OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
for the
U. S. ATOMIC ENERGY COMMISSION

OAK RIDGE NATIONAL LABORATORY LIBRARY
3 4456 0023086 3

ORNL - TM - 271

cy 99

OR GLS,

A GENERAL FORTRAN LEAST SQUARES PROGRAM

William R. Busing
Henri A. Levy

NOTICE This document contains information of a preliminary nature and was prepared primarily for internal use at the Oak Ridge National Laboratory. It is subject to revision or correction and therefore does not represent a final report.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

ORNL-TM-271

Contract No. W-7405-eng-26

OR GLS,

A GENERAL FORTRAN LEAST SQUARES PROGRAM

by

William R. Busing and Henri A. Levy
Chemistry Division

June, 1962

DATE ISSUED

AUG - 7 1962

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

OAK RIDGE NATIONAL LABORATORY LIBRARY
3 4456 0023086 3

CONTENTS

Abstract 1

Introduction 2

General Description 3

Data Input 5

Tapes Required 8

Subroutines to be Supplied by the User 9

Card Decks Provided 11

Library Subroutines 12

Glossary of Symbols 12

Symbolic Program Listing 16

Example of Program Output 35

Distribution 40

ABSTRACT

This report describes a computer program which will adjust the parameters of an arbitrary function to fit a set of observed values by the method of least squares. The form of this function is to be defined in terms of a subroutine prepared by the user. The derivatives needed for the method of least squares are either obtained numerically by the program or calculated analytically by the user's subroutine. Most of the program is written in the Fortran language to facilitate any desired modifications and to permit its use on various machines. Instructions are included for the use of the program, which is available in card form from the authors.

INTRODUCTION

The computer program to be described will adjust the parameters of an arbitrary function to obtain a least-squares fit to a set of observations. The function involved may have any form which can be defined by a subprogram, prepared by the user, to obtain its value for a given set of trial parameters and independent variables. The derivatives needed for the method of least squares are either obtained numerically by the program or calculated analytically by the user's subroutine.

The input data to each job include a set of observations, each with its corresponding independent variables, and, if desired, its estimated standard error. The latter determines the weight of the observation unless the use of unit weights is specified. The program also reads a set of trial parameters and an indication of which of these are to be adjusted. If numerical differentiation is to be performed, a parameter increment to be used in this process is associated with each parameter to be varied.

More than one cycle of refinement will be required to converge on the final solution unless the function to be fitted happens to be linear in the variable parameters. The program allows the user to specify the number of cycles to be performed in each job and also permits him to provide a test to terminate the calculation after fewer cycles if appropriate. Provision is made to transfer the parameters from one job to another by means of either magnetic tape or punched cards.

A list comparing the observed and calculated function is put out together with an over-all agreement factor before each cycle of refinement and once more after the last adjustment. The old and new parameters with their calculated standard errors are listed after each cycle, and the correlation matrix is put out at the end of each job.

The program has been used successfully for crystal structure refinements involving more than ninety variables and over two thousand observations. Most of it is written in Fortran to facilitate any desired modifications and to permit its use on various machines. Both symbolic and column binary cards are available from the authors.

GENERAL DESCRIPTION

It is expected that the Fortran listing and the glossary of symbols which are provided will serve as a complete description of the program. The form of the input is described in detail in a separate section, and an example of such input, together with the corresponding output, is also given. This section is therefore intended to serve only as a brief summary of the method.

Of fundamental importance is the user's subroutine CALC which, during each cycle, is entered once for each observation to obtain YC, the value of the function based on the current parameters and the NX independent variables associated with the observation. For each observation the program stores in the array DV the derivatives of YC with respect to those parameters P which are to be varied. If the user elects to have these derivatives obtained numerically, he must associate with each P(I) a parameter increment DP(I). For each of the NV variables the program adds DP(I) to P(I) and re-enters CALC to obtain YD, the function based on the parameters with one incremented. The required derivative is then taken as DV(I) = (YD-YC)/DP(I).

Alternatively, the user may elect to include the analytical calculation of the derivatives in subroutine CALC, and this will save appreciable machine time in problems with complicated functions and many variables. In this case the subroutine is entered only once for each observation, and the derivatives with respect to every possible variable are stored in the array DC at the same time that YC is calculated. The program later selects from this array the derivatives with respect to those parameters to be varied in a particular job.

It is possible to use a combination of numerical and programmed derivatives by specifying numerical derivatives but setting to zero the parameter increments associated with some variables. When the program finds such a zero increment, it assumes that a programmed derivative is to be used for that variable.

Additional flexibility is provided by an optional user's subroutine PRELIM which is entered once at the beginning of each job. This may be used to read various constants, make preliminary computations, and otherwise prepare for the function calculation. It may also be used for data

processing, weight calculation, or other modification of the observation input.

For each cycle the matrix and vector of the normal equations are stored by computing the contributions of one observation at a time. The calculated function and the required derivatives are obtained as described above, and a line of output comparing the observation with its calculated value is put out. The term (SQRTW*DV(J))*(SQRTW*DV(K)) is then added to AM(JK), the J,Kth element of the matrix, where SQRTW is the square root of the weight of the observation. The contribution to the vector element V(J) is (SQRTW*DV(J))*(SQRTW*(YO-YC)), and that to the agreement factor SIG is (SQRTW*(YO-YC))**2. Here YO is used as an abbreviation for YO(I), the Ith observed value of the function.

This process is repeated until the contributions from all the observations have been obtained. At this point an agreement factor, the standard error of an observation of unit weight, SQRTF(SIG/(NO-NV)), is computed and put out.

The storage scheme used for the matrix AM is described in the glossary. To make efficient use of memory space, only the upper triangular part of this symmetric matrix is stored. Furthermore, to conform to the requirements of the existing matrix inverter, SMI, the matrix is stored forward in core or backward in the normal Fortran indexing system.

Before the matrix is inverted it is tested for zero diagonal elements which would indicate a singular matrix with one or more zero row-columns. This would be the result if the derivatives with respect to the corresponding parameters were zero for all observations. A singular matrix due to the attempt to vary sets of parameters with one or more redundancies will be found in the course of the inversion. In case of either type of singularity, the job is terminated with the appropriate comment.

The matrix inversion procedure is described in detail elsewhere (W. R. Busing and H. A. Levy, Comm. ACM, 1962. To be published.) It involves the diagonalization of the matrix by a series of congruent transformations, inversion by taking reciprocals of the diagonal elements, and a sequence of reverse transformations. Upon completion of the process the inverse matrix has replaced the original one in the array AM.

The vector is then multiplied by the inverse matrix to obtain the parameter changes, PD. An estimated new value of the agreement factor SIG is obtained by subtracting from it PD(I)*V(I) summed over the NV variables, and a revised SQRTF(SIG/(NO-NV)) is computed. The entire list of parameters is then put out showing the changes which were made and the estimated standard errors associated with these variables. The latter are computed as SQRTF(DIAG(J)*SIG/(NO-NV)) where DIAG is an array of the diagonal elements of the inverse matrix. It should be noted that these estimates are exact only if the function is linear in the parameters, are approximately correct for converging nonlinear functions, but may be grossly incorrect if the calculation is diverging.

At this point the program enters a subroutine TEST which may be provided at the option of the user. This routine may be used to determine whether the new parameter values are reasonable, modify them if necessary, or terminate the job. It may also be used to test the agreement factors from several cycles so that the job may be terminated when convergence is achieved. Unless the job is ended by TEST or because of a singular matrix, the above procedure will be repeated for the specified number of cycles, and then a final calculation and output of YC will be made.

At the end of the job, unless a singular matrix has been found, the program computes the correlation matrix by dividing each inverse matrix element AM(IJ) by SQRTF(DIAG(I)*DIAG(J)). Only the upper triangular part of this symmetric matrix is reported, and the other elements appear as zero in the listing.

DATA INPUT

*The limitations marked with an asterisk depend only on the dimensions with which the program is compiled.

1. Title card. FORMAT (12A6)

Columns	
1-72	TITLE consisting of any desired Hollerith information. This will be put out as a heading on each section of output.

2. Control card. FORMAT (7I3)

Columns	
1-3	NC, the number of cycles to be run on this job. Calculated values of YC will be listed NC + 1 times. If NC = 0 one list of calculated YC will be put out, but no refinement will be made.

4-6	NV, the number of parameters to be varied. If NC = 0 then NV is irrelevant. $1 \leqslant NV \leqslant 100$.*
7-9	NX, the number of independent variables associated with each observation. $1 \leqslant NX \leqslant 5$.*
10-12	ID, the derivative indicator. ID = 0 indicates that the required derivatives have been programmed by the user. ID = 1 indicates that the required derivatives will be calculated numerically except for parameters which have DP(I) = 0.
13-15	IW, the weight indicator. IW = 0 indicates that individual standard errors will be supplied by the user for each observation. IW = 1 indicates that the program is to weight each observation at unity.
16-18	IP, the parameter input indicator. IP = 0 indicates that trial parameters are supplied as input data. IP > 0 indicates that the program is to read the input parameters from a private tape using those from cycle IP of a previous job.
19-21	IT, the auxiliary output indicator. If IT = 0 the corrected parameters are not to be saved for later use. If IT = 1 the corrected parameters are to be written on a private tape. If IT = 2 the corrected parameters are to be written on an auxiliary output tape to be punched on cards off-line.

3. Trial parameter cards. FORMAT (I3/(8F9.4))
These are to be provided only when IP = 0 on the control card.

First card.
Columns

1-3	NP, the total number of parameters to be read (including those to be varied and those to be held constant). $1 \leqslant NP \leqslant 200$.*

Second card.
Columns

1-9	P(1), the trial value of the first parameter, etc.
10-18	P(2)
19-27	P(3)
.	.
.	.
64-72	P(8)

Third card.

Columns	
1-9	P(9)
10-18	P(10)
.	.
.	.
	P(NP)

4. Observation cards. FORMAT (I1,E8.4,7E9.4/(8E9.4))
Include one or more cards for each of NO observations. $1 \leqslant NO \leqslant 999$.*

Columns	
1	Blank
2-9	YO, the observed value of the dependent variable.
10-18	SIGYO, the standard error of this observation. If IW = 1 on the control card this field is irrelevant.
19-27	X(1), the first independent variable.
28-36	X(2), the second independent variable.
.	.
.	.
.	X(NX), the last independent variable. Note that these fields can be used to input any numbers which pertain to an individual observation. (If it is desired to make NX > 5 then the program must be recompiled with altered dimension statements. If NX = 6 then a second card which is blank must be supplied for each observation unless the FORMAT statement is changed.)

5. Observation termination card. FORMAT (I1)

Column	
1	ISENT = 1 as sentinel for end of observation deck. (If NX $\geqslant$ 6 then blank cards must be added so that the termination includes as many cards as an observation.)

6. Key integer cards. FORMAT (72I1)
These are omitted if NC = 0. Otherwise one card is included for each 72 trial parameters (or fraction thereof) read.

First card.

Column	
1	KI(1) = 0 if P(1) is not to be varied. KI(1) = 1 if P(1) is to be varied.

2	KI(2) associated in the same way with P(2), etc.
.	.
.	.
72	KI(72)

Second card.
Column

1	KI(73)
.	.
.	.
	KI(NP)

7. Parameter increment cards. FORMAT (8E9.4)
These cards are included only if both NC $\geqslant$ 1 and ID = 1, that is, if some of the least squares derivatives are to be computed numerically.

First cards.
Columns

1-9	DP(1), the parameter increment associated with P(1). If the derivative of YC with respect to P(1) is to be determined numerically, DP(1) is the parameter increment which will be added to P(1). If KI(I) = 0 then DP(I) is irrelevant. If KI(I) = 1 and DP(I) = 0 then the program will expect the derivative with respect to P(I) to be calculated by the user's subprogram, CALC.
10-18	DP(2), the parameter increment associated with P(2), etc.
.	.
.	.
64-72	DP(8)

Second card.
Columns

1-9	DP(9)
.	.
.	.
	DP(NP)

8. Any data to be read by the user's subroutine PRELIM.

TAPES REQUIRED

Listed here are the monitor tape control cards required for operation at the Oak Ridge Central Data Processing Facility. At other installations the necessary tapes should be specified appropriately.

*TAPE(4, Reel number, SAVE)

This is required only if IP > 0 indicating that the initial values of the trial parameters are to be taken from this tape, which was written on a previous job.

*TAPE(5, POOL, SAVE)

This is required only if IT = 1 indicating that the adjusted parameters are to be written on this tape after each cycle. This tape is initially rewound and an end-of-file is written upon completion of the job.

*TAPE(6, AUXOUT)

This is required only if IT = 2 indicating that the adjusted parameters are to be written on this tape after each cycle. Cards suitable for input to another job will then be punched off-line. This tape is not rewound and no end-of-file is written on it by the program.

*TAPE(9, OUTPUT)

*TAPE(10, INPUT)

SUBROUTINES TO BE SUPPLIED BY THE USER

SUBROUTINE CALC(XI,Y,P,D)

This subroutine must be supplied by the user to evaluate the function and to calculate the necessary derivatives if these are to be programmed.

The argument XI is used as a vector of the NX independent variables for one observation. This vector represents column I of the two dimensional calling program array X, and the CALL statement for observation I uses the argument X(1,I). If NX > 1 then XI must be included in a DIMENSION statement. Note that this array may be used to convey to the subroutine any information which pertains to a particular observation.

Y is the single valued function to be calculated. The calling program uses either YC or YD as the corresponding argument.

P is the array of trial parameters some of which are to be varied. It should be included in a DIMENSION statement. This array may also be used to convey constants or instructions to the subroutine, but such parameters should not be adjusted.

D is the array in which derivatives are to be stored if they are calculated by this subroutine. It is in one to one correspondence with

the array P. The calling program refers to it as DC or DD. The array should be included in a DIMENSION statement.

If COMMON storage is used for communication with subroutine PRELIM (see below) then care should be taken to include the COMMON and DIMENSION statements from the calling program.

The user must program the calculation of Y from the independent variables XI and the parameters P. If derivatives are programmed, then $\partial Y/\partial P(J)$ should be stored in D(J), etc. Only derivatives with respect to parameters to be varied need be programmed, but storing derivatives which will not be used is permitted. Programming the derivative calculation will save appreciable machine time on problems with complicated functions and many variables. The derivative programming can often be checked by comparing the results of a least-squares cycle which uses it with those of the same cycle using numerical differentiation.

The usual RETURN and END statements are added, and the compiled program is inserted before the transfer card in the program deck.

SUBROUTINE PRELIM

This optional subroutine is entered once after all the input has been read but before the initial values of the trial parameters are put out. It may be used to read additional input, make preliminary calculations, and otherwise prepare subroutine CALC for the function computation. In its present form the main program provides no arguments for PRELIM, and it is expected that COMMON storage will be used to communicate with CALC.

The subroutine must include COMMON and DIMENSION statements exactly as they appear in the main program, preceding any COMMON statements inserted by the user.

The usual RETURN and END statements are added, and the compiled program is substituted for the dummy program which is included with the card deck provided.

SUBROUTINE TEST

This optional subroutine is entered once at the end of each cycle after the parameters have been adjusted and listed but before they are put out on tape or cards for use in another job. It may be used to test

whether the new parameter values are reasonable, modify them if desired, or terminate the job. It may also be used to test for convergence of the least-squares procedure.

No arguments are provided by the calling program in its present form, but communication may be made by means of COMMON storage.

The subroutine must include COMMON and DIMENSION statements exactly as they appear in the main program, preceding any COMMON statements inserted by the user.

Before TEST is called, the main program sets ISTOP to zero. If the job is to be terminated, TEST should set ISTOP to a non-zero integer. When a job is terminated in this way, the value of ISTOP is given in the output listing so that it may be used as an indicator to identify one of several reasons for stopping.

The array SQSIG may be used as the basis of a test for convergence. When TEST is called, SQSIG(1) contains the estimated agreement factor SQRTF(SIG/(NO-NV)) for the new parameters. For comparison SQSIG(2) contains the same quantity from the previous cycle. On the first cycle of each job SQSIG(2) is zero.

The usual RETURN and END statements are added, and the compiled program is substituted for the dummy routine which is included in the card deck provided.

CARD DECKS PROVIDED

Subprogram	Type	Symbolic card numbers	Column binary card numbers*
Calling program	Fortran	1 - 384	691 - 756
PRELIM (dummy)	Fortran	385 - 389	757 - 758
TEST (dummy)	Fortran	390 - 394	759 - 760
SMI	FAP	395 - 647	761 - 774
CALC (example)	Fortran	648 - 666	775 - 779

Library subroutines to be inserted here if not supplied by monitor system.

Transfer card	667
Data for example	668 - 690

*These column binary cards were compiled or assembled on an IBM 7090. For use on a 704 the calling program should be recompiled, but the remaining subprograms which are included here should be satisfactory.

LIBRARY SUBROUTINES

At the Oak Ridge Central Data Processing Facility all necessary subroutines, except those described above, are supplied from the monitor library tape. At other installations the following subroutines should be provided: Fortran input-output routines, SQRT, FPTRP, ERROR, and EXIT.

FPTRP initializes a floating trap routine so that underflows are set to zero and overflows cause a transfer to ERROR. ERROR terminates the calculation and initiates an optional memory dump. A job is normally ended by calling EXIT.

GLOSSARY OF SYMBOLS

*Indicates input data.

A. Single Storage Variables

* NC	Number of cycles of refinement to be performed in this job. The program puts out YC, the values of the calculated function, NC + 1 times. If NC = 0, YC is calculated, but no refinement occurs.
* NV	Number of parameters to be varied. If NC = 0 then NV is irrelevant.
* NX	Number of independent variables associated with each observation.
* ID	Derivative calculation indicator. If ID = 0 it is assumed that the user's subroutine CALC calculates the derivatives and stores them in DC. If ID = 1 derivatives are to be calculated numerically (except for those parameters for which DP(I) = 0).
* IW	Unit weight indicator. If IW = 1 all observations are assigned unit weights. If IW = 0 then the weights are taken as 1.0/SIGYO(I)**2.
* IP	Parameter input indicator. If IP = 0 the parameters P are to be read from cards. If IP > 0 then the parameters are to be taken from the magnetic tape output of cycle IP of a previous job.
* IT	Parameter output indicator. If IT = 0 parameters are not to be written on tape for later use, if IT = 1 they are to be written on a private tape, and it IT = 2 they are written on the monitor auxiliary tape in such a way as to yield punched

	cards. The private tape is initially rewound and is terminated by an end-of-file while the auxiliary tape is not.
* NP	Total number of parameters including those to be varied as well as those to be held constant.
NO	Number of observations.
IC	Identifying number of a particular cycle in this job.
NCY	NC + 1, the number of cycles plus one. This is the number of times the list of YC will be put out.
SIG	(SQRTW*(YO-YC))**2 summed over all observations.
SQRTW	Square root of the weight for each observation.
YC	Calculated value of the function stored by subroutine CALC.
YD	Calculated value of the function as stored by subroutine CALC for computing numerical derivatives.
DY	YO-YC
WDY	(YO-YC)/SIGYO(I)
PSAVE	Parameter saved while original is incremented for numerical differentiation.
NM	(NV*(NV + 1))/2, the number of elements in the matrix.
SIGP	Standard error of a parameter.
ISTOP	Stop indicator set $\neq$ 0 by subroutine TEST to indicate that no further cycles are to be run on this job. Otherwise ISTOP = 0.
* ISENT	Sentinel set at 1 to end observation deck.
DPK	DP(K) saved for derivative calculation.
PDI	PD(I)
JK	Index used so that AM(JK) is a_{jk}.
IJ	Index used so that AM(IJ) is a_{ij}.
IJD	Increment subtracted from IJ to step down a column of matrix AM(IJ).

POLD	Parameter before correction is added. Saved for output.
II	Index used so that AM(II) is diagonal element a_{ii}.
IID	Increment subtracted from II to step down diagonal of matrix AM(II).
ISING	Singularity indicator set at 1 if a zero diagonal element is found in the original matrix or if a diagonal element becomes zero or negative during inversion by SMI. Otherwise ISING = 0.
NPCD	Multiple of 8 greater than or equal to NP.
NT	Number of private or auxiliary tape used for output of parameters to be saved.

B. Arrays With Their Minimum Dimensions.

* TITLE(12)	Alphanumeric title read at start of problem and transcribed to the output.
* P(NP)	List of NP parameters, some of which will be varied.
* DP(NP)	List of increments to be used if numerical differentation is to be performed.
* KI(NP)	Key integers corresponding to the parameters. KI(I) = 1 if P(I) is to be varied. Otherwise KI(I) = 0.
* X(NX,NO)	NX independent variables for each of NO observations.
* YO(NO)	NO observed dependent variables.
* SIGYO(NO)	Standard errors of the NO observations.
AM((NV*(NV+3))/2)	Matrix of the normal equations. This area is also used for the inverse matrix. Only (NV*(NV+1))/2 words are used for the matrix, but NV more are used by the inverter. Only the upper right triangle of the matrix is stored, and this is stored forward in the memory - i.e., backward in the Fortran indexing system. If a_{ij} represents a matrix element than a_{11} is at AM((NV*(NV+1))/2), a_{12} at AM((NV*(NV+1))/2 - 1), etc., a_{22} is at AM((NV*(NV+1))/2 - NV), and $a_{NV,NV}$ is at AM(1). For example if NV = 4 the storage is as illustrated:

a_{11} = AM(10)	a_{12} = AM(9)	a_{13} = AM(8)	a_{14} = AM(7)
	a_{22} = AM(6)	a_{23} = AM(5)	a_{24} = AM(4)
		a_{33} = AM(3)	a_{34} AM(2)
			a_{44} = AM(1)

V(NV)	Vector of the normal equations.
DC(NP)	Calculated derivatives of YC with respect to P. If derivatives are programmed they are stored here by the user's subroutine.
DV(NV)	Derivatives of those parameters which are to be varied multiplied by the square root of the weight.
PD(NV)	Calculated parameter changes for those parameters which were varied.
DIAG(NV)	Diagonal elements of the inverse matrix. These are used for calculating the standard errors of the parameters which were varied.
DD(NP)	Irrelevant derivatives calculated by CALC on entry for numerical derivatives. This array is needed because both numerical and calculated derivatives may be used in the same problem.
SQSIG(2)	SQSIG(1) is the error of fit, SQRTF(SIG/FLOATF(NO-NV)). SQSIG(2) is SQSIG(1) saved from the previous cycle of this job. SQSIG(2) will be set to zero for the first cycle of each job.
ROW(NV)	A row of the correlation matrix ready for output.

```
*TYPE(FORTRAN)                                                          ORGLS  1
C     OR GLS, GENERAL FORTRAN LEAST SQUARES                             ORGLS  2
      COMMON NC,NV,NX,ID,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC          ORGLS  3
      COMMON SQRTW,DY,WDY,DPK,PSAVE,YD,JK,ISING,II,IID,PDI,IJ,IJD,POLD  ORGLS  4
      COMMON SIGP,ISTOP,NT,NPCD                                         ORGLS  5
      COMMON TITLE,P,X,YO,SIGYO,KI,DP,SQSIG,AM,V,DC,DV,DD,DIAG,PD,ROW   ORGLS  6
                                                                        ORGLS  7
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#200,NO(MAX)#1000,NX(MAX)#5     ORGLS  8
      DIMENSION TITLE(12),P(200),X(5,1000),YO(1000),SIGYO(1000),KI(200) ORGLS  9
      DIMENSION DP(200),SQSIG(2),AM(5150),V(100),DC(200),DV(100),DD(200)ORGLS 10
      DIMENSION DIAG(100),PD(100),ROW(100)                              ORGLS 11
                                                                        ORGLS 12
C     FORMAT STATEMENTS                                                 ORGLS 13
00051 FORMAT(12A6)                                                      ORGLS 14
00052 FORMAT(1H112A6)                                                   ORGLS 15
00053 FORMAT(24I3)                                                      ORGLS 16
00054 FORMAT(32H0NUMBER OF CYCLES IN THIS JOB ISI2/37H0NUMBER OF PARAMETORGLS 17
     1ERS TO BE VARIED ISI3/51H0NUMBER OF INDEPENDENT VARIABLES PER OBSEORGLS 18
     2RVATION ISI2)                                                     ORGLS 19
00058 FORMAT(31H0DERIVATIVES PROGRAMMED BY USER)                        ORGLS 20
00059 FORMAT(57H0NUMERICAL DERIVATIVES UNLESS PARAMETER INCREMENT IS ZERORGLS 21
     10)                                                                ORGLS 22
00061 FORMAT(31H0WEIGHTS TO BE SUPPLIED BY USER)                        ORGLS 23
00062 FORMAT(34H0UNIT WEIGHTS TO BE SET BY PROGRAM)                     ORGLS 24
00063 FORMAT(36H0PARAMETERS TO BE READ AS INPUT DATA)                   ORGLS 25
00064 FORMAT(34H0PARAMETERS TO BE TAKEN FROM CYCLEI2,16H OF PREVIOUS JOBORGLS 26
     1)                                                                 ORGLS 27
00066 FORMAT(I3,81X/(8F9.4,12X))                                        ORGLS 28
00067 FORMAT(29H0NUMBER OF PARAMETERS READ ISI3)                        ORGLS 29
00068 FORMAT(I1,E8.4,7E9.4/(8E9.4))                                     ORGLS 30
00069 FORMAT(31H0NUMBER OF OBSERVATIONS READ ISI4)                      ORGLS 31
00070 FORMAT(72I1)                                                      ORGLS 32
00071 FORMAT(8E9.4)                                                     ORGLS 33
00072 FORMAT(46H0CALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI2)       ORGLS 34
00073 FORMAT(59H0   Y(OBS)   Y(CALC)   OBS-CALC   SIG(O) (O-C)/SIG(O)  XORGLS 35
     1(I)/1H )                                                          ORGLS 36
00079 FORMAT(1H 11F10.4)                                                ORGLS 37
00080 FORMAT(51H0AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE I2/ ORGLS 38
```

```
     120HOSUM(W*(O-C)**2) IS E11.4/35HOSQRTF(SUM(W*(O-C)**2)/(NO-NV)) ISORGLS 39
     2 F10.4)                                                         ORGLS 40
00081 FORMAT(60HOESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CORGLS 41
     1YCLE I2/20HOSUM(W*(O-C)**2) IS E11.4/35HOSQRTF(SUM(W*(O-C)**2)/(NOORGLS 42
     2-NV)) IS F10.4)                                                 ORGLS 43
00083 FORMAT(62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARORGLS 44
     1AMETERI3,16H OF THOSE VARIED)                                   ORGLS 45
00085 FORMAT(40H SINGULARITY RETURN FROM MATRIX INVERTER)             ORGLS 46
00086 FORMAT(37HOPARAMETERS AFTER LEAST SQUARES CYCLEI2/43HO        OLD ORGLS 47
     1    CHANGE      NEW       ERROR/1H )                            ORGLS 48
00088 FORMAT(1H I3,F10.4,10X,F10.4)                                   ORGLS 49
00089 FORMAT(1H I3,4F10.4)                                            ORGLS 50
00090 FORMAT(66HOSUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED ORGLS 51
     1FOR REASONI2)                                                   ORGLS 52
00092 FORMAT(11HOINPUT DATA/30HO  I     P(I)  KI(I)     DP(I)/1H )    ORGLS 53
00093 FORMAT(1H I3,F10.4,I4,3X,E11.4)                                 ORGLS 54
00094 FORMAT(51HOCORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE)  ORGLS 55
00095 FORMAT(51HOCORRECTED PARAMETERS TO BE WRITTEN ON PRIVATE TAPE)  ORGLS 56
00096 FORMAT(51HOCORRECTED PARAMETERS TO BE WRITTEN FOR CARD OUTPUT)  ORGLS 57
00097 FORMAT(19HOCORRELATION MATRIX)                                  ORGLS 58
00098 FORMAT(1HOI3,10F9.4/(1H 3X,10F9.4))                             ORGLS 59
                                                                      ORGLS 60
C     READ TITLE AND CONTROL CARD                                     ORGLS 61
      READ INPUT TAPE 10,00051,(TITLE(I),I#1,12)                      ORGLS 62
      WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                     ORGLS 63
      DUMMY#FPTRPF( 0,-1)                                             ORGLS 64
      READ INPUT TAPE 10,00053,NC,NV,NX,ID,IW,IP,IT                   ORGLS 65
      WRITE OUTPUT TAPE 9,00054,NC,NV,NX                              ORGLS 66
      IF(ID)00206,00204,00206                                         ORGLS 67
                                                                      ORGLS 68
00204    WRITE OUTPUT TAPE 9,00058                                    ORGLS 69
         GO TO 00207                                                  ORGLS 70
                                                                      ORGLS 71
00206    WRITE OUTPUT TAPE 9,00059                                    ORGLS 72
                                                                      ORGLS 73
00207 IF(IW)00210,00208,00210                                         ORGLS 74
                                                                      ORGLS 75
00208    WRITE OUTPUT TAPE 9,00061                                    ORGLS 76
```

```
      GO TO 00211                                                       ORGLS 77
                                                                        ORGLS 78
00210 WRITE OUTPUT TAPE 9,00062                                         ORGLS 79
                                                                        ORGLS 80
00211 IF(IP)00212,00212,00214                                           ORGLS 81
                                                                        ORGLS 82
00212 WRITE OUTPUT TAPE 9,00063                                         ORGLS 83
      GO TO 00215                                                       ORGLS 84
                                                                        ORGLS 85
00214 WRITE OUTPUT TAPE 9,00064,IP                                      ORGLS 86
                                                                        ORGLS 87
00215 IF(IT-1)00216,00218,00221                                         ORGLS 88
                                                                        ORGLS 89
00216 WRITE OUTPUT TAPE 9,00094                                         ORGLS 90
      GO TO 00301                                                       ORGLS 91
                                                                        ORGLS 92
00218 WRITE OUTPUT TAPE 9,00095                                         ORGLS 93
      REWIND 5                                                          ORGLS 94
      GO TO 00301                                                       ORGLS 95
                                                                        ORGLS 96
00221 WRITE OUTPUT TAPE 9,00096                                         ORGLS 97
                                                                        ORGLS 98
C     READ TRIAL PARAMETERS                                             ORGLS 99
00301 IF(IP)00401,00401,00501                                           ORGLS100
                                                                        ORGLS101
00401 READ INPUT TAPE 10,00066,NP,(P(I),I#1,NP)                         ORGLS102
      GO TO 00601                                                       ORGLS103
                                                                        ORGLS104
00501 REWIND 4                                                          ORGLS105
      DO 00503 J#1,IP                                                   ORGLS106
                                                                        ORGLS107
00503    READ INPUT TAPE 4,00066,NP,(P(I),I#1,NP)                       ORGLS108
                                                                        ORGLS109
00601 WRITE OUTPUT TAPE 9,00067,NP                                      ORGLS110
                                                                        ORGLS111
C     READ OBSERVATIONS TO SENTINEL                                     ORGLS112
      J#0                                                               ORGLS113
                                                                        ORGLS114
```

```
00801     J#J+1                                                          ORGLS115
          READ INPUT TAPE 10,00068,ISENT,YO(J),SIGYO(J),(X(I,J),I#1,NX)  ORGLS116
          IF(ISENT)00801,00801,01101                                     ORGLS117
                                                                         ORGLS118
01101 NO#J-1                                                             ORGLS119
      WRITE OUTPUT TAPE 9,00069,NO                                       ORGLS120
                                                                         ORGLS121
C     READ KEY INTEGERS AND PARAMETER INCREMENTS IF SPECIFIED            ORGLS122
      IF(NC)01601,01601,01301                                            ORGLS123
                                                                         ORGLS124
01301     READ INPUT TAPE 10,00070,(KI(I),I#1,NP)                        ORGLS125
          IF(ID)01501,01601,01501                                        ORGLS126
                                                                         ORGLS127
01501         READ INPUT TAPE 10,00071,(DP(I),I#1,NP)                    ORGLS128
                                                                         ORGLS129
C     INITIALIZE PROBLEM AND ENTER SUBROUTINE PRELIM IF PROVIDED         ORGLS130
01601 NM#(NV*(NV+1))/2                                                   ORGLS131
      SQSIG(1)#0.0                                                       ORGLS132
      CALL PRELIM                                                        ORGLS133
                                                                         ORGLS134
C     PUT OUT TRIAL PARAMETERS, KEY INTEGERS, AND PARAMETER INCREMENTS   ORGLS135
      WRITE OUTPUT TAPE 9,00092                                          ORGLS136
      DO 01653 I#1,NP                                                    ORGLS137
                                                                         ORGLS138
01653     WRITE OUTPUT TAPE 9,00093,I,P(I),KI(I),DP(I)                   ORGLS139
                                                                         ORGLS140
C     START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF Y     ORGLS141
      NCY#NC+1                                                           ORGLS142
      DO 08501 IC#1,NCY                                                  ORGLS143
                                                                         ORGLS144
C         CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE                     ORGLS145
          IF(IC-NCY)01851,02001,02001                                    ORGLS146
                                                                         ORGLS147
01851         DO 01852 I#1,NM                                            ORGLS148
                                                                         ORGLS149
01852             AM(I)#0.0                                              ORGLS150
                                                                         ORGLS151
              DO 01902 I#1,NV                                            ORGLS152
```

```
                                                                        ORGLS153
01902          V(I)#0.0                                                 ORGLS154
                                                                        ORGLS155
C        INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF Y(CALC)ORGLS156
02001    SQSIG(2)#SQSIG(1)                                              ORGLS157
         SIG#0.0                                                        ORGLS158
         WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                    ORGLS159
         WRITE OUTPUT TAPE 9,00072,IC                                   ORGLS160
         WRITE OUTPUT TAPE 9,00073                                      ORGLS161
                                                                        ORGLS162
C        START LOOP THROUGH NO OBSERVATIONS                             ORGLS163
02201    DO 05101 I#1,NO                                                ORGLS164
                                                                        ORGLS165
C           ENTER USERS SUBROUTINE TO COMPUTE Y(CALC) AND DERIVATIVES   ORGLS166
            CALL CALC(X(1,I),YC,P,DC)                                   ORGLS167
                                                                        ORGLS168
C           OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM Y(OBS)-Y(CALC)  ORGLS169
            IF(IW)02601,02501,02601                                     ORGLS170
                                                                        ORGLS171
02501          SQRTW#1.0/SIGYO(I)                                       ORGLS172
               GO TO 02701                                              ORGLS173
                                                                        ORGLS174
02601          SIGYO(I)#1.0                                             ORGLS175
               SQRTW#1.0                                                ORGLS176
                                                                        ORGLS177
02701       DY#YO(I)-YC                                                 ORGLS178
            WDY#SQRTW*DY                                                ORGLS179
            SIG#SIG+WDY*WDY                                             ORGLS180
                                                                        ORGLS181
C           PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE OBSERVATION   ORGLS182
            WRITE OUTPUT TAPE 9,00079,YO(I),YC,DY,SIGYO(I),WDY,(X(J,I), ORGLS183
     1                                                     J#1,NX)      ORGLS184
                                                                        ORGLS185
C           BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF Y     ORGLS186
            IF(IC-NCY)03001,05101,05101                                 ORGLS187
                                                                        ORGLS188
C              START LOOP TO STORE AN ARRAY OF NV DERIVATIVES           ORGLS189
03001          J#1                                                      ORGLS190
```

```
                DO 0401 K#1,NP                                          ORGLS191
                                                                        ORGLS192
                   IF(KI(K))0401,0401,0320I                             ORGLS193
                                                                        ORGLS194
0320I                 IF(ID)0340I,0330I,0340I                           ORGLS195
                                                                        ORGLS196
C                        OBTAIN DERIVATIVE FROM THOSE PROGRAMMED BY USER ORGLS197
0330I                    DV(J)#SQRTW*DC(K)                              ORGLS198
                         GO TO 0400I                                    ORGLS199
                                                                        ORGLS200
C                        OBTAIN DERIVATIVE NUMERICALLY UNLESS PARAMETER ORGLS201
C                                                INCREMENT IS ZERO      ORGLS202
0340I                    DPK#DP(K)                                      ORGLS203
                         IF(DPK)0360I,0330I,0360I                       ORGLS204
                                                                        ORGLS205
0360I                       PSAVE#P(K)                                  ORGLS206
                            P(K)#PSAVE+DPK                              ORGLS207
                            CALL CALC(X(1,I),YD,P,DD)                   ORGLS208
                            DV(J)#SQRTW*(YD-YC)/DPK                     ORGLS209
                            P(K)#PSAVE                                  ORGLS210
                                                                        ORGLS211
0400I              J#J+1                                                ORGLS212
0401I              CONTINUE                                             ORGLS213
C                  END LOOP TO OBTAIN DERIVATIVES                       ORGLS214
                                                                        ORGLS215
C               START LOOP TO STORE MATRIX AND VECTOR. SEE GLOSSARY FOR ORGLS216
C                                                STORAGE SCHEME         ORGLS217
                JK#NM                                                   ORGLS218
                DO 0500I J#1,NV                                         ORGLS219
                                                                        ORGLS220
0430I              IF(DV(J))0450I,0440I,0450I                           ORGLS221
                                                                        ORGLS222
C                     BY-PASS IF DERIVATIVE IS ZERO                     ORGLS223
0440I                 JK#JK-NV+J-1                                      ORGLS224
                      GO TO 0500I                                       ORGLS225
                                                                        ORGLS226
0450I                 DO 0480I K#J,NV                                   ORGLS227
                                                                        ORGLS228
```

```
                    AM(JK)#AM(JK)+DV(J)*DV(K)                          ORGLS229
                    JK#JK-1                                            ORGLS230
04801               CONTINUE                                           ORGLS231
                                                                       ORGLS232
                 V(J)#V(J)+DV(J)*WDY                                   ORGLS233
05001            CONTINUE                                              ORGLS234
C                END LOOP TO STORE MATRIX AND VECTOR                   ORGLS235
                                                                       ORGLS236
05101         CONTINUE                                                 ORGLS237
C             END LOOP THROUGH NO OBSERVATIONS                         ORGLS238
                                                                       ORGLS239
C        COMPUTE AND PUT OUT AGREEMENT FACTORS                         ORGLS240
         SQSIG(I)#SQRTF(SIG/FLOATF(NO-NV))                             ORGLS241
         WRITE OUTPUT TAPE 9,00080,IC,SIG,SQSIG(I)                     ORGLS242
                                                                       ORGLS243
C        BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL CYCLE  ORGLS244
         IF(IC-NCY)05401,08701,08701                                   ORGLS245
                                                                       ORGLS246
C           START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT               ORGLS247
05401       ISING#0                                                    ORGLS248
            II#NM                                                      ORGLS249
            IID#NV                                                     ORGLS250
            DO 05801 I#1,NV                                            ORGLS251
                                                                       ORGLS252
               IF(AM(II))05701,05601,05701                             ORGLS253
                                                                       ORGLS254
05601             ISING#1                                              ORGLS255
                  WRITE OUTPUT TAPE 9,00083,I                          ORGLS256
                                                                       ORGLS257
05701          II#II-IID                                               ORGLS258
               IID#IID-1                                               ORGLS259
05801          CONTINUE                                                ORGLS260
C              END LOOP TO TEST FOR ZERO DIAGONAL ELEMENT              ORGLS261
                                                                       ORGLS262
C           TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND           ORGLS263
            IF(ISING)10301,06001,10301                                 ORGLS264
                                                                       ORGLS265
C              ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE         ORGLS266
```

```
06001          CALL SMI(AM(NM),NV,ISING)                                ORGLS267
               IF(ISING)06201,06301,06201                               ORGLS268
                                                                        ORGLS269
C                 TERMINATE JOB IF SINGULAR MATRIX WAS FOUND            ORGLS270
06201             WRITE OUTPUT TAPE 9,00085                             ORGLS271
                  GO TO 10301                                           ORGLS272
                                                                        ORGLS273
C                 START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR       ORGLS274
C                                              PARAMETER CHANGES        ORGLS275
06301             DO 07201 I#1,NV                                       ORGLS276
                                                                        ORGLS277
                     PDI#0.0                                            ORGLS278
                     IJ#NM-I+1                                          ORGLS279
                     IJD#NV-1                                           ORGLS280
                     DO 07001 J#1,NV                                    ORGLS281
                                                                        ORGLS282
                        PDI#PDI+AM(IJ)*V(J)                             ORGLS283
                        IF(J-I)06701,06801,06901                        ORGLS284
                                                                        ORGLS285
06701                      IJ#IJ-IJD                                    ORGLS286
                           IJD#IJD-1                                    ORGLS287
                           GO TO 07001                                  ORGLS288
                                                                        ORGLS289
C                          SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX     ORGLS290
06801                      DIAG(I)#AM(IJ)                               ORGLS291
                                                                        ORGLS292
06901                      IJ#IJ-1                                      ORGLS293
07001                      CONTINUE                                     ORGLS294
                                                                        ORGLS295
                     PD(I)#PDI                                          ORGLS296
                     SIG#SIG-PDI*V(I)                                   ORGLS297
07201                CONTINUE                                           ORGLS298
C                    END LOOP FOR MATRIX VECTOR MULTIPLICATION          ORGLS299
                                                                        ORGLS300
C                 RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG         ORGLS301
                  SQSIG(1)#SQRTF(SIG/FLOATF(NO-NV))                     ORGLS302
                                                                        ORGLS303
C                 PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS      ORGLS304
```

```
                WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)          ORGLS305
                WRITE OUTPUT TAPE 9,00086,IC                         ORGLS306
C               START LOOP TO CORRECT AND PUT OUT PARAMETERS         ORGLS307
                                                                     ORGLS308
                J#1                                                  ORGLS309
                DO 08001 I#1,NP                                      ORGLS310
                                                                     ORGLS311
                   IF(KI(I))07601,07601,07701                        ORGLS312
                                                                     ORGLS313
07601                 WRITE OUTPUT TAPE 9,00088,I,P(I),P(I)          ORGLS314
                      GO TO 08001                                    ORGLS315
                                                                     ORGLS316
07701                 POLD#P(I)                                      ORGLS317
                      P(I)#POLD+PD(J)                                ORGLS318
                      SIGP#SQRTF(DIAG(J))*SQSIG(I)                   ORGLS319
                      WRITE OUTPUT TAPE 9,00089,I,POLD,PD(J),P(I),SIGPORGLS320
                      J#J+1                                          ORGLS321
                                                                     ORGLS322
08001              CONTINUE                                          ORGLS323
C                  END LOOP TO CORRECT AND PUT OUT PARAMETERS        ORGLS324
                                                                     ORGLS325
C               PUT OUT ESTIMATED AGREEMENT FACTORS                  ORGLS326
                WRITE OUTPUT TAPE 9,00081,IC,SIG,SQSIG(I)            ORGLS327
                                                                     ORGLS328
C               ENTER USERS SUBROUTINE TO TEST AND MODIFY PARAMETERS ORGLS329
C                                                 OR END JOB         ORGLS330
                ISTOP#0                                              ORGLS331
                CALL TEST                                            ORGLS332
                                                                     ORGLS333
C               WRITE CORRECTED PARAMETERS ON AUXILIARY TAPE IF      ORGLS334
C                                                DESIRED             ORGLS335
08201           IF(IT)08202,08301,08202                              ORGLS336
                                                                     ORGLS337
08202              NT#IT+4                                           ORGLS338
                   NPCD#8*((NP-1)/8+1)                               ORGLS339
                   WRITE OUTPUT TAPE NT,00066,NP,(P(I),I#1,NPCD)     ORGLS340
                                                                     ORGLS341
C               TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST  ORGLS342
```

```
08301              IF(ISTOP)08401,08501,08401                          ORGLS343
                                                                       ORGLS344
08401                 WRITE OUTPUT TAPE 9,00090,ISTOP                  ORGLS345
                      GO TO 08701                                      ORGLS346
                                                                       ORGLS347
08501                 CONTINUE                                         ORGLS348
C                     END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y   ORGLS349
                                                                       ORGLS350
C     TERMINATE JOB                                                    ORGLS351
08701 IF(NC)10501,10501,08801                                          ORGLS352
                                                                       ORGLS353
C        CALCULATE AND PUT OUT CORRELATION MATRIX                      ORGLS354
08801    WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                   ORGLS355
         WRITE OUTPUT TAPE 9,00097                                     ORGLS356
         DO 09101 I#1,NV                                               ORGLS357
                                                                       ORGLS358
            DIAG(I)#1.0/SQRTF(DIAG(I))                                 ORGLS359
09101       CONTINUE                                                   ORGLS360
                                                                       ORGLS361
         IJ#NM                                                         ORGLS362
         DO 10201 I#1,NV                                               ORGLS363
                                                                       ORGLS364
            DO 09601 J#1,NV                                            ORGLS365
                                                                       ORGLS366
               ROW(J)#0.0                                              ORGLS367
09601          CONTINUE                                                ORGLS368
                                                                       ORGLS369
            DO 10001 J#I,NV                                            ORGLS370
                                                                       ORGLS371
               ROW(J)#AM(IJ)*DIAG(I)*DIAG(J)                           ORGLS372
               IJ#IJ-1                                                 ORGLS373
10001          CONTINUE                                                ORGLS374
                                                                       ORGLS375
            WRITE OUTPUT TAPE 9,00098,I,(ROW(J),J#1,NV)                ORGLS376
10201       CONTINUE                                                   ORGLS377
                                                                       ORGLS378
10301 IF(IT-1)10501,10401,10501                                        ORGLS379
                                                                       ORGLS380
```

```
10401     END FILE 5                                                    ORGLS381
                                                                        ORGLS382
10501 CALL EXIT                                                         ORGLS383
      END(0,1,0,0,0)                                                    ORGLS384


*TYPE(FORTRAN)                                                          ORGLS385
C     DUMMY SUBROUTINE PRELIM                                           ORGLS386
      SUBROUTINE PRELIM                                                 ORGLS387
      RETURN                                                            ORGLS388
      END                                                               ORGLS389


*TYPE(FORTRAN)                                                          ORGLS390
C     DUMMY SUBROUTINE TEST                                             ORGLS391
      SUBROUTINE TEST                                                   ORGLS392
      RETURN                                                            ORGLS393
      END                                                               ORGLS394


*TYPE(FAP)                                                              ORGLS395
       COUNT   230                                                      ORGLS396
       REM SYMMETRIC MATRIX INVERSE. SEE GLOSSARY FOR STORAGE SCHEME.   ORGLS397
       REM FOR USE ON 704, 709, OR 7090.                                ORGLS398
       REM WRITTEN IN FAP FOR ASSEMBLY ON 709 OR 7090.                  ORGLS399
       ENTRY   SMI                                                      ORGLS400
 SMI   SXD T13,1                                                        ORGLS401
       SXD T14,2                                                        ORGLS402
       LFTM                                                             ORGLS403
       TNO *+1                        OVERFLOW TOGGLES                  ORGLS404
       CAL 1,4                                                          ORGLS405
       COM                                                              ORGLS406
       PAX 0,2                                                          ORGLS407
       TXI *+1,2,1                                                      ORGLS408
       CLA 2,4                                                          ORGLS409
```

```
        STA Y1                                                  ORGLS410
        CLA 3,4                                                 ORGLS411
        STA Y28                                                 ORGLS412
        STA SINGI                                               ORGLS413
Y1      CLA 0                   ADD SET                         ORGLS414
        PDX 0,1                                                 ORGLS415
        STD Y27                                                 ORGLS416
        SXD T1,4                                                ORGLS417
Y2      SXD Y25,1               Y2                              ORGLS418
        SXD T2,1                                                ORGLS419
        SXD T3,2                                                ORGLS420
        STZ T4                  Y3                              ORGLS421
        STZ T5,                                                 ORGLS422
        LXD T4,4                                                ORGLS423
Y4      SXD Y7,1                Y4                              ORGLS424
        CLA 0,2                 Y5                              ORGLS425
        SSP                                                     ORGLS426
        FSB T4                                                  ORGLS427
        TMI Y7                                                  ORGLS428
        CLA 0,2                 Y6                              ORGLS429
        SSP                                                     ORGLS430
        STO T4                                                  ORGLS431
        SXD T5,4                                                ORGLS432
Y7      TIX Y8,2,0              Y7   DEC SET Y4,DELTA           ORGLS433
        HTR Y8                                                  ORGLS434
Y8      TNX Y10,1,1             Y8                              ORGLS435
        TXI Y4,4,1              Y9                              ORGLS436
Y10     CAL T3                  Y10                             ORGLS437
        ADD T2                                                  ORGLS438
        PDX 0,4                                                 ORGLS439
        CLA T5                                                  ORGLS440
        STO 0,4                                                 ORGLS441
        TSX X1,4                Y11                             ORGLS442
        LXD T3,2                Y12                             ORGLS443
        CLA 0,2                                                 ORGLS444
        TZE SING                                                ORGLS445
        TMI SING                                                ORGLS446
        CLA FLONE               Y13                             ORGLS447
```

```
        FDP 0,2                                                 ORGLS448
        STQ 0,2                                                 ORGLS449
        CLS 0,2                                                 ORGLS450
        STO T6                                                  ORGLS451
        CLA PON                 Y14                             ORGLS452
        SUB T3                                                  ORGLS453
        ARS 18                                                  ORGLS454
        STA Y16A                     SETS ADDRESSES             ORGLS455
        STA Y19                         AT M                    ORGLS456
        CLA PON                                                 ORGLS457
        SUB T3                                                  ORGLS458
        ADD T2                                                  ORGLS459
        ARS 18                                                  ORGLS460
        STA Y16                      SETS ADDRESSES             ORGLS461
        STA Y19A                        AT M+N                  ORGLS462
        LXD T2,1                                                ORGLS463
        LXD T2,2                                                ORGLS464
        CLA T3                                                  ORGLS465
        SUB T2                                                  ORGLS466
        PDX 0,4                                                 ORGLS467
Y15     TNX Y17,1,1             Y15                             ORGLS468
Y16     LDQ 0,1                 Y16  ADD SET Y14,M+N            ORGLS469
        FMP T6                                                  ORGLS470
        TNO Y16A                                                ORGLS471
        SXD T12,4                                               ORGLS472
        TSX OFL,4                                               ORGLS473
        LXD T12,4                                               ORGLS474
Y16A    STO 0,1                      ADD SET Y14,M              ORGLS475
DT1     TNX Y15,0,0                  DEC FOR T1,C(I4)           ORGLS476
Y17     TNX Y24,2,1             Y17                             ORGLS477
        PXD 0,2                 Y18                             ORGLS478
        PDX 0,1                                                 ORGLS479
Y19     LDQ 0,1                 Y19  ADD SET Y14,M              ORGLS480
Y19A    FMP 0,2                      ADD SET Y14,M+N            ORGLS481
        TNO Y19B                                                ORGLS482
        SXD T12,4                                               ORGLS483
        TSX OFL,4                                               ORGLS484
        LXD T12,4                                               ORGLS485
```

```
Y19B   FAD 0,4                                                  ORGLS486
       TNO Y19C                                                 ORGLS487
       SXD T12,4                                                ORGLS488
       TSX OFL,4                                                ORGLS489
       LXD T12,4                                                ORGLS490
Y19C   STO 0,4                                                  ORGLS491
       TXI Y20,4,-1                                             ORGLS492
Y20    TNX Y17,1,1          Y20                                 ORGLS493
       TNX Y19,0,0                                              ORGLS494
Y24    LXD T3,2             Y24                                 ORGLS495
       LXD T2,1                                                 ORGLS496
       TNX Y26,1,1                                              ORGLS497
Y25    TIX Y2,2,0           Y25  DEC SET Y2                     ORGLS498
       HTR Y2                                                   ORGLS499
Y26    TXI Y26A,1,1         Y26                                 ORGLS500
Y26A   SXD Y29,1                                                ORGLS501
Y27    TXL Y29,1,0          Y27  DEC SET Y1,0                   ORGLS502
       LXD T1,4             Y28                                 ORGLS503
       LXD T13,1                                                ORGLS504
       LXD T14,2                                                ORGLS505
Y28    STZ 0                ADD SET                             ORGLS506
       EFTM                                                     ORGLS507
       TRA 4,4              NORMAL RETURN                       ORGLS508
Y29    TXI Y29A,2,0         Y29  DEC SET Y26                    ORGLS509
Y29A   SXD T3,2                                                 ORGLS510
       SXD T2,1                                                 ORGLS511
       CLA PON              Y30                                 ORGLS512
       SUB T3                                                   ORGLS513
       ARS 18                                                   ORGLS514
       STA Y35                   SETS ADDRESSES                 ORGLS515
       STA Y38                      AT M                        ORGLS516
       STA Y39                                                  ORGLS517
       STA Y39B                                                 ORGLS518
       STA Y39C                                                 ORGLS519
       CLA PON                                                  ORGLS520
       SUB T3                                                   ORGLS521
       ADD T2                                                   ORGLS522
       ARS 18                                                   ORGLS523
```

```
        STA Y31                     SETS ADDRESSES                  ORGLS524
        STA Y36                        AT M+N                       ORGLS525
        STA Y36A                                                    ORGLS526
        STA Y38B                                                    ORGLS527
        STA Y38C                                                    ORGLS528
        STA Y39A                                                    ORGLS529
        CLA T2                                                      ORGLS530
        SUB ONE                                                     ORGLS531
        PDX 0,1                     SETS INDEXES                    ORGLS532
        PDX 0,2                        AT M-N                       ORGLS533
Y31     STZ 0,1                 Y31 ADD SET Y30,M+N                 ORGLS534
        TIX Y31,1,1             Y32                                 ORGLS535
        CLA T3                  Y33                                 ORGLS536
        SUB T2                                                      ORGLS537
        PDX 0,4                                                     ORGLS538
Y34     PXD 0,2                 Y34                                 ORGLS539
        PDX 0,1                                                     ORGLS540
Y35     LDQ 0,2                 Y35 ADD SET Y30,M                   ORGLS541
        FMP 0,4                                                     ORGLS542
        TNO Y36                                                     ORGLS543
        SXD T12,4                                                   ORGLS544
        TSX OFL,4                                                   ORGLS545
        LXD T12,4                                                   ORGLS546
Y36     FAD 0,1                 Y36 ADD SET Y30,M+N                 ORGLS547
        TNO Y36A                                                    ORGLS548
        SXD T12,4                                                   ORGLS549
        TSX OFL,4                                                   ORGLS550
        LXD T12,4                                                   ORGLS551
Y36A    STO 0,1                     ADD SET Y30,M+N                 ORGLS552
        TXI Y37,4,-1                                                ORGLS553
Y37     TNX Y39,1,1             Y37                                 ORGLS554
Y38     LDQ 0,1                 Y38 ADD SET Y30,M                   ORGLS555
        FMP 0,4                                                     ORGLS556
        TNO Y38B                                                    ORGLS557
        SXD T12,4                                                   ORGLS558
        TSX OFL,4                                                   ORGLS559
        LXD T12,4                                                   ORGLS560
Y38B    FAD 0,2                     ADD SET Y30,M+N                 ORGLS561
```

```
        TNO Y38C                                                ORGLS562
        SXD T12,4                                               ORGLS563
        TSX OFL,4                                               ORGLS564
        LXD T12,4                                               ORGLS565
Y38C    STO 0,2                 ADD SET Y30,M+N                 ORGLS566
        TNX Y35,0,0                                             ORGLS567
Y39     LDQ 0,2                 Y39  ADD SET Y30,M              ORGLS568
Y39A    FMP 0,2                      ADD SET Y30,M+N            ORGLS569
        TNO Y39B                                                ORGLS570
        SXD T12,4                                               ORGLS571
        TSX OFL,4                                               ORGLS572
        LXD T12,4                                               ORGLS573
Y39B    FAD 0                        ADD SET Y30,M              ORGLS574
        TNO Y39C                                                ORGLS575
        SXD T12,4                                               ORGLS576
        TSX OFL,4                                               ORGLS577
        LXD T12,4                                               ORGLS578
Y39C    STO 0                        ADD SET Y30,M              ORGLS579
        TIX Y34,2,1             Y40  GO TO Y50                  ORGLS580
        CAL T3                  Y50                             ORGLS581
        ADD T2                                                  ORGLS582
        PDX 0,4                                                 ORGLS583
        CAL 0,4                                                 ORGLS584
        SLW T5                                                  ORGLS585
        TSX X1,4                Y51                             ORGLS586
        LXD T3,2                Y52                             ORGLS587
        LXD T2,1                                                ORGLS588
DT12    TNX Y26,0,0                  DEC FOR T12                ORGLS589
SING    PXD 0,2                 SINGULARITY RETURN              ORGLS590
        LXD T13,1                                               ORGLS591
        LXD T14,2                                               ORGLS592
        LXD T1,4                                                ORGLS593
        CLA ONE                                                 ORGLS594
SING1   STO 0                   ADD SET                         ORGLS595
        EFTM                                                    ORGLS596
        TRA 4,4                 ERROR RETURN                    ORGLS597
OFL     ARS 1                   OVERFLOW-UNDERFLOW              ORGLS598
        PBT                                                     ORGLS599
```

```
DT13   TNX OFL+5,0,0              DEC FOR T13,C(I1)                ORGLS600
       PXD 0,0,0                                                   ORGLS601
       TRA 1,4                                                     ORGLS602
       PXD 0,4                                                     ORGLS603
       SSM                                                         ORGLS604
DT14   TNX SING+1,0,0             DEC FOR T14,C(I2)                ORGLS605
X1     CLA T5                 X1                                  ORGLS606
       TZE 1,4                                                     ORGLS607
       SXD T12,4              X2                                  ORGLS608
       LXD T2,1                                                    ORGLS609
       LXD T3,2                                                    ORGLS610
       CAL T3                                                      ORGLS611
       SUB T5                                                      ORGLS612
       PDX 0,4                                                     ORGLS613
       STD X6                                                      ORGLS614
X3     CAL 0,2                X3                                  ORGLS615
       LDQ 0,4                                                     ORGLS616
       SLW 0,4                                                     ORGLS617
       STQ 0,2                                                     ORGLS618
       TNX X9,1,1             X4                                  ORGLS619
       SXD X8,1               X5                                  ORGLS620
X6     TXH X8,2,0             X6    DEC SET X2                    ORGLS621
       CAL ONE                X7                                  ORGLS622
       STD X8                                                      ORGLS623
X8     TIX X8A,4,0            X8    DEC SET X5,X7                 ORGLS624
       HTR 0                                                       ORGLS625
X8A    TXI X3,2,-1                                                 ORGLS626
X9     LXD T3,2               X9                                  ORGLS627
       LXD X6,4                                                    ORGLS628
       CAL 0,2                                                     ORGLS629
       LDQ 0,4                                                     ORGLS630
       SLW 0,4                                                     ORGLS631
       STQ 0,2                                                     ORGLS632
       LXD T12,4              X10                                 ORGLS633
       TRA 1,4                                                     ORGLS634
ONE    PZE 0,0,1              ONE                                 ORGLS635
FLONE  DEC 1.0                FLONE                               ORGLS636
PON    PON 0,0,0              LGNO                                ORGLS637
```

```
T2     PZE 0,0,0          T2, N                                    ORGLS638
T3     PZE 0,0,0          T3,-M                                    ORGLS639
T4     PZE 0,0,0          T4,X    T6,-B11                          ORGLS640
T5     PZE 0,0,0          T5,J                                     ORGLS641
T1     SYN DT1            C(I4)                                    ORGLS642
T6     SYN T4             -B11                                     ORGLS643
T12    SYN DT12           C(I4) FOR SR                             ORGLS644
T13    SYN DT13           C(I1)                                    ORGLS645
T14    SYN DT14           C(I2)                                    ORGLS646
       END 0                                                       ORGLS647


*TYPE(FORTRAN)                                                     ORGLS648
C      EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTSORGLS649
                                                                   ORGLS650
C      P(1) AND P(2) ARE FIXED PARAMETERS.                         ORGLS651
C      P(1) IS THE X VALUE OF THE FIRST END POINT.                 ORGLS652
C      P(2) IS THE INTERVAL IN X COVERED BY EACH SEGMENT.          ORGLS653
C      P(3),P(4), ETC. ARE THE Y VALUES OF THE END POINTS. THESE   ORGLS654
C         WILL BE ADJUSTED BY LEAST SQUARES.                       ORGLS655
                                                                   ORGLS656
       SUBROUTINE CALC(X,Y,P,D)                                    ORGLS657
                                                                   ORGLS658
       DIMENSION P(10)                                             ORGLS659
                                                                   ORGLS660
       Z#X-P(1)                                                    ORGLS661
       I#Z/P(2)                                                    ORGLS662
       F#Z/P(2)-FLOATF(I)                                          ORGLS663
       Y#P(I+3)+(P(I+4)-P(I+3))*F                                  ORGLS664
       RETURN                                                      ORGLS665
       END                                                         ORGLS666


*DATA                                                              ORGLS667
EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS. ORGLS668
  1  6  1  1  1  0  0                                              ORGLS669
```

```
 8                                                                                  ORGLS670
    10.0      5.0      4.4      5.5      8.4     13.2     16.3     17.3ORGLS671
     4.7               10.8                                                         ORGLS672
     4.7               12.2                                                         ORGLS673
     5.1               13.8                                                         ORGLS674
     5.6               15.6                                                         ORGLS675
     6.5               17.4                                                         ORGLS676
     7.2               18.4                                                         ORGLS677
     8.3               19.8                                                         ORGLS678
     9.9               21.4                                                         ORGLS679
    10.4               22.2                                                         ORGLS680
    12.1               24.0                                                         ORGLS681
    13.4               25.2                                                         ORGLS682
    15.1               27.2                                                         ORGLS683
    15.9               28.8                                                         ORGLS684
    16.2               30.0                                                         ORGLS685
    17.0               32.2                                                         ORGLS686
    17.1               34.2                                                         ORGLS687
1                                                                                   ORGLS688
00111111                                                                            ORGLS689
       0         0     0.01     0.01     0.01     0.01     0.01     0.01ORGLS690
```

```
EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

NUMBER OF CYCLES IN THIS JOB IS 1

NUMBER OF PARAMETERS TO BE VARIED IS  6

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 1

NUMERICAL DERIVATIVES UNLESS PARAMETER INCREMENT IS ZERO

UNIT WEIGHTS TO BE SET BY PROGRAM

PARAMETERS TO BE READ AS INPUT DATA

CORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE

NUMBER OF PARAMETERS READ IS  8

NUMBER OF OBSERVATIONS READ IS  16

INPUT DATA

  I      P(I)  KI(I)      DP(I)

  1    10.0000   0     0.
  2     5.0000   0     0.
  3     4.4000   1     1.0000E-02
  4     5.5000   1     1.0000E-02
  5     8.4000   1     1.0000E-02
  6    13.2000   1     1.0000E-02
  7    16.3000   1     1.0000E-02
  8    17.3000   1     1.0000E-02
```

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 1

Y(OBS)	Y(CALC)	OBS-CALC	SIG(O)	(O-C)/SIG(O)	X(I)
4.7000	4.5760	0.1240	1.0000	0.1240	10.8000
4.7000	4.8840	-0.1840	1.0000	-0.1840	12.2000
5.1000	5.2360	-0.1360	1.0000	-0.1360	13.8000
5.6000	5.8480	-0.2480	1.0000	-0.2480	15.6000
6.5000	6.8920	-0.3920	1.0000	-0.3920	17.4000
7.2000	7.4720	-0.2720	1.0000	-0.2720	18.4000
8.3000	8.2840	0.0160	1.0000	0.0160	19.8000
9.9000	9.7440	0.1560	1.0000	0.1560	21.4000
10.4000	10.5120	-0.1120	1.0000	-0.1120	22.2000
12.1000	12.2400	-0.1400	1.0000	-0.1400	24.0000
13.4000	13.3240	0.0760	1.0000	0.0760	25.2000
15.1000	14.5640	0.5360	1.0000	0.5360	27.2000
15.9000	15.5560	0.3440	1.0000	0.3440	28.8000
16.2000	16.3000	-0.1000	1.0000	-0.1000	30.0000
17.0000	16.7400	0.2600	1.0000	0.2600	32.2000
17.1000	17.1400	-0.0400	1.0000	-0.0400	34.2000

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.9042E 00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.3007

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

	OLD	CHANGE	NEW	ERROR
1	10.0000		10.0000	
2	5.0000		5.0000	
3	4.4000	0.1615	4.5615	0.2275
4	5.5000	-0.3648	5.1352	0.1767
5	8.4000	-0.0886	8.3114	0.1489
6	13.2000	0.1295	13.3295	0.1552
7	16.3000	0.2280	16.5280	0.1588
8	17.3000	-0.0067	17.2933	0.2372

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.4651E-00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.2157

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 2

Y(OBS)	Y(CALC)	OBS-CALC	SIG(O)	(O-C)/SIG(O)	X(I)
4.7000	4.6533	0.0467	1.0000	0.0467	10.8000
4.7000	4.8139	-0.1139	1.0000	-0.1139	12.2000
5.1000	4.9975	0.1025	1.0000	0.1025	13.8000
5.6000	5.5163	0.0837	1.0000	0.0837	15.6000
6.5000	6.6598	-0.1598	1.0000	-0.1598	17.4000
7.2000	7.2950	-0.0950	1.0000	-0.0950	18.4000
8.3000	8.1843	0.1157	1.0000	0.1157	19.8000
9.9000	9.7164	0.1836	1.0000	0.1836	21.4000
10.4000	10.5193	-0.1193	1.0000	-0.1193	22.2000
12.1000	12.3258	-0.2258	1.0000	-0.2258	24.0000
13.4000	13.4574	-0.0574	1.0000	-0.0574	25.2000
15.1000	14.7368	0.3632	1.0000	0.3632	27.2000
15.9000	15.7604	0.1396	1.0000	0.1396	28.8000
16.2000	16.5280	-0.3280	1.0000	-0.3280	30.0000
17.0000	16.8647	0.1353	1.0000	0.1353	32.2000
17.1000	17.1709	-0.0709	1.0000	-0.0709	34.2000

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

SUM(W*(O-C)**2) IS 0.4651E-00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.2157

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CORRELATION MATRIX

1	1.0000	-0.4062	0.1268	-0.0353	0.0083	-0.0023
2	0.	1.0000	-0.3120	0.0869	-0.0204	0.0058
3	0.	0.	1.0000	-0.2787	0.0652	-0.0185
4	0.	0.	0.	1.0000	-0.2341	0.0664
5	0.	0.	0.	0.	1.0000	-0.2836
6	0.	0.	0.	0.	0.	1.0000