTINUE
C        CALCULATE S VECTOR
    9 CALL B(R,S(I))
      RETURN
      END
```

ABSNT

Purpose:
Test missing or zero values for each observation in matrix A.

Usage:
CALL ABSNT (A, S, NO, NV)

Description of parameters:

A	-	Observation matrix, NO by NV.
S	-	Output vector of length NO indicating the following codes for each observation: 1 There is not a missing or zero value. 0 At least one value is missing or zero.
NO	-	Number of observations.
NV	-	Number of variables for each observation.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
A test is made for each row (observation) of the matrix A. If there is not a missing or zero value, 1 is placed in S(J). If at least one value is missing or zero, 0 is placed in S(J).

```
      SUBROUTINE ABSNT(A,S,NO,NV)
      DIMENSION A(1),S(1)
      DO 20 J=1,NO
      IJ=J-NO
      S(J)=1.0
      DO 10 I=1,NV
      IJ=IJ+NO
      IF(A(IJ)) 10,5,10
    5 S(J)=0
      GO TO 20
   10 CONTINUE
   20 CONTINUE
      RETURN
      END
```

TAB1

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 of the i-th 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:

$$\text{Total:} \quad T = \sum_{i=1}^{n} X_{ij} \qquad (3)$$

where j = selected variable

$$\text{Mean:} \quad \bar{X} = \frac{T}{n} \qquad (4)$$

Standard deviation:

$$s = \sqrt{\frac{\sum_{i=1}^{n} X_{ij}^2 - \left(\sum_{i=1}^{n} X_{ij}\right)^2 / n}{n-1}} \qquad (5)$$

Subroutine TAB1

Purpose:
Tabulate for one variable in an observation matrix (or a matrix subset), the frequency and percent frequency over given class intervals. In addition, calculate for the same variable the total, average, standard deviation, minimum, and maximum.

Usage:

CALL TAB1 (A, S, NOVAR, UBO, FREQ, PCT, STATS, NO, NV)

Description of parameters:

A	-	Observation matrix, NO by NV.
S	-	Input vector giving subset of A. Only those observations with a corresponding non-zero S(J) are considered. Vector length is NO.
NOVAR	-	The variable to be tabulated.
UBO	-	Input vector giving 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 uses the minimum and maximum values of the variable. Number of intervals, UBO(2), must include two cells for values under and above limits. Vector length is 3.
FREQ	-	Output vector of frequencies. Vector length is UBO(2).
PCT	-	Output vector of relative frequencies. Vector length is UBO(2).
STATS	-	Output vector of summary statistics, i.e., total, average, standard deviation, minimum and maximum. Vector length is 5.
NO	-	Number of observations.
NV	-	Number of variables for each observation.

Remarks:

None.

Subroutines and function subprograms required:

None.

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.

```
      SUBROUTINE TAB1(A,S,NOVAR,UBO,FREQ,PCT,STATS,NO,NV)
      DIMENSION A(1),S(1),UBO(3),FREQ(1),PCT(1),STATS(5)
      DIMENSION WBO(3)
      DO 5 I=1,3
    5 WBO(I)=UBO(I)
C        CALCULATE MIN AND MAX
      VMIN=1.0E38
      VMAX=-1.0E38
      IJ=NO*(NOVAR-1)
      DO 30 J=1,NO
      IJ=IJ+1
      IF(S(J)) 10,30,10
   10 IF(A(IJ)-VMIN) 15,20,20
   15 VMIN=A(IJ)
   20 IF(A(IJ)-VMAX) 30,30,25
   25 VMAX=A(IJ)
   30 CONTINUE
      STATS(4)=VMIN
      STATS(5)=VMAX
C        DETERMINE LIMITS
      IF(UBO(1)-UBO(3)) 40,35,40
   35 UBO(1)=VMIN
      UBO(3)=VMAX
   40 INN=UBO(2)
C        CLEAR OUTPUT AREAS
      DO 45 I=1,INN
      FREQ(I)=0.0
   45 PCT(I)=0.0
      DO 50 I=1,3
   50 STATS(I)=0.0
C        CALCULATE INTERVAL SIZE
      SINT=ABS((UBO(3)-UBO(1))/(UBO(2)-2.0))
C        TEST SUBSET VECTOR
      SCNT=0.0
      IJ=NO*(NOVAR-1)
      DO 75 J=1,NO
      IJ=IJ+1
      IF(S(J)) 55,75,55
   55 SCNT=SCNT+1.0
C        DEVELOP TOTAL AND FREQUENCIES
      STATS(1)=STATS(1)+A(IJ)
      STATS(3)=STATS(3)+A(IJ)*A(IJ)
      TEMP=UBO(1)-SINT
      INTX=INN-1
      DO 60 I=1,INTX
      TEMP=TEMP+SINT
      IF(A(IJ)-TEMP) 70,60,60
   60 CONTINUE
      IF(A(IJ)-TEMP) 75,65,65
   65 FREQ(INN)=FREQ(INN)+1.0
      GO TO 75
   70 FREQ(I)=FREQ(I)+1.0
   75 CONTINUE
C        CALCULATE RELATIVE FREQUENCIES
      DO 80 I=1,INN
   80 PCT(I)=FREQ(I)*100.0/SCNT
C        CALCULATE MEAN AND STANDARD DEVIATION
      IF(SCNT-1.0) 85,85,90
   85 STATS(2)=0.0
      STATS(3)=0.0
      GO TO 95
   90 STATS(2)=STATS(1)/SCNT
      STATS(3)=SQRT(ABS((STATS(3)-STATS(1)*STATS(1)/SCNT)/(SCNT-1.0)))
   95 DO 100 I=1,3
  100 UBO(I)=WBO(I)
      RETURN
      END
```

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 5.

Symbols $\geq$ and $<$ in Figure 5 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:

$$P_{ij} = \frac{100F_{ij}}{N} \qquad (2)$$

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:

$$s = \sqrt{\frac{\sum_{i=1}^{n} X_i^2 - \left(\sum_{i=1}^{n} X_i\right)^2 / n}{n-1}} \qquad (4)$$

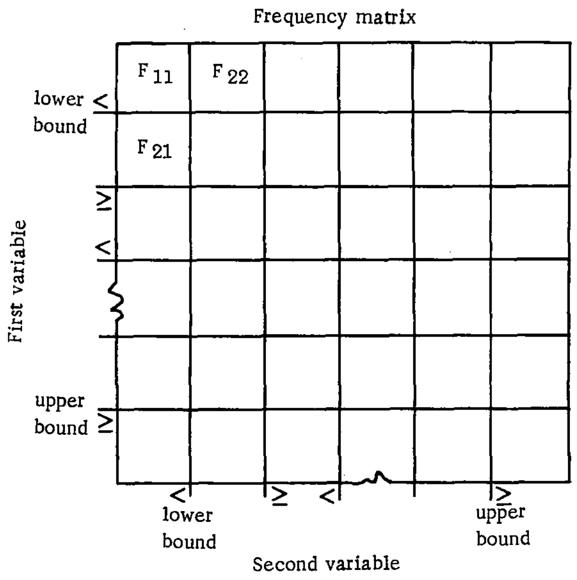


Figure 5. Frequency matrix

Subroutine TAB2

Purpose:
Perform 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	-	Observation matrix, NO by NV
S	-	Input vector giving subset of A. Only those observations with a corresponding non-zero S(J) are considered. Vector length is NO.
NOV	-	Variables to be cross-tabulated. NOV(1) is variable 1, NOV(2) is variable 2. Vector length is 2.

UBO	-	3 by 2 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 variable 1, the program uses the minimum and maximum values on each variable. Number of intervals must include two cells for under and above limits.
FREQ	-	Output matrix of frequencies in the two-way classification. Order of matrix is INT1 by INT2, where INT1 is the number of intervals of variable 1 and INT2 is the number of intervals of variable 2. INT1 and INT2 must be specified in the second position of respective column of UBO matrix.
PCT	-	Output matrix of percent frequencies, same order as FREQ.
STAT1	-	Output matrix summarizing totals, means, and standard deviations for each class interval of variable 1. Order of matrix is 3 by INT1.
STAT2	-	Same as STAT1 but over variable 2. Order of matrix is 3 by INT2.
NO	-	Number of observations.
NV	-	Number of variables for each observation.

Remarks:
None.

Subroutines and function subprograms required:
None.

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.

```
      SUBROUTINE TAB2(A,S,NOV,UBO,FREQ,PCT,STAT1,STAT2,NO,NV)
      DIMENSION A(1),S(1),NOV(2),UBO(3,2),FREQ(1),PCT(1),STAT1(1),
     1STAT2(2),SINT(2)
      DIMENSION WBO(3,2)
      DO 5 I=1,3
      DO 5 J=1,2
    5 WBO(I,J)=UBO(I,J)
C        DETERMINE LIMITS
      DO 40 I=1,2
      IF(UBO(1,I)-UBO(3,I))40,10,40
   10 VMIN=1.0E38
      VMAX=-1.0E38
      IJ=NO*(NOV(I)-1)
      DO 35 J=1,NO
      IJ=IJ+1
      IF(S(J)) 15,35,15
   15 IF(A(IJ)-VMIN) 20,25,25
   20 VMIN=A(IJ)
   25 IF(A(IJ)-VMAX) 35,35,30
   30 VMAX=A(IJ)
   35 CONTINUE
      UBO(1,I)=VMIN
      UBO(3,I)=VMAX
   40 CONTINUE
C        CALCULATE INTERVAL SIZE
   45 DO 50 I=1,2
   50 SINT(I)=ABS((UBO(3,I)-UBO(1,I))/(UBO(2,I)-2.0))
C        CLEAR OUTPUT AREAS
      INT1=UBO(2,1)
      INT2=UBO(2,2)
      INTT=INT1*INT2
      DO 55 I=1,INTT
      FREQ(I)=0.0
   55 PCT(I)=0.0
      INTY=3*INT1
      DO 60 I=1,INTY
   60 STAT1(I)=0.0
      INTZ=3*INT2
      DO 65 I=1,INTZ
   65 STAT2(I)=0.0
C        TEST SUBSET VECTOR
      SCNT=0.0
      INTY=INT1-1
      INTX=INT2-1
      IJ=NO*(NOV(1)-1)
      IJX=NO*(NOV(2)-1)
      DO 95 J=1,NO
      IJ=IJ+1
      IJX=IJX+1
      IF(S(J)) 70,95,70
   70 SCNT=SCNT+1.0
C        CALCULATE FREQUENCIES
      TEMP1=UBO(1,1)-SINT(1)
      DO 75 IY=1,INTY
      TEMP1=TEMP1+SINT(1)
      IF(A(IJ)-TEMP1) 80,75,75
   75 CONTINUE
      IY=INT1
   80 IYY=3*(IY-1)+1
      STAT1(IYY)=STAT1(IYY)+A(IJ)
      IYY=IYY+1
      STAT1(IYY)=STAT1(IYY)+1.0
      IYY=IYY+1
      STAT1(IYY)=STAT1(IYY)+A(IJ)*A(IJ)
      TEMP2=UBO(1,2)-SINT(2)
      DO 85 IX=1,INTX
      TEMP2=TEMP2+SINT(2)
      IF(A(IJX)-TEMP2) 90,85,85
   85 CONTINUE
      IX=INT2
   90 IJF=INT1*(IX-1)+IY
      FREQ(IJF)=FREQ(IJF)+1.0
      IX=3*(IX-1)+1
      STAT2(IX)=STAT2(IX)+A(IJX)
      IX=IX+1
      STAT2(IX)=STAT2(IX)+1.0
      IX=IX+1
      STAT2(IX)=STAT2(IX)+A(IJX)*A(IJX)
   95 CONTINUE
C        CALCULATE PERCENT FREQUENCIES
      DO 100 I=1,INTT
  100 PCT(I)=FREQ(I)*100.0/SCNT
C        CALCULATE TOTALS, MEANS, STANDARD DEVIATIONS
      IXY=-1
      DO 120 I=1,INT1
      IXY=IXY+3
      ISD=IXY+1
      TEMP1=STAT1(IXY)
      SUM=STAT1(IXY-1)
      IF(TEMP1-1.0) 120,105,110
  105 STAT1(ISD)=0.0
      GO TO 115
  110 STAT1(ISD)=SQRT(ABS((STAT1(ISD)-SUM*SUM/TEMP1)/(TEMP1-1.0)))
  115 STAT1(IXY)=SUM/TEMP1
  120 CONTINUE
      IXX=-1
      DO 140 I=1,INT2
      IXX=IXX+3
      ISD=IXX+1
      TEMP2=STAT2(IXX)
      SUM=STAT2(IXX-1)
      IF(TEMP2-1.0) 140,125,130
  125 STAT2(ISD)=0.0
      GO TO 135
  130 STAT2(ISD)=SQRT(ABS((STAT2(ISD)-SUM*SUM/TEMP2)/(TEMP2-1.0)))
  135 STAT2(IXX)=SUM/TEMP2
  140 CONTINUE
      DO 150 I=1,3
      DO 150 J=1,2
  150 UBO(I,J)=WBO(I,J)
      RETURN
      END
```

SUBMX

Purpose:
Based on vector S derived from subroutine SUBST or ABSNT, this subroutine copies from a larger matrix of observation data a subset matrix of those observations which have satisfied certain condition. This subroutine is normally used prior to statistical analyses (e.g., multiple regression, factor analysis).

Usage:
CALL SUBMX (A,D,S,NO,NV,N)

Description of parameters:

A	-	Input matrix of observations, NO by NV.
D	-	Output matrix of observations, N by NV.
S	-	Input vector of length NO containing the codes derived from subroutine SUBST or ABSNT.
NO	-	Number of observations.
NV	-	Number of variables.
N	-	Output variable containing the number of non-zero codes in vector S.

Remarks:
Matrix D can be in the same location as matrix A.

Subroutines and function subprograms required:
None.

Method:
If S(I) contains a non-zero code, I-th observation is copied from the input matrix to the output matrix.

```
      SUBROUTINE SUBMX (A,D,S,NO,NV,N)
      DIMENSION A(1),D(1),S(1)
      L=0
      LL=0
      DO 20 J=1,NV
      DO 15 I=1,NO
      L=L+1
      IF(S(I)) 15, 15, 10
   10 LL=LL+1
      D(LL)=A(L)
   15 CONTINUE
   20 CONTINUE
C        COUNT NON-ZERO CODES IN VECTOR S
      N=0
      DO 30 I=1,NO
      IF(S(I)) 30, 30, 25
   25 N=N+1
   30 CONTINUE
      RETURN
      END
```

MOMEN

This subroutine 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:

$$n = (UBO_3 - UBO_1)/UBO_2 \qquad (1)$$

where UBO_1 = given lower bound

UBO_2 = given class interval

UBO_3 = given upper bound

and the total frequency as follows:

$$T = \sum_{i=1}^{n} F_i \qquad (2)$$

where F_i = frequency count in i-th interval.

Then, the following are computed:

First Moment (Mean):

$$ANS_1 = \frac{\sum_{i=1}^{n} F_i \left[UBO_1 + (i-0.5)\, UBO_2\right]}{T} \qquad (3)$$

j-th Moment (Variance):

$$ANS_j = \frac{\sum_{i=1}^{n} F_i \left[UBO_1 + (i-0.5)\, UBO_2 - ANS_1\right]^j}{T} \qquad (4)$$

$j = 2, 3, 4$

These moments are biased and not corrected for grouping

Subroutine MOMEN

Purpose:

To find the first four moments for grouped data on equal class intervals.

Usage:

CALL MOMEN (F,UBO,NOP,ANS)

Description of Parameters:

F	-	Grouped data (frequencies). Given as a vector of length (UBO(3)-UBO(1))/UBO(2)
UBO	-	3 cell vector, UBO(1) is lower bound and UBO(3) upper bound on data. UBO(2) is class interval. Note that UBO(3) must be greater than UBO(1).
NOP	-	Option parameter. If NOP = 1, ANS(1) = MEAN. If NOP = 2, ANS(2) = second moment. If NOP = 3, ANS(3) = third moment. If NOP = 4, ANS(4) = fourth moment. If NOP = 5, all four moments are filled in.
ANS	-	Output vector of length 4 into which moments are put.

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.

Subroutines and function subprograms required:

None.

Method:

Refer to M. G. Kendall, 'The Advanced Theory of Statistics', V.1, Hafner Publishing Company, 1958, Chapter 3.

```
      SUBROUTINE MOMEN (F,UBO,NOP,ANS)
      DIMENSION F(1),UBO(3),ANS(4)
      DO 100 I=1,4
  100 ANS(I)=0.0
C        CALCULATE THE NUMBER OF CLASS INTERVALS
      N=(UBO(3)-UBO(1))/UBO(2)+0.5
C        CALCULATE TOTAL FREQUENCY
      T=0.0
      DO 110 I=1,N
  110 T=T+F(I)
      IF(NOP-5) 130, 120, 115
  115 NOP=5
  120 JUMP=1
      GO TO 150
  130 JUMP=2
C        FIRST MOMENT
  150 DO 160 I=1,N
      FI=I
  160 ANS(1)=ANS(1)+F(I)*(UBO(1)+(FI-0.5)*UBO(2))
      ANS(1)=ANS(1)/T
      GO TO (350,200,250,300,200), NOP
C        SECOND MOMENT
  200 DO 210 I=1,N
      FI=I
  210 ANS(2)=ANS(2)+F(I)*(UBO(1)+(FI-0.5)*UBO(2)-ANS(1))**2
      ANS(2)=ANS(2)/T
      GO TO (250,350), JUMP
C        THIRD MOMENT
  250 DO 260 I=1,N
      FI=I
  260 ANS(3)=ANS(3)+F(I)*(UBO(1)+(FI-0.5)*UBO(2)-ANS(1))**3
      ANS(3)=ANS(3)/T
      GO TO (300,350), JUMP
C        FOURTH MOMENT
  300 DO 310 I=1,N
      FI=I
  310 ANS(4)=ANS(4)+F(I)*(UBO(1)+(FI-0.5)*UBO(2)-ANS(1))**4
      ANS(4)=ANS(4)/T
  350 RETURN
      END
```

TTSTT

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:

$$SA^2 = \frac{\sum_{i=1}^{NA} (A_i - \bar{A})^2}{NA - 1}; \qquad SB^2 = \frac{\sum_{i=1}^{NB} (B_i - \bar{B})^2}{NB - 1} \tag{2}$$

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).

The subroutine computes:

$$ANS = \frac{\bar{B} - A}{SB} \cdot \sqrt{NB} \quad \text{(t-statistic)} \tag{3}$$

$$NDF = NB - 1 \quad \text{(degrees of freedom)} \tag{4}$$

Hypothesis: $\mu_A = \mu_B;\ \sigma_A^2 = \sigma_B^2$ (Option 2):

The subroutine computes:

$$ANS = \frac{\bar{B} - \bar{A}}{S} \cdot \frac{1}{\sqrt{\frac{1}{NA} + \frac{1}{NB}}} \quad \text{(t-statistic)} \tag{5}$$

$$NDF = NA + NB - 2 \quad \text{(degrees of freedom)} \tag{6}$$

$$\text{where } S = \sqrt{\frac{(NA - 1)SA^2 + (NB - 1)SB^2}{NA + NB - 2}} \tag{7}$$

Hypothesis: $\mu_A = \mu_B \left(\sigma_A^2 \neq \sigma_B^2\right)$ (Option 3):

The subroutine computes:

$$ANS = \frac{\bar{B} - \bar{A}}{\sqrt{\frac{SA^2}{NA} + \frac{SB^2}{NB}}} \quad \text{(t-statistic)} \tag{8}$$

$$NDF = \frac{\left(\frac{SA^2}{NA} + \frac{SB^2}{NB}\right)^2}{\left(\frac{SA^2}{NA}\right)^2 \Big/ (NA+1) + \left(\frac{SB^2}{NB}\right)^2 \Big/ (NB+1)} - 2 \qquad (9)$$

(degrees of freedom)

Note: The program returns a rounded NDF, not a truncated NDF.

Hypothesis: $\mu_A = \mu_B$ (no assumption on σ^2) (Option 4):

The subroutine computes:

$$ANS = \frac{\bar{D}}{SD} \cdot \sqrt{NB} \qquad \text{(t-statistic)} \qquad (10)$$

$$NDF = NB - 1 \qquad \text{(degrees of freedom)} \qquad (11)$$

where $\bar{D} = \bar{B} - \bar{A}$ (12)

$$SD = \sqrt{\frac{\sum_{i=1}^{NB} (B_i - A_i - \bar{D})^2}{NB - 1}} \qquad (13)$$

$NA = NB$

Subroutine TTSTT

Purpose:
To find certain T-statistics on the means of populations.

Usage:
CALL TTSTT (A,NA,B,NB,NOP,NDF,ANS)

Description of parameters:

A	-	Input vector of length NA containing data.
NA	-	Number of observations in A.
B	-	Input vector of length NB containing data.
NB	-	Number of observations in B.
NOP	-	Options for various hypotheses:
		NOP=1--- That population mean of B = given value 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 that the variance of B is not equal to the variance of A.
		NOP=4--- That population mean of B = population mean of A, given no information about variances of A and B. (Set NA=NB.)
NDF	-	Output variable containing degrees of freedom associated with T-statistic calculated.
ANS	-	T-statistic for given hypothesis.

Remarks:
NA and NB must be greater than 1, 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.

Subroutines and function subprograms required:
None.

Method:
Refer to Ostle, Bernard, 'Statistics in Research', Iowa State College Press, 1954, Chapter 5.

```
      SUBROUTINE TTSTT (A,NA,B,NB,NOP,NDF,ANS)
      DIMENSION A(1),B(1)
C        INITIALIZATION
      NDF=0
      ANS=0.0
C        CALCULATE THE MEAN OF A
      AMEAN=0.0
      DO 110 I=1,NA
  110 AMEAN=AMEAN+A(I)
      FNA=NA
      AMEAN=AMEAN/FNA
C        CALCULATE THE MEAN OF B
  115 BMEAN=0.0
      DO 120 I=1,NB
  120 BMEAN=BMEAN+B(I)
      FNB=NB
      BMEAN=BMEAN/FNB
      IF(NOP-4) 122, 180, 200
  122 IF(NOP-1) 200, 135, 125
C        CALCULATE THE VARIANCE OF A
  125 SA2=0.0
      DO 130 I=1,NA
  130 SA2=SA2+(A(I)-AMEAN)**2
      SA2=SA2/(FNA-1.0)
C        CALCULATE THE VARIANCE OF B
  135 SB2=0.0
      DO 140 I=1,NB
  140 SB2=SB2+(B(I)-BMEAN)**2
      SB2=SB2/(FNB-1.0)
      GO TO (150,160,170), NOP
C        OPTION 1
  150 ANS=((BMEAN-AMEAN)/SQRT(SB2))*SQRT(FNB)
      NDF=NB-1
      GO TO 200
C        OPTION 2
  160 NDF=NA+NB-2
      FNDF=NDF
      S=SQRT(((FNA-1.0)*SA2+(FNB-1.0)*SB2)/FNDF)
      ANS=((BMEAN-AMEAN)/S)*(1.0/SQRT(1.0/FNA+1.0/FNB))
      GO TO 200
C        OPTION 3
  170 ANS=(BMEAN-AMEAN)/SQRT(SA2/FNA+SB2/FNB)
      A1=(SA2/FNA+SB2/FNB)**2
      A2=(SA2/FNA)**2/(FNA+1.0)+(SB2/FNB)**2/(FNB+1.0)
      NDF=A1/A2-2.0+0.5
      GO TO 200
C        OPTION 4
  180 SD=0.0
      D=BMEAN-AMEAN
      DO 190 I=1,NB
  190 SD=SD+(B(I)-A(I)-D)**2
      SD=SQRT(SD/(FNB-1.0))
      ANS=(D/SD)*SQRT(FNB)
      NDF=NB-1
  200 RETURN
      END
```

CORRE

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:

$$S_{jk} = \sum_{i=1}^{n} \left(X_{ij} - T_j\right) \left(X_{ik} - T_k\right) - \frac{\sum_{i=1}^{n} \left(X_{ij} - T_j\right) \sum_{i=1}^{n} \left(X_{ik} - T_k\right)}{n} \qquad (1)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

$$T_j = \frac{\sum_{i=1}^{m} X_{ij}}{m} \qquad (2)$$

(These temporary means T_j are subtracted from the data in equation (1) to obtain computational accuracy.)

Means: $$\bar{X}_j = \frac{\sum_{i=1}^{n} X_{ij}}{n} \qquad (3)$$

where j = 1, 2, ..., m

Correlation coefficients:

$$r_{jk} = \frac{S_{jk}}{\sqrt{S_{jj}}\ \sqrt{S_{kk}}} \qquad (4)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

Standard deviations:

$$s_j = \frac{\sqrt{S_{jj}}}{\sqrt{n-1}} \qquad (5)$$

where j = 1, 2, ..., m

Subroutine CORRE

Purpose:
Compute means, standard deviations, sums of cross-products of deviations, and correlation coefficients.

Usage:
CALL CORRE (N, M, IO, X, XBAR, STD, RX, R, B, D, T)

Description of parameters:

N	-	Number of observations.
M	-	Number of variables.
IO	-	Option code for input data. 0 If data are to be read in from input device in the special subroutine named data. (See "subroutines and function subprograms required" below.) 1 If all data are already in core.
X	-	If IO=0, the value of X is 0.0. If IO=1, X is the input matrix (N by M) containing data.
XBAR	-	Output vector of length M containing means.
STD	-	Output vector of length M containing standard deviations.
RX	-	Output matrix (M by M) containing sums of cross-products of deviations from means.
R	-	Output matrix (only upper triangular portion of the symmetric matrix of M by M) containing correlation coefficients. (Storage mode of 1)
B	-	Output vector of length M containing the diagonal of the matrix of sums of cross-products of deviations from means.
D	-	Working vector of length M.
T	-	Working vector of length M.

Remarks:
None.

Subroutines and function subprograms required:
DATA(M,D) - This subroutine must be provided by the user.
(1) If IO=0, this subroutine is expected to furnish an observation in vector D from an external input device.

(2) If IO=1, this subroutine is not used by CORRE but must exist in job deck. If user has not supplied a subroutine named DATA, the following is suggested.

```
SUBROUTINE DATA
RETURN
END
```

Method:

Product-moment correlation coefficients are computed.

```
      SUBROUTINE CORRE (N,M,IO,X,XBAR,STD,RX,R,B,D,T)
      DIMENSION X(1),XBAR(1),STD(1),RX(1),R(1),B(1),D(1),T(1)
C        INITIALIZATION
      DO 100 J=1,M
      B(J)=0.0
  100 T(J)=0.0
      K=(M*M+M)/2
      DO 102 I=1,K
  102 R(I)=0.0
      FN=N
      L=0
      IF(IO) 105, 127, 105
C        DATA ARE ALREADY IN CORE
  105 DO 108 J=1,M
      DO 107 I=1,N
      L=L+1
  107 T(J)=T(J)+X(L)
      XBAR(J)=T(J)
  108 T(J)=T(J)/FN
      DO 115 I=1,N
      JK=0
      L=I-N
      DO 110 J=1,M
      L=L+N
      D(J)=X(L)-T(J)
  110 B(J)=B(J)+D(J)
      DO 115 J=1,M
      DO 115 K=1,J
      JK=JK+1
  115 R(JK)=R(JK)+D(J)*D(K)
      GO TO 205
C        READ OBSERVATIONS AND CALCULATE TEMPORARY
C        MEANS FROM THESE DATA IN T(J)
  127 IF(N-M) 130, 130, 135
  130 KK=N
      GO TO 137
  135 KK=M
  137 DO 140 I=1,KK
      CALL DATA (M,D)
      DO 140 J=1,M
      T(J)=T(J)+D(J)
      L=L+1
  140 RX(L)=D(J)
      FKK=KK
      DO 150 J=1,M
      XBAR(J)=T(J)
  150 T(J)=T(J)/FKK
C        CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS
C        FROM TEMPORARY MEANS FOR M OBSERVATIONS
      L=0
      DO 180 I=1,KK
      JK=0
      DO 170 J=1,M
      L=L+1
  170 D(J)=RX(L)-T(J)
      DO 180 J=1,M
      B(J)=B(J)+D(J)
      DO 180 K=1,J
      JK=JK+1
  180 R(JK)=R(JK)+D(J)*D(K)
      IF(N-KK) 205, 205, 185
C        READ THE REST OF OBSERVATIONS ONE AT A TIME, SUM
C        THE OBSERVATION, AND CALCULATE SUMS OF CROSS-
C        PRODUCTS OF DEVIATIONS FROM TEMPORARY MEANS
  185 KK=N-KK
      DO 200 I=1,KK
      JK=0
      CALL DATA (M,D)
      DO 190 J=1,M
      XBAR(J)=XBAR(J)+D(J)
      D(J)=D(J)-T(J)
  190 B(J)=B(J)+D(J)
      DO 200 J=1,M
      DO 200 K=1,J
      JK=JK+1
  200 R(JK)=R(JK)+D(J)*D(K)
C        CALCULATE MEANS
  205 JK=0
      DO 210 J=1,M
      XBAR(J)=XBAR(J)/FN
C        ADJUST SUMS OF CROSS-PRODUCTS OF DEVIATIONS
C        FROM TEMPORARY MEANS
      DO 210 K=1,J
      JK=JK+1
  210 R(JK)=R(JK)-B(J)*B(K)/FN
C        CALCULATE CORRELATION COEFFICIENTS
      JK=0
      DO 220 J=1,M
      JK=JK+J
  220 STD(J)= SQRT( ABS(R(JK)))
      DO 230 J=1,M
      DO 230 K=J,M
      JK=J+(K*K-K)/2
      L=M*(J-1)+K
      RX(L)=R(JK)
      L=M*(K-1)+J
      RX(L)=R(JK)
      IF(STD(J)*STD(K))225,222,225
  222 R(JK)=0.0
      GO TO 230
  225 R(JK)=R(JK)/(STD(J)*STD(K))
  230 CONTINUE
C        CALCULATE STANDARD DEVIATIONS
      FN=SQRT(FN-1.0)
      DO 240 J=1,M
  240 STD(J)=STD(J)/FN
C        COPY THE DIAGONAL OF THE MATRIX OF SUMS OF CROSS-PRODUCTS OF
C        DEVIATIONS FROM MEANS.
      L=-M
      DO 250 I=1,M
      L=L+M+1
  250 B(I)=RX(L)
      RETURN
      END
```

Statistics - Multiple Linear Regression

In the Scientific Subroutine Package, multiple linear regression is normally performed by calling four subroutines in sequence.

1. CORRE - to find means, standard deviations, and correlation matrix
2. ORDER - to choose a dependent variable and a subset of independent variables from a larger set of variables
3. MINV - to invert the correlation matrix of the subset selected by ORDER
4. MULTR - to compute the regression coefficients, b_0, b_1, b_2, ..., b_m, and various confidence measures

The subroutine CORRE works in either of two ways: (1) it expects all observations in *core*, *or* (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the description of subroutine CORRE).

ORDER

Purpose:
Construct from a larger matrix of correlation coefficients a subset matrix of intercorrelations among independent variables and a vector of intercorrelations of independent variables with dependent variable. This subroutine is normally used in the performance of multiple and polynomial regression analyses.

Usage:
CALL ORDER (M, R, NDEP, K, ISAVE, RX, RY)

Description of parameters:

M	-	Number of variables and order of matrix R.
R	-	Input matrix containing correlation coefficients. This subroutine expects only upper triangular portion of the symmetric matrix to be stored (by column) in R. (Storage mode of 1.)
NDEP	-	The subscript number of the dependent variable.
K	-	Number of independent variables to be included in the forthcoming regression.
ISAVE	-	Input vector of length K+1 containing, in ascending order, the subscript numbers of K independent variables to be included in the forthcoming regression. Upon returning to the calling routine, this vector contains, in addition, the subscript number of the dependent variable in K+1 position.
RX	-	Output matrix (K by K) containing intercorrelations among independent variables to be used in forthcoming regression.
RY	-	Output vector of length K containing intercorrelations of independent variables with dependent variables.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
From the subscript numbers of the variables to be included in the forthcoming regression, the subroutine constructs the matrix RX and the vector RY.

```
      SUBROUTINE ORDER (M,R,NDEP,K,ISAVE,RX,RY)
      DIMENSION R(1),ISAVE(1),RX(1),RY(1)
C        COPY INTERCORRELATIONS OF INDEPENDENT VARIABLES
C        WITH DEPENDENT VARIABLE
      MM=0
      DO 130 J=1,K
      L2=ISAVE(J)
      IF(NDEP-L2) 122, 123, 123
  122 L=NDEP+(L2*L2-L2)/2
      GO TO 125
  123 L=L2+(NDEP*NDEP-NDEP)/2
  125 RY(J)=R(L)
C        COPY A SUBSET MATRIX OF INTERCORRELATIONS AMONG
C        INDEPENDENT VARIABLES
      DO 130 I=1,K
      L1=ISAVE(I)
      IF(L1-L2) 127, 128, 128
  127 L=L1+(L2*L2-L2)/2
      GO TO 129
  128 L=L2+(L1*L1-L1)/2
  129 MM=MM+1
  130 RX(MM)=R(L)
C        PLACE THE SUBSCRIPT NUMBER OF THE DEPENDENT
C        VARIABLE IN ISAVE(K+1)
      ISAVE(K+1)=NDEP
      RETURN
      END
```

MULTR

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 ith independent variable with dependent variable

r_{ij}^{-1} = the inverse of intercorrelation r_{ij}

$i, j = 1, 2, \ldots, k$ imply independent variables

r_{iy} and r_{ij}^{-1} are input to this subroutine.

Then, the regression coefficients are calculated as follows:

$$b_j = \beta_j \cdot \frac{s_y}{s_j} \qquad (2)$$

where s_y = standard deviation of dependent variable

s_j = standard deviation of jth independent variable

$j = 1, 2, \ldots, k$

s_y and s_j are input to this subroutine.

The intercept is found by the following equation:

$$b_0 = \overline{Y} - \sum_{j=1}^{k} b_j \cdot \overline{X}_j \qquad (3)$$

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:

$$R^2 = \sum_{i=1}^{k} \beta_i r_{iy} \qquad (4)$$

and taking the square root of R^2:

$$R = \sqrt{R^2} \qquad (5)$$

The sum of squares attributable to the regression is found by:

$$SSAR = R^2 \cdot D_{yy} \qquad (6)$$

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:

$$SSDR = D_{yy} - SSAR \qquad (7)$$

Then, the F-value for the analysis of variance is calculated as follows:

$$F = \frac{SSAR/k}{SSDR/(n-k-1)} = \frac{SSAR(n-k-1)}{SSDR(k)} \qquad (8)$$

Certain other statistics are calculated as follows:

Variance and standard error of estimate:

$$S^2_{y.12\ldots k} = \frac{SSDR}{n-k-1} \qquad (9)$$

where n = number of observations

$$S_{y.12\ldots k} = \sqrt{S^2_{y.12\ldots k}} \qquad (10)$$

Standard deviations of regression coefficients:

$$S_{b_j} = \sqrt{\frac{r_{jj}^{-1}}{D_{jj}} \cdot S^2_{y.12\ldots k}} \qquad (11)$$

where D_{jj} = sum of squares of deviations from mean for jth independent variable. D_{jj} is input to this subroutine.

$j = 1, 2, \ldots, k$

Computed t:

$$t_j = \frac{b_j}{S_{b_j}} \qquad (12)$$

$j = 1, 2, \ldots, k$

Subroutine MULTR

Purpose:

Perform a multiple linear regression analysis for a dependent variable and a set of independent variables. This subroutine is normally used in the performance of multiple and polynomial regression analyses.

Usage:

CALL MULTR (N, K, XBAR, STD, D, RX, RY, ISAVE, B, SB, T, ANS)

Description of parameters:

N	-	Number of observations.
K	-	Number of independent variables in this regression.
XBAR	-	Input vector of length M containing means of all variables. M is number of variables in observations.
STD	-	Input vector of length M containing standard deviations of all variables.
D	-	Input vector of length M containing the diagonal of the matrix of sums of cross-products of deviations from means for all variables.
RX	-	Input matrix (K by K) containing the inverse of intercorrelations among independent variables.
RY	-	Input vector of length K containing intercorrelations of independent variables with dependent variable.
ISAVE	-	Input vector of length K+1 containing subscripts of independent variables in ascending order. The subscript of the dependent variable is stored in the last, K+1, position.
B	-	Output vector of length K containing regression coefficients.
SB	-	Output vector of length K containing standard deviations of regression coefficients.
T	-	Output vector of length K containing T-values.
ANS	-	Output vector of length 10 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:

N must be greater than K+1.

Subroutines and function subprograms required:

None.

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.

```
      SUBROUTINE MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS)
      DIMENSION XBAR(1),STD(1),D(1),RX(1),RY(1),ISAVE(1),B(1),SB(1),
     1          T(1),ANS(10)
      MM=K+1
C        BETA WEIGHTS
      DO 100 J=1,K
  100 B(J)=0.0
      DO 110 J=1,K
      L1=K*(J-1)
      DO 110 I=1,K
      L=L1+I
  110 B(J)=B(J)+RY(I)*RX(L)
      RM=0.0
      BO=0.0
      L1=ISAVE(MM)
C        COEFFICIENT OF DETERMINATION
      DO 120 I=1,K
      RM=RM+B(I)*RY(I)
C        REGRESSION COEFFICIENTS
      L=ISAVE(I)
      B(I)=B(I)*(STD(L1)/STD(L))
C        INTERCEPT
  120 BO=BO+B(I)*XBAR(L)
      BO=XBAR(L1)-BO
C        SUM OF SQUARES ATTRIBUTABLE TO REGRESSION
      SSAR=RM*D(L1)
C        MULTIPLE CORRELATION COEFFICIENT
  122 RM= SQRT( ABS(RM))
C        SUM OF SQUARES OF DEVIATIONS FROM REGRESSION
      SSDR=D(L1)-SSAR
C        VARIANCE OF ESTIMATE
      FN=N-K-1
      SY=SSDR/FN
C        STANDARD DEVIATIONS OF REGRESSION COEFFICIENTS
      DO 130 J=1,K
      L1=K*(J-1)+J
      L=ISAVE(J)
  125 SB(J)= SQRT( ABS((RX(L1)/D(L))*SY))
C        COMPUTED T-VALUES
  130 T(J)=B(J)/SB(J)
C        STANDARD ERROR OF ESTIMATE
  135 SY= SQRT( ABS(SY))
C        F VALUE
      FK=K
      SSARM=SSAR/FK
      SSDRM=SSDR/FN
      F=SSARM/SSDRM
      ANS(1)=BO
      ANS(2)=RM
      ANS(3)=SY
      ANS(4)=SSAR
      ANS(5)=FK
      ANS(6)=SSARM
      ANS(7)=SSDR
      ANS(8)=FN
      ANS(9)=SSDRM
      ANS(10)=F
      RETURN
      END
```

Statistics - Polynomial Regression

Polynomial regression is a statistical technique for finding the coefficients, $b_0, b_1, b_2, \ldots, b_m$, in the functional relationship of the form:

$$y = b_0 + b_1 x + b_2 x^2 + \ldots + b_m x^m$$

between a dependent variable y and a single independent variable x.

In the Scientific Subroutine Package, polynomial regression is normally performed by calling the following four subroutines in sequence:

1. GDATA - to generate the powers of the independent variable and find means, standard deviations, and correlation matrix
2. ORDER - to choose a dependent variable and subset of independent variables from a larger set of variables
3. MINV - to invert the correlation coefficient matrix
4. MULTR - to compute the regression coefficients, $b_0, b_1, b_2, \ldots, b_m$, and various confidence measures

The special subroutine PLOT may be used to plot Y values and Y estimates.

GDATA

This subroutine generates independent variables up to the mth power (the highest degree polynomial specified) and calculates means, standard deviations, sums of cross-products of deviations from means, and product moment correlation coefficients.

X_{i1} denotes the ith case of the independent variable;

X_{ip} denotes the ith case of the dependent variable,

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

n - number of cases (observations)

$p = m + 1$

m = highest degree polynomial specified

The subroutine GDATA generates powers of the independent variable as follows:

$$\begin{aligned} X_{i2} &= X_{i1} \cdot X_{i1} \\ X_{i3} &= X_{i2} \cdot X_{i1} \\ X_{i4} &= X_{i3} \cdot X_{i1} \\ &\cdot \\ &\cdot \\ &\cdot \\ X_{im} &= X_{i,m-1} \cdot X_{i1} \end{aligned} \qquad (1)$$

where i and m are as defined as above.

Then, the following are calculated:

Means:

$$\bar{X}_j = \frac{\sum_{i=1}^{n} X_{ij}}{n} \qquad (2)$$

where $j = 1, 2, \ldots, p$

Sums of cross-products of deviations from means:

$$D_{jk} = \sum_{i=1}^{n}\left(X_{ij} - \bar{X}_j\right)\left(X_{ik} - \bar{X}_k\right) - \frac{\sum_{i=1}^{n}\left(X_{ij} - \bar{X}_j\right) \sum_{i=1}^{n}\left(X_{ik} - \bar{X}_k\right)}{n} \qquad (3)$$

where j = 1, 2, ..., p; k = 1, 2, ..., p.

Correlation coefficients:

$$r_{ij} = \frac{D_{ij}}{\sqrt{D_{ii}}\ \sqrt{D_{jj}}} \qquad (4)$$

where i = 1, 2, ..., p; j = 1, 2, ..., p.

Standard deviations:

$$s_j = \frac{\sqrt{D_{jj}}}{\sqrt{n-1}} \qquad (5)$$

where j = 1, 2, ..., p

Subroutine GDATA

Purpose:
Generate independent variables up to the M^th^ power (the highest degree polynomial specified) and compute means, standard deviations, and correlation coefficients. This subroutine is normally called before subroutines ORDER, MINV and MULTR in the performance of a polynomial regression.

Usage:
CALL GDATA (N, M, X, XBAR, STD, D, SUMSQ)

Description of parameters:

N	-	Number of observations.
M	-	The highest degree polynomial to be fitted.
X	-	Input matrix (N by M+1). When the subroutine is called, data for the independent variable are stored in the first column of matrix X, and data for the dependent variable are stored in the last column of the matrix. Upon returning to the calling routine, generated powers of the independent variable are stored in columns 2 through M.
XBAR	-	Output vector of length M+1 containing means of independent and dependent variables.
STD	-	Output vector of length M+1 containing standard deviations of independent and dependent variables.
D	-	Output matrix (only upper triangular portion of the symmetric matrix of M+1 by M+1) containing correlation coefficients. (Storage Mode of 1.)
SUMSQ	-	Output vector of length M+1 containing sums of products of deviations from means of independent and dependent variables.

Remarks:
N must be greater than M+1.
If M is equal to 5 or greater, single precision may not be sufficient to give satisfactory computational results.

Subroutines and function subprograms required:
None.

Method:
Refer to B. Ostle, 'Statistics in Research', The Iowa State College Press, 1954, Chapter 6.

```
      SUBROUTINE GDATA (N,M,X,XBAR,STD,D,SUMSQ)
      DIMENSION X(1),XBAR(1),STD(1),D(1),SUMSQ(1)
C        GENERATE INDEPENDENT VARIABLES
      IF (M-1 ) 105,105,90
   90 L1=0
      DO 100 I=2,M
      L1=L1+N
      DO 100 J=1,N
      L=L1+J
      K=L-N
  100 X(L)=X(K)*X(J)
C        CALCULATE MEANS
  105 MM=M+1
      DF=N
      L=0
      DO 115 I=1,MM
      XBAR(I)=0.0
      DO 110 J=1,N
      L=L+1
  110 XBAR(I)=XBAR(I)+X(L)
  115 XBAR(I)=XBAR(I)/DF
      DO 130 I=1,MM
  130 STD(I)=0.0
C        CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS
      L=((MM+1)*MM)/2
      DO 150 I=1,L
  150 D(I)=0.0
      DO 170 K=1,N
      L=0
      DO 170 J=1,MM
      L2=N*(J-1)+K
      T2=X(L2)-XBAR(J)
      STD(J)=STD(J)+T2
      DO 170 I=1,J
      L1=N*(I-1)+K
      T1=X(L1)-XBAR(I)
      L=L+1
  170 D(L)=D(L)+T1*T2
      L=0
      DO 175 J=1,MM
      DO 175 I=1,J
      L=L+1
  175 D(L)=D(L)-STD(I)*STD(J)/DF
      L=0
      DO 180 I=1,MM
      L=L+I
      SUMSQ(I)=D(L)
  180 STD(I)= SQRT( ABS(D(L)))
C        CALCULATE CORRELATION COEFFICIENTS
      L=0
      DO 190 J=1,MM
      DO 190 I=1,J
      L=L+1
  190 D(L)=D(L)/(STD(I)*STD(J))
C        CALCULATE STANDARD DEVIATIONS
      DF=SQRT(DF-1.0)
      DO 200 I=1,MM
  200 STD(I)=STD(I)/DF
      RETURN
      END
```

In the Scientific Subroutine Package, canonical correlation analysis is normally performed by calling the following five subroutines:

1. CORRE - to compute means, standard deviations, and correlation matrix
2. MINV - to invert a part of the correlation matrix
3. EIGEN - to compute eigenvalues and eigenvectors
4. NROOT - to compute eigenvalues and eigenvectors of real nonsymmetric matrix of the form $B^{-1} A$
5. CANOR - to compute canonical correlations and coefficients

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the description of subroutine CORRE).

CANOR

This subroutine performs a canonical correlation analysis between two sets of variables.

The matrix of intercorrelations, R, is partitioned into four submatrices:

$$R = \left[\begin{array}{c|c} R_{11} & R_{12} \\ \hline R_{21} & R_{22} \end{array}\right] \tag{1}$$

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:

$$\left| R_{22}^{-1} R_{21} R_{11}^{-1} R_{12} - \lambda I \right| = 0 \tag{2}$$

is then solved for all values of λ, eigenvalues, in the following matrix operation:

$$T = R_{11}^{-1} R_{12} \tag{3}$$

$$A = R_{21} T \tag{4}$$

The subroutine NROOT 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:

$$\text{CANR} = \sqrt{\lambda_i} \tag{5}$$

where λ_i = ith eigenvalue

Chi-square:

$$\chi^2 = -\left[n - 0.5\,(p + q + 1)\right] \log_e \Lambda \tag{6}$$

where n = number of observations

$$\Lambda = \prod_{j=1}^{q} (1 - \lambda_j);$$

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 $\{t_{jk}\} = T = R_{11}^{-1} R_{12}$

$j = 1, 2, \ldots, p$

Subroutine CANOR

Purpose:

Compute the canonical correlations between two sets of variables. CANOR is normally preceded by a call to subroutine CORRE.

Usage:

CALL CANOR (N, MP, MQ, RR, ROOTS, WLAM, CANR, CHISQ, NDF, COEFR, COEFL, R)

Description of parameters:

N	-	Number of observations.
MP	-	Number of left hand variables.
MQ	-	Number of right hand variables.
RR	-	Input matrix (only upper triangular portion of the symmetric matrix of M by M, where M = MP + MQ) containing correlation coefficients. (Storage mode of 1.)
ROOTS	-	Output vector of length MQ containing eigenvalues computed in the NROOT subroutine.
WLAM	-	Output vector of length MQ containing lambda.
CANR	-	Output vector of length MQ containing canonical correlations.
CHISQ	-	Output vector of length MQ containing the values of chi-squares.
NDF	-	Output vector of length MQ containing the degrees of freedom associated with chi-squares.
COEFR	-	Output matrix (MQ by MQ) containing MQ sets of right hand coefficients columnwise.
COEFL	-	Output matrix (MP by MQ) containing MQ sets of left hand coefficients columnwise.
R	-	Work matrix (M by M).

Remarks:

The number of left hand variables (MP) should be greater than or equal to the number of right hand variables (MQ). The values of canonical correlation, lambda, chi-square, degrees of freedom, and canonical coefficients are computed only for those eigenvalues in roots which are greater than zero.

Subroutines and function subprograms required:

MINV

NROOT (which, in turn, calls the subroutine EIGEN.)

Method:

Refer to W. W. Cooley and P. R. Lohnes, 'Multivariate Procedures for the Behavioral Sciences', John Wiley and Sons, 1962, Chapter 3.

```
      SUBROUTINE CANOR (N,MP,MQ,RR,ROOTS,WLAM,CANR,CHISQ,NDF,COEFR,
     1                  COEFL,R)
      DIMENSION RR(1),ROOTS(1),WLAM(1),CANR(1),CHISQ(1),NDF(1),COEFR(1),
     1          COEFL(1),R(1)
C        PARTITION INTERCORRELATIONS AMONG LEFT HAND VARIABLES, BETWEEN
C        LEFT AND RIGHT HAND VARIABLES, AND AMONG RIGHT HAND VARIABLES.
      M=MP+MQ
      N1=0
      DO 105 I=1,M
      DO 105 J=1,M
      IF(I-J) 102, 103, 103
  102 L=I+(J*J-J)/2
      GO TO 104
  103 L=J+(I*I-I)/2
  104 N1=N1+1
  105 R(N1)=RR(L)
      L=MP
      DO 108 J=2,MP
      N1=M*(J-1)
      DO 108 I=1,MP
      L=L+1
      N1=N1+1
  108 R(L)=R(N1)
      N2=MP+1
      L=0
      DO 110 J=N2,M
      N1=M*(J-1)
      DO 110 I=1,MP
      L=L+1
      N1=N1+1
  110 COEFL(L)=R(N1)
      L=0
      DO 120 J=N2,M
      N1=M*(J-1)+MP
      DO 120 I=N2,M
      L=L+1
      N1=N1+1
  120 COEFR(L)=R(N1)
C        SOLVE THE CANINICAL EQUATION
      L=MP*MP+1
      K=L+MP
      CALL MINV (R,MP,DET,R(L),R(K))
C        CALCULATE T = INVERSE OF R11 * R12
      DO 140 I=1,MP
      N2=0
      DO 130 J=1,MQ
      N1=I-MP
      ROOTS(J)=0.0
      DO 130 K=1,MP
      N1=N1+MP
      N2=N2+1
  130 ROOTS(J)=ROOTS(J)+R(N1)*COEFL(N2)
      L=I-MP
      DO 140 J=1,MQ
      L=L+MP
  140 R(L)=ROOTS(J)
C        CALCULATE A = R21 * T
      L=MP*MQ
      N3=L+1
      DO 160 J=1,MQ
      N1=0
      DO 160 I=1,MQ
      N2=MP*(J-1)
      SUM=0.0
      DO 150 K=1,MP
      N1=N1+1
      N2=N2+1
  150 SUM=SUM+COEFL(N1)*R(N2)
      L=L+1
  160 R(L)=SUM
C        CALCULATE EIGENVALUES WITH ASSOCIATED FIGENVECTORS OF THE
C        INVERSE OF R22 * A
      L=L+1
      CALL NROOT (MQ,R(N3),COEFR,ROOTS,R(L))
C        FOR EACH VALUE OF I = 1, 2, ...., MQ, CALCULATE THE FOLLOWING
C        STATISTICS
      DO 210 I=1,MQ
C        TEST WHETHER EIGENVALUE IS GREATER THAN ZERO
      IF(ROOTS(I)) 220, 220, 165
C        CANONICAL CORRELATION
  165 CANR(I)= SQRT(ROOTS(I))
C        CHI-SQUARE
      WLAM(I)=1.0
      DO 170 J=I,MQ
  170 WLAM(I)=WLAM(I)*(1.0-ROOTS(J))
      FN=N
      FMP=MP
      FMQ=MQ
      BAT = WLAM(I)
  175 CHISQ(I) = -(FN-0.5*(FMP+FMQ+1.0))*ALOG(BAT)
C        DEGREES OF FREEDOM FOR CHI-SQUARE
      N1=I-1
      NDF(I)=(MP-N1)*(MQ-N1)
C        I-TH SET OF RIGHT HAND COEFFICIENTS
      N1=MQ*(I-1)
      N2=MQ*(I-1)+L-1
      DO 180 J=1,MQ
      N1=N1+1
      N2=N2+1
  180 COEFR(N1)=R(N2)
C        I-TH SET OF LEFT HAND COEFFICIENTS
      DO 200 J=1,MP
      N1=J-MP
      N2=MQ*(I-1)
      K=MP*(I-1)+J
      COEFL(K)=0.0
      DO 190 JJ=1,MQ
      N1=N1+MP
      N2=N2+1
  190 COEFL(K)=COEFL(K)+R(N1)*COEFR(N2)
  200 COEFL(K)=COEFL(K)/CANR(I)
  210 CONTINUE
  220 RETURN
      END
```

NROOT

This subroutine calculates the eigenvalues, λ_i, and the matrix of eigenvectors, V, of a real square nonsymmetric matrix of the special form $B^{-1}A$, where both B and A are real symmetric matrices and B is positive-definite. This subroutine is normally called by the subroutine CANOR in performing a canonical correlation analysis. The computational steps are as follows.

A symmetric matrix (storage mode 1) is formed by using the upper triangle elements of the square matrix B. Then, the eigenvalues, h_i, and the matrix of eigenvectors, H, of the symmetric matrix are calculated by the subroutine EIGEN.

The reciprocal of square root of each eigenvalue is formed as follows:

$$\mu_i = \frac{1}{\sqrt{h_i}} \tag{1}$$

where i = 1, 2, ..., m

m = order of matrix B

The matrix $B^{-1/2}$ is formed by multiplying the j^{th} column vector of H by μ_j, where j = 1, 2, ..., m.

The symmetric matrix $S = (B^{-1/2})' AB^{-1/2}$ is formed in the following two matrix multiplications:

$$Q = (B^{-1/2})' A \tag{2}$$

$$S = QB^{-1/2} \tag{3}$$

and eigenvalues, λ_i , and the matrix of eigenvectors, M, of S are calculated by the subroutine EIGEN.

The matrix $W = B^{-1/2}M$ is formed, and the vectors in W are normalized to form the matrix of eigenvectors, V, by the following equation:

$$V_{ij} = \frac{W_{ij}}{\sqrt{SUMV_j}} \tag{4}$$

where i = 1, 2, ..., m

j = 1, 2, ..., m

$$SUMV_j = \sum_{i=1}^{m} W_{ij}^2 \tag{5}$$

Subroutine NROOT

Purpose:

Compute eigenvalues and eigenvectors of a real nonsymmetric matrix of the form B-inverse times A. This subroutine is normally called by subroutine CANOR in performing a canonical correlation analysis.

Usage:

CALL NROOT (M, A, B, XL, X)

Description of parameters:

M	-	Order of square matrices A, B, and X.
A	-	Input matrix (M by M).
B	-	Input matrix (M by M).
XL	-	Output vector of length M containing eigenvalues of B-inverse times A.
X	-	Output matrix (M by M) containing eigenvectors columnwise.

Remarks:

None.

Subroutines and function subprograms required:

EIGEN

Method:

Refer to W. W. Cooley and P. R. Lohnes, 'Multivariate Procedures for the Behavioral Sciences', John Wiley and Sons, 1962, Chapter 3.

```
      SUBROUTINE NROOT (M,A,B,XL,X)
      DIMENSION A(1),B(1),XL(1),X(1)
C        COMPUTE EIGENVALUES AND EIGENVECTORS OF B
      K=1
      DO 100 J=2,M
      L=M*(J-1)
      DO 100 I=1,J
      L=L+1
      K=K+1
  100 B(K)=B(L)
C        THE MATRIX B IS A REAL SYMMETRIC MATRIX.
      MV=0
      CALL EIGEN (B,X,M,MV)
C        FORM RECIPROCALS OF SQUARE ROOT OF EIGENVALUES.  THE RESULTS
C        ARE PREMULTIPLIED BY THE ASSOCIATED EIGENVECTORS.
      L=0
      DO 110 J=1,M
      L=L+J
  110 XL(J)=1.0/ SQRT( ABS(B(L)))
      K=0
      DO 115 J=1,M
      DO 115 I=1,M
      K=K+1
  115 B(K)=X(K)*XL(J)
C        FORM (B**(-1/2))PRIME * A * (B**(-1/2))
      DO 120 I=1,M
      N2=0
      DO 120 J=1,M
      N1=M*(I-1)
      L=M*(J-1)+I
      X(L)=0.0
      DO 120 K=1,M
      N1=N1+1
      N2=N2+1
  120 X(L)=X(L)+B(N1)*A(N2)
      L=0
      DO 130 J=1,M
      DO 130 I=1,J
      N1=I-M
      N2=M*(J-1)
      L=L+1
      A(L)=0.0
      DO 130 K=1,M
      N1=N1+M
      N2=N2+1
  130 A(L)=A(L)+X(N1)*B(N2)
C        COMPUTE EIGENVALUES AND EIGENVECTORS OF A
      CALL EIGEN (A,X,M,MV)
      L=0
      DO 140 I=1,M
      L=L+I
  140 XL(I)=A(L)
C        COMPUTE THE NORMALIZED EIGENVECTORS
      DO 150 I=1,M
      N2=0
      DO 150 J=1,M
      N1=I-M
      L=M*(J-1)+I
      A(L)=0.0
      DO 150 K=1,M
      N1=N1+M
      N2=N2+1
  150 A(L)=A(L)+B(N1)*X(N2)
      L=0
      K=0
      DO 180 J=1,M
      SUMV=0.0
      DO 170 I=1,M
      L=L+1
  170 SUMV=SUMV+A(L)*A(L)
  175 SUMV= SQRT(SUMV)
      DO 180 I=1,M
      K=K+1
  180 X(K)=A(K)/SUMV
      RETURN
      END
```

Statistics - Analysis of Variance

In the Scientific Subroutine Package, analysis of variance is normally performed by calling the following three subroutines in sequence:

1. AVDAT - to place data in properly distributed positions of storage
2. AVCAL - to apply the operators sigma and delta in order to compute deviates for analysis of variance
3. MEANQ - to pool the deviates and compute sums of squares, degrees of freedom, and mean squares

AVDAT

This subroutine places data for analysis of variance in properly distributed positions of storage.

The size of data array X, required for an analysis of variance problem, is calculated as follows:

$$n = \prod_{i=1}^{k} (L_i + 1) \qquad (1)$$

where L_i = number of levels of ith factor

k = number of factors

The input data placed in the lower part of the array X are moved temporarily to the upper part of the array. From there, the data are redistributed according to the equation (4) below. Prior to that, multipliers, s_j, to be used in finding proper positions of storage, are calculated as follows:

$$s_1 = 1 \qquad (2)$$

$$s_j = \prod_{i=1}^{j-1} (L_i + 1) \qquad (3)$$

where $J = 2, 3, \ldots, k$

Then, a position for each data point is calculated by the following equation:

$$S = KOUNT_1 + \sum_{j=2}^{k} s_j \cdot (KOUNT_j - 1) \qquad (4)$$

where $KOUNT_j$ = value of jth subscript of the data to be stored.

The subroutine increments the value(s) of subscript(s) after each data point is stored.

Subroutine AVDAT

Purpose:

Place data for analysis of variance in properly distributed positions of storage. This subroutine is normally followed by calls to AVCAL and MEANQ subroutines in the performance of analysis of variance for a complete factorial design.

Usage:

CALL AVDAT (K, LEVEL, N, X, L, ISTEP, KOUNT)

Description of parameters:

K	-	Number of variables (factors) K must be greater than 1.
LEVEL	-	Input vector of length K containing levels (categories) within each variable.
N	-	Total number of data points read in.
X	-	When the subroutine is called, this vector contains data in locations X(1) through X(N). Upon returning to the calling routine, the vector contains the data in properly redistributed locations of vector X. The length of vector X is calculated by (1) adding one to each level of variable and (2) obtaining the cumulative product of all levels. (The length of X = (LEVEL(1)+ 1)*(LEVEL(2)+ 1)* ...*(LEVEL(K)+ 1).)
L	-	Output variable containing the position in vector X where the last input data is stored.
ISTEP	-	Output vector of length K containing control steps which are used to locate data in proper positions of vector X.
KOUNT	-	Working vector of length K.

Remarks:

Input data must be arranged in the following manner. Consider the 3-variable analysis of variance design, where one variable has 3 levels and the other two variables have 2 levels. The data may be represented in the form X(I, J, K), I=1, 2, 3 J=1, 2 K=1, 2. In arranging data, the inner subscript, namely I, changes first. When I=3, the next inner subscript, J, changes and so on until I=3, J=2, and K=2.

Subroutines and function subprograms required:
None.

Method:
The method is based on the technique discussed by H. D. Hartley in 'Mathematical Methods for Digital Computers', edited by A. Ralston and H. Wilf, John Wiley and Sons, 1962, Chapter 20.

```
      SUBROUTINE AVDAT (K,LEVEL,N,X,L,ISTEP,KOUNT)
      DIMENSION LEVEL(1),X(1),ISTEP(1),KOUNT(1)
C        CALCULATE TOTAL DATA AREA REQUIRED
      M=LEVEL(1)+1
      DO 105 I=2,K
  105 M=M*(LEVEL(I)+1)
C        MOVE DATA TO THE UPPER PART OF THE ARRAY X
C        FOR THE PURPOSE OF REARRANGEMENT
      N1=M+1
      N2=N+1
      DO 107 I=1,N
      N1=N1-1
      N2=N2-1
  107 X(N1)=X(N2)
C        CALCULATE MULTIPLIERS TO BE USED IN FINDING STORAGE LOCATIONS
C        FOR INPUT DATA
      ISTEP(1)=1
      DO 110 I=2,K
  110 ISTEP(I)=ISTEP(I-1)*(LEVEL(I-1)+1)
      DO 115 I=1,K
  115 KOUNT(I)=1
C        PLACE DATA IN PROPER LOCATIONS
      N1=N1-1
      DO 135 I=1,N
      L=KOUNT(1)
      DO 120 J=2,K
  120 L=L+ISTEP(J)*(KOUNT(J)-1)
      N1=N1+1
      X(L)=X(N1)
      DO 130 J=1,K
      IF(KOUNT(J)-LEVEL(J)) 124, 125, 124
  124 KOUNT(J)=KOUNT(J)+1
      GO TO 135
  125 KOUNT(J)=1
  130 CONTINUE
  135 CONTINUE
      RETURN
      END
```

AVCAL

This subroutine 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 ath level of factor A, the bth level of factor B, and the cth level of factor C. The symbols A, B, and C will also denote the number of levels for each factor so that a = 1, 2, ..., A; b = 1, 2, ..., B; and c = 1, 2, ..., C.

With regard to the first factor A,

operator $\sum_{a} \equiv$	sum over all levels a = 1, 2, ..., A, holding the other subscripts at constant levels, and
operator $\underset{a}{\Delta} \equiv$	multiply all items by A and subtract the result of $\sum_{a}$ from all items

In mathematical notations, these operators are defined as follows:

$$\sum_{a} x_{abc} \equiv X_{.bc} \equiv \sum_{a=1}^{A} x_{abc} \qquad (1)$$

$$\underset{a}{\Delta}\, x_{abc} \equiv A\, x_{abc} - X_{.bc} \qquad (2)$$

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 in the subroutine MEANQ.

Subroutine AVCAL

Purpose:
Perform the calculus of a factorial experiment using operator sigma and operator delta. This subroutine is preceded by subroutine ADVAT and followed by subroutine MEANQ in the performance of analysis of variance for a complete factorial design.

Usage:

CALL AVCAL (K, LEVEL, X, L, ISTEP, LASTS)

Description of parameters:

K		Number of variables (factors). K must be greater than 1.
LEVEL	-	Input vector of length K containing levels (categories) within each variable.
X	-	Input vector containing data. Data have been placed in vector X by subroutine AVDAT. The length of X is (LEVEL(1)+ 1)*(LEVEL(2)+ 1)*... *(LEVEL(K)+ 1).
L	-	The position in vector X where the last input data is located. L has been calculated by subroutine AVDAT.
ISTEP	-	Input vector of length K containing storage control steps which have been calculated by subroutine AVDAT.
LASTS	-	Working vector of length K.

Remarks:

This subroutine must follow subroutine AVDAT.

Subroutines and function subprograms required:

None.

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.

```
      SUBROUTINE AVCAL (K,LEVEL,X,L,ISTEP,LASTS)
      DIMENSION LEVEL(1),X(1),ISTEP(1),LASTS(1)
C        CALCULATE THE LAST DATA POSITION OF EACH FACTOR
      LASTS(1)=L+1
      DO 145 I=2,K
  145 LASTS(I)=LASTS(I-1)+ISTEP(I)
C        PERFORM CALCULUS OF OPERATION
  150 DO 175 I=1,K
      L=1
      LL=1
      SUM=0.0
      NN=LEVEL(I)
      FN=NN
      INCRE=ISTEP(I)
      LAST=LASTS(I)
C        SIGMA OPERATION
  155 DO 160 J=1,NN
      SUM=SUM+X(L)
  160 L=L+INCRE
      X(L)=SUM
C        DELTA OPERATION
      DO 165 J=1,NN
      X(LL)=FN*X(LL)-SUM
  165 LL=LL+INCRE
      SUM=0.0
      IF(L-LAST) 167, 175, 175
  167 IF(L-LAST+INCRE) 168, 169, 170
  168 L=L+INCRE
      LL=LL+INCRE
      GO TO 155
  170 L=L+INCRE+1-LAST
      LL=LL+INCRE+1-LAST
      GO TO 155
  175 CONTINUE
      RETURN
      END
```

MEANQ

This subroutine performs the mean square operation for the general k-factor experiment in the following two steps:

1. Square each value of deviates for analysis of variance stored in the array X (the result of the operators Σ and Δ applied in the subroutine AVCAL).

2. Add the squared value into summation storage. In a three-factor experiment, for example, the squared value is added into one of seven storages ($7 = 2^3 - 1$) as shown in the first column of Table 1. The symbols A, B, and C in the first column denote factor A, factor B, and factor C.

After the mean square operation is completed for all values in the storage array X, the subroutine forms sums of squares of analysis of variance by dividing the totals of squared values by proper divisors. These divisors for the three-factor experiment mentioned above are shown in the second column of Table 1. The symbols A, B, and C in the second column denote the number of levels for each factor.

The subroutine, then, forms mean squares by dividing sums of squares by degrees of freedom. The third column of the summary table shows the degrees of freedom. The symbols A, B, and C denote the number of levels for each factor.

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)

Subroutine MEANQ

Purpose:

Compute sum of squares, degrees of freedom, and mean square using the mean square operator. This subroutine normally follows calls to AVDAT and AVCAL subroutines in the performance of analysis of variance for a complete factorial design.

Usage:

CALL MEANQ (K, LEVEL, X, GMEAN, SUMSQ, NDF, SMEAN, MSTEP, KOUNT, LASTS)

Description of parameters:

K	-	Number of variables (factors). K must be greater than 1.
LEVEL	-	Input vector of length K containing levels (categories) within each variable.
X	-	Input vector containing the result of the sigma and delta operators. The length of X is (LEVEL(1)+ 1)*(LEVEL(2)+ 1)*...*(LEVEL(K)+ 1).
GMEAN	-	Output variable containing grand mean.
SUMSQ	-	Output vector containing sums of squares. The length of SUMSQ is 2 to the K^{th} power minus one, (2**K)-1.
NDF	-	Output vector containing degrees of freedom. The length of NDF is 2 to the K^{th} power minus one, (2**K)-1.
SMEAN	-	Output vector containing mean squares. The length of SMEAN is 2 to the K^{th} power minus one, (2**K)-1.
MSTEP	-	Working vector of length K.
KOUNT	-	Working vector of length K.
LASTS	-	Working vector of length K.

Remarks:
This subroutine must follow subroutine AVCAL.

Subroutines and function subprograms required:
None.

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.

```
      SUBROUTINE MEANQ (K,LEVEL,X,GMEAN,SUMSQ,NDF,SMEAN,MSTEP,KOUNT,    MEANQ  1
     1                  LASTS)                                          MEANQ  2
      DIMENSION LEVEL(1),X(1),SUMSQ(1),NDF(1),SMEAN(1),MSTEP(1),        MEANQ  3
     1          KOUNT(1),LASTS(1)                                       MEANQ  4
C        CALCULATE TOTAL NUMBER OF DATA                                 MEANQ  5
      N=LEVEL(1)                                                        MEANQ  6
      DO 150 I=2,K                                                      MEANQ  7
  150 N=N*LEVEL(I)                                                      MEANQ  8
C        SET UP CONTROL FOR MEAN SQUARE OPERATOR                        MEANQ  9
      LASTS(1)=LEVEL(1)                                                 MEANQ 10
      DO 178 I=2,K                                                      MEANQ 11
  178 LASTS(I)=LEVEL(I)+1                                               MEANQ 12
      NN=1                                                              MEANQ 13
C        CLEAR THE AREA TO STORE SUMS OF SQUARES                        MEANQ 14
      LL=(2**K)-1                                                       MEANQ 15
      MSTEP(1)=1                                                        MEANQ 16
      DO 180 I=2,K                                                      MEANQ 17
  180 MSTEP(I)=MSTEP(I-1)*2                                             MEANQ 18
      DO 185 I=1,LL                                                     MEANQ 19
  185 SUMSQ(I)=0.0                                                      MEANQ 20
C        PERFORM MEAN SQUARE OPERATOR                                   MEANQ 21
      DO 190 I=1,K                                                      MEANQ 22
  190 KOUNT(I)=0                                                        MEANQ 23
  200 L=0                                                               MEANQ 24
      DO 260 I=1,K                                                      MEANQ 25
      IF(KOUNT(I)-LASTS(I)) 210, 250, 210                               MEANQ 26
  210 IF(L) 220, 220, 240                                               MEANQ 27
  220 KOUNT(I)=KOUNT(I)+1                                               MEANQ 28
      IF(KOUNT(I)-LEVEL(I)) 230, 230, 250                               MEANQ 29
  230 L=L+MSTEP(I)                                                      MEANQ 30
      GO TO 260                                                         MEANQ 31
  240 IF(KOUNT(I)-LEVEL(I)) 230, 260, 230                               MEANQ 32
  250 KOUNT(I)=0                                                        MEANQ 33
  260 CONTINUE                                                          MEANQ 34
      IF(L) 285, 285, 270                                               MEANQ 35
  270 SUMSQ(L)=SUMSQ(L)+X(NN)*X(NN)                                     MEANQ 36
      NN=NN+1                                                           MEANQ 37
      GO TO 200                                                         MEANQ 38
C        CALCULATE THE GRAND MEAN                                       MEANQ 39
  285 FN=N                                                              MEANQ 40
      GMEAN=X(NN)/FN                                                    MEANQ 41
C        CALCULATE FIRST DIVISOR REQUIRED TO FORM SUM OF SQUARES AND    MEANQ 42
C        DIVISOR, WHICH IS EQUAL TO DEGREES OF FREEDOM, REQUIRED TO FORMMEANQ 43
C        MEAN SQUARES                                                   MEANQ 44
      DO 310 I=2,K                                                      MEANQ 45
  310 MSTEP(I)=0                                                        MEANQ 46
      NN=0                                                              MEANQ 47
      MSTEP(1)=1                                                        MEANQ 48
  320 ND1=1                                                             MEANQ 49
      ND2=1                                                             MEANQ 50
      DO 340 I=1,K                                                      MEANQ 51
      IF(MSTEP(I)) 330, 340, 330                                        MEANQ 52
  330 ND1=ND1*LEVEL(I)                                                  MEANQ 53
      ND2=ND2*(LEVEL(I)-1)                                              MEANQ 54
  340 CONTINUE                                                          MEANQ 55
      FN1=ND1                                                           MEANQM01
      FN1=FN*FN1                                                        MEANQM02
      FN2=ND2                                                           MEANQ 57
      NN=NN+1                                                           MEANQ 58
      SUMSQ(NN)=SUMSQ(NN)/FN1                                           MEANQ 59
      NDF(NN)=ND2                                                       MEANQ 60
      SMEAN(NN)=SUMSQ(NN)/FN2                                           MEANQ 61
      IF(NN-LL) 345, 370, 370                                           MEANQ 62
  345 DO 360 I=1,K                                                      MEANQ 63
      IF(MSTEP(I)) 347, 350, 347                                        MEANQ 64
  347 MSTEP(I)=0                                                        MEANQ 65
      GO TO 360                                                         MEANQ 66
  350 MSTEP(I)=1                                                        MEANQ 67
      GO TO 320                                                         MEANQ 68
  360 CONTINUE                                                          MEANQ 69
  370 RETURN                                                            MEANQ 70
      END                                                               MEANQ 71
```

Statistics - Discriminant Analysis

In the Scientific Subroutine Package, discriminant analysis is normally performed by calling the following three subroutines in sequence:

1. DMATX - to compute means of variables in each group and a pooled dispersion matrix
2. MINV - to invert the pooled dispersion matrix
3. DISCR - to compute coefficients of discriminant functions and evaluate the functions for each observation (individual)

DMATX

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, ..., g, the subroutine calculates means and sums of cross-products of deviations from means as follows:

Means:

$$\bar{x}_{jk} = \frac{\sum_{i=1}^{n_k} x_{ijk}}{n_k} \qquad (1)$$

where n_k = sample size in the k^{th} group

$j = 1, 2, \ldots, m$ are variables

Sum of cross-products of deviations from means:

$$S_k = \left\{ s^k_{j\ell} \right\} = \sum (x_{ijk} - \bar{x}_{jk})(x_{i\ell k} - \bar{x}_{\ell k}) \qquad (2)$$

where $j = 1, 2, \ldots, m$

$\ell = 1, 2, \ldots, m$

The pooled dispersion matrix is calculated as follows:

$$D = \frac{\sum_{k=1}^{g} S_k}{\sum_{k=1}^{g} n_k - g} \qquad (3)$$

where g = number of groups

Subroutine DMATX

Purpose:

Compute means of variables in each group and a pooled dispersion matrix for all the groups. Normally this subroutine is used in the performance of discriminant analysis.

Usage:

CALL DMATX (K,M,N,X,XBAR,D,CMEAN)

Description of parameters:

K	- Number of groups.
M	- Number of variables (must be the same for all groups).
N	- Input vector of length K containing sample sizes of groups.
X	- Input vector containing data in the manner equivalent to a 3-dimensional FORTRAN array, X(1,1,1), X(2,1,1), X(3,1,1), etc. The first subscript is case number, the second subscript is variable number and the third subscript is group number. The length of vector X is equal to the total number of data points, T*M, where T = N(1)+N(2)+ ... +N(K).
XBAR	- Output matrix (M by K) containing means of variables in K groups.
D	- Output matrix (M by M) containing pooled dispersion.
CMEAN	- Working vector of length M.

Remarks:

The number of variables must be greater than or equal to the number of groups.

Subroutines and function subprograms required:

None.

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, Section 6.6-6.8.

```
      SUBROUTINE DMATX (K,M,N,X,XBAR,D,CMEAN)
      DIMENSION N(1),X(1),XBAR(1),D(1),CMEAN(1)
      MM=M*M
      DO 100 I=1,MM
  100 D(I)=0.0
C        CALCULATE MEANS
      N4=0
      L=0
      LM=0
      DO 160 NG=1,K
      N1=N(NG)
      FN=N1
      DO 130 J=1,M
      LM=LM+1
      XBAR(LM)=0.0
      DO 120 I=1,N1
      L=L+1
  120 XBAR(LM)=XBAR(LM)+X(L)
  130 XBAR(LM)=XBAR(LM)/FN
C        CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS
      LMEAN=LM-M
      DO 150 I=1,N1
      LL=N4+I-N1
      DO 140 J=1,M
      LL=LL+N1
      N2=LMEAN+J
  140 CMEAN(J)=X(LL)-XBAR(N2)
      LL=0
      DO 150 J=1,M
      DO 150 JJ=1,M
      LL=LL+1
  150 D(LL)=D(LL)+CMEAN(J)*CMEAN(JJ)
  160 N4=N4+N1*M
C        CALCULATE THE POOLED DISPERSION MATRIX
      LL=-K
      DO 170 I=1,K
  170 LL=LL+N(I)
      FN=LL
      DO 180 I=1,MM
  180 D(I)=D(I)/FN
      RETURN
      END
```

DISCR

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:

$$\bar{x}_j = \frac{\sum_{k=1}^{g} n_k \bar{x}_{jk}}{\sum_{k=1}^{g} n_k} \qquad (1)$$

where g = number of groups

$j = 1, 2, \ldots, m$ are variables

n_k = sample size in the kth group

$\bar{x}_{jk}$ = mean of jth variable in kth group

Generalized Mahalanobis D^2 statistics, V:

$$V = \sum_{i=1}^{m}\sum_{j=1}^{m} d_{ij} \sum_{k=1}^{g} n_k (\bar{x}_{ik} - \bar{x}_i)\ (\bar{x}_{jk} - \bar{x}_j) \qquad (2)$$

where d_{ij} = the inverse element of the pooled dispersion matrix D

V can be used as chi-square (under assumption of normality) with $m(g-1)$ degrees of freedom to test the hypothesis that the mean values are the same in all the g groups for these m variables.

For each discriminant function $k* = 1, 2, \ldots, g$, the following statistics are calculated:

Coefficients:

$$C_{ik*} = \sum_{j=1}^{m} d_{ij} \bar{x}_{jk} \qquad (3)$$

where $i = 1, 2, \ldots, m$

$k = k*$

Constant:

$$C_{ok*} = -1/2 \sum_{j=1}^{m} \sum_{l=1}^{m} d_{jl} \bar{x}_{jk} \bar{x}_{lk} \qquad (4)$$

For each ith case in each kth group, the following calculations are performed:

Discriminant functions:

$$f_{k*} = \sum_{j=1}^{m} C_{jk} x_{ijk} + C_{ok*} \qquad (5)$$

where $k* = 1, 2, \ldots, g$

Probability associated with largest discriminant function:

$$P_L = \frac{1}{\sum_{k*=1}^{g} e^{(f_{k*} - f_L)}} \qquad (6)$$

where f_L = the value of the largest discriminant function

L = the subscript of the largest discriminant function

Subroutine DISCR

Purpose:
Compute a set of linear functions which serve as indices for classifying an individual into one of several groups. Normally this subroutine is used in the performance of discriminant analysis.

Usage:
CALL DISCR (K, M, N, X, XBAR, D, CMEAN, V, C, P, LG)

Description of parameters:

K	- Number of groups. K must be greater than 1.
M	- Number of variables.
N	- Input vector of length K containing sample sizes of groups.
X	- Input vector containing data in the manner equivalent to a 3-dimensional FORTRAN array, X(1,1,1), X(2,1,1), X(3,1,1), etc. The first

		subscript is case number, the second subscript is variable number and the third subscript is group number. The length of vector X is equal to the total number of data points, T*M, where T = N(1) + N(2) + ... + N(K).
XBAR	-	Input matrix (M by K) containing means of M variables in K groups.
D	-	Input matrix (M by M) containing the inverse of pooled dispersion matrix.
CMEAN	-	Output vector of length M containing common means.
V	-	Output variable containing generalized Mahalanobis D-square.
C	-	Output matrix (M+1 by K) containing the coefficients of discriminant functions. The first position of each column (function) contains the value of the constant for that function.
P	-	Output 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 2-dimensional area (the first subscript is case number, and the second subscript is group number). Vector P has length equal to the total number of cases, T (T = N(1) + N(2) + ... + N(K)).
LG	-	Output vector containing the subscripts of the largest discriminant functions stored in vector P. The length of vector LG is the same as the length of vector P.

Remarks:

The number of variables must be greater than or equal to the number of groups.

Subroutines and function subprograms required:

None.

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.

```
      SUBROUTINE DISCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG)
      DIMENSION N(1),X( 1),XBAR(1),D(1),CMEAN(1),C(1),P(1),LG(1)
C        CALCULATE COMMON MEANS
      N1=N(1)
      DO 100 I=2,K
  100 N1=N1+N(I)
      FNT=N1
      DO 110 I=1,K
  110 P(I)=N(I)
      DO 130 I=1,M
      CMEAN(I)=0
      N1=I-M
      DO 120 J=1,K
      N1=N1+M
  120 CMEAN(I)=CMEAN(I)+P(J)*XBAR(N1)
  130 CMEAN(I)=CMEAN(I)/FNT
C        CALCULATE GENERALIZED MAHALANOBIS D SQUARE
      L=0
      DO 140 I=1,K
      DO 140 J=1,M
      L=L+1
  140 C(L)=XBAR(L)-CMEAN(J)
      V=0.0
      L=0
      DO 160 J=1,M
      DO 160 I=1,M
      N1=I-M
      N2=J-M
      SUM=0.0
      DO 150 IJ=1,K
      N1=N1+M
      N2=N2+M
  150 SUM=SUM+P(IJ)*C(N1)*C(N2)
      L=L+1
  160 V=V+D(L)*SUM
C        CALCULATE THE COEFFICIENTS OF DISCRIMINANT FUNCTIONS
      N2=0
      DO 190 KA=1,K
      DO 170 I=1,M
      N2=N2+1
  170 P(I)=XBAR(N2)
      IQ=(M+1)*(KA-1)+1
      SUM=0.0
      DO 180 J=1,M
      N1=J-M
      DO 180 L=1,M
      N1=N1+M
  180 SUM=SUM+D(N1)*P(J)*P(L)
      C(IQ)=-(SUM/2.0)
      DO 190 I=1,M
      N1=I-M
      IQ=IQ+1
      C(IQ)=0.0
      DO 190 J=1,M
      N1=N1+M
  190 C(IQ)=C(IQ)+D(N1)*P(J)
C        FOR EACH CASE IN EACH GROUP, CALCULATE..
C        DISCRIMINANT FUNCTIONS
      LBASE=0
      N1=0
      DO 270 KG=1,K
      NN=N(KG)
      DO 260 I=1,NN
      L=I-NN+LBASE
      DO 200 J=1,M
      L=L+NN
  200 D(J)=X(L)
      N2=0
      DO 220 KA=1,K
      N2=N2+1
      SUM=C(N2)
      DO 210 J=1,M
      N2=N2+1
  210 SUM=SUM+C(N2)*D(J)
  220 XBAR(KA)=SUM
C        THE LARGEST DISCRIMINANT FUNCTION
      L=1
      SUM=XBAR(1)
      DO 240 J=2,K
      IF(SUM-XBAR(J)) 230, 240, 240
  230 L=J
      SUM=XBAR(J)
  240 CONTINUE
C        PROBABILITY ASSOCIATED WITH THE LARGEST DISCRIMINANT FUNCTION
      PL=0.0
      DO 250 J=1,K
  250 PL=PL+ EXP(XBAR(J)-SUM)
      N1=N1+1
      LG(N1)=L
  260 P(N1)=1.0/PL
  270 LBASE=LBASE+NN*M
      RETURN
      END
```

Statistics - Factor Analysis

Factor analysis is a method of analyzing the intercorrelations within a set of variables. It determines whether the variance in the original set of variables can be accounted for adequately by a smaller number of basic categories, namely factors.

In the Scientific Subroutine Package, factor analysis is normally performed by calling the following five subroutines in sequence:

1. CORRE - to find means, standard deviations, and correlation matrix
2. EIGEN - to compute eigenvalues and associated eigenvectors of the correlation matrix
3. TRACE - to select the eigenvalues that are greater than or equal to the control value specified by the user
4. LOAD - to compute a factor matrix
5. VARMX - to perform varimax rotation of the factor matrix

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the description of subroutine CORRE).

TRACE

This subroutine finds k, the number of eigenvalues that are greater than or equal to the value of a specified constant. The given eigenvalues λ_1, λ_2, ..., λ_m must be arranged in descending order.

Cumulative percentage for these 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 TRACE

Purpose:

Compute cumulative percentage of eigenvalues greater than or equal to a constant specified by the user. This subroutine normally occurs in a sequence of calls to subroutines CORRE, EIGEN, TRACE, LOAD, and VARMX in the performance of a factor analysis.

Usage:

CALL TRACE (M,R,CON,K,D)

Description of parameters:

M	- Number of variables.
R	- Input matrix (symmetric and stored in compressed form with only upper triangle by column in core) containing eigenvalues in diagonal. Eigenvalues are arranged in descending order. The order of matrix R is M by M. Only M*(M+1)/2 elements are in storage. (Storage mode of 1.)
CON	- A constant used to decide how many eigenvalues to retain. Cumulative percentage of eigenvalues which are greater than or equal to this value is calculated.
K	- Output variable containing the number of eigenvalues greater than or equal to CON. (K is the number of factors.)
D	- Output vector of length M containing cumulative percentage of eigenvalues which are greater than or equal to CON.

Remarks:
None.

Subroutines and function subprograms required:
None.

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.

```
      SUBROUTINE TRACE (M,R,CON,K,D)
      DIMENSION R(1),D(1)
      FM=M
      L=0
      DO 100 I=1,M
      L=L+I
  100 D(I)=R(L)
      K=0
C        TEST WHETHER I-TH EIGENVALUE IS GREATER
C        THAN OR EQUAL TO THE CONSTANT
      DO 110 I=1,M
      IF(D(I)-CON) 120, 105, 105
  105 K=K+1
  110 D(I)=D(I)/FM
C        COMPUTE CUMULATIVE PERCENTAGE OF EIGENVALUES
  120 DO 130 I=2,K
  130 D(I)=D(I)+D(I-1)
      RETURN
      END
```

LOAD

This subroutine calculates the coefficients of each factor by multiplying the elements of each normalized eigenvector by the square root of the corresponding eigenvalue.

$$a_{ij} = v_{ij} \cdot \sqrt{\lambda_j} \qquad (1)$$

where $i = 1, 2, \ldots, m$ are variables

$j = 1, 2, \ldots, k$ are eigenvalues retained (see the subroutine TRACE)

$k \leq m$

Subroutine LOAD

Purpose:
Compute a factor matrix (loading) from eigenvalues and associated eigenvectors. This subroutine normally occurs in a sequence of calls to subroutines CORRE, EIGEN, TRACE, LOAD, and VARMX in the performance of a factor analysis.

Usage:
CALL LOAD (M, K, R, V)

Description of parameters:

M	-	Number of variables.
K	-	Number of factors.
R	-	A matrix (symmetric and stored in compressed form with only upper triangle by column in core) containing eigenvalues in diagonal. Eigenvalues are arranged in descending order, and first K eigenvalues are used by this subroutine. The order of matrix R is M by M. Only M*(M+1)/2 elements are in storage. (Storage mode of 1.)
V	-	When this subroutine is called, matrix V (M by M) contains eigenvectors columnwise. Upon returning to the calling program, matrix V contains a factor matrix (M by K).

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:

Normalized eigenvectors are converted to the factor pattern by multiplying the elements of each vector by the square root of the corresponding eigenvalue.

```
      SUBROUTINE LOAD (M,K,R,V)
      DIMENSION R(1),V(1)
      L=0
      JJ=0
      DO 160 J=1,K
      JJ=JJ+J
  150 SQ= SQRT(R(JJ))
      DO 160 I=1,M
      L=L+1
  160 V(L)=SQ*V(L)
      RETURN
      END
```

VARMX

This subroutine performs orthogonal rotations on a m by k factor matrix such that:

$$\sum_j \left\{ m \sum_i \left(a_{ij}^2 / h_i^2 \right)^2 - \left[\sum_i \left(a_{ij}^2 / h_i^2 \right) \right] \right\}^2 \tag{1}$$

is a maximum, where i = 1, 2, ..., m are variables, j = 1, 2, ..., k are factors, a_{ij} is the loading for the ith variable on the jth factor, and h_i^2 is the communality of the ith variable defined below.

Communalities:

$$h_i^2 = \sum_{j=1}^{k} a_{ij}^2 \tag{2}$$

where i = 1, 2, ..., m

Normalized factor matrix:

$$b_{ij} = a_{ij} / \sqrt{h_i^2} \tag{3}$$

where i = 1, 2, ..., m

j = 1, 2, ..., k

Variance for factor matrix:

$$V_c = \sum_j \left\{ \left[m \sum_i \left(b_{ij}^2 \right)^2 - \left(\sum_i b_{ij}^2 \right)^2 \right] \Big/ m^2 \right\} \tag{4}$$

where c = 1, 2, ... (iteration cycle)

Convergence test:

$$\text{If } V_c - V_{c-1} \leq 10^{-7} \tag{5}$$

four successive times, the program stops rotation and performs the 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.

Assume 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:

$$\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ x_m & y_m \end{bmatrix} \cdot \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} = \begin{bmatrix} X_1 & Y_1 \\ X_2 & Y_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ X_m & Y_m \end{bmatrix} \qquad (6)$$

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 as follows:

A. Calculation of NUM and DEN:

$$A = \sum_i (x_i + y_i)(x_i - y_i)$$

$$B = 2 \sum_i x_i y_i$$

$$C = \sum_i \left[(x_i + y_i)(x_i - y_i) + 2x_i y_i\right] \qquad (7)$$

$$\left[(x_i + y_i)(x_i - y_i) - 2x_i y_i\right]$$

$$D = 4 \sum_i (x_i + y_i)(x_i - y_i) x_i y_i$$

$$NUM = D - 2AB/m$$

$$DEN = C - [(A + B)(A - B)]/m$$

B. Comparison of NUM and DEN:

The following four cases may arise:

NUM < DEN, go to B1 below.

NUM > DEN, go to B2 below.

(NUM + DEN) $\geq \epsilon$*, go to B3 below.

(NUM + DEN) $< \epsilon$, skip to the next rotation.

* ϵ is a small tolerance factor.

B1: $\tan 4\theta = |NUM|/|DEN|$ (8)

If $\tan 4\theta < \epsilon$ and

(i) DEN is positive, skip to the next rotation.

(ii) DEN is negative, set $\cos\phi = \sin\phi = (\sqrt{2})/2$ and go to E below.

If $\tan 4\theta \geq \epsilon$, calculate:

$$\cos 4\theta = 1\Big/\sqrt{1 + \tan^2 4\theta} \qquad (9)$$

$$\sin 4\theta = \tan 4\theta \cdot \cos 4\theta \qquad (10)$$

and go to C below.

B2: $\text{ctn}\,4\theta = |NUM|/|DEN|$ (11)

If $\text{ctn}\,4\theta < \epsilon$, set $\cos 4\theta = 0$ and $\sin 4\theta = 1$. Go to C below.

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 C below.

B3: Set $\cos 4\theta = \sin 4\theta = (\sqrt{2})/2$ and go to C below.

C. Determining $\cos\theta$ and $\sin\theta$:

$$\cos 2\theta = \sqrt{(1 + \cos 4\theta)/2} \qquad (14)$$

$$\sin 2\theta = \sin 4\theta / 2\cos 2\theta \qquad (15)$$

$$\cos\theta = \sqrt{(1 + \cos 2\theta)/2} \qquad (16)$$

$$\sin\theta = \sin 2\theta / 2\cos\theta \qquad (17)$$

D. Determining $\cos\phi$ and $\sin\phi$:

D1: If DEN is positive, set

$$\cos\phi = \cos\theta \qquad (18)$$

$$\sin\phi = \sin\theta \qquad (19)$$

and go to (D2) below.

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 (D2) below.

D2: If NUM is positive, set

$$\cos\phi = |\cos\phi| \qquad (22)$$

$$\sin\phi = |\sin\phi| \qquad (23)$$

and go to (E) below.

If NUM is negative, set

$$\cos\phi = |\cos\phi| \qquad (24)$$

$$\sin\phi = -|\sin\phi| \qquad (25)$$

E. Rotation:

$$X_i = x_i\cos\phi + y_i\sin\phi \qquad (26)$$

$$Y_i = x_i\sin\phi + y_i\cos\phi \qquad (27)$$

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 (equation 4).

Denormalization:

$$a_{ij} = b_{ij} \cdot h_i \qquad (28)$$

where $i = 1, 2, \ldots, m$

$j = 1, 2, \ldots, k$

Check on communalities:

Final communalities $$f_i^2 = \sum_{j=1}^{k} a_{ij}^2 \qquad (29)$$

Difference $$d_i = h_i^2 - f_i^2 \qquad (30)$$

where $i = 1, 2, \ldots, m$

Subroutine VARMX

Purpose:

Perform orthogonal rotations of a factor matrix. This subroutine normally occurs in a sequence of calls to subroutines CORRE, EIGEN, TRACE, LOAD, VARMX in the performance of a factor analysis.

Usage:

CALL VARMX (M, K, A, NC, TV, H, F, D)

Description of parameters:

M -	Number of variables and number of rows of matrix A.
K -	Number of factors.
A -	Input is the original factor matrix, and output is the rotated factor matrix. The order of matrix A is M by K.
NC -	Output variable containing the number of iteration cycles performed.
TV -	Output 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 subroutine is 50. Therefore, the length of vector TV is 51.
H -	Output vector of length M containing the original communalities.
F -	Output vector of length M containing the final communalities.
D -	Output vector of length M containing the differences between the original and final communalities.

Remarks:

If variance computed after each iteration cycle does not increase for four successive times, the subroutine stops rotation.

Subroutines and function subprograms required:

None.

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.

```
      SUBROUTINE VARMX (M,K,A,NC,TV,H,F,D)
      DIMENSION A(1),TV(1),H(1),F(1),D(1)
C          INITIALIZATION
      EPS=0.00116
      TVLT=0.0
      LL=K-1
      NV=1
      NC=0
      FN=M
      FFN=FN*FN
      CONS=0.7071066
C          CALCULATE ORIGINAL COMMUNALITIES
      DO 110 I=1,M
      H(I)=0.0
      DO 110 J=1,K
      L=M*(J-1)+I
  110 H(I)=H(I)+A(L)*A(L)
C          CALCULATE NORMALIZED FACTOR MATRIX
      DO 120 I=1,M
  115 H(I)= SQRT(H(I))
      DO 120 J=1,K
      L=M*(J-1)+I
  120 A(L)=A(L)/H(I)
      GO TO 132
C          CALCULATE VARIANCE FOR FACTOR MATRIX
  130 NV=NV+1
      TVLT=TV(NV-1)
  132 TV(NV)=0.0
      DO 150 J=1,K
      AA=0.0
      BB=0.0
      LB=M*(J-1)
      DO 140 I=1,M
      L=LB+I
      CC=A(L)*A(L)
      AA=AA+CC
  140 BB=BB+CC*CC
  150 TV(NV)=TV(NV)+(FN*BB-AA*AA)/FFN
      IF(NV-51) 160, 430, 430
C          PERFORM CONVERGENCE TEST
  160 IF((TV(NV)-TVLT)-(1.E-7)) 170, 170, 190
  170 NC=NC+1
      IF(NC-3) 190, 190, 430
C          ROTATION OF TWO FACTORS CONTINUES UP TO
C          THE STATEMENT 120.
  190 DO 420 J=1,LL
      L1=M*(J-1)
      II=J+1
C          CALCULATE NUM AND DEN
      DO 420 KI=II,K
      L2=M*(KI-1)
      AA=0.0
      BB=0.0
      CC=0.0
      DD=0.0
      DO 230 I=1,M
      L3=L1+I
      L4=L2+I
      U=(A(L3)+A(L4))*(A(L3)-A(L4))
      T=A(L3)*A(L4)
      T=T+T
      CC=CC+(U+T)*(U-T)
      DD=DD+2.0*U*T
      AA=AA+U
  230 BB=BB+T
      T=DD-2.0*AA*BB/FN
      B=CC-(AA*AA-BB*BB)/FN
C          COMPARISON OF NUM AND DEN
      IF(T-B) 280, 240, 320
  240 IF((T+B)-EPS) 420, 250, 250
C          NUM + DEN IS GREATER THAN OR EQUAL TO THE
C          TOLERANCE FACTOR
  250 COS4T=CONS
      SIN4T=CONS
      GO TO 350
C          NUM IS LESS THAN DEN
  280 TAN4T= ABS(T)/ ABS(B)
      IF(TAN4T-EPS) 300, 290, 290
  290 COS4T=1.0/ SQRT(1.0+TAN4T*TAN4T)
      SIN4T=TAN4T*COS4T
      GO TO 350
  300 IF(B) 310, 420, 420
  310 SINP=CONS
      COSP=CONS
      GO TO 400
C          NUM IS GREATER THAN DEN
  320 CTN4T= ABS(T/B)
      IF(CTN4T-EPS) 340, 330, 330
  330 SIN4T=1.0/ SQRT(1.0+CTN4T*CTN4T)
      COS4T=CTN4T*SIN4T
      GO TO 350
  340 COS4T=0.0
      SIN4T=1.0
C          DETERMINE COS THETA AND SIN THETA
  350 COS2T= SQRT((1.0+COS4T)/2.0)
      SIN2T=SIN4T/(2.0*COS2T)
  355 COST= SQRT((1.0+COS2T)/2.0)
      SINT=SIN2T/(2.0*COST)
C          DETERMINE COS PHI AND SIN PHI
      IF(B) 370, 370, 360
  360 COSP=COST
      SINP=SINT
      GO TO 380
  370 COSP=CONS*COST+CONS*SINT
  375 SINP= ABS(CONS*COST-CONS*SINT)
  380 IF(T) 390, 390, 400
  390 SINP=-SINP
C          PERFORM ROTATION
  400 DO 410 I=1,M
      L3=L1+I
      L4=L2+I
      AA=A(L3)*COSP+A(L4)*SINP
      A(L4)=-A(L3)*SINP+A(L4)*COSP
  410 A(L3)=AA
  420 CONTINUE
      GO TO 130
C          DENORMALIZE VARIMAX LOADINGS
  430 DO 440 I=1,M
      DO 440 J=1,K
      L=M*(J-1)+I
  440 A(L)=A(L)*H(I)
C          CHECK ON COMMUNALITIES
      NC=NV-1
      DO 450 I=1,M
  450 H(I)=H(I)*H(I)
      DO 470 I=1,M
      F(I)=0.0
      DO 460 J=1,K
      L=M*(J-1)+I
  460 F(I)=F(I)+A(L)*A(L)
  470 D(I)=H(I)-F(I)
      RETURN
      END
```

Statistics - Time Series

AUTO

This subroutine calculates the autocovariances for lags 0, 1, 2, ..., (L-1), given a time series of observations A_1, A_2, ..., A_n and a number L.

$$R_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_i - \text{AVER}) \; (A_{i+j-1} - \text{AVER}) \quad (1)$$

where $\text{AVER} = \frac{1}{n} \sum_{i=1}^{n} A_i$

n = number of observations in time series A.

j = 1, 2, 3, ..., L represent time lags 0, 1, 2, ..., (L-1).

Subroutine AUTO

Purpose:
To find autocovariances of series A for lags 0 to L-1.

Usage:
CALL AUTO (A, N, L, R)

Description of parameters:

A -	Input vector of length N containing the time series whose autocovariance is desired.
N -	Length of the vector A.
L -	Autocovariance is calculated for lags of 0, 1, 2,..., L-1.
R -	Output vector of length L containing autocovariances of series A.

Remarks:
The length of R is different from the length of A. N must be greater than L. Otherwise, R(1) is set to zero and this routine exits.

Subroutines and function subprograms required:
None.

Method:
The method described by R. B. Blackman and J. W. Tukey in The Measurement of Power Spectra, Dover Publications, Inc., New York, 1959.

```
      SUBROUTINE AUTO (A,N,L,R)                                         AUTO   1
      DIMENSION A(1),R(1)                                               AUTO   2
C        CALCULATE AVERAGE OF TIME SERIES A                             AUTO   3
      AVER=0.0                                                          AUTO   4
      IF(N-L) 50,50,100                                                 AUTO M01
   50 R(1)=0.0                                                          AUTO M02
      RETURN                                                            AUTO M03
  100 DO 110 I=1,N                                                      AUTO M04
  110 AVER=AVER+A(I)                                                    AUTO   6
      FN=N                                                              AUTO   7
      AVER=AVER/FN                                                      AUTO   8
C        CALCULATE AUTOCOVARIANCES                                      AUTO  11
      DO 130 J=1,L                                                      AUTO  12
      NJ=N-J+1                                                          AUTO  13
      SUM=0.0                                                           AUTO  14
      DO 120 I=1,NJ                                                     AUTO  15
      IJ=I+J-1                                                          AUTO  16
  120 SUM=SUM+(A(I)-AVER)*(A(IJ)-AVER)                                  AUTO M05
      FNJ=NJ                                                            AUTO  18
  130 R(J)=SUM/FNJ                                                      AUTO M06
      RETURN                                                            AUTO  20
      END                                                               AUTO  21
```

CROSS

This subroutine calculates the crosscovariances of series B lagging and leading A, given two time series $A_1, A_2, \ldots, A_n$ and $B_1, B_2, \ldots, B_n$ and given a number L.

(a) B lags A:

$$R_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_i - \text{AVERA})(B_{i+j-1} - \text{AVERB}) \tag{1}$$

(b) B leads A:

$$S_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_{i+j-1} - \text{AVERA})(B_i - \text{AVERB}) \tag{2}$$

where $\text{AVERA} = \frac{1}{n} \sum_{i=1}^{n} A_i$

$$\text{AVERB} = \frac{1}{n} \sum_{i=1}^{n} B_i$$

n = number of observations in each series.

j = 1, 2, ..., L represent time lags (or leads) of 0, 1, 2, ..., (L-1).

Subroutine CROSS

Purpose:
To find the crosscovariances of series A with series B (which leads and lags A).

Usage:
CALL CROSS (A, B, N, L, R, S)

Description of parameters:
- A - Input vector of length N containing first time series.
- B - Input vector of length N containing second time series.
- N - Length of series A and B.
- L - Crosscovariance is calculated for lags and leads of 0, 1, 2, ..., L-1.

R - Output vector of length L containing cross-covariances of A with B, where B lags A.
S - Output vector of length L containing cross-covariances of A with B, where B leads A.

Remarks:
N must be greater than L. If not, R(1) and S(1) are set to zero and this routine exits.

Subroutines and function subprograms required:
None.

Method:
The method is described by R. B. Blackman and J. W. Tukey in The Measurement of Power Spectra, Dover Publications, Inc., New York, 1959.

```
      SUBROUTINE CROSS (A,B,N,L,R,S)
      DIMENSION A(1),B(1),R(1),S(1)
C        CALCULATE AVERAGES OF SERIES A AND B
      FN=N
      AVERA=0.0
      AVERB=0.0
      IF(N-L)50,50,100
   50 R(1)=0.0
      S(1)=0.0
      RETURN
  100 DO 110 I=1,N
      AVERA=AVERA+A(I)
  110 AVERB=AVERB+B(I)
      AVERA=AVERA/FN
      AVERB=AVERB/FN
C        CALCULATE CROSSCOVARIANCES OF SERIES A AND B
      DO 130 J=1,L
      NJ=N-J+1
      SUMR=0.0
      SUMS=0.0
      DO 120 I=1,NJ
      IJ=I+J-1
      SUMR=SUMR+(A(I)-AVERA)*(B(IJ)-AVERB)
  120 SUMS=SUMS+(A(IJ)-AVERA)*(B(I)-AVERB)
      FNJ=NJ
      R(J)=SUMR/FNJ
  130 S(J)=SUMS/FNJ
      RETURN
      END
```

SMO

This subroutine calculates the smoothed or filtered series, given a time series $A_1, A_2, \ldots, A_n$, a selection integer L, and a weighting series $W_1, W_2, \ldots, W_m$.

$$R_i = \sum_{j=1}^{m} A_p \cdot W_j \tag{1}$$

where $p = j \cdot L - L + k$

$k = i - IL + 1$

$i = IL$ to IH

$$IL = \frac{L(m-1)}{2} + 1 \tag{2}$$

$$IH = n - \frac{L(m-1)}{2} \tag{3}$$

L = a given selection integer. For example, L = 4 applies weights to every 4th item of the time series.

m = number of weights. Must be an odd integer. (If m is an even integer, any fraction resulting from the calculation of $\frac{L(m-1)}{2}$ in (2) and (3) above will be truncated.

n = number of items in the time series.

From IL to IH elements of the vector R are filled with the smoothed series and other elements with zeros.

Subroutine SMO

Purpose:
To smooth or filter series A by weights W.

Usage:
CALL SMO (A,N,W,M,L,R)

Description of parameters:
A - Input vector of length N containing time series data.
N - Length of series A.
W - Input vector of length M containing weights.

M - Number of items in weight vector. M must be an odd integer. (If M is an even integer, any fraction resulting from the calculation of (L*(M-1))/2 in (1) and (2) below will be truncated.)

L - Selection integer. For example, L=12 means that weights are applied to every 12th item of A. L=1 applies weights to successive items of A. For monthly data, L=12 gives year-to-year averages and L=1 gives month-to-month averages.

R - Output vector of length N. From IL to IH elements of the vector R are filled with the smoothed series and other elements with zero, where

IL=(L*(M-1))/2+1 .... (1)

IH=N-(L*(M-1))/2 .... (2)

Remarks:

N must be greater than or equal to the product of L*M.

Subroutines and function subprograms required:

None.

Method:

Refer to the article 'FORTRAN Subroutines for Time Series Analysis', by J. R. Healy and B. P. Bogert, Communications of ACM, V.6, No. 1, Jan., 1963.

```
      SUBROUTINE SMO (A,N,W,M,L,R)
      DIMENSION A(1),W(1),R(1)
C        INITIALIZATION
      DO 110 I=1,N
  110 R(I)=0.0
      IL=(L*(M-1))/2+1
      IH=N-(L*(M-1))/2
C        SMOOTH SERIES A BY WEIGHTS W
      DO 120 I=IL,IH
      K=I-IL+1
      DO 120 J=1,M
      IP=(J*L)-L+K
  120 R(I)=R(I)+A(IP)*W(J)
      RETURN
      END
```

EXSMO

This subroutine 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 subroutine 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 subroutine (see below).

(a) Find S_i for one period ahead

$$S_i = A + B + .5C \qquad (1)$$

(b) Update coefficients A, B, and C

$$A = X_i + (1-\alpha)^3 \ (S_i - X_i) \qquad (2)$$

$$B = B + C - 1.5\,(\alpha^2)\,(2-\alpha)\,(S_i - X_i) \qquad (3)$$

$$C = C - (\alpha^3)\,(S_i - X_i) \qquad (4)$$

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:

$$C = X_1 - 2X_2 + X_3 \qquad (5)$$

$$B = X_2 - X_1 - 1.5C \qquad (6)$$

$$A = X_1 - B - 0.5C \qquad (7)$$

Subroutine EXSMO

Purpose:

To find the triple exponential smoothed series S of the given series X.

Usage:

CALL EXSMO (X,NX,AL,A,B,C,S)

Description of parameters:

X - Input vector of length NX containing time series data which is to be exponentially smoothed.

NX	-	The number of elements in X.
AL	-	Smoothing constant alpha. AL must be greater than zero and less than one.
A, B, C	-	Coefficients of the prediction equation where S is predicted T periods hence by A + B*T + C*T*T/2. As input: If A=B=C=0, program will provide initial values. If at least one of A, B, C is not zero, program will take given values as initial values. As output: A, B, C, contain latest, updated coefficients of prediction.
S	-	Output vector of length NX containing triple exponentially smoothed time series.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Refer to R. G. Brown, 'Smoothing, Forecasting and Prediction of Discrete Time Series', Prentice-Hall, N.J., 1963, pp. 140 to 144.

```
      SUBROUTINE EXSMO (X,NX,AL,A,B,C,S)                                EXSMO  1
      DIMENSION X(1),S(1)                                               EXSMO  2
C        IF A=B=C=0.0, GENERATE INITIAL VALUES OF A, B, AND C           EXSMO  3
      IF(A) 140, 110, 140                                               EXSMO  4
  110 IF(B) 140, 120, 140                                               EXSMO  5
  120 IF(C) 140, 130, 140                                               EXSMO  6
  130 L1=1                                                              EXSMOM01
      L2=2                                                              EXSMOM02
      L3=3                                                              EXSMOM03
      C=X(L1)-2.0*X(L2)+X(L3)                                           EXSMOM04
      B=X(L2)-X(L1)-1.5*C                                               EXSMOM05
      A=X(L1)-B-0.5*C                                                   EXSMOM06
  140 BE=1.0-AL                                                         EXSMO 10
      BECUB=BE*BE*BE                                                    EXSMO 11
      ALCUB=AL*AL*AL                                                    EXSMO 12
C        DO THE FOLLOWING FOR I=1 TO NX                                 EXSMO 13
      DO 150 I=1,NX                                                     EXSMO 14
C        FIND S(I) FOR ONE PERIOD AHEAD                                 EXSMO 15
      S(I)=A+B+0.5*C                                                    EXSMO 16
C        UPDATE COEFFICIENTS A, B, AND C                                EXSMO 17
      DIF=S(I)-X(I)                                                     EXSMO 18
      A=X(I)+BECUB*DIF                                                  EXSMO 19
      B=B+C-1.5*AL*AL*(2.0-AL)*DIF                                      EXSMO 20
  150 C=C-ALCUB*DIF                                                     EXSMO 21
      RETURN                                                            EXSMO 22
      END                                                               EXSMO 23
```

Statistics - Nonparametric

CHISQ

This subroutine calculates degrees of freedom and chi-square for a given contingency table A of observed frequencies with n rows (conditions) and m columns (groups). The degrees of freedom are:

$$\text{d.f.} = (n-1)\ (m-1) \qquad (1)$$

If one or more cells have an expected value of less than 1, chi-square is computed and the error code is set to 1.

The following totals are computed:

$$T_i = \sum_{j=1}^{m} A_{ij};\ i = 1, 2, \ldots, n \text{ (row totals)} \qquad (2)$$

$$T_j = \sum_{i=1}^{n} A_{ij};\ j = 1, 2, \ldots, m \text{ (column totals)} \qquad (3)$$

$$GT = \sum_{i=1}^{n} T_i \text{ (grand total)} \qquad (4)$$

Chi-square is obtained for two cases:

(a) for 2 x 2 table:

$$\chi^2 = \frac{GT\left(\left| A_{11}A_{22} - A_{12}A_{21} \right| - \frac{GT}{2}\right)^2}{(A_{11}+A_{12})(A_{21}+A_{22})(A_{11}+A_{21})(A_{12}+A_{22})} \qquad (5)$$

(b) for other contingency tables:

$$\chi^2 = \sum_{i=1}^{n} \sum_{j=1}^{m} \frac{\left(A_{ij} - E_{ij}\right)^2}{E_{ij}} \qquad (6)$$

where $E_{ij} = \dfrac{T_i T_j}{GT}$

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

$j = 1, 2, \ldots, m$

Subroutine CHISQ

Purpose:
Compute chi-square from a contingency table.

Usage:
CALL CHISQ(A, N, M, CS, NDF, IERR, TR, TC)

Description of parameters:

A	-	Input matrix, N by M, containing contingency table.
N	-	Number of rows in A.
M	-	Number of columns in A.
CS	-	Chi-square (output).
NDF	-	Number of degrees of freedom (output).
IERR	-	Error code (output): 0 - Normal case. 1 - Expected value less than 1.0 in one or more cells. 3 - Number of degrees of freedom is zero.
TR	-	Work vector of length N.
TC	-	Work vector of length M.

Remarks:

Chi-square is set to zero if either N or M is one (error code 3).

Subroutines and function subprograms required:
None.

Method:
Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 6 and Chapter 8.

```
      SUBROUTINE CHISQ(A,N,M,CS,NDF,IERR,TR,TC)                         CHISQ   1
      DIMENSION A(1),TR(1),TC(1)                                        CHISQ   2
      NM=N*M                                                            CHISQ   3
      IERR=0                                                            CHISQ   4
      CS=0.0                                                            CHISQ   5
C        FIND DEGREES OF FREEDOM                                        CHISQ   6
      NDF=(N-1)*(M-1)                                                   CHISQ   7
      IF(NDF) 5,5,10                                                    CHISQ   8
    5 IERR=3                                                            CHISQ   9
      RETURN                                                            CHISQ  10
C        COMPUTE TOTALS OF ROWS                                         CHISQ  25
   10 DO 90 I=1,N                                                       CHISQM01
      TR(I)=0.0                                                         CHISQ  27
      IJ=I-N                                                            CHISQ  28
      DO 90 J=1,M                                                       CHISQ  29
      IJ=IJ+N                                                           CHISQ  30
   90 TR(I)=TR(I)+A(IJ)                                                 CHISQ  31
C        COMPUTE TOTALS OF COLUMNS                                      CHISQ  32
      IJ=0                                                              CHISQ  33
      DO 100 J=1,M                                                      CHISQ  34
      TC(J)=0.0                                                         CHISQ  35
      DO 100 I=1,N                                                      CHISQ  36
      IJ=IJ+1                                                           CHISQ  37
  100 TC(J)=TC(J)+A(IJ)                                                 CHISQ  38
C        COMPUTE GRAND TOTAL                                            CHISQ  39
      GT=0.0                                                            CHISQ  40
      DO 110 I=1,N                                                      CHISQ  41
  110 GT=GT+TR(I)                                                       CHISQ  42
C        COMPUTE CHI SQUARE FOR 2 BY 2 TABLE (SPECIAL CASE)             CHISQ  43
      IF(NM-4) 130,120,130                                              CHISQ  44
  120 L1=1                                                              CHISQM04
      L2=2                                                              CHISQM05
      L3=3                                                              CHISQM06
      L4=4                                                              CHISQM07
      CS=GT*(ABS(A(L1)*A(L4)-A(L2)*A(L3))-GT/2.0)**2/(TC(L1)*TC(L2)     CHISQM08
     1*TR(L1)*TR(L2))                                                   CHISQM09
      RETURN                                                            CHISQ  47
C        COMPUTE CHI SQUARE FOR OTHER CONTINGENCY TABLES                CHISQ  48
  130 IJ=0                                                              CHISQ  49
      DO 140 J=1,M                                                      CHISQ  50
      DO 140 I=1,N                                                      CHISQ  51
      IJ=IJ+1                                                           CHISQ  52
      E=TR(I)*TC(J)/GT                                                  CHISQ  53
      IF(E-1.0) 135, 140, 140                                           CHISQM02
  135 IERR=1                                                            CHISQM03
  140 CS=CS+(A(IJ)-E)*(A(IJ)-E)/E                                       CHISQ  54
      RETURN                                                            CHISQ  55
      END                                                               CHISQ  56
```

UTEST

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 smaller group preceding 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

$U = n_1 n_2 - U'$

$$\text{if } U' < U, \text{ set } U = U' \qquad (2)$$

A correction factor for ties is obtained:

$$T = \sum \frac{t^3 - t}{12} \qquad (3)$$

where t = number of observations tied for a given rank

The standard deviation is computed for two cases:

(a) if T = 0

$$s = \sqrt{\frac{n_1 n_2 (n_1 + n_2 + 1)}{12}} \qquad (4)$$

(b) if T > 0

$$s = \sqrt{\left(\frac{n_1 n_2}{N(N-1)}\right)\left(\frac{N^3 - N}{12} - T\right)} \qquad (5)$$

where N = total number of cases $(n_1 + n_2)$

The significance of U is then tested:

$$Z = \frac{U - \bar{X}}{s} \qquad (6)$$

where $\bar{X}$ = mean $= \frac{n_1 n_2}{2}$

Z is set to zero if n_2 is less than 20.

Subroutine UTEST

Purpose:
Test whether two independent groups are from the same population by means of Mann-Whitney U-test.

Usage:
CALL UTEST(A, R, N1, N2, U, Z)

Description of parameters:

A	-	Input vector of cases consisting of two independent groups. Smaller group precedes larger group. Length is N1+N2.
R	-	Output vector of ranks. Smallest value is ranked 1, largest is ranked N. Ties are assigned average of tied ranks. Length is N1+N2.
N1	-	Number of cases in smaller group.
N2	-	Number of cases in larger group.
U	-	Statistic used to test homogeneity of the two groups (output).
Z	-	Measure of significance of U in terms of normal distribution (output).

Remarks:
Z is set to zero if N2 is less than 20.

Subroutines and function subprograms required:
RANK
TIE

Method:
Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 6.

```
      SUBROUTINE UTEST(A,R,N1,N2,U,Z)
      DIMENSION A(1),R(1)
C        RANK SCORES FROM BOTH GROUP TOGETHER IN ASCENDING ORDER, AND
C        ASSIGN TIED OBSERVATIONS AVERAGE OF TIED RANKS
      N=N1+N2
      CALL RANK(A,R,N)
      Z=0.0
C        SUM RANKS IN LARGER GROUP
      R2=0.0
      NP=N1+1
      DO 10 I=NP,N
   10 R2=R2+R(I)
C        CALCULATE U
      FNX=N1*N2
      FN=N
      FN2=N2
      UP=FNX+FN2*((FN2+1.0)/2.0)-R2
      U=FNX-UP
      IF(UP-U) 20,30,30
   20 U=UP
C        TEST FOR N2 LESS THAN 20
   30 IF(N2-20) 80,40,40
C        COMPUTE STANDARD DEVIATION
   40 KT=1
      CALL TIE(R,N,KT,TS)
      IF(TS) 50,60,50
   50 S=SQRT((FNX/(FN*(FN-1.0)))*(((FN*FN*FN-FN)/12.0)-TS))
      GO TO 70
   60 S=SQRT(FNX*(FN+1.0)/12.0)
C        COMPUTE Z
   70 Z=(U-FNX*0.5)/S
   80 RETURN
      END
```

TWOAV

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:

$$R_j = \sum_{i=1}^{n} A_{ij} \tag{1}$$

Friedman's statistic is then computed:

$$\chi_r^2 = \frac{12}{nm(m+1)} \sum_{j=1}^{m} (R_j)^2 - 3n(m+1) \tag{2}$$

The degrees of freedom are:

$$d.f = m - 1 \tag{3}$$

Subroutine TWOAV

Purpose:

Test whether a number of samples are from the same population by the Friedman two-way analysis of variance test.

Usage:

CALL TWOAV(A, R, N, M, W, XR, NDF, NR)

Description of parameters:

A	-	Input matrix, N by M, of original data.
R	-	Output matrix, N by M, of ranked data.
N	-	Number of groups.
M	-	Number of cases in each group.
W	-	Work area of length 2*M.
XR	-	Friedman statistic (output).
NDF	-	Number of degrees of freedom (output).
NR	-	Code: 0 for unranked data in A; 1 for ranked data in A (input).

Remarks:

None.

Subroutines and function subprograms required:

Rank.

Method:

Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 7.

```
      SUBROUTINE TWOAV (A,R,N,M,W,XR,NDF,NR)
      DIMENSION A(1),R(1),W(1)
C        DETERMINE WHETHER DATA IS RANKED
      IF(NR-1) 10, 30, 10
C        RANK DATA IN EACH GROUP AND ASSIGN TIED OBSERVATIONS AVERAGE
C        OF TIED RANK
   10 DO 20 I=1,N
      IJ=I-N
      IK=IJ
      DO 15 J=1,M
      IJ=IJ+N
   15 W(J)=A(IJ)
      CALL RANK (W,W(M+1),M)
      DO 20 J=1,M
      IK=IK+N
      IW=M+J
   20 R(IK)=W(IW)
      GO TO 35
   30 NM=N*M
      DO 32 I=1,NM
   32 R(I)=A(I)
C        CALCULATE SUM OF SQUARES OF SUMS OF RANKS
   35 RTSQ=0.0
      IR=0
      DO 50 J=1,M
      RT=0.0
      DO 40 I=1,N
      IR=IR+1
   40 RT=RT+R(IR)
   50 RTSQ=RTSQ+RT*RT
C        CALCULATE FRIEDMAN TEST VALUE, XR
      FNM=N*(M+1)
      FM=M
      XR=(12.0/(FM*FNM))*RTSQ-3.0*FNM
C        FIND DEGREES JF FREEDOM
      NDF=M-1
      RETURN
      END
```

QTEST

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:

$$L_i = \sum_{j=1}^{m} A_{ij} \text{ (row totals)} \qquad (1)$$

where i = 1, 2, ..., n

$$G_j = \sum_{i=1}^{n} A_{ij} \text{ (column totals)} \qquad (2)$$

where j = 1, 2, ..., m

The Cochran Q statistic is computed:

$$Q = \frac{(m-1)\left[m \sum_{j=1}^{m} G_j^2 - \left(\sum_{j=1}^{m} G_j\right)^2\right]}{m \sum_{i=1}^{n} L_i - \sum_{i=1}^{n} L_i^2} \qquad (3)$$

The degrees of freedom are:

$$d.f = m - 1 \qquad (4)$$

Subroutine QTEST

Purpose:
Test whether three or more matched groups of dichotomous data differ significantly by the Cochran Q-test.

Usage:
CALL QTEST(A, N, M, Q, NDF)

Description of parameters:

A	-	Input matrix, N by M, of dichotomous data (0 and 1).
N	-	Number of sets in each group.
M	-	Number of groups.
Q	-	Cochran Q statistic (output).
NDF	-	Number of degrees of freedom (output).

Remarks:
M must be three or greater.

Subroutines and function subprograms required:
None.

Method:
Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 7.

```
      SUBROUTINE QTEST(A,N,M,Q,NDF)
      DIMENSION A(1)
C        COMPUTE SUM OF SQUARES OF ROW TOTALS, RSQ, AND GRAND TOTAL OF
C        ALL ELEMENTS, GD
      RSQ=0.0
      GD=0.0
      DO 20 I=1,N
      TR=0.0
      IJ=I-N
      DO 10 J=1,M
      IJ=IJ+N
   10 TR=TR+A(IJ)
      GD=GD+TR
   20 RSQ=RSQ+TR*TR
C        COMPUTE SUM OF SQUARES OF COLUMN TOTALS, CSQ
      CSQ=0.0
      IJ=0
      DO 40 J=1,M
      TC=0.0
      DO 30 I=1,N
      IJ=IJ+1
   30 TC=TC+A(IJ)
   40 CSQ=CSQ+TC*TC
C        COMPUTE COCHRAN Q TEST VALUE
      FM=M
      Q=(FM-1.0)*(FM*CSQ-GD*GD)/(FM*GD-RSQ)
C        FIND DEGREES OF FREEDOM
      NDF=M-1
      RETURN
      END
```

SRANK

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:

$$T_a = \sum \frac{t^3 - t}{12} \text{ over variable A}$$

$$T_b = \sum \frac{t^3 - t}{12} \text{ over variable B} \qquad (2)$$

where t = number of observations tied for a given rank

The Spearman rank correlation coefficient is then computed for the following two cases:

(a) if T_a and T_b are zero,

$$r_s = 1 - \frac{6D}{n^3 - n} \qquad (3)$$

(b) if T_a and/or T_b are not zero,

$$r_s = \frac{X + Y - D}{2\sqrt{XY}} \qquad (4)$$

where $X = \frac{n^3 - n}{12} - T_a$ (5)

$$Y = \frac{n^3 - n}{12} - T_b \qquad (6)$$

The statistic used to measure the significance of r_s is:

$$t = r_s \sqrt{\frac{n - 2}{1 - r_s^2}} \qquad (7)$$

The degrees of freedom are:

$$\text{d.f.} = n - 2 \qquad (8)$$

Subroutine SRANK

Purpose:
Test correlation between two variables by means of Spearman rank correlation coefficient.

Usage:
CALL SRANK(A, B, R, N, RS, T, NDF, NR)

Description of parameters:

A	-	Input vector of N observations for first variable.
B	-	Input vector of N observations for second variable.
R	-	Output vector for ranked data, length is 2*N. Smallest observation is ranked 1, largest is ranked N. Ties are assigned average of tied ranks.
N	-	Number of observations.
RS	-	Spearman rank correlation coefficient (output).
T	-	Test of significance of RS (output).
NDF	-	Number of degrees of freedom (output).
NR	-	Code: 0 for unranked data in A and B; 1 for ranked data in A and B (input).

Remarks:
T is set to zero if N is less than ten.

Subroutines and function subprograms required:
RANK
TIE

Method:
Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 9.

```
      SUBROUTINE SRANK(A,B,R,N,RS,T,NDF,NR)                              SRANK   1
      DIMENSION A(1),B(1),R(1)                                           SRANK   2
      D=N                                                                SRANKM01
      FNNN=D*D*D-D                                                       SRANKM02
C        DETERMINE WHETHER DATA IS RANKED                                SRANK   4
      IF(NR-1) 5, 10, 5                                                  SRANK   5
C        RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS       SRANK   6
C        AVERAGE OF TIED RANKS                                           SRANK   7
    5 CALL RANK (A,R,N)                                                  SRANK   8
```

```
      CALL RANK (B,R(N+1),N)
      GO TO 40
C        MOVE RANKED DATA TO R VECTOR
   10 DO 20 I=1,N
   20 R(I)=A(I)
      DO 30 I=1,N
      J=I+N
   30 R(J)=B(I)
C        COMPUTE SUM OF SQUARES OF RANK DIFFERENCES
   40 D=0.0
      DO 50 I=1,N
      J=I+N
   50 D=D+(R(I)-R(J))*(R(I)-R(J))
C        COMPUTE TIED SCORE INDEX
      KT=1
      CALL TIE (R,N,KT,TSA)
      CALL TIE (R(N+1),N,KT,TSB)
C        COMPUTE SPEARMAN RANK CORRELATION COEFFICIENT
      IF(TSA) 60,55,60
   55 IF(TSB) 60,57,60
   57 RS=1.0-6.0*D/FNNN
      GO TO 70
   60 X=FNNN/12.0-TSA
      Y=X+TSA-TSB
      RS=(X+Y-D)/(2.0*(SQRT(X*Y)))
C        COMPUTE T AND DEGREES OF FREEDOM IF N IS 10 OR LARGER
      T=0.0
   70 IF(N-10) 80,75,75
   75 T=RS*SQRT(FLOAT(N-2)/(1.0-RS*RS))
   80 NDF=N-2
      RETURN
      END
```

KRANK

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:

$$T_a = \sum \frac{t(t-1)}{2} \text{ for variable A}$$

$$T_b = \sum \frac{t(t-1)}{2} \text{ for variable B} \qquad (1)$$

where t = number of observations tied for a given rank

The Kendall rank correlation coefficient is then computed for the following two cases:

(a) 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 as follows: selecting each rank in turn, add 1 for each larger rank to its right, subtract 1 for each smaller rank to its right.

(b) 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 significance of τ can be measured by:

$$z = \frac{\tau}{s} \qquad (5)$$

Subroutine KRANK

Purpose:

Test correlation between two variables by means of Kendall rank correlation coefficient.

Usage:

CALL KRANK(A, B, R, N, TAU, SD, Z, NR)

Description of parameters:

A	-	Input vector of N observations for first variable.
B	-	Input vector of N observations for second variable.
R	-	Output vector of ranked data of length 2*N. Smallest observation is ranked 1, largest is ranked N. Ties are assigned average of tied ranks.
N	-	Number of observations.
TAU	-	Kendall rank correlation coefficient (output).
SD	-	Standard deviation (output).
Z	-	Test of significance of TAU in terms of normal distribution (output).
NR	-	Code: 0 for unranked data in A and B; 1 for ranked data in A and B (input).

Remarks:

SD and Z are set to zero if N is less than ten.

Subroutines and function subprograms required:

RANK
TIE

Method:

Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 9.

```
      SUBROUTINE KRANK(A,B,R,N,TAU,SD,Z,NR)
      DIMENSION A(1),B(1),R(1)
      SD=0.0
      Z=0.0
      FN=N
      FN1=N*(N-1)
C        DETERMINE WHETHER DATA IS RANKED
      IF(NR-1) 5, 10, 5
C        RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS
C        AVERAGE OF TIED RANKS
    5 CALL RANK (A,R,N)
      CALL RANK (B,R(N+1),N)
      GO TO 40
C        MOVE RANKED DATA TO R VECTOR
   10 DO 20 I=1,N
   20 R(I)=A(I)
      DO 30 I=1,N
      J=I+N
   30 R(J)=B(I)
C        SORT RANK VECTOR R IN SEQUENCE OF VARIABLE A
   40 ISORT=0
      DO 50 I=2,N
      IF(R(I)-R(I-1)) 45,50,50
   45 ISORT=ISORT+1
      RSAVE=R(I)
      R(I)=R(I-1)
      R(I-1)=RSAVE
      I2=I+N
      SAVER=R(I2)
      R(I2)=R(I2-1)
      R(I2-1)=SAVER
   50 CONTINUE
      IF(ISORT) 40,55,40
C        COMPUTE S ON VARIABLE B. STARTING WITH THE FIRST RANK, ADD 1
C        TO S FOR EACH LARGER RANK TO ITS RIGHT AND SUBTRACT 1 FOR EACH
C        SMALLER RANK.  REPEAT FOR ALL RANKS.
   55 S=0.0
      NM=N-1
      DO 60 I=1,NM
      J=N+I
      DO 60 L=I,N
      K=N+L
      IF(R(K)-R(J)) 56,60,57
   56 S=S-1.0
      GO TO 60
   57 S=S+1.0
   60 CONTINUE
C        COMPUTE TIED SCORE INDEX FOR BOTH VARIABLES
      KT=2
      CALL TIE(R,N,KT,TA)
      CALL TIE(R(N+1),N,KT,TB)
C        COMPUTE TAU
      IF(TA) 70,65,70
   65 IF(TB) 70,67,70
   67 TAU=S/(0.5*FN1)
      GO TO 90
   70 TAU=S/((SQRT(0.5*FN1-TA))*(SQRT(0.5*FN1-TB)))
C        COMPUTE STANDARD DEVIATION AND Z IF N IS 10 OR LARGER
   80 IF(N-10) 90,85,85
   85 SD=(SQRT((2.0*(FN+FN+5.0))/(9.0*FN1)))
      Z=TAU/SD
   90 RETURN
      END
```

WTEST

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:

$$T = \sum_{i=1}^{n} \frac{t^3 - t}{12} \qquad (1)$$

where t = number of observations tied for a given rank

Sums of ranks are calculated:

$$Y_j = \sum_{i=1}^{n} R_{ij} \qquad (2)$$

where j = 1, 2, ..., m

From these, the mean of sums of ranks is found:

$$\bar{R} = \frac{\sum_{j=1}^{m} Y_j}{m} \qquad (3)$$

The sum of squares of deviations is derived:

$$s = \sum_{j=1}^{m} (Y_j - \bar{R})^2 \qquad (4)$$

The Kendall coefficient of concordance is then computed:

$$W = \frac{s}{\frac{1}{12}n^2 (m^3 - m) - nT} \qquad (5)$$

For m larger than 7, chi-square is:

$$\chi^2 = n(m-1)W \qquad (6)$$

The degrees of freedom are:

$$\text{d.f.} = n - 1 \qquad (7)$$

Subroutine WTEST

Purpose:

Test degree of association among a number of variables by the Kendall coefficient of concordance.

Usage:

CALL WTEST (A, R, N, M, WA, W, CS, NDF, NR)

Description of parameters:

A	-	Input matrix, N by M, of original data.
R	-	Output matrix, N by M, of ranked data. Smallest value is ranked 1; largest is ranked N. Ties are assigned average of tied ranks.
N	-	Number of variables.
M	-	Number of cases.
WA	-	Work area vector of length 2*M.
W	-	Kendall coefficient of concordance (output).
CS	-	Chi-square (output).
NDF	-	Number of degrees of freedom (output).
NR	-	Code: 0 for unranked data in A; 1 for ranked data in A (input).

Remarks:

Chi-square is set to zero if M is 7 or smaller.

Subroutines and function subprograms required:

RANK
TIE

Method:

Described in S. Siegel, 'Nonparametric Statistics for the Behavioral Sciences', McGraw-Hill, New York, 1956, Chapter 9.

```
      SUBROUTINE WTEST (A,R,N,M,WA,W,CS,NDF,NR)
      DIMENSION A(1),R(1),WA(1)
      FM=M
      FN=N
C        DETERMINE WHETHER DATA IS RANKED
C        RANK DATA FOR ALL VARIABLES ASSIGNING TIED OBSERVATIONS AVERAGE
C        OF TIED RANKS AND COMPUTE CORRECTION FOR TIED SCORES
      T=0.0
      KT=1
      DO 20 I=1,N
      IJ=I-N
      IK=IJ
      IF(NR-1) 5,2,5
    2 DO 3 J=1,M
      IJ=IJ+N
      K=M+J
    3 WA(K)=A(IJ)
      GO TO 15
    5 DO 10 J=1,M
      IJ=IJ+N
   10 WA(J)=A(IJ)
      CALL RANK(WA,WA(M+1),M)
   15 CALL TIE(WA(M+1),M,KT,TI)
      T=T+TI
      DO 20 J=1,M
      IK=IK+N
      IW=M+J
   20 R(IK)=WA(IW)
C        CALCULATE VECTOR OF SUMS OF RANKS
      IR=0
      DO 40 J=1,M
      WA(J)=0.0
      DO 40 I=1,N
      IR=IR+1
   40 WA(J)=WA(J)+R(IR)
C        COMPUTE MEAN OF SUMS OF RANKS
      SM=0.0
      DO 50 J=1,M
   50 SM=SM+WA(J)
      SM=SM/FM
C        COMPUTE SUM OF SQUARES OF DEVIATIONS
      S=0.0
      DO 60 J=1,M
   60 S=S+(WA(J)-SM)*(WA(J)-SM)
C        COMPUTE W
      W=S/(((FN*FN)*(FM*FM*FM-FM)/12.0)-FN*T)
C        COMPUTE DEGREES OF FREEDOM AND CHI-SQUARE IF M IS OVER 7
      CS=0.0
      NDF=0
      IF(M-7) 70,70,65
   65 CS=FN*(FM-1.0)*W
      NDF=M-1
   70 RETURN
      END
```

RANK

Purpose:
Rank a vector of values.

Usage:
CALL RANK(A, R, N)

Description of parameters:
- A - Input vector of N values.
- R - Output vector of length N. Smallest value is ranked 1; largest is ranked N. Ties are assigned average of tied ranks.
- N - Number of values.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Vector is searched for successively larger elements. If ties occur, they are located and their rank value computed. For example, if two values are tied for sixth rank, they are assigned a rank of 6.5 (=(6+7)/2).

```
      SUBROUTINE RANK(A,R,N)
      DIMENSION A(1),R(1)
C        INITIALIZATION
      DO 10 I=1,N
   10 R(I)=0.0
C        FIND RANK OF DATA
      DO 100 I=1,N
C        TEST WHETHER DATA POINT IS ALREADY RANKED
      IF(R(I)) 20, 20, 100
C        DATA POINT TO BE RANKED
   20 SMALL=0.0
      EQUAL=0.0
      X=A(I)
      DO 50 J=1,N
      IF(A(J)-X) 30, 40, 50
C        COUNT NUMBER OF DATA POINTS WHICH ARE SMALLER
   30 SMALL=SMALL+1.0
      GO TO 50
C        COUNT NUMBER OF DATA POINTS WHICH ARE EQUAL
   40 EQUAL=EQUAL+1.0
      R(J)=-1.0
   50 CONTINUE
C        TEST FOR TIE
      IF(EQUAL-1.0) 60, 60, 70
C        STORE RANK OF DATA POINT WHERE NO TIE
   60 R(I)=SMALL+1.0
      GO TO 100
C        CALCULATE RANK OF TIED DATA POINTS
   70 P=SMALL+(EQUAL+1.0)/2.0
      DO 90 J=I,N
      IF(R(J)+1.0) 90, 80, 90
   80 R(J)=P
   90 CONTINUE
  100 CONTINUE
      RETURN
      END
```

TIE

Purpose:
Calculate correction factor due to ties.

Usage:
CALL TIE(R, N, KT, T)

Description of parameters:
- R - Input vector of ranks of length N containing values 1 to N.
- N - Number of ranked values.
- KT - Input code for calculation of correction factor:
  - 1 Solve equation 1.
  - 2 Solve equation 2.
- T - Correction factor (output):
  - 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:
None.

Subroutines and function subprograms required:
None.

Method:
Vector is searched for successively larger ranks. Ties are counted and correction factor 1 or 2 summed.

```
      SUBROUTINE TIE(R,N,KT,T)
      DIMENSION R(1)
C        INITIALIZATION
      T=0.0
      Y=0.0
    5 X=1.0E38
      IND=0
C        FIND NEXT LARGEST RANK
      DO 30 I=1,N
      IF(R(I)-Y) 30,30,10
   10 IF(R(I)-X) 20,30,30
   20 X=R(I)
      IND=IND+1
   30 CONTINUE
C        IF ALL RANKS HAVE BEEN TESTED, RETURN
      IF(IND) 90,90,40
   40 Y=X
      CT=0.0
C        COUNT TIES
      DO 60 I=1,N
      IF(R(I)-X) 60,50,60
   50 CT=CT+1.0
   60 CONTINUE
C        CALCULATE CORRECTION FACTOR
      IF(CT) 70,5,70
   70 IF(KT-1) 75,80,75
   75 T=T+CT*(CT-1.)/2.0
      GO TO 5
   80 T=T+(CT*CT*CT-CT)/12.0
      GO TO 5
   90 RETURN
      END
```

RANDU

Purpose:

Computes uniformly distributed random floating point numbers between 0 and 1.0 and integers in the range 0 to 2**15.

Usage:

CALL RANDU(IX, IY, YFL)

Description of parameters:

IX	- For the first entry this must contain any odd positive integer less than 32,768. After the first entry, IX should be the previous value of IY computed by this subroutine.
IY	- A resultant integer random number required for the next entry to this subroutine. The range of this number is from zero to 2**15.
YFL	- The resultant uniformly distributed, floating point, random number in the range 0 to 1.0.

Remarks:

This subroutine is specific to the IBM 1130. This subroutine should not repeat its cycle in less than 2 to the 13th entries.

Note: If random bits are needed, the high order bits of IY should be chosen.

Subroutines and function subprograms required:

None.

Method:

Power residue method discussed in IBM manual Random Number Generation and Testing (C20-8011).

```
      SUBROUTINE RANDU(IX,IY,YFL)
      IY=IX*899
      IF(IY)5,6,6
    5 IY=IY+32767+1
    6 YFL=IY
      YFL=YFL/32767.
      RETURN
      END
```

GAUSS

This subroutine computes a normally distributed random number with a given mean and standard deviation.

An approximation to normally distributed random numbers Y can be found from a sequence of uniform random numbers* using the formula:

$$Y = \frac{\sum_{i=1}^{K} X_i - \frac{K}{2}}{\sqrt{K/12}} \tag{1}$$

where X_i is a uniformly distributed random number, $0 < X_i < 1$

K is the number of values X_i to be used

Y approaches a true normal distribution asympototically as K approaches infinity. For this subroutine, K was chosen as 12 to reduce execution time. Equation (1) thus becomes:

$$Y = \sum_{i=1}^{12} X_i - 6.0$$

The adjustment for the required mean and standard deviation is then

$$Y' = Y * S + AM \tag{2}$$

where Y' is the required normally distributed random number

S is the required standard deviation

AM is the required mean

* R. W. Hamming, Numerical Methods for Scientists and Engineers, McGraw-Hill, N.Y., 1962, pages 34 and 389.

Subroutine GAUSS

Purpose:
Computes a normally distributed random number with a given mean and standard deviation.

Usage:
CALL GAUSS(IX, S, AM, V)

Description of parameters:

IX	-	IX must contain an odd positive integer less than 32,768. Thereafter it will contain a uniformly distributed integer random number generated by the subroutine for use on the next entry to the subroutine.
S	-	The desired standard deviation of the normal distribution.
AM	-	The desired mean of the normal distribution.
V	-	The value of the computed normal random variable.

Remarks:
This subroutine uses RANDU which is machine specific.

Subroutines and function subprograms required:
RANDU

Method:
Uses 12 uniform random numbers to compute normal random numbers by central limit theorem. The result is then adjusted to match the given mean and standard deviation. The uniform random numbers computed within the subroutine are found by the power residue method.

```
      SUBROUTINE GAUSS(IX,S,AM,V)                                       GAUSS   1
      A=0.0                                                             GAUSS   2
      DO 50 I=1,12                                                      GAUSS   3
      CALL RANDU(IX,IY,Y)                                               GAUSS   4
      IX=IY                                                             GAUSS   5
   50 A=A+Y                                                             GAUSS   6
      V=(A-6.0)*S+AM                                                    GAUSS   7
      RETURN                                                            GAUSS   8
      END                                                               GAUSS   9
```

Mathematics - Special Matrix Operations

MINV

Purpose:
Invert a matrix.

Usage:
CALL MINV(A,N,D,L,M)

Description of parameters:

A	-	Input matrix, destroyed in computation and replaced by resultant inverse.
N	-	Order of matrix A.
D	-	Resultant determinant.
L	-	Work vector of length N.
M	-	Work vector of length N.

Remarks:
Matrix A must be a general matrix.

Subroutines and function subprograms required:
None.

Method:
The standard Gauss-Jordan method is used. The determinant is also calculated. A determinant with absolute value less than 10**(-20) indicates singularity. The user may wish to change this.

```
      SUBROUTINE MINV(A,N,D,L,M)                                        MINV   1
      DIMENSION A(1),L(1),M(1)                                          MINV   2
C        SEARCH FOR LARGEST ELEMENT                                     MINV   3
      D=1.0                                                             MINV   4
      NK=-N                                                             MINV   5
      DO 80 K=1,N                                                       MINV   6
      NK=NK+N                                                           MINV   7
      L(K)=K                                                            MINV   8
      M(K)=K                                                            MINV   9
      KK=NK+K                                                           MINV  10
      BIGA=A(KK)                                                        MINV  11
      DO 20 J=K,N                                                       MINV  12
      IZ=N*(J-1)                                                        MINV  13
      DO 20 I=K,N                                                       MINV  14
      IJ=IZ+I                                                           MINV  15
   10 IF( ABS(BIGA)- ABS(A(IJ))) 15,20,20                               MINV  16
   15 BIGA=A(IJ)                                                        MINV  17
      L(K)=I                                                            MINV  18
      M(K)=J                                                            MINV  19
   20 CONTINUE                                                          MINV  20
C        INTERCHANGE ROWS                                               MINV  21
      J=L(K)                                                            MINV  22
      IF(J-K) 35,35,25                                                  MINV  23
   25 KI=K-N                                                            MINV  24
      DO 30 I=1,N                                                       MINV  25
      KI=KI+N                                                           MINV  26
      HOLD=-A(KI)                                                       MINV  27
      JI=KI-K+J                                                         MINV  28
      A(KI)=A(JI)                                                       MINV  29
   30 A(JI) =HOLD                                                       MINV  30
C        INTERCHANGE COLUMNS                                            MINV  31
   35 I=M(K)                                                            MINV  32
      IF(I-K) 45,45,38                                                  MINV  33
   38 JP=N*(I-1)                                                        MINV  34
      DO 40 J=1,N                                                       MINV  35
      JK=NK+J                                                           MINV  36
      JI=JP+J                                                           MINV  37
      HOLD=-A(JK)                                                       MINV  38
      A(JK)=A(JI)                                                       MINV  39
   40 A(JI) =HOLD                                                       MINV  40
C        DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS        MINV  41
C        CONTAINED IN BIGA)                                             MINV  42
   45 IF(ABS(BIGA)-1.E-20)46,46,48                                      MINV M03
   46 D=0.0                                                             MINV  44
      RETURN                                                            MINV  45
   48 DO 55 I=1,N                                                       MINV  46
      IF(I-K) 50,55,50                                                  MINV  47
   50 IK=NK+I                                                           MINV  48
      A(IK)=A(IK)/(-BIGA)                                               MINV  49
   55 CONTINUE                                                          MINV  50
C        REDUCE MATRIX                                                  MINV  51
      DO 65 I=1,N                                                       MINV  52
      IK=NK+I                                                           MINV  53
      HOLD=A(IK)
      IJ=I-N
      DO 65 J=1,N
      IJ=IJ+N
      IF(I-K) 60,65,60
   60 IF(J-K) 62,65,62
   62 KJ=IJ-I+K
      A(IJ)=HOLD*A(KJ)+A(IJ)
   65 CONTINUE
C        DIVIDE ROW BY PIVOT
      KJ=K-N
      DO 75 J=1,N
      KJ=KJ+N
      IF(J-K) 70,75,70
   70 A(KJ)=A(KJ)/BIGA
   75 CONTINUE
C        PRODUCT OF PIVOTS
      D=D*BIGA
C        REPLACE PIVOT BY RECIPROCAL
      A(KK)=1.0/BIGA
   80 CONTINUE
C        FINAL ROW AND COLUMN INTERCHANGE
      K=N
  100 K=(K-1)
      IF(K) 150,150,105
  105 I=L(K)
      IF(I-K) 120,120,108
  108 JQ=N*(K-1)
      JR=N*(I-1)
      DO 110 J=1,N
      JK=JQ+J
      HOLD=A(JK)
      JI=JR+J
      A(JK)=-A(JI)
  110 A(JI) =HOLD
  120 J=M(K)
      IF(J-K) 100,100,125
  125 KI=K-N
      DO 130 I=1,N
      KI=KI+N
      HOLD=A(KI)
      JI=KI-K+J
      A(KI)=-A(JI)
  130 A(JI) =HOLD
      GO TO 100
  150 RETURN
      END
```

EIGEN

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:

$$\nu_I = \left\{ \sum_{i \le k} 2A_{ik}^2 \right\}^{1/2} \tag{1}$$

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:

$$\nu_F = \frac{\nu_I \times 10^{-6}}{N} \tag{2}$$

This final norm is set sufficiently small that the requirement that any off-diagonal element A_{lm} shall 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:

$$\lambda = -A_{lm} \tag{3}$$

$$\mu = 1/2\,(A_{ll} - A_{mm}) \tag{4}$$

$$\omega = \text{sign}\,(\mu)\,\frac{\lambda}{\sqrt{\lambda^2 + \mu^2}} \tag{5}$$

$$\sin\,\Theta = \frac{\omega}{\sqrt{2\,(1 + \sqrt{1 - \omega^2})}} \tag{6}$$

$$\cos\,\Theta = \sqrt{1 - \sin^2\Theta} \tag{7}$$

$$B = A_{il} \cos\Theta - A_{im} \sin\Theta \tag{8}$$

$$C = A_{il} \sin\Theta + A_{im} \cos\Theta \tag{9}$$

$$B = R_{il} \cos\Theta - R_{im} \sin\Theta \tag{10}$$

$$R_{im} = R_{il} \sin\Theta + R_{im} \cos\Theta \tag{11}$$

$$R_{il} = B \tag{12}$$

$$A_{ll} = A_{il} \cos^2\Theta + A_{mm} \sin^2\Theta - 2A_{lm} \sin\Theta \cos\Theta \tag{13}$$

$$A_{mm} = A_{ll} \sin^2\Theta + A_{mm} \cos^2\Theta + 2A_{lm} \sin\Theta \cos\Theta \tag{14}$$

$$A_{lm} = (A_{ll} - A_{mm}) \sin\Theta \cos\Theta + A_{lm} (\cos^2\Theta - \sin^2\Theta) \tag{15}$$

The above calculations are repeated until all of the pivotal elements are less than the threshold.

Subroutine EIGEN

Purpose:
Compute eigenvalues and eigenvectors of a real symmetric matrix.

Usage:
CALL EIGEN(A, R, N, MV)

Description of parameters:

- A - Original matrix (symmetric), destroyed in computation. Resultant eigenvalues are developed in diagonal of matrix A in descending order.
- R - Resultant matrix of eigenvectors (stored columnwise, in same sequence as eigenvalues).
- N - Order of matrices A and R.
- MV - Input code:
  - 0 Compute eigenvalues and eigenvectors.
  - 1 Compute eigenvalues only (R need not be dimensioned but must still appear in calling sequence).

Remarks:
Original matrix A must be real symmetric (storage mode=1). Matrix A cannot be in the same location as matrix R.

Subroutines and function subprograms required:
None.

Method:
Diagonalization method originated by Jacobi and adapted by von Neumann for large 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.

```
      SUBROUTINE EIGEN(A,R,N,MV)
      DIMENSION A(1),R(1)
C        GENERATE IDENTITY MATRIX
      IF(MV-1) 10,25,10
   10 IQ=-N
      DO 20 J=1,N
      IQ=IQ+N
      DO 20 I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE
C        COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)
   25 ANORM=0.0
      DO 35 I=1,N
      DO 35 J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*SQRT(ANORM)
      ANRMX=ANORM*1.0E-6/FLOAT(N)
C        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR
      IND=0
      THR=ANORM
   45 THR=THR/FLOAT(N)
   50 L=1
   55 M=L+1
C        COMPUTE SIN AND COS
   60 MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
   62 IF( ABS(A(LM))-THR) 130,65,65
   65 IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
   68 Y=-A(LM)/ SQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
   70 Y=-Y
   75 SINX=Y/ SQRT(2.0*(1.0+( SQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
   78 COSX= SQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS =SINX*COSX
C        ROTATE L AND M COLUMNS
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO 125 I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
   80 IF(I-M) 85,115,90
   85 IM=I+MQ
      GO TO 95
   90 IM=M+IQ
   95 IF(I-L) 100,105,105
  100 IL=I+LQ
      GO TO 110
  105 IL=L+IQ
  110 X=A(IL)*COSX-A(IM)*SINX
      A(IM)=A(IL)*SINX+A(IM)*COSX
      A(IL)=X
  115 IF(MV-1) 120,125,120
  120 ILR=ILQ+I
      IMR=IMQ+I
      X=R(ILR)*COSX-R(IMR)*SINX
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX
      R(ILR)=X
  125 CONTINUE
      X=2.0*A(LM)*SINCS
      Y=A(LL)*COSX2+A(MM)*SINX2-X
      X=A(LL)*SINX2+A(MM)*COSX2+X
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
      A(LL)=Y
      A(MM)=X
C        TESTS FOR COMPLETION
C        TEST FOR M = LAST COLUMN
  130 IF(M-N) 135,140,135
  135 M=M+1
      GO TO 60
C        TEST FOR L = SECOND FROM LAST COLUMN
  140 IF(L-(N-1)) 145,150,145
  145 L=L+1
      GO TO 55
  150 IF(IND-1) 160,155,160
  155 IND=0
      GO TO 50
C        COMPARE THRESHOLD WITH FINAL NORM
  160 IF(THR-ANRMX) 165,165,45
C        SORT EIGENVALUES AND EIGENVECTORS
  165 IQ=-N
      DO 185 I=1,N
      IQ=IQ+N
      LL=I+(I*I-I)/2
      JQ=N*(I-2)
      DO 185 J=I,N
      JQ=JQ+N
      MM=J+(J*J-J)/2
      IF(A(LL)-A(MM)) 170,185,185
  170 X=A(LL)
      A(LL)=A(MM)
      A(MM)=X
      IF(MV-1) 175,185,175
  175 DO 180 K=1,N
      ILR=IQ+K
      IMR=JQ+K
      X=R(ILR)
      R(ILR)=R(IMR)
  180 R(IMR)=X
  185 CONTINUE
      RETURN
      END
```

GMADD

Purpose:
Add two general matrices to form resultant general matrix.

Usage:
CALL GMADD(A, B, R, N, M)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A, B, R.
M	-	Number of columns in A, B, R.

Remarks:
All matrices must be stored as general matrices.

Subroutines and function subprograms required:
None.

Method:
Addition is performed element by element.

```
      SUBROUTINE GMADD(A,B,R,N,M)
      DIMENSION A(1),B(1),R(1)
C        CALCULATE NUMBER OF ELEMENTS
      NM=N*M
C        ADD MATRICES
      DO 10 I=1,NM
   10 R(I)=A(I)+B(I)
      RETURN
      END
```

GMSUB

Purpose:
Subtract one general matrix from another to form resultant matrix.

Usage:
CALL GMSUB(A, B, R, N, M)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A, B, R.
M	-	Number of columns in A, B, R.

Remarks:
All matrices must be stored as general matrices.

Subroutines and function subprograms required:
None.

Method:
Matrix B elements are subtracted from corresponding matrix A elements.

```
      SUBROUTINE GMSUB(A,B,R,N,M)
      DIMENSION A(1),B(1),R(1)
C        CALCULATE NUMBER OF ELEMENTS
      NM=N*M
C        SUBTRACT MATRICES
      DO 10 I=1,NM
   10 R(I)=A(I)-B(I)
      RETURN
      END
```

GMPRD

Purpose:
Multiply two general matrices to form a resultant general matrix.

Usage:
CALL GMPRD(A, B, R, N, M, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A.
M	-	Number of columns in A and rows in B.
L	-	Number of columns in B.

Remarks:
All matrices must be stored as general matrices.
Matrix R cannot be in the same location as matrix A.
Matrix R cannot be in the same location as matrix B.
Number of columns of matrix A must be equal to the number of rows of matrix B.

Subroutines and function subprograms required:
None.

Method:
The M by L matrix B is premultiplied by the N by M matrix A and the result is stored in the N by L matrix R.

```
      SUBROUTINE GMPRD(A,B,R,N,M,L)
      DIMENSION A(1),B(1),R(1)
      IR=0
      IK=-M
      DO 10 K=1,L
      IK=IK+M
      DO 10 J=1,N
      IR=IR+1
      JI=J-N
      IB=IK
      R(IR)=0
      DO 10 I=1,M
      JI=JI+N
      IB=IB+1
   10 R(IR)=R(IR)+A(JI)*B(IB)
      RETURN
      END
```

GMTRA

Purpose:
Transpose a general matrix.

Usage:
CALL GMTRA(A, R, N, M)

Description of parameters:

A	-	Name of matrix to be transposed.
R	-	Name of resultant matrix.
N	-	Number of rows of A and columns of R.
M	-	Number of columns of A and rows of R.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrices A and R must be stored as general matrices.

Subroutines and function subprograms required:
None.

Method:
Transpose N by M matrix A to form M by N matrix R.

```
      SUBROUTINE GMTRA(A,R,N,M)
      DIMENSION A(1),R(1)
      IR=0
      DO 10 I=1,N
      IJ=I-N
      DO 10 J=1,M
      IJ=IJ+N
      IR=IR+1
   10 R(IR)=A(IJ)
      RETURN
      END
```

GTPRD

Purpose:
Premultiply a general matrix by the transpose of another general matrix.

Usage:
CALL GTPRD(A, B, R, N, M, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A and B.
M	-	Number of columns in A and rows in R.
L	-	Number of columns in B and R.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrix R cannot be in the same location as matrix B.
All matrices must be stored as general matrices.

Subroutines and function subprograms required:
None.

Method:
Matrix transpose of A is not actually calculated. Instead, elements of matrix A are taken columnwise rather than rowwise for postmultiplication by matrix B.

```
      SUBROUTINE GTPRD(A,B,R,N,M,L)
      DIMENSION A(1),B(1),R(1)
      IR=0
      IK=-N
      DO 10 K=1,L
      IJ=0
      IK=IK+N
      DO 10 J=1,M
      IB=IK
      IR=IR+1
      R(IR)=0
      DO 10 I=1,N
      IJ=IJ+1
      IB=IB+1
   10 R(IR)=R(IR)+A(IJ)*B(IB)
      RETURN
      END
```

MADD

Purpose:
Add two matrices element by element to form resultant matrix.

Usage:
CALL MADD(A, B, R, N, M, MSA, MSB)

Description of parameters:

A	-	Name of input matrix.
B	-	Name of input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A, B, R.
M	-	Number of columns in A, B, R.
MSA	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
MSB	-	Same as MSA except for matrix B.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Storage mode of output matrix is first determined. Addition of corresponding elements is then performed.
The following table shows the storage mode of the output matrix for all combinations of input matrices:

A	B	R
General	General	General
General	Symmetric	General
General	Diagonal	General
Symmetric	General	General
Symmetric	Symmetric	Symmetric
Symmetric	Diagonal	Symmetric
Diagonal	General	General
Diagonal	Symmetric	Symmetric
Diagonal	Diagonal	Diagonal

```
      SUBROUTINE MADD(A,B,R,N,M,MSA,MSB)
      DIMENSION A(1),B(1),R(1)
C        DETERMINE STORAGE MODE OF OUTPUT MATRIX
      IF(MSA-MSB) 7,5,7
    5 CALL LOC(N,M,NM,N,M,MSA)
      GO TO 100
    7 MTEST=MSA*MSB
      MSR=0
      IF(MTEST) 20,20,10
   10 MSR=1
   20 IF(MTEST-2) 35,35,30
   30 MSR=2
C        LOCATE ELEMENTS AND PERFORM ADDITION
   35 DO 90 J=1,M
      DO 90 I=1,N
      CALL LOC(I,J,IJR,N,M,MSR)
      IF(IJR) 40,90,40
   40 CALL LOC(I,J,IJA,N,M,MSA)
      AEL=0.0
      IF(IJA) 50,60,50
   50 AEL=A(IJA)
   60 CALL LOC(I,J,IJB,N,M,MSB)
      BFL=0.0
      IF(IJB) 70,80,70
   70 BFL=B(IJB)
   80 R(IJR)=AEL+BEL
   90 CONTINUE
      RETURN
C        ADD MATRICES FOR OTHER CASES
  100 DO 110 I=1,NM
  110 R(I)=A(I)+B(I)
      RETURN
      END
```

MSUB

Purpose:
Subtract two matrices element by element to form resultant matrix.

Usage:
CALL MSUB(A, B, R, N, M, MSA, MSB)

Description of parameters:

A	-	Name of input matrix.
B	-	Name of input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A, B, R.
M	-	Number of columns in A, B, R.
MSA	-	One digit number for storage mode of matrix A:
		0 - General.
		1 - Symmetric.
		2 - Diagonal.
MSB	-	Same as MSA except for matrix B.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Structure of output matrix is first determined. Subtraction of matrix B elements from corresponding matrix A elements is then performed. The following table shows the storage mode of the output matrix for all combinations of input matrices:

A	B	R
General	General	General
General	Symmetric	General
General	Diagonal	General
Symmetric	General	General
Symmetric	Symmetric	Symmetric
Symmetric	Diagonal	Symmetric
Diagonal	General	General
Diagonal	Symmetric	Symmetric
Diagonal	Diagonal	Diagonal

```
      SUBROUTINE MSUB(A,B,R,N,M,MSA,MSB)
      DIMENSION A(1),B(1),R(1)
C        DETERMINE STORAGE MODE OF OUTPUT MATRIX
      IF(MSA-MSB) 7,5,7
    5 CALL LOC(N,M,NM,N,M,MSA)
      GO TO 100
    7 MTEST=MSA*MSB
      MSR=0
      IF(MTEST) 20,20,10
   10 MSR=1
   20 IF(MTEST-2) 35,35,30
   30 MSR=2
C        LOCATE ELEMENTS AND PERFORM SUBTRACTION
   35 DO 90 J=1,M
      DO 90 I=1,N
      CALL LOC(I,J,IJR,N,M,MSR)
      IF(IJR) 40,90,40
   40 CALL LOC(I,J,IJA,N,M,MSA)
      AEL=0.0
      IF(IJA) 50,60,50
   50 AEL=A(IJA)
   60 CALL LOC(I,J,IJB,N,M,MSB)
      BEL=0.0
      IF(IJB) 70,80,70
   70 BEL=B(IJB)
   80 R(IJR)=AEL-BEL
   90 CONTINUE
      RETURN
C        SUBTRACT MATRICES FOR OTHER CASES
  100 DO 110 I=1,NM
  110 R(I)=A(I)-B(I)
      RETURN
      END
```

MPRD

Purpose:
Multiply two matrices to form a resultant matrix.

Usage:
CALL MPRD(A, B, R, N, M, MSA, MSB, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A and R.
M	-	Number of columns in A and rows in B.
MSA	-	One digit number for storage mode of matrix A:
		0 - General.
		1 - Symmetric.
		2 - Diagonal.
MSB	-	Same as MSA except for matrix B.
L	-	Number of columns in B and R.

Remarks:
Matrix R cannot be in the same location as matrices A or B.
Number of columns of matrix A must be equal to number of rows of matrix B.

Subroutines and function subprograms required:
LOC

Method:
The M by L matrix B is premultiplied by the N by M matrix A and the result is stored in the N by L matrix R. This is a row into column product.
The following table shows the storage mode of the output matrix for all combinations of input matrices:

A	B	R
General	General	General
General	Symmetric	General
General	Diagonal	General
Symmetric	General	General
Symmetric	Symmetric	General
Symmetric	Diagonal	General
Diagonal	General	General
Diagonal	Symmetric	General
Diagonal	Diagonal	Diagonal

```
      SUBROUTINE MPRD(A,B,R,N,M,MSA,MSB,L)
      DIMENSION A(1),B(1),R(1)
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL
      MS=MSA*10+MSB
      IF(MS-22) 30,10,30
   10 DO 20 I=1,N
   20 R(I)=A(I)*B(I)
      RETURN
C        ALL OTHER CASES
   30 IR=1
      DO 90 K=1,L
      DO 90 J=1,N
      R(IR)=0
      DO 80 I=1,M
      IF(MS) 40,60,40
   40 CALL LOC(J,I,IA,N,M,MSA)
      CALL LOC(I,K,IB,M,L,MSB)
      IF(IA) 50,80,50
   50 IF(IB) 70,80,70
   60 IA=N*(I-1)+J
      IB=M*(K-1)+I
   70 R(IR)=R(IR)+A(IA)*B(IB)
   80 CONTINUE
   90 IR=IR+1
      RETURN
      END
```

MTRA

Purpose:
Transpose a matrix.

Usage:
CALL MTRA(A, R, N, M, MS)

Description of parameters:

A	-	Name of matrix to be transposed.
R	-	Name of output matrix.
N	-	Number of rows of A and columns of R.
M	-	Number of columns of A and rows of R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in the same location as matrix A.

Subroutines and function subprograms required:
MCPY

Method:
Transpose N by M matrix A to form M by N matrix R by moving each row of A into the corresponding column of R. If matrix A is symmetric or diagonal, matrix R is the same as A.

```
      SUBROUTINE MTRA(A,R,N,M,MS)
      DIMENSION A(1),R(1)
C        IF MS IS 1 OR 2, COPY A
      IF(MS) 10,20,10
   10 CALL MCPY(A,R,N,N,MS)
      RETURN
C        TRANSPOSE GENERAL MATRIX
   20 IR=0
      DO 30 I=1,N
      IJ=I-N
      DO 30 J=1,M
      IJ=IJ+N
      IR=IR+1
   30 R(IR)=A(IJ)
      RETURN
      END
```

TPRD

Purpose:
Transpose a matrix and postmultiply by another to form a resultant matrix.

Usage:
CALL TPRD(A, B, R, N, M, MSA, MSB, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A and B.
M	-	Number of columns in A and rows in R.
MSA	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
MSB	-	Same as MSA except for matrix B.
L	-	Number of columns in B and R.

Remarks:
Matrix R cannot be in the same location as matrices A or B.

Subroutines and function subprograms required:
LOC

Method:
Matrix transpose of A is not actually calculated. Instead, elements in matrix A are taken columnwise rather than rowwise for multiplication by matrix B.
The following table shows the storage mode of the output matrix for all combinations of input matrices:

A	B	R
General	General	General
General	Symmetric	General
General	Diagonal	General
Symmetric	General	General
Symmetric	Symmetric	General
Symmetric	Diagonal	General
Diagonal	General	General
Diagonal	Symmetric	General
Diagonal	Diagonal	Diagonal

```
      SUBROUTINE TPRD(A,B,R,N,M,MSA,MSB,L)
      DIMENSION A(1),B(1),R(1)
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL
      MS=MSA*10+MSB
      IF(MS-22) 30,10,30
   10 DO 20 I=1,N
   20 R(I)=A(I)*B(I)
      RETURN
C        MULTIPLY TRANSPOSE OF A BY B
   30 IR=1
      DO 90 K=1,L
      DO 90 J=1,M
      R(IR)=0.0
      DO 80 I=1,N
      IF(MS) 40,60,40
   40 CALL LOC(I,J,IA,N,M,MSA)
      CALL LOC(I,K,IB,N,L,MSB)
      IF(IA) 50,80,50
   50 IF(IB) 70,80,70
   60 IA=N*(J-1)+I
      IB=N*(K-1)+I
   70 R(IR)=R(IR)+A(IA)*B(IB)
   80 CONTINUE
   90 IR=IR+1
      RETURN
      END
```

MATA

Purpose:
Premultiply a matrix by its transpose to form a symmetric matrix.

Usage:
CALL MATA(A, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A.
M	-	Number of columns in A. Also number of rows and number of columns of R.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrix R is always a symmetric matrix with a storage mode=1.

Subroutines and function subprograms required:
LOC

Method:
Calculation of (A transpose A) results in a symmetric matrix regardless of the storage mode of the input matrix. The elements of matrix A are not changed.

```
      SUBROUTINE MATA(A,R,N,M,MS)
      DIMENSION A(1),R(1)
      DO 60 K=1,M
      KX=(K*K-K)/2
      DO 60 J=1,M
      IF(J-K) 10,10,60
   10 IR=J+KX
      R(IR)=0
      DO 60 I=1,N
      IF(MS) 20,40,20
   20 CALL LOC(I,J,IA,N,M,MS)
      CALL LOC(I,K,IB,N,M,MS)
      IF(IA) 30,60,30
   30 IF(IB) 50,60,50
   40 IA=N*(J-1)+I
      IB=N*(K-1)+I
   50 R(IR)=R(IR)+A(IA)*A(IB)
   60 CONTINUE
      RETURN
      END
```

SADD

Purpose:
Add a scalar to each element of a matrix to form a resultant matrix.

Usage:
CALL SADD(A, C, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
R	-	Name of output matrix.
N	-	Number of rows in matrix A and R.
M	-	Number of columns in matrix A and R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Scalar is added to each element of matrix.

```
      SUBROUTINE SADD(A,C,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        ADD SCALAR
      DO 1 I=1,IT
    1 R(I)=A(I)+C
      RETURN
      END
```

SSUB

Purpose:
Subtract a scalar from each element of a matrix to form a resultant matrix.

Usage:
CALL SSUB(A, C, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
R	-	Name of output matrix.
N	-	Number of rows in matrix A and R.
M	-	Number of columns in matrix A and R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Scalar is subtracted from each element of matrix.

```
      SUBROUTINE SSUB(A,C,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        SUBTRACT SCALAR
      DO 1 I=1,IT
    1 R(I)=A(I)-C
      RETURN
      END
```

SMPY

Purpose:
Multiply each element of a matrix by a scalar to form a resultant matrix.

Usage:
CALL SMPY(A, C, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
R	-	Name of output matrix.
N	-	Number of rows in matrix A and R.
M	-	Number of columns in matrix A and R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Scalar is multiplied by each element of matrix.

```
      SUBROUTINE SMPY(A,C,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        MULTIPLY BY SCALAR
      DO 1 I=1,IT
    1 R(I)=A(I)*C
      RETURN
      END
```

SDIV

Purpose:
Divide each element of a matrix by a scalar to form a resultant matrix.

Usage:
CALL SDIV(A, C, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
R	-	Name of output matrix.
N	-	Number of rows in matrix A and R.
M	-	Number of columns in matrix A and R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
If scalar is zero, division is performed only once to cause floating-point overflow condition.

Subroutines and function subprograms required:
LOC

Method:
Each element of matrix is divided by scalar.

```
      SUBROUTINE SDIV(A,C,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        DIVIDE BY SCALAR (IF SCALAR IS ZERO, DIVIDE ONLY ONCE)
      IF(C) 2,1,2
    1 IT=1
    2 DO 3 I=1,IT
    3 R(I)=A(I)/C
      RETURN
      END
```

RADD

Purpose:
Add row of one matrix to row of another matrix.

Usage:
CALL RADD(A, IRA, R, IRR, N, M, MS, L)

Description of parameters:

A	-	Name of input matrix.
IRA	-	Row in matrix A to be added to row IRR of matrix R.
R	-	Name of output matrix.
IRR	-	Row in matrix R where summation is developed.
N	-	Number of rows in A.
M	-	Number of columns in A and R.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
L	-	Number of rows in R.

Remarks:
Matrix R must be a general matrix.
Matrix R cannot be in the same location as matrix A unless A is general.

Subroutines and function subprograms required:
LOC

Method:
Each element of row IRA of matrix A is added to corresponding element of row IRR of matrix R.

```
      SUBROUTINE RADD(A,IRA,R,IRR,N,M,MS,L)
      DIMENSION A(1),R(1)
      IR=IRR-L
      DO 2 J=1,M
      IR=IR+L
C        LOCATE INPUT ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(IRA,J,IA,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IA) 1,2,1
C        ADD ELEMENTS
    1 R(IR)=R(IR)+A(IA)
    2 CONTINUE
      RETURN
      END
```

CADD

Purpose:
Add column of one matrix to column of another matrix.

Usage:
CALL CADD(A, ICA, R, ICR, N, M, MS, L)

Description of parameters:

A	-	Name of input matrix.
ICA	-	Column in matrix A to be added to column ICR of R.
R	-	Name of output matrix.
ICR	-	Column in matrix R where summation is developed.
N	-	Number of rows in A and R.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
L	-	Number of columns in R.

Remarks:
Matrix R must be a general matrix.
Matrix R cannot be in the same location as matrix A unless A is general.

Subroutines and function subprograms required:
LOC

Method:
Each element of column ICA of matrix A is added to corresponding element of column ICR of matrix R.

```
      SUBROUTINE CADD(A,ICA,R,ICR,N,M,MS,L)
      DIMENSION A(1),R(1)
      IR=N*(ICR-1)
      DO 2 I=1,N
      IR=IR+1
C        LOCATE INPUT ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,ICA,IA,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IA) 1,2,1
C        ADD ELEMENTS
    1 R(IR)=R(IR)+A(IA)
    2 CONTINUE
      RETURN
      END
```

SRMA

Purpose:
Multiply row of matrix by a scalar and add to another row of the same matrix.

Usage:
CALL SRMA(A, C, N, M, LA, LB)

Description of parameters:

A	-	Name of matrix.
C	-	Scalar.
N	-	Number of rows in A.
M	-	Number of columns in A.
LA	-	Row in A to be multiplied by scalar.
LB	-	Row in A to which product is added. If 0 is specified, product replaces elements in row LA.

Remarks:
Matrix A must be a general matrix.

Subroutines and function subprograms required:
None.

Method:
Each element of row LA is multiplied by scalar C and the product is added to the corresponding element of row LB. Row LA remains unaffected by the operation.
If parameter LB contains zero, multiplication by the scalar is performed and the product replaces elements in row LA.

```
      SUBROUTINE SRMA(A,C,N,M,LA,LB)
      DIMENSION A(1)
      LAJ=LA-N
      LBJ=LB-N
      DO 3 J=1,M
C        LOCATE ELEMENT IN BOTH ROWS
      LAJ=LAJ+N
      LBJ=LBJ+N
C        CHECK LB FOR ZERO
      IF(LB) 1,2,1
C        IF NOT, MULTIPLY BY CONSTANT AND ADD TO OTHER ROW
    1 A(LBJ)=A(LAJ)*C+A(LBJ)
      GO TO 3
C        OTHERWISE, MULTIPLY ROW BY CONSTANT
    2 A(LAJ)=A(LAJ)*C
    3 CONTINUE
      RETURN
      END
```

SCMA

Purpose:
Multiply column of,matrix by a scalar and add to another column of the same matrix.

Usage:
CALL SCMA(A, C, N, LA, LB)

Description of parameters:

A	-	Name of matrix.
C	-	Scalar.
N	-	Number of rows in A.
LA	-	Column in A to be multiplied by scalar.
LB	-	Column in A to which product is added. If 0 is specified, product replaces elements in LA.

Remarks:
Matrix A must be a general matrix.

Subroutines and function subprograms required:
None.

Method:
Each element of column LA is multiplied by scalar C and the product is added to the corresponding element of column LB. Column LA remains unaffected by the operation.
If parameter LB contains zero, multiplication by the scalar is performed and the product replaces elements in LA.

```
      SUBROUTINE SCMA(A,C,N,LA,LB)
      DIMENSION A(1)
C        LOCATE STARTING POINT OF BOTH COLUMNS
      ILA=N*(LA-1)
      ILB=N*(LB-1)
      DO 3 I=1,N
      ILA=ILA+1
      ILB=ILB+1
C        CHECK LB FOR ZERO
      IF(LB) 1,2,1
C        IF NOT MULTIPLY BY CONSTANT AND ADD TO SECOND COLUMN
    1 A(ILB)=A(ILA)*C+A(ILB)
      GO TO 3
C        OTHERWISE, MULTIPLY COLUMN BY CONSTANT
    2 A(ILA)=A(ILA)*C
    3 CONTINUE
      RETURN
      END
```

RINT

Purpose:
Interchange two rows of a matrix.

Usage:
CALL RINT(A, N, M, LA, LB)

Description of parameters:

A	-	Name of matrix.
N	-	Number of rows in A.
M	-	Number of columns in A.
LA	-	Row to be interchanged with row LB.
LB	-	Row to be interchanged with row LA.

Remarks:
Matrix A must be a general matrix.

Subroutines and function subprograms required:
None.

Method:
Each element of row LA is interchanged with corresponding element of row LB.

```
      SUBROUTINE RINT(A,N,M,LA,LB)
      DIMENSION A(1)
      LAJ=LA-N
      LBJ=LB-N
      DO 3 J=1,M
C        LOCATE ELEMENTS IN BOTH ROWS
      LAJ=LAJ+N
      LBJ=LBJ+N
C        INTERCHANGE ELEMENTS
      SAVE=A(LAJ)
      A(LAJ)=A(LBJ)
    3 A(LBJ)=SAVE
      RETURN
      END
```

CINT

Purpose:
Interchange two columns of a matrix.

Usage:
CALL CINT(A,N,LA,LB)

Description of parameters:

A	-	Name of matrix.
N	-	Number of rows in A.
LA	-	Column to be interchanged with column LB.
LB	-	Column to be interchanged with column LA.

Remarks:
Matrix A must be a general matrix.

Subroutines and function subprograms required:
None.

Method:
Each element of column LA is interchanged with corresponding element of column LB.

```
      SUBROUTINE CINT(A,N,LA,LB)
      DIMENSION A(1)
C        LOCATE STARTING POINT OF BOTH COLUMNS
      ILA=N*(LA-1)
      ILB=N*(LB-1)
      DO 3 I=1,N
      ILA=ILA+1
      ILB=ILB+1
C        INTERCHANGE ELEMENTS
      SAVE=A(ILA)
      A(ILA)=A(ILB)
    3 A(ILB)=SAVE
      RETURN
      END
```

RSUM

Purpose:
Sum elements of each row to form column vector.

Usage:
CALL RSUM (A,R,N,M,MS)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of vector of length N.
N	-	Number of rows in A.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Vector R cannot be in the same location as matrix A unless A is general.

Subroutines and function subprograms required:
LOC

Method:
Elements are summed across each row into a corresponding element of output column vector R.

```
      SUBROUTINE RSUM(A,R,N,M,MS)
      DIMENSION A(1),R(1)
      DO 3 I=1,N
C        CLEAR OUTPUT LOCATION
      R(I)=0.0
      DO 3 J=1,M
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,J,IJ,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 2,3,2
C        ACCUMULATE IN OUTPUT VECTOR
    2 R(I)=R(I)+A(IJ)
    3 CONTINUE
      RETURN
      END
```

CSUM

Purpose:
Sum elements of each column to form row vector.

Usage:
CALL CSUM(A, R, N, M, MS)

Description of parameters:

A	- Name of input matrix.
R	- Name of vector of length M.
N	- Number of rows in A.
M	- Number of columns in A.
MS	- One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Vector R cannot be in the same location as matrix A unless A is general.

Subroutines and function subprograms required:
LOC

Method:
Elements are summed down each column into a corresponding element of output row vector R.

```
      SUBROUTINE CSUM(A,R,N,M,MS)
      DIMENSION A(1),R(1)
      DO 3 J=1,M
C        CLEAR OUTPUT LOCATION
      R(J)=0.0
      DO 3 I=1,N
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,J,IJ,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 2,3,2
C        ACCUMULATE IN OUTPUT VECTOR
    2 R(J)=R(J)+A(IJ)
    3 CONTINUE
      RETURN
      END
```

RTAB

The function of this subroutine is graphically displayed by Figure 6 (see description under "Method").

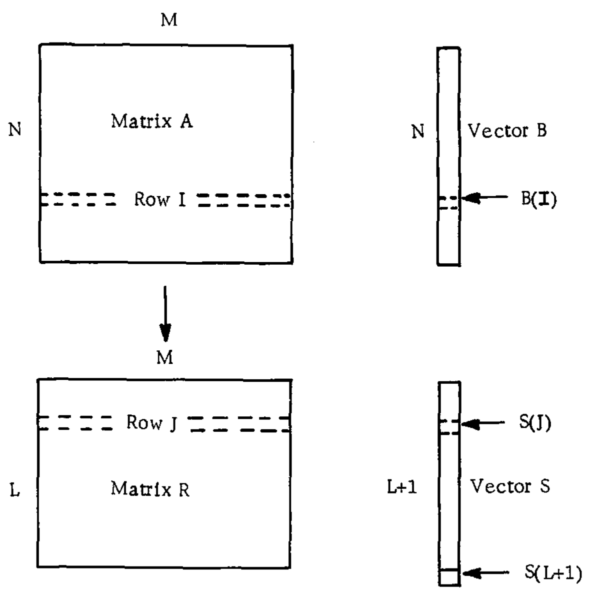


Figure 6. Row tabulation

Subroutine RTAB

Purpose:
Tabulate rows of a matrix to form a summary matrix.

Usage:
CALL RTAB(A, B, R, S, N, M, MS, L)

Description of parameters:

A	- Name of input matrix.
B	- Name of input vector of length N containing key.
R	- Name of output matrix containing summary of row data. It is initially set to zero by this subroutine.
S	- Name of output vector of length L+1 containing counts.
N	- Number of rows in A.
M	- Number of columns in A and R.
L	- Number of rows in R.
MS	- One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R is always a general matrix.

Subroutines and function subprograms required:
LOC
RADD

Method:
Rows of data in matrix A are tabulated using the key contained in vector B. The floating point number in B(I) is truncated to form J. The I^{th} row of A is added to the J^{th} row of R, element by element, and one is added to S(J). If J is not between one and L, one is added to S(L+1). This procedure is repeated for every element in vector B. Upon completion, the output matrix R contains a summary of row data as specified by vector B. Each element in vector S contains a count of the number of rows of A used to form the corresponding row of R. Element S(L+1) contains a count of the number of rows of A not included in R as a result of J being less than one or greater than L.

```
      SUBROUTINE RTAB(A,B,R,S,N,M,MS,L)
      DIMENSION A(1),B(1),R(1),S(1)
C        CLEAR OUTPUT AREAS
      CALL LOC(M,L,IT,M,L,0)
      DO 10 IR=1,IT
   10 R(IR)=0.0
      DO 20 IS=1,L
   20 S(IS)=0.0
      S(L+1)=0.0
      DO 60 I=1,N
C        TEST FOR THE KEY OUTSIDE THE RANGE
      IF(B(I)) 50,50,30
   30 E=L
      IF(B(I)-E) 40,40,50
   40 JR=B(I)
C        ADD ROW OF A TO ROW OF R AND 1 TO COUNT
      CALL RADD(A,I,R,JR,N,M,MS,L)
      S(JR)=S(JR)+1.0
      GO TO 60
   50 S(L+1)=S(L+1)+1.0
   60 CONTINUE
      RETURN
      END
```

CTAB

The function of this subroutine is graphically displayed by Figure 7 (see description under "Method").

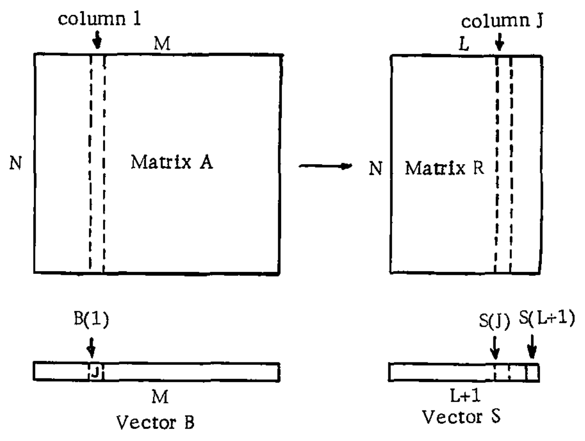


Figure 7. Column tabulation

Subroutine CTAB

Purpose:
Tabulate columns of a matrix to form a summary matrix.

Usage:
CALL CTAB(A,B,R,S,N,M,MS,L)

Description of parameters:

A	-	Name of input matrix.
B	-	Name of input vector of length M containing key.
R	-	Name of output matrix containing summary of column data. It is initially set to zero by this subroutine.
S	-	Name of output vector of length L+1 containing counts.
N	-	Number of rows in A and R.
M	-	Number of columns in A.
L	-	Number of columns in R.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R is always a general matrix.

Subroutines and function subprograms required:
LOC
CADD

Method:

Columns of data in matrix A are tabulated using the key contained in vector B. The floating-point number in B(I) is truncated to form J. The I^{th} column of A is added to the J^{th} column of matrix R and one is added to S(J). If the value of J is not between one and M, one is added to S(L+ 1). Upon completion, the output matrix R contains a summary of column data as specified by vector B. Each element in vector S contains a count of the number of columns of A used to form R. Element S(L+ 1) contains the number of columns of A not included in R as a result of J being less than one or greater than L.

```
      SUBROUTINE CTAB(A,B,R,S,N,M,MS,L)
      DIMENSION A(1),B(1),R(1),S(1)
C        CLEAR OUTPUT AREAS
      CALL LOC(N,L,IT,N,L,0)
      DO 10 IR=1,IT
   10 R(IR)=0.0
      DO 20 IS=1,L
   20 S(IS)=0.0
      S(L+1)=0.0
      DO 60 I=1,M
C        TEST FOR THE KEY OUTSIDE THE RANGE
      IF(B(I)) 50,50,30
   30 E=L
      IF(B(I)-E) 40,40,50
   40 JR=B(I)
C        ADD COLUMN OF A TO COLUMN OF R AND 1 TO COUNT
      CALL CADD(A,I,R,JR,N,M,MS,L)
      S(JR)=S(JR)+1.0
      GO TO 60
   50 S(L+1)=S(L+1)+1.0
   60 CONTINUE
      RETURN
      END
```

RSRT

Purpose:
Sort rows of a matrix.

Usage:
CALL RSRT(A, B, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix to be sorted.
B	-	Name of input vector which contains sorting key.
R	-	Name of sorted output matrix.
N	-	Number of rows in A and R and length of B.
M	-	Number of columns in A and R.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrix R is always a general matrix. .
N must be greater than 1. This routine sorts into ascending order. Sorting into descending order requires changing card RSRT 013 to read IF(R(I-1)-R(I)) 30, 40, 40

Subroutines and function subprograms required:
LOC

Method:
Rows of input matrix A are sorted to form output matrix R. The sorted row sequence is determined by the values of elements in column vector B. The lowest valued element in B will cause the corresponding row of A to be placed in the first row of R. The highest valued element of B will cause the corresponding row of A to be placed in the last row of R. If duplicate values exist in B, the corresponding rows of A are moved to R in the same order as in A.

```
      SUBROUTINE RSRT(A,B,R,N,M,MS)                                     RSRT   1
      DIMENSION A(1),B(1),R(1)                                          RSRT   2
C        MOVE SORTING KEY VECTOR TO FIRST COLUMN OF OUTPUT MATRIX       RSRT   3
C        AND BUILD ORIGINAL SEQUENCE LIST IN SECOND COLUMN              RSRT   4
      DO 10 I=1,N                                                       RSRT   5
      R(I)=B(I)                                                         RSRT   6
      I2=I+N                                                            RSRT   7
   10 R(I2)=I                                                           RSRT   8
C        SORT ELEMENTS IN SORTING KEY VECTOR (ORIGINAL SEQUENCE LIST    RSRT   9
C        IS RESEQUENCED ACCORDINGLY)                                    RSRT  10
      L=N+1                                                             RSRT M01
   20 ISORT=0                                                           RSRT  11
      L=L-1                                                             RSRT M02
      DO 40 I=2,L                                                       RSRT M03
      IF(R(I)-R(I-1)) 30,40,40                                          RSRT  13
   30 ISORT=1                                                           RSRT M04
      RSAVE=R(I)                                                        RSRT  15
      R(I)=R(I-1)                                                       RSRT  16
      R(I-1)=RSAVE                                                      RSRT  17
      I2=I+N                                                            RSRT  18
      SAVER=R(I2)                                                       RSRT  19
      R(I2)=R(I2-1)                                                     RSRT  20
      R(I2-1)=SAVER                                                     RSRT  21
   40 CONTINUE                                                          RSRT  22
      IF(ISORT) 20,50,20                                                RSRT  23
C        MOVE ROWS FROM MATRIX A TO MATRIX R (NUMBER IN SECOND COLUMN   RSRT  24
C        OF R REPRESENTS ROW NUMBER OF MATRIX A TO BE MOVED)            RSRT  25
   50 DO 80 I=1,N                                                       RSRT  26
C        GET ROW NUMBER IN MATRIX A                                     RSRT  27
      I2=I+N                                                            RSRT  28
      IN=R(I2)                                                          RSRT  29
      IR=I-N                                                            RSRT  30
      DO 80 J=1,M                                                       RSRT  31
C        LOCATE ELEMENT IN OUTPUT MATRIX                                RSRT  32
      IR=IR+N                                                           RSRT  33
C        LOCATE ELEMENT IN INPUT MATRIX                                 RSRT  34
      CALL LOC(IN,J,IA,N,M,MS)                                          RSRT  35
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RSRT  36
      IF(IA) 60,70,60                                                   RSRT  37
C        MOVE ELEMENT TO OUTPUT MATRIX                                  RSRT  38
   60 R(IR)=A(IA)                                                       RSRT  39
      GO TO 80                                                          RSRT  40
   70 R(IR)=0                                                           RSRT  41
   80 CONTINUE                                                          RSRT  42
      RETURN                                                            RSRT  43
      END                                                               RSRT  44
```

CSRT

Purpose:
    Sort columns of a matrix.

Usage:
    CALL CSRT(A, B, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix to be sorted.
B	-	Name of input vector which contains sorting key.
R	-	Name of sorted output matrix.
N	-	Number of rows in A and R.
M	-	Number of columns in A and R and length of B.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
    Matrix R cannot be in the same location as matrix A.
    Matrix R is always a general matrix.
    N must be greater than 1. This routine sorts into ascending order. Sorting into descending order requires changing card CSRT 016 to read IF(R(IP)-R(IQ)) 30, 40, 40

Subroutines and function subprograms required:
    LOC
    CCPY

Method:
    Columns of input matrix A are sorted to form output matrix R. The sorted column sequence is determined by the values of elements in row vector B. The lowest valued element in B will cause the corresponding column of A to be placed in the first column of R. The highest valued element of B will cause the corresponding row of A to be placed in the last column of R. If duplicate values exist in B, the corresponding columns of A are moved to R in the same order as in A.

```
      SUBROUTINE CSRT(A,B,R,N,M,MS)                                     CSRT   1
      DIMENSION A(1),B(1),R(1)                                          CSRT   2
C        MOVE SORTING KEY VECTOR TO FIRST ROW OF OUTPUT MATRIX          CSRT   3
C        AND BUILD ORIGINAL SEQUENCE LIST IN SECOND ROW                 CSRT   4
      IK=1                                                              CSRT   5
      DO 10 J=1,M                                                       CSRT   6
      R(IK)=B(J)                                                        CSRT   7
      R(IK+1)=J                                                         CSRT   8
   10 IK=IK+N                                                           CSRT   9
C        SORT ELEMENTS IN SORTING KEY VECTOR (ORIGINAL SEQUENCE LIST    CSRT  10
C        IS RESEQUENCED ACCORDINGLY)                                    CSRT  11
      L=M+1                                                             CSRT M01
   20 ISORT=0                                                           CSRT  12
      L=L-1                                                             CSRT M02
      IP=1                                                              CSRT  13
      IQ=N+1                                                            CSRT  14
      DO 50 J=2,L                                                       CSRT M03
      IF(R(IQ)-R(IP)) 30,40,40                                          CSRT  16
   30 ISORT=1                                                           CSRT M04
      RSAVE=R(IQ)                                                       CSRT  18
      R(IQ)=R(IP)                                                       CSRT  19
      R(IP)=RSAVE                                                       CSRT  20
      SAVER=R(IQ+1)                                                     CSRT  21
      R(IQ+1)=R(IP+1)                                                   CSRT  22
      R(IP+1)=SAVER                                                     CSRT  23
   40 IP=IP+N                                                           CSRT  24
      IQ=IQ+N                                                           CSRT  25
   50 CONTINUE                                                          CSRT  26
      IF(ISORT) 20,60,20                                                CSRT  27
C        MOVE COLUMNS FROM MATRIX A TO MATRIX R (NUMBER IN SECOND ROW   CSRT  28
C        OF R REPRESENTS COLUMN NUMBER OF MATRIX A TO BE MOVED)         CSRT  29
   60 IQ=-N                                                             CSRT  30
      DO 70 J=1,M                                                       CSRT  31
      IQ=IQ+N                                                           CSRT  32
C        GET COLUMN NUMBER IN MATRIX A                                  CSRT  33
      I2=IQ+2                                                           CSRT  34
      IN=R(I2)                                                          CSRT  35
C        MOVE COLUMN                                                    CSRT  36
      IR=IQ+1                                                           CSRT  37
      CALL CCPY(A,IN,R(IR),N,M,MS)                                      CSRT  38
   70 CONTINUE                                                          CSRT  39
      RETURN                                                            CSRT  40
      END                                                               CSRT  41
```

RCUT

Purpose:
Partition a matrix between specified rows to form two resultant matrices.

Usage:
CALL RCUT (A, L, R, S, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
L	-	Row of A above which partitioning takes place.
R	-	Name of matrix to be formed from upper portion of A.
S	-	Name of matrix to be formed from lower portion of A.
N	-	Number of rows in A.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in same location as matrix A.
Matrix S cannot be in same location as matrix A.
Matrix R cannot be in same location as matrix S.
Matrix R and matrix S are always general matrices.

Subroutines and function subprograms required:
LOC

Method:
Elements of matrix A above row L are moved to form matrix R of L-1 rows and M columns. Elements of matrix A in row L and below are moved to form matrix S of N-L+1 rows and M columns.

```
      SUBROUTINE RCUT(A,L,R,S,N,M,MS)
      DIMENSION A(1),R(1),S(1)
      IR=0
      IS=0
      DO 70 J=1,M
      DO 70 I=1,N
C        FIND LOCATION IN OUTPUT MATRIX AND SET TO ZERO
      IF(I-L) 20,10,10
   10 IS=IS+1
      S(IS)=0.0
      GO TO 30
   20 IR=IR+1
      R(IR)=0.0
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
   30 CALL LOC(I,J,IJ,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 40,70,40
C        DETERMINE WHETHER ABOVE OR BELOW L
   40 IF(I-L) 60,50,50
   50 S(IS)=A(IJ)
      GO TO 70
   60 R(IR)=A(IJ)
   70 CONTINUE
      RETURN
      END
```

CCUT

Purpose:
Partition a matrix between specified columns to form two resultant matrices.

Usage:
CALL CCUT (A, L, R, S, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
L	-	Column of A to the left of which partitioning takes place.
R	-	Name of matrix to be formed from left portion of A.
S	-	Name of matrix to be formed from right portion of A.
N	-	Number of rows in A.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in same location as matrix A.
Matrix S cannot be in same location as matrix A.
Matrix R cannot be in same location as matrix S.
Matrix R and matrix S are always general matrices.

Subroutines and function subprograms required:
LOC

Method:
Elements of matrix A to the left of column L are moved to form matrix R of N rows and L-1 columns. Elements of matrix A in column L and to the right of L are moved to form matrix S of N rows and M-L+1 columns.

```
      SUBROUTINE CCUT(A,L,R,S,N,M,MS)
      DIMENSION A(1),R(1),S(1)
      IR=0
      IS=0
      DO 70 J=1,M
      DO 70 I=1,N
C        FIND LOCATION IN OUTPUT MATRIX AND SET TO ZERO
      IF(J-L) 20,10,10
   10 IS=IS+1
      S(IS)=0.0
      GO TO 30
   20 IR=IR+1
      R(IR)=0.0
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
   30 CALL LOC(I,J,IJ,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 40,70,40
C        DETERMINE WHETHER RIGHT OR LEFT OF L
   40 IF(J-L) 60,50,50
   50 S(IS)=A(IJ)
      GO TO 70
   60 R(IR)=A(IJ)
   70 CONTINUE
      RETURN
      END
```

RTIE

Purpose:

Adjoin two matrices with same column dimension to form one resultant matrix. (See Method.)

Usage:

CALL RTIE(A, B, R, N, M, MSA, MSB, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A.
M	-	Number of columns in A, B, R.
MSA	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
MSB	-	Same as MSA except for matrix B.
L	-	Number of rows in B.

Remarks:

Matrix R cannot be in the same location as matrices A or B.
Matrix R is always a general matrix.
Matrix A must have the same number of columns as matrix B.

Subroutines and function subprograms required:

LOC

Method:

Matrix B is attached to the bottom of matrix A. The resultant matrix R contains N+ L rows and M columns.

```
      SUBROUTINE RTIE(A,B,R,N,M,MSA,MSB,L)
      DIMENSION A(1),B(1),R(1)
      NN=N
      IR=0
      NX=NN
      MSX=MSA
      DO 9 J=1,M
      DO 8 II=1,2
      DO 7 I=1,NN
      IR=IR+1
      R(IR)=0.0
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,J,IJ,NN,M,MSX)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 2,7,2
C        MOVE ELEMENT TO MATRIX R
    2 GO TO(3,4),II
    3 R(IR)=A(IJ)
      GO TO 7
    4 R(IR)=B(IJ)
    7 CONTINUE
C        REPEAT ABOVE FOR MATRIX B
      MSX=MSB
    8 NN=L
C        RESET FOR NEXT COLUMN
      MSX=MSA
    9 NN=NX
      RETURN
      END
```

CTIE

Purpose:

Adjoin two matrices with same row dimension to form one resultant matrix. (See Method.)

Usage:

CALL CTIE(A, B, R, N, M, MSA, MSB, L)

Description of parameters:

A	-	Name of first input matrix.
B	-	Name of second input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A, B, R.
M	-	Number of columns in A.
MSA	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
MSB	-	Same as MSA except for matrix B.
L	-	Number of columns in B.

Remarks:

Matrix R cannot be in the same location as matrices A or B.
Matrix R is always a general matrix.
Matrix A must have the same number of rows as matrix B.

Subroutines and function subprograms required:

LOC

Method:

Matrix B is attached to the right of matrix A. The resultant matrix R contains N rows and M+ L columns.

```
      SUBROUTINE CTIE(A,B,R,N,M,MSA,MSB,L)
      DIMENSION A(1),B(1),R(1)
      MM=M
      IR=0
      MSX=MSA
      DO 6 JJ=1,2
      DO 5 J=1,MM
      DO 5 I=1,N
      IR=IR+1
      R(IR)=0.0
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,J,IJ,N,MM,MSX)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IJ) 2,5,2
C        MOVE ELEMENT TO MATRIX R
    2 GO TO(3,4),JJ
    3 R(IR)=A(IJ)
      GO TO 5
    4 R(IR)=B(IJ)
    5 CONTINUE
C        REPEAT ABOVE FOR MATRIX B
      MSX=MSB
      MM=L
    6 CONTINUE
      RETURN
      END
```

MCPY

Purpose:
Copy entire matrix.

Usage:
CALL MCPY (A, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of output matrix.
N	-	Number of rows in A or R.
M	-	Number of columns in A or R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Each element of matrix A is moved to the corresponding element of matrix R.

```
      SUBROUTINE MCPY(A,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        COPY MATRIX
      DO 1 I=1,IT
    1 R(I)=A(I)
      RETURN
      END
```

XCPY

Purpose:
Copy a portion of a matrix.

Usage:
CALL XCPY(A, R, L, K, NR, MR, NA, MA, MS)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of output matrix.
L	-	Row of A where first element of R can be found.
K	-	Column of A where first element of R can be found.
NR	-	Number of rows to be copied into R.
MR	-	Number of columns to be copied into R.
NA	-	Number of rows in A.
MA	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrix R is always a general matrix.

Subroutines and function subprograms required:
LOC

Method:
Matrix R is formed by copying a portion of matrix A. This is done by extracting NR rows and MR columns of matrix A, starting with element at row L, column K.

```
      SUBROUTINE XCPY(A,R,L,K,NR,MR,NA,MA,MS)
      DIMENSION A(1),R(1)
C        INITIALIZE
      IR=0
      L2=L+NR-1
      K2=K+MR-1
      DO 5 J=K,K2
      DO 5 I=L,L2
      IR=IR+1
      R(IR)=0.0
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,J,IA,NA,MA,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IA) 4,5,4
    4 R(IR)=A(IA)
    5 CONTINUE
      RETURN
      END
```

RCPY

Purpose:
Copy specified row of a matrix into a vector.

Usage:
CALL RCPY (A, L, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
L	-	Row of A to be moved to R.
R	-	Name of output vector of length M.
N	-	Number of rows in A.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Elements of row L are moved to corresponding positions of vector R.

```
      SUBROUTINE RCPY(A,L,R,N,M,MS)
      DIMENSION A(1),R(1)
      DO 3 J=1,M
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(L,J,LJ,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(LJ) 1,2,1
C        MOVE ELEMENT TO R
    1 R(J)=A(LJ)
      GO TO 3
    2 R(J)=0.0
    3 CONTINUE
      RETURN
      END
```

CCPY

Purpose:
Copy specified column of a matrix into a vector.

Usage:
CALL CCPY(A, L, R, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
L	-	Column of A to be moved to R.
R	-	Name of output vector of length N.
N	-	Number of rows in A.
M	-	Number of columns in A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Elements of column L are moved to corresponding positions of vector R.

```
      SUBROUTINE CCPY(A,L,R,N,M,MS)
      DIMENSION A(1),R(1)
      DO 3 I=1,N
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,L,IL,N,M,MS)
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX
      IF(IL) 1,2,1
C        MOVE ELEMENT TO R
    1 R(I)=A(IL)
      GO TO 3
    2 R(I)=0.0
    3 CONTINUE
      RETURN
      END
```

DCPY

Purpose:
Copy diagonal elements of a matrix into a vector.

Usage:
CALL DCPY (A, R, N, MS)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of output vector of length N.
N	-	Number of rows and columns in matrix A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Input matrix must be a square matrix.

Subroutines and function subprograms required:
LOC

Method:
Elements on diagonal of matrix are moved to corresponding positions of vector R.

```
      SUBROUTINE DCPY(A,R,N,MS)
      DIMENSION A(1),R(1)
      DO 3 J=1,N
C        LOCATE DIAGONAL ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(J,J,IJ,N,N,MS)
C        MOVE DIAGONAL ELEMENT TO VECTOR R
    3 R(J)=A(IJ)
      RETURN
      END
```

SCLA

Purpose:
Set each element of a matrix equal to a given scalar.

Usage:
CALL SCLA (A, C, N, M, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
N	-	Number of rows in matrix A.
M	-	Number of columns in matrix A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
LOC

Method:
Each element of matrix A is replaced by Scalar C.

```
      SUBROUTINE SCLA(A,C,N,M,MS)
      DIMENSION A(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        REPLACE BY SCALAR
      DO 1 I=1,IT
    1 A(I)=C
      RETURN
      END
```

DCLA

Purpose:
Set each diagonal element of a matrix equal to a scalar.

Usage:
CALL DCLA (A, C, N, MS)

Description of parameters:

A	-	Name of input matrix.
C	-	Scalar.
N	-	Number of rows and columns in matrix A.
MS	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Input matrix must be a square matrix.

Subroutines and function subprograms required:
LOC

Method:
Each element on diagonal of matrix is replaced by scalar C.

```
      SUBROUTINE DCLA(A,C,N,MS)
      DIMENSION A(1)
      DO 3 I=1,N
C        LOCATE DIAGONAL ELEMENT FOR ANY MATRIX STORAGE MODE
      CALL LOC(I,I,ID,N,N,MS)
C        REPLACE DIAGONAL ELEMENTS
    3 A(ID)=C
      RETURN
      END
```

MSTR

Purpose:
Change storage mode of a matrix.

Usage:
CALL MSTR(A, R, N, MSA, MSR)

Description of parameters:

A	-	Name of input matrix.
R	-	Name of output matrix.
N	-	Number of rows and columns in A and R.
MSA	-	One digit number for storage mode of matrix A: 0 - General. 1 - Symmetric. 2 - Diagonal.
MSR	-	Same as MSA except for matrix R.

Remarks:
Matrix R cannot be in the same location as matrix A.
Matrix A must be a square matrix.

Subroutines and function subprograms required:
LOC

Method:
Matrix A is restructured to form matrix R.

MSA	MSR	
0	0	Matrix A is moved to matrix R.
0	1	The upper triangle elements of a general matrix are used to form a symmetric matrix.
0	2	The diagonal elements of a general matrix are used to form a diagonal matrix.
1	0	A symmetric matrix is expanded to form a general matrix.
1	1	Matrix A is moved to matrix R.
1	2	The diagonal elements of a symmetric matrix are used to form a diagonal matrix.
2	0	A diagonal matrix is expanded by inserting missing zero elements to form a general matrix.
2	1	A diagonal matrix is expanded by inserting missing zero elements to form a symmetric matrix.
2	2	Matrix A is moved to matrix R.

```
      SUBROUTINE MSTR(A,R,N,MSA,MSR)
      DIMENSION A(1),R(1)
      DO 20 I=1,N
      DO 20 J=1,N
C        IF R IS GENERAL, FORM ELEMENT
      IF(MSR) 5,10,5
C        IF IN LOWER TRIANGLE OF SYMMETRIC OR DIAGONAL R, BYPASS
    5 IF(I-J) 10,10,20
   10 CALL LOC(I,J,IR,N,N,MSR)
C        IF IN UPPER AND OFF DIAGONAL  OF DIAGONAL R, BYPASS
      IF(IR) 20,20,15
C        OTHERWISE, FORM R(I,J)
   15 R(IR)=0.0
      CALL LOC(I,J,IA,N,N,MSA)
C        IF THERE IS NO A(I,J), LEAVE R(I,J) AT 0.0
      IF(IA) 20,20,18
   18 R(IR)=A(IA)
   20 CONTINUE
      RETURN
      END
```

MFUN

Purpose:
Apply a function to each element of a matrix to form a resultant matrix.

Usage:

CALL MFUN (A, F, R, N, M, MS)

An external statement must precede call statement in order to identify parameter F as the name of a function.

Description of parameters:

A	-	Name of input matrix.
F	-	Name of FORTRAN-furnished or user function subprogram.
R	-	Name of output matrix.
N	-	Number of rows in matrix A and R.
M	-	Number of columns in matrix A and R.
MS	-	One digit number for storage mode of matrix A (and R): 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
Precision is dependent upon precision of function used.

Subroutines and function subprograms required:
LOC
F (see Description of Parameters)

Method:
Function F is applied to each element of matrix A to form matrix R.

```
      SUBROUTINE MFUN(A,F,R,N,M,MS)
      DIMENSION A(1),R(1)
C        COMPUTE VECTOR LENGTH, IT
      CALL LOC(N,M,IT,N,M,MS)
C        BUILD MATRIX R FOR ANY STORAGE MODE
      DO 5 I=1,IT
      B=A(I)
    5 R(I)=F(B)
      RETURN
      END
```

Function RECP

Purpose:
Calculate reciprocal of an element. This is a FORTRAN function subprogram which may be used as an argument by subroutine MFUN.

Usage:
RECP(E)

Description of parameters:
E - Matrix element.

Remarks:
Reciprocal of zero is taken to be 1.0E38.

Subroutines and function subprograms required:
None.

Method:
Reciprocal of element E is placed in RECP.

```
      FUNCTION RECP(E)
      BIG=1.0E38
C        TEST ELEMENT FOR ZERO
      IF(E) 1,2,1
C        IF NON-ZERO, CALCULATE RECIPROCAL
    1 RECP=1.0/E
      RETURN
C        IF ZERO, SET EQUAL TO INFINITY
    2 RECP=SIGN(BIG,E)
      RETURN
      END
```

LOC

Purpose:
Compute a vector subscript for an element in a matrix of specified storage mode.

Usage:
CALL LOC (I, J, IR, N, M, MS)

Description of parameters:

I	-	Row number of element.
J	-	Column number of element.
IR	-	Resultant vector subscript.
N	-	Number of rows in matrix.
M	-	Number of columns in matrix.
MS	-	One digit number for storage mode of matrix: 0 - General. 1 - Symmetric. 2 - Diagonal.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:

MS=0	Subscript is computed for a matrix with N*M elements in storage (general matrix).
MS=1	Subscript is computed for a matrix with N*(N+1)/2 in storage (upper triangle of symmetric matrix). If element is in lower triangular portion, subscript is corresponding element in upper triangle.
MS=2	Subscript is computed for a matrix with N elements in storage (diagonal elements of diagonal matrix). If element is not on diagonal (and therefore not in storage), IR is set to zero.

```
      SUBROUTINE LOC(I,J,IR,N,M,MS)
      IX=I
      JX=J
      IF(MS-1) 10,20,30
   10 IRX=N*(JX-1)+IX
      GO TO 36
   20 IF(IX-JX) 22,24,24
   22 IRX=IX+(JX*JX-JX)/2
      GO TO 36
   24 IRX=JX+(IX*IX-IX)/2
      GO TO 36
   30 IRX=0
      IF(IX-JX) 36,32,36
   32 IRX=IX
   36 IR=IRX
      RETURN
      END
```

ARRAY

Purpose:
Convert data array from single to double dimension or vice versa. This subroutine is used to link the user program which has double dimension arrays and the SSP subroutines which operate on arrays of data in a vector fashion.

Usage:
CALL ARRAY (MODE, I, J, N, M, S, D)

Description of parameters:

MODE	-	Code indicating type of conversion: 1 - From single to double dimension. 2 - From double to single dimension.
I	-	Number of rows in actual data matrix.
J	-	Number of columns in actual data matrix.
N	-	Number of rows specified for the matrix D in dimension statement.
M	-	Number of columns specified for the matrix D in dimension statement.
S	-	If MODE=1, this vector contains, as input, a data matrix of size I by J in consecutive locations columnwise. If MODE=2, it contains a data matrix of the same size as output. The length of vector S is IJ, where IJ=I*J.
D	-	If MODE=1, this matrix (N by M) contains, as output, a data matrix of size I by J in first I rows and J columns. If MODE=2, it contains a data matrix of the same size as input.

Remarks:
Vector S can be in the same location as matrix D. Vector S is referred as a matrix in other SSP routines, since it contains a data matrix. This subroutine converts only general data matrices (storage mode of 0).

Subroutines and function subroutines required:
None.

Method:
Refer to the discussion on variable data size in the section describing overall rules for usage in this manual.

```
      SUBROUTINE ARRAY (MODE,I,J,N,M,S,D)
      DIMENSION S(1),D(1)
      NI=N-I
C        TEST TYPE OF CONVERSION
      IF(MODE-1) 100, 100, 120
C        CONVERT FROM SINGLE TO DOUBLE DIMENSION
  100 IJ=I*J+1
      NM=N*J+1
      DO 110 K=1,J
      NM=NM-NI
      DO 110 L=1,I
      IJ=IJ-1
      NM=NM-1
  110 D(NM)=S(IJ)
      GO TO 140
C        CONVERT FROM DOUBLE TO SINGLE DIMENSION
  120 IJ=0
      NM=0
      DO 130 K=1,J
      DO 125 L=1,I
      IJ=IJ+1
      NM=NM+1
  125 S(IJ)=D(NM)
  130 NM=NM+NI
  140 RETURN
      END
```

Mathematics — Integration and Differentiation

QSF

This subroutine performs the integration of an equidistantly tabulated function by Simpson's rule. To compute the vector of integral values:

$$\left.\begin{aligned} z_i = z(x_i) &= \int_a^{x_i} y(x)\,dx \\ \text{with } x_i &= a + (i-1)\,h \end{aligned}\right\}\ (i = 1,2,\ldots,n)$$

for a table of function values y_i $(i = 1,2,\ldots,n)$, given at equidistant points $x_i = a + (i-1)\,h$ $(i = 1,2,\ldots,n)$, Simpson's rule together with Newton's 3/8 rule or a combination of these two rules is used. Local truncation error is of the order h^5 in all cases with more than three points in the given table. Only z_2 has a truncation error of the order h^4 if there are only three points in the given table. No action takes place if the table consists of less than three sample points.

The function is assumed continuous and differentiable (three or four times, depending on the rule used).

Formulas used in this subroutine (z_j are integral values, y_j function values) are:

$$z_j = z_{j-1} + \frac{h}{3}(1.25\,y_{j-1} + 2y_j - 0.25\,y_{j+1}) \qquad (1)$$

$$z_j = z_{j-2} + \frac{h}{3}(y_{j-2} + 4y_{j-1} + y_j) \quad \text{(Simpson's rule)} \qquad (2)$$

$$z_j = z_{j-3} + \frac{3}{8}h\,(y_{j-3} + 3y_{j-2} + 3y_{j-1} + y_j) \qquad (3)$$

(Newton's 3/8 rule)

$$z_j = z_{j-5} + \frac{h}{3}(y_{j-5} + 3.875\,y_{j-4} + 2.625\,y_{j-3} + 2.625\,y_{j-2} + 3.875\,y_{j-1} + y_j) \qquad (4)$$

[combination of (2) and (3)]

Sometimes formula (2) is used in the following form:

$$z_j = z_{j+2} - \frac{h}{3}(y_j + 4\,y_{j+1} + y_{j+2}) \qquad (5)$$

Local truncation errors of formulas (1)...(4) are, respectively:

$$R_1 = \frac{1}{24}h^4\,y'''(\xi_1) \qquad (\xi_1 \epsilon [x_{j-1}, x_{j+1}]\ )$$

$$R_2 = -\frac{1}{90}h^5\,y''''(\xi_2) \qquad (\xi_2 \epsilon [x_{j-2}, x_j])$$

$$R3 = -\frac{3}{80}h^5\,y''''(\xi_3) \qquad (\xi_3 \epsilon [x_{j-3}, x_j])$$

$$R_4 = -\frac{1}{144}h^5\,y''''(\xi_4) \qquad (\xi_4 \epsilon [x_{j-5}, x_j])$$

However, these truncation errors may accumulate. For reference see:

(1) F.B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 71-76.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 214-221.

Subroutine QSF

Purpose:
To compute the vector of integral values for a given equidistant table of function values.

Usage:
CALL QSF(H,Y,Z,NDIM)

Description of parameters:

H	-	The increment of argument values.
Y	-	The input vector of function values.
Z	-	The resulting vector of integral values. Z may be identical to Y.
NDIM	-	The dimension of vectors Y and Z.

Remarks:
No action in case NDIM less then 3.

Subroutines and function subprograms required:
None

Method:
Beginning with Z(1) = 0, evaluation of vector Z is done by means of Simpson's rule together with Newton's 3/8 rule or a combination of these two rules. Truncation error is of order H**5 (that is, fourth-order method). Only in case NDIM=3 truncation error of Z(2) is of order H**4.

```
      SUBROUTINE QSF(H,Y,Z,NDIM)
      DIMENSION Y(1),Z(1)
      HT=.3333333*H
      L1=1
      L2=2
      L3=3
      L4=4
      L5=5
      L6=6
      IF(NDIM-5)7,8,1
C     NDIM IS GREATER THAN 5. PREPARATIONS OF INTEGRATION LOOP
    1 SUM1=Y(L2)+Y(L2)
      SUM1=SUM1+SUM1
      SUM1=HT*(Y(L1)+SUM1+Y(L3))
      AUX1=Y(L4)+Y(L4)
      AUX1=AUX1+AUX1
      AUX1=SUM1+HT*(Y(L3)+AUX1+Y(L5))
      AUX2=HT*(Y(L1)+3.875*(Y(L2)+Y(L5))+2.625*(Y(L3)+Y(L4))+Y(L6))
      SUM2=Y(L5)+Y(L5)
      SUM2=SUM2+SUM2
      SUM2=AUX2-HT*(Y(L4)+SUM2+Y(L6))
      Z(L1)=0.
      AUX=Y(L3)+Y(L3)
      AUX=AUX+AUX
      Z(L2)=SUM2-HT*(Y(L2)+AUX+Y(L4))
      Z(L3)=SUM1
      Z(L4)=SUM2
      IF(NDIM-6)5,5,2
C     INTEGRATION LOOP
    2 DO 4 I=7,NDIM,2
      SUM1=AUX1
      SUM2=AUX2
      AUX1=Y(I-1)+Y(I-1)
      AUX1=AUX1+AUX1
      AUX1=SUM1+HT*(Y(I-2)+AUX1+Y(I))
      Z(I-2)=SUM1
      IF(I-NDIM)3,6,6
    3 AUX2=Y(I)+Y(I)
      AUX2=AUX2+AUX2
      AUX2=SUM2+HT*(Y(I-1)+AUX2+Y(I+1))
    4 Z(I-1)=SUM2
    5 Z(NDIM-1)=AUX1
      Z(NDIM)=AUX2
      RETURN
    6 Z(NDIM-1)=SUM2
      Z(NDIM)=AUX1
      RETURN
C     END OF INTEGRATION LOOP
    7 IF(NDIM-3)12,11,8
C     NDIM IS EQUAL TO 4 OR 5
    8 SUM2=1.125*HT*(Y(L1)+Y(L2)+Y(L2)+Y(L2)+Y(L3)+Y(L3)+Y(L3)+Y(L4))
      SUM1=Y(L2)+Y(L2)
      SUM1=SUM1+SUM1
      SUM1=HT*(Y(L1)+SUM1+Y(L3))
      Z(L1)=0.
      AUX1=Y(L3)+Y(L3)
      AUX1=AUX1+AUX1
      Z(L2)=SUM2-HT*(Y(L2)+AUX1+Y(L4))
      IF(NDIM-5)10,9,9
    9 AUX1=Y(L4)+Y(L4)
      AUX1=AUX1+AUX1
      Z(L5)=SUM1+HT*(Y(L3)+AUX1+Y(L5))
   10 Z(L3)=SUM1
      Z(L4)=SUM2
      RETURN
C     NDIM IS EQUAL TO 3
   11 SUM1=HT*(1.25*Y(L1)+Y(L2)+Y(L2)-.25*Y(L3))
      SUM2=Y(L2)+Y(L2)
      SUM2=SUM2+SUM2
      Z(L3)=HT*(Y(L1)+SUM2+Y(L3))
      Z(L1)=0.
      Z(L2)=SUM1
   12 RETURN
      END
```

This subroutine performs the integration of a given function by the trapezoidal rule together with Romberg's extrapolation method in order to compute an approximation for:

$$y = \int_a^b f(x)\,dx \tag{1}$$

Successively dividing the interval $[a,b]$ into 2^i equidistant subintervals $(i = 0,1,2,\ldots)$ and using the following notations:

$$h_i = \frac{b-a}{2^i}\ ;\ x_{i,k} = a + k\,.\,h_i,\ f_{i,k} = f(x_{i,k})$$

$$(k = 0,1,2,\ldots,2^i)$$

the trapezoidal rule gives approximations $T_{o,i}$ to the integral value y:

$$T_{o,i} = h_i\left\{\sum_{k=0}^{2^i} f_{i,k} - \frac{1}{2}(f(a) + f(b))\right\} \tag{2}$$

Then the following can be written:

$$T_{o,i} = y + \sum_{r=1}^{\infty} C_{o,2r}\cdot h_i^{2r}$$

with unknown coefficients $C_{o,2r}$ which do not depend on i. Thus there is a truncation error of the order h_i^2.

Knowing two successive approximations, $T_{o,i}$ and $T_{o,i+1}$, an extrapolated value can be generated:

$$T_{1,i} = T_{o,\,i+1} + \frac{T_{o,i+1} - T_{o,i}}{2^2 - 1} \tag{3}$$

This is a better approximation to y because:

$$T_{1,i} = y + \frac{1}{2^2-1}\sum_{r=1}^{\infty} C_{o,2r}\,(2^2\,h_{i+1}^{2r} - h_i^{2r})$$

Noting that $2^2\,h_{i+1}^2 - h_i^2 = 0$ and setting:

$$C_{1,2r} = \frac{1}{2^2-1}\,(2^2 - 2^{2r})\,.\,C_{o,2r}$$

$T_{1,i}$ 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 $T_{o,\,i+2}$ also, $T_{1,\,i+1}$ can be generated (formula 3), and:

$$T_{2,i} = T_{1,\,i+1} + \frac{T_{1,i+1} - T_{1,i}}{2^4 - 1} \tag{4}$$

Thus:

$$T_{2,i} = y + \sum_{r=3}^{\infty} C_{2,2r}\cdot h_{i+2}^{2r}$$

with $C_{2,2r} = \dfrac{1}{2^4-1}\,(2^4 - 2^{2r})\,C_{1,2r}$

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.

The subroutine uses the scheme shown in the figure below for computation of T-values and generates the upward diagonal in the one-dimensional storage array AUX, using the general formula:

$$T_{k,j} = T_{k-1,j+1} + \frac{T_{k-1,j+1} - T_{k-1,j}}{2^{2k}-1} \quad (k+j=i, \qquad (5)$$

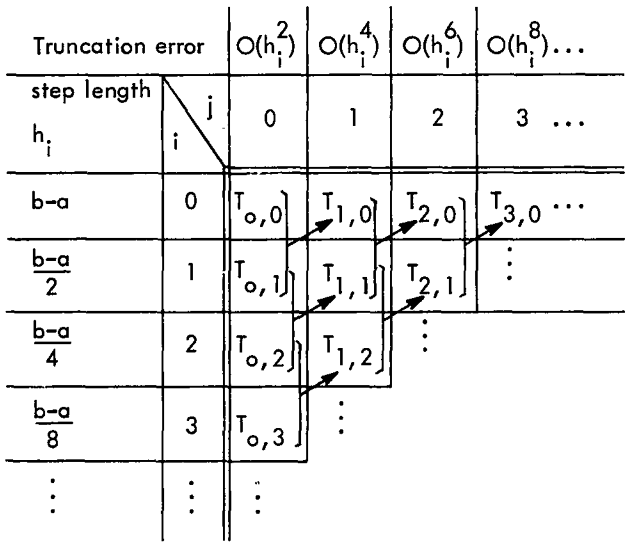
$$j = i-1, i-2, \ldots, 2, 1, 0)$$

and storing:

$T_{o,i}$ into AUX (i+1)

$T_{1,i-1}$ into AUX (i) ....

$T_{k,0}$ into AUX (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 QATR

Purpose:

To compute an approximation for integral (FCT(X), summed over X from XL to XU).

Usage:

CALL QATR(XL, XU, EPS, NDIM, FCT, Y, IER, AUX) Parameter FCT required an EXTERNAL statement.

Description of parameters:

XL	-	The lower bound of the interval.
XU	-	The upper bound of the interval.
EPS	-	The upper bound of the absolute error.
NDIM	-	The dimension of the auxiliary storage array AUX. NDIM-1 is the maximal number of bisections of the interval (XL, XU).
FCT	-	The name of the external function subprogram used.
Y	-	The resulting approximation for the integral value.
IER	-	A resulting error parameter.
AUX	-	An auxiliary storage array with dimension NDIM.

Remarks:

Error parameter IER is coded in the following form:

IER=0	-	It was possible to reach the required accuracy. No error.
IER=1	-	It is impossible to reach the required accuracy because of rounding errors.
IER=2	-	It was impossible to check accuracy because NDIM is less than 5, or the required accuracy could not be reached within NDIM-1 steps. NDIM should be increased.

Subroutines and function subprograms required:

The external function subprogram FCT(X) must be coded by the user. Its argument X should not be destroyed.

Method:

Evaluation of Y is done by means of the trapezoidal rule in connection with Romberg's principle. On return Y contains the best possible approximation of the integral value and vector AUX the upward diagonal of the Romberg scheme. Components AUX(I) (I=1, 2,..., IEND, with IEND less than or equal to NDIM) become approximation to the integral value with decreasing accuracy by multiplication by (XU-XL).

For reference see:

1. 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.

2. Bauer, Algorithm 60, CACM, Vol. 4, Iss. 6 (1961), pp. 255.

```
      SUBROUTINE QATR(XL,XU,EPS,NDIM,FCT,Y,IER,AUX)
      DIMENSION AUX(1)
C     PREPARATIONS OF ROMBERG-LOOP
      AUX(1)=.5*(FCT(XL)+FCT(XU))
      H=XU-XL
      IF(NDIM-1)8,8,1
    1 IF(H)2,10,2
C     NDIM IS GREATER THAN 1 AND H IS NOT EQUAL TO 0.
    2 HH=H
      E=EPS/ABS(H)
      DELT2=0.
      P=1.
      JJ=1
      DO 7 I=2,NDIM
      Y=AUX(1)
      DELT1=DELT2
      HD=HH
      HH=.5*HH
      P=.5*P
      X=XL+HH
      SM=0.
      DO 3 J=1,JJ
      SM=SM+FCT(X)
    3 X=X+HD
      AUX(I)=.5*AUX(I-1)+P*SM
C     A NEW APPROXIMATION OF INTEGRAL VALUE IS COMPUTED BY MEANS OF
C     TRAPEZOIDAL RULE.
C     START OF ROMBERGS EXTRAPOLATION METHOD.
      Q=1.
      JI=I-1
      DO 4 J=1,JI
      II=I-J
      Q=Q+Q
      Q=Q+Q
    4 AUX(II)=AUX(II+1)+(AUX(II+1)-AUX(II))/(Q-1.)
C     END OF ROMBERG-STEP
      DELT2=ABS(Y-AUX(1))
      IF(I-5)7,5,5
    5 IF(DELT2-E)10,10,6
    6 IF(DELT2-DELT1)7,11,11
    7 JJ=JJ+JJ
    8 IER=2
    9 Y=H*AUX(1)
      RETURN
   10 IER=0
      GO TO 9
   11 IER=1
      Y=H*Y
      RETURN
      END
```

Mathematics - Ordinary Differential Equations

RK1

This subroutine integrates a given function using the Runge-Kutta technique and produces the final computed value of the integral.

The ordinary differential equation:

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

with initial condition $y(x_0) = y_0$ is solved numerically using a fourth-order Runge-Kutta integration process. This is a single-step method in which the value of y at $x = x_n$ is used to compute $y_{n+1} = y(x_{n+1})$ and earlier values y_{n-1}, y_{n-2}, etc., are not used.

The relevant formulae are:

$$y_{n+1} = y_n + 1/6\,[k_0 + 2k_1 + 2k_2 + k_3] \tag{2}$$

where we define, for step size h

$$\left\{\begin{aligned} k_0 &= hf(x_n, y_n) \\ k_1 &= hf(x_n + h/2, y_n + k_0/2) \\ k_2 &= hf(x_n + h/2, y_n + k_1/2) \\ k_3 &= hf(x_n + h, y_n + k_2) \end{aligned}\right. \tag{3}$$

Subroutine RK1

Purpose:

Integrates a first order differential equation DY/DX=FUN(X,Y) up to a specified final value.

Usage:

CALL RK1(FUN,HI,XI,YI,XF,YF,ANSX,ANSY,IER)

Description of parameters:

FUN	-	User-supplied function subprogram with arguments X,Y which gives DY/DX.
HI	-	The step size.
XI	-	Initial value of X.
YI	-	Initial value of Y where YI=Y(XI).
XF	-	Final value of X.
YF	-	Final value of Y.
ANSX	-	Resultant final value of X.
ANSY	-	Resultant final value of Y. Either ANSX will equal XF or ANSY will equal YF depending on which is reached first.
IER	-	Error code:

IER=0	No error.
IER=1	Step size is zero.

Remarks:

If XI is greater than XF, ANSX=XI and ANSY=YI.

If H is zero, IER is set to one, ANSX is set to XI, and ANSY is set to zero.

Subroutines and function subprograms required:

FUN is a two argument function subprogram furnished by the user: DY/DX=FUN (X,Y). Calling program must have FORTRAN external statement containing names of function subprograms listed in call to RK1.

Method:

Uses fourth-order Runge-Kutta integration process on a recursive basis as shown in F. B. Hildebrand, 'Introduction to Numerical Analysis', McGraw-Hill, 1956. Process is terminated and final value adjusted when either XF or YF is reached.

```
      SUBROUTINE RK1(FUN,HI,XI,YI,XF,YF,ANSX,ANSY,IER)
C        IF XF IS LESS THAN OR EQUAL TO XI, RETURN XI,YI AS ANSWER
      IF(XF-XI) 11,11,12
   11 ANSX=XI
      ANSY=YI
      RETURN
C        TEST INTERVAL VALUE
   12 H=HI
      IF(HI) 16,14,20
   14 IER=1
      ANSX=XI
      ANSY=0.0
      RETURN
   16 H=-HI
C        SET XN=INITIAL X,YN=INITIAL Y
   20 XN=XI
      YN=YI
C        INTEGRATE ONE TIME STEP
      HNEW=H
      JUMP=1
      GO TO 170
   25 XN1=XX
      YN1=YY
C        COMPARE XN1 (=X(N+1)) TO X FINAL AND BRANCH ACCORDINGLY
      IF(XN1-XF)50,30,40
C        XN1=XF, RETURN (XF,YN1) AS ANSWER
   30 ANSX=XF
      ANSY=YN1
      GO TO 160
C        XN1 GREATER THAN XF, SET NEW STEP SIZE AND INTEGRATE ONE STEP
C        RETURN RESULTS OF INTEGRATION AS ANSWER
   40 HNEW=XF-XN
      JUMP=2
      GO TO 170
   45 ANSX=XX
      ANSY=YY
      GO TO 160
C        XN1 LESS THAN X FINAL, CHECK IF (YN,YN1) SPAN Y FINAL
   50 IF((YN1-YF)*(YF-YN))60,70,110
```

```
C          YN1 AND YN DO NOT SPAN YF. SET (XN,YN) AS (XN1,YN1) AND REPEAT
   60 YN=YN1
      XN=XN1
      GO TO 170
C          EITHER YN OR YN1 =YF. CHECK WHICH AND SET PROPER (X,Y) AS ANSWER
   70 IF(YN1-YF)80,100,80
   80 ANSY=YN
      ANSX=XN
      GO TO 160
  100 ANSY=YN1
      ANSX=XN1
      GO TO 160
C          YN AND YN1 SPAN YF. TRY TO FIND X VALUE ASSOCIATED WITH YF
  110 DO 140 I=1,10
C          INTERPOLATE TO FIND NEW TIME STEP AND INTEGRATE ONE STEP
C          TRY TEN INTERPOLATIONS AT MOST
      HNEW=((YF-YN )/(YN1-YN))*(XN1-XN)
      JUMP=3
      GO TO 170
  115 XNEW=XX
      YNEW=YY
C          COMPARE COMPUTED Y VALUE WITH YF AND BRANCH
      IF(YNEW-YF)120,150,130
C          ADVANCE, YF IS BETWEEN YNEW AND YN1
  120 YN=YNEW
      XN=XNEW
      GO TO 140
C          ADVANCE, YF IS BETWEEN YN AND YNEW
  130 YN1=YNEW
      XN1=XNEW
  140 CONTINUE
C          RETURN (XNEW,YF) AS ANSWER
  150 ANSX=XNEW
      ANSY=YF
  160 RETURN
  170 H2=HNEW/2.0
      T1=HNEW*FUN(XN,YN)
      T2=HNEW*FUN(XN+H2,YN+T1/2.0)
      T3=HNEW*FUN(XN+H2,YN+T2/2.0)
      T4=HNEW*FUN(XN+HNEW,YN+T3)
      YY=YN+(T1+2.0*T2+2.0*T3+T4)/6.0
      XX=XN+HNEW
      GO TO (25,45,115), JUMP
      END
```

RK2

This subroutine integrates a given function using the Runge-Kutta technique and produces tabulated values of the computed integral.

The ordinary differential equation:

$$\frac{dy}{dx} = f(x,y) \qquad (1)$$

with initial condition $y(x_0) = y_0$ is solved numerically using a fourth-order Runge-Kutta integration process. This is a single-step method in which the value of y at $x = x_n$ is used to compute $y_{n+1} = y(x_{n+1})$ and earlier values y_{n-1}, y_{n-2}, etc., are not used.

The relevant formulae are:

$$y_{n+1} = y_n + 1/6\left[k_0 + 2k_1 + 2k_2 + k_3\right] \qquad (2)$$

where we define, for step size h

$$\left\{\begin{aligned} k_0 &= hf(x_n, y_n) \\ k_1 &= hf(x_n + h/2, y_n + k_0/2) \\ k_2 &= hf(x_n + h/2, y_n + k_1/2) \\ k_3 &= hf(x_n + h, y_n + k_2) \end{aligned}\right. \qquad (3)$$

Subroutine RK2

Purpose:

Integrates a first-order differential equation DY/DX=FUN(X, Y) and produces a table of integrated values.

Usage:

CALL RK2(FUN, H, XI, YI, K, N, VEC)

Description of parameters:

FUN	-	User-supplied function subprogram with arguments X, Y which gives DY/DX.
H	-	Step size.
XI	-	Initial value of X.
YI	-	Initial value of Y where YI=Y(XI).
K	-	The interval at which computed values are to be stored.
N	-	The number of values to be stored.
VEC	-	The resultant vector of length N in which computed values of Y are to be stored.

Remarks:

None.

Subroutines and function subprograms required:

FUN - User-supplied function subprogram for DY/DX.

Calling program must have FORTRAN EXTERNAL statement containing names of function subprograms listed in call to RK2.

Method:

Fourth-order Runge-Kutta integration on a recursive basis as shown in F. B. Hildebrand, 'Introduction to Numerical Analysis', McGraw-Hill, New York, 1956.

```
      SUBROUTINE RK2(FJN,H,XI,YI,K,N,VEC)
      DIMENSION VEC(1)
      H2=H/2.
      Y=YI
      X=XI
      DO 2 I=1,N
      DO 1 J=1,K
      T1=H*FUN(X,Y)
      T2=H*FUN(X+H2,Y+T1/2.)
      T3=H*FUN(X+H2,Y+T2/2.)
      T4=H*FUN(X+H,Y+T3)
      Y= Y+(T1+2.*T2+2.*T3+T4)/6.
    1 X=X+H
    2 VEC(I)=Y
      RETURN
      END
```

RKGS

This subroutine uses the Runge-Kutta method for the solution of initial-value problems.

The purpose of the Runge-Kutta method is to obtain an approximate solution of a system of first-order ordinary differential equations with given initial values. It is a fourth-order integration procedure which is stable and self-starting; that is, only the functional values at a single previous point are required to obtain the functional values ahead. For this reason it is easy to change the step size h at any step in the calculations. On the other hand, each Runge-Kutta step requires the evaluation of the right-hand side of the system four times, which is a great disadvantage compared with other methods of the same order of accuracy, especially predictor-corrector methods. Another disadvantage of the method is that neither the truncation errors nor estimates of them are obtained in the calculation procedure. Therefore, control of accuracy and adjustment of the step size h is done by comparison of the results due to double and single step size 2h and h.

Given the system of first-order ordinary differential equations:

$$y_1' = \frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$
$$y_2' = \frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$
$$\ldots\ldots\ldots\ldots$$
$$y_n' = \frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

and the initial values:

$$y_1(x_0) = y_{1,0},\ y_2(x_0) = y_{2,0},\ \ldots,\ y_n(x_0) = y_{n,0}$$

and using the following vector notations:

$$Y(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \bullet \\ \bullet \\ \bullet \\ y_n(x) \end{pmatrix},\quad F(x, Y) = \begin{pmatrix} f_1(x, Y) \\ f_2(x, Y) \\ \bullet \\ \bullet \\ \bullet \\ f_n(x, Y) \end{pmatrix},\quad Y_0 = \begin{pmatrix} y_{1,0} \\ y_{2,0} \\ \bullet \\ \bullet \\ \bullet \\ y_{n,0} \end{pmatrix}$$

where Y, F and Y_0 are column vectors, the given problem appears as follows:

$$Y' = \frac{dY}{dx} = F(x, Y) \text{ with } Y(x_0) = Y_0$$

With respect to storage requirements and compensation of accumulated roundoff errors, Gill's modification of the classical Runge-Kutta formulas is preferred. Thus, starting at x_0 with $Y(x_0) = Y_0$ and vector $Q_0 = 0$, the resulting vector $Y_4 = Y(x_0 + h)$ is computed by the following formulas:

$$K_1 = hF(x_0, Y_0) \quad ; Y_1 = Y_0 + \frac{1}{2}(K_1 - 2Q_0)$$
$$Q_1 = Q_0 + 3\left[\frac{1}{2}(K_1 - 2Q_0)\right] - \frac{1}{2}K_1$$
$$K_2 = hF(x_0 + \frac{h}{2}, Y_1) \ ; Y_2 = Y_1 + (1 - \sqrt{\tfrac{1}{2}})(K_2 - Q_1)$$
$$Q_2 = Q_1 + 3\left[(1 - \sqrt{\tfrac{1}{2}})(K_2 - Q_1)\right] - (1 - \sqrt{\tfrac{1}{2}})K_2 \qquad (1)$$
$$K_3 = hF(x_0 + \frac{h}{2}, Y_2) \ ; Y_3 = Y_2 + (1 + \sqrt{\tfrac{1}{2}})(K_3 - Q_2)$$
$$Q_3 = Q_2 + 3\left[(1 + \sqrt{\tfrac{1}{2}})(K_3 - Q_2)\right] - (1 + \sqrt{\tfrac{1}{2}})K_3$$
$$K_4 = hF(x_0 + h, Y_3) \ ; Y_4 = Y_3 + \frac{1}{6}(K_4 - 2Q_3)$$
$$Q_4 = Q_3 + 3\left[\frac{1}{6}(K_4 - 2Q_3)\right] - \frac{1}{2}K_4$$

where K_1, K_2, K_3, K_4, Y_1, Y_2, Y_3, Y_4, Q_1, Q_2, Q_3, Q_4 are all column vectors with n components. If the procedure were carried out with infinite precision (that is, no rounding errors), vector Q_4 defined above would be zero. In practice this is not true, and Q_4 represents approximately three times the roundoff error in Y_4 accumulated during one step. To compensate for this accumulated roundoff, Q_4 is used as Q_0 for the next step. Also $(x_0 + h)$ and Y_4 serve as x_0 and Y_0 respectively at the next step.

For initial control of accuracy, an approximation for $Y(x_0 + 2h)$ called $Y^{(2)}(x_0 + 2h)$ is computed using the step size 2h, and then an approximation called $Y^{(1)}(x_0 + 2h)$, using two times the step size h. From these two approximations, a test value δ for accuracy is generated in the following way:

$$\delta = \frac{1}{15} \sum_{i=1}^{n} a_i \cdot \left| y_i^{(1)} - y_i^{(2)} \right| \qquad (2)$$

where the coefficients a_i are error-weights specified in the input of the procedure.

Test value δ is an approximate measure for the local truncation error at point x_0+2h. If δ is greater than a given tolerance ϵ_2, increment h is halved and the procedure starts again at the point x_0. If δ is less than ϵ_2, the results $Y^{(1)}(x_0+h)$ and $Y^{(1)}(x_0+2h)$

are assumed to be correct. They are then handed, together with $x_0 + h$ and $x_0 + 2h$ and the derivatives at these points -- that is, the values of $F[x_0 + h, Y^{(1)}(x_0+h)]$ and $F[x_0+2h, Y^{(1)}(x_0+2h)]$ respectively -- to a user-supplied output subroutine.

If δ is less than $\epsilon_1 = \epsilon_2/50$, the next step is carried out with the doubled increment. However, care is taken in the procedure that the increment never becomes greater than the increment h specified as an input parameter, and further that all points $x_0 + jh$ (where $j = 1, 2, \ldots$) which are situated between the lower and upper bound of the integration interval are included in the output. Finally, the increment of the last step of the procedure is chosen in such a way that the upper bound of the integration interval is reached exactly.

The entire input of the procedure is:

1. Lower and upper bound of the integration interval, initial increment of the independent variable, upper bound ϵ_2 of the local truncation error.
2. Initial values of the dependent variables and weights for the local truncation errors in each component of the dependent variables.
3. The number of differential equations in the system.
4. As external subroutine subprograms, the computation of the right-hand side of the system of differential equations; for flexibility in output, an output subroutine.
5. An auxiliary storage array named AUX with 8 rows and n columns.

Output is done in the following way. If a set of approximations to the dependent variables Y(x) is found to be of sufficient accuracy, it is handed -- together with x, the derivative $F[x, Y(x)]$, the number of bisections of the initial increment, the number of differential equations, the lower and upper bound of the interval, the initial step size, error bound ϵ_2, and a parameter for terminating subroutine RKGS -- to the output subroutine. Because of this output subroutine, the user has the opportunity to choose his own output format, to handle the output values as he wants, to change the upper error bound, and to terminate subroutine RKGS at any output point. In particular, the user is able to drop the output of some intermediate points, printing only the result values at the special points $x_0 + nh$ $(n = 0, 1, 2, \ldots)$. The user may also perform intermediate computation using the integration results before continuing the process.

For better understanding of the flowchart and of the FORTRAN program, the following figure shows the allocation of special intermediate result vectors within the storage array AUX.

For reference see A. Ralston/H. S. Wilf, Mathematical Methods for Digital Computers, Wiley, New York/London, 1960, pp. 110-120.

AUX

function vector Y(x)	1. row (AUX (1) in flowchart)
derivative vector F(x, Y(x))	2. row (AUX (2) in flowchart)
vector of accumulated roundoff at point x	3. row (AUX (3) in flowchart)
function vector Y(x+2h) for testing purposes	4. row (AUX (4) in flowchart)
function vector Y(x+h)	5. row (AUX (5) in flowchart)
vector of accumulated roundoff at point x+h	6. row (AUX (6) in flowchart)
derivative vector F(x+h, Y(x+h))	7. row (AUX (7) in flowchart)
vector of error weights multiplied by 1/15	8. row (AUX (8) in flowchart)

Storage allocation in auxiliary storage array AUX (RKGS)

Subroutine RKGS

Purpose:
To solve a system of first-order ordinary differential equations with given initial values.

Usage:
CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT, OUTP,AUX) Parameters FCT and OUTP require an external statement.

Description of parameters:

PRMT	-	An input and output vector with dimension greater than or equal to 5, which specifies the parameters of the interval and of accuracy and which serves for communication between the output subroutine (furnished by the user) and subroutine RKGS. Except for PRMT(5), the components are not destroyed by subroutine RKGS and they are:
PRMT(1)	-	Lower bound of the interval (input).
PRMT(2)	-	Upper bound of the interval (input).
PRMT(3)	-	Initial increment of the independent variable (input).
PRMT(4)	-	Upper error bound (input). If absolute error is greater than PRMT(4), the increment gets halved. If the increment is less than PRMT(3) and absolute error less than PRMT(4)/50, the increment gets doubled. The user may change PRMT(4) in his output subroutine.

PRMT(5)	-	No input parameter. Subroutine RKGS initializes PRMT(5)=0. If the user wants to terminate subroutine RKGS at any output point, he must change PRMT(5) to nonzero in subroutine OUTP. Further components of vector PRMT can be made available if its dimension is defined greater than 5. However subroutine RKGS does not require this. Nevertheless, they may be useful for handling result values to the main program (calling RKGS) which are obtained by special manipulations with output data in subroutine OUTP.
Y	-	Input vector of initial values (destroyed). On return, Y is the resultant vector of dependent variables computed at intermediate points X.
DERY	-	Input vector of error weights (destroyed). The sum of its components must equal 1. On return, DERY is the vector of derivatives of function values Y at points X.
NDIM	-	An input value which specifies the number of equations in the system.
IHLF	-	An output value which specifies the number of bisections of the initial increment. When IHLF is greater than 10, subroutine RKGS exits to the main program with error message IHLF=11. Other error messages are: IHLF=12; PRMT(3)=0 or PRMT(1)=PRMT(2) IHLF=13; SIGN(PRMT(3)) is not equal to SIGN(PRMT(2)-PRMT(1)).
FCT	-	The name of the external subroutine used. This subroutine computes the right-hand side, DERY, of the system for given values X and Y. Its parameter list must be X, Y, DERY. Subroutine FCT should not destroy X and Y.
OUTP	-	The name of the external output subroutine used. Its parameter list must be X, Y, DERY, IHLF, NDIM, PRMT. None of these parameters (except, if necessary, PRMT(4), PRMT(5),...) should be changed by subroutine OUTP. If PRMT(5) is changed to nonzero, subroutine RKGS is terminated.
AUX	-	An auxiliary storage array with 8 rows and NDIM columns.

Remarks:

The procedure terminates and returns to the calling program, if

1. More than 10 bisections of the initial increment are necessary to get satisfactory accuracy (error message IHLF=11).
2. The initial increment is equal to 0 or has the wrong sign (error messages IHLF=12 or IHLF=13).
3. The integration interval is exhausted.
4. Subroutine OUTP has changed PRMT(5) to nonzero.

Subroutines and function subprograms required:

The external subroutines FCT(X, Y, DERY) and OUTP(X, Y, DERY, IHLF, NDIM, PRMT) must be furnished by the user.

Method:

Evaluation is done by means of fourth-order Runge-Kutta formulae using the modification due to Gill. Accuracy is tested comparing the results of the procedure with the increment.

Subroutine RKGS automatically adjusts the increment during the whole computation by halving or doubling. If more than 10 bisections of the increment are necessary to get satisfactory accuracy, the subroutine returns with error message IHLF=11 to the main program.

To get full flexibility in output, an output subroutine must be furnished by the user.

```
      SUBROUTINE RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(5)
      DO 1 I=1,NDIM
    1 AUX(8,I)=.06666667*DERY(I)
      X=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      PRMT(5)=0.
      CALL FCT(X,Y,DERY)
C     ERROR TEST
      IF(H*(XEND-X))38,37,2
C     PREPARATIONS FOR RUNGE-KUTTA METHOD
    2 A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP
      DO 3 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
      AUX(3,I)=0.
    3 AUX(6,I)=0.
      IREC=0
      H=H+H
      IHLF=-1
      ISTEP=0
      IEND=0
C     START OF A RUNGE-KUTTA STEP
    4 IF((X+H-XEND)*H)7,6,5
    5 H=XEND-X
    6 IEND=1
C     RECORDING OF INITIAL VALUES OF THIS STEP
    7 CALL OUTP(X,Y,DERY,IREC,NDIM,PRMT)
      IF(PRMT(5))40,8,40
    8 ITEST=0
    9 ISTEP=ISTEP+1
C     START OF INNERMOST RUNGE-KUTTA LOOP
      J=1
   10 AJ=A(J)
      BJ=B(J)
      CJ=C(J)
      DO 11 I=1,NDIM
      R1=H*DERY(I)
      R2=AJ*(R1-BJ*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1
      IF(J-4)12,15,15
   12 J=J+1
      IF(J-3)13,14,13
   13 X=X+.5*H
   14 CALL FCT(X,Y,DERY)
      GOTO 10
C     END OF INNERMOST RUNGE-KUTTA LOOP
C     TEST OF ACCURACY
   15 IF(ITEST)16,16,20
C     IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY
   16 DO 17 I=1,NDIM
   17 AUX(4,I)=Y(I)
      ITEST=1
      ISTEP=ISTEP+ISTEP-2
   18 IHLF=IHLF+1
      X=X-H
      H=.5*H
      DO 19 I=1,NDIM
      Y(I)=AUX(1,I)
      DERY(I)=AUX(2,I)
   19 AUX(6,I)=AUX(3,I)
      GOTO 9
C     IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE
   20 IMOD=ISTEP/2
      IF(ISTEP-IMOD-IMOD)21,23,21
   21 CALL FCT(X,Y,DERY)
      DO 22 I=1,NDIM
      AUX(5,I)=Y(I)
   22 AUX(7,I)=DERY(I)
      GOTO 9
C     COMPUTATION OF TEST VALUE DELT
   23 DELT=0.
      DO 24 I=1,NDIM
   24 DELT=DELT+AUX(8,I)*ABS(AUX(4,I)-Y(I))
      IF(DELT-PRMT(4))28,28,25
C     ERROR IS TOO GREAT
   25 IF(IHLF-10)26,36,36
   26 DO 27 I=1,NDIM
   27 AUX(4,I)=AUX(9,I)
      ISTEP=ISTEP+ISTEP-4
      X=X-H
      IEND=0
      GOTO 18
C     RESULT VALUES ARE GOOD
   28 CALL FCT(X,Y,DERY)
      DO 29 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
      AUX(3,I)=AUX(6,I)
      Y(I)=AUX(5,I)
   29 DERY(I)=AUX(7,I)
      CALL OUTP(X-H,Y,DERY,IHLF,NDIM,PRMT)
      IF(PRMT(5))40,30,40
   30 DO 31 I=1,NDIM
      Y(I)=AUX(1,I)
   31 DERY(I)=AUX(2,I)
      IREC=IHLF
      IF(IEND)32,32,39
C     INCREMENT GETS DOUBLED
   32 IHLF=IHLF-1
      ISTEP=ISTEP/2
      H=H+H
      IF(IHLF)4,33,33
   33 IMOD=ISTEP/2
      IF(ISTEP-IMOD-IMOD)4,34,4
   34 IF(DELT-.02*PRMT(4))35,35,4
   35 IHLF=IHLF-1
      ISTEP=ISTEP/2
      H=H+H
      GOTO 4
C     RETURNS TO CALLING PROGRAM
   36 IHLF=11
      CALL FCT(X,Y,DERY)
      GOTO 39
   37 IHLF=12
      GOTO 39
   38 IHLF=13
   39 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
   40 RETURN
      END
```

Mathematics - Fourier Analysis

FORIF

This subroutine produces the Fourier coefficients for a given periodic function.

Given:
1. A function f(x) for values of x between 0 and 2π
2. N - the spacing desired such that the interval is $2\pi/(2N+1)$
3. M - the desired order of the Fourier coefficients, $0 \leq M \leq N$.

The coefficients of the Fourier series that approximate the given function are calculated as follows:

$$C_1 = \cos\left(\frac{2\pi}{2N+1}\right) \tag{1}$$

$$S_1 = \sin\left(\frac{2\pi}{2N+1}\right) \tag{2}$$

$$U_2 = 0$$

$$U_1 = 0$$

$$C = 1$$

$$S = 0$$

$$J = 1$$

The following recursive sequence is used to compute U_0, U_1, and U_2:

$$U_0 = f\left(\frac{2m\pi}{2N+1}\right) + 2\,C\,U_1 - U_2 \tag{3}$$

$$U_2 = U_1$$

$$U_1 = U_0$$

for values of m = 2N, 2N-1, ..., 1

The coefficients are then:

$$A_J = \frac{2}{2N+1}\left(f(0) + C\,U_1 - U_2\right) \tag{4}$$

$$B_J = \frac{2}{2N+1}\,S\,U_1 \tag{5}$$

The values of C and S are updated to:

$$Q = C_1\,C - S_1\,S$$

$$S = C_1\,S + S_1\,C$$

$$C = Q$$

J is stepped by 1 and the sequence starting at equation (3) is now repeated until M+1 pairs of coefficients have been computed.

Subroutine FORIF

Purpose:

Fourier analysis of a given periodic function in the range 0-2π.

Computes the coefficients of the desired number of terms in the Fourier series F(X) = A(0) + SUM(A(K)COS KX+B(K)SIN KX) where K=1, 2, ..., M to approximate the computed values of a given function subprogram.

Usage:
CALL FORIF(FUN, N, M, A, B, IER)

Description of parameters:

FUN	-	Name of function subprogram to be used for computing data points.
N	-	Defines the interval such that 2N+1 points are taken over the interval $(0, 2\pi)$. The spacing is thus $2\pi/(2N+1)$.
M	-	The maximum order of the harmonics to be fitted.
A	-	Resultant vector of Fourier cosine coefficients of length M+1; i.e., $A_0, \ldots, A_M$.
B	-	Resultant vector of Fourier sine coefficients of length M+1; i.e., $B_0, \ldots, B_M$.
IER	-	Resultant error code where:

IER=0	No error.
IER=1	N not greater than or equal to M.
IER=2	M less than 0.

Remarks:
M must be greater than or equal to zero.
N must be greater than or equal to M.
The first element in vector B is zero in all cases.

Subroutines and function subprograms required:
FUN - Name of user function subprogram used for computing data points.
Calling program must have FORTRAN EXTERNAL statement containing names of function subprograms listed in call to FORIF.

Method:
Uses recursive technique described in A. Ralston, H. Wilf, 'Mathematical Methods for Digital Computers', John Wiley and Sons, New York, 1960, Chapter 24. The method of indexing through the procedure has been modified to simplify the computation.

```
      SUBROUTINE FORIF(FUN,N,M,A,B,IER)
      DIMENSION A(1),B(1)
C        CHECK FOR PARAMETER ERRORS
      IER=0
   20 IF(M) 30,40,40
   30 IER=2
      RETURN
   40 IF(M-N) 60,60,50
   50 IER=1
      RETURN
C        COMPUTE AND PRESET CONSTANTS
   60 AN=N
      COEF=2.0/(2.0*AN+1.0)
      CONST=3.141593*COEF
      S1=SIN(CONST)
      C1=COS(CONST)
      C=1.0
      S=0.0
      J=1
      FUNZ=FUN(0.0)
   70 U2=0.0
      U1=0.0
      AI=2*N
C        FORM FOURIER COEFFICIENTS RECURSIVELY
   75 X=AI*CONST
      U0=FUN(X)+2.0*C*U1-U2
      U2=U1
      U1=U0
      AI=AI-1.0
      IF(AI) 80,80,75
   80 A(J)=COEF*(FUNZ+C*U1-U2)
      B(J)=COEF*S*U1
      IF(J-(M+1)) 90,100,100
   90 Q=C1*C-S1*S
      S=C1*S+S1*C
      C=Q
      J=J+1
      GO TO 70
  100 A(1)=A(1)*0.5
      RETURN
      END
```

FORIT

This subroutine produces the Fourier coefficients of a tabulated function.

Given:
1. Tabulated values of a function f(x) for x between 0 and 2π in steps of $2\pi/(2N+1)$
2. N such that there are 2N+1 tabulated data points: $2K\pi/2N+1$, $K = 0, 1, 2, \ldots, 2N$
3. M - the desired order of the Fourier coefficients where $0 \leq M \leq N$

The coefficients of the Fourier series which approximate the given function are calculated as follows:

$$C_1 = \cos\left(\frac{2\pi}{2N+1}\right) \tag{1}$$

$$S_1 = \sin\left(\frac{2\pi}{2N+1}\right) \tag{2}$$

$$U_2 = 0$$

$$U_1 = 0$$

$$C = 1$$

$$S = 0$$

$$J = 1$$

The following recursive sequence is used to compute U_0, U_1, and U_2:

$$U_0 = f\left(\frac{2m\pi}{2N+1}\right) + 2\,C\,U_1 - U_2 \tag{3}$$

$$U_2 = U_1$$

$$U_1 = U_0$$

for values of m = 2N, 2N-1, ..., 1

The coefficients are then:

$$A_J = \frac{2}{2N+1}\left(f(0) + C\,U_1 - U_2\right) \tag{4}$$

$$B_J = \frac{2}{2N+1} S U_1 \qquad (5)$$

The values of C and S are updated to:

$$Q = C_1 C - S_1 S$$

$$S = C_1 S + S_1 C$$

$$C = Q$$

J is stepped by 1 and the sequence starting at equation (3) is now repeated until M+1 pairs of coefficients have been computed.

Subroutine FORIT

Purpose:
Fourier analysis of a periodically tabulated function.
Computes the coefficients of the desired number of terms in the Fourier series F(X) = A(0)+ SUM(A(K)COS KX+B(K)SIN KX) where K=1, 2, . . . , M to approximate a given set of periodically tabulated values of a function.

Usage:
CALL FORIT(FNT, N, M, A, B, IER)

Description of parameters:

FNT	-	Vector of tabulated function values of length 2N+1.
N	-	Defines the interval such that 2N+1 points are taken over the interval $(0, 2\pi)$. The spacing is thus $2\pi/(2N+1)$.
M	-	Maximum order of harmonics to be fitted.
A	-	Resultant vector of Fourier cosine coefficients of length M+1; i.e., $A_0, \ldots, A_M$.
B	-	Resultant vector of Fourier sine coefficients of length M+1; i.e., $B_0, \ldots, B_M$.
IER	-	Resultant error code where:

IER=0	No error.
IER=1	N not greater or equal to M.
IER=2	M less than 0.

Remarks:
M must be greater than or equal to zero.
N must be greater than or equal to M.
The first element of vector B is zero in all cases.

Subroutines and function subprograms required:
None.

Method:
Uses recursive technique described in A. Ralston, H. Wilf, 'Mathematical Methods for Digital Computers', John Wiley and Sons, New York, 1960, Chapter 24. The method of indexing through the procedure has been modified to simplify the computation.

```
      SUBROUTINE FORIT(FNT,N,M,A,B,IER)
      DIMENSION A(1),B(1),FNT(1)
C        CHECK FOR PARAMETER ERRORS
      IER=0
   20 IF(M) 30,40,40
   30 IER=2
      RETURN
   40 IF(M-N) 60,60,50
   50 IER=1
      RETURN
C        COMPUTE AND PRESET CONSTANTS
   60 AN=N
      COEF=2.0/(2.0*AN+1.0)
      CONST=3.141593*COEFF
      S1=SIN(CONST)
      C1=COS(CONST)
      C=1.0
      S=0.0
      J=1
      FNTZ=FNT(1)
   70 U2=0.0
      U1=0.0
      I=2*N+1
C        FORM FOURIER COEFFICIENTS RECURSIVELY
   75 U0=FNT(I)+2.0*C*U1-U2
      U2=U1
      U1=U0
      I=I-1
      IF(I-1) 80,80,75
   80 A(J)=COEF*(FNTZ+C*U1-U2)
      B(J)=COEF*S*U1
      IF(J-(M+1)) 90,100,100
   90 Q=C1*C-S1*S
      S=C1*S+S1*C
      C=Q
      J=J+1
      GO TO 70
  100 A(1)=A(1)*0.5
      RETURN
      END
```

Mathematics - Special Operations and Functions

GAMMA

This subroutine computes the value of the gamma function for a given argument x.

Calculation of the Gamma Function. $\Gamma(x)$ is defined for $x > 0$ by:

$$\Gamma(x) = \int_0^\infty t^{x-1} \cdot e^{-t} \, dt \qquad (1)$$

This function satisfies the recurrence relation:

$$\Gamma(x) = (x-1) \cdot \Gamma(x-1) \qquad (2)$$

which defines $\Gamma(x)$ for any x not a negative integer.

Note that when x is a positive integer $\Gamma(x) = (x-1)!$

To compute $\Gamma(x)$ for $x > 1$, apply the recurrence (2), r times until $1 < x - r = y \leq 2$. Thus, for $x > 1$

$$\Gamma(x) = (x-1)(x-2) \ldots (x-r)\,\Gamma(y) \qquad (3)$$

$\Gamma(y)$ is computed from the following formula:

$$\Gamma(y) \approx 1 - 0.57710166(y-1) + 0.98585399(y-1)^2 - 0.87642182(y-1)^3 + 0.83282120(y-1)^4$$

$$- 0.56847290(y-1)^5 + 0.25482049(y-1)^6$$

$$- 0.05149930(y-1)^7 \qquad (4)$$

For $x < 1$, the recurrence (2) is taken in the direction of decreasing n, giving

$$\Gamma(x) = \frac{\Gamma(y)}{x(x+1)(x+2)\ldots(x+r-1)} \qquad (5)$$

where $1 < x + r = y \leq 2$.

As before, $\Gamma(y)$ is computed using equation (4).

Subroutine GAMMA

Purpose:
Computes the gamma function for a given argument.

Usage:
CALL GAMMA(XX, GX, IER)

Description of parameters:

XX	-	The argument for the gamma function.	
GX	-	The resultant gamma function value.	
IER	-	Resultant error code where:	
		IER= 0	No error.
		IER= 1	XX is within .000001 of being a negative integer.
		IER= 2	XX is greater than 34.5 GX is set to 1.0E38

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
The recursion relation and polynomial approximation by C. Hastings, Jr., 'Approximations for Digital Computers', Princeton University Press, 1955.

```
      SUBROUTINE GAMMA(XX,GX,IER)
      IF(XX-34.5)6,6,4
    4 IER=2
      GX=1.E38
      RETURN
    6 X=XX
      ERR=1.0E-6
      IER=0
      GX=1.0
      IF(X-2.0)50,50,15
   10 IF(X-2.0)110,110,15
   15 X=X-1.0
      GX=GX*X
      GO TO 10
   50 IF(X-1.0)60,120,110
C        SEE IF X IS NEAR NEGATIVE INTEGER OR ZERO
   60 IF(X-ERR)62,62,80
   62 K=X
      Y=FLOAT(K)-X
      IF(ABS(Y)-ERR)130,130,64
   64 IF(1.0-Y-ERR)130,130,70
C        X NOT NEAR A NEGATIVE INTEGER OR ZERO
   70 IF(X-1.0)80,80,110
   80 GX=GX/X
      X=X+1.0
      GO TO 70
  110 Y=X-1.0
      GY=1.0+Y*(-0.5771017+Y*(+0.9858540+Y*(-0.8764218+Y*(+0.8328212+
     1Y*(-0.5684729+Y*(+0.2548205+Y*(-0.05149930)))))))
      GX=GX*GY
  120 RETURN
  130 IER=1
      RETURN
      END
```

LEP

This subroutine computes the values of the Legendre polynomials for a given argument x and orders zero up to N. The Legendre polynomial $P_n(x)$ satisfies the recurrence equation

$$P_{n+1}(x) = ((2n+1) \cdot x \cdot P_n(x) - n \cdot P_{n-1}(x))/(n+1)$$

with starting values $P_0(x) = 1$, $P_1(x) = x$.

For reasons of economy and numerical stability the recurrence equation is used in the form:

$$P_{n+1}(x) = x \cdot P_n(x) - P_{n-1}(x) + x \cdot P_n(x)$$

$$- (x \cdot P_n(x) - P_{n-1}(x))/(n+1)$$

For large values of n the last term is negligible, giving the approximation:

$$P_{n+1}(x) = 2 \cdot x \cdot P_n(x) - P_{n-1}(x)$$

This form shows that roundoff errors grow at worst linearly, assuming that the argument x is absolutely less than one.

If e_{n+r} is the error in $P_{n+r}(x)$ due to a single rounding error e in $P_n(x)$, the approximation is

$$e_{n+r+1} = 2x \cdot e_{n+r} - e_{n+r-1}$$

with initial conditions $e_n = e$, $e_{n-1} = 0$. The solution of this difference equation has its maximum for $|x| = 1$:

$$e_{n-1} = 0,\ e_n = e,\ |e_{n+1}| = 2e,\ \ldots,\ |e_{n+r}|$$

$$= (r + 1)e$$

The order is assumed to be zero for negative values of N.

Subroutine LEP

Purpose:
Compute the values of the Legendre polynomials P(N,X) for argument value X and orders 0 to N.

Usage:
CALL LEP(Y,X,N)

Description of parameters:

Y	-	Result vector of dimension N+1 containing the values of Legendre polynomials of order 0 to N for given argument X. Values are ordered from low to high order.
X	-	Argument of Legendre polynomial.
N	-	Order of Legendre polynomial.

Remarks:
N less than 0 is treated as if N were 0.

Subroutines and function subprograms required:
None.

Method:
Evaluation is based on the recurrence equation for Legendre polynomials P(N,X);
P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1), where the first term in brackets is the order, and the second is the argument.
Starting values are P(0,X)=1, P(1,X)=X.

```
      SUBROUTINE LEP(Y,X,N)
      DIMENSION Y(1)
C        TEST OF ORDER
      L1=1
      L2=2
      Y(L1)=1.0
      IF(N)1,1,2
    1 RETURN
    2 Y(L2)=X
      IF(N-1)1,1,3
    3 DO 4 I=2,N
      G=X*Y(I)
    4 Y(I+1)=G-Y(I-1)  -(G-Y(I-1))/FLOAT(I)+G
      RETURN
      END
```

BESJ

This subroutine computes the J Bessel function for a given argument and integer order by using the recurrence relationship:

$$F_{n+1}(x) + F_{n-1}(x) = \left(\frac{2n}{x}\right) F_n(x) \qquad (1)$$

The desired Bessel function is:

$$J_n(x) = \frac{F_n(x)}{\alpha} \qquad (2)$$

where

$$\alpha = F_0(x) + 2 \sum_{m=1}^{M-2} F_{2m}(x) \qquad (3)$$

M is initialized at M_0.

M_0 is the greater of M_A and M_B where:

$M_A = [x+6]$ if $x < 5$ and $M_A = [1.4x+60/x]$ if $x \geq 5$.

$M_B = [n+x/4+2]$

$F_{M-2}, F_{M-3}, \ldots, F_2, F_1, F_0$ is evaluated using equation (1) with $F_M = 0$ and $F_{M-1} = 10^{-30}$.

α and $J_n(x)$ are then computed using equations (3) and (2) respectively.

The computation is repeated for M+3.

The values of $J_n(x)$ for M and M+3 are compared:

$$\text{If } \left| J_n(x)_M - J_n(x)_{M+3} \right| \leq \delta \left| J_n(x)_{M+3} \right|$$

this value is accepted as $J_n(x)$; if not, the computation is repeated by adding 3 to M and using this as a new value for M. If M reaches M_{MAX} before the desired accuracy is obtained, execution is terminated. M_{MAX} is defined as:

$$M_{MAX} = \begin{cases} \left[20 + 10x - \frac{x^2}{3}\right] & \text{for } x \leq 15 \\ [90 + x/2] & \text{for } x > 15 \end{cases} \qquad (4)$$

Subroutine BESJ

Purpose:
Compute the J Bessel function for a given argument and order.

Usage:
CALL BESJ(X, N, BJ, D, IER)

Description of parameters:

X	-	The argument of the J Bessel function desired.
N	-	The order of the J Bessel function desired.
BJ	-	The resultant J Bessel function.
D	-	Required accuracy.
IER	-	Resultant error code where:

IER= 0	No error.
IER= 1	N is negative.
IER= 2	X is negative or zero.
IER= 3	Required accuracy not obtained.
IER= 4	Range of N compared to X not correct. (See Remarks.)

Remarks:
N must be greater than or equal to zero, but it must be less than

20+10*X-X** 2/3	for X less than or equal to 15;
90+X/2	for X greater than 15.

Subroutines and function subprograms required:
None.

Method:
Recurrence relation technique described by H. Goldstein and R.M. Thaler, 'Recurrence Techniques for the Calculation of Bessel Functions', M.T.A.C., V.13, pp.102-108 and I.A. Stegun and M. Abramowitz, 'Generation of Bessel Functions on High Speed Computers', M.T.A.C., V.11, 1957, pp.255-257.

```
      SUBROUTINE BESJ(X,N,BJ,D,IER)
      BJ=.0
      IF(N)10,20,20
   10 IER=1
      RETURN
   20 IF(X)30,30,31
   30 IER=2
      RETURN
   31 IF(X-15.)32,32,34
   32 NTEST=20.+10.*X-X** 2/3
      GO TO 36
   34 NTEST=90.+X/2.
   36 IF(N-NTEST)40,38,38
   38 IER=4
      RETURN
   40 IER=0
      N1=N+1
      BPREV=.0
C        COMPUTE STARTING VALUE OF M
      IF(X-5.)50,60,60
   50 MA=X+6.
      GO TO 70
   60 MA=1.4*X+60./X
   70 MB=N+IFIX(X)/4+2
      MZERO=MA
      IF(MA-MB)80,90,90
   80 MZERO=MB
C        SET UPPER LIMIT OF M
   90 MMAX=NTEST
  100 DO 190 M=MZERO,MMAX,3
C        SET F(M),F(M-1)
      FM1=1.0E-28
      FM=.0
      ALPHA=.0
      IF(M-(M/2)*2)120,110,120
  110 JT=-1
      GO TO 130
  120 JT=1
  130 M2=M-2
      DO 160 K=1,M2
      MK=M-K
      BMK=2.*FLOAT(MK)*FM1/X-FM
      FM=FM1
      FM1=BMK
      IF(MK-N-1)150,140,150
  140 BJ=BMK
  150 JT=-JT
      S=1+JT
  160 ALPHA=ALPHA+BMK*S
      BMK=2.*FM1/X-FM
      IF(N)180,170,180
  170 BJ=BMK
  180 ALPHA=ALPHA+BMK
      BJ=BJ/ALPHA
      IF(ABS(BJ-BPREV)-ABS(D*BJ))200,200,190
  190 BPREV=BJ
      IER=3
  200 RETURN
      END
```

BESY

This subroutine computes the Y Bessel function for a given argument x and order n. The recurrence relation:

$$Y_{n+1}(x) = \left(\frac{2n}{x}\right) \cdot Y_n(x) - Y_{n-1}(x) \qquad (1)$$

is used for this evaluation.

For $x > 4$

$$Y_0(x) = \sqrt{\frac{2}{\pi x}}\left(P_0(x)\sin\left(x-\frac{\pi}{4}\right) + Q_0(x)\cos\left(x-\frac{\pi}{4}\right)\right) \qquad (2)$$

$$Y_1(x) = \sqrt{\frac{2}{\pi x}}\left(-P_1(x)\cos\left(x-\frac{\pi}{4}\right) + Q_1(x)\sin\left(x-\frac{\pi}{4}\right)\right) \qquad (3)$$

$P_0(x)$, $Q_0(x)$, $P_1(x)$, and $Q_1(x)$ are:

$$\frac{1}{\sqrt{2\pi}} P_0\left(\frac{4}{t}\right) = 0.3989422793 - 0.0017530620t^2 + 0.0001734300t^4 - 0.0000487613t^6 + 0.0001735665t^8 - 0.0000037043t^{10} \qquad (4)$$

$$\frac{1}{t\sqrt{2\pi}} Q_0\left(\frac{4}{t}\right) = -0.124669441 + 0.0004564324t^2 - 0.0000869791t^4 + 0.0000342468t^6 - 0.0000142078t^8 + 0.0000032312t^{10} \qquad (5)$$

$$\frac{1}{\sqrt{2\pi}} P_1\left(\frac{4}{t}\right) = 0.3989422819 + 0.0029218256t^2 - 0.0002232030t^4 + 0.0000580759t^6 - 0.0000200920t^8 + 0.0000042414t^{10} \qquad (6)$$

$$\frac{1}{t\sqrt{2\pi}} Q_1\left(\frac{4}{t}\right) = 0.0374008364 - 0.0006390400t^2 + 0.0001064741t^4 - 0.0000398708t^6 + 0.0000162200t^8 - 0.0000036594t^{10} \qquad (7)$$

where $t = \frac{4}{x}$

For $x \leq 4$

$$Y_0(x) = \frac{2}{\pi}\sum_{m=0}^{15} (-1)^m \left(\frac{x}{2}\right)^{2m} \frac{1}{(m!)^2} \left[\log\frac{x}{2} + \gamma - H_m\right] \qquad (8)$$

where

$$H_m = \sum_{r=1}^{m} \frac{1}{r} \text{ if } m \geq 1 = 0 \quad \text{if } m = 0 \qquad (9)$$

and γ = Euler's constant = 0.5772156649

$$Y_1(x) = -\frac{2}{\pi x} + \frac{2}{\pi}\sum_{m=1}^{16} (-1)^{m+1}\left(\frac{x}{2}\right)^{2m-1} \frac{1}{m!\,(m-1)!} \cdot \left[\log\frac{x}{2} + \gamma - H_m + \frac{1}{2m}\right] \qquad (10)$$

Subroutine BESY

Purpose:
Compute the Y Bessel function for a given argument and order.

Usage:
CALL BESY(X, N, BY, IER)

Description of parameters:

X	-	The argument of the Y Bessel function desired.
N	-	The order of the Y Bessel function desired.

BY	-	The resultant Y Bessel function.
IER	-	Resultant error code where:

IER= 0	No error.
IER= 1	N is negative.
IER= 2	X is negative or zero.
IER= 3	BY is greater than 10**36.

Remarks:

Very small values of X may cause the range of the library function ALOG to be exceeded. For N > 30 and X ≤ 5, this condition may occur.
X must be greater than zero.
N must be greater than or equal to zero.

Subroutines and function subprograms required:
None.

Method:

Recurrence relation and polynomial approximation technique as described by A.J.M. Hitchcock, 'Polynomial Approximations to Bessel Functions of Order Zero and One and to Related Functions', M.T.A.C., V.11, 1957, pp.86-88, and G.N. Watson, 'A Treatise on the Theory of Bessel Functions', Cambridge University Press, 1958 p. 62.

```
      SUBROUTINE BESY(X,N,BY,IER)
C        CHECK FOR ERRORS IN N AND X
      IF(N)180,10,10
   10 IER=0
      IF(X)190,190,20
C        BRANCH IF X LESS THAN OR EQUAL 4
   20 IF(X-4.0)40,40,30
C       COMPUTE Y0 AND Y1 FOR X GREATER THAN 4
   30 T1=4.0/X
      T2=T1*T1
      P0=((((-.0000037043*T2+.0000173565)*T2-.0000487613)*T2
     1  +.00017343)*T2-.001753062)*T2+.3989423
      Q0=((((.0000032312*T2-.0000142078)*T2+.0000342468)*T2
     1  -.0000869791)*T2+.0004564324)*T2-.01246694
      P1=((((.0000042414*T2-.0000200920)*T2+.0000580759)*T2
     1  -.000223203)*T2+.002921826)*T2+.3989423
      Q1=((((-.0000036594*T2+.00001622)*T2-.0000398708)*T2
     1  +.0001064741)*T2-.0006390400)*T2+.03740084
      A=2.0/SQRT(X)
      B=A*T1
      C=X-.7853982
      Y0=A*P0*SIN(C)+B*Q0*COS(C)
      Y1=-A*P1*COS(C)+B*Q1*SIN(C)
      GO TO 90
C       COMPUTE Y0 AND Y1 FOR X LESS THAN OR EQUAL TO 4
   40 XX=X/2.
      X2=XX*XX
      T=ALOG(XX)+.5772157
      SUM=0.
      TERM=T
      Y0=T
      DO 70 L=1,15
      IF(L-1)50,60,50
   50 SUM=SUM+1./FLOAT(L-1)
   60 FL=L
      TS=T-SUM
      TERM=(TERM*(-X2)/FL**2)*(1.-1./(FL*TS))
   70 Y0=Y0+TERM
      TERM = XX*(T-.5)
      SUM=0.
      Y1=TERM
      DO 80 L=2,16
      SUM=SUM+1./FLOAT(L-1)
      FL=L
      FL1=FL-1.
      TS=T-SUM
      TERM=(TERM*(-X2)/(FL1*FL))*((TS-.5/FL)/(TS+.5/FL1))
   80 Y1=Y1+TERM
      PI2=.6366198
      Y0=PI2*Y0
      Y1=-PI2/X+PI2*Y1
C          CHECK IF ONLY Y0 OR Y1 IS DESIRED
   90 IF(N-1)100,100,130
C          RETURN EITHER Y0 OR Y1 AS REQUIRED
  100 IF(N)110,120,110
  110 BY=Y1
      GO TO 170
  120 BY=Y0
      GO TO 170
C        PERFORM RECURRENCE OPERATIONS TO FIND YN(X)
  130 YA=Y0
      YB=Y1
      K=1
  140 T=FLOAT(2*K)/X
      YC=T*YB-YA
      IF(ABS(YC)-1.0E36)145,145,141
  141 IER=3
      RETURN
  145 K=K+1
      IF(K-N)150,160,150
  150 YA=YB
      YB=YC
      GO TO 140
  160 BY=YC
  170 RETURN
  180 IER=1
      RETURN
  190 IER=2
      RETURN
      END
```

BESI

This subroutine computes the I Bessel function for a given argument x and order n.

For $x \leq 12$ or $\leq n$

$$I_n(x) = \left(\frac{x}{2}\right)^n \frac{1}{n!} \sum_{s=0}^{30} \left(\frac{x}{2}\right)^{2s} \frac{n!}{s!(n+s)!} \qquad (1)$$

For $x > 12$ and $> n$

$$I_n(x) = \frac{e^x}{\sqrt{2\pi x}} \sum_{m=0}^{30} (8x)^{-m} \cdot \frac{1}{m!}$$

$$\prod_{K=1}^{m} \left((2K-1)^2 - 4n^2\right) \qquad (2)$$

Subroutine BESI

Purpose:
Compute the I Bessel function for a given argument and order.

Usage:
CALL BESI(X, N, BI, IER)

Description of parameters:

X	-	The argument of the I Bessel function desired.
N	-	The order of the I Bessel function desired.
BI	-	The resultant I Bessel function.
IER	-	Resultant error code where:

IER= 0	No error.
IER= 1	N is negative.
IER= 2	X is negative.
IER= 3	BI is less than 1.0E-36, and is set to zero.
IER= 4	X is greater than 60 and and greater than N.

Remarks:
X and N must be greater than zero.

Subroutines and function subprograms required:
None.

Method:
Computes the I^{th} Bessel function using series or asymptotic approximations depending on the range of the arguments.

```
      SUBROUTINE BESI(X,N, BI,IER)
C        CHECK FOR ERRORS IN N AND X AND EXIT IF ANY ARE PRESENT
      IER=0
      BI=1.0
      IF(N)150,15,10
   10 IF(X)160,20,20
   15 IF(X)160,17,20
   17 RETURN
C        DEFINE TOLERANCE
   20 TOL=1.E-6
C        IF ARGUMENT GT 12 AND GT N, USE ASYMPTOTIC FORM
      IF(X-12.)40,40,30
   30 IF(X-FLOAT(N))40,40,110
C        COMPUTE FIRST TERM OF SERIES AND SET INITIAL VALUE OF THE SUM
   40 XX=X/2.
   50 TERM=1.0
      IF(N) 70,70,55
   55 DO 60 I=1,N
      FI=I
      IF(ABS(TERM)-1.E-36)56,60,60
   56 IER=3
      BI=0.0
      RETURN
   60 TERM=TERM*XX/FI
   70 BI=TERM
      XX=XX*XX
C        COMPUTE TERMS,STOPPING WHEN ABS(TERM) LE ABS(SUM OF TERMS)
C        TIMES TOLERANCE
      DO 90 K=1,1000
      IF(ABS(TERM)-ABS(BI*TOL))100,100,80
   80 FK=K*(N+K)
      TERM=TERM*(XX/FK)
   90 BI=BI+TERM
C        RETURN BI AS ANSWER
  100 RETURN
C        X GT 12 AND X GT N, SO USE ASYMPTOTIC APPROXIMATION
  110 FN=4*N*N
      IF(X- 60.0)115,111,111
  111 IER=4
      RETURN
  115 XX=1./(8.*X)
      TERM=1.
      BI=1.
      DO 130 K=1,30
      IF(ABS(TERM)-ABS(TOL*BI))140,140,120
  120 FK=(2*K-1)**2
      TERM=TERM*XX*(FK-FN)/FLOAT(K)
  130 BI=BI+TERM
C        SIGNIFICANCE LOST AFTER 30 TERMS,TRY SERIES
      GO TO 40
  140 PI=3.141592653
      BI=BI*EXP(X)/SQRT(2.*PI*X)
      GO TO 100
  150 IER=1
      GO TO 100
  160 IER=2
      GO TO 100
      END
```

BESK

This subroutine computes the K Bessel function for a given argument x and order n.

The recurrence relation:

$$K_{n+1}(x) = \frac{2n}{x} K_n(x) + K_{n-1}(x) \tag{1}$$

is used for this evaluation.

The initial values K_0 and K_1 are found as follows:

For $x > 1$

$$K_0(x) = e^{-x} \sqrt{\frac{\pi}{2x}}\, G_0(x) \tag{2}$$

$$K_1(x) = e^{-x} \sqrt{\frac{\pi}{2x}}\, G_1(x) \tag{3}$$

where $x = 1/t$ for $t < 1$

$$\begin{aligned} G_0\left(\frac{1}{t}\right)\cdot\sqrt{\frac{\pi}{2}} = {} & 1.2533141373 && -0.1566641816t \\ & +0.0881112782t^2 && -0.0913909546t^3 \\ & +0.1344596228t^4 && -0.2299850328t^5 \\ & +0.3792409730t^6 && -0.5247277331t^7 \\ & +0.5575368367t^8 && -0.4262632912t^9 \\ & +0.2184518096t^{10} && -0.0668097672t^{11} \\ & +0.0091893830t^{12} \end{aligned} \tag{4}$$

$$\begin{aligned} G_1\left(\frac{1}{t}\right)\cdot\sqrt{\frac{\pi}{2}} = {} & 1.2533141373 && +0.4699927013t \\ & -0.1468582957t^2 && +0.1280426636t^3 \\ & -0.1736431637t^4 && +0.2847618149t^5 \\ & -0.4594342117t^6 && +0.6283380681t^7 \\ & -0.6632295430t^8 && +0.5050238576t^9 \\ & -0.2581303765t^{10} && +0.0788000118t^{11} \\ & -0.0108241775t^{12} \end{aligned} \tag{5}$$

For $x \leq 1$

$$\gamma = \text{Euler's constant} = 0.5772156649 \tag{6}$$

$$K_0(x) = -\left(\gamma + \log\frac{x}{2}\right) + \sum_{s=1}^{6} \left(\frac{x}{2}\right)^{2s} \frac{1}{(s!)^2} \left[H_s - \left(\gamma + \log\frac{x}{2}\right)\right] \tag{7}$$

where

$$H_s = \sum_{r=1}^{s} \frac{1}{r} \tag{8}$$

$$K_1(x) = \frac{1}{x} + \sum_{s=1}^{8} \left(\frac{x}{2}\right)^{2s-1} \frac{1}{(s!)^2} \left[\frac{1}{2} + s \cdot \left(\gamma + \log\frac{x}{2} - H_s\right)\right] \tag{9}$$

Subroutine BESK

Purpose:
Compute the K Bessel function for a given argument and order.

Usage:
CALL BESK(X, N, BK, IER)

Description of parameters:

X	-	The argument of the K Bessel function desired.
N	-	The order of the K Bessel function desired.
BK	-	The resultant K Bessel function.
IER	-	Resultant error code where:

IER= 0	No error.
IER= 1	N is negative.
IER= 2	X is zero or negative.
IER= 3	X is greater than 60. Machine range exceeded.
IER= 4	BK is greater than 1. E36.

Remarks:
N must be greater than or equal to zero.

Subroutines and function subprograms required:
None.

Method:
Computes zero-order and first-order Bessel functions using series approximations and then computes N^{th} order function using recurrence relation.

Recurrence relation and polynomial approximation technique as described by A. J. M. Hitchcock, 'Polynomial Approximations to Bessel Functions of Order Zero and One and to Related Functions', M.T.A.C., V.11, 1957, pp. 86-88, and G. N. Watson, 'A Treatise on the Theory of Bessel Functions', Cambridge University Press, 1958, p. 62.

```
      SUBROUTINE BESK(X,N,BK,IER)
      DIMENSION T(12)
      BK=.0
      IF(N)10,11,11
   10 IER=1
      RETURN
   11 IF(X)12,12,20
   12 IER=2
      RETURN
   20 IF(X- 60.0)22,22,21
   21 IER=3
      RETURN
   22 IER=0
      IF(X-1.)36,36,25
   25 A=EXP(-X)
      B=1./X
      C=SQRT(B)
      T(1)=B
      DO 26 L=2,12
   26 T(L)=T(L-1)*B
      IF(N-1)27,29,27
C        COMPUTE KO USING POLYNOMIAL APPROXIMATION
   27 G0=A*(1.25331414-.15666418*T(1)+.088111278*T(2)-.091390954*T(3)
     2+.13445962*T(4)-.22998503*T(5)+.37924097*T(6)-.52472773*T(7)
     3+.55753684*T(8)-.42626329*T(9)+.21845181*T(10)-.066809767*T(11)
     4+.009189383*T(12))*C
      IF(N)20,28,29
   28 BK=G0
      RETURN
C        COMPUTE K1 USING POLYNOMIAL APPROXIMATION
   29 G1=A*(1.2533141+.46999270*T(1)-.14685830*T(2)+.12804266*T(3)
     2-.17364316*T(4)+.28476181*T(5)-.45943421*T(6)+.62833807*T(7)
     3-.66322954*T(8)+.50502386*T(9)-.25813038*T(10)+.078800012*T(11)
     4-.010824177*T(12))*C
      IF(N-1)20,30,31
   30 BK=G1
      RETURN
C        FROM KO,K1 COMPUTE KN USING RECURRENCE RELATION
   31 DO 35 J=2,N
      GJ=2.*(FLOAT(J)-1.)*G1/X+G0
      IF(GJ-1.0E36)33,33,32
   32 IER=4
      GO TO 34
   33 G0=G1
   35 G1=GJ
   34 BK=GJ
      RETURN
   36 B=X/2.
      A=.57721566+ALOG(B)
      C=B*B
      IF(N-1)37,43,37
C        COMPUTE KO USING SERIES EXPANSION
   37 G0=-A
      X2J=1.
      FACT=1.
      HJ=.0
      DO 40 J=1,6
      RJ=1./FLOAT(J)
      X2J=X2J*C
      FACT=FACT*RJ*RJ
      HJ=HJ+RJ
   40 G0=G0+X2J*FACT*(HJ-A)
      IF(N)43,42,43
   42 BK=G0
      RETURN
C        COMPUTE K1 USING SERIES EXPANSION
   43 X2J=B
      FACT=1.
      HJ=1.
      G1=1./X+X2J*(.5+A-HJ)
      DO 50 J=2,8
      X2J=X2J*C
      RJ=1./FLOAT(J)
      FACT=FACT*RJ*RJ
      HJ=HJ+RJ
   50 G1=G1+X2J*FACT*(.5+(A-HJ)*FLOAT(J))
      IF(N-1)31,52,31
   52 BK=G1
      RETURN
      END
```

CEL1

This subroutine computes the complete elliptic integral of the first kind. This is defined as:

$$K(k) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-k^2 \sin^2 t}} \quad . \quad 0 \le k < 1$$

An equivalent definition is:

$$K(k) = \int_0^{\infty} \frac{dx}{\sqrt{(1+x^2)\,(1+k_c^2 x^2)}}$$

where k_c is the complementary modulus:

$$k_c^2 + k^2 = 1, \; 0 < k_c^2 \le 1$$

The subroutine CELI1 calculates K (k) for given modulus k.

The calculation of RES = K (k) is based on the process of the Arithmetic-Geometric Mean.

Starting with the pair of numbers:

$$a_0 = 1, \; g_0 = k_c$$

the sequences of numbers (a_n), (g_n) are generated using the definition:

$$a_n = \frac{1}{2}(a_{n-1} + g_{n-1}), \quad g_n = \sqrt{a_{n-1}\, g_{n-1}}$$

This iterative process is stopped at the Nth step, when $a_N = g_N$.

If D is the number of decimal digits in the mantissa of floating-point numbers, then the equality $a_N = g_N$ must be interpreted as $|a_N - g_N|$ is less than $a_N \cdot 10^{-D}$.

Since the sequences (a_n), (g_n) converge quadratically to the same limit (Arithmetico-Geometrical mean) the test for the end of iteration 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 geometrical mean.

The value of $K(k) = \dfrac{\pi}{2\, a_N}$.

Subroutine CEL1

Purpose:
Calculate complete elliptic integral of first kind.

Usage:
CALL CEL1 (RES, AK, IER)

Description of parameters:

RES - Result value.
AK - Modulus (input).
IER - Resultant error code where:
 IER=0 No error.
 IER=1 AK not in range -1 to +1.

Remarks:

For AK=+1, -1 the result is set to 1. E38.
For modulus AK and complementary modulus CK, equation AK*AK+CK*CK=1.0 is used.
AK must be in the range -1 to +1.

Subroutines and function subprograms required:

None.

Method:

Landen's transformation is used for calculation.
Reference:
R. Bulirsch, 'Numerical Calculation of Elliptic Integrals and Elliptic Functions', Handbook Series Special Functions, Numerische Mathematik Vol. 7, 1965, pp. 78-90.

```
      SUBROUTINE CEL1(RES,AK,IER)
      IER=0
C     TEST MODULUS
      GEO=1.-AK*AK
      IF(GEO)1,2,3
    1 IER=1
      RETURN
C     SET RESULT VALUE =OFLOW
    2 RES=1.E38
      RETURN
    3 GEO=SQRT(GEO)
      ARI=1.
    4 AARI=ARI
      TEST=AARI*1.E-4
      ARI=GEO+ARI
C     TEST OF ACCURACY
      IF(AARI-GEO-TEST)6,6,5
    5 GEO=SQRT(AARI*GEO)
      ARI=0.5*ARI
      GO TO 4
    6 RES=3.141593  /ARI
      RETURN
      END
```

CEL2

This subroutine computes the generalized complete elliptic integral of the second kind. This is defined as

$$\text{cel } 2\ (k;\ A, B) = \int_0^{\pi/2} \frac{A + (B-A)\sin^2 t}{\sqrt{1 - k^2 \sin^2 t}}\, dt.$$

Equivalent is the definition:

$$\text{cel } 2\ (k;\ A, B) = \int_0^{\infty} \frac{A + Bx^2}{(1+x^2)\sqrt{(1+x^2)(1+k_c^2 x^2)}}\, dx,$$

where k_c is the complementary modulus:

$$k_c^2 + k^2 = 1,\ 0 < k_c^2 \leq 1$$

The subroutine CELI2 calculates cel 2 (k; A, B) for given modulus k, and constants A, B.

The calculation of RES = cel 2 (k, A, B) is based on the process of the Arithmetic-Geometric Mean.

Starting with the pair of numbers:

$$a_0 = 1,\ g_0 = k_c$$

the sequences of numbers (a_n), (g_n) are generated using for definition:

$$a_n = (a_{n-1} + g_{n-1}),\ g_n = 2\sqrt{a_{n-1}\, g_{n-1}}$$

This iteration process is stopped at the N^th step, when $a_N = g_N$.

Further needed are the sequences

(A_i), (B_i) defined by means of:

$$A_0 = A,\ B_0 = B$$

$$A_n = B_{n-1}/a_{n-1} + A_{n-1}$$

$$B_n = 2\,(B_{n-1} + g_{n-1} \cdot A_{n-1})$$

If D is the number of decimal digits in the mantissa of floating-point numbers, the iteration process is stopped as soon as $(a_{N-1} - g_{N-1})$ is less than $a_{N-1} \cdot 10^{-D/2}$.

Since (a_n), (g_n) converge quadratically to the same limit (Arithmetico-Geometrical mean) this implies that $(a_N - g_N)$ is less than $a_N \cdot 10^{-D}$.

The value of cel 2 (k; A, B) $= \frac{\pi}{4} \cdot \frac{A_{N+1}}{a_N}$

Subroutine CEL2

Purpose:
Computes the generalized complete elliptic integral of second kind.

Usage:
CALL CEL2(RES, AK, A, B, IER)

Description of parameters:

RES	-	Result value.
AK	-	Modulus (input).
A	-	Constant term in numerator.
B	-	Factor of quadratic term in numerator.
IER	-	Resultant error code where:
		IER=0 No error.
		IER=1 AK not in range -1 to +1.

Remarks:
For AK = +1, -1, the result value is set to 1.E38 if B is positive, to -1.E38 if B is negative.
Special cases are:
K(K) obtained with A = 1, B = 1.
E(K) obtained with A = 1, B = CK*CK where CK is complementary modulus.
B(K) obtained with A = 1, B = 0.
D(K) obtained with A = 0, B = 1
where K, E, B, D define special cases of the generalized complete elliptic integral of second kind in the usual notation, and the argument K of these functions means the modulus.

Subroutines and function subprograms required:
None.

Method:
Definition:
RES= integral((A+ B*T*T)/(SQRT((1+ T*T)*(1+ (CK*T)**2))*(1+ T*T)) summed over T from 0 to infinity).
Evaluation:
Landen's transformation is used for calculation.
Reference:
R. Bulirsch, 'Numerical Calculation of Elliptic Integrals and Elliptic Functions', Handbook Series Special Functions, Numerische Mathematik Vol. 7, 1965, pp. 78-90.

```
      SUBROUTINE CEL2(RES,AK,A,B,IER)
      IER=0
C     TEST MODULUS
      GEO=1.-AK*AK
      IF(GEO)1,2,6
    1 IER=1
      RETURN
C     SET RESULT VALUE = OVERFLOW
    2 IF(B)3,5,4
    3 RES=-1.E38
      RETURN
    4 RES=1.E38
      RETURN
    5 RES=A
      RETURN
C     COMPUTE INTEGRAL
    6 GEO=SQRT(GEO)
      ARI=1.
      AA=A
      AN=A+B
      W=B
    7 W=W+AA*GEO
      W=W+W
      AA=AN
      AARI=ARI
      ARI=GEO+ARI
      AN=W/ARI+AN
C     TEST OF ACCURACY
      IF(AARI-GEO-1.E-4*AARI)9,9,8
    8 GEO=SQRT(GEO*AARI)
      GEO=GEO+GEO
      GO TO 7
    9 RES=.7853982 *AN/ARI
      RETURN
      END
```

EXPI

This subroutine computes the exponential integral in the range from -4 to infinity.

For positive x, the exponential integral is defined as:

$$E_1(x) = \int_x^\infty \frac{e^{-t}}{t}\,dt, \quad x > 0$$

This function, $E_1(x)$, may be analytically continued throughout the complex plane, and defines a multivalued complex function. However, for any given real argument, this extended multivalued function has a unique real part. The subroutine EXPI computes this unique real number for $x \geq -4$, $x \neq 0$.

For negative x, the real part of the extended exponential integral function is equal to $-E_i(-x)$,

where

$$E_i(y) = -\int_{-y}^\infty \frac{e^{-t}}{t}\,dt, \quad y > 0$$

($\int$ denotes Cauchy principal value.)

For x = 0, a singularity of the function, the program returns 1.0×10^{38}.

No action is taken in case of an argument less than -4.

Polynomial approximations which are close to Chebyshev approximations over their respective ranges are used for calculation.

1. Approximation in the range $x \geq 4$.

A polynomial approximation is obtained by means of truncation of the Expansion of $E_1(x)$ in terms of shifted Chebyshev Polynomials T_n^*

$$E_1(x) = \frac{e^{-x}}{x} \sum_{n=0}^{\infty} A_n T_n^*\left(\frac{4}{x}\right), \quad \text{for } 4 \leq x < \infty$$

The coefficients A_n are given in the article by Luke/Wimp. *

Using only nine terms of the above infinite series results in a truncation error $\epsilon(x)$ with:

$$|\epsilon(x)| < \frac{e^{-x}}{x} \sum_{v=9}^{\infty} |A_v| < \frac{e^{-x}}{x} \cdot 0.82 \cdot 10^{-8}$$

Transformation of the shifted Chebyshev polynominals to ordinary polynomials finally leads to the approximation:

$$\text{EXPI}(x) = e^{-x}\left(\frac{4}{x}\right) \sum_{v=0}^{\infty} a_v \left(\frac{4}{x}\right)^v \quad \text{for } x \geq 4$$

The coefficients of this approximation given to eight signification digits are:

a_0	=	0.24999 999
a_1	=	-0.06249 8588
a_2	=	0.03120 8561
a_3	=	-0.02295 1979
a_4	=	0.02041 2099
a_5	=	-0.01755 5779
a_6	=	0.01172 3273
a_7	=	-0.00493 62007
a_8	=	0.00094 42761 4

2. Approximation in the range $|x| \leq 4$.

A polynomial approximation is obtained by means of telescoping of the Taylor series of the function:

$$\int_0^x \frac{(e^{-t}-1)}{t}\,dt = -\ln x - C - E_1(x),$$

where C = 0.57721 56649 is Euler's constant.

This results in the approximation:

$$\text{EXPI}(x) = -\ln|x| + \sum_{v=0}^{14} b_v x^v$$

*Luke/Wimp, "Jacobi Polynomial expansion of a generalized hypergeometric function over a semi-infinite ray", Math. Comp., Vol. 17, 1963, Iss. 84, p. 400.

with a truncation error E absolutely less than 3×10^{-8}.

The coefficients of this approximation given to eight significant digits are:

b_0	=	-0.57721 566
b_1	=	1.00000 00
b_2	=	-0.25000 000
b_3	=	0.05555 5520
b_4	=	-0.01041 6662
b_5	=	0.00166 66906
b_6	=	-0.00023 14839 2
b_7	=	0.00002 83375 90
b_8	=	-0.00000 30996 040
b_9	=	0.00000 03072 6221
b_{10}	=	-0.00000 00276 35830
b_{11}	=	0.00000 00021 91569 9
b_{12}	=	-0.00000 00001 68265 92
b_{13}	=	0.00000 00000 15798 675
b_{14}	=	-0.00000 00000 01031 7602

Subroutine EXPI

Purpose:
Computes the exponential integral in the range -4 to infinity.

Usage:
CALL EXPI(RES, X, IER)

Description of parameters:

RES	-	Result value.
X	-	Argument of exponential integral.

IER	-	Resultant error code where:
		IER=0 No error.
		IER=1 X less than -4.

Remarks:
For X = 0 the result value is set to 1.E38.
For X less than -4 calculation is bypassed.
The argument remains unchanged.

Subroutines and function subprograms required:
None.

Method:
Definition:
RES=integral(EXP(-T)/T, summed over T from X to infinity).
Evaluation:
Two different polynomial approximations are used for X greater than 4 and for ABS(X) equal or less than 4.
Reference:
Luke and Wimp, 'Jacobi Polynomial Expansions of a Generalized Hypergeometric Function over a Semi-Infinite Range', Mathematical Tables and Other Aids to Computation, Vol. 17, 1963, Issue 84, pp. 395-404.

```
      SUBROUTINE EXPI(RES,X,IER)
C        TEST OF RANGE
      IER=0
      IF(X-4.) 10,10,20
   10 IF(X+4.) 55,30,30
C        ARGUMENT IS GREATER THAN 4
   20 ARG=4./X
      RES=EXP(-X)*((((((((.00094427614*ARG-.0049362007)*ARG+.011723273)
     1 *ARG-.01755779)*ARG+.020412099)*ARG-.022951979)*ARG+.031208561)
     2 *ARG-.06249858)*ARG+.24999999)*ARG
      RETURN
C        ARGUMENT IS ABSOLUTELY LESS OR EQUAL 4
   30 IF(X) 40,50,40
   40 RES=-ALOG(ABS(X))-(((((((((((((.10317602E-11*X-.15798675E-10)*X+
     1.16826592E-9)*X-.21915699E-8)*X+.27635830E-7)*X-.30726221E-6)*X+
     2.30996040E-5)*X-.28337590E-4)*X+.23148392E-3)*X-.0016666906)*X+
     3.010416662)*X-.05555520)*X+.25)*X-1.0)*X-.57721566
      RETURN
   50 RES=1.E38
      RETURN
C        ARGUMENT IS LESS THAN -4.
   55 IER=1
      RETURN
      END
```

SICI

This subroutine computes the sine and cosine integrals. These integrals are defined as:

$$\mathrm{Si}(x) = \int_{\infty}^{x} \frac{\sin(t)}{t}\,dt, \; x \geq 0$$

and

$$\mathrm{Ci}(x) = \int_{\infty}^{x} \frac{\cos(t)}{t}\,dt, \; x > 0$$

The subroutine SICI calculates both Si (x) and Ci (x) for a given argument x. Two different approximations are used for the ranges $|x| \leq 4$ and $4 < |x| < \infty$. Negative values of the argument x are handled by means of the following symmetries:

$$\mathrm{Si}(-x) = -\pi - \mathrm{Si}(x)$$

Real part of

$$\mathrm{Ci}(-x) = \mathrm{Ci}(x), \; x > 0 \text{ (see discussion of EXPI).}$$

For x = 0, a singularity of Ci (x), the routine returns -1.0×10^{38}.

Polynomial approximations that are close to Chebyshev approximations over their respective ranges are used for calculation.

1. Approximation in the range $|x| > 4$.

The sine and cosine integrals are closely related to the confluent hypergeometric function:

$$Y(x) = -ix\,\Psi(1, 1; -ix).$$

We have:

$$\mathrm{Si}(x) + i\,\mathrm{Ci}(x) = \frac{\pi}{2} + ie^{ix}\,\Psi(1, 1; -ix).$$

Setting:

$$ix\,\Psi(1, 1; ix) = \sum_{n=0}^{\infty} (A_n + i B_n)\, T_n^*\left(\frac{4}{x}\right)$$

*Luke/Wimp, "Jacobi Polynomial expansion of a generalized hypergeometric function over a semi-infinite ray", Math. Comp. Vol. 17, 1963, Iss. 84, p. 402.

we get the expansions:

$$\mathrm{Si}(x) = \sum_{n=0}^{\infty} \left(\frac{A_n \cdot \cos x}{x} + \frac{B_n \cdot \sin x}{x}\right) T_n^*\left(\frac{4}{x}\right)$$

$$\mathrm{Ci}(x) = \sum_{n=0}^{\infty} \left(\frac{B_n \cdot \cos x}{x} - \frac{A_n \cdot \sin x}{x}\right) T_n\left(\frac{4}{x}\right)$$

in terms of shifted Chebyshev polynomials T_n^*.

The coefficients A_n and B_n are given in the article by Luke/Wimp.*

Using only ten terms of the above infinite series results in a truncation error E (x) with:

$$|E(x)| < \frac{1}{x} \cdot 2.3 \cdot 10^{-8}$$

Transformation of the shifted Chebyshev polynomials to ordinary polynomials finally leads to the approximations:

$$\mathrm{Si}(x) = -\left(\frac{4}{x}\right) \cdot (\cos x \cdot V(x) + \sin x \cdot U(x))$$

$$\mathrm{Ci}(x) = \left(\frac{4}{x}\right) \cdot (\sin x \cdot V(x) - \cos x \cdot U(x)),$$

where

$$V(x) = \sum_{n=0}^{10} a_n \cdot \left(\frac{4}{x}\right)^n$$

$$U(x) = \sum_{n=0}^{9} b_n \cdot \left(\frac{4}{x}\right)^n$$

The coefficients of these expansions given to eight significant digits are:

a_0	=	0.25000 000
b_0	=	0.00000 00002 58398 86
a_1	=	-0.00000 06646 4406
b_1	=	0.06250 0111
a_2	=	-0.03122 4178
b_2	=	-0.00001 13495 79

a_3	=	-0.00037 64000 3
b_3	=	-0.02314 6168
a_4	=	0.02601 2930
b_4	=	-0.00333 25186
a_5	=	-0.00794 55563
b_5	=	0.04987 7159
a_6	=	-0.04400 4155
b_6	=	-0.07261 6418
a_7	=	0.07902 0335
b_7	=	0.05515 0700
a_8	=	-0.06537 2834
b_8	=	-0.02279 1426
a_9	=	0.02819 1786
b_9	=	0.00404 80690
a_{10}	=	-0.00510 86993

2. Approximation in the range $|x| \leq 4.$

A polynomial approximation for Si (x) is obtained by means of telescoping of the Taylor series:

$$\mathrm{Si}(x) = -\frac{\pi}{2} + \int_0^x \frac{\sin t}{t}\, dt$$

$$= -\frac{\pi}{2} + x \cdot \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n+1) \cdot (2n+1)!}$$

This results in the approximation:

$$\mathrm{Si}(x) = -\frac{\pi}{2} + x \cdot \sum_{n=0}^{6} a_v (x^2)^v ,$$

with a truncation error E absolutely less than $|X| \cdot 1.4 \cdot 10^{-9}$.

Similarly an approximation for Ci (x) is obtained by means of telescoping of the Taylor series:

$$\mathrm{Ci}(x) - C - \ln(x) = \sum_{n=1}^{\infty} \frac{(-1)^n x^{2n}}{2N \cdot (2n)!}$$

This results in the approximation:

$$\mathrm{Ci}(x) = C + \ln|x| - x^2 \cdot \sum_{n=0}^{5} b_n (x^2)^n ,$$

with a truncation error E absolutely less than $x^2 \cdot 5.6 \cdot 10^{-9}$.

The coefficients of these approximations given to eight significant decimal digits are:

C	=	0.57721 566
a_0	=	1.00000 00
b_0	=	0.24999 999
a_1	=	-0.05555 5547
b_1	=	-0.01041 6642
a_2	=	0.00166 66582
b_2	=	0.00023 14630 3
a_3	=	-0.00002 83414 60
b_3	=	-0.00000 30952 207
a_4	=	0.00000 03056 1233
b_4	=	0.00000 00269 45842
a_5	=	-0.00000 00022 23263 3
b_5	=	-0.00000 00001 38698 51
a_6	=	-0.00000 00000 09794 2154

Subroutine SICI

Purpose:
Computes the sine and cosine integral.

Usage:
CALL SICI(SI, CI, X)

Description of parameters:
SI - The resultant value SI(X).
CI - The resultant value CI(X).
X - The argument of SI(X) and CI(X).

Remarks:
The argument value remains unchanged.

Subroutines and function subprograms required:
None.

Method:
Definition:
SI(X)=integral (SIN(T)/T, summed over T from infinity to X).
CI(X)=integral (COS(T)/T, summed over T from infinity to X).
Evaluation:
Reduction of range using symmetry.
Different approximations are used for ABS(X) greater than 4 and for ABS(X) less than 4.
Reference:
Luke and Wimp, 'Polynomial Approximations to Integral Transforms', Mathematical Tables and Other Aids to Computation, Vol. 15, 1961, Issue 74, pp. 174-178.

```
      SUBROUTINE SICI(SI,CI,X)                                          SICI
C        TEST ARGUMENT RANGE                                            SICI
      Z=ABS(X).                                                         SICI
      IF(Z-4.) 10,10,50                                                 SICI
C        Z IS NOT GREATER THAN 4                                        SICI
   10 Y=Z*Z                                                             SICI
      SI=-1.5707963+X*(((((.97942154E-11*Y-.22232633E-8)*Y+.30561233E-5SICI
     1)*Y-.28341460E-4)*Y+.16666582E-2)*Y-.55555547E-1)*Y+1.)          SICI
C        TEST FOR LOGARITHMIC SINGULARITY                               SICI
      IF(Z) 30,20,30                                                    SICI
   20 CI=-1.E38                                                         SICI
      RETURN                                                            SICI
   30 CI=0.57721566+ALOG(Z)-Y*(((((-.13869851E-9*Y+.26945842E-7)*Y-     SICI
     1.30952207E-5)*Y+.23146303E-3)*Y-.10416642E-1)*Y+.24999999)        SICI
   40 RETURN                                                            SICI
C        Z IS GREATER THAN 4.                                           SICI
   50 SI=SIN(Z)                                                         SICI
      Y=COS(Z)                                                          SICI
      Z=4./Z                                                            SICI
     0U=((((((((.40480590E-2*Z-.02279426)*Z+.05515070)*Z-.07261642)*7SICI
     1+.04987716)*Z-.33325186E-2)*Z-.02314617)*Z-.11349579E-4)*Z       SICI
     2+.06250011)*Z+.25839886E-9                                        SICI
     0V=((((((((-.0051086993*Z+.02819179)*Z-.06537283)*Z+.07902034)*SICI
     1Z-.04400416)*Z-.00079455563)*Z+.02601293)*Z-.37640003E-3)*Z       SICI
     2-.03122418)*Z-.66464406E-6)*Z+.25000000                           SICI
      CI=Z*(SI*V-Y*U)                                                   SICI
      SI=-Z*(SI*U+Y*V)                                                  SICI
C        TEST FOR NEGATIVE ARGUMENT                                     SICI
      IF(X) 60,40,40                                                    SICI
C        X IS LESS THAN -4.                                             SICI
   60 SI=-3.1415927-SI                                                  SICI
      RETURN                                                            SICI
      END                                                               SICI
```

CS

This subroutine computes the Fresnel integrals for a given value of the argument x. The Fresnel integrals are defined as:

$$C(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \frac{\cos(t)}{\sqrt{t}}\, dt$$

and

$$S(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \frac{\sin(t)}{\sqrt{t}}\, dt.$$

The subroutine CS calculates both C(x) and S(x) for a given argument x.

In case of a negative argument x the absolute value of x is taken as argument for C and for S.

Polynomial approximations that are close to Chebyshev approximations over their respective ranges are used for calculation.

1. Approximation in the range $|x| > 4$.

The Fresnel integrals C(x) and S(x) are closely related to the confluent hypergeometric function:

$$Y(x) = \sqrt{xi}\, \psi\left(\frac{1}{2}, \frac{1}{2}; xi\right) = xi\, \psi\left(1, \frac{3}{2}; xi\right).$$

We have:

$$C(x) = \frac{1}{2} + \frac{1}{\sqrt{8\pi}} \sqrt{\frac{4}{x}}\,(\sin(x)\,\mathrm{Re}(Y) - \cos(x)\,\mathrm{Im}(Y))$$

$$S(x) = \frac{1}{2} - \frac{1}{\sqrt{8\pi}} \sqrt{\frac{4}{x}}\,(\cos(x)\,\mathrm{Re}(Y) + \sin(x)\,\mathrm{Im}(Y))$$

The expansions of real part Re (Y) and complex part Im (Y) in terms of shifted Chebyshev polynomials T_n^* over the range $4 \leq x < \infty$ are easily obtained using the method of computation described by Luke/Wimp.*

By means of truncation of the infinite series:

$$\mathrm{Re}\,(Y\,(x)) = \sum_{v=0}^{\infty} A_v T_v^* \left(\frac{4}{x}\right)$$

$$\mathrm{Im}\,(Y\,(x)) = \sum_{v=0}^{\infty} B_v T_v^* \left(\frac{4}{x}\right)$$

*Luke/Wimp, "Jacobi Polynomial expansion of a generalized hypergeometric function over a semi-infinite ray", Math. Comp., Vol. 17, 1963, Iss. 84, pp. 395-404.

beyond the eighth and ninth term respectively we get approximations with errors $E_c(x)$ and $E_s(x)$ where both errors are absolutely less than:

$$\epsilon = \sqrt{\frac{4}{x}} \cdot 1.3 \cdot 10^{-8}$$

Transformation of the shifted Chebyshev polynomials to ordinary polynomials finally leads to the approximations:

$$C(x) = \frac{1}{2} + \sqrt{\frac{4}{x}}\,(\sin(x) \cdot P(x) + \cos(x) \cdot Q(x))$$

$$S(x) = \frac{1}{2} + \sqrt{\frac{4}{x}}\,(-\cos(x) \cdot P(x) + \sin(x) \cdot Q(x))$$

where

$$P(x) = \sum_{0}^{7} a_v \left(\frac{4}{x}\right)^v$$

$$Q(x) = \sum_{0}^{8} b_v \left(\frac{4}{x}\right)^v.$$

The coefficients a_v and b_v are given to eight significant decimal digits:

a_0	=	0.19947 115
b_0	=	-0.00000 00044 44090 9
a_1	=	-0.00000 12079 984
b_1	=	-0.02493 3215
a_2	=	-0.00931 49105
b_2	=	-0.00001 60642 81
a_3	=	-0.00040 27145 0
b_3	=	0.00597 21508
a_4	=	0.00742 82459
b_4	=	-0.00030 95341 2
a_5	=	-0.00727 16901
b_5	=	-0.00679 28011
a_6	=	0.00340 14090
b_6	=	0.00797 09430
a_7	=	-0.00066 33925 6
b_7	=	-0.00416 92894
b_8	=	0.00087 68258

2. <u>Approximation in the range $0 \leqq x \leqq 4$.</u>

Approximations for C(x) and S(x) in the range $0 \leqq x \leqq 4$ were obtained by means of telescoping of the respective Taylor series expansions:

$$C(x) = \sqrt{\frac{2}{\pi}} \cdot \sqrt{x} \cdot \sum_{v=0}^{\infty} \frac{(-1)^v x^{2v}}{(4v+1)\,(2v)!}$$

$$S(x) = \sqrt{\frac{2}{\pi}} \cdot \sqrt{x^3} \cdot \sum_{v=0}^{\infty} \frac{(-1)^v x^{2v}}{(4v+3)\,(2v+1)!}$$

This leads finally to the following approximations:

$$C(x) = \sqrt{x} \sum_{v=0}^{6} c_v \cdot (x^2)^v$$

$$S(x) = x\sqrt{x} \sum_{v=0}^{5} d_v (x^2)^v ,$$

with respective errors $E_c(x)$ and $E_s(x)$, where

$$\left|E_c(x)\right| < \sqrt{x} \cdot 2.6 \cdot 10^{-8}$$

$$\left|E_s(x)\right| < x\sqrt{x} \cdot 3.5 \cdot 10^{-8}$$

The coefficients c_v and d_v are given below to eight significant decimal digits:

c_0	=	0.79788 455
d_0	=	0.26596 149
c_1	=	-0.07978 8405
d_1	=	-0.01899 7110

$c_2 = 0.00369\ 38586$

$d_2 = 0.00060\ 43537\ 1$

$c_3 = -0.00008\ 52246\ 22$

$d_3 = -0.00001\ 05258\ 53$

$c_4 = 0.00000\ 11605\ 284$

$d_4 = 0.00000\ 01122\ 5331$

$c_5 = -0.00000\ 00101\ 40729$

$d_5 = -0.00000\ 00006\ 67774\ 47$

$c_6 = 0.00000\ 00000\ 50998\ 348$

Subroutine CS

Purpose:
Computes the Fresnel integrals.

Usage:
CALL CS (C,S,X)

Description of parameters:

C - The resultant value C(X).
S - The resultant value S(X).
X - The argument of Fresnel integrals.
    If X is negative, the absolute value is used.

Remarks:
The argument value X remains unchanged.

Subroutines and function subprograms required:
None.

Method:
Definition:
C(X)=integral (COS(T)/SQRT(2*PI*T) summed over T from 0 to X).
S(X)=integral (SIN(T)/SQRT(2*PI*T) summed over T from 0 to X).
Evaluation:
Using different approximations for X less than 4 and X greater than 4.
Reference:
'Computation of Fresnel Integrals' by Boersma, Mathematical Tables and Other Aids to Computation, Vol. 14, 1960, No. 72, p. 380.

```
      SUBROUTINE CS(C,S,X)
      Z=ABS(X)
    2 IF(Z-4.) 3,3,4
C        X IS NOT GREATER THAN 4
    3 C=SQRT(Z)
      S=Z*C
      Z=Z*Z
      C=C*((((((.50998348E-10*Z-.10140729E-7)*Z+.11605284E-5)*Z
     1 -.85224622E-4)*Z+.369938586E-2)*Z-.079788405)*Z+.79788455)
      S=S*(((((-.66777447E-9*Z+.11225331E-6)*Z-.10525853E-4)*Z
     1 +.60435371E-3)*Z-.18997110E-1)*Z+.26596149)
      RETURN
C        X IS GREATER THAN 4
    4 D=COS(Z)
      S=SIN(Z)
      Z=4./Z
      A=(((((((.87682593E-3*Z-.41692894E-2)*Z+.79709430E-2)*Z-
     1.67928011F-2)*Z-.30953412E-3)*Z+.59721508E-2)*Z-.16064281E-4)*Z-
     2.024933215)*Z-.44440909E-8
      B=((((((-.66339256E-3*Z+.34014090E-2)*Z-.72716901E-2)*Z+
     1.74282459E-2)*Z-.40271450E-3)*Z-.93149105E-2)*Z-.12079984E-5)*Z+
     2.19947111
      Z=SQRT(Z)
      C=.5+Z*(D*A+S*B)
      S=.5+Z*(S*A-D*B)
      RETURN
      END
```

SIMQ

Purpose:
    Obtain solution of a set of simultaneous linear equations, AX=B.

Usage:
    CALL SIMQ(A,B,N,KS)

Description of parameters:

A	-	Matrix of coefficients stored columnwise. These are destroyed in the computation. The size of matrix A is N by N.
B	-	Vector of original constants (length N). These are replaced by final solution values, vector X.
N	-	Number of equations and variables. N must be greater than 1.
KS	-	Output digit: 0 For a normal solution. 1 For a singular set of equations.

Remarks:
    Matrix A must be general.
    If matrix is singular, solution values are meaningless.
    An alternative solution may be obtained by using matrix inversion (MINV) and matrix product (GMPRD).

Subroutines and function subprograms required:
    None.

Method:
    Method of solution is by elimination using largest pivotal divisor. Each stage of elimination consists of interchanging rows when necessary to avoid division by zero or small elements.
    The forward solution to obtain variable N is done in N stages. The back solution for the other variables is calculated by successive substitutions. Final solution values are developed in vector B, with variable 1 in B(1), variable 2 in B(2),........, variable N in B(N).
    If no pivot can be found exceeding a tolerance of 0.0, the matrix is considered singular and KS is set to 1. This tolerance can be modified by replacing the first statement.

```
      SUBROUTINE SIMQ(A,B,N,KS)
      DIMENSION A(1),B(1)
C        FORWARD SOLUTION
      TOL=0.0
      KS=0
      JJ=-N
      DO 65 J=1,N
      JY=J+1
      JJ=JJ+N+1
      BIGA=0
      IT=JJ-J
      DO 30 I=J,N
C        SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
      IJ=IT+I
      IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30
   20 BIGA=A(IJ)
      IMAX=I
   30 CONTINUE
C        TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX)
      IF(ABS(BIGA)-TOL) 35,35,40
   35 KS=1
      RETURN
C        INTERCHANGE RJWS IF NECESSARY
   40 I1=J+N*(J-2)
      IT=IMAX-J
      DO 50 K=J,N
      I1=I1+N
      I2=I1+IT
      SAVE=A(I1)
      A(I1)=A(I2)
      A(I2)=SAVE
C        DIVIDE EQUATIJN BY LEADING COEFFICIENT
   50 A(I1)=A(I1)/BIGA
      SAVE=B(IMAX)
      B(IMAX)=B(J)
      B(J)=SAVE/BIGA
C        ELIMINATE NEXT VARIABLE
      IF(J-N) 55,70,55
   55 IQS=N*(J-1)
      DO 65 IX=JY,N
      IXJ=IQS+IX
      IT=J-IX
      DO 60 JX=JY,N
      IXJX=N*(JX-1)+IX
      JJX=IXJX+IT
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))
   65 B(IX)=B(IX)-(B(J)*A(IXJ))
C        BACK SOLUTION
   70 NY=N-1
      IT=N*N
      DO 80 J=1,NY
      IA=IT-J
      IB=N-'
      IC='
      DO 80 K=1,J
      B(IB)=B(IB)-A(IA)*B(IC)
      IA=IA-N
   80 IC=IC-1
      RETURN
      END
```

RTWI

This subroutine refines the initial guess x_0 of a root of the general nonlinear equation $x = f(x)$. Wegstein's iteration scheme is used in order to get accelerated convergence in case of a function $f(x)$, which has at least continuous first derivative in the range in which iteration moves.

Following Figure 8, set $x_1 = y_0 = f(x_0)$ and $y_1 = f(x_1)$.

Refinement of x_1 is done by determination of the intersection of the linear function $y = x$ and the secant through the points (x_0, y_0) and (x_1, y_1), thus getting:

$$x_2 = x_1 + \frac{x_1 - x_0}{\dfrac{x_0 - y_0}{x_1 - y_1} - 1}$$

and $y_2 = f(x_2)$

The next step is done by starting at (x_2, y_2) and setting:

$$x_3 = x_2 + \frac{x_2 - x_1}{\dfrac{x_1 - y_1}{x_2 - y_2} - 1}$$

$$y_3 = f(x_3)$$

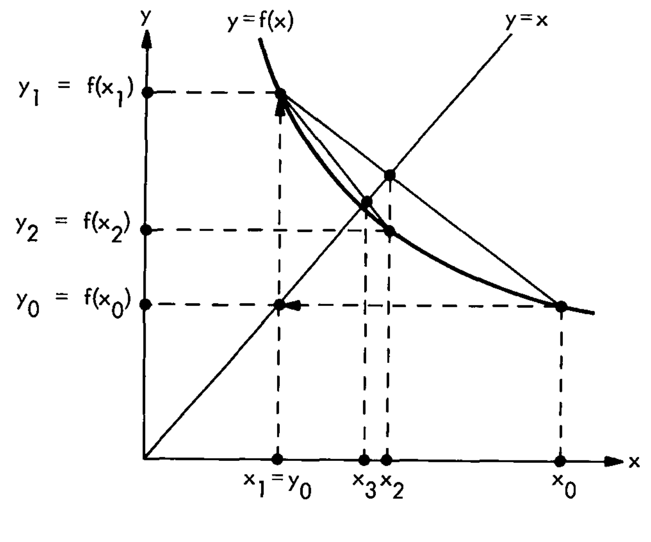


Figure 8. Wegstein's iterative method

It can be seen that this determines the intersection between $y = x$ and the secant through the points (x_1, y_1) and (x_2, y_2). Therefore Wegstein's iteration scheme is often called the secant modification of the normal iteration scheme $x_{i+1} = f(x_i)$.

Repeating these steps, the result is the iteration scheme:

$$\left.\begin{aligned} x_{i+1} &= x_i + \frac{x_i - x_{i-1}}{\dfrac{x_{i-1} - y_{i-1}}{x_i - y_i} - 1} \\ y_{i+1} &= f(x_{i+1}) \end{aligned}\right\} (i = 1, 2, \dots) \quad (1)$$

Each step requires one evaluation of f(x).

This iterative procedure is terminated if the following two conditions are satisfied:

$$\left.\begin{aligned} &\delta_1 \leq \text{ and } \delta_2 \leq 10 \cdot \varepsilon \\ &\text{with } \delta_1 = \begin{cases} \left|\dfrac{x_{i+1} - x_i}{x_{i+1}}\right| & \text{if } |x_{i+1}| > 1 \\ |x_{i+1} - x_i| & \text{if } |x_{i+1}| \leqq 1, \end{cases} \\ &\delta_2 = \begin{cases} \left|\dfrac{x_{i+1} - y_{i+1}}{x_{i+1}}\right| & \text{if } |x_{i+1}| > 1 \\ |x_{i+1} - y_{i+1}| & \text{if } |x_{i+1}| \leqq 1 \end{cases} \end{aligned}\right\} (2)$$

and tolerance ε given by input.

The procedure described above may not converge within a specified number of iteration steps. Reasons for this behavior, which is indicated by an error message may be:

1. Too few iteration steps are specified.
2. The initial guess x_0 is too far away from any root.
3. The tolerance ε is too small with respect to roundoff errors.
4. The root to be determined is of multiplicity greater than one.

Furthermore, the procedure fails if at any iteration step the denominator of equation (1) becomes zero. This is also indicated by an error message. This failure may have two reasons:

1. The secant has the slope 1, either exactly or due to roundoff errors. In both cases it is probable that there is at least one point ξ in the range in which iteration moves with $f'(\xi) = 1$.
2. $x_i = x_{i-1}$ and $x_i \neq y_i = f(x_i)$. This case is possible due to roundoff errors or to a very steep slope of the secant.

Subroutine RTWI

Purpose:

To solve general nonlinear equations of the form X=FCT(X) by means of Wegstein's iteration method.

Usage:

CALL RTWI (X, VAL, FCT, XST, EPS, IEND, IER)
Parameter FCT requires an EXTERNAL statement.

Description of parameters:

X	-	Resultant root of equation X=FCT(X).
VAL	-	Resultant value of X-FCT(X) at root X.
FCT	-	Name of the external function subprogram used.
XST	-	Input value which specifies the initial guess of the root X.
EPS	-	Input value which specifies the upper bound of the error of result X.
IEND	-	Maximum number of iteration steps specified.
IER	-	Resultant error parameter coded as follows:

IER=0	-	no error
IER=1	-	no convergence after IEND iteration steps
IER=2	-	at some iteration step the denominator of iteration formula was equal to zero

Remarks:

The procedure is bypassed and gives the error message IER=2 if at any iteration steps the denominator of the iteration formula is equal to zero. That means that there is at least one point in the range in which iteration moves with the derivative of FCT(X) equal to 1.

Subroutines and function subprograms required:

The external function subprogram FCT(X) must be furnished by the user.

Method:

Solution of equation X=FCT(X) is done by means of Wegstein's iteration method, which starts at the initial guess XST of a root X. One iteration step requires one evaluation of FCT(X). For test on satisfactory accuracy see formula (2) of mathematical description.

For reference, see:

1. G. N. Lance, Numerical Methods for High Speed Computers, Iliffe, London, 1960, pp. 134-138.
2. J. Wegstein, "Algorithm 2," CACM, Vol. 3, Iss. 2 (1960), pp. 74.
3. H. C. Thacher, "Algorithm 15," CACM, Vol. 3, Iss. 8 (1960), pp. 475.
4. J. G. Herriot, "Algorithm 26," CACM, Vol. 3, Iss. 11 (1960), pp. 603.

```
      SUBROUTINE RTWI(X,VAL,FCT,XST,EPS,IEND,IER)
C     PREPARE ITERATION
      IER=0
      TOL=XST
      X=FCT(TOL)
      A=X-XST
      B=-A
      TOL=X
      VAL=X-FCT(TOL)
C     START ITERATION LOOP
      DO 6 I=1,IEND
      IF(VAL)1,7,1
C     EQUATION IS NOT SATISFIED BY X
    1 B=B/VAL-1.
      IF(B)2,8,2
C     ITERATION IS POSSIBLE
    2 A=A/B
      X=X+A
      B=VAL
      TOL=X
      VAL=X-FCT(TOL)
C     TEST ON SATISFACTORY ACCURACY
      TOL=EPS
      D=ABS(X)
      IF(D-1.)4,4,3
    3 TOL=TOL*D
    4 IF(ABS(A)-TOL)5,5,6
    5 IF(ABS(VAL)-10.*TOL)7,7,6
    6 CONTINUE
C     END OF ITERATION LOOP
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.
      IER=1
    7 RETURN
C     ERROR RETURN IN CASE OF ZERO DIVISOR
    8 IER=2
      RETURN
      END
```

RTMI

This subroutine determines a root of the general nonlinear equation $f(x) = 0$ in the range of x from x_{li} up to x_{ri} (x_{li}, x_{ri} given by input) by means of Mueller's iteration scheme of successive bisection and inverse parabolic interpolation. The procedure assumes $f(x_{li}) \cdot f(x_{ri}) \leq 0$.

Starting with $x_l = x_{li}$ and $x_r = x_{ri}$ and following Fig. 9, one iteration step is described.

First, the middle of the interval $x_l \ldots x_r$ is computed:

$$x_m = \frac{1}{2}(x_l + x_r).$$

In case $f(x_m) \cdot f(x_r) < 0$, x_l and x_r are interchanged to ensure that $f(x_m) \cdot f(x_r) > 0$.

In case

$$2\,f(x_m)\left[f(x_m)-f(x_l)\right] - f(x_r)\left[f(x_r) - f(x_l)\right] \geq 0 \tag{1}$$

x_r is replaced by x_m and the bisection step is repeated. If, after a specified number of successive bisections, inequality (1) is still satisfied, the procedure is bypassed and an error message is given.

In Fig. 9, the second bisection step leads to a configuration which does not satisfy inequality (1). Thus by inverse parabolic interpolation:

$$\Delta x = f(x_l)\,\frac{x_m - x_l}{f(x_m)-f(x_l)}\left\{1 + f(x_m)\,\frac{f(x_r) - 2\,f(x_m)+f(x_l)}{\left[f(x_r)-f(x_m)\right]\left[f(x_r)-f(x_l)\right]}\right\} \tag{2}$$

$$\text{and } x = x_l - \Delta x$$

and x is sure to be situated between x_l and x_m

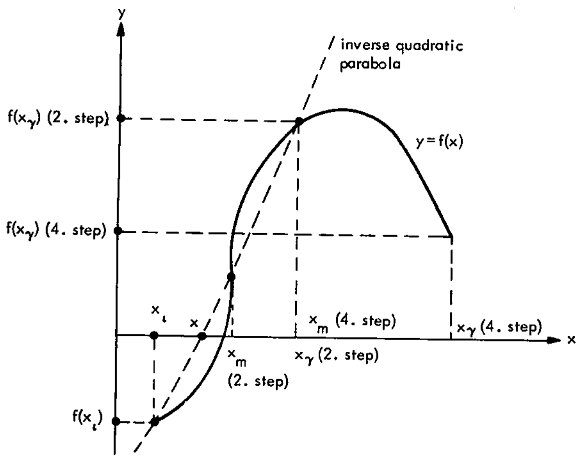


Figure 9. Mueller's iterative method

Now, for the next iteration step, x becomes x_l and x_m becomes x_r if $f(x) \cdot f(x_l) > 0$, or x becomes x_r if $f(x) \cdot f(x_l) < 0$.

Convergence is either quadratic or linear if the multiplicity of the root to be determined is equal to one or greater than one respectively, and if f(x) can be differentiated continuously at least twice in the range $x_{li} \cdots x_{ri}$. Each iteration step requires two evaluations of f(x).

This iterative procedure is terminated if either the two conditions (checked in bisection loop)

$$\left.\begin{aligned} &|x_r - x_l| \leq \varepsilon \cdot \max(1, |x_r|) \\ \text{and} \quad &|f(x_r) - f(x_l)| \leq 100 \cdot \varepsilon \end{aligned}\right\} \tag{3}$$

or the two conditions (checked after inverse parabolic interpolation)

$$\left.\begin{aligned} &|\Delta x| \leq \varepsilon \cdot \max(1, |x|) \\ \text{and} \quad &|f(x)| \leq 100 \cdot \varepsilon \end{aligned}\right\} \tag{4}$$

are satisfied, where tolerance ε is given by input.

The procedure described above may not converge within a specified number of iteration steps followed by the same number of successive bisections. Reasons for this behaviour, which is indicated by an error message, may be:

1. Too few iteration steps are specified.
2. The initial interval $x_{li} \cdots x_{ri}$ is too long.
3. The tolerance ε is too small with respect to roundoff errors.

Furthermore, the procedure is bypassed, also giving an error message, if the basic assumption $f(x_{li}) \cdot f(x_{ri}) \leq 0$ is not satisfied.

For reference see G. K. Kristiansen, "Zero of Arbitrary Function", BIT, vol. 3 (1963), pp. 205-206.

Subroutine RTMI

Purpose:
To solve general nonlinear equations of the form FCT(X)=0 by means of Mueller's iteration method.

Usage:
CALL RTMI(X, F, FCT, XLI, XRI, EPS, IEND, IER)
Parameter FCT requires an EXTERNAL statement.

Description of parameters:

X	-	Resultant root of equation FCT(X)=0.
F	-	Resultant function value at root X.
FCT	-	Name of the external function subprogram used.
XLI	-	Input value which specifies the initial left bound of the root X.
XRI	-	Input value which specifies the initial right bound of the root X.
EPS	-	Input value which specifies the upper bound of the error of result X.
IEND	-	Maximum number of iteration steps specified.
IER	-	Resultant error parameter coded as follows:

IER=0	-	no error
IER=1	-	no convergence after IEND iteration steps followed by IEND successive steps of bisection
IER=2	-	basic assumption FCT(XLI) *FCT(XRI) less than or equal to zero is not satisfied

Remarks:
The procedure assumes that function values at initial bounds XLI and XRI have not the same sign. If this basic assumption is not satisfied by input values XLI and XRI, the procedure is bypassed and gives the error message IER=2.

Subroutines and function subprograms required:
The external function subprogram FCT(X) must be furnished by the user.

Method:
Solution of equation FCT(X)=0 is done by means of Mueller's iteration method of successive bisections and inverse parabolic interpolation, which starts at the initial bounds XLI and XRI. Convergence is quadratic if the derivative of FCT(X) at root X is not equal to zero. One iteration step requires two evaluations of FCT(X). For test on satisfactory accuracy see formulae (3, 4) of mathematical description.

```
      SUBROUTINE RTMI(X,F,FCT,XLI,XRI,EPS,IEND,IER)
C     PREPARE ITERATION
      IER=0
      XL=XLI
      XR=XRI
      X=XL
      TOL=X
      F=FCT(TOL)
      IF(F)1,16,1
    1 FL=F
      X=XR
      TOL=X
      F=FCT(TOL)
      IF(F)2,16,2
    2 FR=F
      IF(SIGN(1.,FL)+SIGN(1.,FR))25,3,25
C     BASIC ASSUMPTION FL*FR LESS THAN 0 IS SATISFIED.
C     GENERATE TOLERANCE FOR FUNCTION VALUES.
    3 I=0
      TOLF=100.*EPS
C     START ITERATION LOOP
    4 I=I+1
C     START BISECTION LOOP
      DO 13 K=1,IEND
      X=.5*(XL+XR)
      TOL=X
      F=FCT(TOL)
      IF(F)5,16,5
    5 IF(SIGN(1.,F)+SIGN(1.,FR))7,6,7
C     INTERCHANGE XL AND XR IN ORDER TO GET THE SAME SIGN IN F AND FR
    6 TOL=XL
      XL=XR
      XR=TOL
      TOL=FL
      FL=FR
      FR=TOL
    7 TOL=F-FL
      A=F*TOL
      A=A+A
      IF(A-FR*(FR-FL))8,9,9
    8 IF(I-IEND)17,17,9
    9 XR=X
      FR=F
C     TEST ON SATISFACTORY ACCURACY IN BISECTION LOOP
      TOL=EPS
      A=ABS(XR)
      IF(A-1.)11,11,10
   10 TOL=TOL*A
   11 IF(ABS(XR-XL)-TOL)12,12,13
   12 IF(ABS(FR-FL)-TOLF)14,14,13
   13 CONTINUE
C     END OF BISECTION LOOP
C     NO CONVERGENCE AFTER IEND ITERATION STEPS FOLLOWED BY IEND
C     SUCCESSIVE STEPS OF BISECTION OR STEADILY INCREASING FUNCTION
C     VALUES AT RIGHT BOUNDS. ERROR RETURN.
      IER=1
   14 IF(ABS(FR)-ABS(FL))16,16,15
   15 X=XL
      F=FL
   16 RETURN
C     COMPUTATION OF ITERATED X-VALUE BY INVERSE PARABOLIC INTERPOLATION
   17 A=FR-F
      DX=(X-XL)*FL*(1.+F*(A-TOL)/(A*(FR-FL)))/TOL
      XM=X
      FM=F
      X=XL-DX
      TOL=X
      F=FCT(TOL)
      IF(F)18,16,18
C     TEST ON SATISFACTORY ACCURACY IN ITERATION LOOP
   18 TOL=EPS
      A=ABS(X)
      IF(A-1.)20,20,19
   19 TOL=TOL*A
   20 IF(ABS(DX)-TOL)21,21,22
   21 IF(ABS(F)-TOLF)16,16,22
C     PREPARATION OF NEXT BISECTION LOOP
   22 IF(SIGN(1.,F)+SIGN(1.,FL))24,23,24
   23 XR=X
      FR=F
      GO TO 4
   24 XL=X
      FL=F
      XR=XM
      FR=FM
      GO TO 4
C     END OF ITERATION LOOP
C     ERROR RETURN IN CASE OF WRONG INPUT DATA
   25 IER=2
      RETURN
      END
```

RTNI

This subroutine refines the initial guess x_0 of a root of the general nonlinear equation $f(x) = 0$. Newton's iteration scheme is used in the following form:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \qquad (i = 0, 1, 2, \ldots) \qquad (1)$$

Convergence is quadratic or linear if the multiplicity of the root to be determined is equal to one or greater than one respectively, and if f(x) can be differentiated continuously at least twice in the range in which iteration moves. Each iteration step requires one evaluation of f(x) and one evaluation of f$'$(x).

This iterative procedure is terminated if the following two conditions are satisfied:

$$\left.\begin{array}{l} \delta \leqq \varepsilon \text{ and } |f(x_{i+1})| \leqq 100 \cdot \varepsilon \\ \text{with} \quad \delta = \begin{cases} \left|\dfrac{x_{i+1} - x_i}{x_{i+1}}\right| & \text{in case of } |x_{i+1}| > 1 \\ |x_{i+1} - x_i| & \text{in case of } |x_{i+1}| \leqq 1 \end{cases} \end{array}\right\} \qquad (2)$$

and tolerance ε given by input.

The procedure described above may not converge within a specified number of iteration steps. Reasons for this behaviour, which is indicated by an error message, may be:

1. Too few iteration steps are specified.
2. The initial guess x_0 is too far away from any root.
3. The tolerance ε is too small with respect to roundoff errors.
4. The root to be determined is of multiplicity greater than one.

Furthermore, the procedure fails and is bypassed if at any iteration step the derivative $f(x_i)$ becomes zero. This is also indicated by an error message.

For reference see:

(1) F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York/Toronto/London, 1956, pp. 447 - 450.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker, Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 12 - 17.

Subroutine RTNI

Purpose:

To solve general nonlinear equations of the form F(X)=0 by means of Newton's iteration method.

Usage:

CALL RTNI (X, F, DERF, FCT, XST, EPS, IEND, IER) Parameter FCT requires an EXTERNAL statement

Description of parameters:

X	-	Resultant root of equation F(X)=0.
F	-	Resultant function value at root X.
DERF	-	Resultant value of derivative at root X.
FCT	-	Name of the external subroutine used. It computes for given argument X the function value F and derivative DERF. Its parameter list must be X, F, DERF.
XST	-	Input value which specifies the initial guess of the root X.
EPS	-	Input value which specifies the upper bound of the error of result X.

IEND	- Maximum number of iteration steps specified.
IER	- Resultant error parameter coded as follows:

IER=0	- no error
IER=1	- no convergence after IEND iteration steps
IER=2	- at some iteration step derivative DERF was equal to zero

Remarks:

The procedure is bypassed and gives the error message IER=2 if at any iteration step the derivative of F(X) is equal to 0. Possibly the procedure would be successful if it were started again with another initial guess XST.

Subroutines and function subprograms required:

The external subroutine FCT(X, F, DERF) must be furnished by the user.

Method:

Solution of the equation F(X)=0 is obtained by means of Newton's iteration method, which starts at the initial guess XST of a root X. Convergence is quadratic if the derivative of F(X) at root X is not equal to zero. One iteration step requires one evaluation of F(X) and one evaluation of the derivative of F(X). For tests on satisfactory accuracy see formula (2) of the mathematical description.

```
      SUBROUTINE RTNI(X,F,DERF,FCT,XST,EPS,IEND,IER)
C     PREPARE ITERATION
      IER=0
      X=XST
      TOL=X
      CALL FCT(TOL,F,DERF)
      TOLF=100.*EPS
C     START ITERATION LOOP
      DO 6 I=1,IEND
      IF(F)1,7,1
C     EQUATION IS NOT SATISFIED BY X
    1 IF(DERF)2,8,2
C     ITERATION IS POSSIBLE
    2 DX=F/DERF
      X=X-DX
      TOL=X
      CALL FCT(TOL,F,DERF)
C     TEST ON SATISFACTORY ACCURACY
      TOL=EPS
      A=ABS(X)
      IF(A-1.)4,4,3
    3 TOL=TOL*A
    4 IF(ABS(DX)-TOL)5,5,6
    5 IF(ABS(F)-TOLF)7,7,6
    6 CONTINUE
C     END OF ITERATION LOOP
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.
      IER=1
    7 RETURN
C     ERROR RETURN IN CASE OF ZERO DIVISOR
    8 IER=2
      RETURN
      END
```

Mathematics - Roots of Polynomial

POLRT

This subroutine computes the real and complex roots of a real polynomial.

Given a polynomial

$$f(z) = \sum_{n=0}^{N} a_n z^n \qquad (1)$$

let

$Z = X + iY$ be a starting value for a root of f(z).

Then:

$$Z^n = (X + iY)^n. \qquad (2)$$

Define X_n as real terms of expanded equation (2).

Define Y_n as imaginary terms of expanded equation (2).

Then for:

$n = 0$

$X_o = 1.0$

$Y_o = 0.0$

$n > 0$

$$X_n = X \cdot X_{n-1} - Y \cdot Y_{n-1} \qquad (3)$$

$$Y_n = X \cdot Y_{n-1} + Y \cdot X_{n-1} \qquad (4)$$

Let U be the real terms of (1).

V be the imaginary terms of (1).

Then:

$$U = \sum_{n=0}^{N} a_n X_n \qquad (5)$$

$$V = \sum_{n=0}^{N} a_n Y_n \qquad (6)$$

or

$$U = a_o + \sum_{n=1}^{N} a_n X_n \qquad (7)$$

$$V = \sum_{n=1}^{N} a_n Y_n \qquad (8)$$

$$\frac{\partial U}{\partial X} = \sum_{n=1}^{N} n \cdot X_{n-1} \cdot a_n \qquad (9)$$

$$\frac{\partial U}{\partial Y} = - \sum_{n=1}^{N} n \, Y_{n-1} \, a_n \qquad (10)$$

Note that equations (3), (4), (7), (8), (9), and (10) can be performed iteratively for n = 1 to N by saving X_{n-1} and Y_{n-1}.

Using the Newton-Raphson method for computing ΔX, ΔY, we have:

$$\Delta X = \left(V\frac{\partial U}{\partial Y} - U\frac{\partial U}{\partial X}\right) \Big/ \left[\left(\frac{\partial U}{\partial X}\right)^2 + \left(\frac{\partial U}{\partial Y}\right)^2\right] \quad (11)$$

$$\Delta Y = -\left(U\frac{\partial U}{\partial Y} + V\frac{\partial U}{\partial X}\right) \Big/ \left[\left(\frac{\partial U}{\partial X}\right)^2 + \left(\frac{\partial U}{\partial Y}\right)^2\right] \quad (12)$$

after applying the Cauchy-Riemann equations.

Thus, for the next iteration:

$$X' = X + \Delta X$$

$$Y' = Y + \Delta Y$$

Subroutine POLRT

Purpose:

Computes the real and complex roots of a real polynomial.

Usage:

CALL POLRT(XCOF, COF, M, ROOTR, ROOTI, IER)

Description of parameters:

XCOF	-	Vector of M+1 coefficients of the polynomial ordered from smallest to largest power.
COF	-	Working vector of length M+1.
M	-	Order of polynomial.
ROOTR	-	Resultant vector of length M containing real roots of the polynomial.
ROOTI	-	Resultant vector of length M containing the corresponding imaginary roots of the polynomial.
IER	-	Error code where:

IER=0	No error.
IER=1	M less than one.
IER=2	M greater than 36.
IER=3	Unable to determine root with 500 iterations on 5 starting values.
IER=4	High order coefficient is zero.

Remarks:

Limited to 36th order polynomial or less. Floating-point overflow may occur for high order polynomials but will not affect the accuracy of the results.

Subroutines and function subprograms required:

None.

Method:

Newton-Raphson iterative technique. The final iterations on each root are performed using the original polynomial rather than the reduced polynomial to avoid accumulated errors in the reduced polynomial.

```
      SUBROUTINE POLRT(XCOF,COF,M,ROOTR,ROOTI,IER)
      DIMENSION XCOF(1),COF(1),ROOTR(1),ROOTI(1)
      IFIT=0
      N=M
      IER=0
      IF(XCOF(N+1)) 10,25,10
   10 IF(N) 15,15,32
C        SET ERROR CODE TO 1
   15 IER=1
   20 RETURN
C        SET ERROR CODE TO 4
   25 IER=4
      GO TO 20
C        SET ERROR CODE TO 2
   30 IER=2
      GO TO 20
   32 IF(N-36) 35,35,30
   35 NX=N
      NXX=N+1
      N2=1
      KJ1 = N+1
      DO 40 L=1,KJ1
      MT=KJ1-L+1
   40 COF(MT)=XCOF(L)
C        SET INITIAL VALUES
   45 XO=.00500101
      YO=0.01000101
C        ZERO INITIAL VALUE COUNTER
      IN=0
   50 X=XO
C        INCREMENT INITIAL VALUES AND COUNTER
      XO=-10.0*YO
      YO=-10.0*X
C        SET X AND Y TO CURRENT VALUE
      X=XO
      Y=YO
      IN=IN+1
      GO TO 59
   55 IFIT=1
      XPR=X
      YPR=Y
C        EVALUATE POLYNOMIAL AND DERIVATIVES
   59 ICT=0
   60 UX=0.0
      UY=0.0
      V =0.0
      YT=0.0
      XT=1.0
      U=COF(N+1)
      IF(U) 65,130,65
   65 DO 70 I=1,N
      L =N-I+1
      XT2=X*XT-Y*YT
      YT2=X*YT+Y*XT
      U=U+COF(L )*XT2
      V=V+COF(L )*YT2
      FI=I
      UX=UX+FI*XT*COF(L )
      UY=UY-FI*YT*COF(L )
      XT=XT2
   70 YT=YT2
      SUMSQ=UX*UX+UY*UY
      IF(SUMSQ) 75,110,75
   75 DX=(V*UY-U*UX)/SUMSQ
      X=X+DX
      DY=-(U*UY+V*UX)/SUMSQ
      Y=Y+DY
   78 IF( ABS(DY)+ ABS(DX)-1.0E-05) 100,80,80
C        STEP ITERATION COUNTER
   80 ICT=ICT+1
      IF(ICT-500) 60,85,85
   85 IF(IFIT) 100,90,100
   90 IF(IN-5) 50,95,95
C        SET ERROR CODE TO 3
   95 IER=3
      GO TO 20
  100 DO 105 L=1,NXX
      MT=KJ1-L+1
      TEMP=XCOF(MT)
      XCOF(MT)=COF(L)
  105 COF(L)=TEMP
      ITEMP=N
      N=NX
      NX=ITEMP
      IF(IFIT) 120,55,120
  110 IF(IFIT) 115,50,115
  115 X=XPR
      Y=YPR
  120 IFIT=0
      IF(X)122,125,122
  122 IF(ABS(Y)-ABS(X)*1.0E-04)135,125,125
  125 ALPHA=X+X
      SUMSQ=X*X+Y*Y
      N=N-2
      GO TO 140
  130 X=0.0
      NX=NX-1
      NXX=NXX-1
  135 Y=0.0
      SUMSQ=0.0
      ALPHA=X
      N=N-1
  140 L1=1
      L2=2
      COF(L2)=COF(L2)+ALPHA*COF(L1)
  145 DO 150 L=2,N
  150 COF(L+1)=COF(L+1)+ALPHA*COF(L)-SUMSQ*COF(L-1)
  155 ROOTI(N2)=Y
      ROOTR(N2)=X
      N2=N2+1
      IF(SUMSQ) 160,165,160
  160 Y=-Y
      SUMSQ=0.0
      GO TO 155
  165 IF(N) 20,20,45
      END
```

PADD

Purpose:
Add two polynomials.

Usage:
CALL PADD(Z, IDIMZ, X, IDIMX, Y, IDIMY)

Description of parameters:

Z	-	Vector of resultant coefficients, ordered from smallest to largest power.
IDIMZ	-	Dimension of Z (calculated).
X	-	Vector of coefficients for first polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X (degree is IDIMX-1).
Y	-	Vector of coefficients for second polynomial, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (degree is IDIMY-1).

Remarks:
Vector Z may be in same location as either vector X or vector Y only if the dimension of that vector is not less than the other input vector.
The resultant polynomial may have trailing zero coefficients.

Subroutines and function subprograms required:
None.

Method:
Dimension of resultant vector IDIMZ is calculated as the larger of the two input vector dimensions. Corresponding coefficients are then added to form Z.

```
      SUBROUTINE PADD(Z,IDIMZ,X,IDIMX,Y,IDIMY)
      DIMENSION Z(1),X(1),Y(1)
C        TEST DIMENSIONS OF SUMMANDS
      NDIM=IDIMX
      IF (IDIMX-IDIMY) 10,20,20
   10 NDIM=IDIMY
   20 IF(NDIM) 90,90,30
   30 DO 80 I=1,NDIM
      IF(I-IDIMX) 40,40,60
   40 IF(I-IDIMY) 50,50,70
   50 Z(I)=X(I)+Y(I)
      GO TO 80
   60 Z(I)=Y(I)
      GO TO 80
   70 Z(I)=X(I)
   80 CONTINUE
   90 IDIMZ=NDIM
      RETURN
      END
```

PADDM

Purpose:
Add coefficients of one polynomial to the product of a factor by coefficients of another polynomial.

Usage:
CALL PADDM(Z, IDIMZ, X, IDIMX, FACT, Y, IDIMY)

Description of parameters:

Z	-	Vector of resultant coefficients, ordered from smallest to largest power.
IDIMZ	-	Dimension of Z (calculated).
X	-	Vector of coefficients for first polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X (degree is IDIMX-1).
FACT	-	Factor to be multiplied by vector Y.
Y	-	Vector of coefficients for second polynomial, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (degree is IDIMY-1).

Remarks:
Vector Z may be in same location as either vector X or vector Y only if the dimension of that vector is not less than the other input vector.
The resultant polynomial may have trailing zero coefficients.

Subroutines and function subprograms required:
None.

Method:
Dimension of resultant vector IDIMZ is calculated as the larger of the two input vector dimensions. Coefficient in vector X is then added to coefficient in vector Y multiplied by factor to form Z.

```
      SUBROUTINE PADDM(Z,IDIMZ,X,IDIMX,FACT,Y,IDIMY)
      DIMENSION Z(1),X(1),Y(1)
C        TEST DIMENSIONS OF SUMMANDS
      NDIM=IDIMX
      IF(IDIMX-IDIMY) 10,20,20
   10 NDIM=IDIMY
   20 IF(NDIM) 90,90,30
   30 DO 80 I=1,NDIM
      IF(I-IDIMX) 40,40,60
   40 IF(I-IDIMY) 50,50,70
   50 Z(I)=FACT*Y(I)+X(I)
      GO TO 80
   60 Z(I)=FACT*Y(I)
      GO TO 80
   70 Z(I)=X(I)
   80 CONTINUE
   90 IDIMZ=NDIM
      RETURN
      END
```

PCLA

Purpose:
Move polynomial X to Y.

Usage:
CALL PCLA(Y, IDIMY, X, IDIMX)

Description of parameters:

Y	-	Vector of resultant coefficients, ordered from smallest to largest power.
IDIMY	-	Dimension of Y.

X	-	Vector of coefficients for polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
IDIMY is replaced by IDIMX and vector X is moved to Y.

```
      SUBROUTINE PCLA (Y,IDIMY,X,IDIMX)
      DIMENSION X(1),Y(1)
      IDIMY=IDIMX
      IF(IDIMX) 30,30,10
   10 DO 20 I=1,IDIMX
   20 Y(I)=X(I)
   30 RETURN
      END
```

PSUB

Purpose:
Subtract one polynomial from another.

Usage:
CALL PSUB(Z, IDIMZ, X, IDIMX, Y, IDIMY)

Description of parameters:

Z	-	Vector of resultant coefficients, ordered from smallest to largest power.
IDIMZ	-	Dimension of Z (calculated).
X	-	Vector of coefficients for first polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X (degree is IDIMX-1).
Y	-	Vector of coefficients for second polynomial, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (degree is IDIMY-1).

Remarks:
Vector Z may be in same location as either vector X or vector Y only if the dimension of that vector is not less than the other input vector. The resultant polynomial may have trailing zero coefficients.

Subroutines and function subprograms required:
None.

Method:
Dimension of resultant vector IDIMZ is calculated as the larger of the two input vector dimensions. Coefficients in vector Y are then subtracted from corresponding coefficients in vector X.

```
      SUBROUTINE PSUB(Z,IDIMZ,X,IDIMX,Y,IDIMY)
      DIMENSION Z(1),X(1),Y(1)
C        TEST DIMENSIONS OF SUMMANDS
      NDIM=IDIMX
      IF (IDIMX-IDIMY) 10,20,20
   10 NDIM=IDIMY
   20 IF (NDIM) 90,90,30
   30 DO 80 I=1,NDIM
      IF (I-IDIMX) 40,40,60
   40 IF (I-IDIMY) 50,50,70
   50 Z(I)=X(I)-Y(I)
      GO TO 80
   60 Z(I)=-Y(I)
      GO TO 80
   70 Z(I)=X(I)
   80 CONTINUE
   90 IDIMZ=NDIM
      RETURN
      END
```

PMPY

Purpose:
Multiply two polynomials.

Usage:
CALL PMPY(Z, IDIMZ, X, IDIMX, Y, IDIMY)

Description of parameters:

Z	-	Vector of resultant coefficients, ordered from smallest to largest power.
IDIMZ	-	Dimension of Z (calculated).
X	-	Vector of coefficients for first polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X (degree is IDIMX-1).
Y	-	Vector of coefficients for second polynomial, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (degree is IDIMY-1).

Remarks:
Z cannot be in the same location as X.
Z cannot be in the same location as Y.

Subroutines and function subprograms required:
None.

Method:
Dimension of Z is calculated as IDIMX+IDIMY-1. The coefficients of Z are calculated as sum of products of coefficients of X and Y, whose exponents add up to the corresponding exponent of Z.

```
      SUBROUTINE PMPY(Z,IDIMZ,X,IDIMX,Y,IDIMY)
      DIMENSION Z(1),X(1),Y(1)
      IF(IDIMX*IDIMY)10,10,20
   10 IDIMZ=0
      GO TO 50
   20 IDIMZ=IDIMX+IDIMY-1
      DO 30 I=1,IDIMZ
   30 Z(I)=0.
      DO 40 I=1,IDIMX
      DO 40 J=1,IDIMY
      K=I+J-1
   40 Z(K)=X(I)*Y(J)+Z(K)
   50 RETURN
      END
```

PDIV

Purpose:
Divide one polynomial by another.

Usage:
CALL PDIV(P, IDIMP, X, IDIMX, Y, IDIMY, TOL, IER)

Description of parameters:

P	- Resultant vector of integral part.
IDIMP	- Dimension of P.
X	- Vector of coefficients for dividend polynomial, ordered from smallest to largest power. It is replaced by remainder after division.
IDIMX	- Dimension of X.
Y	- Vector of coefficients for divisor polynomial, ordered from smallest to largest power.
IDIMY	- Dimension of Y.
TOL	- Tolerance value below which coefficients are eliminated during normalization.
IER	- Error code. 0 is normal, 1 is for zero divisor.

Remarks:
The remainder R replaces X.
The divisor Y remains unchanged.
If dimension of Y exceeds dimension of X, IDIMP is set to zero and calculation is bypassed.

Subroutines and function subprograms required:
PNORM

Method:
Polynomial X is divided by polynomial Y giving integer part P and remainder R such that
X = P*Y + R.
Divisor Y and remainder vector get normalized.

```
      SUBROUTINE PDIV(P,IDIMP,X,IDIMX,Y,IDIMY,TOL,IER)
      DIMENSION P(1),X(1),Y(1)
      CALL PNORM (Y,IDIMY,TOL)
      IF(IDIMY) 50,50,10
   10 IDIMP=IDIMX-IDIMY+1
      IF(IDIMP) 20,30,50
C        DEGREE OF DIVISOR WAS GREATER THAN DEGREE OF DIVIDEND
   20 IDIMP=0
   30 IER=0
   40 RETURN
C        Y IS ZERO POLYNOMIAL
   50 IER=1
      GO TO 40
C        START REDUCTION
   60 IDIMX=IDIMY-1
      I=IDIMP
   70 II=I+IDIMX
      P(I)=X(II)/Y(IDIMY)
C        SUBTRACT MULTIPLE OF DIVISOR
      DO 80 K=1,IDIMX
      J=K-1+I
      X(J)=X(J)-P(I)*Y(K)
   80 CONTINUE
      I=I-1
      IF(I) 90,90,70
C        NORMALIZE REMAINDER POLYNOMIAL
   90 CALL PNORM(X,IDIMX,TOL)
      GO TO 30
      END
```

PQSD

Purpose:
Perform quadratic synthetic division.

Usage:
CALL PQSD(A, B, P, Q, X, IDIMX)

Description of parameters:

A	- Coefficient of Z in remainder (calculated).
B	- Constant term in remainder (calculated).
P	- Coefficient of Z in quadratic polynomial.
Q	- Constant term in quadratic polynomial.
X	- Coefficient vector for given polynomial, ordered from smallest to largest power.
IDIMX	- Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
The linear remainder A*Z+B.

```
      SUBROUTINE PQSD(A,B,P,Q,X,IDIMX)
      DIMENSION X(1)
      A=0.
      B=0.
      J=IDIMX
    1 IF(J)3,3,2
    2 Z=P*A+B
      B=Q*A+X(J)
      A=Z
      J=J-1
      GO TO 1
    3 RETURN
      END
```

PVAL

Purpose:
Evaluate a polynomial for a given value of the variable.

Usage:
CALL PVAL(RES, ARG, X, IDIMX)

Description of parameters:

RES	- Resultant value of polynomial.
ARG	- Given value of the variable.
X	- Vector of coefficients, ordered from smallest to largest power.
IDIMX	- Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Evaluation is done by means of nested multiplication.

```
      SUBROUTINE PVAL(RES,ARG,X,IDIMX)
      DIMENSION X(1)
      RES=0.
      J=IDIMX
    1 IF(J)3,3,2
    2 RES=RES*ARG+X(J)
      J=J-1
      GO TO 1
    3 RETURN
      END
```

PVSUB

Purpose:
Substitute variable of a polynomial by another polynomial.

Usage:
CALL PVSUB(Z, IDIMZ, X, IDIMX, Y, IDIMY, WORK1, WORK2)

Description of parameters:

Z	-	Vector of coefficients for resultant polynomial, ordered from smallest to largest power.
IDIMZ	-	Dimension of Z.
X	-	Vector of coefficients for original polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.
Y	-	Vector of coefficients for polynomial which is substituted for variable, ordered from smallest to largest power.
IDIMY	-	Dimension of Y.
WORK1	-	Working storage array (same dimension as Z).
WORK2	-	Working storage array (same dimension as Z).

Remarks:
None.

Subroutines and function subprograms required:
PMPY
PADDM
PCLA

Method:
Variable of polynomial X is substituted by polynomial Y to form polynomial Z. Dimension of new polynomial is (IDIMX-1)*(IDIMY-1)+1. Subroutine requires two work areas.

```
      SUBROUTINE PVSUB(Z,IDIMZ,X,IDIMX,Y,IDIMY,WORK1,WORK2)
      DIMENSION Z(1),X(1),Y(1),WORK1(1),WORK2(1)
C        TEST OF DIMENSIONS
      IF (IDIMX-1) 1,3,3
    1 IDIMZ=0
    2 RETURN
    3 IDIMZ=1
      Z(1)=X(1)
      IF (IDIMY*IDIMX-IDIMY) 2,2,4
    4 IW1=1
      WORK1(1)=1.
      DO 5 I=2,IDIMX
      CALL PMPY(WORK2,IW2,Y,IDIMY,WORK1,IW1)
      CALL PCLA(WORK1,IW1,WORK2,IW2)
      FACT=X(I)
      CALL PADDM(Z,IDIMZ,Z,IDIMZ,FACT,WORK1,IW1)
    5 CONTINUE
      GO TO 2
      END
```

PCLD

Purpose:
Shift of origin (complete linear synthetic division).

Usage:
CALL PCLD(X, IDIMX, U)

Description of parameters:

X	-	Vector of coefficients, ordered from smallest to largest power. It is replaced by vector of transformed coefficients.
IDIMX	-	Dimension of X.
U	-	Shift parameter.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Coefficient vector X(I) of polynomial P(Z) is transformed so that Q(Z)=P(Z-U) where Q(Z) denotes the polynomial with transformed coefficient vector.

```
      SUBROUTINE PCLD (X,IDIMX,U)
      DIMENSION X(1)
      K=1
    1 J=IDIMX
    2 IF (J-K) 4,4,3
    3 X(J-1)=X(J-1)+U*X(J)
      J=J-1
      GO TO 2
    4 K=K+1
      IF (IDIMX-K) 5,5,1
    5 RETURN
      END
```

PILD

Purpose:
Evaluate polynomial and its first derivative for a given argument.

Usage:
CALL PILD(POLY, DVAL, ARGUM, X, IDIMX)

Description of parameters:

POLY	-	Value of polynomial.
DVAL	-	Derivative.
ARGUM	-	Argument.
X	-	Vector of coefficients for polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
PQSD

Method:
Evaluation is done by means of subroutine PQSD (quadratic synthetic division).

```
      SUBROUTINE PILD (POLY,DVAL,ARGUM,X,IDIMX)
      DIMENSION X(1)
      P=ARGUM+ARGUM
      Q=-ARGUM*ARGUM
      CALL PQSD (DVAL,POLY,P,Q,X,IDIMX)
      POLY=ARGUM*DVAL+POLY
      RETURN
      END
```

PDER

Purpose:
Find derivative of a polynomial.

Usage:
CALL PDER(Y, IDIMY, X, IDIMX)

Description of parameters:

Y	-	Vector of coefficients for derivative, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (equal to IDIMX-1).
X	-	Vector of coefficients for original polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Dimension of Y is set at dimension of X less one. Derivative is then calculated by multiplying coefficients by their respective exponents.

```
      SUBROUTINE PDER(Y,IDIMY,X,IDIMX)
      DIMENSION X(1),Y(1)
C        TEST OF DIMENSION
      IF (IDIMX-1) 3,3,1
    1 IDIMY=IDIMX-1
      EXPT=0.
      DO 2 I=1,IDIMY
      EXPT=EXPT+1.
    2 Y(I)=X(I+1)*EXPT
      GO TO 4
    3 IDIMY=0
    4 RETURN
      END
```

PINT

Purpose:
Find integral of a polynomial with constant of integration equal to zero.

Usage:
CALL PINT(Y, IDIMY, X, IDIMX)

Description of parameters:

Y	-	Vector of coefficients for integral, ordered from smallest to largest power.
IDIMY	-	Dimension of Y (equal to IDIMX+1).
X	-	Vector of coefficients for original polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.

Remarks:
None.

Subroutines and function subprograms required:
None.

Method:
Dimension of Y is set at dimension of X plus one, and the constant term is set to zero. Integral is then calculated by dividing coefficients by their respective exponents.

```
      SUBROUTINE PINT(Y,IDIMY,X,IDIMX)
      DIMENSION X(1),Y(1)
      IDIMY=IDIMX+1
      Y(1)=0.
      IF(IDIMX)1,1,2
    1 RETURN
    2 EXPT=1.
      DO 3 I=2,IDIMY
      Y(I)=X(I-1)/EXPT
    3 EXPT=EXPT+1.
      GO TO 1
      END
```

PGCD

Purpose:
Determine greatest common divisor of two polynomials.

Usage:
CALL PGCD(X, IDIMX, Y, IDIMY, WORK, EPS, IER)

Description of parameters:

X	-	Vector of coefficients for first polynomial, ordered from smallest to largest power.
IDIMX	-	Dimension of X.
Y	-	Vector of coefficients for second polynomial, ordered from smallest to largest power. This is replaced by greatest common divisor.
IDIMY	-	Dimension of Y.
WORK	-	Working storage array.
EPS	-	Tolerance value below which coefficient is eliminated during normalization.
IER	-	Resultant error code where:

IER=0	No error.
IER=1	X or Y is zero polynomial.

Remarks:

IDIMX must be greater than IDIMY.

IDIMY=1 on return means X and Y are prime, the GCD is a constant.

Subroutines and function subprograms required:

PDIV

PNORM

Method:

Greatest common divisor of two polynomials X and Y is determined by means of Euclidean algorithm. Coefficient vectors X and Y are destroyed and greatest common divisor is generated in Y.

```
      SUBROUTINE PGCD(X,IDIMX,Y,IDIMY,WORK,EPS,IER)
      DIMENSION X(1),Y(1),WORK(1)
C        DIMENSION REQUIRED FOR VECTOR NAMED  WORK  IS   IDIMX-IDIMY+1
    1 CALL PDIV(WORK,NDIM,X,IDIMX,Y,IDIMY,EPS,IER)
      IF(IER) 5,2,5
    2 IF(IDIMX) 5,5,3
C        INTERCHANGE X AND Y
    3 DO 4 J=1,IDIMY
      WORK(1)=X(J)
      X(J)=Y(J)
    4 Y(J)=WORK(1)
      NDIM=IDIMX
      IDIMX=IDIMY
      IDIMY=NDIM
      GO TO 1
    5 RETURN
      END
```

PNORM

Purpose:

Normalize coefficient vector of a polynomial.

Usage:

CALL PNORM(X, IDIMX, EPS)

Description of parameters:

X	-	Vector of original coefficients, ordered from smallest to largest power. It remains unchanged.
IDIMX	-	Dimension of X. It is replaced by final dimension.
EPS	-	Tolerance below which coefficient is eliminated.

Remarks:

If all coefficients are less than EPS, result is a zero polynomial with IDIMX=0 but vector X remains intact.

Subroutines and function subprograms required:

None.

Method:

Dimension of vector X is reduced by one for each trailing coefficient with an absolute value less than or equal to EPS.

```
      SUBROUTINE PNORM(X,IDIMX,EPS)
      DIMENSION X(1)
    1 IF(IDIMX) 4,4,2
    2 IF(ABS(X(IDIMX))-EPS) 3,3,4
    3 IDIMX=IDIMX-1
      GO TO 1
    4 RETURN
      END
```

APPENDIX A: ALPHABETIC GUIDE TO SUBROUTINES AND SAMPLE PROGRAMS, WITH STORAGE REQUIREMENTS

The following alphabetic index lists the number of characters of storage required by each of the subroutines in the Scientific Subroutine Package. The figures given were obtained by using 1130 Monitor FORTRAN, Version 2, Modification Level 1. Storage requirements are not given for the sample subroutines.

Name	Storage Required (Words)	Page
ABSNT	94	16
ADSAM		179
ANOVA		164
ARRAY	198	86
AUTO	180	46
AVCAL	268	35
AVDAT	326	34
BESI	414	03
BESJ	448	99
BESK	844	104
BESY	704	101
BOOL		145
BOUND	206	14
CADD	92	72
CANOR	1132	30
CCPY	78	82
CCUT	162	79
CEL1	126	105
CEL2	200	106
CHISQ	490	50
CINT	96	74
CORRE	1164	23
CROSS	248	47
CS	310	112
CRST	306	78
CSUM	98	75
CTAB	198	76
CTIE	166	80
DASCR		144
DATA		151 160 173
DCLA	50	84
DCPY	58	83
DISCR	980	39
DMATX	422	38
EIGEN	1058	62
EXPI	262	108
EXPON		175
EXSMO	274	49
FACTO		172
FORIF	292	95
FORIT	284	96
FUN		184
GAMMA	260	97
GAUSS	68	60
GDATA	668	28

Name	Storage Required (Words)	Page	Name	Storage Required (Words)	Page
GMADD	52	64	MULTR	518	26
GMPRD	156	65	NROOT	752	32
GMSUB	52	64	ORDER	206	25
GMTRA	88	65	PADD	110	122
GTPRD	152	66	PADDM	118	122
HIST		145	PCLA	48	122
KRANK	524	56	PCLD	74	125
LEP	132	98	PDER	88	126
LOAD	98	42	PDIV	198	124
LOC	108	86	PILD	56	125
MADD	226	66	PINT	88	126
MATA	194	69	PGCD	108	126
MATIN		145 179 190	PLOT		156
			PMPY	142	123
MCANO		159	PNORM	48	127
MCPY	52	81	POLRG		155
MDISC		168	POLRT	820	120
MEANQ	560	36	PSUB	112	123
MFUN	66	85	PQSD	78	124
MINV	784	61	PVAL	54	124
MOMEN	404	20	PVSUB	132	125
MPRD	230	67	QATR	386	88
MSTR	116	84	QDINT		182
MSUB	226	67	QSF	806	87
MTRA		68	QTEST	232	54
MXOUT		80 91	RADD	90	71

Name	Storage Required (Words)	Page	Name	Storage Required (Words)	Page
RANDU	52	60	SIMQ	540	115
RANK	216	59	SMO	166	48
RCPY	78	82	SMPRT		186
RCUT	162	79	SMPY	56	70
RECP	44	85	SOLN		190
REGRE		150	SRANK	378	55
RINT	94	73	SRMA	108	72
RKGS	1174	92	SSUB	56	70
RKINT		184	SUBMX	134	20
RK1	468	90	SUBST	224	15
RK2	210	91	TAB1	612	16
RSUM	98	74	TAB2	1140	18
RSRT	308	77	TALLY	356	13
RTAB	198	75	TIE	196	59
RTIE	178	80	TPRD	230	68
RTMI	536	117	TRACE	160	41
RTNI	172	119	TTSTT	538	21
RTWI	208	116	TWOAV	324	53
SADD	56	69	UTEST	242	52
SCLA	52	83	VARMX	1186	43
SCMA	110	73	WTEST	498	58
SDIV	66	71	XCPY	128	81
SICI	366	110			

APPENDIX B: ACCURACY OF SUBROUTINES

The subroutines in SSP can be broken down into three major categories from the standpoint of accuracy. They are: subroutines having little or no affect on accuracy; subroutines whose accuracy is dependent on the characteristics of the input data; and subroutines in which definite statements on accuracy can be made.

SUBROUTINES HAVING 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:

TALLY	totals, means, standard deviations, minimums, and maximums
BOUND	selection of observations within bounds
SUBST	subset selection from observation matrix
ABSNT	detection of missing data
TAB1	tabulation of data (1 variable)
TAB2	tabulation of data (2 variables)
SUBMX	build subset matrix
MOMEN	first four moments
TTSTT	tests on population means
ORDER	rearrangement of intercorrelations
AVDAT	data storage allocation
TRACE	cumulative percentage of eigenvalues
CHISQ	χ^2 test for a contingency table
UTEST	Mann-Whitney U-test
TWOAV	Friedman two-way analysis of variance
QTEST	Cochran Q-test
SRANK	Spearman rank correlation
KRANK	Kendall rank correlation
WTEST	Kendall coefficient of concordance
RANK	rank observations
TIE	calculation of ties in ranked observations
RANDU	uniform random numbers
GAUSS	normal random numbers
GMADD	add two general matrices
GMSUB	subtract two general matrices
GMPRD	product of two general matrices
GMTRA	transpose of a general matrix
GTPRD	transpose product of two general matrices
MADD	add two matrices
MSUB	subtract two matrices
MPRD	matrix product (row into column)
MTRA	transpose a matrix
TPRD	transpose a product
MATA	transpose product of matrix by itself
SADD	add scalar to matrix
SSUB	subtract scalar from a matrix
SMPY	matrix multiplied by a scalar
SDIV	matrix divided by a scalar
RADD	add row of one matrix to row of another matrix
CADD	add column of one matrix to column of another matrix
SRMA	scalar multiply row and add to another row
SCMA	scalar multiply column and add to another column
RINT	interchange two rows
CINT	interchange two columns
RSUM	sum the rows of a matrix
CSUM	sum the columns of a matrix
RTAB	tabulate the rows of a matrix
CTAB	tabulate the columns of a matrix
RSRT	sort matrix rows
CSRT	sort matrix columns
RCUT	partition row-wise
CCUT	partition column-wise
RTIE	adjoin two matrices row-wise
CTIE	adjoin two matrices column-wise
MCPY	matrix copy
XCPY	copy submatrix from given matrix
RCPY	copy row of matrix into vector
CCPY	copy column of matrix into vector
DCPY	copy diagonal of matrix into vector
SCLA	matrix clear and add scalar
DCLA	replace diagonal with scalar

MSTR	storage conversion
MFUN	matrix transformation by a function
RECP	reciprocal function for MFUN
LOC	location in compressed-stored matrix
CONVT	single precision, double precision conversion
ARRAY	vector storage--double dimensioned conversion
PADD	add two polynomials
PADDM	multiply polynomial by constant and add to another polynomial
PCLA	replace one polynomial by another
PSUB	subtract one polynomial from another
PMPY	multiply two polynomials
PDIV	divide one polynomial by another
PQSD	quadratic synthetic division of a polynomial
PVAL	value of a polynomial
PVSUB	substitute variable of polynomial by another polynomial
PCLD	complete linear division
PILD	evaluate polynomial and its first derivative
PDER	derivative of a polynomial
PINT	integral of a polynomial
PGCD	greatest common divisor of two polynomials
PNORM	normalize coefficient vector of polynomial

SUBROUTINES WHOSE ACCURACY IS DATA DEPENDENT

The accuracy of the following subroutines cannot be predicted because it is dependent 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 analyses considerations. It cannot be assumed that the results are accurate simply because subroutine execution is completed. Subroutines in this category are:

CORRE	means, standard deviations, and correlations
MULTR	multiple regression and correlation
GDATA	data generation
CANOR	canonical correlation
NROOT	eigenvalues and eigenvectors of a special nonsymmetric matrix
AVCAL	Σ and Δ operation
MEANQ	mean square operation
DMATX	means and dispersion matrix
DISCR	discriminant functions
LOAD	factor loading
VARMX	varimax rotation
AUTO	autocovariances
CROSS	crosscovariances
SMO	application of filter coefficients (weights)
EXSMO	triple exponential smoothing
MINV	matrix inversion
EIGEN	eigenvalues and eigenvectors of a real, symmetric matrix
SIMQ	solution of simultaneous linear, algebraic equations
QSF	integral of tabulated function by Simpson's Rule
QATR	integral of given function by trapezoidal rule
RK1	integral of first-order differential equation by Runge-Kutta method
RK2	tabulated integral of first-order differential equation by Runge-Kutta method
RKGS	solution of a system of first-order differential equations by Runge-Kutta method
FORIF	Fourier analysis of a given function
FORIT	Fourier analysis of a tabulated function
RTWI	refine estimate of root by Wegstein's iteration
RTMI	determine root within a range by Mueller's iteration
RTNI	refine estimate of root by Newton's iteration
POLRT	real and complex roots of polynomial

SUBROUTINES WITH DEFINITE ACCURACY CHARACTERISTICS

This table was developed by comparing floating-point results from the subroutines with the tables given in Abramowitz and Stegun*. In certain cases the reference table gave results in fixed-point form. In these cases the maximum differences below are given in terms of number of decimal places (d.p.) which agreed, rather than number of significant digits (s.d.) which agree. 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	Remarks	Allowable Parameter Range	Range Checked with references*	Maximum Difference s.d.=significant digits d.p.=decimal places
GAMMA	$\Gamma(x)$ (gamma)		$x \leq 34.5$, and x not within 10^{-6} of zero or a negative integer	x = .1 (.1) 3	2 in 6th s.d.
				x = 1 (1) 34	1 in 6th s.d.
LEP	$P_n(x)$ (Legendre)		$-1 \leq x \leq 1$	x = 0 (.2) 1 n = 2, 3	3 in 6th s.d.
			$n \geq 0$	n = 9, 10	1 in 5th s.d.
BESJ	$J_n(x)$ (Bessel)	(The accuracy Factor, D, used in the program was 10^{-5}.)	$x > 0$; $n > 0$	x = 1 (1) 17 n = 0, 1, 2	8 in 6th s.d.
			when $x \leq 15$; $n < 20 + 10x - x^{2/3}$	n = 3 (1) 9 x = 1 (1) n-2	1 in 5th s.d.
			when $x > 15$, $n < 90 + x/2$	n = 3 (1) 9 x = n - 1 (1) 20	1 in 5th d.p.
				x = 1, 2, 5, 10, 50 n = 10 (10) 50**	3 in 6th s.d.
BESY	$Y_n(x)$ (Bessel)		$n \geq 0$ $x > 0$	x = 1 (1) 17 n = 0, 1, 2	9 in 6th s.d.
				n = 3 (1) 9 x = 1 (1) n-2	1 in 5th s.d.
				n = 3 (1) 9 x = n-1 (1) 20	1 in 5th d.p.
				x = 1, 2, 5, 10, 50 n = 10 (10) 50**	3 in 5th s.d.
BESI	$I_n(x)$ (Bessel)	(Table values are $e^{-x}I_n(x)$. maximum difference is for these values)	$x > 0$ $0 \leq n \leq 30$	x = 1 (1) 20 n = 0, 1	8 in 7th s.d.
				x = 5 (1) 20 n = 2	6 in 7th s.d.
				x = 1 (1) 20 n = 3 (1) 9	1 in 5th s.d.
		(Table values are $I_n(x)$)		x = 1, 2, 5, 10 n = 10, 20, 30**	8 in 7th s.d.

Subroutines with Definite Accuracy Characteristics (continued)

Name	Functions	Remarks	Allowable Parameter Range	Range Checked with references*	Maximum Difference s.d.=significant digits d.p.=decimal places
BESK	$K_n(x)$ (Bessel)	(Table values are $e^x K_n(x)$. These were used for maximum differences)	$x > 0$ $n \geq 0$	x = 1 (1) 20 n = 0, 1	8 in 7th s.d.
				x = 5 (1) 20 n = 2	9 in 7th s.d.
				x = 1 (1) 20 n = 3 (1) 9	1 in 5th s.d.
		(Tabled values are $K_n(x)$		x = 1,2,5,10,50 n = 10 (10) 50**	1 in 6th s.d.
CEL1	K (k) (elliptic 1st integral)	(Tabled values are K(m); $m = k^2$	$-1 \leq k \leq 1$	m = 0 (.1) .9	1 in 7th s.d.
CEL2	(Generalized Integral of 2nd kind)	K(m) when A = B = 1	$-1 \leq k \leq 1$	m = 0 (.1) .9	1 in 7th s.d.
		E(m) when A = 1, $B = ck^2$ where $m = k^2$		m = 0 (.1) .9	1 in 7th s.d.
EXPI	Exponential Integral	-Ei (-x) when $X < 0$	$x \geq -4$	x = -.5 (.-5) -2	0 in 7th s.d.
				x = -2.5 (-.5) -4	1 in 7th s.d.***
		$E_1(x)$ when $x > 0$		x = .5 (.5) 2	2 in 7th s.d.
				x = 2.5 (.5) 4	6 in 5th s.d.***
				x = 4.5 (.5) 8	3 in 7th s.d.***
SICI	$s_i(x)$ (sine integral)		none	x = 1 (1) 10 x = 10 π	3 in 7th s.d. 0 in 7th s.d.
SICI	C i (x) (cosine integral)		none	x = 1 (1) 10 x = 10 π	3 in 7th s.d. 0 in 5th s.d.
CS	$C_2(u)$ (Fresnel) $\mu = \frac{1}{2}\pi x^2$		none	x = .1, .3, .6, .8	1 in 6th s.d.
				x = 1 (1) 5	2 in 7th s.d.
CS	$S_2(u)$ (Fresnel) $\mu = \frac{1}{2}\pi x^2$		none	x = .1, .3, .6, .8	1 in 4th s.d.
				x = 1 (1) 5	3 in 7th s.d.

*Handbook of Mathematical Functions, Abramowitz and Stegun, National Bureau of Standards publication.
**Results outside the range of the 1130 are set to zero or machine infinity. Results are subject to compatability of x and n.
***Tabled results, used for maximum difference, were given for $xe^xE_i(-x)$ and $xe^xE_1(x)$

APPENDIX C: TIMING

1. Sample program SOLN was chosen to exemplify the overall timing of a problem. In all cases the 1442 Card Reader, Model 7, is used for input and all necessary subroutines are already on disk. (Core speed: 3.6μs.)
   a. Compile time, using a LIST ALL card (gives a program listing of its 56 cards and a memory map which includes variable allocations, statement allocations, features supported, called subprograms, integer constants, and core requirements), requires 1 minute 32 seconds on the 1132 Printer. (Compile time, minus the LIST ALL card, requires 36 seconds.)
   b. To store the program on disk takes 10 seconds.
   c. After the XEQ control card is read, the computer uses 17 seconds to locate the necessary subprograms and the main program, and to load them in core.
   d. Execution time is four seconds. Output printing time is 53 seconds on an 1132 Printer and 3 minutes 32 seconds on the console typewriter.
2. To illustrate the computational time used by an IBM 1130 computer, the following program was selected:

```
      DIMENSION A(1600),L(40),M(40)
      IX=3
    2 PAUSE 1
      DO 1 I=1,1600
      CALL RANDU (IX,IY,Y)
      IX=IY
    1 A(I)=Y
      PAUSE 2
      CALL MINV (A,10,D,L,M)
      PAUSE 3
      CALL MINV (A,15,D,L,M)
      PAUSE 4
      CALL MINV (A,20,D,L,M)
      PAUSE 5
      CALL MINV (A,30,D,L,M)
      PAUSE 6
      CALL MINV (A,40,D,L,M)
      PAUSE 7
      GO TO 2
      END
```

   a. RANDU - random number generator subroutine. To generate 1600 numbers, using subroutine RANDU, execution time is 5 seconds.
   b. MINV - matrix inversion subroutine. Matrix inversion, using subroutine MINV, is performed on five different sized matrices, with the following results in execution time:

      (1) The 10 x 10 matrix uses 4 seconds.
      (2) The 15 x 15 matrix uses 12 seconds.
      (3) The 20 x 20 matrix uses 27 seconds.
      (4) The 30 x 30 matrix uses 1 minute 28 seconds.
      (5) The 40 x 40 matrix uses 3 minutes 27 seconds.

SAMPLE PROBLEM TIMING

The table below gives sample problem times from the reading of the XEQ card to the printing, on the 1132 Printer, of the last output line:

Problem	Time
DASCR	2 min. 20 sec. (5 min. 30 sec. using the console typewriter)
ADSAM	1 min. 25 sec.
ANOVA	55 sec.
EXPON	1 min. 5 sec.
FACTO	1 min. 55 sec.
MCANO	1 min. 55 sec.
MDISC	2 min. 12 sec.
POLRG	2 min. 53 sec.
QDINT	30 sec.
REGRE	2 min. 25 sec.
RKINT	55 sec.
SMPRT	30 sec.
SOLN	1 min. 15 sec.

APPENDIX D: SAMPLE PROGRAMS

This appendix describes a set of sample programs designed to illustrate typical applications of the scientific subroutines. The sample programs also make use of certain user-written special sample subroutines. Such subroutines are, of course, to be taken only as typical solutions to the problem under consideration, each user being urged to tailor such subroutines to his own specific requirements.

A "Guide to the Sample Programs" immediately follows this introduction. The guide indicates the location of the sample program (if any) calling a particular subroutine of the SSP or referencing a special sample subroutine. The SSP listings are not repeated in this appendix; to locate such listings refer to "Guide to Subroutines" in the introduction.

Listings of the special sample subroutines (HIST, MATIN, PLOT, MXOUT, BOOL, DATA, and FUN) are provided immediately following each sample program. The subroutines DATA, MATIN, and MXOUT are used with several sample programs, and for purposes of clarity the listings of these special user-written routines are repeated with each sample program.

GUIDE TO THE SAMPLE PROGRAMS

SAMPLE PROGRAM DESCRIPTION

The specific requirements for each sample program, including problem description, subroutines, program capacity, input, output, operating instructions, error messages, program modifications, and timing, as well as listings of data inputs and program results, are given in the documentations of the individual sample programs.

There are, however, several significant facts, which apply to all these sample programs.

1. Data input to programs produced by 1130 FORTRAN is required to be right justified within a field, even if the data includes decimal points. Only leading blanks are permitted.

2. All sample programs as distributed will run on an 8K Model IIB with 1132 Printer and 1442 Card Read Punch, Model 6 or 7. If the user has different

card I/O devices, he must change the *IOCS card and the first READ instruction of each sample program to conform to his configuration.

3. All of the output format statements in the sample main programs and the sample subroutines specify the console typewriter as the output device. However, the logical unit numbers for input and output are optional. The first card of the sample problem data deck defines the input/output units for a specific run, and is read from the principal card reader by the sample main program. Format for this card is as follows:

Column 2 contains the logical unit number for output

Column 4 contains the logical unit number for input

4. The IOCS card, included with each sample main program, specifies three devices (CARD, TYPEWRITER, 1132 PRINTER). The user should include only those I/O devices employed by the program, thus eliminating any unnecessary Monitor subroutines.

5. Since core storage for the IBM 1130 Model II B computer is 8K, only a limited number of the sample programs have ample storage area for increases in dimension statements. The majority of the programs are now dimensioned so near maximum storage size that any increases in the dimension would create system overlays (SOCAL's) or would necessitate the use of a LOCAL overlay area.

6. For each sample program given below, there is a schematic diagram showing deck setup. This schematic gives a general description of deck requirements. Specific details pertaining to three different situations should be understood. To follow the discussion of the three cases for all sample programs, consider Figure 10.

a. Initial run of a sample program under the disk monitor system: All required monitor control cards are distributed with decks. If the deck setup given in Figure 10 is used, the final card of the routine DASCR, the //XEQ card (which is a monitor control card), should be taken out of the routine DASCR and placed after the *STORE card which has stored the routine LOC on the disk. With this change, DASCR will be compiled, stored on disk (with all of its required routines), and then will execute. After this initial run is complete, the second case can be considered (b, below).

b. After the initial run of a sample program under the disk monitor system, following runs can be made by using only the //XEQ card and any required *LOCAL cards, followed by data. This case assumes that all routines are on the disk.

c. Running sample programs under Card FORTRAN (1130-FO-001) (non-disk system): All monitor control cards (see the Application Directory) must now be removed from decks. Using Figure 10, consider that the labeled decks refer to object programs which were previously compiled using Card FORTRAN (C26-3629). With this consideration, noting the binary loaders and library required as stated under "Object Deck Loading Procedures" in the 1130 Card/Paper Tape Programming System Operator's Guide, and with decks in Figure 10 order, DASCR will run.

NOTE: Remarks in (a) above about changes in placement of //XEQ cards pertain also to any required *LOCAL cards, which must succeed the //XEQ cards.

A fourth situation may also be considered. If the user has all subroutines stored on the disk, and none of the sample problems are on the disk, then any individual sample problem will run as it was distributed in card form.

A LOCAL card, following the XEQ Monitor control card, allows the user to designate all subroutines to be loaded into a LOCAL overlay area on call at execution time. For the function of SOCAL and the use of LOCAL, the reader is referred to IBM 1130 Disk Monitor System, Version 2, Programming and Operator's Guide (C26-3717). The sample programs employ the LOCAL facility.

DATA SCREENING

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, DASCR, and six subroutines:

SUBST, TAB1, LOC } are from the Scientific Subroutine Package

MATIN	is a sample input routine
HIST	is a sample program for plotting a histogram
BOOL	refer to subroutine SUBST

Capacity

The maximum size of matrix of observations has been set at 1000 elements, the number of observations at 200, and the number of conditions at 21. Therefore, if a problem satisfies the above conditions, no modification to the sample program is necessary. However, if the maximum sizes must be increased, the dimension statements in the sample main program must be modified to handle this particular problem. The general rules for program modification are described later.

Input

One I/O Specification card defines input/output units (see "Sample Program Descriptions".)

A parameter card with the following format must precede each matrix of observations:

Columns	Contents	For Sample Problem
1 - 2	Blank	
3 - 6	Up to four digit identification code (numeric only)	0001
7 - 10	Number of observations	0100
11 - 14	Number of variables	0004

Matrix of Observations

Each matrix of observations must be followed by a card with a 9 punch in column 1.

The condition matrix and bounds data are preceded by a parameter card containing the number of conditions and the variable to be selected for analysis:

Columns	Contents	For Sample Problem
1 - 2	Number of conditions	02
3 - 4	Variable to be selected	03

UBO Vector

A card with an asterisk in column 1 must follow the UBO vector. A blank card after the last set of input data terminates the run.

Data Cards

1. The observation matrix: Data cards have seven fields of ten columns each, starting in column one. The decimal point may appear anywhere in a field or may be omitted, if the number is an integer. However, all numbers must be right justified even if the decimal point is punched. 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 the next card.
2. The condition matrix (see description in the subroutine SUBST): Each ten-column field contains a condition to be satisfied. The first two columns contain the variable number (right justified), the third column the relational code, and the last seven columns of each field a floating-point number. There may be as many as seven conditions per card and a total of three cards or 21 conditions.
3. The UBO vector (see description in the subroutine TAB1): The UBO vector is punched in three fields of ten columns each as a floating-point number.

Deck Setup

The deck setup is shown in Figure 10.

Sample

A listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The output consists of the subset vector showing which observations are rejected (zero) and accepted (nonzero), summary statistics for the selected variable, and a histogram of frequencies versus intervals for that variable.

Sample

The output listing for the sample problem is shown in Figure 11.

Program Modification

Noting that storage problems may result, as previously discussed in "Sample Program Description", program capacity can be increased or decreased by making changes to the DIMENSION statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statement of the main program, DASCR.
   a. The dimension of array A must be greater than or equal to the number of elements in the observation matrix. For the sample problems the value is 400.

b. The dimension of array C must be greater than or equal to the number of conditions, c times 3. For the sample problem this product is 6 = 2 x 3.

c. The dimension of array S must be greater than or equal to the number of observations, m. Since there are 100 observations in the sample problem the value of m is 100.

d. The dimension of array R must be greater than or equal to the number of conditions, c. For the sample problem the value of c is 2.

e. The dimensions of array FREQ and PCT must be greater than or equal to the number of intervals for the selected variable. For the sample problem this value is 20.

2. Insert the dimension size for A in the third argument of the CALL MATIN statement (following statement 24).

3. Subroutine BOOL can be replaced if the user wishes to use a different boolean expression (see description in subroutine SUBST). The boolean expression provided in the sample program is for both conditions to be satisfied:

T = R (1) * R (2)

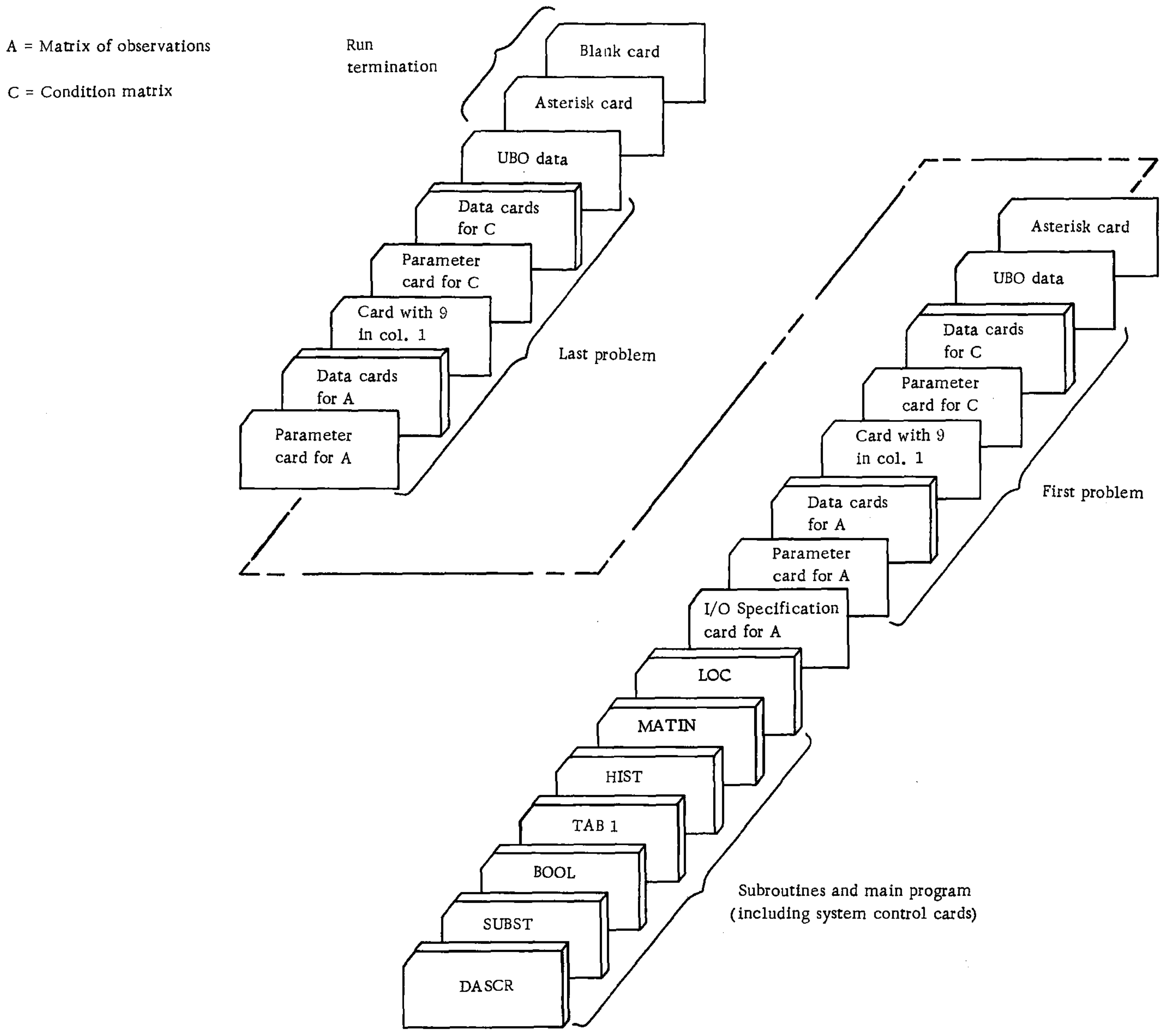


Figure 10. Deck setup (data screening)

```
DATA SCREENING PROBLEM  1      48  1.
                               49  1.
SUBSET VECTOR                  50  1.
                               51  0.0
                               52  1.
                               53  1.
 1  1.                         54  1.
 2  0.0                        55  1.
 3  1.                         56  1.
 4  1.                         57  1.
 5  1.                         58  1.
 6  1.                         59  1.
 7  1.                         60  1.
 8  1.                         61  1.
 9  1.                         62  1.
10  1.                         63  1.
11  1.                         64  1.
12  0.0                        65  1.
13  1.                         66  1.
14  1.                         67  1.
15  0.0                        68  1.
16  1.                         69  1.
17  1.                         70  1.
18  1.                         71  1.
19  1.                         72  1.
20  1.                         73  1.
21  1.                         74  1.
22  1.                         75  1.
23  1.                         76  1.
24  1.                         77  1.
25  0.0                        78  0.0
26  1.                         79  1.
27  1.                         80  1.
28  1.                         81  1.
29  1.                         82  1.
30  1.                         83  1.
31  1.                         84  1.
32  1.                         85  1.
33  1.                         86  1.
34  0.0                        87  0.0
35  1.                         88  0.0
36  1.                         89  1.
37  1.                         90  1.
38  1.                         91  1.
39  1.                         92  1.
40  1.                         93  1.
41  0.0                        94  1.
42  1.                         95  1.
43  1.                         96  1.
44  1.                         97  1.
45  1.                         98  1.
46  1.                         99  1.
47  1.                        100  1.


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
 ------------------------------------------------------------------------------------------
   23                                      *
   22                                      *
   21                                      *
   20                                      *
   19                                      *
   18                                      *
   17                                      *
   16                                      *
   15                                      *
   14                                      *   *
   13                                      *   *
   12                                      *   *
   11                                      *   *
   10                                  *   *   *
    9                                  *   *   *
    8                                  *   *   *   *
    7                                  *   *   *   *
    6                                  *   *   *   *
    5                                  *   *   *   *
    4                          *   *   *   *   *   *   *
    3                      *   *   *   *   *   *   *   *   *                           *
    2          *   *       *   *   *   *   *   *   *   *   *   *       *               *
    1      *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *
 ------------------------------------------------------------------------------------------

INTERVAL       1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
CLASS

END OF CASE
```

Figure 11. Output listing

Operating Instructions

The sample program for data screening is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix: DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX. GO ON TO NEXT CASE.
2. Number of data cards does not correspond to that required by parameter card: INCORRECT NUMBER OF DATA CARDS FOR MATRIX. EXECUTION TERMINATED.

Error condition 1 allows the computer run to continue. Error condition 2, however, terminates execution and requires another run to process succeeding cases.

Sample Main Program for Data Screening - DASCR

Purpose:

Perform data screening calculations on a set of observations.

Remarks:

I/O specifications transmitted to subroutines by COMMON.

Input Card:

Column 2 MX - Logical unit number for output.

Column 4 MY - Logical unit number for input.

Subroutines and function subprograms required:

SUBST
TAB1
LOC
BOOL
HIST
MATIN

Method:

Derive a subset of observations satisfying certain conditions on the variables. For this subset, the frequency of a selected variable over given class intervals is obtained. This is plotted in the form of a histogram. Total, average, standard deviation, minimum, and maximum are also calculated.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR DATA SCREENING - DASCR
      EXTERNAL BOOL
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        MAXIMUM NUMBER OF ELEMENTS OF THE OBSERVATION MATRIX.
      DIMENSION A(1000)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF CONDITIONS TIMES 3.
      DIMENSION C(63)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 3.
      DIMENSION UBO(3)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF OBSERVATIONS.
      DIMENSION S(200)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF CONDITIONS.
      DIMENSION R(21)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF INTERVALS FOR THE SELECTED VARIABLE.
      DIMENSION FREQ(20),PCT(20)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 5.
      DIMENSION STATS(5)
      COMMON MX,MY
   10 FORMAT(////23H DATA SCREENING PROBLEM,I3)
   11 FORMAT(//45H DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)
   12 FORMAT(//21H EXECUTION TERMINATED)
   13 FORMAT(//43H INCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)
   14 FORMAT(//19H GO ON TO NEXT CASE)
   15 FORMAT(//12H END OF CASE)
   16 FORMAT(7(F2.0,F1.0,F7.0))
   17 FORMAT(3F10.0)
   18 FORMAT(//14H SUBSET VECTOR,///)
   19 FORMAT(I6,F5.0)
   20 FORMAT(////33H SUMMARY STATISTICS FOR VARIABLE ,I3)
   21 FORMAT(//8H TOTAL =,F10.3,2X,9HAVERAGE =,F10.3,2X,20HSTANDARD DEVI
     1ATION =,F10.3,2X,9HMINIMUM =,F10.3,2X,9HMAXIMUM =,F10.3)
   22 FORMAT(2I2)
      KC=0
C        READ I/O UNIT NUMBERS
      READ(2,22)MX,MY
   24 KC=KC+1
      CALL MATIN(ICOD,A,1000,NO,NV,MS,IER)
      IF(NO) 25,50,25
   25 IF(IER-1) 40,30,35
   30 WRITE(MX,11) ICOD
      WRITE(MX,14)
      GO TO 24
   35 WRITE(MX,13)
      WRITE(MX,12)
      GO  TO 60
   40 READ(MY,22)NC,NOVAR
      JC=NC*3
      READ(MY,16)(C(I),I=1,JC)
      READ(MY,17)(UBO(I),I=1,3)
      CALL SUBST(A,C,R,BOOL,S,NO,NV,NC)
      WRITE(MX,10)KC
      WRITE(MX,18)
      DO 50 I=1,NO
   50 WRITE(MX,19)I,S(I)
      CALL TAB1(A,S,NOVAR,UBO,FREQ,PCT,STATS,NO,NV)
      WRITE(MX,20) NOVAR
      WRITE(MX,21)(STATS(I),I=1,5)
      JZ=UBO(2)
      CALL HIST(KC,FREQ,JZ)
      WRITE(MX,15)
      GO TO 24
   60 STOP
      END
// DUP
*STORE      WS  UA  DASCR
// XEQ DASCR
```

```
1 2
 000101000004
       46         64        173        12
       24         72        170         8
       32         71        154        16
       41         68        129        10
       50         65        192         9
       63         75        203        12
       29         70        122        14
       28         64        136        13
       52         77        147        11
       36         67        153        18
       31         68        165         9
       72         70        178        10
       53         71        205        14
       21         65        219        12
       49         63        150         6
       28         62        160        16
       53         72        161        13
       47         73        142        15
       37         67        193        18
       64         68        156        14
       65         60        114        10
       62         64        153        12
       19         68        225         9
       46         67        158        11
       33         72        121         4
       37         65        132        13
       41         76        148        16
       52         71        123        16
       29         68        128        14
       32         65        155        17
       24         72        172        16
       56         73        163        10
       63         65        158        11
       67         69        146         2
       58         66        171         9
       41         65        153        12
       49         66        165        14
       52         72        172        16
       23         78        183        15
       56         71        195        16
       52         68        118         7
       40         66        165        14
       39         68        215        16
       23         71        154        12
       56         65        149        10
       25         65        162        16
       37         68        152        16
       46         70        159        15
       41         69        137        14
```

```
      62        71        163       12                                 52
      29        72        191        4                                 53
      19        68        168       10                                 54
      46        63        158       16                                 55
      37        64        139       18                                 56
      34        68        156       10                                 57
      64        67        153       12                                 58
      57        67        141       13                                 59
      32        68        157       17                                 60
      29        70        183       15                                 61
      53        72        164       18                                 62
      47        72        156       18                                 63
      56        73        160       16                                 64
      61        74        169       12                                 65
      21        68        161       10                                 66
      25        76        178       11                                 67
      23        72        157       16                                 68
      29        68        186       16                                 69
      39        70        159       14                                 70
      42        70        154       10                                 71
      56        62        159       12                                 72
      63        70        177       12                                 73
      51        71        161        9                                 74
      41        66        158       10                                 75
      33        69        158       16                                 76
      37        68        157       16                                 77
      25        70        163       15                                 78
      63        68        159       12                                 79
      53        71        202        6                                 80
      51        72        167       14                                 81
      47        73        164       14                                 82
      39        75        151       12                                 83
      28        68        166       10                                 84
      64        69        156       16                                 85
      55        67        144       16                                 86
      51        66        177       10                                 87
      46        65        157       12                                 88
      72        66        125       10                                 89
      66        65        131       12                                 90
      28        74        149       18                                 91
      27        71        168       11                                 92
      23        72        158       12                                 93
      23        72        163       12                                 94
      60        68        157        9                                 95
      30        66        142       10                                 96
      39        67        162       16                                 97
      46        74        154       16                                 98
      50        68        158       10                                 99
      61        66        161       14                                100
      36        64        157       15                                101
      32        71        156       16                                102
9                                                                     103
0203                                                                  104
 12       65 46       8                                               105
         120         20       210                                     106
*                                                                     107
                                                                      108
```

USER-SUPPLIED SPECIAL SUBROUTINE - BOOL

THIS SPECIAL SUBROUTINE ILLUSTRATES AN EXTERNAL SUBROUTINE CALLED BY SUBROUTINE SUBST.

IF DIFFERENT PROPOSITIONS ARE USED FOR DIFFERENT PROBLEMS IN THE SAME RUN, DIFFERENT SUBROUTINES WITH APPROPRIATE PROPOSITIONS MUST BE COMPILED UNDER DIFFERENT NAMES. IF SO, THESE SUBROUTINE NAMES MUST BE DEFINED BY AN EXTERNAL STATEMENT APPEARING IN THE MAIN PROGRAM WHICH CALLS SUBST. THEN, FOR EACH PROBLEM, SUBST IS CALLED WITH A PROPER SUBROUTINE NAME IN ITS ARGUMENT LIST.

```
      SUBROUTINE BOOL(R,T)                                              BOOL   1
      DIMENSION R(1)                                                    BOOL   2
      L1=1                                                              BOOL M01
      L2=2                                                              BOOL M02
      T=R(L1)*R(L2)                                                     BOOL M03
      RETURN                                                            BOOL   4
      END                                                               BOOL   5
```

SUBROUTINE HIST

PURPOSE
   PRINT A HISTOGRAM OF FREQUENCIES VERSUS INTERVALS

USAGE
   CALL HIST(NU,FREQ,IN)

DESCRIPTION OF PARAMETERS

```
   NU   - HISTOGRAM NUMBER (3 DIGITS MAXIMUM)
   FREQ - VECTOR OF FREQUENCIES
   IN   - NUMBER OF INTERVALS AND LENGTH OF FREQ (MAX IS 20)
          NORMALLY, FREQ(1) CONTAINS THE FREQUENCY SMALLER THAN
          THE LOWER BOUND AND FREQ(IN) CONTAINS THE FREQUENCY
          LARGER THAN THE UPPER BOUND
```

REMARKS
   FREQUENCIES MUST BE POSITIVE NUMBERS

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   NONE

METHOD
   THE LARGEST FREQUENCY IS DETERMINED AND SCALING IS USED
   IF REQUIRED

```
      SUBROUTINE HIST(NU,FREQ,IN)                                       HIST   1
      DIMENSION JOUT(20),FREQ(20)                                       HIST   2
      COMMON MX,MY                                                      HIST   3
    1 FORMAT(6H EACH ,A1,8H EQUALS ,I2,7H POINTS,/)                     HIST   4
    2 FORMAT(I6,4X,20(4X,A1))                                           HIST   5
    3 FORMAT(//9H INTERVAL,4X,19(I2,3X),I2)                             HIST   6
    4 FORMAT(///,47X,11H HISTOGRAM ,I3)                                 HIST   7
    5 FORMAT(//10H FREQUENCY,20I5)                                      HIST   8
    6 FORMAT(6H CLASS)                                                  HIST   9
    7 FORMAT(113H     --------------------------------------------------HIST  10
     1------------------------------------------------------------)     HIST  11
    8 FORMAT(2A1)                                                       HIST  12
      READ(MY,8) K,NOTH                                                 HIST  13
C        PRINT TITLE AND FREQUENCY VECTOR                               HIST  14
      WRITE(MX,4) NU                                                    HIST  15
      DO 12 I=1,IN                                                      HIST  16
   12 JOUT(I)=FREQ(I)                                                   HIST  17
      WRITE(MX,5)(JOUT(I),I=1,IN)                                       HIST  18
      WRITE(MX,7)                                                       HIST  19
C        FIND LARGEST FREQUENCY                                         HIST  20
      FMAX=0.0                                                          HIST  21
      DO 20 I=1,IN                                                      HIST  22
      IF(FREQ(I)-FMAX) 20,20,15                                         HIST  23
   15 FMAX=FREQ(I)                                                      HIST  24
   20 CONTINUE                                                          HIST  25
C        SCALE IF NECESSARY                                             HIST  26
      JSCAL=1                                                           HIST  27
      IF(FMAX-50.0) 40,40,30                                            HIST  28
   30 JSCAL=(FMAX+49.0)/50.0                                            HIST  29
      WRITE(MX,1)K,JSCAL                                                HIST  30
C        CLEAR OUTPUT AREA TO BLANKS                                    HIST  31
   40 DO 50 I=1,IN                                                      HIST  32
   50 JOUT(I)=NOTH                                                      HIST  33
C        LOCATE FREQUENCIES IN EACH INTERVAL                            HIST  34
      MAX=FMAX/FLOAT(JSCAL)                                             HIST  35
      DO 80 I=1,MAX                                                     HIST  36
      X=MAX-(I-1)                                                       HIST  37
      DO 70 J=1,IN                                                      HIST  38
      IF(FREQ(J)/FLOAT(JSCAL)-X) 70,60,60                               HIST  39
   60 JOUT(J)=K                                                         HIST  40
   70 CONTINUE                                                          HIST  41
      IX=X*FLOAT(JSCAL)                                                 HIST  42
C        PRINT LINE OF FREQUENCIES                                      HIST  43
   80 WRITE(MX,2)IX,(JOUT(J),J=1,IN)                                    HIST  44
C        GENERATE CONSTANTS                                             HIST  45
      DO 90 I=1,IN                                                      HIST  46
   90 JOUT(I)=I                                                         HIST  47
C        PRINT INTERVAL NUMBERS                                         HIST  48
      WRITE(MX,7)                                                       HIST  49
      WRITE(MX,3)(JOUT(J),J=1,IN)                                       HIST  50
      WRITE(MX,6)                                                       HIST  51
      RETURN                                                            HIST  52
      END                                                               HIST  53
```

SUBROUTINE MATIN

PURPOSE
   READS CONTROL CARD AND MATRIX DATA ELEMENTS FROM LOGICAL
   UNIT 5

USAGE
   CALL MATIN(ICODE,A,ISIZE,IROW,ICOL,IS,IER)

DESCRIPTION OF PARAMETERS

```
   ICODE-UPON RETURN, ICODE WILL CONTAIN FOUR DIGIT
          IDENTIFICATION CODE FROM MATRIX PARAMETER CARD
   A    -DATA AREA FOR INPUT MATRIX
   ISIZE-NUMBER OF ELEMENTS DIMENSIONED BY USER FOR AREA A
   IROW -UPON RETURN, IROW WILL CONTAIN ROW DIMENSION FROM
         MATRIX PARAMETER CARD
   ICOL -UPON RETURN, ICOL WILL CONTAIN COLUMN DIMENSION FROM
         MATRIX PARAMETER CARD
   IS   -UPON RETURN, IS WILL CONTAIN STORAGE MODE CODE FROM
         MATRIX PARAMETER CARD WHERE
         IS=0 GENERAL MATRIX
         IS=1 SYMMETRIC MATRIX
         IS=2 DIAGONAL MATRIX
   IER  -UPON RETURN, IER WILL CONTAIN AN ERROR CODE WHERE
         IER=0    NO ERROR
         IER=1    ISIZE IS LESS THAN NUMBER OF ELEMENTS IN
                  INPUT MATRIX
         IER=2    INCORRECT NUMBER OF DATA CARDS
```

REMARKS
   NONE

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   LOC

METHOD

```
   SUBROUTINE ASSUMES THAT INPUT MATRIX CONSISTS OF PARAMETER
   CARD FOLLOWED BY DATA CARDS
   PARAMETER CARD HAS THE FOLLOWING FORMAT
      COL. 1- 2 BLANK
      COL. 3- 6 UP TO FOUR DIGIT IDENTIFICATION CODE
      COL. 7-10 NUMBER OF ROWS IN MATRIX
      COL.11-14 NUMBER OF COLUMNS IN MATRIX
      COL.15-16 STORAGE MODE OF MATRIX WHERE
           0 - GENERAL MATRIX
           1 - SYMMETRIC MATRIX
           2 - DIAGONAL MATRIX
   DATA CARDS ARE ASSUMED TO HAVE SEVEN FIELDS OF TEN COLUMNS
   EACH.  DECIMAL POINT MAY APPEAR ANYWHERE IN A FIELD.  IF NO
   DECIMAL POINT IS INCLUDED, IT IS ASSUMED THAT THE DECIMAL
   POINT IS AT THE END OF THE 10 COLUMN FIELD. NUMBER IN EACH
   FIELD MAY BE PRECEDED BY BLANKS.  DATA ELEMENTS MUST BE
   PUNCHED BY ROW.  A ROW MAY CONTINUE FROM CARD TO CARD.
   HOWEVER EACH NEW ROW MUST START IN THE FIRST FIELD OF THE
   NEXT CARD.  ONLY THE UPPER TRIANGULAR PORTION OF A SYMMETRIC
   OR THE DIAGONAL ELEMENTS OF A DIAGONAL MATRIX ARE CONTAINED
   ON DATA CARDS.  THE FIRST ELEMENT OF EACH NEW ROW WILL BE
   THE DIAGONAL ELEMENT FOR A MATRIX WITH  SYMMETRIC OR
   DIAGONAL STORAGE MODE. COLUMNS 71-80 OF DATA CARDS MAY BE
   USED FOR IDENTIFICATION, SEQUENCE NUMBERING, ETC..
   THE LAST DATA CARD FOR ANY MATRIX MUST BE FOLLOWED BY A CARD
   WITH A 9 PUNCH IN COLUMN 1.
```

```
      SUBROUTINE MATIN(ICODE,   A,ISIZE,IROW,ICOL,IS,IER)               MATIN  1
      DIMENSION A(1)                                                    MATIN  2
      DIMENSION CARD(8)                                                 MATIN  3
      COMMON MX,MY                                                      MATIN  4
    1 FORMAT(7F10.0)                                                    MATIN  5
    2 FORMAT(I6,2I4,I2)                                                 MATIN  6
    3 FORMAT(I1)                                                        MATIN  7
      IDC=7                                                             MATIN  8
      IER=0                                                             MATIN  9
      READ( MY,2)ICODE,IROW,ICOL,IS                                     MATIN 10
      CALL LOC(IROW,ICOL,ICNT,IROW,ICOL,IS)                             MATIN 11
      IF(ISIZE-ICNT)6,7,7                                               MATIN 12
    6 IER=1                                                             MATIN 13
    7 IF (ICNT)38,38,8                                                  MATIN 14
    8 ICOLT=ICOL                                                        MATIN 15
      IROCR=1                                                           MATIN 16
C        COMPUTE NUMBER OF CARDS FOR THIS ROW                           MATIN 17
   11 IRCDS=(ICOLT-1)/IDC+1                                             MATIN 18
      IF(IS-1)15,15,12                                                  MATIN 19
   12 IRCDS=1                                                           MATIN 20
C        SET UP LOOP FOR NUMBER OF CARDS IN ROW                         MATIN 21
   15 DO 31 K=1,IRCDS                                                   MATIN 22
      READ(MY,1)(CARD(I),I=1,IDC)                                       MATIN 23
C        SKIP THROUGH DATA CARDS IF INPUT AREA TOO SMALL                MATIN 24
      IF(IER)16,16,31                                                   MATIN 25
   16 L=0                                                               MATIN 26
C        COMPUTE COLUMN NUMBER FOR FIRST FIELD IN CURRENT CARD          MATIN 27
      JS=(K-1)*IDC+ICOL-ICOLT+1                                         MATIN 28
      JE=JS+IOC-1                                                        MATIN 29
      IF(IS-1)19,19,17                                                   MATIN 30
   17 JE=JS                                                              MATIN 31
C        SET UP LOOP FOR DATA ELEMENTS  WITHIN CARD                      MATIN 32
   19 DO 30 J=JS,JE                                                      MATIN 33
      IF(J-ICOL)20,20,31                                                 MATIN 34
   20 CALL LOC(IROCR ,J,IJ,IROW,ICOL,IS)                                 MATIN 35
      L=L+1                                                              MATIN 36
   30 A(IJ)=CARD(L)                                                      MATIN 37
   31 CONTINUE                                                           MATIN 38
      IROCR=IROCR+1                                                      MATIN 39
      IF(IROW-IROCR) 38,35,35                                            MATIN 40
   35 IF(IS-1)37,36,36                                                   MATIN 41
   36 ICOLT=ICOLT-1                                                      MATIN 42
   37 GO TO 11                                                           MATIN 43
   38 READ(MY,3)ICARD                                                    MATIN 44
      IF(ICARD-9)39,40, 39                                               MATIN 45
   39 IER=2                                                              MATIN 46
   40 RETURN                                                             MATIN 47
      END                                                                MATIN 48
```

MULTIPLE LINEAR REGRESSION

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 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 second, third, and fifth variables are used to predict the dependent variable in the second analysis.

Table 2. 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 sample program consists of a main routine, REGRE, and five subroutines:

CORRE ORDER MINV MULTR	are from the Scientific Subroutine Package
DATA	is a special input subroutine

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 21 variables, including both independent and dependent variables.
2. Up to 99,999 observations, if observations are read into the computer one at a time by the special input subroutine named DATA. If all data are to be stored in core prior to the calculation of correlation coefficients, the limitation on the number of observations depends on the size of core storage available for input data.
3. (12F6.0) format for input data cards.

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 22 variables, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

One I/O Specification card defines input/output units (see "Sample Program Descriptions").

One control card is required for each problem and is read by the main program, REGRE. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE

Columns	Contents	For Sample Problem
7 - 11	Number of observations	00030
12 - 13	Number of variables	06
14 - 15	Number of selection cards (see below)	02

Leading zeros are not required to be keypunched, but all numbers must be right-justified, even if a decimal point is included.

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 (12F6.0). 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.

Selection Card

The selection card is used to specify a dependent variable and a set of independent variables in a multiple linear 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.

The selection card is prepared as follows:

Columns	Contents	For Sample Problem Selection 1	For Sample Problem Selection 2
1 - 2	Option code for table of residuals 00 if it is not desired 01 if it 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	05	03
5 - 6 (cont)	(the subscript numbers of individual variables are specified below)		
7 - 8	1st independent variable included	01	02
9 - 10	2nd independent variable included	02	03
11 - 12	3rd independent variable included	03	05
13 - 14	4th independent variable included	04	
15 - 16	5th independent variable included	05	
etc.			

The input format of (36I2) is used for the selection card.

Deck Setup

Deck setup is shown in Figure 12.

The repetition of the data cards following a selection card is dependent upon the option code for the table of residuals. If the table is required (option 01), the data must be repeated; if the table is not required (option 00), card G immediately follows card E.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The output of the sample program for multiple linear regression includes:

1. Means
2. Standard deviations
3. Correlation coefficients between the independent variables and the dependent variable
4. Regression coefficients
5. Standard errors of regression coefficients
6. Computed t-values
7. Intercept
8. Multiple correlation coefficients

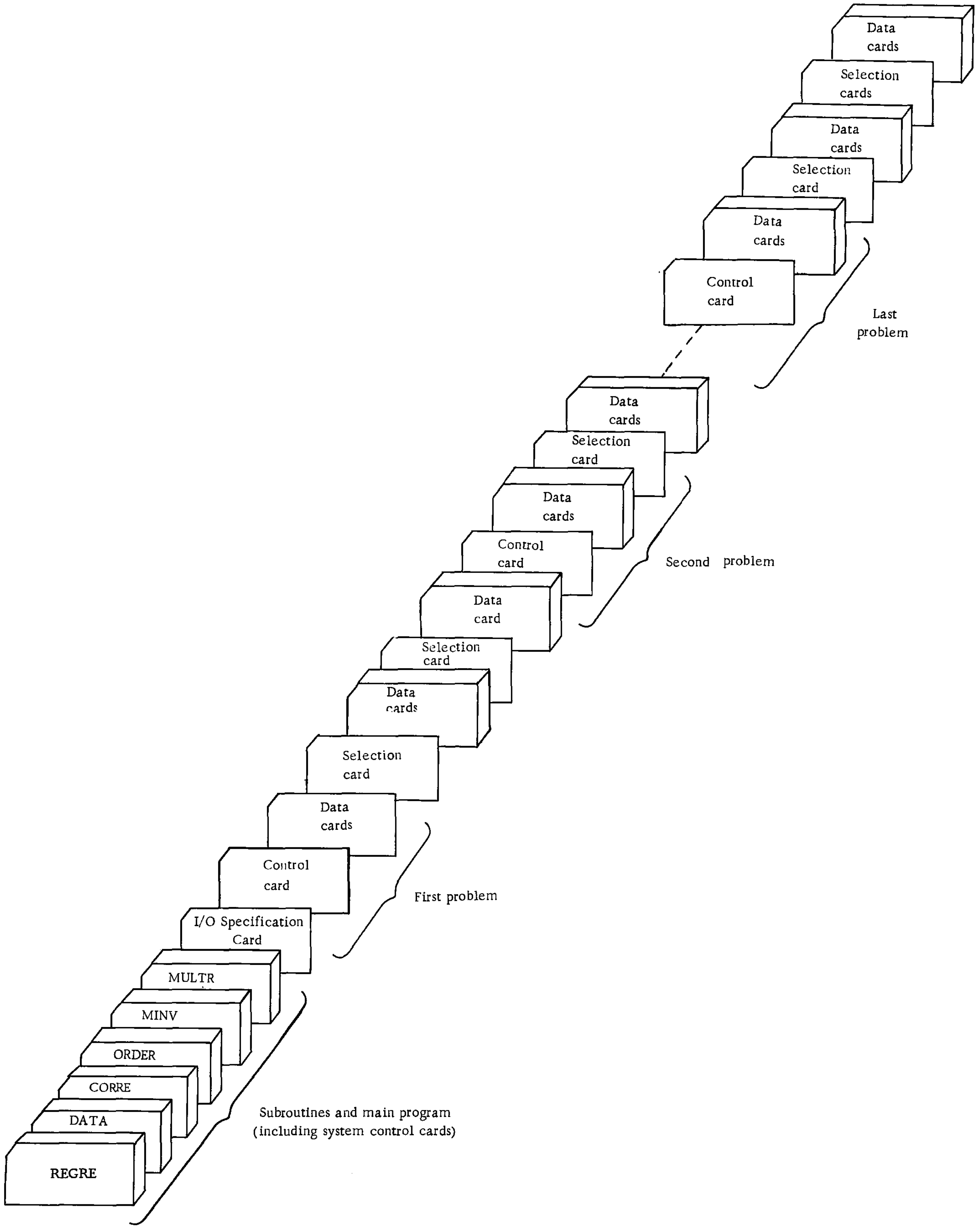


Figure 12. Deck setup (multiple linear regression)

9. Standard error of estimate
10. Analysis of variance for the multiple regression
11. Table of residuals (optional)

Sample

The output listing for the sample problem is shown in Figure 13.

<u>Program Modification</u>

Noting that storage problems may result, as previously discussed in "Sample Program Description", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, REGRE:
   a. The dimension of arrays XBAR, STD, D, RY, ISAVE, B, SB, T, and W must be greater than or equal to the number of variables, m. Since there are six variables in the sample problem the value of m is 6.
   b. The dimension of array RX must be greater than or equal to the product of m x m. For the sample problem this product is 36 = 6 x 6.
   c. The dimension of array R must be greater than or equal to (m + 1) m/2. For the sample problem this number is 21 = (6 + 1) 6/2.

```
MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 1


VARIABLE      MEAN        STANDARD      CORRELATION    REGRESSION    STD. ERROR     COMPUTED
  NO.                     DEVIATION       X VS Y       COEFFICIENT   OF REG.COEF.   T VALUE

   1       43.13333       6.52175        0.28422        0.01242       0.03634       0.34172

   2      316.16668     114.42994        0.42189        0.00738       0.00186       3.96545

   3      241.80001      36.43074        0.11900        0.01504       0.00634       2.36882

   4      105.66667      17.65638        0.37822        0.00150       0.03678       0.04101

   5       34.13333      15.97569        0.39412        0.04918       0.04141       1.18782

DEPENDENT

   6        2.26666       1.41258


INTERCEPT                    -6.07935

MULTIPLE CORRELATION          0.73575

STD. ERROR OF ESTIMATE        1.05161


                    ANALYSIS OF VARIANCE FOR THE REGRESSION

    SOURCE OF VARIATION         DEGREES      SUM OF          MEAN              F VALUE
                               OF FREEDOM    SQUARES         SQUARES

ATTRIBUTABLE TO REGRESSION         5        31.32517        6.26503           5.66512
DEVIATION FROM REGRESSION         24        26.54149        1.10589

    TOTAL                         29        57.86666


MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 1


               TABLE OF RESIDUALS

CASE NO.      Y VALUE     Y ESTIMATE     RESIDUAL
    1         1.00000      0.48089        0.51910
    2         2.00000      1.77669        0.22330
    3         2.00000      2.14585       -0.14585
    4         0.00000      0.82879       -0.82879
    5         2.00000      1.90522        0.09477
    6         2.00000      1.52124        0.47875
    7         3.00000      3.46447       -0.46447
    8         2.00000      2.25886       -0.25886
    9         3.00000      3.80259       -0.80259
   10         0.00000      1.02042       -1.02042
   11         4.00000      2.49735        1.50264
   12         1.00000      2.00065       -1.00065
   13         1.00000      2.00735       -1.00735
   14         1.00000      1.15307       -0.15307
   15         3.00000      2.90445        0.09554
   16         2.00000      1.83531        0.16468
   17         3.00000      2.56004        0.43995
   18         4.00000      3.45229        0.54770
   19         4.00000      3.62661        0.37338
   20         3.00000      2.68067        0.31932
   21         4.00000      3.64886        0.35113
   22         4.00000      1.86541        2.13458
   23         1.00000      2.09862       -1.09862
   24         0.00000      1.97217       -1.97217
   25         4.00000      1.41253        2.58746
   26         1.00000      1.88026       -0.88026
   27         3.00000      2.27646        0.72353
   28         4.00000      4.51080       -0.51080
   29         4.00000      3.95746        0.04253
   30         0.00000      0.45457       -0.45457


MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 2


VARIABLE      MEAN        STANDARD      CORRELATION    REGRESSION    STD. ERROR     COMPUTED
  NO.                     DEVIATION       X VS Y       COEFFICIENT   OF REG.COEF.   T VALUE

   2      316.16668     114.42994        0.42189        0.00743       0.00172       4.31764

   3      241.80001      36.43074        0.11900        0.01497       0.00551       2.71693

   5       34.13333      15.97569        0.39412        0.05362       0.01258       4.26263

DEPENDENT


   6        2.26666       1.41258


INTERCEPT                    -5.53530

MULTIPLE CORRELATION          0.73423

STD. ERROR OF ESTIMATE        1.01281


                    ANALYSIS OF VARIANCE FOR THE REGRESSION

    SOURCE OF VARIATION         DEGREES      SUM OF          MEAN              F VALUE
                               OF FREEDOM    SQUARES         SQUARES

ATTRIBUTABLE TO REGRESSION         3        31.19601       10.39867          10.13718
DEVIATION FROM REGRESSION         26        26.67065        1.02579

    TOTAL                         29        57.86666


MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 2


               TABLE OF RESIDUALS

CASE NO.      Y VALUE     Y ESTIMATE     RESIDUAL
    1         1.00000      0.59868        0.40131
    2         2.00000      1.88362        0.11637
    3         2.00000      2.26619       -0.26619
    4         0.00000      0.90703       -0.90703
    5         2.00000      1.99812        0.00187
    6         2.00000      1.58407        0.41592
    7         3.00000      3.49858       -0.49858
    8         2.00000      2.23347       -0.23347
    9         3.00000      3.85875       -0.85875
   10         0.00000      0.98943       -0.98943
   11         4.00000      2.51254        1.48745
   12         1.00000      1.95925       -0.95925
   13         1.00000      2.04998       -1.04998
   14         1.00000      1.10725       -0.10725
   15         3.00000      2.91951        0.08048
   16         2.00000      1.76538        0.23461
   17         3.00000      2.54052        0.45947
   18         4.00000      3.36591        0.63408
   19         4.00000      3.67961        0.32038
   20         3.00000      2.65434        0.34565
   21         4.00000      3.70045        0.29954
   22         4.00000      1.84628        2.15371
   23         1.00000      2.06899       -1.06899
   24         0.00000      1.95640       -1.95640


   25         4.00000      1.34019        2.65980
   26         1.00000      1.79816       -0.79816
   27         3.00000      2.24542        0.75458
   28         4.00000      4.41268       -0.41268
   29         4.00000      3.92577        0.07423
   30         0.00000      0.33331       -0.33331
```

Figure 13. Output listing

2. Changes in the input format statement of the special input subroutine, DATA:

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 may be keypunched in six 3-column fields, and, if so, the format is changed to (6F3.0).

The special input subroutine, DATA, 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.

Operating Instructions

The sample program for multiple linear regression is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following error conditions will result in messages:

1. The number of selection cards is not specified on the control card: NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED.
2. The matrix of correlation coefficients is singular: THE MATRIX IS SINGULAR. THIS SELECTION IS SKIPPED.

Error condition 2 allows the computer run to continue; however, error condition 1 terminates execution of the job.

Sample Main Program for Multiple Regression - REGRE

Purpose:

(1) Read the problem parameter card for a multiple regression, (2) Read subset selection cards, (3) Call the subroutines to calculate means, standard deviations, simple and multiple correlation coefficients, regression coefficients. T-values, and analysis of variance for multiple regression, and (4) Print the results.

Remarks:

The number of observations, N, must be greater than M+1, where M is the number of variables. If subset selection cards are not present, the program can not perform multiple after returning from subroutine MINV, the value of determinant (DET) is tested to check whether the correlation matrix is singular. If DET is compared against a small constant, this test may also be used to check near-singularity.

I/O specifications transmitted to subroutines by COMMON.

Input card:

Column 2 MX - Logical unit number for output.

Column 4 MY - Logical unit number for input.

Subroutines and function subprograms required:

CORRE (which, in turn, calls the subroutine named DATA)
ORDER
MINV
MULTR

Method:

Refer to B. Ostle, 'Statistics in Research', The Iowa State College Press', 1954, Chapter 8.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR MULTIPLE REGRESSION - REGRE
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF VARIABLES,M.
      DIMENSION XBAR(21),STD(21),D(21),RY(21),ISAVE(21),B(21),
     1SB(21),T(21),W(21)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OF M*M.
      DIMENSION RX(441)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO
C        (M+1)*M/2.
      DIMENSION R(231)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 10.
      DIMENSION ANS(10)
      COMMON MX,MY
      READ(2,15)MX,MY
   15 FORMAT(2I2)
    1 FORMAT(A4,A2,I5,2I2)
    2 FORMAT(////25H MULTIPLE REGRESSION.....A4,A2//6X,14HSELECTION.....
     1I2//)
    3 FORMAT(//9H VARIABLE,5X,4HMEAN,6X,8HSTANDARD,6X,11HCORRELATION,4X,
     110HREGRESSION,4X,10HSTD. ERROR,5X,8HCOMPUTED/6H   NO.,18X,9HDEVIAT
     2ION,7X,6HX VS Y,7X,11HCOEFFICIENT,3X,12HOF REG.COEF.,3X,7HT VALUE)
    4 FORMAT(/,I4,6F14.5)
    5 FORMAT(//,10H DEPENDENT)
    6 FORMAT(///10H INTERCEPT,13X,F13.5//23H MULTIPLE CORRELATION  ,F13.
     15//23H STD. ERROR OF ESTIMATE,F13.5//)
    7 FORMAT(//,21X,39HANALYSIS OF VARIANCE FOR THE REGRESSION//5X,19HSO
     1URCE OF VARIATION,7X,7HDEGREES,7X,6HSUM OF,10X,4HMEAN,13X,7HF VALU
     2E/30X,10HOF FREEDOM,4X,7HSQUARES,9X,7HSQUARES)
    8 FORMAT(/30H ATTRIBUTABLE TO REGRESSION   ,I6,3F16.5/30H DEVIATION
     1FROM REGRESSION     ,I6,2F16.5)
    9 FORMAT(/5X,5HTOTAL,19X,I6,F16.5)
   10 FORMAT(36I2)
   11 FORMAT(/,15X,18HTABLE OF RESIDUALS//9H CASE NO.,5X,7HY VALUE,5X,10
     1HY ESTIMATE,6X,8HRESIDUAL)
   12 FORMAT(I6,F15.5,2F14.5)
   13 FORMAT(////53H NUMBER OF SELECTIONS NOT SPECIFIED.  JOB TERMINATED
     1.)
   14 FORMAT(//52H THE MATRIX IS SINGULAR.  THIS SELECTION IS SKIPPED.)
C        READ PROBLEM PARAMETER CARD
  100 READ (MY,1) PR,PR1,N,M,NS
C        PR........PROBLEM NUMBER (MAY BE ALPHAMERIC)
C        PR1.......PROBLEM NUMBER (CONTINUED)
C        N.........NUMBER OF OBSERVATIONS
C        M.........NUMBER OF VARIABLES
C        NS........NUMBER OF SELECTIONS
      IO=0
      X=0.0
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,D,B,T)
C        TEST NUMBER OF SELECTIONS
      IF(NS) 108, 108, 109
  108 WRITE (MX,13)
      GO TO 300
  109 DO 200 I=1,NS
      WRITE (MX,2) PR,PR1,I
C        READ SUBSET SELECTION CARD
      READ (MY,10)NRESI,NDEP,K,(ISAVE(J),J=1,K)
C        NRESI.....OPTION CODE FOR TABLE OF RESIDUALS
C                  0  IF IT IS NOT DESIRED.
C                  1  IF IT IS DESIRED.
C        NDEP......DEPENDENT VARIABLE
C        K.........NUMBER OF INDEPENDENT VARIABLES INCLUDED
C        ISAVE.....A VECTOR CONTAINING THE INDEPENDENT VARIABLES
C                    INCLUDED
      CALL ORDER (M,R,NDEP,K,ISAVE,RX,RY)
      CALL MINV (RX,K,DET,B,T)
C        TEST SINGULARITY OF THE MATRIX INVERTED
      IF(DET) 112, 110, 112
  110 WRITE (MX,14)
      GO TO 200
  112 CALL MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS)
C        PRINT MEANS, STANDARD DEVIATIONS, INTERCORRELATIONS BETWEEN
C        X AND Y, REGRESSION COEFFICIENTS, STANDARD DEVIATIONS OF
C        REGRESSION COEFFICIENTS, AND COMPUTED T.VALUES
      MM=K+1
      WRITE (MX,3)
      DO 115 J=1,K
      L=ISAVE(J)
  115 WRITE (MX,4) L,XBAR(L),STD(L),RY(J),B(J),SB(J),T(J)
      WRITE (MX,5)
      L=ISAVE(MM)
      WRITE (MX,4) L,XBAR(L),STD(L)
C        PRINT INTERCEPT, MULTIPLE CORRELATION COEFFICIENT, AND
C        STANDARD ERROR OF ESTIMATE
      WRITE (MX,6) ANS(1),ANS(2),ANS(3)
```

```
C        PRINT ANALYSIS OF VARIANCE FOR THE REGRESSION
      WRITE (MX,7)
      L=ANS(8)
      WRITE (MX,8) K,ANS(4),ANS(6),ANS(10),L,ANS(7),ANS(9)
      L=N-1
      SUM=ANS(4)+ANS(7)
      WRITE (MX,9) L,SUM
      IF(NRESI) 200, 200, 120
C        PRINT TABLE OF RESIDUALS
  120 WRITE(MX,2)PR,PR1,I
      WRITE (MX,11)
      MM=ISAVE(K+1)
      DO  140 II=1,N
      CALL DATA(M,W)
      SUM=ANS(1)
      DO 130 J=1,K
      L=ISAVE(J)
  130 SUM=SUM+W(L)*B(J)
      RESI=W(MM)-SUM
  140 WRITE (MX,12) II,W(MM),SUM,RESI
  200 CONTINUE
      GO TO 100
  300 STOP
      END
```

```
 1 2
SAMPLE000300602
    29    289    216     85     14      1
    30    391    244     92     16      2
    30    424    246     90     18      2
    30    313    239     91     10      0
    35    243    275     95     30      2
    35    365    219     95     21      2
    43    396    267    100     39      3
    43    356    274     79     19      2
    44    346    255    126     56      3
    44    156    258     95     28      0
    44    278    249    110     42      4
    44    349    252     88     21      1
    44    141    236    129     56      1
    44    245    236     97     24      1
    45    297    256    111     45      3
    45    310    262     94     20      2
    49    151    339     96     35      3
    45    370    357     88     15      4
    45    379    198    147     64      4
    45    463    206    105     31      3
    45    316    245    132     60      4
    45    280    225    108     36      4
    44    395    215    101     27      1
    49    139    220    136     59      0
    49    245    205    113     37      4
    49    373    215     88     25      1
    51    224    215    118     54      3
    51    677    210    116     33      4
    51    424    210    140     59      4
    51    150    210    105     30      0
0106050102030405
    29    289    216     85     14      1
    30    391    244     92     16      2
    30    424    246     90     18      2
    30    313    239     91     10      0
    35    243    275     95     30      2
    35    365    219     95     21      2
    43    396    267    100     39      3
    43    356    274     79     19      2
    44    346    255    126     56      3
    44    156    258     95     28      0
    44    278    249    110     42      4
    44    349    252     88     21      1
    44    141    236    129     56      1
    44    245    236     97     24      1
    45    297    256    111     45      3
    45    310    262     94     20      2
    45    151    339     96     35      3
    45    370    357     88     15      4
    45    379    198    147     64      4
    45    463    206    105     31      3
    45    316    245    132     60      4
    45    280    225    108     36      4
    44    395    215    101     27      1
    49    139    220    136     59      0
    49    245    205    113     37      4
    49    373    215     88     25      1
    51    224    215    118     54      3
    51    677    210    116     33      4
    51    424    210    140     59      4
    51    150    210    105     30      0
010603020305
    29    289    216     85     14      1
    30    391    244     92     16      2
    30    424    246     90     18      2
    30    313    239     91     10      0
    35    243    275     95     30      2
    35    365    219     95     21      2
    43    396    267    100     39      3
    43    356    274     79     19      2
    44    346    255    126     56      3
    44    156    258     95     28      0
    44    278    249    110     42      4
    44    349    252     88     21      1
    44    141    236    129     56      1
    44    245    236     97     24      1
    45    297    256    111     45      3
    45    310    262     94     20      2
    45    151    339     96     35      3
    45    370    357     88     15      4
    45    379    198    147     64      4
    45    463    206    105     31      3
    45    316    245    132     60      4
    45    280    225    108     36      4
    44    395    215    101     27      1
    49    139    220    136     59      0
    49    245    205    113     37      4
    49    373    215     88     25      1
    51    224    215    118     54      3
    51    677    210    116     33      4
    51    424    210    140     59      4
    51    150    210    105     30      0
```

```
SAMPLE INPUT SUBROUTINE - DATA

PURPOSE
   READ AN OBSERVATION (M DATA VALUES) FROM INPUT DEVICE.
   THIS SUBROUTINE IS CALLED BY THE SUBROUTINE CORRE AND MUST
   BE PROVIDED BY THE USER.  IF SIZE AND LOCATION OF DATA
   FIELDS ARE DIFFERENT FROM PROBLEM TO PROBLEM, THIS SUB-
   ROUTINE MUST BE RECOMPILED WITH A PROPER FORMAT STATEMENT.

USAGE
   CALL DATA (M,D)

DESCRIPTION OF PARAMETERS
   M - THE NUMBER OF VARIABLES IN AN OBSERVATION.
   D - OUTPUT VECTOR OF LENGTH M CONTAINING THE OBSERVATION
       DATA.

REMARKS
   THE TYPE OF CONVERSION SPECIFIED IN THE FORMAT MUST BE
   EITHER F OR E.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   NONE
```

```
      SUBROUTINE DATA (M,D)
      DIMENSION D(1)
      COMMON MX,MY
    1 FORMAT(12F6.0)
C        READ AN OBSERVATION FROM INPUT DEVICE.
      READ (MY,1) (D(I),I=1,M)
      RETURN
      END
```

POLYNOMIAL REGRESSION

Problem Description

Powers of an independent variable are generated to calculate polynomials of successively increasing degrees. If there is no reduction in the residual sum of squares between two successive degrees of polynomials, the program terminates the problem before completing the analysis for the highest degree polynomial specified.

The sample problem for polynomial regression consists of 15 observations, as presented in Table 3. The highest degree polynomial specified for this problem is 4.

Table 3. Sample Data for Polynomial Regression

X	Y
1	10
2	16
3	20
4	23
5	25
6	26
7	30
8	36
9	48
10	62
11	78
12	94
13	107
14	118
15	127

Program

Description

The polynomial regression sample program consists of a main routine, POLRG, and five subroutines:

GDATA ORDER MINV MULTR	are from the Scientific Subroutine Package
PLOT	is a special plot subroutine

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 50 observations
2. Up to 6th degree polynomials
3. (2F 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 there are more than 60 observations or if greater than 7th degree polynomial is desired, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the sample main program must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, POLRG. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 11	Number of observations	00015
12 - 13	Highest degree polynomial to be fitted	04
14	Option code for plotting Y values and Y estimates: 0 if it is not desired 1 if it is desired	1

Leading zeros are not required to be keypunched; but numbers must be right-justified in fields.

Data Cards

Since input data are read into the computer one observation at a time, each pair of X and Y data in Table 3 is keypunched in that order on a separate card using the format (2F 6.0).

Plot Option Card

A card containing b12...9 (blank followed by numbers 1 through 9) in columns 1 to 10 is necessary after each set of data if plotting is required (option 1). If plotting is not required (option 0), this card must be omitted.

Deck Setup

Deck setup is shown in Figure 14.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The output of the sample program for polynomial regression includes:

1. Regression coefficients for successive degree polynomial
2. Analysis-of-variance table for successive degree polynomial
3. Table of residuals for the final degree polynomial (included with plot)
4. Plot of Y values and Y estimates (optional)

Sample

The output listing for the sample problem is shown in Figure 15.

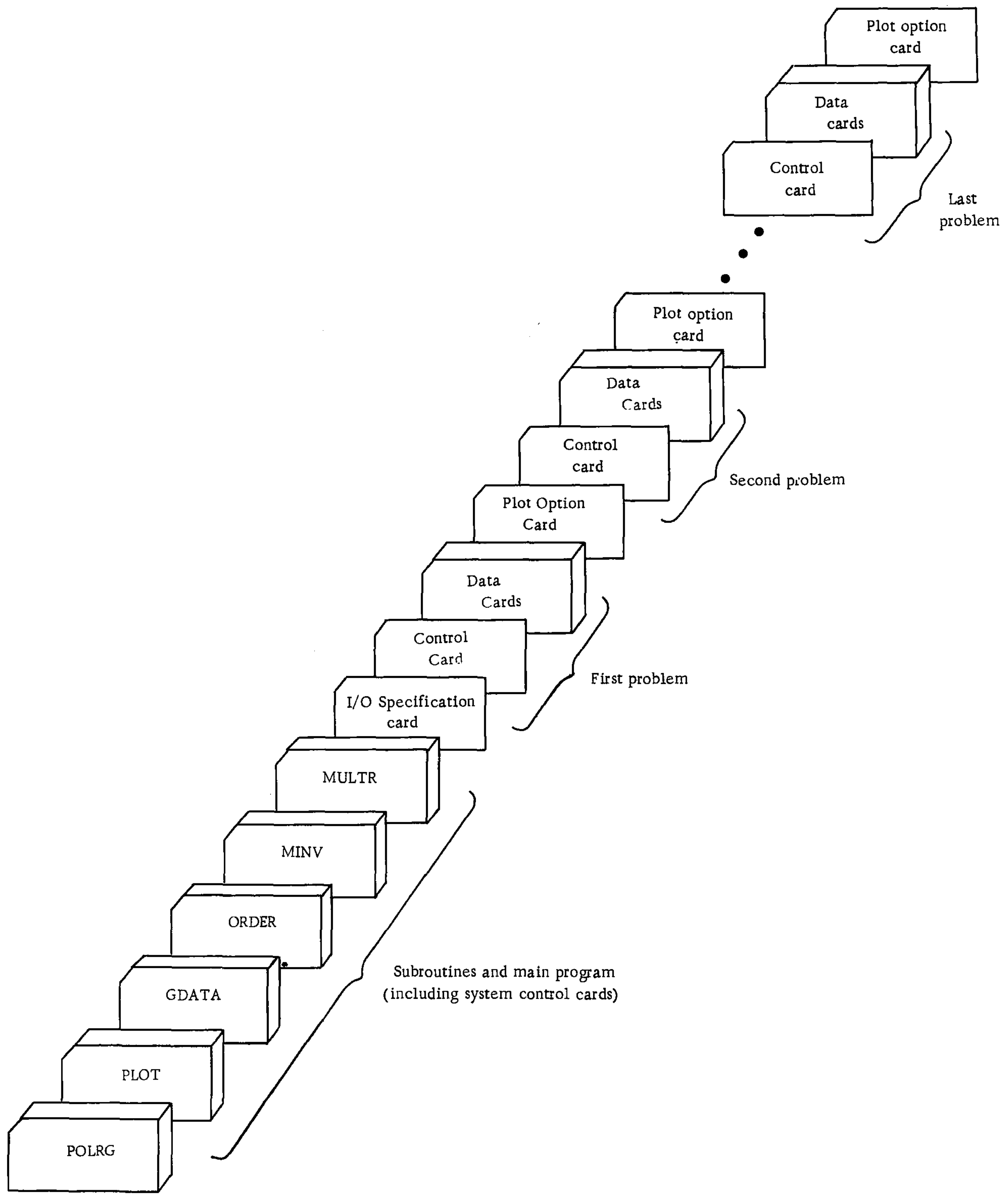


Figure 14. Deck setup (polynomial regression)

Program Modification

Noting that storage problems may result, as previously discussed in "Sample Program Description", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, POLRG:
   a. The dimension of array X must be greater than or equal to the product of n (m + 1), where n is the number of observations and m is the highest degree polynomial to be fitted. Since there are 15 observations and the highest degree polynomial specified is 4, the product is 75 = 15 (4 + 1).
   b. The dimension of array DI must be greater than or equal to the product of m x m. For the sample problem this product is 16 = 4 x 4.
   c. The dimension of array D must be greater than or equal to (m + 2) (m + 1)/2. For the sample problem this number is 15 = (4 + 2) (4 + 1)/2.
   d. The dimension of arrays B, E, SB, and T must be greater than or equal to the highest degree polynomial to be fitted, m. For the sample problem the value of m is 4.
   e. The dimension of arrays XBAR, STD, COE, SUMSQ and ISAVE must be greater than or equal to (m + 1). For the sample problem this value is 5 = (4 + 1).
   f. The dimension of array P must be greater than or equal to 3n. For the sample problem this value is 45 = 3(15). The array P is used when a plot of Y values and Y estimates is desired.
2. Changes in the input format statement of the main program, POLRG:

   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 may be keypunched in two 3-column fields, and if so the format is changed to (2F 3.0).

```
POLYNOMIAL REGRESSION.....SAMPLE

NUMBER OF OBSERVATION,    15

POLYNOMIAL REGRESSION OF DEGREE  1

  INTERCEPT      -13.87616

  REGRESSION COEFFICIENTS
    8.56785

                    ANALYSIS OF VARIANCE FOR   1  DEGREE POLYNOMIAL

    SOURCE OF VARIATION       DEGREE OF     SUM OF       MEAN          F       IMPROVEMENT IN TERMS
                               FREEDOM      SQUARES      SQUARE       VALUE     OF SUM OF SQUARES

 DUE TO REGRESSION,               1      20554.28520  20554.28520  135.56591       20554.28520
  DEVIATION ABOUT REGRESSION     13       1971.03930    151.61840
       TOTAL                     14      22525.32427

POLYNOMIAL REGRESSION OF DEGREE  2

  INTERCEPT       15.07238

  REGRESSION COEFFICIENTS
   -1.64922      0.63856

                    ANALYSIS OF VARIANCE FOR   2  DEGREE POLYNOMIAL

    SOURCE OF VARIATION       DEGREE OF     SUM OF       MEAN          F       IMPROVEMENT IN TERMS
                               FREEDOM      SQUARES      SQUARE       VALUE     OF SUM OF SQUARES

 DUE TO REGRESSION,               2      22236.39849  11118.19926  461.77386        1682.11352
  DEVIATION ABOUT REGRESSION     12        288.92584     24.07715
       TOTAL                     14      22525.32427

POLYNOMIAL REGRESSION OF DEGREE  3

  INTERCEPT       18.52303

  REGRESSION COEFFICIENTS
   -3.88201      0.97641     -0.01408

                    ANALYSIS OF VARIANCE FOR   3  DEGREE POLYNOMIAL

    SOURCE OF VARIATION       DEGREE OF     SUM OF       MEAN          F       IMPROVEMENT IN TERMS
                               FREEDOM      SQUARES      SQUARE       VALUE     OF SUM OF SQUARES

 DUE TO REGRESSION,               3      22245.30083   7415.09962  291.28314           8.90234
  DEVIATION ABOUT REGRESSION     11        280.02349     25.45667
       TOTAL                     14      22525.32427

POLYNOMIAL REGRESSION OF DEGREE  4

  INTERCEPT      -5.55942

  REGRESSION COEFFICIENTS
   19.71618     -5.18033      0.57106     -0.01829

                    ANALYSIS OF VARIANCE FOR   4  DEGREE POLYNOMIAL

    SOURCE OF VARIATION       DEGREE OF     SUM OF       MEAN          F       IMPROVEMENT IN TERMS
                               FREEDOM      SQUARES      SQUARE       VALUE     OF SUM OF SQUARES

 DUE TO REGRESSION,               4      22391.92976   5597.98243  419.65600         146.62893
  DEVIATION ABOUT REGRESSION     10        133.39456     13.33945
       TOTAL                     14      22525.32427


POLYNOMIAL REGRESSION.....SAMPLE

POLYNOMIAL REGRESSION OF DEGREE  4

                    TABLE OF RESIDUALS

OBSERVATION NO.     X VALUE      Y VALUE      Y ESTIMATE     RESIDUAL

      1             1.00000     10.00000        9.53319      0.46680
      2             2.00000     16.00000       17.43140     -1.43139
      3             3.00000     20.00000       20.90693     -0.90693
      4             4.00000     23.00000       22.28845      0.71155
      5             5.00000     25.00000       23.46550      1.53449
      6             6.00000     26.00000       25.88856      0.11143
      7             7.00000     30.00000       30.56892     -0.56892
      8             8.00000     36.00000       38.07897     -2.07896
      9             9.00000     46.00000       46.55179     -0.55178
     10            10.00000     62.00000       61.68150      0.31850
     11            11.00000     78.00001       76.72306      1.27694
     12            12.00000     94.00001       92.49252      1.50749
     13            13.00000    107.00001      107.36628     -0.36627
     14            14.00000    118.00001      119.28244     -1.28242
     15            15.00000    127.00001      125.73935      1.26066
```

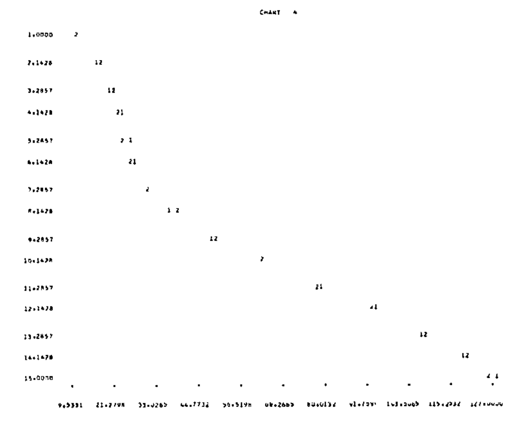


Figure 15. Output listing

Operating Instructions

The sample program for polynomial regression is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Sample Main Program for Polynomial Regression - POLRG

Purpose:

(1) Read the problem parameter card for a polynomial regression, (2) Call subroutines to perform the analysis, (3) Print the regression coefficients and analysis of variance table for polynomials of successively increasing degrees, and (4) Optionally print the table of residuals and a plot of Y values and Y estimates.

Remarks:

I/O specifications transmitted to subroutines by COMMON.

Input card:

Column 2	MX -	Logical unit number for output.
Column 4	MY -	Logical unit number for input.

The number of observations, N, must be greater than M+1, where M is the highest degree polynomial specified. If there is no reduction in the residual sum of squares between two successive degrees of the polynomials, the program terminates the problem before completing the analysis for the highest degree polynomial specified.

Subroutines and function subprograms required:

GDATA
ORDER
MINV
MULTR
PLOT (A special PLOT subroutine provided for the sample program.)

Method:

Refer to B. Ostle, 'Statistics in Research', The Iowa State College Press, 1954, chapter 6.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR POLYNOMIAL REGRESSION - POLRG
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OF N*(M+1), WHERE N IS THE NUMBER OF OBSERVATIONS AND
C        M IS THE HIGHEST DEGREE POLYNOMIAL SPECIFIED.
      DIMENSION X(350)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OF M*M.
      DIMENSION DI(36)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO
C        (M+2)*(M+1)/2.
      DIMENSION D(28)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO M.
      DIMENSION B(6),SB(6),T(6),E(6)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO
C        (M+1).
      DIMENSION XBAR(7),STD(7),COE(7),SUMSQ(7),ISAVE(7)
C        THE FOLLOWIN DIMENSION MUST BE GREATER THAN OR EQUAL TO 10.
      DIMENSION ANS(10)
C        THE FOLLOWING DIMENSION WILL BE USED IF THE PLOT OF OBSERVED
C        DATA AND ESTIMATES IS DESIRED. THE SIZE OF THE DIMENSION, IN
C        THIS CASE, MUST BE GREATER THAN OR EQUAL TO N*3. OTHERWISE,
C        THE SIZE OF DIMENSION MAY BE SET TO 1.
      DIMENSION P(150)
      COMMON MX,MY
    1 FORMAT(A4,A2,I5,I2,I1)
    2 FORMAT(2F6.0)
    3 FORMAT(////27H POLYNOMIAL REGRESSION......A4,A2/)
    4 FORMAT(//23H NUMBER OF OBSERVATION,I6//)
    5 FORMAT(//32H POLYNOMIAL REGRESSION OF DEGREE,I3)
    6 FORMAT(//12H   INTERCEPT,F15.5)
    7 FORMAT(//26H   REGRESSION COEFFICIENTS/(10F12.5))
    8 FORMAT(///24X,24HANALYSIS OF VARIANCE FOR,I4,19H  DEGREE POLYNOMIA
     1L/)
    9 FORMAT(///,5X,19HSOURCE OF VARIATION,7X,9HDEGREE OF,7X,6HSUM OF,
     19X,4HMEAN,10X,1HF,9X,20HIMPROVEMENT IN TERMS/33X,7HFREEDOM,8X,
     27HSQUARES,7X,6HSQUARE,7X,5HVALUE,8X,17HOF SUM OF SQUARES)
   10 FORMAT(//20H  DUE TO REGRESSION,12X,I6,F17.5,F14.5,F13.5,F20.5)
   11 FORMAT(32H   DEVIATION ABOUT REGRESSION   ,I6,F17.5,F14.5)
   12 FORMAT(8X,5HTOTAL,19X,I6,F17.5///)
   13 FORMAT(//17H   NO IMPROVEMENT)
   14 FORMAT(////27X,18HTABLE OF RESIDUALS//16H OBSERVATION NO.,5X,7HX V
     1ALUE,7X,7HY VALUE,7X,10HY ESTIMATE,7X,8HRESIDUAL/)
   15 FORMAT(/,3X,I6,F18.5,F14.5,F17.5,F15.5)
   16 FORMAT(2I2)
      READ(2,16)MX,MY
C        READ PROBLEM PARAMETER CARD
  100 READ (MY,1) PR,PR1,N,M,NPLOT
C        PR....PROBLEM NUMBER (MAY BE ALPHAMERIC)
C        PR1...PROBLEM NUMBER (CONTINUED)
C        N.....NUMBER OF OBSERVATIONS
C        M.....HIGHEST DEGREE POLYNOMIAL SPECIFIED
C        NPLOT.OPTION CODE FOR PLOTTING
C                0  IF PLOT IS NOT DESIRED.
C                1  IF PLOT IS DESIRED.
C        PRINT PROBLEM NUMBER AND N.
      WRITE (MX,3) PR,PR1
      WRITE (MX,4) N
C        READ INPUT DATA
      L=N*M
      DO 110 I=1,N
      J=L+I
C        X(I) IS THE INDEPENDENT VARIABLE, AND X(J) IS THE DEPENDENT
C        VARIABLE.
  110 READ (MY,2) X(I),X(J)
      CALL GDATA (N,M,X,XBAR,STD,D,SUMSQ)
      MM=M+1
      SUM=0.0
      NT=N-1
      DO 200 I=1,M
      ISAVE(I)=I
C        FORM SUBSET OF CORRELATION COEFFICIENT MATRIX
      CALL ORDER (MM,D,MM,I,ISAVE,DI,E)
C        INVERT THE SUBMATRIX OF CORRELATION COEFFICIENTS
      CALL MINV (DI,I,DET,B,T)
      CALL MULTR (N,I,XBAR,STD,SUMSQ,DI,E,ISAVE,B,SB,T,ANS)
C        PRINT THE RESULT OF CALCULATION
      WRITE (MX,5) I
      IF(ANS(7))140,130,130
  130 SUMIP=ANS(4)-SUM
      IF(SUMIP) 140, 140, 150
  140 WRITE(MX,13)
      GO TO 210
  150 WRITE(MX,6)ANS(1)
      WRITE (MX,7) (B(J),J=1,I)
      WRITE (MX,8) I
      WRITE (MX,9)
      SUM=ANS(4)
      WRITE (MX,10) I,ANS(4),ANS(6),ANS(10),SUMIP
      NI=ANS(8)
      WRITE (MX,11) NI,ANS(7),ANS(9)
      WRITE (MX,12) NT,SUMSQ(MM)
C        SAVE COEFFICIENTS FOR CALCULATION OF Y ESTIMATES
      COE(1)=ANS(1)
      DO 160 J=1,I
  160 COE(J+1)=B(J)
      LA=I
  200 CONTINUE
C        TEST WHETHER PLOT IS DESIRED
  210 IF(NPLOT) 100, 100, 220
C        CALCULATE ESTIMATES
  220 NP3=N+N
      DO 230 I=1,N
      NP3=NP3+1
      P(NP3)=COE(1)
      L=I
      DO 230 J=1,LA
      P(NP3)=P(NP3)+X(L)*COE(J+1)
  230 L=L+N
C        COPY OBSERVED DATA
      N2=N
       L=N*M
      DO 240 I=1,N
      P(I)=X(I)
      N2=N2+1
      L=L+1
  240 P(N2)=X(L)
C        PRINT TABLE OF RESIDUALS
      WRITE (MX,3) PR,PR1
      WRITE (MX,5) LA
      WRITE (MX,14)
      NP2=N
      NP3=N+N
      DO 250 I=1,N
      NP2=NP2+1
      NP3=NP3+1
      RESID=P(NP2)-P(NP3)
  250 WRITE (MX,15) I,P(I),P(NP2),P(NP3),RESID
      CALL PLOT (LA,P,N,3,0,1)
      GO TO 100
      END
```

```
 1 2
SAMPLE00015041
     1     10
     2     16
     3     20
     4     23
     5     25
     6     26
     7     30
     8     36
     9     48
    10     62
    11     78
    12     94
    13    107
    14    118
    15    127
123456789
```

```
        SUBROUTINE PLOT

        PURPOSE
           PLOT SEVERAL CROSS-VARIABLES VERSUS A BASE VARIABLE

        USAGE
           CALL PLOT (NO,A,N,M,NL,NS)

        DESCRIPTION OF PARAMETERS
           NO - CHART NUMBER (3 DIGITS MAXIMUM)
           A  - MATRIX OF DATA TO BE PLOTTED. FIRST COLUMN REPRESENTS
                BASE VARIABLE AND SUCCESSIVE COLUMNS ARE THE CROSS-
                VARIABLES (MAXIMUM IS 9).
           N  - NUMBER OF ROWS IN MATRIX A
           M  - NUMBER OF COLUMNS IN MATRIX A (EQUAL TO THE TOTAL
                NUMBER OF VARIABLES). MAXIMUM IS 10.
           NL - NUMBER OF LINES IN THE PLOT. IF 0 IS SPECIFIED, 50
                LINES ARE USED.
           NS - CODE FOR SORTING THE BASE VARIABLE DATA IN ASCENDING
                ORDER
                  0  SORTING IS NOT NECESSARY (ALREADY IN ASCENDING
                     ORDER).
                  1  SORTING IS NECESSARY.

        REMARKS
           NONE

        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
           NONE
```

```
      SUBROUTINE PLOT(NO,A,N,M,NL,NS)
      DIMENSION OUT(101),YPR(11),ANG(9),A(1)
      COMMON MX,MY
    1 FORMAT (///,60X,7H CHART ,I3,//)
    2 FORMAT (1X,F11.4,5X,101A1)
    3 FORMAT (2X)
    5 FORMAT(10A1)
    7 FORMAT(     16X,101H.          .          .          .          .
     1          .          .          .          .          .)
    8 FORMAT (//,9X,11F10.4)
      NLL=NL
      IF(NS) 16, 16, 10
C        SORT BASE VARIABLE DATA IN ASCENDING ORDER
   10 DO 15 I=1,N
      DO 14 J=I,N
      IF(A(I)-A(J)) 14, 14, 11
   11 L=I-N
      LL=J-N
      DO 12 K=1,M
      L=L+N
      LL=LL+N
      F=A(L)
      A(L)=A(LL)
   12 A(LL)=F
   14 CONTINUE
   15 CONTINUE
C        TEST NLL
   16 IF(NLL) 20, 18, 20
   18 NLL=50
C        PRINT TITLE
   20 WRITE(MX,1)NO
C        READ BLANK AND DIGITS FOR PRINTING
      READ(MY,5) BLANK,(ANG(I),I=1,9)
C        FIND SCALE FOR BASE VARIABLE
      XSCAL=(A(N)-A(1))/(FLOAT(NLL-1))
C        FIND SCALE FOR CROSS-VARIABLES
      M1=N+1
      M2=M*N
      YMIN=A(M1)
      YMAX=YMIN
      DO 40 J=M1,M2
      IF(A(J)-YMIN) 28,26,26
   26 IF(A(J)-YMAX) 40,40,30
   28 YMIN=A(J)
      GO TO 40
   30 YMAX=A(J)
   40 CONTINUE
      YSCAL=(YMAX-YMIN)/100.0
C        FIND BASE VARIABLE PRINT POSITION
      XB=A(1)
      L=1
      MYX = M-1
      I=1
   45 F=I-1
      XPR=XB+F*XSCAL
      IF(A(L)-XPR) 50,50,70
C        FIND CROSS-VARIABLES
   50 DO 55 IX=1,101
   55 OUT(IX)=BLANK
      DO 60 J=1,MYX
      LL=L+J*N
      JP=((A(LL)-YMIN)/YSCAL)+1.0
      OUT(JP)=ANG(J)
   60 CONTINUE
C        PRINT LINE AND CLEAR, OR SKIP
      WRITE(MX,2)XPR,(OUT(IZ),IZ=1,101)
      L=L+1
      GO TO 80
   70 WRITE(MX,3)
   80 I=I+1
      IF(I-NLL)45,84,86
   84 XPR=A(N)
      GO TO 50
C        PRINT CROSS-VARIABLES NUMBERS
   86 WRITE(MX,7)
      YPR(1)=YMIN
      DO 90 KN=1,9
   90 YPR(KN+1)=YPR(KN)+YSCAL*10.0
      YPR(11)=YMAX
      WRITE(MX,8)(YPR(IP),IP=1,11)
      RETURN
      END
```

CANONICAL CORRELATION

Problem Description

An analysis of the interrelations between two sets of variables measured on the same subjects is performed by this program. 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 4. These two sets of measurements have been made on 23 subjects.

Table 4. 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 sample program consists of a main routine, MCANO, and six subroutines:

CORRE CANOR MINV NROOT EIGEN	are from the Scientific Subroutine Package
DATA	is a special input subroutine

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 9 variables, including both the first set of variables (that is, left-hand variables) and the second set of variables (that is, right-hand variables). The number of variables in the first set must be greater than or equal to the number of variables in the second set.
2. Up to 99,999 observations.
3. (12F 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 there are more than 9 variables, dimension statements in the sample main program must be modified to handle the particular problem. Similarly, if input data cards are prepared using a different format, the input format in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, MCANO. 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

*The number of variables in the first set must be greater than or equal to the number of variables in the second set.

Leading zeros are not required to be keypunched; but must be right-justified within fields.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 4 is keypunched on a separate card using the format (12F 6.0). This format assumes twelve 6-column fields per card.

Deck Setup

Deck setup is shown in Figure 16.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

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 and degrees of freedom
7. Coefficients for left- and right-hand variables

Sample

The output listing for the sample problem is shown in Figure 17 of this sample program.

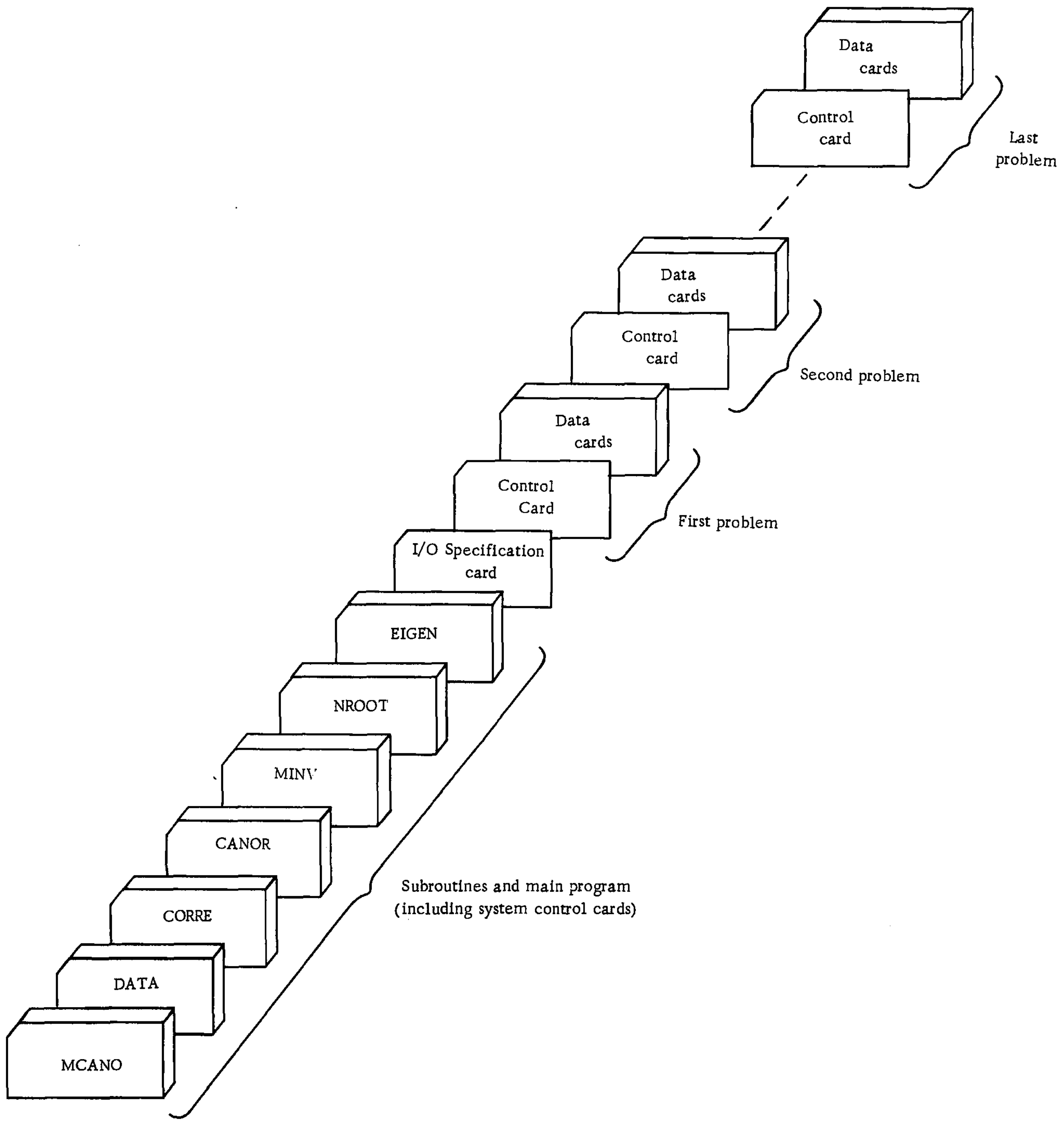
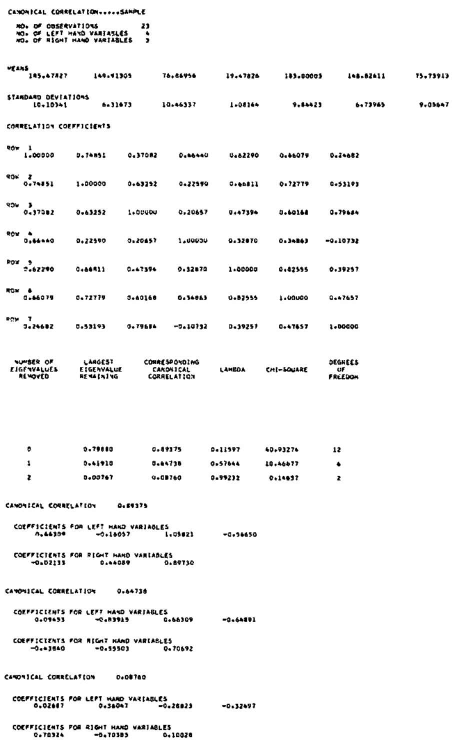


Figure 16. Deck setup (canonical correlation)

Program Modification

Noting that storage problems may result, as previously described in "Sample Program Descriptions", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize



```
CANONICAL CORRELATION.....SAMPLE

  NO. OF OBSERVATIONS          23
  NO. OF LEFT HAND VARIABLES    4
  NO. OF RIGHT HAND VARIABLES   3


MEANS
    185.47827    149.91305    76.86956    19.47826    183.00003    148.82611    75.73913

STANDARD DEVIATIONS
     10.10341      6.31673    10.46337     1.08164      9.64423      6.73965     9.05647

CORRELATION COEFFICIENTS

ROW  1
    1.00000    0.74851    0.37082    0.66440    0.62290    0.66079    0.24682

ROW  2
    0.74851    1.00000    0.63252    0.22590    0.66811    0.72779    0.53193

ROW  3
    0.37082    0.63252    1.00000    0.20657    0.47394    0.60168    0.79684

ROW  4
    0.66440    0.22590    0.20657    1.00000    0.32870    0.34863   -0.10732

ROW  5
    0.62290    0.66811    0.47394    0.32870    1.00000    0.82555    0.39257

ROW  6
    0.66079    0.72779    0.60168    0.34863    0.82555    1.00000    0.47657

ROW  7
    0.24682    0.53193    0.79684   -0.10732    0.39257    0.47657    1.00000


  NUMBER OF       LARGEST      CORRESPONDING                              DEGREES
 EIGENVALUES     EIGENVALUE      CANONICAL        LAMBDA     CHI-SQUARE      OF
   REMOVED       REMAINING      CORRELATION                               FREEDOM




     0            0.79880        0.89375        0.11597     40.93276        12

     1            0.41910        0.64738        0.57644     10.46677         6

     2            0.00767        0.08760        0.99232      0.14857         2

CANONICAL CORRELATION       0.89375

  COEFFICIENTS FOR LEFT HAND VARIABLES
      0.66309       -0.16057        1.05821       -0.56650

  COEFFICIENTS FOR RIGHT HAND VARIABLES
     -0.02133        0.44089        0.89730

CANONICAL CORRELATION       0.64738

  COEFFICIENTS FOR LEFT HAND VARIABLES
      0.09453       -0.83915        0.66309       -0.64891

  COEFFICIENTS FOR RIGHT HAND VARIABLES
     -0.43640       -0.55503        0.70692

CANONICAL CORRELATION       0.08760

  COEFFICIENTS FOR LEFT HAND VARIABLES
      0.02687        0.36047       -0.26825       -0.32497

  COEFFICIENTS FOR RIGHT HAND VARIABLES
      0.70324       -0.70383        0.10028
```

Figure 17. Output listing

the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, MCANO:
   a. The dimension of arrays XBAR, STD, CANR, CHISQ, and NDF must be greater than or equal to the total number of variables m (m = p + q, where p is the number of left-hand variables and q is the number of right-hand variables). Since there are seven variables, four on left and three on right, the value of m is 7.
   b. The dimension of array RX must be greater than or equal to the product of m x m. For the sample problem this product is 49 = 7 x 7.
   c. The dimension of array R must be greater than or equal to (m + 1)m/2. For the sample problem this number is 28 = (7 + 1)7/2.
   d. The dimension of array COEFL must be greater than or equal to the product of p x q. For the sample problem this product is 12 = 4 x 3.
   e. The dimension of array COEFR must be greater than or equal to the product of q x q. For the sample problem this product is 9 = 3 x 3.
2. Changes in the input format statement of the special input subroutine, DATA:

   Only the format statement for input data may be changed. For example, 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 may be keypunched in seven 3-column fields, and if so, the format would be changed to (7F 3.0). Note that the current input format statement will allow a maximum of twelve variables per card. The special input subroutine, DATA, 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.

Operating Instructions

The sample program for canonical correlation is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Sample Main Program for Canonical Correlation - MCANO

Purpose:

(1) Read the problem parameter card for a canonical correlation, (2) Call two subroutines to calculate simple correlations, canonical correlations, chi-squares, degrees of freedom for chi-squares, and coefficients for left and right hand variables, namely canonical variates, and (3) Print the results.

Remarks:

I/O specifications transmitted to subroutines by COMMON.

Input card:

Column 2	MX -	Logical unit number for output.
Column 4	MY -	Logical unit number for input.

The number of left-hand variables must be greater than or equal to the number of right-hand variables.

Subroutines and function subprograms required:

CORRE	(which, in turn, calls the input subroutine named DATA.)
CANOR	(which, in turn, calls the subroutines MINV and NROOT. NROOT, in turn, calls the subroutine EIGEN.)

Method:

Refer to W. W. Cooley and P. R. Lohnes, 'Multivariate Procedures for the Behavioral Sciences', John Wiley and Sons, 1962, chapter 3.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C          SAMPLE MAIN PROGRAM FOR CANONICAL CORRELATION - MCANO           MCANO  1
C          THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE   MCANO  2
C          TOTAL NUMBER OF VARIABLES M (M=MP+MQ, WHERE MP IS THE NUMBER    MCANO  3
C          OF LEFT HAND VARIABLES, AND MQ IS THE NUMBER OF RIGHT HAND      MCANO  4
C          VARIABLES).                                                     MCANO  5
      DIMENSION XBAR(9),STD(9),CANR(9),CHISQ(9),NDF(9)                     MCANO  6
C          THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE    MCANO  7
C          PRODUCT OF M*M.                                                 MCANO  8
      DIMENSION RX(81)                                                     MCANO  9
C          THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO        MCANO 10
C          (M+1)*M/2.                                                      MCANO 11
      DIMENSION R(45)                                                      MCANO 12
C          THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE    MCANO 13
C          PRODUCT OF MP*MQ.                                               MCANO 14
      DIMENSION COEFL(81)                                                  MCANO 15
C          THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE    MCANO 16
C          PRODUCT OF MQ*MQ.                                               MCANO 17
      DIMENSION COEFR(25)                                                  MCANO 18
       COMMON MX,MY                                                        MCANO 19
    1 FORMAT(A4,A2,I5,2I2)                                                 MCANO 20
    2 FORMAT(////27H CANONICAL CORRELATION.....,A4,A2//22H   NO. OF OBSEMCANO 21
     1RVATIONS,8X,I4/29H    NO. OF LEFT HAND VARIABLES,I5/30H    NO. OF RIMCANO 22
     2GHT HAND VARIABLES,I4/)                                              MCANO 23
    3 FORMAT(//6H MEANS/(8F15.5))                                          MCANO 24
    4 FORMAT(//20H STANDARD DEVIATIONS/(8F15.5))                           MCANO 25
    5 FORMAT(//25H CORRELATION COEFFICIENTS)                               MCANO 26
    6 FORMAT(//4H ROW,I3/(10F12.5))                                        MCANO 27
    7 FORMAT(////12H    NUMBER OF,7X,7HLARGEST,7X,13HCORRESPONDING,31X,7HMCANO 28
     1DEGREES/13H   EIGENVALUES,5X,10HEIGENVALUE,7X,9HCANONICAL,7X,6HLAMBMCANO 29
     2DA,5X,10HCHI-SQUARE,7X,2HOF/4X,7HREMOVED,7X,9HREMAINING,7X,11HCORRMCANO 30
     3ELATION,32X,7HFREEDOM/)                                              MCANO 31
    8 FORMAT(/I7,F19.5,F16.5,2F14.5,5X,I5)                                 MCANO 32
    9 FORMAT(///22H CANONICAL CORRELATION,F12.5)                           MCANO 33
   10 FORMAT(//39H    COEFFICIENTS FOR LEFT HAND VARIABLES/(8F15.5))       MCANO 34
   11 FORMAT(//40H    COEFFICIENTS FOR RIGHT HAND VARIABLES/(8F15.5))      MCANO 35
   12 FORMAT(2I2)                                                          MCANO 36
      READ(2,12)MX,MY                                                      MCANO 37
C          READ PROBLEM PARAMETER CARD                                     MCANO 38
  100 READ (MY,1)PR,PR1,N,MP,MQ                                            MCANO 39
C          PR.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                     MCANO 40
C          PR1......PROBLEM NUMBER (CONTINUED)                             MCANO 41
C          N........NUMBER OF OBSERVATIONS                                 MCANO 42
C          MP.......NUMBER OF LEFT HAND VARIABLES                          MCANO 43
C          MQ.......NUMBER OF RIGHT HAND VARIABLES                         MCANO 44
      WRITE (MX,2)PR,PR1,N,MP,MQ                                           MCANO 45
      M=MP+MQ                                                              MCANO 46
      IO=0                                                                 MCANO 47
      X=0.0                                                                MCANO 48
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,CANR,CHISQ,COEFL)                 MCANO 49
C          PRINT MEANS, STANDARD DEVIATIONS, AND CORRELATION               MCANO 50
C          COEFFICIENTS OF ALL VARIABLES                                   MCANO 51
      WRITE (MX,3)(XBAR(I),I=1,M)                                          MCANO 52
      WRITE (MX,4)(STD(I),I=1,M)                                           MCANO 53
      WRITE (MX,5)                                                         MCANO 54
      DO 160 I=1,M                                                         MCANO 55
      DO 150 J=1,M                                                         MCANO 56
      IF(I-J) 120, 130, 130                                                MCANO 57
  120 L=I+(J*J-J)/2                                                        MCANO 58
      GO TO 140                                                            MCANO 59
  130 L=J+(I*I-I)/2                                                        MCANO 60
  140 CANR(J)=R(L)                                                         MCANO 61
  150 CONTINUE                                                             MCANO 62
  160 WRITE (MX,6)I,(CANR(J),J=1,M)                                        MCANO 63
      CALL CANOR (N,MP,MQ,R,XBAR,STD,CANR,CHISQ,NDF,COEFR,COEFL,RX)        MCANO 64
C          PRINT EIGENVALUES, CANONICAL CORRELATIONS, LAMBDA, CHI-SQUARES MCANO 65
C          DEGREES OF FREEDOMS                                             MCANO 66
      WRITE (MX,7)                                                         MCANO 67
      DO 170 I=1,MQ                                                        MCANO 68
      N1=I-1                                                               MCANO 69
C          TEST WHETHER EIGENVALUE IS GREATER THAN ZERO                    MCANO 70
      IF(XBAR(I)) 165, 165, 170                                            MCANO 71
  165 MM=N1                                                                MCANO 72
      GO TO 175                                                            MCANO 73
  170 WRITE (MX,8)N1,XBAR(I),CANR(I),STD(I),CHISQ(I),NDF(I)                MCANO 74
      MM=MQ                                                                MCANO 75
C          PRINT CANONICAL COEFFICIENTS                                    MCANO 76
  175 N1=0                                                                 MCANO 77
      N2=0                                                                 MCANO 78
      DO 200 I=1,MM                                                        MCANO 79
      WRITE (MX,9)CANR(I)                                                  MCANO 80
      DO 180 J=1,MP                                                        MCANO 81
      N1=N1+1                                                              MCANO 82
  180 XBAR(J)=COEFL(N1)                                                    MCANO 83
      WRITE (MX,10)(XBAR(J),J=1,MP)                                        MCANO 84
      DO 190 J=1,MQ                                                        MCANO 85
      N2=N2+1                                                              MCANO 86
  190 XBAR(J)=COEFR(N2)                                                    MCANO 87
      WRITE (MX,11)(XBAR(J),J=1,MQ)                                        MCANO 88
  200 CONTINUE                                                             MCANO 89
      GO TO 100                                                            MCANO 90
      END                                                                  MCANO 91
// DUP
*STORE      WS  UA  MCANO
// XEQ MCANO   01
*LOCALMCANO,CORRE,CANOR
```

```
 1 2                                                         1
SAMPLE000250403                                              2
   191    155    65    19   179   145    70                  3
   195    149    70    20   201   152    69                  4
   181    148    71    19   185   149    75                  5
   183    153    82    18   188   149    86                  6
   176    144    67    18   171   142    71                  7
   208    157    81    22   192   152    77                  8
   189    150    75    21   190   149    72                  9
   197    159    90    20   189   152    82                 10
   188    152    76    19   197   159    84                 11
   192    150    78    20   187   151    72                 12
   179    158    99    18   186   148    89                 13
   183    147    65    18   174   147    70                 14
   174    150    71    19   185   152    65                 15
   190    159    91    19   195   157    99                 16
   188    151    98    20   187   158    87                 17
   163    137    59    18   161   130    63                 18
   195    155    85    20   183   158    81                 19
   196    153    80    21   173   148    74                 20
   181    145    77    20   182   146    70                 21
   175    140    70    19   165   137    81                 22
   192    154    69    20   185   152    63                 23
   174    143    79    20   178   147    73                 24
   176    139    70    20   176   143    69                 25
```

```
        SAMPLE INPUT SUBROUTINE - DATA

        PURPOSE
           READ AN OBSERVATION (M DATA VALUES) FROM INPUT DEVICE.
           THIS SUBROUTINE IS CALLED BY THE SUBROUTINE CORRE AND MUST
           BE PROVIDED BY THE USER.  IF SIZE AND LOCATION OF DATA
           FIELDS ARE DIFFERENT FROM PROBLEM TO PROBLEM, THIS SUB-
           ROUTINE MUST BE RECOMPILED WITH A PROPER FORMAT STATEMENT.

        USAGE
           CALL DATA (M,D)

        DESCRIPTION OF PARAMETERS
           M - THE NUMBER OF VARIABLES IN AN OBSERVATION.
           D - OUTPUT VECTOR OF LENGTH M CONTAINING THE OBSERVATION
               DATA.

        REMARKS
           THE TYPE OF CONVERSION SPECIFIED IN THE FORMAT MUST BE
           EITHER F OR E.

        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
           NONE
```

```
      SUBROUTINE DATA (M,D)                                     DATA   1
      DIMENSION D(1)                                            DATA   2
      COMMON MX,MY                                              DATA   3
    1 FORMAT(12F6.0)                                            DATA   4
C        READ AN OBSERVATION FROM INPUT DEVICE.                 DATA   5
      READ (MY,1) (D(I),I=1,M)                                  DATA   6
      RETURN                                                    DATA   7
      END                                                       DATA   8
```

ANALYSIS OF VARIANCE

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 reducing them first 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 present in Table 5. 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 5. 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

*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.

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 5 may be represented in the form:

$$x_{abcr} \quad \text{where} \quad \begin{aligned} a &= 1,2,3,4 \\ b &= 1,2,3 \\ c &= 1,2,3 \\ r &= 1,2 \end{aligned}$$

The general principle of the analysis-of-variance procedure used in the program is to perform first a formal factorial analysis and then 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 sample program consists of a main routine, ANOVA, and three subroutines:

$$\left.\begin{array}{l} \text{AVDAT} \\ \text{AVCAL} \\ \text{MEANQ} \end{array}\right\} \text{are from the Scientific Subroutine Package}$$

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to six-factor factorial experiment
2. Up to a total of 1600 data points. The total number of core locations for data points in a problem is calculated as follows:

$$T = \prod_{i=1}^{k} (\text{LEVEL}_i + 1)$$

where LEVEL_i = number of levels of i^{th} factor
k = number of factors
Π = notation for repeated products

3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than six factors or if the total number of data points is more than 1800, dimension statements in the sample main program must be modified. Similarly, if input data cards are prepared using a different format, the input format statement in the sample main program must be modified. The general rules for program modifications are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, ANOVA. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 8	Number of factors	04
9 - 15	Blank	
16	Label for the first factor	A
17 - 20	Number of levels of the first factor	0004
21	Label for the second factor	B
22 - 25	Number of levels of the second factor	0003
26	Label for the third factor	C
27 - 30	Number of levels of the third factor	0003
31	Label for the fourth factor	R
32 - 35	Number of levels of the fourth factor	0002
66	Label for the eleventh factor (if present)	
67 - 70	Number of levels of the eleventh factor	

If there are more than eleven factors, continue to the second card in the same manner.

Columns	Contents
1	Label for the twelfth factor
2 - 5	Number of levels for the twelfth factor
.	
.	
.	
etc.	

Leading zeros are not required to be keypunched.

Data Cards

Data are keypunched in the following order: X_{1111}, X_{2111}, X_{3111}, X_{4111}, X_{1211}, X_{2211}, X_{3211}, . . . , X_{4332}. In other words, the innermost subscript is changed first; namely, the first factor, and then second, third, and fourth subscripts. In the sample problem, the first subscript corresponds to factor A and the second, third, and fourth subscripts to factors B, C, and R. Since the number of data fields per cards is twelve, implied by the format (12F6.0), each row in Table 5 is keypunched on a separate card.

Deck Setup

Deck setup is shown in Figure 18.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

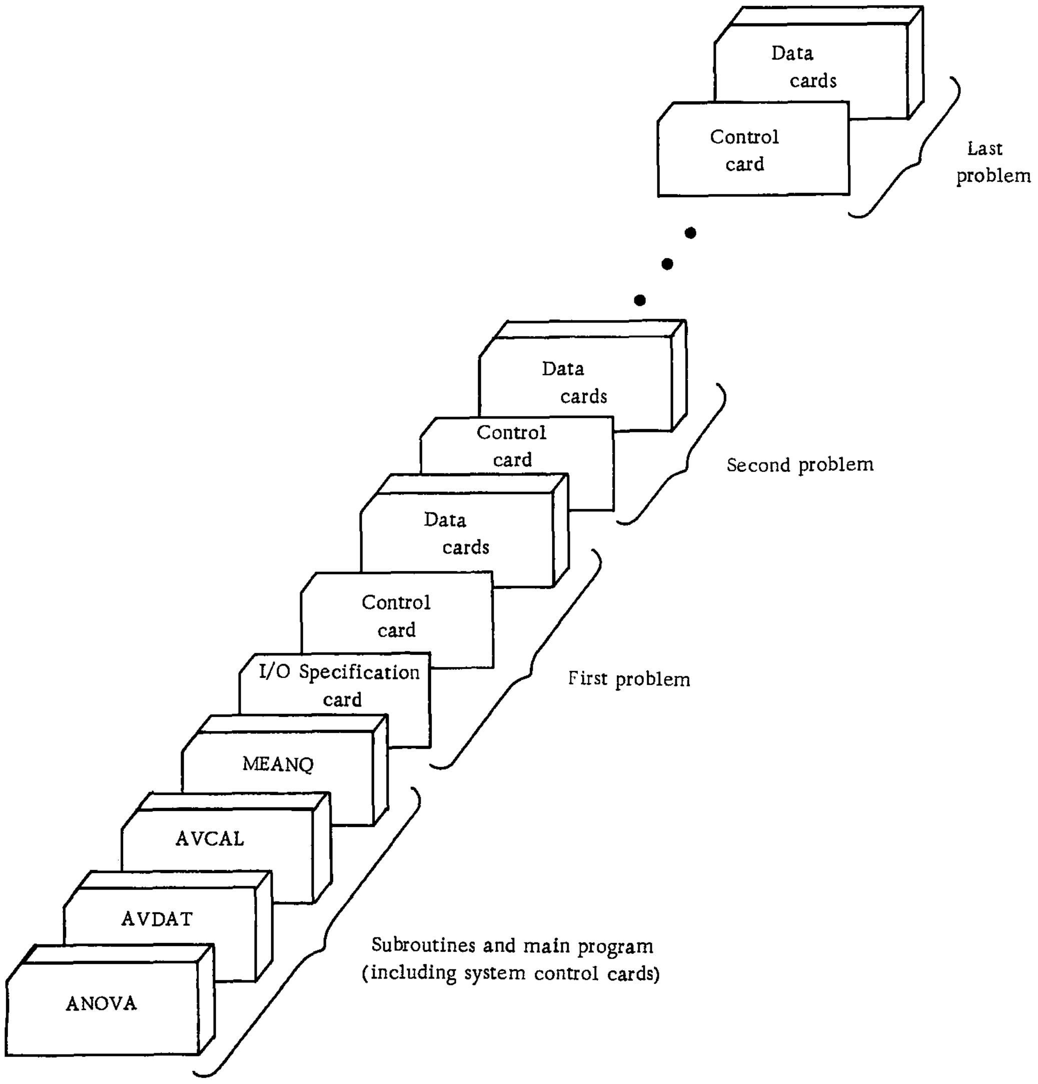


Figure 18. Deck setup (analysis of variance)

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 as presented in Table 6.

Table 6. 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)

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 19. 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 19. Since these data are purely hypothetical, interpretations of the various effects are not made.

Sample

The output listing for the sample problem is shown in Figure 19.

```
ANALYSIS OF VARIANCE.....SAMPLE


LEVELS OF FACTORS
  A          4
  B          3
  C          3
  R          2


GRAND MEAN               9.40277



SOURCE OF                  SUMS OF       DEGREES OF       MEAN
VARIATION                  SQUARES        FREEDOM        SQUARES

 A                       229.04168           3          76.34722
 B                       722.69445           2         361.34722
 AB                     1382.08349           6         230.34722
 C                        55.11111           2          27.55555
 AC                       42.00000           6           7.00000
 BC                       13.13888           4           3.28472
 ABC                     140.75003          12          11.72916
 R                       141.68057           1         141.68057
 AR                       18.81944           3           6.27314
 BR                        6.02777           2           3.01388
 ABR                     176.97222           6          29.49536
 CR                       40.77777           2          20.38888
 ACR                      50.55555           6           8.42592
 BCR                      62.63889           4          15.65972
 ABCR                    151.02780          12          12.58564

 TOTAL                  3233.31641          71
```

Figure 19. Output listing

Program Modification

Noting that storage problems may result, as previously described in "Sample Program Description", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, ANOVA:
   a. The dimension of array X must be greater than or equal to the total number of data points as calculated by the formula in the program capacity section above. For the sample problem the total number of data points is 240 = (4+1)(3+1)(3+1)(2+1).
   b. The dimension of arrays HEAD, LEVEL, ISTEP, KOUNT, and LASTS must be greater than or equal to the number of factors, k. Since there are four factors in the sample problem (4 = 3 original factors + 1 pseudo factor) the value of k is 4.
   c. The dimension of arrays SUMSQ, NDF, and SMEAN must be greater than or equal to n = 2^k-1, where k is the number of factors. For the sample problem the value of n is 15 = 2^4-1.
2. Change in the input format statement of the main program, ANOVA:
   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 data may be keypunched in a two-column field, and, if so, the format is changed to (12F2.0). This format assumes twelve 2-column fields per card, beginning in column 1.

Operating Instructions

The sample analysis-of-variance program is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Sample Main Program for Analysis of Variance - ANOVA

Purpose:

(1) Read the problem parameter card for analysis of variance, (2) Call the subroutines for the calculation of sums of squares, degrees of freedom and mean square, and (3) Print factor levels, grand mean, and analysis of variance table.

Remarks:

The program handles only complete factorial designs. Therefore, other experimental design must be reduced to this form prior to the use of the program.
I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

AVDAT
AVCAL
MEANQ

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.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR ANALYSIS OF VARIANCE - ANOVA
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        CUMULATIVE PRODUCT OF EACH FACTOR LEVEL PLUS ONE (LEVEL(I)+1)
C        FOR I=1 TO K, WHERE K IS THE NUMBER OF FACTORS..
      DIMENSION X(1600)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF FACTORS..
      DIMENSION HEAD(6),LEVEL(6),ISTEP(6),KOUNT(6),LASTS(6)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO 2 TO
C        THE K-TH POWER MINUS 1, ((2**K)-1)..
      DIMENSION SUMSQ(63),NDF(63),SMEAN(63)
C        THE FOLLOWING DIMENSION IS USED TO PRINT FACTOR LABELS IN
C        ANALYSIS OF VARIANCE TABLE AND IS FIXED
      DIMENSION FMT(15)
    1 FORMAT(A4,A2,I2,A4,3X,11(A1,I4)/(A1,I4,A1,I4,A1,I4,A1,I4,A1,I4))
    2 FORMAT(////26H ANALYSIS OF VARIANCE.....A4,A2//)
    3 FORMAT(//18H LEVELS OF FACTORS/(3X,A1,7X,I4))
    4 FORMAT(////11H GRAND MEAN,F20.5////)
    5 FORMAT(//10H SOURCE OF,18X,7HSUMS OF,10X,10HDEGREES OF,9X,4HMEAN/
     110H VARIATION,18X,7HSQUARES,11X,7HFREEDOM,10X,7HSQUARES/)
    6 FORMAT(2X,15A1,F20.5,10X,I6,F20.5)
    7 FORMAT(/7H  TOTAL,10X,F20.5,10X,I6)
    8 FORMAT(12F6.0)
    9 FORMAT(2I2)
C        ...............................................................
      READ(2,9)MX,MY
C        READ PROBLEM PARAMETER CARD
  100 READ (MY,1)PR,PR1,K,BLANK,(HEAD(I),LEVEL(I),I=1,K)
C        PR.....PROBLEM NUMBER (MAY BE ALPHAMERIC)
C        PR1....PROBLEM NUMBER (CONTINUED)
C        K......NUMBER OF FACTORS
C        BLANK..BLANK FIELD
C        HEAD...FACTOR LABELS
C        LEVEL..LEVELS OF FACTORS
C        PRINT PROBLEM NUMBER AND LEVELS OF FACTORS
      WRITE (MX,2)PR,PR1
      WRITE (MX,3)(HEAD(I),LEVEL(I),I=1,K)
C        CALCULATE TOTAL NUMBER OF DATA ELEMENTS
      N=LEVEL(1)
      DO 102 I=2,K
  102 N=N*LEVEL(I)
C        READ ALL INPUT DATA
      READ (MY,8)(X(I),I=1,N)
      CALL AVDAT (K,LEVEL,N,X,L,ISTEP,KOUNT)
      CALL AVCAL (K,LEVEL,X,L,ISTEP,LASTS)
      CALL MEANQ (K,LEVEL,X,GMEAN,SUMSQ,NDF,SMEAN,ISTEP,KOUNT,LASTS)
C        PRINT GRAND MEAN
      WRITE (MX,4)GMEAN
C        PRINT ANALYSIS OF VARIANCE TABLE
      WRITE (MX,5)
      LL=(2**K)-1
      ISTEP(1)=1
      DO 105 I=2,K
  105 ISTEP(I)=0
      DO 110 I=1,15
  110 FMT(I)=BLANK
      NN=0
      SUM=0.0
  120 NN=NN+1
      L=0
      DO 140 I=1,K
      FMT(I)=BLANK
      IF(ISTEP(I)) 130, 140, 130
  130 L=L+1
      FMT(L)=HEAD(I)
  140 CONTINUE
      WRITE (MX,6)(FMT(I),I=1,15),SUMSQ(NN),NDF(NN),SMEAN(NN)
      SUM=SUM+SUMSQ(NN)
      IF(NN-LL) 145, 170, 170
  145 DO 160 I=1,K
      IF(ISTEP(I)) 147, 150, 147
  147 ISTEP(I)=0
      GO TO 160
  150 ISTEP(I)=1
      GO TO 120
  160 CONTINUE
  170 N=N-1
      WRITE (MX,7)SUM,N
      GO TO 100
      END
// DUP
*STORE      WS  UA  ANOVA
// XEQ ANOVA
```

```
 1 2
SAMPLE04        A0004B0003C0003R0002
     3    10     9     8    24     8     9     3     2     8     9     8
     4    12     3     9    22     7    16     2     2     2     7     2
     5    10     5     8    23     9    17     3     2     8     6     3
     2    14     9    13    29    16    11     3     2     7     5     3
     7    11     5     8    28    18    10     6     6     6     5     9
     9    10    27     8    28    16    11     7     8     9     8    15
```

DISCRIMINANT ANALYSIS

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 value is the largest.

The sample problem for discriminant analysis consists of four groups of observations as presented in Table 7. 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 is six in all groups.

Program

Description

The discriminant analysis sample program consists of a main routine, MDISC, and three subroutines:

DMATX
MINV } are from the Scientific Subroutine Package
DISCR

Table 7. **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 four groups
2. Up to ten variables
3. Up to a total number of 100 observations in all groups combined.
4. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than four groups, more than ten variables, or more than 100 observations, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format statement in the sample main program must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, MDISC. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 8	Number of groups	04
9 - 10	Number of variables	06
11 - 15	Number of observations in first group	00008
16 - 20	Number of observations in second group	00007
21 - 25	Number of observations in third group	00007
26 - 30	Number of observations in fourth group	00008
.		
.		
65 - 70	Number of observations in twelfth group (if present)	

If there are more than twelve groups in the problem, continue to the second card in the same manner.

Columns	Contents
1 - 5	Number of observations in thirteenth group
6 - 10	Number of observations in fourteenth group

Leading zeros are not required to be keypunched, but numbers must be right-justified in fields.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 7 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

Deck Setup

Deck setup is shown in Figure 20.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

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. Generalized Mahalanobis D-square
5. Constant and coefficients of each discriminant function

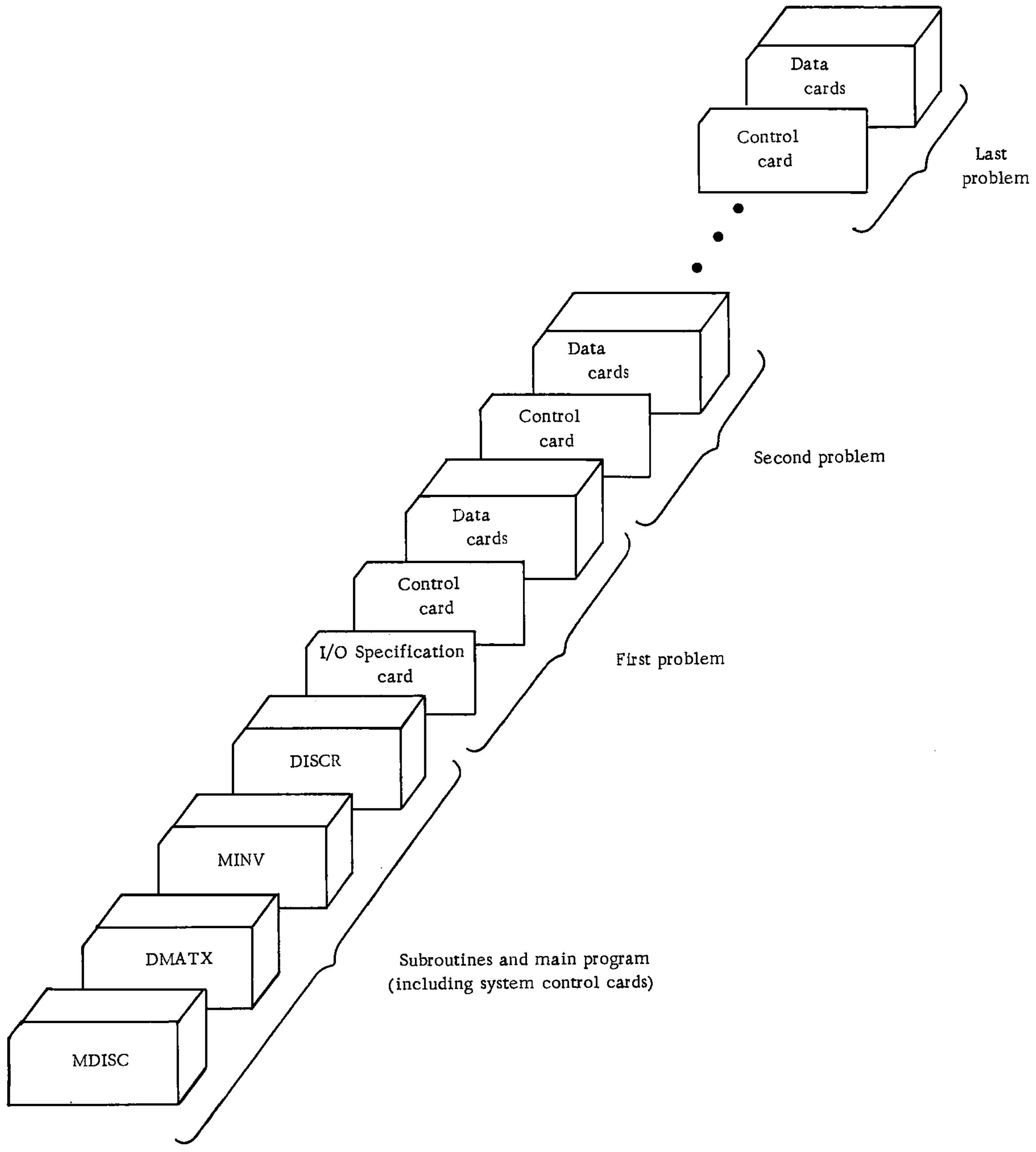


Figure 20. Deck setup (discriminant analysis)

6. Probability associated with the largest discriminant function evaluated for each observation.

Sample

The output listing for the sample problem is shown in Figure 21.

Program Modification

Noting that storage problems may result, as previously discussed in "Sample Program Description", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, MDISC:
    a. The dimension of array N must be greater than or equal to the number of groups, k. Since there are four groups in the sample problem the value of k is 4.
    b. The dimension of array CMEAN must be greater than or equal to the number of variables, m. Since there are six variables in the sample problem the value of m is 6.
    c. The dimension of array XBAR must be greater than or equal to the product of m times k. For the sample problem this product is 24 = 6 x 4.
    d. The dimension of array C must be greater than or equal to the product of (m+1)k. For the sample problem this product is 28 = (6+1)4.
    e. The dimension of array D must be greater than or equal to the product of m times m. For the sample problem this product is 36 = 6 x 6.
    f. The dimension of arrays P and LG must be greater than or equal to the total number of observations in all groups combined, t. For the sample problem this total is 30 = 8 + 7 + 7 + 8.
    g. The dimension of array X must be greater than or equal to the total number of data points that is equal to the product of t

```
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
       7.14285      8.57143      9.57143      7.85714     20.14286     12.57143

GROUP  3  MEANS
       7.85714      7.85714      8.85714      9.28571     17.42857     10.14285

GROUP  4  MEANS
       7.75000      8.00000      6.75000      7.37500     21.37500      9.25000

POOLED DISPERSION MATRIX

ROW  1
      19.61880    -11.16208     -5.21496     -6.09889    -22.74861     -9.54051

ROW  2
     -11.16208     11.94504      5.61812      1.91758     22.60987     10.66757

ROW  3
      -5.21496      5.61812     39.45945      3.93681     16.23487      9.34546

ROW  4
      -6.09889      1.91758      3.93681      9.83309      4.62156      3.83790

ROW  5



     -22.74861     22.60987     16.23487      4.62156     62.78635     30.18268

ROW  6
      -9.54051     10.66757      9.34546      3.83790     30.18268     29.57484


COMMON MEANS
       7.66666      7.96666      7.33333      7.89999     19.39999     10.13333


GENERALIZED MAHALANOBIS D-SQUARE       12.78067


DISCRIMINANT FUNCTION  1

     CONSTANT   *   COEFFICIENTS

    -28.49425   *           2.63868      2.12202     -0.17167      1.91198      0.58476     -0.40476

DISCRIMINANT FUNCTION  2

     CONSTANT   *   COEFFICIENTS

    -29.21008   *           2.61928      2.25227     -0.04816      1.88318      0.43732     -0.21783

DISCRIMINANT FUNCTION  3

     CONSTANT   *   COEFFICIENTS

    -31.86424   *           2.74448      2.39585     -0.06456      2.13259      0.42619     -0.32718

DISCRIMINANT FUNCTION  4

     CONSTANT   *   COEFFICIENTS

    -30.82023   *           2.71858      2.03934     -0.13351      1.94538      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                   0.37043                        1
      3                   0.36260                        1




      4                   0.44189                        1
      5                   0.34453                        1
      6                   0.44216                        3
      7                   0.31786                        2
      8                   0.29272                        2

GROUP  2
                  PROBABILITY ASSOCIATED WITH         LARGEST
 OBSERVATION     LARGEST DISCRIMINANT FUNCTION      FUNCTION NO.
      1                   0.51027                        2
      2                   0.50061                        3
      3                   0.34760                        4
      4                   0.43131                        3
      5                   0.44281                        4
      6                   0.36406                        2
      7                   0.28514                        2

GROUP  3
                  PROBABILITY ASSOCIATED WITH         LARGEST
 OBSERVATION     LARGEST DISCRIMINANT FUNCTION      FUNCTION NO.
      1                   0.67612                        3
      2                   0.46628                        2
      3                   0.54634                        2
      4                   0.66689                        3
      5                   0.30599                        2
      6                   0.33043                        4
      7                   0.39006                        3

GROUP  4
                  PROBABILITY ASSOCIATED WITH         LARGEST
 OBSERVATION     LARGEST DISCRIMINANT FUNCTION      FUNCTION NO.
      1                   0.33727                        4
      2                   0.37474                        1
      3                   0.62340                        4
      4                   0.45696                        1
      5                   0.52173                        2
      6                   0.34061                        4
      7                   0.43135                        4
      8                   0.27848                        1
```

Figure 21. Output listing

times m. For the sample this product is 180 = 30 x 6.

2. Changes in the input format statement of the main program, MDISC:

   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 may be keypunched in two-column fields, and, if so, the format is changed to (6F2.0). This format assumes six 2-column fields per card, beginning in column 1.

Operating Instructions

The sample program for discriminant analysis is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Sample Main Program for Discriminant Analysis - MDISC

Purpose:

(1) Read the problem parameter card and data for discriminant analysis, (2) Call three subroutines to calculate variable means in each group, pooled dispersion matrix, common means of variables, generalized Mahalanobis D square, coefficients of discriminant functions, and probability associated with largest discriminant function of each case in each group, and (3) Print the results.

Remarks:

The number of variables must be greater than or equal to the number of groups.

I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

DMATX
MINV
DISCR

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, section 6.6-6.8.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR DISCRIMINANT ANALYSIS - MDISC           MDISC   1
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC   2
C        NUMBER OF GROUPS, K..                                           MDISC   3
      DIMENSION N(4)                                                     MDISC   4
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC   5
C        NUMBER OF VARIABLES, M..                                        MDISC   6
      DIMENSION CMEAN(10)                                                MDISC   7
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC   8
C        PRODUCT OF M*K..                                                MDISC   9
      DIMENSION XBAR(40)                                                 MDISC  10
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC  11
C        PRODUCT OF (M+1)*K..                                            MDISC  12
      DIMENSION C(44)                                                    MDISC  13
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC  14
C        PRODUCT OF M*M..                                                MDISC  15
      DIMENSION D(100)                                                   MDISC  16
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE  MDISC  17
C        TOTAL OF SAMPLE SIZES OF K GROUPS COMBINED, T (T = N(1)+N(2)+..MDISC  18
C        +N(K))..                                                        MDISC  19
      DIMENSION P(100),LG(100)                                           MDISC  20
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE   MDISC  21
C        TOTAL DATA POINTS WHICH IS EQUAL TO THE PRODUCT OF T*M..        MDISC  22
      DIMENSION X(1000)                                                  MDISC  23
C        ...............................................................MDISC  24
    1 FORMAT(A4,A2,2I2,12I5/(14I5))                                      MDISC  25
    2 FORMAT(////27H DISCRIMINANT ANALYSIS.....A4,A2//19H  NUMBER OF GRMDISC  26
     1OUPS,7X,I3/22H  NUMBER OF VARIABLES,I7/17H  SAMPLE SIZES../12X, MDISC  27
     25HGROUP)                                                           MDISC  28
    3 FORMAT(12X,I3,8X,I4)                                               MDISC  29
    4 FORMAT(//2X)                                                       MDISC  30
    5 FORMAT(12F6.0)                                                     MDISC  31
    6 FORMAT(//6H GROUP,I3,7H  MEANS/(8F15.5))                           MDISC  32
    7 FORMAT(///25H POOLED DISPERSION MATRIX)                            MDISC  33
    8 FORMAT(//4H ROW,I3/(8F15.5))                                       MDISC  34
    9 FORMAT(////13H COMMON MEANS/(8F15.5))                              MDISC  35
   10 FORMAT(////33H GENERALIZED MAHALANOBIS D-SQUARE,F15.5//)           MDISC  36
   11 FORMAT(//22H DISCRIMINANT FUNCTION,I3//6X,27HCONSTANT   *   COEFFIMDISC  37
     1CIENTS//F14.5,7H    *    ,7F14.5/(22X,7F14.5))                     MDISC  38
   12 FORMAT(////60H EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH OBSMDISC  39
     1ERVATION)                                                          MDISC  40
   13 FORMAT(//6H GROUP,I3/19X,27HPROBABILITY ASSOCIATED WITH,11X,7HLARGMDISC  41
     1EST/13H  OBSERVATION,5X,29HLARGEST DISCRIMINANT FUNCTION,8X,12HFUNMDISC  42
     2CTION NO.)                                                         MDISC  43
   14 FORMAT(I7,20X,F8.5,20X,I6)                                         MDISC  44
   15 FORMAT(2I2)                                                        MDISC  45
C        ...............................................................MDISC  46
      READ(2,15)MX,MY                                                    MDISC  47
C        READ PROBLEM PARAMETER CARD                                     MDISC  48
  100 READ(MY,1)PR,PR1,K,M,(N(I),I=1,K)                                  MDISC  49
C        PR.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                     MDISC  50
C        PR1......PROBLEM NUMBER (CONTINUED)                             MDISC  51
C        K........NUMBER OF GROUPS                                       MDISC  52
C        M........NUMBER OF VARIABLES                                    MDISC  53
C        N........VECTOR OF LENGTH K CONTAINING SAMPLE SIZES             MDISC  54
      WRITE (MX,2) PR,PR1,K,M                                            MDISC  55
      DO 110 I=1,K                                                       MDISC  56
  110 WRITE (MX,3) I,N(I)                                                MDISC  57
      WRITE (MX,4)                                                       MDISC  58
C        READ DATA                                                       MDISC  59
      L=0                                                                MDISC  60
      DO 130 I=1,K                                                       MDISC  61
      N1=N(I)                                                            MDISC  62
      DO 120 J=1,N1                                                      MDISC  63
      READ (MY,5) (CMEAN(IJ),IJ=1,M)                                     MDISC  64
      L=L+1                                                              MDISC  65
      N2=L-N1                                                            MDISC  66
      DO 120 IJ=1,M                                                      MDISC  67
      N2=N2+N1                                                           MDISC  68
  120 X(N2)=CMEAN(IJ)                                                    MDISC  69
  130 L=N2                                                               MDISC  70
      CALL DMATX (K,M,N,X,XBAR,D,CMEAN)                                  MDISC  71
C        PRINT MEANS AND POOLED DISPERSION MATRIX                        MDISC  72
      L=0                                                                MDISC  73
      DO 150 I=1,K                                                       MDISC  74
      DO 140 J=1,M                                                       MDISC  75
      L=L+1                                                              MDISC  76
  140 CMEAN(J)=XBAR(L)                                                   MDISC  77
  150 WRITE (MX,6) I,(CMEAN(J),J=1,M)                                    MDISC  78
      WRITE (MX,7)                                                       MDISC  79
      DO 170 I=1,M                                                       MDISC  80
      L=I-M                                                              MDISC  81
      DO 160 J=1,M                                                       MDISC  82
      L=L+M                                                              MDISC  83
  160 CMEAN(J)=D(L)                                                      MDISC  84
  170 WRITE (MX,8) I,(CMEAN(J),J=1,M)                                    MDISC  85
      CALL MINV (D,M,DET,CMEAN,C)                                        MDISC  86
      CALL DISCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG)                         MDISC  87
C        PRINT COMMON MEANS                                              MDISC  88
      WRITE(MX,9) (CMEAN(I),I=1,M)                                       MDISC  89
C        PRINT GENERALIZED MAHALANOBIS D-SQUARE                          MDISC  90
      WRITE (MX,10) V                                                    MDISC  91
C        PRINT CONSTANTS AND COEFFICIENTS OF DISCRIMINANT FUNCTIONS      MDISC  92
      N1=1                                                               MDISC  93
      N2=M+1                                                             MDISC  94
      DO 180 I=1,K                                                       MDISC  95
      WRITE (MX,11) I,(C(J),J=N1,N2)                                     MDISC  96
      N1=N1+(M+1)                                                        MDISC  97
  180 N2=N2+(M+1)                                                        MDISC  98
C        PRINT EVALUATION OF CLASSIFICATION FUNCTIONS FO EACH            MDISC  99
C        OBSERVATION                                                     MDISC100
      WRITE (MX,12)                                                      MDISC101
      N1=1                                                               MDISC102
      N2=N(1)                                                            MDISC103
      DO 210 I=1,K                                                       MDISC104
      WRITE (MX,13) I                                                    MDISC105
      L=0                                                                MDISC106
      DO 190 J=N1,N2                                                     MDISC107
      L=L+1                                                              MDISC108
  190 WRITE (MX,14) L,P(J),LG(J)                                         MDISC109
      IF(I-K) 200, 100, 100                                              MDISC110
  200 N1=N1+N(I)                                                         MDISC111
      N2=N2+N(I+1)                                                       MDISC112
  210 CONTINUE                                                           MDISC113
      STOP                                                               MDISC114
      END                                                                MDISC115
// DUP
*STORE      WS  UA  MDISC
// XEQ MDISC   01
*LOCALMDISC,DMATX,MINV,DISCR
```

```
 1 2                                                                            1
SAMPLE0406000080000700007000008                                                  2
     3    10     9     8    24     8                                            3
     4    12     3     8    22     7                                            4
     9     3     2     8     9     8                                            5
    16     2     2     2     7     2                                            6
     5    10     5     8    23     9                                            7
    17     3     2     8     6     3                                            8
     2    10     9     8    29    16                                            9
     7    10     5     8    28    18                                           10
     9    10    27     8    28    16                                           11
    11     7     8     9     8    15                                           12
     8    10     2     8    27    16                                           13
     1     6     8    14    14    13                                           14
     7     8     9     6    18     2                                           15
```

7	9	8	2	19	9	16
7	10	5	8	27	17	17
3	11	9	15	20	10	18
9	4	10	7	9	9	19
4	13	10	7	21	15	20
8	5	16	16	16	7	21
6	9	10	5	23	11	22
8	10	5	8	27	16	23
17	3	2	7	6	3	24
3	10	8	8	23	8	25
4	12	3	8	23	7	26
9	3	2	8	21	7	27
15	2	2	2	7	2	28
9	10	26	8	27	16	29
8	9	2	8	26	16	30
7	8	6	9	18	2	31
7	10	5	8	26	16	32

FACTOR ANALYSIS

Problem Description

A principal component solution and the varimax rotation of the factor matrix are performed. Principal component 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 factor analysis consists of 23 observations with nine variables as presented in Table 8. 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.

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 factor analysis sample program consists of a main routine, FACTO, and six subroutines:

CORRE EIGEN TRACE LOAD VARMX	are from the Scientific Subroutine Package
DATA	is a special input subroutine

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 29 variables
2. Up to 99,999 observations
3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 30 variables, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format statement in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, FACTO. 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	09
14 - 19	Value used to limit the number of eigenvalues of	0001.0

Columns	Contents	For Sample Problem
14 - 19 (cont)	correlation coefficients. Only those eigenvalues greater than or equal to this value are retained in the analysis. (A decimal point must be specified.)	

Leading zeros are not required to be keypunched, but numbers must be right-justified in fields.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 8 is keypunched on a separate card using the format (12F6.0). 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

Deck setup is shown in Figure 22.

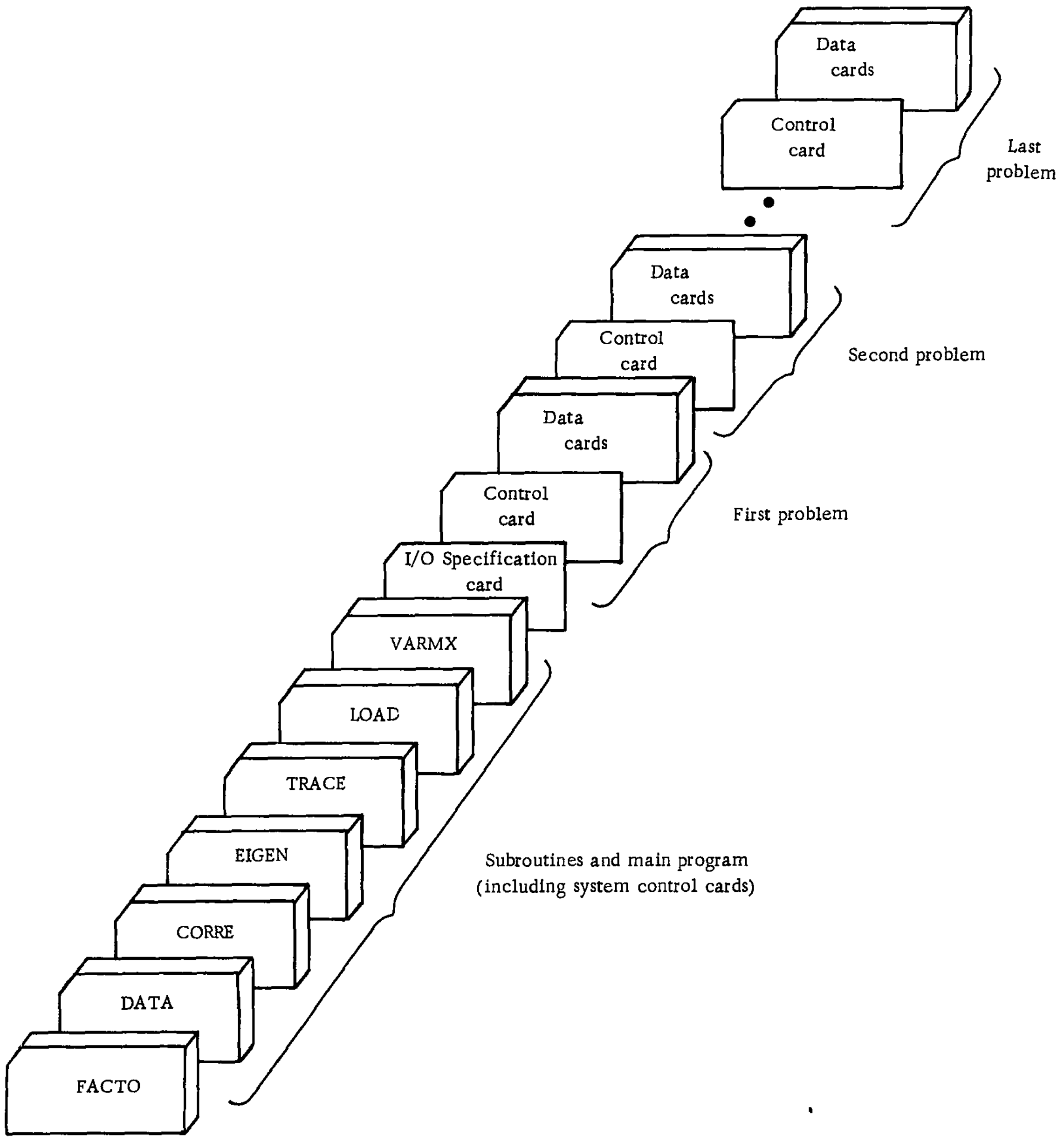


Figure 22. Deck setup (factor analysis)

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The output of the sample program for factor 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 the 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 23.

Program Modification

Noting that storage problems may result, as previously described in "Sample Program Description", program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, FACTO:
   a. The dimension of arrays B, D, S, T, and XBAR must be greater than or equal to the number of variables, m. Since there are nine variables in the sample problem the value of m is 9.
   b. The dimension of array V must be greater than or equal to the product of m times m. For the sample problem this product is 81 = 9 x 9.
   c. The dimension of array R must be greater than $\frac{(m+1)m}{2}$

```
FACTOR ANALYSIS.....SAMPLE

  NO. OF CASES        23
  NO. OF VARIABLES     9


MEANS
      9.30434     12.60869     23.00000     18.00000     12.86956     34.82608     54.00000     19.39130
     25.13043

STANDARD DEVIATIONS
      2.70411      4.59979      5.33427      8.33393      3.13780      9.29149     14.87828      5.56563
      6.09249

CORRELATION COEFFICIENTS

ROW  1
    1.00000    0.34986    0.11974    0.12101    0.21917   -0.09548    0.20901   -0.12908    0.05817

ROW  2
    0.34986    1.00000    0.41311    0.35572   -0.08242   -0.09100    0.29622   -0.32044    0.35387

ROW  3
    0.11974    0.41311    1.00000    0.41512   -0.43178   -0.08345   -0.10251    0.03215    0.27832

ROW  4
    0.12101    0.35572    0.41512    1.00000   -0.31287   -0.50364    0.49855    0.22539    0.59890

ROW  5
    0.21917   -0.08242   -0.43178   -0.31287    1.00000   -0.22999    0.03310   -0.00475   -0.30341

ROW  6
   -0.09548   -0.09100   -0.08345   -0.50364   -0.22999    1.00000   -0.44520   -0.25440   -0.37456

ROW  7
    0.20901    0.29622   -0.10251    0.49855    0.03310   -0.44520    1.00000   -0.28049    0.60123

ROW  8
   -0.12908   -0.32044    0.03215    0.22539   -0.00475   -0.25440   -0.28049    1.00000    0.13515




ROW  9
    0.05817    0.35387    0.27832    0.59890   -0.30341   -0.37456    0.60123    0.13515    1.00000


EIGENVALUES
    2.94988    1.64370    1.55516    1.06581

CUMULATIVE PERCENTAGE OF EIGENVALUES
    0.32776    0.51039    0.68319    0.80161


EIGENVECTORS

VECTOR  1
    0.16437    0.34835    0.28797    0.49660   -0.16806   -0.32921    0.39935    0.01287    0.47516

VECTOR  2
    0.34836    0.06551   -0.44646   -0.11893    0.61209   -0.26427    0.38859   -0.24844   -0.06013

VECTOR  3
   -0.29899   -0.46825   -0.23533    0.17377    0.14467   -0.43545    0.01880    0.61587    0.12470

VECTOR  4
    0.54440    0.16909    0.38288    0.04162    0.30536   -0.16163   -0.43410    0.40283   -0.23788


FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
    0.28231    0.44663   -0.37286    0.56203

VARIABLE  2
    0.59830    0.08399   -0.58393    0.17456

VARIABLE  3
    0.49459   -0.57240   -0.29347    0.39526

VARIABLE  4
    0.85293   -0.15248    0.21670    0.04297

VARIABLE  5
   -0.28865    0.78475    0.18042    0.31525

VARIABLE  6
   -0.56543   -0.33882   -0.54303   -0.16686




VARIABLE  7
    0.68589    0.49821    0.02344   -0.44816

VARIABLE  8
    0.02211   -0.31852    0.76802    0.41587

VARIABLE  9
    0.81613   -0.07710    0.15550   -0.24559


ITERATION       VARIANCES
  CYCLE
    0            0.211288
    1            0.336136
    2            0.397020
    3            0.403003
    4            0.405175
    5            0.405528
    6            0.405580
    7            0.405587
    8            0.405587
    9            0.405587
   10            0.405587
   11            0.405587
   12            0.405587


ROTATED FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
    0.05497    0.07183   -0.05578    0.85017

VARIABLE  2
    0.29328   -0.39652   -0.35580    0.60549

VARIABLE  3
    0.05113   -0.82493    0.15068    0.32984

VARIABLE  4
    0.74040   -0.41401    0.24579    0.13971

VARIABLE  5
   -0.09090    0.80662    0.13524    0.39228

VARIABLE  6
   -0.68285   -0.21579   -0.44983   -0.20502

VARIABLE  7
    0.86996    0.18299   -0.34918    0.08830

VARIABLE  8
    0.03602   -0.05499    0.91375   -0.15962

VARIABLE  9
    0.80531   -0.32759    0.00993   -0.02379


CHECK ON COMMUNALITIES

VARIABLE        ORIGINAL          FINAL          DIFFERENCE
    1            0.73409         0.73409          0.00000
    2            0.73648         0.73647          0.00000
    3            0.81464         0.81463          0.00000
    4            0.79954         0.79953          0.00000
    5            0.83109         0.83106          0.00001
    6            0.75725         0.75724          0.00000
    7            0.92006         0.92005          0.00001
    8            0.86476         0.86475          0.00001
    9            0.75651         0.75650          0.00000
```

Figure 23. Output listing

For the sample problem, this number is

$$45 = \frac{(9+1)9}{2}$$

2. Changes in the input format statement of the special input subroutine, DATA:
   a. 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 may be keypunched in two-column fields, and, if so, the format is changed to (9F2. 0). This format assumes nine 2-column fields per card, beginning in column 1.
   b. The special input subroutine, DATA, 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.

Operating Instructions

The sampleprogram for factor analysis is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

If the number of factors to be rotated is one or zero, the following message will be printed:

ONLY____FACTOR RETAINED, NO ROTATION.

The program skips rotation and goes to the next problem if it is present.

Sample Main Program for Factor Analysis - FACTO

Purpose:

(1) Read the problem parameter card, (2) Call five subroutines to perform a principal component solution and the varimax rotation of a factor matrix, and (3) Print the results.

Remarks:

I/O specifications transmitted to subroutines by COMMON.

Input card:

Column 2 MX -	Logical unit number for output.
Column 4 MY -	Logical unit number for input.

Subroutines and function subprograms required:
(which, in turn, calls the subroutine named DATA.)

CORRE
EIGEN
TRACE
LOAD
VARMX

Method:

Refer to "BMD Computer Programs Manual", edited by W. J. Dixon, UCLA, 1964.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C         SAMPLE MAIN PROGRAM FOR FACTOR ANALYSIS - FACTO
C         THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C         NUMBER OF VARIABLES, M..
      DIMENSION B(29),D(29),S(29),T(29),XBAR(29)
C         THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C         PRODUCT OF M*M..
      DIMENSION V(841)
C         THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO
C         (M+1)*M/2..
      DIMENSION R(435)
C         THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 51..
          DIMENSION TV(51)
      COMMON MX,MY
    1 FORMAT(////21H FACTOR ANALYSIS.....A4,A2//3X,12HNO. OF CASES,4X,
     1I6/3X,16HNO. OF VARIABLES,I6/)
    2 FORMAT(//6H MEANS/(8F15.5))
    3 FORMAT(//20H STANDARD DEVIATIONS/(8F15.5))
    4 FORMAT(//25H CORRELATION COEFFICIENTS)
    5 FORMAT(//4H ROW,I3/(10F12.5))
    6 FORMAT(///12H EIGENVALUES/(10F12.5))
    7 FORMAT(//37H CUMULATIVE PERCENTAGE OF EIGENVALUES/(10F12.5))
    8 FORMAT(///13H EIGENVECTORS)
    9 FORMAT(//7H VECTOR,I3/(10F12.5))
   10 FORMAT(///16H FACTOR MATRIX (,I3,9H FACTORS))
   11 FORMAT(//9H VARIABLE,I3/(10F12.5))
   12 FORMAT(///10H ITERATION,7X, 9HVARIANCES/8H   CYCLE)
   13 FORMAT(I6,F20.6)
   14 FORMAT(///24H ROTATED FACTOR MATRIX (,I3,9H FACTORS))
   15 FORMAT(//9H VARIABLE,I3/(10F12.5))
   16 FORMAT(///23H CHECK ON COMMUNALITIES//9H VARIABLE,7X,8HORIGINAL,
     112X,5HFINAL,10X,10HDIFFERENCE)
   17 FORMAT(I6,3F18.5)
   18 FORMAT(A4,A2,I5,I2,F6.0)
   19 FORMAT(//5H ONLY,I2,30H FACTOR RETAINED. NO ROTATION )
   20 FORMAT(2I2)
      READ(2,20)MX,MY
C         READ PROBLEM PARAMETER CARD
  100 READ (MY,18)PR,PR1,N,M,CON
C         PR.........PROBLEM NUMBER (MAY BE ALPHAMERIC)
C         PR1........PROBLEM NUMBER (CONTINUED)
C         N..........NUMBER OF CASES
C         M..........NUMBER OF VARIABLES
C         CON........CONSTANT USED TO DECIDE HOW MANY EIGENVALUES
C                    TO RETAIN
      WRITE (MX,1)PR,PR1,N,M
      IO=0
      X=0.0
      CALL CORRE (N,M,IO,X,XBAR,S,V,R,D,B,T)
C         PRINT MEANS
      WRITE (MX,2)(XBAR(J),J=1,M)
C         PRINT STANDARD DEVIATIONS
      WRITE (MX,3)(S(J),J=1,M)
C         PRINT CORRELATION COEFFICIENTS
      WRITE (MX,4)
      DO 120 I=1,M
      DO 110 J=1,M
      IF(I-J) 102, 104, 104
  102 L=I+(J*J-J)/2
      GO TO 110
  104 L=J+(I*I-I)/2
  110 D(J)=R(L)
  120 WRITE (MX,5)I,(D(J),J=1,M)
      MV=0
      CALL EIGEN (R,V,M,MV)
      CALL TRACE (M,R,CON,K,D)
C         PRINT EIGENVALUES
      DO 130 I=1,K
      L=I+(I*I-I)/2
  130 S(I)=R(L)
      WRITE (MX,6)(S(J),J=1,K)
C         PRINT CUMULATIVE PERCENTAGE OF EIGENVALUES
      WRITE (MX,7)(D(J),J=1,K)
C         PRINT EIGENVECTORS
      WRITE (MX,8)
      L=0
      DO 150 J=1,K
      DO 140 I=1,M
      L=L+1
  140 D(I)=V(L)
  150 WRITE (MX,9)J,(D(I),I=1,M)
      CALL LOAD (M,K,R,V)
C         PRINT FACTOR MATRIX
      WRITE (MX,10)K
      DO 180 I=1,M
      DO 170 J=1,K
      L=M*(J-1)+I
  170 D(J)=V(L)
  180 WRITE (MX,11)I,(D(J),J=1,K)
      IF(K-1) 185, 185, 188
  185 WRITE (MX,19)K
      GO TO 100
  188 CALL VARMX (M,K,V,NC,TV,B,T,D)
```

```
C         PRINT VARIANCES
      NV=NC+1
      WRITE (MX,12)
      DO 190 I=1,NV
      NC=I-1
  190 WRITE (MX,13)NC,TV(I)
C         PRINT ROTATED FACTUR MATRIX
      WRITE (MX,14)K
      DO 220 I=1,M
      DO 210 J=1,K
      L=M*(J-1)+I
  210 S(J)=V(L)
  220 WRITE(MX,15)I,(S(J),J=1,K)
C         PRINT COMMUNALITIES
      WRITE (MX,16)
      DO 230 I=1,M
  230 WRITE (MX,17)I,B(I),T(I),D(I)
      GO TO 100
      END
// DUP
*STORE      WS  UA  FACTO
// XEQ FACTO   01
*LOCALFACTO,CORRE,EIGEN,TRACE,LOAD,VARMX
```

```
 1 2
SAMPLE00023090001.0
     7     7     9     7    15    36    60    15    24
    13    18    25    15    13    35    61    18    30
     9    18    24    23    12    43    62    14    31
     7    13    25    36    11    12    63    26    32
     6     8    20     7    15    46    18    28    15
    10    12    30    11    10    42    27    12    17
     7     6    11     7    15    35    60    20    25
    16    19    25    16    13    30    64    20    30
     9    22    26    24    13    40    66    15    32
     8    15    26    30    13    10    66    25    34
     8    10    20     8    17    40    20    30    18
     9    12    28    11     8    45    30    15    19
    11    17    21    30    10    45    60    17    30
     9    16    26    27    14    31    59    19    17
    10    15    24    18    12    29    48    18    26
    11    11    30    19    19    26    57    20    30
    16     9    16    20    18    31    60    21    17
     9     8    19    14    16    33    67     9    19
     7    18    22     9    15    37    62    11    20
     8    11    23    18     9    36    61    22    24
     6     6    27    23     7    40    55    24    31
    10     9    26    26    10    37    57    27    29
     8    10    26    15    11    42    59    20    28
```

```
SAMPLE INPUT SUBROUTINE - DATA

PURPOSE
   READ AN OBSERVATION (M DATA VALUES) FROM INPUT DEVICE.
   THIS SUBROUTINE IS CALLED BY THE SUBROUTINE CORRE AND MUST
   BE PROVIDED BY THE USER.  IF SIZE AND LOCATION OF DATA
   FIELDS ARE DIFFERENT FROM PROBLEM TO PROBLEM, THIS SUB-
   ROUTINE MUST BE RECOMPILED WITH A PROPER FORMAT STATEMENT.

USAGE
   CALL DATA (M,D)

DESCRIPTION OF PARAMETERS
   M - THE NUMBER OF VARIABLES IN AN OBSERVATION.
   D - OUTPUT VECTOR OF LENGTH M CONTAINING THE OBSERVATION
       DATA.

REMARKS
   THE TYPE OF CONVERSION SPECIFIED IN THE FORMAT MUST BE
   EITHER F OR E.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   NONE
```

```
      SUBROUTINE DATA (M,D)
      DIMENSION D(1)
      COMMON MX,MY
    1 FORMAT(12F6.0)
C        READ AN OBSERVATION FROM INPUT DEVICE.
      READ (MY,1) (D(I),I=1,M)
      RETURN
      END
```

TRIPLE EXPONENTIAL SMOOTHING

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 a main routine, EXPON, and one subroutine, EXSMO, from the Scientific Subroutine Package.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 1000 data points in a given time series
2. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 1000 data points, the dimension statement in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the sample main program must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

One control card is required for each problem and is read by the main program, EXPON. 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, $(0.0 < \alpha < 1.0)$	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

Leading zeros are not required to be keypunched, but numbers must be right-justified in fields.

Data Cards

Time series data are keypunched using the format (12F6.0). This format assumes that each data point is keypunched in a six-column field and twelve fields per card.

Deck Setup

Deck setup is shown in Figure 24.

Sample

The listing of input cards for the sample problem is presented at the end of the sample main program.

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 25.

Program Modification

Noting that storage problems may result, as previously discussed in "Sample Program Description", program capacity can be increased or decreased by making changes in the dimension statement. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statement of the main program, EXPON:

The dimension of arrays X and S must be greater than or equal to the number of data points in time series, NX. Since there are 38 data points in the sample problem, the value of NX is 38.

2. Changes in the input format statement of the main program, EXPON:

Only the format statement for input data may be changed. Since sample data are three-digit numbers, rather than using six-column fields as in the sample program, each data point may be keypunched in a three-column field and 24 fields per card. If so, the format is changed to (24F3.0).

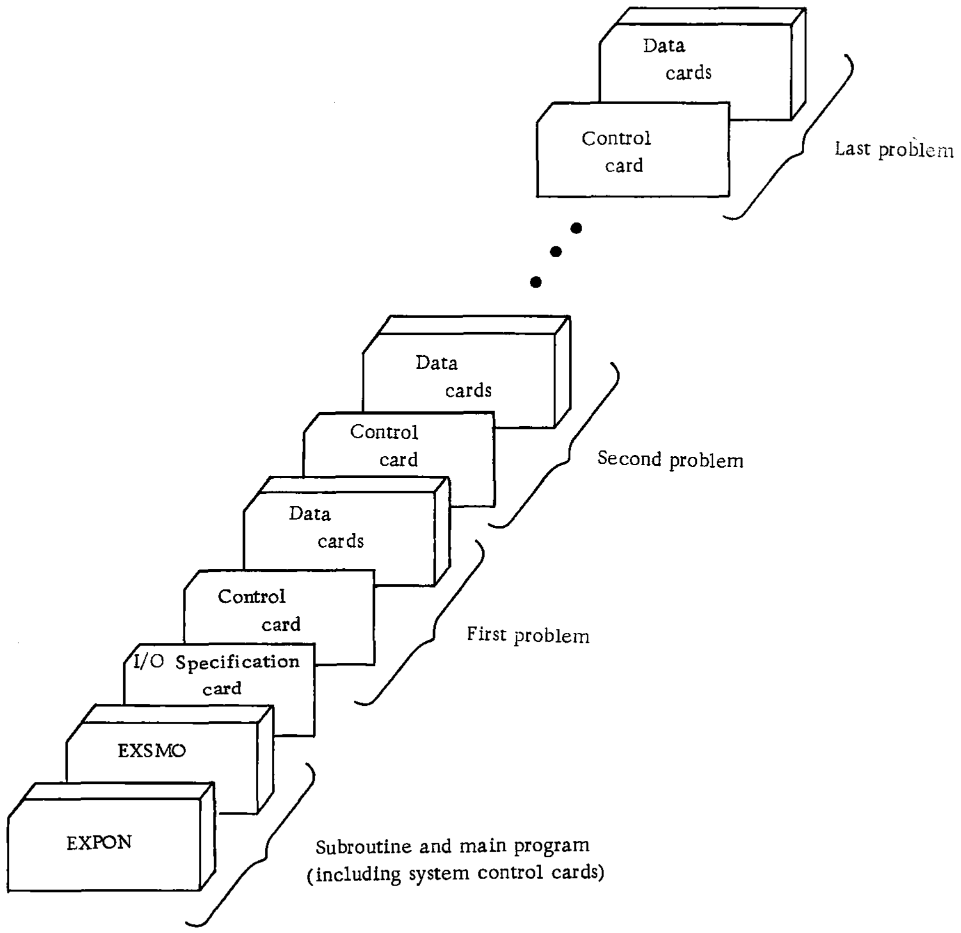


Figure 24. Deck setup (triple exponential smoothing)

```
TRIPLE EXPONENTIAL SMOOTHING.....SAMPLE

NUMBER OF DATA POINTS    38
SMOOTHING CONSTANT    0.100


COEFFICIENTS              A                B                C


ORIGINAL              0.00000          0.00000          0.00000


UPDATED             484.80169          1.71278          0.04165



                          SMOOTHED DATA
       INPUT DATA          (FORECAST)
        430.00006          430.00006
        426.00006          426.00006
        422.00006          422.00006
        419.00006          418.00006
        414.00006          414.29998
        413.00006          410.23993
        412.00006          407.08990
        409.00006          404.66839
        411.00006          402.22406
        417.00006          401.25134
        422.00006          402.64642
        430.00006          405.61694
        438.00006          410.71417
        441.00006          417.47027
        447.00006          423.99908
        455.00006          431.18335
        461.00006          439.43420
        453.00006          447.87902
        448.00006          452.21600
        449.00006          454.10571
        454.00006          455.80731
        463.00006          458.54632
        470.00006          463.30535
        472.00006          469.06439
        476.00006          474.09521
        481.00006          479.11016
        483.00006          484.38598
        487.00006          488.94592
        491.00006          493.50836
        492.00006          498.05432
        485.00006          501.66992
        486.00006          502.12536
        482.00006          502.44427
        479.00006          501.16723






        479.00006          498.92730
        476.00006          496.84124
        472.00006          494.00787
        470.00006          490.30413
```

Figure 25. Output listing

Operating Instructions

The sample program for triple exponential smoothing is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Sample Main Program for Triple Exponential Smoothing - EXPON

Purpose:

(1) Read the problem parameter card and a time series, (2) Call the subroutine EXSMO to smooth the time series, and (3) Print the result.

Remarks:

A smoothing constant specified in the problem parameter card must be greater than zero but less than one in order to obtain reasonable results.

I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

EXSMO.

Method:

Refer to R. G. Brown, "Smoothing, Forecasting and Prediction of Discrete Time Series", Prentice-Hall, N. J., 1963, pp. 140 to 144.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE MAIN PROGRAM FOR TRIPLE EXPONENTIAL SMOOTHING - EXPON
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF DATA POINTS IN A GIVEN TIME SERIES.
      DIMENSION X(1000),S(1000)
    1 FORMAT(A4,A2,I4,F5.0,3F10.0)
    2 FORMAT(12F6.0)
    3 FORMAT(////34H TRIPLE EXPONENTIAL SMOOTHING.....,A4,A2//22H NUMBER
     1 OF DATA POINTS,I6/19H SMOOTHING CONSTANT,F9.3/)
    4 FORMAT(//13H COEFFICIENTS,9X,1HA,14X,1HB,14X,1HC)
    5 FORMAT(//9H ORIGINAL,F19.5,2F15.5)
    6 FORMAT(//8H UPDATED,F20.5,2F15 .5/)
    7 FORMAT(//27X,13HSMOOTHED DATA/7X,10HINPUT DATA,12X,10H(FORECAST))
    8 FORMAT(F17.5,8X,F15.5)
    9 FORMAT(2I2)
      READ(2,9)MX,MY
C        READ PROBLEM PARAMETER CARD
  100 READ (MY,1) PR,PR1,NX,AL,A,B,C
C        PR......PROBLEM NUMBER (MAY BE ALPHAMERIC)
C        PR1.....PROBLEM NUMBER (CONTINUED)
C        NX......NUMBER OF DATA POINTS IN TIME SERIES
C        AL......SMOOTHING CONSTANT
C        A,B,C...COEFFICIENTS OF THE PREDICTION EQUATION
      WRITE (MX,3) PR,PR1,NX,AL
C        PRINT ORIGINAL COEFFICIENTS
      WRITE (MX,4)
      WRITE (MX,5) A,B,C
C        READ TIME SERIES DATA
      READ (MY,2) (X(I),I=1,NX)
      CALL EXSMO (X,NX,AL,A,B,C,S)
C        PRINT UPDATED COEFFICIENTS
      WRITE (MX,6) A,B,C
C        PRINT INPUT AND SMOOTHED DATA
      WRITE (MX,7)
      DO 200 I=1,NX
  200 WRITE (MX,8) X(I),S(I)
      GO TO 100
      END
// DUP
*STORE      WS  UA  EXPON
// XEQ EXPON
```

```
 1 2
SAMPLE  38  0.1        0.0        0.0        0.0
   430   426   422   419   414   413   412   409   411   417   422   430
   438   441   447   455   461   453   448   449   454   463   470   472
   476   481   483   487   491   492   485   486   482   479   479   476
   472   470
```

MATRIX ADDITION

Problem Description

An input matrix is added to another input matrix to form a resultant matrix. Each set of input matrices and the corresponding output matrix is printed. The procedure is repeated until all sets of input matrices have been processed.

Program

Description

The matrix addition sample program consists of a main routine, ADSAM, and four subroutines:

MADD LOC	are from the Scientific Subroutine Package
MATIN MXOUT	are sample subroutines for matrix input and output

Capacity

Matrix size has arbitrarily been set at 650 data elements. Therefore, if a problem satisfies the above condition, no modification in the sample program is necessary. However, if there are more than 650 elements, the dimension statement in the sample main program must be modified to handle this particular problem. The general rules for program modification are described later.

Input

I/O Specification Card

Each input matrix must be preceded by a control card with the following format:

Columns	Contents	For Sample Problem
1 - 2	Blank	
3 - 6	Up to four-digit identification code	0001
7 - 10	Number of rows in matrix	0008
11 - 14	Number of columns in matrix	0011
15 - 16	Storage mode of matrix 0 for general matrix 1 for symmetric matrix 2 for diagonal matrix	0

Each input matrix must be followed by a card with a 9-punch in column 1.

Data Cards

Data cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in a field, or may be omitted; however, all numbers must be right-justified. The number in each field may be preceded by blanks. Data elements must be punched by row. A row may continue from card to card. However, each new row must start in the first field of the next card. Only the upper triangular portion of a symmetric or the diagonal elements of a diagonal matrix are contained on data cards. The first element of each new row will be the diagonal element for a matrix with symmetric or diagonal storage mode. Columns 71-80 of data cards may be used for identification, sequence numbering, etc.

A blank card after the last pair of input matrices terminates the run.

Deck Setup

The deck setup is shown in Figure 26.

Sample

A listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

Both sets of input matrices and the output matrix are printed. The resultant matrix is printed for any sized array as a general matrix regardless of the storage mode. Each seven-column grouping is headed with the matrix code number, dimensions, and storage mode. Columns and rows are headed with their respective number. The code number for the output matrix is derived by adding the code numbers for the input matrices.

Sample

The output listing for the sample problem is shown in Figure 27.

Program Modification

Noting that storage problems may result, as previously described in "Sample Program Description", the maximum matrix size acceptable to the sample

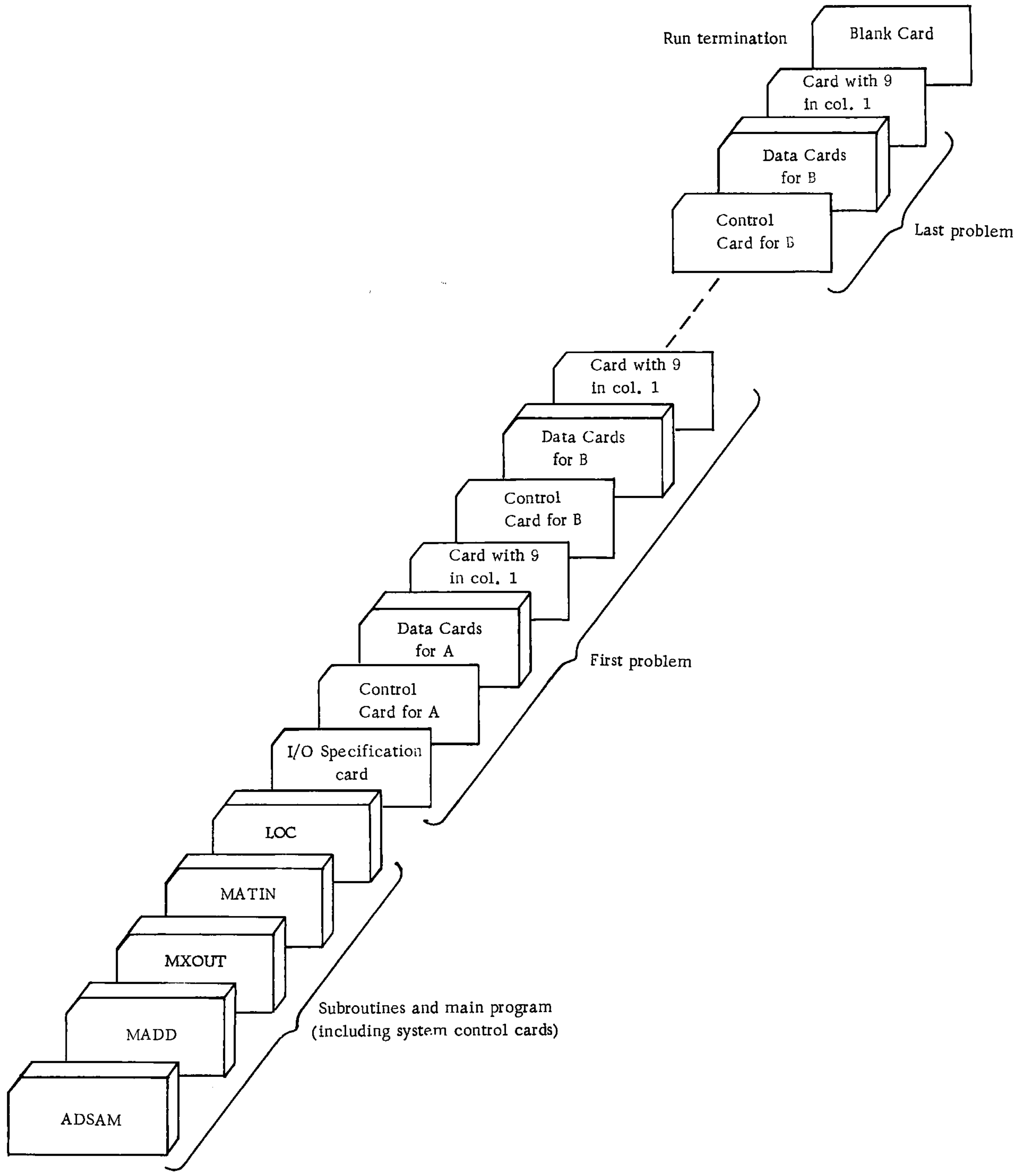


Figure 26. Deck setup (matrix addition)

program may be increased or decreased by making the following changes in ADSAM:

1. Modify the DIMENSION statement to reflect the number of elements for A, B, and R.
2. Insert the same number in the third parameter of the two CALL MATIN statements (20 and 45).

The output listing is set for 120 print positions across the page and double spacing. This can be changed by means of the last two arguments in the three CALL MXOUT statements in ADSAM (statements 40, 80, 90).

Operating Instructions

The matrix addition sample program is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix: DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX (matrix code no.). GO ON TO NEXT CASE.
2. Input matrices do not have the same dimensions: MATRIX DIMENSIONS NOT CONSISTENT. GO ON TO NEXT CASE.
3. Number of data cards does not correspond to that required by parameter card: INCORRECT NUMBER OF DATA CARDS FOR MATRIX (matrix code no.). EXECUTION TERMINATED.

Error conditions 1 and 2 allow the computer run to continue. Error condition 3, however, terminates execution and requires another run to process succeeding cases.

```
MATRIX     1        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       1             2             3             4             5             6
  ROW  1    0.760100E 00  0.627180E 00  0.100000E 01  0.708684E 00  0.405851E 00  0.314260E-02
  ROW  2    0.664408E 00  0.100000E 01  0.627180E 00  0.619465E 00  0.354757E 00  0.274700E-02
  ROW  3    0.100000E 01  0.664408E 00  0.760100E 00  0.750750E 00  0.429942E 00  0.332910E-02
  ROW  4    0.696326E 00  0.574558E 00  0.657310E 00  0.649224E 00  0.371800E 00  0.287890E-02
  ROW  5    0.744684E 00  0.614459E 00  0.702958E 00  0.694310E 00  0.397620E 00  0.307890E-02
  ROW  6    0.675176E 00  0.557106E 00  0.637344E 00  0.629504E 00  0.360507E 00  0.279150E-02
  ROW  7    0.332910E-02  0.274700E-02  0.314260E-02  0.310390E-02  0.177760E-02  0.100000E 01
  ROW  8    0.429942E 00  0.354757E 00  0.405851E 00  0.400859E 00  0.100000E 01  0.177760E-02

MATRIX     1        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       7             8             9             10            11
  ROW  1    0.687660E 00  0.675176E 00  0.863591E 00  0.744684E 00  0.696326E 00
  ROW  2    0.601087E 00  0.557106E 00  0.712572E 00  0.614459E 00  0.574558E 00
  ROW  3    0.728478E 00  0.637344E 00  0.815202E 00  0.702958E 00  0.657310E 00
  ROW  4    0.629964E 00  0.629504E 00  0.805174E 00  0.694310E 00  0.649224E 00
  ROW  5    0.673713E 00  0.360507E 00  0.461109E 00  0.397620E 00  0.371800E 00
  ROW  6    0.610829E 00  0.279150E-02  0.357050E-02  0.307890E-02  0.287890E-02
  ROW  7    0.301190E-02  0.610829E 00  0.781287E 00  0.673713E 00  0.629964E 00
  ROW  8    0.388967E 00  0.100000E 01  0.724121E 00  0.624418E 00  0.583870E 00

MATRIX     2        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       1             2             3             4             5             6



  ROW  1    0.750750E 00  0.619465E 00  0.708684E 00  0.100000E 01  0.400859E 00  0.310390E-02
  ROW  2    0.744684E 00  0.614459E 00  0.702958E 00  0.694310E 00  0.397620E 00  0.307890E-02
  ROW  3    0.863591E 00  0.712572E 00  0.815202E 00  0.805174E 00  0.461109E 00  0.357050E-02
  ROW  4    0.696326E 00  0.574558E 00  0.657310E 00  0.649224E 00  0.371800E 00  0.287890E-02
  ROW  5    0.675176E 00  0.557106E 00  0.637344E 00  0.629504E 00  0.360507E 00  0.279150E-02
  ROW  6    0.744684E 00  0.614459E 00  0.702958E 00  0.694310E 00  0.397620E 00  0.307890E-02
  ROW  7    0.863591E 00  0.712572E 00  0.815202E 00  0.805174E 00  0.461109E 00  0.357050E-02
  ROW  8    0.760100E 00  0.627180E 00  0.100000E 01  0.708684E 00  0.405851E 00  0.314260E-02

MATRIX     2        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       7             8             9             10            11
  ROW  1    0.679201E 00  0.724121E 00  0.100000E 01  0.798668E 00  0.746805E 00
  ROW  2    0.673713E 00  0.624418E 00  0.798668E 00  0.100000E 01  0.643978E 00
  ROW  3    0.781287E 00  0.583870E 00  0.746805E 00  0.643978E 00  0.100000E 01
  ROW  4    0.629964E 00  0.100000E 01  0.664408E 00  0.760100E 00  0.750750E 00
  ROW  5    0.610829E 00  0.728478E 00  0.601087E 00  0.687660E 00  0.679201E 00
  ROW  6    0.673713E 00  0.429942E 00  0.354757E 00  0.405851E 00  0.400859E 00
  ROW  7    0.781287E 00  0.760100E 00  0.627180E 00  0.100000E 01  0.708684E 00
  ROW  8    0.687660E 00  0.696326E 00  0.574558E 00  0.657310E 00  0.649224E 00

MATRIX     3        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       1             2             3             4             5             6
  ROW  1    0.151085E 01  0.124664E 01  0.170868E 01  0.170868E 01  0.806711E 00  0.624650E-02
  ROW  2    0.140909E 01  0.161445E 01  0.133013E 01  0.131377E 01  0.752377E 00  0.582590E-02
  ROW  3    0.186359E 01  0.137698E 01  0.157530E 01  0.155592E 01  0.891052E 00  0.689959E-02
  ROW  4    0.139265E 01  0.114911E 01  0.131462E 01  0.129844E 01  0.743600E 00  0.575780E-02
  ROW  5    0.141986E 01  0.117156E 01  0.134030E 01  0.132381E 01  0.758127E 00  0.587040E-02
  ROW  6    0.141986E 01  0.117156E 01  0.134030E 01  0.132381E 01  0.758127E 00  0.587040E-02



  ROW  7    0.866920E 00  0.715319E 00  0.818344E 00  0.808277E 00  0.462887E 00  0.100357E 01
  ROW  8    0.119004E 01  0.981937E 00  0.140585E 01  0.110954E 01  0.140585E 01  0.492020E-02

MATRIX     3        8 ROWS      11 COLUMNS       STORAGE MODE 0
     COLUMN       7             8             9             10            11
  ROW  1    0.136686E 01  0.139929E 01  0.186359E 01  0.154335E 01  0.144313E 01
  ROW  2    0.127480E 01  0.118152E 01  0.151124E 01  0.161445E 01  0.121853E 01
  ROW  3    0.150976E 01  0.122121E 01  0.156200E 01  0.134693E 01  0.165731E 01
  ROW  4    0.125992E 01  0.162950E 01  0.146958E 01  0.145441E 01  0.139997E 01
  ROW  5    0.128434E 01  0.108898E 01  0.106219E 01  0.108528E 01  0.105100E 01
  ROW  6    0.128434E 01  0.432734E 00  0.358327E 00  0.408930E 00  0.403738E 00
  ROW  7    0.784299E 00  0.137093E 01  0.140846E 01  0.167371E 01  0.133864E 01
  ROW  8    0.107662E 01  0.169632E 01  0.129868E 01  0.128172E 01  0.123309E 01

END OF CASE
```

Figure 27. Output listing

Sample Main Program for Matrix Addition - ADSAM

Purpose:
Matrix addition sample program.

Remarks:
I/O specifications transmitted to subroutines by COMMON.
Input card:
Column 2 MX - Logical unit number for output.
Column 4 MY - Logical unit number for input.

Subroutines and function subprograms required:
MADD
MATIN
MXOUT
LOC

Method:
Two input matrices are read from the standard input device. They are added and the resultant matrix is listed on the standard output device. This can be repeated for any number of pairs of matrices until a blank card is encountered.

```
// FOR

*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C         SAMPLE MAIN PROGRAM FOR MATRIX ADDITION - ADSAM
C         MATRICES ARE DIMENSIONED FOR 1000 ELEMENTS. THEREFORE, PRODUCT
C         OF NUMBER OF ROWS BY NUMBER OF COLUMNS CANNOT EXCEED 1000.
      DIMENSION A(650),B(650),R(650)
      COMMON MX,MY
   10 FORMAT(////16H MATRIX ADDITION)
   11 FORMAT(//45H DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)
   12 FORMAT(//21H EXECUTION TERMINATED)
   13 FORMAT(//33H MATRIX DIMENSIONS NOT CONSISTENT)
   14 FORMAT(//43H INCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)
   15 FORMAT(//19H GO ON TO NEXT CASE)
   16 FORMAT(//12H END OF CASE)
   17 FORMAT(2I2)
      READ(2,17)MX,MY
      WRITE(MX,10)
   20 CALL MATIN(ICODA,A, 100,NA,MA,MSA,IER)
      IF( NA ) 25,95,25
   25 IF(IER-1) 40,30,35
   30 WRITE(MX,11) ICODA
      GO TO 45
   35 WRITE(MX,14) ICODA
   37 WRITE(MX,12)
      GO TO 95
   40 CALL MXOUT(ICODA,A,NA,MA,MSA,60,120,2)
   45 CALL MATIN(ICODB,B, 100,NB,MB,MSB,IER)
      IF(IER-1) 60,50,55
   50 WRITE(MX,11)ICODB
      WRITE(MX,15)
      GO TO 20
   55 WRITE(MX,14) ICODB
      GO TO 37
   60 IF(NA-NB) 75,70,75
   70 IF(MA-MB) 75,80,75
   75 WRITE(MX,13)
      WRITE(MX,15)
      GO TO 20
   80 CALL MXOUT(ICODB,B,NB,MB,MSB,60,120,2)
      ICODR=ICODA+ICODB
      CALL MADD(A,B,R,NA,MA,MSA,MSB)
      MSR=MSA
      IF(MSA-MSB) 90,90,85
   85 MSR=MSB
   90 CALL MXOUT(ICODR,R,NA,MA,MSR,60,120,2)
      WRITE(MX,16)
      GO TO 20
   95 STOP
      END
// DUP
*STORE      WS  UA  ADSAM
// XEQ ADSAM
```

```
1 2
 00010008001100
0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
0.6751766 0.8635910 0.7446845 0.6963269
0.6644085 1.0000000 0.6271802 0.6194650 0.3547574 0.0027470 0.6010878
0.5571068 0.7125728 0.6144597 0.5745585
1.0000000 0.6644085 0.7601008 0.7507505 0.4299425 0.0033291 0.7284786
0.6373449 0.8152021 0.7029582 0.6573101
0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
0.6295047 0.8051740 0.6943108 0.6492243
0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
0.3605070 0.4611099 0.3976204 0.3718001
0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296
0.0027915 0.0035705 0.0030789 0.0028789
0.0033291 0.0027470 0.0031426 0.0031039 0.0017776 1.0000000 0.0030119
0.6108296 0.7812874 0.6737132 0.6299642
0.4299425 0.3547574 0.4058519 0.4008593 1.0000000 0.0017776 0.3889673
1.0000000 0.7241215 0.6244183 0.5838704
9
 00020008001100
0.7507505 0.6194650 0.7086843 1.0000000 0.4008593 0.0031039 0.6792011
0.7241215 1.0000000 0.7986682 0.7468050
0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
0.6244183 0.7986682 1.0000000 0.6439786
0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874
0.5838704 0.7468050 0.6439786 1.0000000
0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
1.0000000 0.6644085 0.7601008 0.7507505 0.4299425 0.0033291 0.7284786
0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296
0.7284786 0.6010878 0.6876602 0.6792011 0.3889673 0.0030119 1.0000000
0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
0.4299425 0.3547574 0.4058519 0.4008593 1.0000000 0.0017776 0.3889673
0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874
0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
9
```

```
   SUBROUTINE MATIN

   PURPOSE
      READS CONTROL CARD AND MATRIX DATA ELEMENTS FROM LOGICAL
      UNIT 5

   USAGE
      CALL MATIN(ICODE,A,ISIZE,IROW,ICOL,IS,IER)

   DESCRIPTION OF PARAMETERS
      ICODE-UPON RETURN, ICODE WILL CONTAIN FOUR DIGIT
            IDENTIFICATION CODE FROM MATRIX PARAMETER CARD
      A    -DATA AREA FOR INPUT MATRIX
      ISIZE-NUMBER OF ELEMENTS DIMENSIONED BY USER FOR AREA A
      IROW -UPON RETURN, IROW WILL CONTAIN ROW DIMENSION FROM
            MATRIX PARAMETER CARD
      ICOL -UPON RETURN, ICOL WILL CONTAIN COLUMN DIMENSION FROM
            MATRIX PARAMETER CARD
      IS   -UPON RETURN, IS WILL CONTAIN STORAGE MODE CODE FROM
            MATRIX PARAMETER CARD WHERE
            IS=0 GENERAL MATRIX
            IS=1 SYMMETRIC MATRIX
            IS=2 DIAGONAL MATRIX
      IER  -UPON RETURN, IER WILL CONTAIN AN ERROR CODE WHERE
            IER=0   NO ERROR
            IER=1   ISIZE IS LESS THAN NUMBER OF ELEMENTS IN
                    INPUT MATRIX
            IER=2   INCORRECT NUMBER OF DATA CARDS

   REMARKS
      NONE

   SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
      LOC

   METHOD
      SUBROUTINE ASSUMES THAT INPUT MATRIX CONSISTS OF PARAMETER
      CARD FOLLOWED BY DATA CARDS
      PARAMETER CARD HAS THE FOLLOWING FORMAT
        COL. 1- 2 BLANK
        COL. 3- 6 UP TO FOUR DIGIT IDENTIFICATION CODE
        COL. 7-10 NUMBER OF ROWS IN MATRIX
        COL.11-14 NUMBER OF COLUMNS IN MATRIX
        COL.15-16 STORAGE MODE OF MATRIX WHERE
             0 - GENERAL MATRIX
             1 - SYMMETRIC MATRIX
             2 - DIAGONAL MATRIX
      DATA CARDS ARE ASSUMED TO HAVE SEVEN FIELDS OF TEN COLUMNS
      EACH.  DECIMAL POINT MAY APPEAR ANYWHERE IN A FIELD.  IF NO
      DECIMAL POINT IS INCLUDED, IT IS ASSUMED THAT THE DECIMAL
      POINT IS AT THE END OF THE 10 COLUMN FIELD. NUMBER IN EACH
      FIELD MAY BE PRECEDED BY BLANKS.  DATA ELEMENTS MUST BE
      PUNCHED BY ROW.  A ROW MAY CONTINUE FROM CARD TO CARD.
      HOWEVER EACH NEW ROW MUST START IN THE FIRST FIELD OF THE
      NEXT CARD.  ONLY THE UPPER TRIANGULAR PORTION OF A SYMMETRIC
      OR THE DIAGONAL ELEMENTS OF A DIAGONAL MATRIX ARE CONTAINED
      ON DATA CARDS.  THE FIRST ELEMENT OF EACH NEW ROW WILL BE
      THE DIAGONAL ELEMENT FOR A MATRIX WITH  SYMMETRIC OR
      DIAGONAL STORAGE MODE. COLUMNS 71-80 OF DATA CARDS MAY BE
      USED FOR IDENTIFICATION, SEQUENCE NUMBERING, ETC..
      THE LAST DATA CARD FOR ANY MATRIX MUST BE FOLLOWED BY A CARD
      WITH A 9 PUNCH IN COLUMN 1.
```

```
      SUBROUTINE MATIN(ICODE,   A,ISIZE,IROW,ICOL,IS,IER)
      DIMENSION A(1)
      DIMENSION CARD(8)
      COMMON MX,MY
    1 FORMAT(7F10.0)
    2 FORMAT(I6,2I4,I2)
    3 FORMAT(I1)
      IDC=7
      IER=0
      READ( MY,2)ICODE,IROW,ICOL,IS
      CALL LOC(IROW,ICOL,ICNT,IROW,ICOL,IS)
      IF(ISIZE-ICNT)6,7,7
    6 IER=1
    7 IF (ICNT)38,38,8
    8 ICOLT=ICOL
      IROCR=1
C        COMPUTE NUMBER OF CARDS FOR THIS ROW
   11 IRCOS=(ICOLT-1)/IDC+1
      IF(IS-1)15,15,12
   12 IRCOS=1
C        SET UP LOOP FOR NUMBER OF CARDS IN ROW
   15 DO 31 K=1,IRCOS
      READ(MY,1)(CARD(I),I=1,IDC)
C        SKIP THROUGH DATA CARDS IF INPUT AREA TOO SMALL
      IF(IER)16,16,31
   16 L=0
C        COMPUTE COLUMN NUMBER FOR FIRST FIELD IN CURRENT CARD
      JS=(K-1)*IDC+ICOL-ICOLT+1
```

```
   SUBROUTINE MXOUT

   PURPOSE
      PRODUCES AN OUTPUT LISTING OF ANY SIZED ARRAY ON
      LOGICAL UNIT 1
```

```
USAGE
   CALL MXOUT(ICODE,A,N,M,MS,LINS,IPOS,ISP)

DESCRIPTION OF PARAMETERS
   ICODE- INPUT CODE NUMBER TO BE PRINTED ON EACH OUTPUT PAGE
   A-NAME OF OUTPUT MATRIX
   N-NUMBER OF ROWS IN A
   M-NUMBER OF COLUMNS IN A
   MS-STORAGE MODE OF A WHERE MS=
           0-GENERAL
           1-SYMMETRIC
           2-DIAGONAL
   LINS-NUMBER OF PRINT LINES ON THE PAGE (USUALLY 60)
   IPOS-NUMBER OF PRINT POSITIONS ACROSS THE PAGE (USUALLY 132)
   ISP-LINE SPACING CODE, 1 FOR SINGLE SPACE, 2 FOR DOUBLE
       SPACE

REMARKS
   NONE

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   LOC

METHOD
   THIS SUBROUTINE CREATES A STANDARD OUTPUT LISTING OF ANY
   SIZED ARRAY WITH ANY STORAGE MODE. EACH PAGE IS HEADED WITH
   THE CODE NUMBER,DIMENSIONS AND STORAGE MODE OF THE ARRAY.
   EACH COLUMN AND ROW IS ALSO HEADED WITH ITS RESPECTIVE
   NUMBER.
```

```
      SUBROUTINE MXOUT (ICODE,A,N,M,MS,LINS,IPOS,ISP)                 MXOUT   1
      DIMENSION A(1),B(8)                                             MXOUT   2
      COMMON MX,MY                                                    MXOUT   3
    1 FORMAT(////5X, 7HMATRIX ,I5,6X,I3,5H ROWS,6X,I3,8H COLUMNS,    MXOUT   4
     18X,13HSTORAGE MODE ,I1,/)                                       MXOUT   5
    2 FORMAT(12X,8HCOLJMN  ,7(3X,I3,10X)//)                           MXOUT   6
    4 FORMAT(7X,4HROW ,I3,7(E16.6))                                   MXOUT   7
    5 FORMAT(/,7X,4HROW ,I3,7(E16.6))                                 MXOUT   8
      J=1                                                             MXOUT   9
C        WRITE HEADING                                                MXOUT  10
      NEND=IPOS/16-1                                                  MXOUT  11
      LEND = (LINS/ISP)-10                                            MXOUT  12
   10 LSTRT=1                                                         MXOUT  13
   20 WRITE(MX,1)ICODE,N,M,MS                                         MXOUT  14
      JNT=J+NEND-1                                                    MXOUT  15
      IF(JNT-M)33,33,32                                               MXOUT  16
   32 JNT=M                                                           MXOUT  17
   33 CONTINUE                                                        MXOUT  18
      WRITE(MX,2)(JCUR,JCUR=J,JNT)                                    MXOUT  19
      LTEND = LSTRT+LEND-1                                            MXOUT  20
      DO 80 L=LSTRT,LTEND                                             MXOUT  21
C        FORM OUTPUT RJW LINE                                         MXOUT  22
      DO 55 K=1,NEND                                                  MXOUT  23
      KK=K                                                            MXOUT  24
      JT = J+K-1                                                      MXOUT  25
      CALL LOC(L,JT,IJNT,N,M,MS)                                      MXOUT  26
      B(K)=0.0                                                        MXOUT  27
      IF(IJNT)50,50,45                                                MXOUT  28
   45 B(K)=A(IJNT)                                                    MXOUT  29
   50 CONTINUE                                                        MXOUT  30
C        CHECK IF LAST COLUMN.  IF YES GO TO 60                       MXOUT  31
      IF(JT-M) 55,60,60                                               MXOUT  32
   55 CONTINUE                                                        MXOUT  33
C        END OF LINE, NOW WRITE                                       MXOUT  34
   60 IF(ISP-1)65,65,70                                               MXOUT  35
   65 WRITE(MX,4)L,(B(JW),JW=1,KK)                                    MXOUT  36
      GO TO 75                                                        MXOUT  37
   70 WRITE(MX,5)L,(B(JW),JW=1,KK)                                    MXOUT  38
C        IF END OF ROWS,GO CHECK COLUMNS                              MXOUT  39
   75 IF(N-L)85,85,80                                                 MXOUT  40
   80 CONTINUE                                                        MXOUT  41
C        WRITE NEW HEADING                                            MXOUT  42
      LSTRT=LSTRT+LEND                                                MXOUT  43
      GO TO 20                                                        MXOUT  44
C        END OF COLUMNS, THEN RETURN                                  MXOUT  45
   85 IF(JT-M)90,95,95                                                MXOUT  46
   90 J=JT+1                                                          MXOUT  47
      GO TO 10                                                        MXOUT  48
   95 RETURN                                                          MXOUT  49
      END                                                             MXOUT  50
```

NUMERICAL QUADRATURE INTEGRATION

Problem Description

The tabulated values of a function for a given spacing are integrated. Multiple sets of tabulated values may be processed.

Program

Description

The numerical quadrature integration program consists of a main routine QDINT, and one subroutine, QSF, from the Scientific Subroutine Package.

Capacity

The capacity of the sample program and the format for data input have been set up as follows:

1. Up to 500 tabulated values of a function
2. (7F10.0) format for input data cards

Therefore, if the problem satisfies the above conditions, no modification to the sample program is necessary. However, if there are more than 500 values to be integrated the dimension statement in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format statement in the sample main program must be modified. The general rules for program modification are described later.

Input

I/O Specification Card

Each integration requires a parameter card with the following format:

Columns	Contents	For Sample Problem
1 - 5	Up to 5-digit numeric identification code	12345
6 - 10	Number of tabulated values for this function	0020
11 - 20	Interval between tabulated values	1.0

The first two parameters consist of up to five digits with no decimal point (FORMAT (2I5)). Note that the second parameter may not exceed 500. The third parameter consists of up to ten digits (FORMAT) (F10.0).

Data Cards

Data cards are assumed to be seven fields of ten columns each. The decimal point may appear anywhere in the field, or be omitted, but the number must be right-justified. The number in each field may be preceded by blanks. Columns 71 through 80 of the data cards may be used for identification, sequence numbering, etc. If there are more than seven tabulated values, the values should continue from card to card with seven values per card, until the number of values specified in the parameter card has been reached.

A blank card following the last set of data terminates the run.

Deck Setup

The deck setup is shown in Figure 28.

Sample

A listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The identification code number, number of tabulated input values, the interval for the tabulated values, and the resultant integral values at each step are printed.

Sample

The output listing for the sample problem is shown in Figure 29.

Program Modification

Noting that storage problems may result, as previously discussed in "Sample Program Description", the maximum number of tabulated values acceptable to the sample program may be increased. Input data in a different format can also be handled by providing a specific format statement.

1. Modify the DIMENSION statement in QDINT so that the size of array Z is equal to the maximum number of tabulated values.

2. Changes to the format of the parameter cards and data cards may be made by modifying FORMAT statements 10 and 32, respectively, in QDINT.

```
INTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBROUTINE QSF

FUNCTION  12345      20 TABULATED VALUES     INTERVAL = 0.10000002E 01

      RESULTANT VALUE OF INTEGRAL AT EACH STEP IS
 0.00000000E 00 0.19999983E 01 0.39999995E 01 0.59999981E 01 0.79999990E 01 0.99999981E 01
 0.11999998E 02 0.13999996E 02 0.15999996E 02 0.17999996E 02 0.19999996E 02 0.21999992E 02
 0.23999992E 02 0.25999988E 02 0.27999988E 02 0.29999984E 02 0.31999984E 02 0.33999984E 02
 0.35999984E 02 0.37999977E 02



INTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBROUTINE QSF

FUNCTION    543      10 TABULATED VALUES     INTERVAL = 0.10000002E 01

      RESULTANT VALUE OF INTEGRAL AT EACH STEP IS
 0.00000000E 00 0.14999959E 01 0.39999995E 01 0.74999952E 01 0.11999998E 02 0.17499996E 02
 0.23999996E 02 0.31499992E 02 0.39999992E 02 0.49499984E 02
```

Figure 29. Output listing

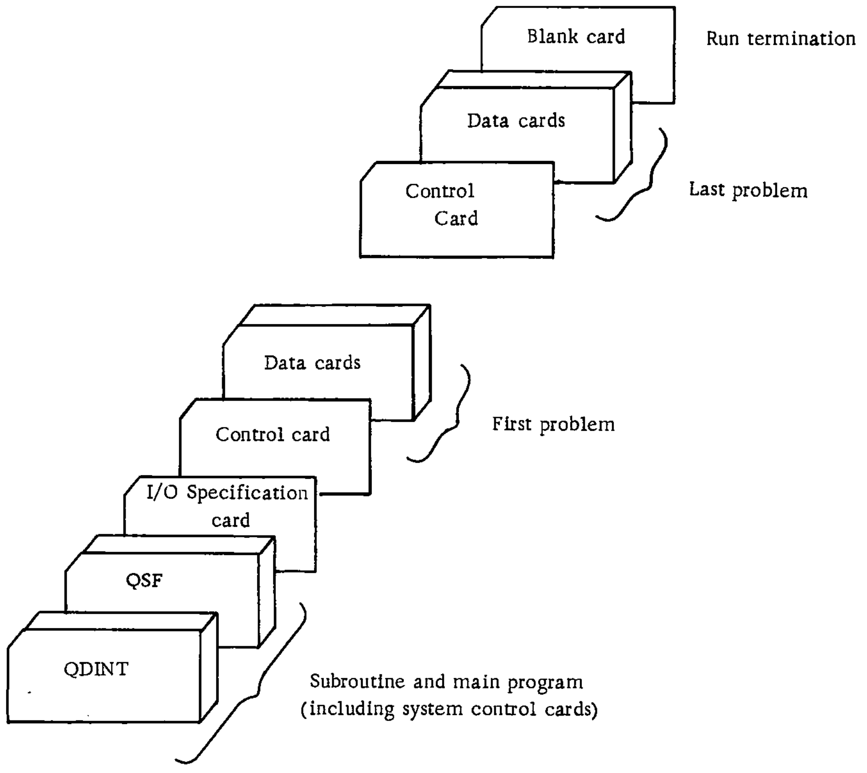


Figure 28. Deck setup (numerical quadrature integration)

Operating Instructions

The numerical quadrature integration sample program is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following conditions will result in error messages:

1. The number of tabulated values specified in the parameter card is less than or equal to two: ILLEGAL CONDITION. NUMBER OF TABULATED VALUES IS LESS THAN THREE.

   The program will continue to read data cards until the next problem is reached.

2. The interval specified in the parameter card is zero: ILLEGAL CONDITION. SPECIFIED INTERVAL IS ZERO.

   The program will continue to read data cards until the next problem is reached.

Sample Program for Integration of a Tabulated Function by Numerical Quadrature - QDINT

Purpose:

Integrates a set of tabulated values for F(X) given the number of values and their spacing.

Remarks:

The number of values must be more than two and the spacing greater than zero.
I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

QSF

Method:

Reads control card containing the code number, number of values, and the spacing of the function values contained on the following data cards. Data cards are then read and integration is performed. More than one control card and corresponding data can be integrated in one run. Execution is terminated by a blank control card.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE PROGRAM FOR INTEGRATION OF A TABULATED FUNCTION BY      QDINT  1
C        NUMERICAL QUADRATURE - QDINT                                   QDINT  2
C        THE FOLLOWING DIMENSION MUST BE AS LARGE AS THE MAXIMUM NUMBER QDINT  3
C        OF TABULATED VALUES TO BE INTEGRATED                           QDINT  4
      DIMENSION Z(500)                                                  QDINT  5
   10 FORMAT (2I5,F10.0)                                                QDINT  6
   20 FORMAT(//////' INTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBQDINTM01
     1ROUTINE QSF' ///11H FUNCTION  ,I5,3X,I5,17H TABULATED VALUES,     QDINTM02
     25X,10HINTERVAL =,E15.8/)                                          QDINTM03
   22 FORMAT(/18H ILLEGAL CONDITION/)                                   QDINT 10
   23 FORMAT(/46H NUMBER OF TABULATED VALUES IS LESS THAN THREE)        QDINTM04
   24 FORMAT(/27H SPECIFIED INTERVAL IS ZERO)                           QDINT 12
   30 FORMAT(/7X,  'RESULTANT VALUE OF INTEGRAL AT EACH STEP IS',/      QDINTM05
     1(1H ,6E15.8))                                                     QDINTM06
   31 FORMAT(2I2)                                                       QDINT 14
   32 FORMAT(7F10.0)                                                    QDINT 15
      READ(2,31)MX,MY                                                   QDINT 16
   35 READ(MY,10)ICOD,NUMBR,SPACE                                       QDINT 17
      IF(ICOD+NUMBR)70,70,38                                            QDINT 18
   70 STOP                                                              QDINT 19
   38 WRITE(MX,20)ICOD,NUMBR,SPACE                                      QDINT 20
      IF(NUMBR-3)100,50,50                                              QDINTM07
   50 READ(MY,32)(Z(I),I=1,NUMBR)                                       QDINT 22
      CALL QSF (SPACE,Z,Z,NUMBR)                                        QDINTM08
      IF(SPACE)60,200,60                                                QDINTM09
   60 WRITE(MX,30)(Z(I),I=1,NUMBR)                                      QDINTM10
      GO TO 35                                                          QDINT 26
  100 WRITE(MX,22)                                                      QDINT 27
      WRITE(MX,23)                                                      QDINT 28
      READ(MY,32)(Z(I),I=1,NUMBR)                                       QDINTM11
      GO TO 35                                                          QDINT 29
  200 WRITE(MX,22)                                                      QDINT 30
      WRITE(MX,24)                                                      QDINT 31
      GO TO 35                                                          QDINT 32
      END                                                               QDINT 33
// DUP
*STORE      WS  UA  QDINT
// XEQ QDINT
```

```
 1 2                                                                        1
12345   20       1.0                                                        2
       2.0       2.0       2.0       2.0       2.0       2.0       2.0      3
       2.0       2.0       2.0       2.0       2.0       2.0       2.0      4
       2.0       2.0       2.0       2.0       2.0       2.0                5
  543   10       1.0                                                        6
       1.0       2.0       3.0       4.0       5.0       6.0       7.0      7
       8.0       9.0      10.0                                              8
                                                                            9
```

RUNGE-KUTTA INTEGRATION

Problem Description

A differential equation of the form:

$$\frac{dy}{dx} = f(x, y)$$

is integrated with initial conditions as specified in a parameter card. The differential equation is defined in the form of a function subprogram that is provided by the user.

Program

Description

The Runge-Kutta integration program consists of a main routine, RKINT, one subroutine, RK2, from the Scientific Subroutine Package, and one user-supplied function subprogram, FUN, which defines the differential equation to be integrated.

Capacity

Up to 500 values of the integral may be tabulated.

Input

I/O Specification Card

Each integration requires a control card with the following format:

Columns	Contents	For Sample Problem
1 - 10	Initial value of $X = X_0$	1.0
11 - 20	Initial value of $Y = Y(X_0)$	0.0

Columns	Contents	For Sample Problem
21 - 30	Step size	0.01
31 - 35	Number of steps required between tabulated values	10
36 - 40	Total number of tabulated values required	30

The first three parameters consist of up to ten digits.

(FORMAT (F10.0))

The last two parameters consist of up to four digits plus a blank.

(FORMAT (15))

Multiple parameter cards may be used.

A blank card terminates the run.

Data Cards

None.

Blank Card

Run termination.

Deck Setup

The deck setup is shown in Figure 30.

Sample

A listing of the input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The values for the initial conditions and the tabulated values of the integral are printed.

Sample

The output listing for the sample problem is shown in Figure 31.

Program Modification

Noting that storage problems may result, as previously described in "Sample Program Description", the maximum number of tabulated values acceptable to the sample program may be increased. Input data in a different format can also be handled by providing a specific format statement.

1. Modify the DIMENSION statement in RKINT so that array A is as large as the number of tabulated values.

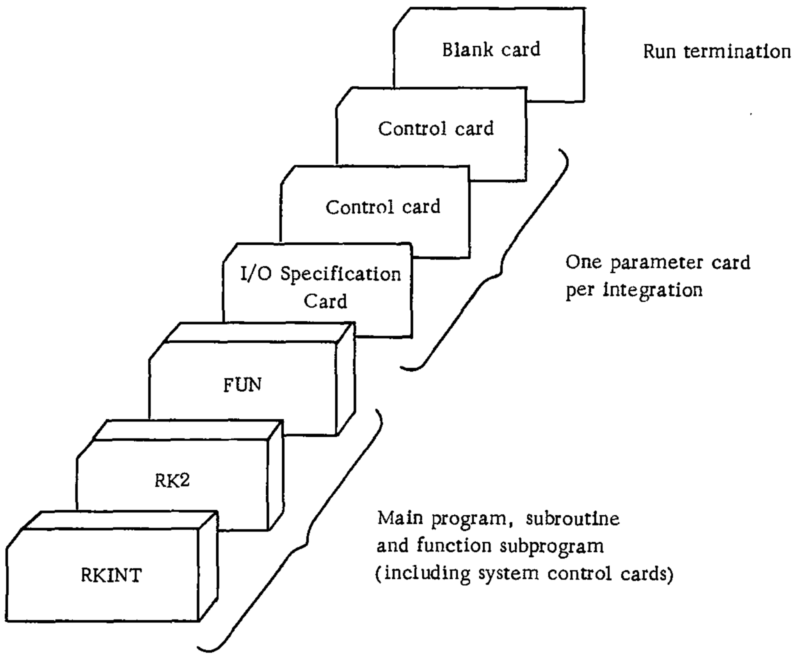

Blank card
Run termination
Control card
Control card
I/O Specification Card
One parameter card per integration
FUN
RK2
RKINT
Main program, subroutine and function subprogram (including system control cards)

Figure 30. Deck setup (Runge-Kutta integration)

```
SOLUTION OF DY/DX=FUN(X,Y) BY RK2 SUBROUTINE

  H=  0.010  X0=  1.000  Y0=  0.000

    X              Y(X)


   1.10          0.95310136E-01
   1.20          0.18232139E 00
   1.30          0.26236397E 00
   1.40          0.33647167E 00
   1.50          0.40546423E 00
   1.60          0.47000247E 00
   1.70          0.53062677E 00
   1.80          0.58778464E 00
   1.90          0.64185142E 00
   2.00          0.69314432E 00
   2.10          0.74193394E 00
   2.20          0.78845346E 00
   2.30          0.83290457E 00
   2.40          0.87546372E 00
   2.50          0.91628539E 00
   2.60          0.95550584E 00
   2.70          0.99324584E 00
   2.80          0.10296125E 01
   2.90          0.10647029E 01
   3.00          0.10986037E 01
   3.10          0.11313924E 01
   3.20          0.11631403E 01
   3.30          0.11939110E 01
   3.40          0.12237627E 01
   3.50          0.12527496E 01
   3.60          0.12809195E 01
   3.70          0.13083176E 01
   3.80          0.13349850E 01
   3.90          0.13609600E 01
   4.00          0.13862772E 01
```

Figure 31. Output listing

2. Changes to the format of the parameter card may be made by modifying FORMAT statement 1.

The user-supplied function subprogram FUN may be replaced by any function subprogram having the same name and parameter list. In this way, the user may define any desired first-order differential equation.

Operating Instructions

The sample program for Runge-Kutta integration is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

None.

Sample Program for Runge-Kutta Integration of a Given Function with Tabulated Output - RKINT

Purpose:

Integrates the function subprogram FUN using the initial conditions contained in control cards. Produces tabulated output.

Remarks:

I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

RK2

FUN - User-supplied function subprogram giving DY/DX=FUN(X, Y)

Method:

Reads control card containing initial values of X and Y, step size, number of steps desired between tabulated values, and number of tabulated values required. Program then enters RK2 to perform integration. Multiple control cards can be used on the same function.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C        SAMPLE PROGRAM FOR RUNGE-KUTTA INTEGRATION OF A GIVEN FUNCTION RKINT  1
C        WITH TABULATED OUTPUT - RKINT                                  RKINT  2
      EXTERNAL FUN                                                      RKINT  3
C        THE FOLLOWING DIMENSION MUST BE AS LARGE AS THE MAXIMUM        RKINT  4
C        NUMBER OF TABULATED VALUES DESIRED                             RKINT  5
      DIMENSION A(500)                                                  RKINT  6
    1 FORMAT (3F10.0,2I5)                                               RKINT  7
    2 FORMAT(////7X,44HSOLUTION OF DY/DX=FUN(X,Y) BY RK2 SUBROUTINE///, RKINT  8
     110X,2HH=,F7.3,2X,3HX0=,F7.3,2X,3HY0=,F7.3///12X,1HX,18X,4HY(X)//) RKINT  9
    3 FORMAT(/10X,F5.2,10X,E15.8)                                       RKINT 10
    4 FORMAT(2I2)                                                       RKINT 11
      READ(2,4)MX,MY                                                    RKINT 12
C        READ CONTROL CARD CONTAINING ITEMS LISTED UNDER METHOD.        RKINT 13
   10 READ(MY,1)X0,Y0,H,JNT,IENT                                        RKINT 14
C        CHECK IF CARD IS BLANK. IF SO, RETURN.                         RKINT 15
      IF(IENT)20,40,20                                                  RKINT 16
C        WRITE HEADING INFORMATION.                                     RKINT 17
   20 WRITE(MX,2)H,X0,Y0                                                RKINT 18
C        PERFORM INTEGRATION                                            RKINT 19
      CALL RK2(FUN,H,X0,Y0,JNT,IENT,A)                                  RKINT 20
C        WRITE OUTPUT                                                   RKINT 21
      STEP=FLOAT(JNT)*H                                                 RKINT 22
      X=X0                                                              RKINT 23
      DO 30 I=1,IENT                                                    RKINT 24
      X = X+STEP+.1E-05                                                 RKINT 25
   30 WRITE(MX,3)X,A(I)                                                 RKINT 26
C        GO BACK AND CHECK FOR ADDITIONAL CONTROL CARD.                 RKINT 27
      GO TO 10                                                          RKINT 28
   40 STOP                                                              RKINT 29
       END                                                              RKINT 30
// DUP
*STORE      WS  UA  RKINT
// XEQ RKINT
```

```
1 2                                                                     1
     1.0       0.0       .01    10    30                                2
                                                                        3
```

```
  FUNCTION FUN(X,Y)                                           FUN    1
  FUN=1./X                                                    FUN    2
  RETURN                                                      FUN    3
  END                                                         FUN    4
```

POLYNOMIAL ROOTS

Problem Description

The real and complex roots are computed for a real polynomial with given coefficients. Multiple sets of coefficients may be processed.

Program

Description

The polynomial roots sample program consists of a main routine, SMPRT, and one subroutine, POLRT, from the Scientific Subroutine Package.

Capacity

Roots for polynomials of order 36 or less may be computed.

Input

I/O Specification Card

Each set of data requires a control card with the following format:

Columns	Contents	For Sample Problem
1	Blank	
2 - 5	Up to four-digit identification code	360
6 - 8	Blank	
9 - 10	Order of polynomial	9

The first parameter consists of up to four digits without decimal point (I4).

The second parameter consists of up to two digits with no decimal point (I2). The order of the polynomial must be less than or equal to 36.

Data Cards

Data cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in the field, or be omitted, but the number must be right-justified. The number in each field may be preceded by blanks. Columns 71 to 80 of the data cards may be used for identification, sequence numbering, etc. If there are more than seven coefficients, the values should continue from card to card with seven values per card until the number of values has been reached that is one greater than the order of the polynomial. The first coefficient is for the constant term of the polynomial and the last coefficient for the highest order term. Fields with zero coefficients may be left blank.

Blank Card

Run termination.

Deck Setup

The deck setup is shown in Figure 32.

Sample

A listing of the input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The identification code, the polynomial order, the input coefficients, and the real and complex roots are printed.

Sample

The output listing of the sample problem is shown in Figure 33.

Program Modification

The maximum order of the polynomial acceptable to the sample program is fixed by the subroutine POLRT. However, input data in a different format can be handled by providing a specific format statement.

1. The sample program can accept polynomials up to the maximum 36th order, which is allowed by the subroutine.
2. Changes to the format of the parameter card and data cards can be made by modifying FORMAT statements 10 and 40, respectively, in main sample program SMPRT.

Operating Instructions

The polynomial roots sample program is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following conditions will result in error messages:

1. The order of the polynomial specified in the control card is less than one: ORDER OF POLYNOMIAL LESS THAN ONE.

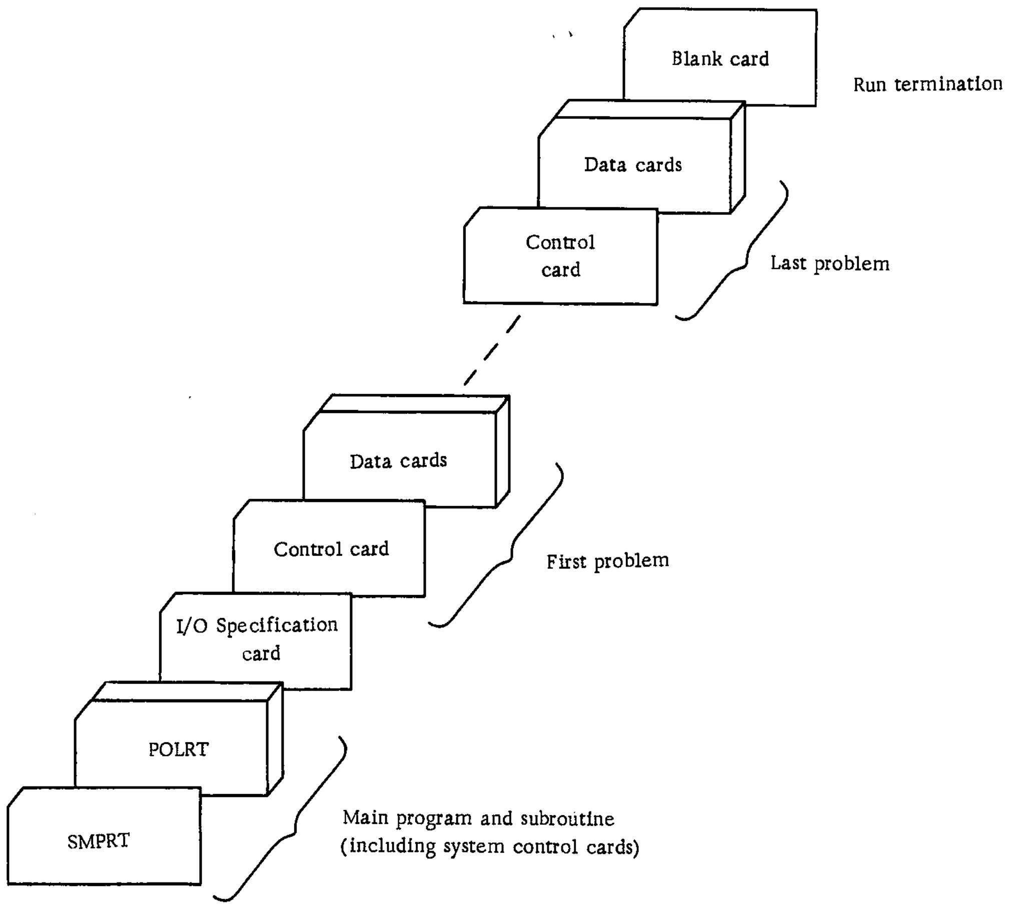


Figure 32. Deck setup (polynomial roots)

The program will go on to the next set of data.

2. The order of the polynomial specified in the control card is greater than 36: ORDER OF POLYNOMIAL GREATER THAN 36.

The program will go on to the next set of data.

```
REAL AND COMPLEX ROOTS OF A POLYNOMIAL USING SUBROUTINE POLRT

FOR POLYNOMIAL   360  OF ORDER   9
THE INPUT COEFFICIENTS ARE

 -0.1000000E 01   0.0000000E 00   0.0000000E 00   0.0000000E 00   0.0000000E 00   0.0000000E 00
  0.1000000E 01   0.0000000E 00   0.0000000E 00   0.1000000E 01


   REAL ROOT      COMPLEX ROOT

  0.2986480E 00   0.1004528E 01
  0.2986480E 00  -0.1004528E 01
 -0.1019270E 01   0.2436272E 00
 -0.1019270E 01  -0.2436272E 00
  0.9105258E 00   0.0000000E 00
  0.7206227E 00  -0.7609007E 00
  0.7206227E 00   0.7609007E 00
 -0.4552629E 00  -0.7885384E 00
 -0.4552629E 00   0.7885384E 00
```

Figure 33. Output listing

3. The subroutine POLRT is unable to determine a root after 500 iterations on eight different starting values: UNABLE TO DETERMINE ROOT. THOSE ALREADY FOUND ARE ...

The program will print all the roots that were computed and then go to the next set of data.

Sample Program for Real and Complex Roots of a Real Polynomial - SMPRT

Purpose:

Computes the real and complex roots of a real polynomial whose coefficients are input.

Remarks:

The order of the polynomial must be greater than one and less than thirty-seven.

I/O logical units determined by MX and MY, respectively.

Subroutines and function subprograms required:

POLRT

Method:

Reads a control card containing the identification code and the order of the polynomial whose coefficients are contained on the following data cards. The coefficients are then read and the roots are computed.

More than one control card and corresponding data can be processed. Execution is terminated by a blank control card.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C         SAMPLE PROGRAM FOR REAL AND COMPLEX ROOTS OF A REAL POLY-      SMPRT  1
C         NOMIAL - SMPRT                                                 SMPRT  2
      DIMENSION A(37),W(37),ROOTR(37),ROOTI(37)                          SMPRT  3
   10 FORMAT(1X,I4,3X,I2)                                                SMPRT  4
   30 FORMAT(////62H REAL AND COMPLEX ROOTS OF A POLYNOMIAL USING SUBROUSMPRT  5
     1TINE POLRT///17H FOR POLYNOMIAL  ,I4,2X,10HOF ORDER  ,I2//27H THE SMPRT  6
     2INPUT COEFFICIENTS ARE//)                                          SMPRT  7
   40 FORMAT(7F10.0)                                                     SMPRT  8
   50 FORMAT(6E16.7)                                                     SMPRT  9
   65 FORMAT(////34H ORDER OF POLYNOMIAL LESS THAN ONE)                  SMPRT 10
   77 FORMAT(////36H ORDER OF POLYNOMIAL GREATER THAN 36)                SMPRT 11
   79 FORMAT(////31H HIGH ORDER COEFFICIENT IS ZERO)                     SMPRT 12
   85 FORMAT(////50H UNABLE TO DETERMINE ROOT. THOSE ALREADY FOUND ARE)  SMPRT 13
   95 FORMAT(////5X,9HREAL ROOT,6X,12HCOMPLEX ROOT//)                    SMPRT 14
   97 FORMAT(2E16.7)                                                     SMPRT 15
   98 FORMAT(2I2)                                                        SMPRT 16
      READ(2,98)MX,MY                                                    SMPRT 17
    5 READ(MY,10)ID,IORD                                                 SMPRT 18
      IF(ID+IORD)100,100,20                                              SMPRT 19
   20 WRITE(MX,30)ID,IORD                                                SMPRT 20
      J=IORD+1                                                           SMPRT 21
      READ(MY,40)(A(I),I=1,J)                                            SMPRT 22
      WRITE(MX,50)(A(I),I=1,J)                                           SMPRT 23
      CALL POLRT(A,W,IORD,ROOTR,ROOTI,IER)                               SMPRT 24
      IF(IER-1)90,60,70                                                  SMPRT 25
   60 WRITE(MX,65)                                                       SMPRT 26
      GO TO 5                                                            SMPRT 27
   70 IF(IER-3)75,80,78                                                  SMPRT 28
   75 WRITE(MX,77)                                                       SMPRT 29
      GO TO 5                                                            SMPRT 30
   78 WRITE(MX,79)                                                       SMPRT 31
      GO TO 5                                                            SMPRT 32
   80 WRITE(MX,85)                                                       SMPRT 33
   90 WRITE(MX,95)                                                       SMPRT 34
      DO 96 I=1,IORD                                                     SMPRT 35
   96 WRITE(MX,97)ROOTR(I),ROOTI(I)                                      SMPRT 36
      GO TO 5                                                            SMPRT 37
  100 STOP                                                               SMPRT 38
      END                                                                SMPRT 39
// DUP
*STORE      WS  UA  SMPRT
// XEQ SMPRT
```

```
1 2                                                                     1
 360    9                                                               2
    -1.0                                                  1.0           3
                        1.0                                             4
                                                                        5
```

SOLUTION OF SIMULTANEOUS EQUATIONS

Problem Description

A solution is obtained for a set of simultaneous equations by the method of elimination using largest pivotal divisor. Both the input data and the solution values are printed. This procedure is repeated until all sets of input data have been processed.

Program

Description

The solution of simultaneous equations sample program consists of a main routine, SOLN, and four subroutines:

SIMQ, LOC } are from the Scientific Subroutine Package

MATIN, MXOUT } are sample subroutines for matrix input and output

Capacity

The sample program will solve for 40 equations. The general rules for program modifications are described later.

Input

I/O Specification Card

A control card with the following format must precede each matrix of coefficients:

Columns	Contents	For Sample Problem
1 - 2	Blank	
3 - 6	Up to four-digit identification code (numeric only)	1
7 - 10	Number of rows in matrix	10
11 - 14	Number of columns in matrix (same as number of rows)	10

Each matrix must be followed by a card with a 9-punch in column 1. This, in turn, is followed by the constant vector.

Data Cards

Data cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in a field, or be omitted, but the number must be right-justified. The number in each field may be preceded by blanks. Equation coefficients must be punched by row. A row may continue from card to card. However, each new row must start in the first field of the next card. The vector of constants is punched in continuous data fields following the 9 card. Columns 71 to 80 of data cards may be used for identification, sequence numbering, etc.

A blank card after the last set of input data terminates the run.

Deck Setup

The deck setup is shown in Figure 34.

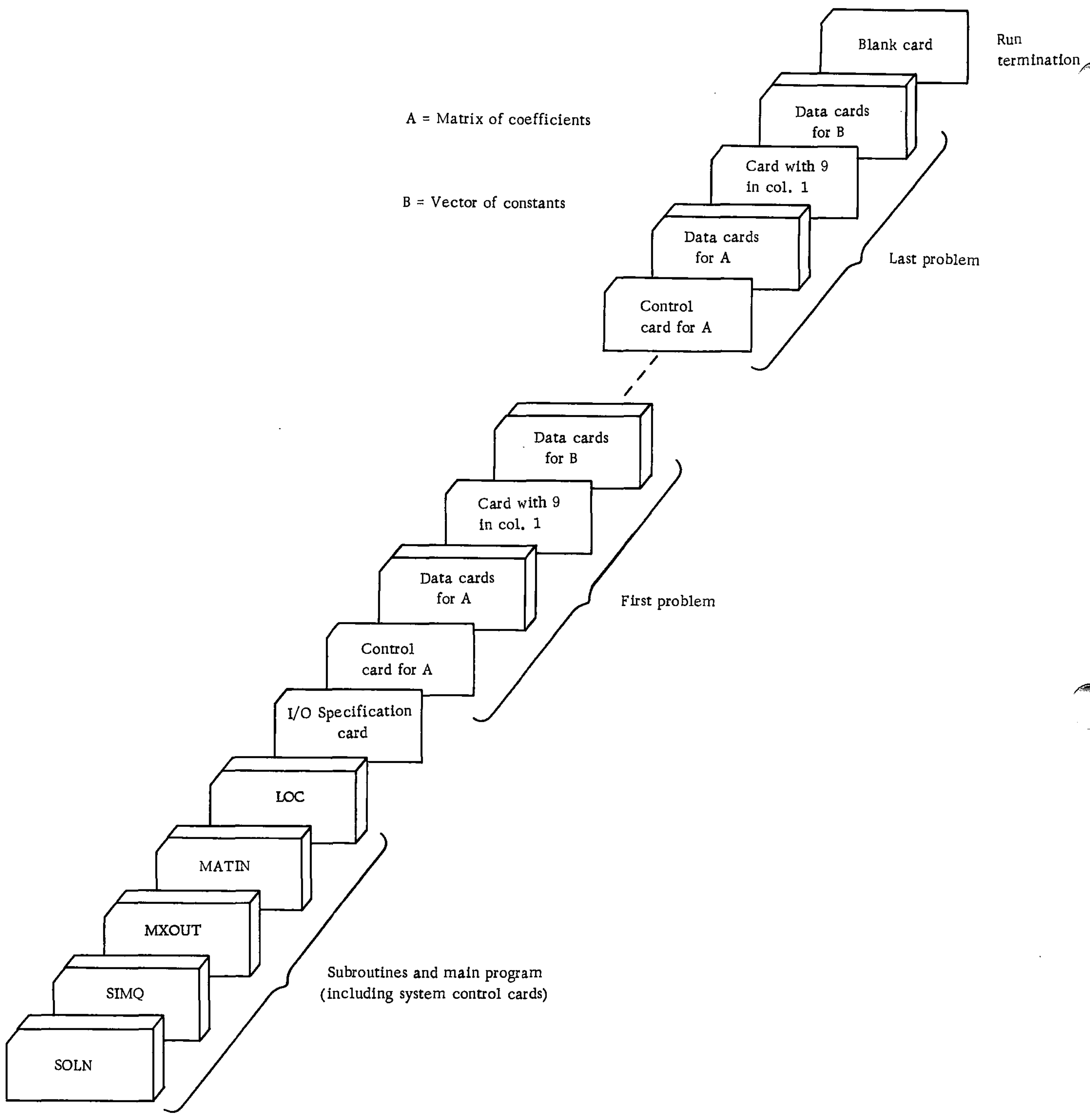


Figure 34. Deck setup (solution of simultaneous equations)

Sample

A listing of input cards for the sample problem is presented at the end of the sample main program.

Output

Description

The original matrix is printed for any sized array. Each six-column grouping is headed with the matrix code number, dimensions, and storage mode (always 0 in this sample program). Columns and rows are headed with their respective number. The original vector of constants is also printed. The solution values are then listed. This output is given for each case to be processed.

Sample

The output listing for the sample problem is shown in Figure 35.

Program Modifications

Noting that storage problems may result, as previously discussed in "Sample Program Description", the size of the maximum problem acceptable to the sample program can be increased. Output of the solution values in a different format can be handled by providing a specific format statement.

1. Changes to the DIMENSION statement of the main program, SOLN. The dimension of array A must be greater than or equal to the maximum number of elements in the matrix (N x N). The dimension of array B must be greater than or equal to N.
2. Insert the same number N in the third argument of the CALL MATIN statement (statement 25) in SOLN.
3. Changes to the format of the solution values may be made by modifying FORMAT statement 21 in SOLN.

```
SOLUTION OF SIMULTANEOUS EQUATIONS


MATRIX    1      10 ROWS      10 COLUMNS      STORAGE MODE 0
     COLUMN      1             2             3             4             5             6
 ROW   1    0.100000E 01  0.664408E 00  0.760100E 00  0.750750E 00  0.429942E 00  0.332910E-02
 ROW   2    0.664408E 00  0.100000E 01  0.627180E 00  0.619465E 00  0.354757E 00  0.274700E-02
 ROW   3    0.760100E 00  0.627180E 00  0.100000E 01  0.708684E 00  0.405851E 00  0.314260E-02
 ROW   4    0.750750E 00  0.619465E 00  0.708684E 00  0.100000E 01  0.400859E 00  0.310390E-02
 ROW   5    0.429942E 00  0.354757E 00  0.405851E 00  0.400859E 00  0.100000E 01  0.177760E-02
 ROW   6    0.332910E-02  0.274700E-02  0.314260E-02  0.310390E-02  0.177760E-02  0.100000E 01
 ROW   7    0.728478E 00  0.601087E 00  0.687660E 00  0.679201E 00  0.388967E 00  0.301190E-02
 ROW   8    0.675176E 00  0.557106E 00  0.637344E 00  0.629504E 00  0.360507E 00  0.279150E-02
 ROW   9    0.863591E 00  0.712572E 00  0.815202E 00  0.805174E 00  0.461109E 00  0.357050E-02
 ROW  10    0.744684E 00  0.614459E 00  0.702958E 00  0.694310E 00  0.397620E 00  0.307890E-02

MATRIX    1      10 ROWS      10 COLUMNS      STORAGE MODE 0
     COLUMN      7             8             9            10
 ROW   1    0.728478E 00  0.675176E 00  0.863591E 00  0.744684E 00
 ROW   2    0.601087E 00  0.557106E 00  0.712572E 00  0.614459E 00
 ROW   3    0.687660E 00  0.637344E 00  0.815202E 00  0.702958E 00
 ROW   4    0.679201E 00  0.629504E 00  0.805174E 00  0.694310E 00
 ROW   5    0.388967E 00  0.360507E 00  0.461109E 00  0.397620E 00
 ROW   6    0.301190E-02  0.279150E-02  0.357050E-02  0.307890E-02
 ROW   7    0.100000E 01  0.610829E 00  0.781287E 00  0.673713E 00
 ROW   8    0.610829E 00  0.100000E 01  0.724121E 00  0.624418E 00
 ROW   9    0.781287E 00  0.724121E 00  0.100000E 01  0.798668E 00



 ROW  10    0.673713E 00  0.624418E 00  0.798668E 00  0.100000E 01


ORIGINAL B VECTOR


   1             0.110000E 03
   2            -0.120000E 03
   3             0.100000E 02
   4             0.145000E 03
   5            -0.500000E 02
   6             0.442000E 02
   7            -0.140000E 02
   8             0.389000E 02
   9             0.220000E 02
  10             0.165000E 04


SOLUTION VALUES


   1            -0.283123E 03
   2            -0.567240E 03
   3            -0.516456E 03
   4            -0.299155E 02
   5            -0.179352E 03
   6             0.435176E 02
   7            -0.479274E 03
   8            -0.230431E 03
   9            -0.210172E 04
  10             0.480974E 04

END OF CASE
```

Figure 35. Output listing

The matrix listing is set for 120 print positions across the page, and double spacing. This can be changed by means of the last two arguments in the CALL MXOUT statement in SOLN (statement 65).

Operating Instructions

The sample program for the solution of simultaneous equations is a standard FORTRAN program. Special operating instructions are not required. Logical unit 2 is used for input, and logical unit 1 is used for output.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix: DIMENSIONED AREA TOO SMALL FOR

INPUT MATRIX (matrix code no.). GO ON TO NEXT CASE.

2. Matrix of coefficients is not square: ROW AND COLUMN DIMENSIONS NOT EQUAL FOR MATRIX (matrix code no.). GO ON TO NEXT CASE.

3. Number of data cards does not correspond to that required by parameter card: INCORRECT NUMBER OF DATA CARDS FOR MATRIX (matrix code no.). EXECUTION TERMINATED.

4. Singular input matrix: MATRIX IS SINGULAR. GO ON TO NEXT CASE.

Error conditions 1, 2, and 4 allow the computer run to continue. Error condition 3, however, terminates execution and requires another run to process succeeding cases.

Sample Main Program - SOLN

Purpose:
Solution of a set of simultaneous equations.

Remarks:
I/O specifications transmitted to subroutines by COMMON.
Input card:

Column 2	MX -	Logical unit number for output.
Column 4	MY -	Logical unit number for input.

Subroutines and function subprograms required:
SIMQ
MATIN
MXOUT
LOC

Method:
A matrix of simultaneous equations coefficients and a vector of constants are read from the standard input device. The solution is obtained and listed on the standard output device. This procedure is repeated for other sets of equations until a blank card is encountered.

```
// FOR
*IOCS(CARD,TYPEWRITER,1132 PRINTER)
*ONE WORD INTEGERS
C         SAMPLE MAIN PROGRAM - SOLN
C         MATRIX IS DIMENSIONED FOR 1600 ELEMENTS. THEREFORE, NUMBER OF
C         EQUATIONS TO BE SOLVED CANNOT EXCEED 40 UNLESS DIMENSION
C         STATEMENT IS CHANGED
      DIMENSION A(1600),B(40)
      COMMON MX,MY
   10 FORMAT(////35H SOLUTION OF SIMULTANEOUS EQUATIONS)
   11 FORMAT(//45H DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)
   12 FORMAT(//21H EXECUTION TERMINATED)
   13 FORMAT(//48H ROW AND COLUMN DIMENSIONS NOT EQUAL FOR MATRIX ,I4)
   14 FORMAT(//43H INCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)
   15 FORMAT(//19H GO ON TO NEXT CASE)
   16 FORMAT(//39H STRUCTURE CODE IS NOT ZERO FOR MATRIX,I4)
   17 FORMAT(////18H ORIGINAL B VECTOR,////)
   18 FORMAT(////16H SOLUTION VALUES,////)
   19 FORMAT(//19H MATRIX IS SINGULAR)
   20 FORMAT(7F10.0)
   21 FORMAT(I6,10X,E16.6)
   22 FORMAT(//12H END OF CASE)
   23 FORMAT(2I2)
      READ(2,23)MX,MY
      WRITE(MX,10)
   25 CALL MATIN (ICOD,A,1600,N,M,MS,IER)
      IF(N) 30,95,30
   30 IF(IER-1) 45,35,40
   35 WRITE(MX,11)ICOD
      GO TO 90
   40 WRITE(MX,14)ICOD
      GO TO 95
   45 IF(N-M) 50,55,50
   50 WRITE(MX,13)ICOD
      GO TO 90
   55 IF(MS) 60,65,60
   60 WRITE(MX,16)ICOD
      GO TO 90
   65 CALL MXOUT(ICOD,A,N,M,MS,60,120,2)
      READ(MY,20)(B(I),I=1,N)
      WRITE(MX,17)
      DO 70 I=1,N
   70 WRITE(MX,21)I,B(I)
      CALL SIMQ(A,B,N,KS)
      IF(KS-1) 80,75,80
   75 WRITE(MX,19)
      WRITE(MX,15)
      GO TO 25
   80 WRITE(MX,18)
      DO 85 I=1,N
   85 WRITE(MX,21)I,B(I)
      WRITE(MX,22)
      GO TO 25
   90 READ(MY,20)(B(I),I=1,N)
      WRITE(MX,15)
      GO TO 25
   95 WRITE(MX,12)
      STOP
      END
// DUP
*STORE      WS  UA  SOLN
// XEQ SOLN
```

```
1 2
 000100100010
1.0000000 0.6644085 0.7601008 0.7507505 0.4299425 0.0033291 0.7284786
0.6751766 0.8635910 0.7446845
0.6644085 1.0000000 0.6271802 0.6194650 0.3547574 0.0027470 0.6010878
0.5571068 0.7125728 0.6144597
0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
0.6373449 0.8152021 0.7029582
0.7507505 0.6194650 0.7086843 1.0000000 0.4008593 0.0031039 0.6792011
0.6295047 0.8051740 0.6943108
0.4299425 0.3547574 0.4058519 0.4008593 1.0000000 0.0017776 0.3889673
0.3605070 0.4611099 0.3976204
0.0033291 0.0027470 0.0031426 0.0031039 0.0017776 1.0000000 0.0030119
0.0027915 0.0035705 0.0030789
0.7284786 0.6010878 0.6876602 0.6792011 0.3889673 0.0030119 1.0000000
0.6108296 0.7812874 0.6737132
0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296
1.0000000 0.7241215 0.6244183
0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874
0.7241215 1.0000000 0.7986682
0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
0.6244183 0.7986682 1.0000000
9
    110.0    -120.0       10.       145.       -50.      44.20      -14.
     38.5       22.     1650.
```

```
SUBROUTINE MATIN

PURPOSE
   READS CONTROL CARD AND MATRIX DATA ELEMENTS FROM LOGICAL
   UNIT 5

USAGE
   CALL MATIN(ICODE,A,ISIZE,IROW,ICOL,IS,IER)

DESCRIPTION OF PARAMETERS
   ICODE-UPON RETURN, ICODE WILL CONTAIN FOUR DIGIT
         IDENTIFICATION CODE FROM MATRIX PARAMETER CARD
   A    -DATA AREA FOR INPUT MATRIX
   ISIZE-NUMBER OF ELEMENTS DIMENSIONED BY USER FOR AREA A
   IROW -UPON RETURN, IROW WILL CONTAIN ROW DIMENSION FROM
         MATRIX PARAMETER CARD
   ICOL -UPON RETURN, ICOL WILL CONTAIN COLUMN DIMENSION FROM
         MATRIX PARAMETER CARD
   IS   -UPON RETURN, IS WILL CONTAIN STORAGE MODE CODE FROM
         MATRIX PARAMETER CARD WHERE
         IS=0 GENERAL MATRIX
         IS=1 SYMMETRIC MATRIX
         IS=2 DIAGONAL MATRIX
   IER  -UPON RETURN, IER WILL CONTAIN AN ERROR CODE WHERE
         IER=0   NO ERROR
         IER=1   ISIZE IS LESS THAN NUMBER OF ELEMENTS IN
                 INPUT MATRIX
         IER=2   INCORRECT NUMBER OF DATA CARDS

REMARKS
   NONE

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   LOC

METHOD
   SUBROUTINE ASSUMES THAT INPUT MATRIX CONSISTS OF PARAMETER
   CARD FOLLOWED BY DATA CARDS
   PARAMETER CARD HAS THE FOLLOWING FORMAT
     COL. 1- 2 BLANK
     COL. 3- 6 UP TO FOUR DIGIT IDENTIFICATION CODE
     COL. 7-10 NUMBER OF ROWS IN MATRIX
     COL.11-14 NUMBER OF COLUMNS IN MATRIX
     COL.15-16 STORAGE MODE OF MATRIX WHERE
          0 - GENERAL MATRIX
          1 - SYMMETRIC MATRIX
          2 - DIAGONAL MATRIX
   DATA CARDS ARE ASSUMED TO HAVE SEVEN FIELDS OF TEN COLUMNS
   EACH.  DECIMAL POINT MAY APPEAR ANYWHERE IN A FIELD.  IF NO
   DECIMAL POINT IS INCLUDED, IT IS ASSUMED THAT THE DECIMAL
   POINT IS AT THE END OF THE 10 COLUMN FIELD. NUMBER IN EACH
   FIELD MAY BE PRECEDED BY BLANKS.  DATA ELEMENTS MUST BE
   PUNCHED BY ROW.  A ROW MAY CONTINUE FROM CARD TO CARD.
   HOWEVER EACH NEW ROW MUST START IN THE FIRST FIELD OF THE
   NEXT CARD.  ONLY THE UPPER TRIANGULAR PORTION OF A SYMMETRIC
   OR THE DIAGONAL ELEMENTS OF A DIAGONAL MATRIX ARE CONTAINED
   ON DATA CARDS.  THE FIRST ELEMENT OF EACH NEW ROW WILL BE
   THE DIAGONAL ELEMENT FOR A MATRIX WITH  SYMMETRIC OR
   DIAGONAL STORAGE MODE. COLUMNS 71-80 OF DATA CARDS MAY BE
   USED FOR IDENTIFICATION, SEQUENCE NUMBERING, ETC..
   THE LAST DATA CARD FOR ANY MATRIX MUST BE FOLLOWED BY A CARD
   WITH A 9 PUNCH IN COLUMN 1.
```

```
      SUBROUTINE MATIN(ICODE,   A,ISIZE,IROW,ICOL,IS,IER)
      DIMENSION A(1)
      DIMENSION CARD(8)
      COMMON MX,MY
    1 FORMAT(7F10.0)
    2 FORMAT(I6,2I4,I2)
    3 FORMAT(I1)
      IDC=7
      IER=0
      READ( MY,2)ICODE,IROW,ICOL,IS
      CALL LOC(IROW,ICOL,ICNT,IROW,ICOL,IS)
      IF(ISIZE-ICNT)6,7,7
    6 IER=1
    7 IF (ICNT)38,38,8
    8 ICOLT=ICOL
      IROCR=1
C         COMPUTE NUMBER OF CARDS FOR THIS ROW
   11 IRCDS=(ICOLT-1)/IDC+1
      IF(IS-1)15,15,12
   12 IRCDS=1
C         SET UP LOOP FOR NUMBER OF CARDS IN ROW
   15 DO 31 K=1,IRCDS
      READ(MY,1)(CARD(I),I=1,IDC)
C         SKIP THROUGH DATA CARDS IF INPUT AREA TOO SMALL
      IF(IER)16,16,31
   16 L=0
C         COMPUTE COLUMN NUMBER FOR FIRST FIELD IN CURRENT CARD
      JS=(K-1)*IDC+ICOL-ICOLT+1
```

```
USAGE
   CALL MXOUT(ICODE,A,N,M,MS,LINS,IPOS,ISP)

DESCRIPTION OF PARAMETERS
   ICODE- INPUT CODE NUMBER TO BE PRINTED ON EACH OUTPUT PAGE
   A-NAME OF OUTPUT MATRIX
   N-NUMBER OF ROWS IN A
   M-NUMBER OF COLUMNS IN A
   MS-STORAGE MODE OF A WHERE MS=
           0-GENERAL
           1-SYMMETRIC
           2-DIAGONAL
   LINS-NUMBER OF PRINT LINES ON THE PAGE (USUALLY 60)
   IPOS-NUMBER OF PRINT POSITIONS ACROSS THE PAGE (USUALLY 132)
   ISP-LINE SPACING CODE, 1 FOR SINGLE SPACE, 2 FOR DOUBLE
        SPACE

REMARKS
   NONE

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
   LOC

METHOD
   THIS SUBROUTINE CREATES A STANDARD OUTPUT LISTING OF ANY
   SIZED ARRAY WITH ANY STORAGE MODE. EACH PAGE IS HEADED WITH
   THE CODE NUMBER,DIMENSIONS AND STORAGE MODE OF THE ARRAY.
   EACH COLUMN AND ROW IS ALSO HEADED WITH ITS RESPECTIVE
   NUMBER.


SUBROUTINE MXOUT

PURPOSE
   PRODUCES AN OUTPUT LISTING OF ANY SIZED ARRAY ON
   LOGICAL UNIT 1
```

```
      SUBROUTINE MXOUT (ICODE,A,N,M,MS,LINS,IPOS,ISP)
      DIMENSION A(1),B(8)
      COMMON MX,MY
    1 FORMAT(////5X, 7HMATRIX ,I5,6X,I3,5H ROWS,6X,I3,8H COLUMNS,
     18X,13HSTORAGE MODE ,I1,/)
    2 FORMAT(12X,8HCOLUMN  ,7(3X,I3,10X)//)
    4 FORMAT(7X,4HROW ,I3,7(E16.6))
    5 FORMAT(/,7X,4HROW ,I3,7(E16.6))
      J=1
C          WRITE HEADING
      NEND=IPOS/16-1
      LEND = (LINS/ISP)-10
   10 LSTRT=1
   20 WRITE(MX,1)ICODE,N,M,MS
      JNT=J+NEND-1
      IF(JNT-M)33,33,32
   32 JNT=M
   33 CONTINUE
      WRITE(MX,2)(JCUR,JCUR=J,JNT)
      LTEND = LSTRT+LEND-1
      DO 80 L=LSTRT,LTEND
C          FORM OUTPUT ROW LINE
      DO 55 K=1,NEND
      KK=K
      JT = J+K-1
      CALL LOC(L,JT,IJNT,N,M,MS)
      B(K)=0.0
      IF(IJNT)50,50,45
   45 B(K)=A(IJNT)
   50 CONTINUE
C          CHECK IF LAST COLUMN.  IF YES GO TO 60
      IF(JT-M) 55,60,60
   55 CONTINUE
C          END OF LINE, NOW WRITE
   60 IF(ISP-1)65,65,70
   65 WRITE(MX,4)L,(B(JW),JW=1,KK)
      GO TO 75
   70 WRITE(MX,5)L,(B(JW),JW=1,KK)
C          IF END OF ROWS,GO CHECK COLUMNS
   75 IF(N-L)85,85,80
   80 CONTINUE
C          WRITE NEW HEADING
      LSTRT=LSTRT+LEND
      GO TO 20
C          END OF COLUMNS, THEN RETURN
   85 IF(JT-M)90,95,95
   90 J=JT+1
      GO TO 10
   95 RETURN
      END
```

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1130 Scientific Subroutine Package
Programmer's Manual
Program Number 1130-CM-02X

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Program Number 1130-CM-02X

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