MULTI-DIMENSIONAL
REGRESSION ANALYSIS'

(USERS' MANUAL FOR PROGRAMS
CURVE AND MULTI)

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1. THEORY

A problem, which is encountered rather frequently in experimental research, is to find a functional expression for a relationship between a number of variables from a set of data obtained by experiments. The most widely used method for solving this problem is the "Least Squares Fit".

The basis of this method is to approximate the data \( D_L(x,y,z) \), (which are assumed to be a function of three independent variables) by a regression function \( \bar{D}(x,y,z) \) in such a way that the sum of squares of the residuals \( r_L(x,y,z) = D_L(x,y,z) - \bar{D}(x,y,z) \) becomes a minimum.

\[
S = \sum_{L=1}^{n} [D_L(x,y,z) - \bar{D}(x,y,z)]^2 = \min
\]

\( n \) = total number of data

For a four-dimensional regression analysis (three independent variables) the regression function has the following form:

\[
\bar{D}(x,y,z) = \sum_{i=1}^{n_i} \sum_{j=1}^{n_j} \sum_{k=1}^{n_k} a_{ijk} \cdot f_i(x) \cdot g_j(y) \cdot h_k(z)
\]

where \( a_{ijk} \) are unknown coefficients of the regression subfunctions \( f_i(x) \), \( g_j(y) \), and \( h_k(z) \).
These coefficients can be determined by minimizing the sum of squares of residuals:

$$\frac{\partial S}{\partial a_{ijk}} = \frac{\partial}{\partial a_{ijk}} \left[ \sum_{L=1}^{n} \left( D_L - \bar{D} \right)^2 \right] = 2 \sum_{L=1}^{n} \left( \bar{D}_L - D \right) \cdot f_i g_j h_k = 0$$

The minimization process leads to a system of \( m \times m \) linear simultaneous equations where \( m \) is the product of the total number of subfunctions \( f_i(x), g_j(y), \) and \( h_k(z) \):

$$m = n_i \times n_j \times n_k$$

Solving these equations gives the regression coefficients \( a_{ijk} \), from which the values of the regression function \( \bar{D}(x, y, z) \) can be determined for arbitrary values of \( x, y, \) and \( z \).

As an illustration of the basic procedure the following equations for a two-dimensional regression analysis (one independent variable \( x \)) are obtained:

$$\bar{D}(x) = \sum_{i=1}^{n_i} a_i f_i(x) = a_1 f_1(x) + a_2 f_2(x) + \ldots + a_{n_i} f_{n_i}(x)$$

$$S = \sum_{L=1}^{n} \left[ D_L(x) - \bar{D}(x) \right]^2$$

$$\frac{\partial S}{\partial a_i} = 2 \sum_{L=1}^{n} \left[ D_L(x) - \bar{D}(x) \right] \frac{\partial \bar{D}(x)}{\partial a_i} = 0$$
The governing equations for the three and four-dimensional regression analysis are found in a way similar to those for a two-dimensional problem.
2. PROGRAM CURVE

2.1 Purpose

The purpose of the program CURVE is a regression analysis of data with one or two independent variables.

This analysis is based on the following regression functions:

One independent variable:

\[ D(x) = \sum_{i=1}^{n_i} a_i f_i(x) \]

Two independent variables:

\[ D(x,y) = \sum_{i=1}^{n_i} \sum_{j=1}^{n_j} a_{ij} f_i(x) g_j(y) \]

The data have to be arranged in the following form:

\[ D(I,J) \quad I = 1, \ldots, NR \text{ subscript related to variable } x \]
\[ J = 1, \ldots, NP \text{ subscript related to variable } y \]

where \( x \) = constant for all values \( D(I, J = 1 \ldots NP) \)

\( y \) = constant for all values \( D(I = 1 \ldots NR, J) \)

For two-dimensional problems (one independent variable) \( y \) is assumed to have a constant value of 1.

By selecting the proper code numbers the following types of regression subfunctions can be utilized:
<table>
<thead>
<tr>
<th>Code Number</th>
<th>( f_j(u) ), ( g_j(u) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>( u )</td>
</tr>
<tr>
<td>3</td>
<td>( \sqrt{u} )</td>
</tr>
<tr>
<td>4</td>
<td>( 1/u )</td>
</tr>
<tr>
<td>5</td>
<td>( u^2 )</td>
</tr>
<tr>
<td>6</td>
<td>( u^3 )</td>
</tr>
<tr>
<td>7</td>
<td>( \log_{10} u )</td>
</tr>
<tr>
<td>8</td>
<td>( 4/u )</td>
</tr>
</tbody>
</table>

Unless special provisions are made the program will in a subsequent step reject data whose residuals after the first least squares fit lie beyond a defined constant band-width. This band-width is twice the standard error of estimate (standard deviation of residuals) multiplied by a factor which has to be specified by the user. In a final step the program will repeat the regression analysis for those data which were not rejected.
2.2 Logical Flow Chart

Two-dimensional Regression

- CURVE
  - CURFIT
    - Outxx

- Solve → UNIFORM
  - Outxx → REJECT
    - Solve → UNIFORM
    - No Data Rejection

Three-dimensional Regression

- Solve → NONUNI
  - Outxx → REJECT
    - Outxx → NONUNI
    - Solve

END
2.3 Description of Subprograms

(1) Main program CURVE

Purpose: Input of data
1. control variables
2. data
3. arguments of variable x (and y)
4. code numbers of regression subfunctions
   \( f_i(x) \) (and \( g_j(y) \))

The source program is written in such a form, that after executing the regression analysis with a certain set of functions \( f_i(x) \) (or \( f_i(x) \) and \( g_j(y) \)) other sets of functions will be read in and the regression analysis will be repeated.

(2) Subprogram CURFIT

Purpose: Calling of regression subroutines in prescribed order (see the logical flow chart)
Output: original data
arguments of variable x (and y)

(3) Subprogram OUTXX

Purpose: print out of arrays (original data, residuals, fitted data), output is printed in columns of 8 (Format E14.4), headings are provided by the calling program
(4) **Subprogram SOLVE**

**Purpose:** Solution of systems of simultaneous equations
(modified version of the matrix pack subroutine)

(5) **Subprogram REJECT**

**Purpose:**
1. calculation of total number of data, sum of squares of residuals, standard error of estimate (standard deviation of residuals) before rejection
2. rejection of data, whose residuals lie beyond a certain (constant) band-width
3. calculation of total number of data, sum of squares and standard error of estimate after rejection

**Output:**
1. residuals before rejection
2. total number of data, sum of squares and standard error before rejection
3. rejected data
4. residuals after rejection
5. total number of data, sum of squares, and standard error after rejection

(6) **Subroutine UNIFORM**

**Purpose:** Two dimensional regression analysis (one independent variable x)
1. scaling of variable x  
   (logarithmic or linear scale)  
2. calculation of values of regression subfunctions $f_i(x)$  
3. generating and solving the system of simultaneous equations for the regression coefficients  
4. calculation of fitted data  
5. calculation of residuals

Output:  
1. list of regression subfunctions $f_i(x)$ and code numbers of selected functions  
2. coefficient matrix and right-hand side of system of simultaneous equations  
3. regression coefficients  
4. fitted data

(7) Subroutine NONUNI  
Purpose: Three dimensional regression analysis (two independent variables x and y)  
1. scaling of variable x  
   (logarithmic or linear scale)  
2. calculation of values of regression subfunctions $f_i(x)$ and $g_j(y)$  
3. generating and solving the system of simultaneous equations for the regression coefficients
4. calculation of fitted data
5. calculation of residuals

Output: 1. list of regression subfunctions \( f_i(x) \), \( g_j(y) \) and code number of selected functions
2. coefficient matrix and right hand side of system of simultaneous equations
3. regression coefficients
4. fitted data

2.4 Input
Card A Control Variables FORMAT (4I5, F10.0)
Cols.

1-5 \( NP = \) maximum number of data per value of variable \( x \)
(NP \( \leq 40 \))

6-10 \( NR = \) maximum number of values for variable \( x \)
(NR \( \leq 165 \))

15 scaling of variable \( x \)
1 \( x' = x \) (linear scale)
2 \( x' = \log_{10} x \) (logarithmic scale)

20 number of independent variables
1 one independent variable \( x \)
2 two independent variables \( x \) and \( y \)

21-30 \( PRO = \) band-width factor for rejection
(PRO = 1.50...2.0)
Card B  Data FORMAT (10F8.0)
Data D(I,J) have to be arranged row by row
D(1,J = 1,2,...,NP)
D(2,J = 1,2,...,NP)

Card C  Arguments of variable x FORMAT (10F8.0)

Two-dimensional regression analysis:
Card D1:  Number of regression subfunctions FORMAT (Il)

NF = total number of regression subfunctions \( f_i(x) \)

NF \( \leq 8 \)

Card E1:  Code numbers for regression subfunctions:

FORMAT (8(Il, lx))

code number i for regression subfunctions \( f_i(x) \) see page 5

In case the regression analysis should be repeated with different types of subfunctions an unrestricted number of cards of type D1 and E1 can be added.

Card F1:  Blank card

Terminal for repetition of regression analysis

Three-dimensional regression analysis:
Card D2:  Arguments of variable y FORMAT (10F8.0)
Card E2: Number of regression subfunctions \( \text{FORMAT (2(I1,lx))} \)

Col. 1 \( NF = \) total number of subfunctions \( f_i(x) \)
\( NF \leq 8 \)

Col. 3 \( NG = \) total number of subfunctions \( g_j(y) \)
\( NG \leq 8 \quad NF \times NG \leq 30 \)

Card F2: Code number of regression subfunctions \( f_i(x) \)
\( \text{FORMAT (8(I1,lx))} \)
see page 5

Card G2: Code number of regression subfunctions \( g_j(y) \)
\( \text{FORMAT (8(I1,lx))} \)
see page 5

In case the regression analysis should be repeated with different types of subfunctions an unrestricted number of cards of type E2, F2, and G2 can be added.

Card H2: Blank Card
Terminal for repetition of regression analysis.

2.5 Limitations, Remarks

(1) Maximum values for control variables

\( NR \leq 165 \) maximum number of arguments for variable \( x \)
\( NP \leq 40 \) maximum number of data per argument of variable \( x \) or maximum number of arguments for variable \( y \) respectively

\( 165 \times 40 = 6600 \) maximum number of data
NF \leq 8 \text{ maximum number of subfunctions } f_i(x)
\NG \leq 8 \text{ maximum number of subfunctions } g_j(y)
\NF \times \NG \leq 30

(2) **Sequence of code numbers**
The code numbers \(i\) (and \(j\)) for the selection of regression subfunctions \(f_i(x)\) (and \(g_j(y)\)) have to be arranged in increasing order, for instance 1, 4, 5 not 1, 5, 4

(3) **Arrangement of data**
\(x(I) = \text{constant for all values } D(I,J = 1 \ldots NP)\)
\(y(J) = \text{constant for all values } D(I=1 \ldots NR, J)\)

(4) **Zero and negative arguments of } x \text{ and } y**
In case the independent variables \(x' = \frac{x}{\log_{10} x}\) and \(y\) have arguments less than or equal to zero, a value of zero is assigned to the following subfunctions:

<table>
<thead>
<tr>
<th>Code Number</th>
<th>(f_i(u), g_j(u))</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>(2\sqrt{u})</td>
</tr>
<tr>
<td>4</td>
<td>(1/u)</td>
</tr>
<tr>
<td>7</td>
<td>(\log_{10} u)</td>
</tr>
<tr>
<td>8</td>
<td>(\sqrt[4]{u})</td>
</tr>
</tbody>
</table>

(5) **Zero values of data**
Zero values of data \(D(I,J) = 0.0\) are considered as missing data. In case it is their true value, a very small quantity should be assigned to them.
(6) Rejection of data
In case the rejection of data and a subsequent second
least squares fit should be suppressed, card CURVE 56
in subprogram CURFIT (NOREJ = 2) has to be replaced
by NOREJ = 1.

(7) Required field length
CM = 100 000

2.6 Nomenclature
Arrays
STR (165,40) Data D(I,J)
AGE (165) Variable X(I)
X (40) Variable Y(J)
RES (165,40) Residuals
ST (165) Fitted data D(I) one independent
variable
DAT (165,40) Fitted data D(I,J) two independent
variables
AG (165) Scaled variable x'(I)
F (8,165) Regression subfunctions f_i(x)
G (8,40) Regression subfunctions g_j(y)
KT (8) code numbers for selected sub-
functions f_i(x)
code numbers for selected subfunctions $g_j(y)$

coefficient matrix for system of simultaneous equations

Variables

\[
\begin{align*}
NR &= \text{total number of arguments for variable } x \\
NP &= \text{total number of arguments for variable } y \text{ or total number of data per argument of variable } x \\
NF &= \text{n}_i = \text{total number of selected subfunctions } f_i(x) \\
NG &= \text{n}_j = \text{total number of selected subfunctions } g_j(y) \\
SNOM &= \text{total number of data} \\
PRO &= \text{band-width factor}
\end{align*}
\]

Branching Indices

\[
\begin{align*}
NSE &= \text{Scaling of variable } x \\
NSE = 1 & \Rightarrow x' = x \text{ (linear scale)} \\
NSE = 2 & \Rightarrow x' = \log_{10} x \text{ (logarithmic scale)} \\
NCODE &= \text{number of independent variables} \\
NCODE = 1 & \Rightarrow \text{one independent variable } x \\
NCODE = 2 & \Rightarrow \text{two independent variables } x \text{ and } y
\end{align*}
\]
NOREJ rejection of data
NOREJ = 1 no rejection of data
NOREJ = 2 rejection of data with subsequent second least squares fit
2.7 PROGRAM LISTING
PROGRAM CURVE (INPUT, TAPE1=INPUT, OUTPUT, TAPE2=OUTPUT)

*********************************************************

* REgression analysis of data with one or two independent variables *

*********************************************************

COMMON/UNIA/STR(165,40), RES(165,40), AGE(165), AG(165), F(8,165),
1ST(165), KT(8), NSE, NCODE, PR, SNOM

COMMON/NON/A/DAT(165,40), G(8*40), X(41), KX(8)

DIMENSION A(30,30)

IO=2

C

INPUT DATA

READ(IN,400) NP,NR,NSE,NCODE,PR

DO 100 I=1,NR

READ(IN,401) (STR(I,N),N=1,NP)

100 CONTINUE

READ(IN,401) (AGE(I), I=1,NR)

GO TO (101,102)NCODE

C

ONE INDEPENDENT VARIABLE


C

101 READ(IN,402) NF.

IF(NF.EQ.0) GO TO 150

READ(IN,403) (KT(J),J=1,NF)

NG=1

NFG=NF

CALL CURFIT(NP,NR,NF,NG,NFG,A)

GO TO 101

C

TWO INDEPENDENT VARIABLES

C

102 READ(IN,401) (X(I),I=1,NP)

103 READ(IN,402) NF,NG

IF(NF.EQ.0) GO TO 150

READ(IN,403) (KT(J),J=1,NF)

READ(IN,403) (KX(I),I=1,NG)

NFG=NF*NG

CALL CURFIT(NP,NR,NF,NG,NFG,A)

GO TO 103

C

400 FORMAT(415,F10.0)

401 FORMAT(10F8.0)

402 FORMAT(11*3X,11)

403 FORMAT(8(I1,1X))

150 CALL EXIT

END
SUBROUTINE CURFIT(NP, NR, NF, NG, NFG, A)

COMMON/UNIA/STR(165, 40), RES(165, 40), AGE(165), AG(165), F(8, 165), 

1ST(165), KT(8), KSE, NCODE, PRO, SNOM

DIMENSION VAR(165)

Č
Č C
Č ONE INDEPENDENT VARIABLE
Č

200 DO 101 I=1, NR
2 DO 101 N=1, NP
3 RES(I,N)=0.0
4
5 101 CONTINUE
6 WRITE(10, 300)
7 WRITE(10, 301)
8 CALL OUTXX(STR, AGE, NP, NR)
9 WRITE(10, 302)
10 CALL UNIFORM(NP, NR, NF, A)
11 GO TO (150, 102) NOREJ
12 WRITE(10, 303)
13 CALL REJECT(NP, NR)
14 WRITE(10, 304)
15 CALL UNIFORM(NP, NR, NF, A)
16 GO TO 150

Č Č TWO INDEPENDENT VARIABLES
Č

200 DO 104 I=1, NR
20 DO 104 N=1, NP
2 RES(I,N)=0.0
3
4 104 CONTINUE
5 WRITE(10, 305)
6 WRITE(10, 301)
7 CALL OUTXX(STR, AGE, NP, NR)
8 WRITE(10, 306)
9 WRITE(10, 307)
10 P=NP
11 NPH=P/2.0+0.6
12 X(NP+1)=0.0
13 DO 105 I=1, NPH
14 J=I+NPH
15 WRITE(10, 308) I, X(I), J, X(J)

5 105 CONTINUE
6 WRITE(10, 302)
7 CALL NONUNI(NP, NR, NF, NG, NFG, A)
8 GO TO (150, 106) NOREJ
9 WRITE(10, 303)
10 CALL REJECT(NP, NR)
11 WRITE(10, 304)
12 CALL NONUNI(NP, NR, NF, NG, NFG, A)
13 300 FORMAT(1H1, //, 51X, "ONE INDEPENDENT VARIABLE", //)
14 301 FORMAT(1H1, //, 10X, 15HORIGINAL DATA ://)
15 302 FORMAT(1H1, //, 10X, 25HFIRST LEAST SQUARES FIT ://)
16 303 FORMAT(1H1, //, 10X, 16HDATA REJECTION ://)
17 304 FORMAT(1H1, //, 10X, 26HSECOND LEAST SQUARES FIT ://)
305 FORMAT(1H1, 'TWO INDEPENDENT VARIABLES', /)
306 FORMAT(10X, 'Y-COORDINATES', /)
307 FORMAT(10X, 2(POI 11X, *Y*, 20X), /)
308 FORMAT(10X, 2(T3, 8X, E11.4, 15X))
150 RETURN
END
SUBROUTINE OUTXX(S,AGE,NP,NR)
DIMENSION S(165,40),AGE(165)

I0=2
DO 100 L=1,NP,8
NA=L
NE=L+7
IF(NE,GT,NP) NE=NP
WRITE(IO,300) (N,N=NA,NE)
WRITE(IO,301)
DO 100 I=1,SR
WRITE(IO,302) AGE(I),(S(I,N),N=NA,NE)
100 CONTINUE

300 FORMAT(/,11X,6X,8(11X,13))
301 FORMAT(/)
302 FORMAT(5X,E12.4,5X,E14.4)
RETURN
END
SUBROUTINE SOLVE(C,R,X,N)
DIMENSION C(N,N),R(N),X(N),A(30,31),IROW(30)

IO=2
M=N+1

DO 100 I=1,N
IROW(I)=1
A(I,M)=8(I)
DO 100 J=1,N
A(I,J)=C(I,J)
100 CONTINUE
DET=1.
DO 106 I=1,N
BIG=0.*0
DO 101 II=1,N
IF(BIG.GE.ABS(A(II,II))) GO TO 101
BIG=ABS(A(II,II))
K=II
101 CONTINUE
IF(BIG.GT.0.*0) GO TO 102
WRITE(IO,300)
CALL EXIT
102 IF(K.EQ.I) GO TO 104
L=IROW(I)
IROW(I)=IROW(K)
IROW(K)=L
DO 103 J=1,M
Z=A(I,J)
A(I,J)=A(K,J)
A(K,J)=Z
103 CONTINUE
104 Z=A(I,I)
DET=Z*DET
DO 105 J=1,M
A(I,J)=A(I,J)/Z
105 CONTINUE
IF(I.EQ.N) GO TO 107
II=I+1
DO 106 K=II,N
Z=A(K,I)
DO 106 J=I,M
A(K,J)=A(K,J)-Z*A(I,J)
106 CONTINUE
107 X(N)=A(N,M)
I=N
108 Z=0.*0
DO 109 J=1,N
Z=Z+A(I-1,J)*X(J)
109 CONTINUE
I=I-1
X(I)=A(I,M)-Z
IF(I.GT.1) GO TO 108
300 FORMAT(///,10X,*SINGULAR COEFFICIENT MATRIX*)
RETURN
END
SUBROUTINE REJECT(NP,NR)
COMMON/UNIA/STR(165,40),RES(165,40),AGE(165),A=165),F(8,165)
C
IST(165),KT(8),NSE,NCODE,PRO,SNO
C
IO=2
WRITE(10,300)
CALL OUTXX(RES,AGE,NP, NR)
C
C
C
C
C
C
DO 100 I=1, NR
DO 100 L=1, NP
SUM=RES(I,L)*RES(I,L)*SUM
100 CONTINUE
WRITE(10,301) SNOM
WRITE(10,302) SUM
STD=SQR(SUM/SNOM)
WRITE(10,303) STD, PRO
C
C
C
C
C
C
C
STD=PRO*STD
WRITE(10,304)
DO 101 I=1, NR
DO 101 L=1, NP
IF(ABS(RES(I,L)) .LE. STD) GO TO 101
SNOM=SNOM-1.0
SUM=SUM-RES(I,L)*RES(I,L)
RES(I,L)=2.0E+300
WRITE(10,305) AGE(I), L
101 CONTINUE
WRITE(10,306)
CALL OUTXX(RES, AGE, NP, NR)
WRITE(10,307) SNOM
WRITE(10,308) SUM
STD=SQR(SUM/SNOM)
WRITE(10,309) STD, PRO
C
300 FORMAT(/,10X, "RESIDUALS BEFORE REJECTION")
301 FORMAT(/,10X, "TOTAL NO. OF DATA BEFORE REJECTION", 14X, F7.0)
302 FORMAT(/,10X, "SUM OF SQUARES BEFORE REJECTION", 13X, E11.4)
303 FORMAT(/,10X, "STANDARD ERROR BEFORE REJECTION", 13X, E11.4, 10X, F7.0)
305 FORMAT(30X, E11.4, 9A, 12)
306 FORMAT(/,10X, "RESIDUALS AFTER REJECTION")
307 FORMAT(/,10X, "TOTAL NO. OF DATA AFTER REJECTION", 14X, F7.0)
308 FORMAT(/,10X, "SUM OF SQUARES AFTER REJECTION", 13X, E11.4)
309 FORMAT(/,10X, "STANDARD ERROR AFTER REJECTION", 13X, E11.4, 10X, F7.0)
1WIDTH FACTOR*5X,F6.3)
RETURN
END
SUBROUTINE UNIFORM(NP,NR,NF,A)
COMMON/UNIAX/STR(165,40),RES(165,40),AGE(165),AG(165),F(8,165),
IST(165),KT(8),NSET,NCODE,PRO,SNOM
DIMENSION A(NF,NF),B(8),R(8)
IO=2
WRITE(IO,300)
WRITE(IO,301)
WRITE(IO,302) (KT(L),L=1,NF)
C
C LOG OR NON-LOG SCALE FOR VARIABLE X
C
GO TO (100,102) NSE
100 DO 101 I=1,NR
AG(I)=AGE(I)
101 CONTINUE
WRITE(IO,303)
GO TO 104
102 DO 103 I=1,NR
AG(I)=0.0
IF(AGE(I).GT.0.0) AG(I)=ALOG10(AGE(I))
103 CONTINUE
WRITE(IO,304)
C
C COMPUTE VALUES OF REGRESSION SUBFUNCTIONS F
C
104 DO 107 I=1,NR
F(1,I)=1.0
F(2,I)=AG(I)
F(5,I)=AG(I)@AG(I)
F(6,I)=F(5,I)@AG(I)
IF(AG(I)@LE.0.0) 105,106
105 F(3,I)=F(4,I)=F(7,I)=F(8,I)=0.0
106 GO TO 107
107 CONTINUE
DO 108 J=1,NF
KK=KT(J)
DO 108 I=1,NR
F(J,I)=F(KK,I)
108 CONTINUE
C
C GENERATE SYSTEM OF SIMULTANEOUS EQUATIONS
C
DO 109 J=1,NF
B(J)=0.0
DO 109 K=1,NF
A(J,K)=0.0
109 CONTINUE
SNOM=0.0
DO 111 I=1,NR
SNOM=SNOM+1.0
IF(STR(I,L)@EQ.0.0) GO TO 111
IF(RES(I,L)@GT.1.0E+300) GO TO 111
111 SNOM=SNOM+1.0
DO 110 J=1,NF
B(J)=STR(I,L)*F(J,I)+B(J)
DO 110 K=1,NF
A(J,K)=F(K,I)*F(J,I)+A(J,K)
110 CONTINUE
111 CONTINUE
.C
 SOLVE SIMULTANEOUS EQUATIONS
 CALL SOLVE(A,B,R,NF)
 WRITE(10,305)
 DO 112 J=1,NF
 WRITE(10,306) B(J),(A(J,K),K=1,NF)
112 CONTINUE
 WRITE(10,307)
 WRITE(10,308) (R(J),J=1,NF)
.C
 COMPUTE FITTED DATA
 DO 114 I=1,NR
 ST(I)=0.0
 DO 113 J=1,NF
 ST(I)=F(J,I)*R(J)+ST(I)
113 CONTINUE
114 CONTINUE
 WRITE(10,309)
 DO 115 I=1,NR
 WRITE(10,310) AGE(I),ST(I)
115 CONTINUE
.C
 COMPUTE RESIDUALS
 DO 116 I=1,NR
 RES(I,L)=0.0
 IF(STR(I,L),NE,0.0) RES(I,L)=STR(I,L)-ST(I)
116 CONTINUE
300 FORMAT(/'10X#LIST OF FUNCTIONS OF X : 1= CONST. 2= X 3=C
 1= SORT(X) 4= 1/X 5= X**2 6= X**3 7= LOG10(X) 8= X**.25,//)
301 FORMAT(37X,46H5- X**2 6- X**3 7- LOG10(X) 8- X**.25,//)
302 FORMAT(10X,21HUSED FUNCTIONS OF X : 5X,8(I1,2X))
303 FORMAT(/'10X#VARIABLE X = X (NON-LOG. SCALE) 8),//)
304 FORMAT(/'10X#VARIABLE X = LOG10(X) 8),//)
305 FORMAT(/'10X#SIMULTANEOUS EQUATIONS 8),//)
306 FORMAT(10X,12.5,10X,8(F12.5,1X))
307 FORMAT(/'10X#34HCOEFFICIENTS A(I) : A(I)*F(I),//)
308 FORMAT(6X,8E15.4)
309 FORMAT(/'10X#13X#FITS DATA,8),//)
310 FORMAT(1X,9X,E11.4))
RETURN
END
SUBROUTINE NONUNI(NP,NR,RF,NG,NFG,A)
COMMON/UNIA/STR(165,40),RES(165,40),AGE(165),AG(165),F(8,165),
IST(165),KT(8),NSE,NCODE,PRO,SNOM
COMMON/NONA/DAT(165,40),G(8,40),X(41),KX(8)
DIMENSION A(NFG,NFG),R(30),B(30)
10=2
WRITE(10,300)
WRITE(10,301)
WRITE(10,302) (KT(L),L=1,NF)
WRITE(10,303)
WRITE(10,304) (KX(L),L=1,NG)
C LOG, OR NON-LOG, SCALE FOR VARIABLE X
GO TO (100,102) NSE
100 DO 101 I=1,NR
AG(I)=AGE(I)
101 CONTINUE
WRITE(10,306)
GO TO 104
102 DO 103 L=1,NR
AG(I)=0.0
IF(AGE(I).LE.0.0) AG(I)=ALOG10(AGE(I))
103 CONTINUE
WRITE(10,307)
C COMPUTE VALUES OF REGRESSION SUBFUNCTIONS F AND G
104 DO 107 I=1,NR
F(1,I)=1.0
F(2,I)=AG(I)
F(5,I)=AG(I)*AG(I)
F(6,I)=AG(I)*F(5,I)
IF(AG(I).LE.0.0) 105,106
105 F(3,I)=F(4,I)=F(7,I)=F(8,I)=0.0
GO TO 107
106 F(3,I)=SQRT(AG(I))
F(4,I)=1.0/AG(I)
F(7,I)=ALOG10(AG(I))
F(8,I)=SQRT(F(3,I))
107 CONTINUE
DO 110 L=1,NF
G(1,L)=1.0
G(2,L)=X(L)
G(5,L)=X(L)*X(L)
G(6,L)=X(L)*G(5,L)
IF(X(L).LE.0.0) 108,109
108 G(3,L)=G(4,L)=G(7,L)=G(8,L)=0.0
GO TO 110
109 G(3,L)=SQRT(X(L))
G(4,L)=1.0/X(L)
G(7,L)=ALOG10(X(L))
G(8,L)=SQRT(G(3,L))
110 CONTINUE
DO 111 J=1,NF
KK=KT(J)
DO 111 I=1,NR
F(J,I)=F(KK,I)
111 CONTINUE

DO 112 J=1,NG
KK=KK(J)
DO 112 L=1,NP
G(J,L)=G(KK,L)
112 CONTINUE

DO 113 J=1,NFG
B(J)=0.0
DO 113 K=1,NFG
A(J,K)=0.0
113 CONTINUE

SNOM=0.0
DO 115 I=1,NR
DO 115 N=1,NP
IF(STR(I,N).EQ.0.0) GO TO 115
IF(RES(I,N).GT.1.0E+300) GO TO 115
SNOM=SNOM+1.0
115 CONTINUE

DO 114 L=1,NG
NV=(J-1)*NG+L
114 CONTINUE

DO 114 JH=1,NF
NH=(JH-1)*NG+NH
114 CONTINUE

B(NV)=STR(I,N)*F(J,I)*G(L,N)+B(NV)
DO 114 JH=1,NF
A(NV,NH)=F(JH,I)*G(LH,N)*F(J,I)*G(L,N)+A(NV,NH)
114 CONTINUE

DO 116 I=1,NF
JE=(I-1)*NG+1
116 CONTINUE

JA=JE*NG+1
WRITE(10,309) R(J),J=JE,JA

DO 117 I=1,NR
DO 117 L=1,NP
DAT(I,L)=0.0
DO 117 J=1,NF
DO 117 K=1,NG
NV=(J-1)*NG+K
DAT(I,L)=F(J,K)*G(K,L)*R(NV)+DAT(I,L)
117 CONTINUE

WRITE(10,310)
CALL OUTXX(DAT,AGE,NP,NR)

DO 117 I=1,NR
DO 117 L=1,NP
DAT(I,L)=0.0
DO 117 J=1,NF
DO 117 K=1,NG
NV=(J-1)*NG+K
DAT(I,L)=F(J,K)*G(K,L)*R(NV)+DAT(I,L)
117 CONTINUE

WRITE(10,310)
CALL OUTXX(DAT,AGE,NP,NR)

SOLVE SIMULTANEOUS EQUATIONS

CALL SOLVE(A,B,R,NFG)
WRITE(10,308)
DO 116 I=1,NF
JE=(I-1)*NG+1
JA=JE*NG+1
WRITE(10,309) R(J),J=JE,JA
116 CONTINUE

COMPUTE FITTED DATA

DO 117 I=1,NR
DO 117 L=1,NP
DAT(I,L)=0.0
DO 117 J=1,NF
DO 117 K=1,NG
NV=(J-1)*NG+K
DAT(I,L)=F(J,K)*G(K,L)*R(NV)+DAT(I,L)
117 CONTINUE

WRITE(10,310)
CALL OUTXX(DAT,AGE,NP,NR)

COMPUTE RESIDUALS
DO 118 I=1,NR
DO 118 L=1,NP
RES(I*L)=0.0
IF(STR(I*L) .NE. '0.0') RES(I*L)=STR(I*L)-DAT(I*L)
118 CONTINUE

300 FORMAT(/'10X,#LIST OF FUNCTIONS OF X: 1- CONST. 2- X 3CURVE463
1- SOR(T(X) 4- 1/X) 5CURVE464
301 FORMAT(37X,46H5- X*2 6- X*3 7- LOG10(X) 8- X**.25,/) CURVE465
302 FORMAT(10X,1HUSED FUNCTIONS OF X :6X,B(I1,2X))
303 FORMAT(/'10X,#LIST OF FUNCTIONS OF Y: 1- CONST. 2- Y)
1- SOR(T(Y) 4- 1/Y) 5CURVE467
304 FORMAT(37X,46H5- Y*2 6- Y*3 7- LOG10(Y) 8- Y**.25,/) CURVE469
305 FORMAT(10X,1HUSED FUNCTIONS OF Y :6X,B(I1,2X))
306 FORMAT(/'10X,#VARIABLE X = X (NON-LOG. SCALE)*/)
307 FORMAT(/'10X,#VARIABLE X = LOG10(X)*/)
308 FORMAT(/'10X,42HCOEFFICIENTS A(I,J) A(I,J)*F(I)*G(J),/) CURVE473
309 FORMAT(6X,8E15.4) CURVE474
310 FORMAT(1H1,/'10X,13HFITTED DATA ://) CURVE475
RETURN
END
3. PROGRAM MULTI

3.1 Purpose

The purpose of the program MULTI is a regression analysis of data with three independent variables $x$, $y$, and $z$. This analysis is based on the following regression functions:

$$D(x,y,z) = \sum_{i=1}^{n_i} \sum_{j=1}^{n_j} \sum_{k=1}^{n_k} a_{ijk} f_i(x) g_j(y) h_k(z)$$

The data have to be arranged in the following form:

$$D(I,J) \quad I = 1, \ldots, NR \quad \text{subscript related to variable } x$$
$$J = 1, \ldots, NP \quad \text{subscript related to variables } y \text{ and } z$$

where $x = \text{constant}$ for all values $D(I,J=1\ldots NP)$

$y = \text{constant}$ for all values $D(I=1\ldots NR,J)$

$z = \text{constant}$

The types of subfunctions, which can be selected for $f_i(x)$, $g_j(y)$, and $h_k(z)$ as well as the information about data rejection are identical to those given on page 5 for program CURVE.
3.2 Logical Flow Chart

- MULTI
- REGRES
- REJECT
- REGRES
- END

No Data Rejection

Solve
Outxx
3.3 Description of Subprograms

(1) Main Program MULTI:
Purpose: Input of data
1. control variables
2. data
3. arguments of variable x, y, and z
4. code numbers for regression subfunctions
   \( f_i(x), g_j(y), \) and \( h_k(z) \)
Calling of regression subroutines in prescribed order

Output: Original data
arguments of variables x, y and z
headings

The source program is written in such a form, that after executing the regression analysis with a certain set of functions \( f_i(x), g_j(y), h_k(z) \) other sets of functions will be read in and the regression analysis will be repeated.

(2) Subprogram REGRES
Purpose: Four-dimensional regression analysis (three independent variables x, y, z)
1. scaling of variable x
   (logarithmic or linear scale)
2. calculation of values of regression subfunctions \( f_i(x), g_j(y), h_k(z) \)
3. generating and solving the system of simultaneous equations for the regression coefficients
4. calculation of fitted data
5. calculation of residuals

Output:
1. list of regression subfunctions \( f_i(x), g_j(y), h_k(z) \) and code numbers of selected functions
2. regression coefficients
3. fitted data

(3) Other subprograms
The remaining subprograms OUTXX, SOLVE, and REJECT, used in this program, are identical to those described on page 7 for program CURVE.

3.4 Input
Card A Control Variables FORMAT (3I5, 5X, F10.0)
Cols.
1-5 \( NP = \) maximum number of values for variable y (or z)
   \( (NP \leq 40) \)
6-10 \( NR = \) maximum number of values for variable x
   \( (NR \leq 140) \)
scaling of variable $x$

1. $x' = x$ (linear scale)
2. $x' = \log_{10} x$ (logarithmic scale)

PRO = band-with factor for rejection

(PRO = 1.5...2.0)

Card B  Data  FORMAT (10F8.0)

Data $D(I,J)$ have to be arranged row by row

$D(1, J=1,2,\ldots,NP)$
$D(2, J=1,2,\ldots,NP)$

Card C  Arguments of variable $x$

Card D  Arguments of variable $y$  FORMAT (10F8.0)

Card E  Arguments of variable $z$

Card F  Number of regression subfunctions  FORMAT (3(I1,1X))

Col. 1  $NF$ = total number of subfunctions $f_i(x)$  $NF \leq 8$

Col. 3  $NG$ = total number of subfunctions $g_j(y)$  $NG \leq 8$

Col. 5  $NH$ = total number of subfunctions $h_k(z)$  $NH \leq 7$

Card G  code numbers of regression subfunctions  $f_i(x)$
Card H  $g_j(y)$
Card I  $h_k(z)$

(see page 5)

FORMAT (8(I1, 1X))

In case the regression analysis should be repeated with different types of subfunctions, an unrestricted number of cards of type G, H, and I can be added.
3.5 Limitations, Remarks

(1) Maximum values for control variables

NR ≤ 140  maximum number of arguments for variable x

NP ≤ 40  maximum number of arguments for variables y and z

140 * 40 = 5600 maximum number of data

NF ≤ 8  maximum number of subfunctions $f_i(x)$

NG ≤ 8  maximum number of subfunctions $g_j(y)$

NH ≤ 7  maximum number of subfunctions $h_k(z)$

NF * NG * NH ≤ 50

(2) Arrangement of data

$X(I) = \text{constant for all values } D(I,J=1,\ldots,NP)$

$Y(J) = \text{constant for all values } D(I=1,\ldots,NR,J)$

$Z(J) = \text{constant for all values } D(I,J=1,\ldots,NP)$

For further limitations and remarks concerning sequence of code numbers, zero and negative arguments of x, y, z, zero values of data, rejection of data, and required field length see page 13.
3.6 Nomenclature

Arrays

<table>
<thead>
<tr>
<th>Array</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>STR (140,40)</td>
<td>data $D(I,J)$</td>
</tr>
<tr>
<td>AGE (140)</td>
<td>variable $X(I)$</td>
</tr>
<tr>
<td>X (40)</td>
<td>variable $Y(J)$</td>
</tr>
<tr>
<td>Y (40)</td>
<td>variable $Z(J)$</td>
</tr>
<tr>
<td>RES (140,40)</td>
<td>residuals</td>
</tr>
<tr>
<td>DAT (140,40)</td>
<td>fitted data $\bar{D}(I,J)$</td>
</tr>
<tr>
<td>AG (140)</td>
<td>scaled variable $x'(I)$</td>
</tr>
<tr>
<td>F(8,140)</td>
<td>regression subfunctions $f_i(x)$</td>
</tr>
<tr>
<td>G(8,40)</td>
<td>regression subfunctions $g_j(y)$</td>
</tr>
<tr>
<td>H(8,40)</td>
<td>regression subfunctions $h_k(z)$</td>
</tr>
<tr>
<td>KT (8)</td>
<td>code numbers for selected subfunctions $f_i(x)$</td>
</tr>
<tr>
<td>KX (8)</td>
<td>code numbers for selected subfunctions $g_j(y)$</td>
</tr>
<tr>
<td>KY (8)</td>
<td>code numbers for selected subfunctions $h_k(z)$</td>
</tr>
<tr>
<td>A (50,50)</td>
<td>coefficient matrix for system of simultaneous equations</td>
</tr>
</tbody>
</table>

Variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>NR</td>
<td>total number of arguments of variable $x$</td>
</tr>
<tr>
<td>NP</td>
<td>total number of arguments of variable $y$ (or $z$)</td>
</tr>
<tr>
<td>NF = $n_i$</td>
<td>total number of selected subfunctions $f_i(x)$</td>
</tr>
<tr>
<td>NG = $n_j$</td>
<td>total number of selected subfunctions $g_j(y)$</td>
</tr>
<tr>
<td>NH = $n_k$</td>
<td>total number of selected subfunctions $h_k(z)$</td>
</tr>
<tr>
<td>SNOM</td>
<td>total number of data</td>
</tr>
<tr>
<td>PRO</td>
<td>band-width factor</td>
</tr>
</tbody>
</table>
Branching Indices

NSE Scaling of variable x
NSE = 1 \( x' = x \) (linear scale)
NSE = 2 \( x' = \log_{10}x \) (logarithmic scale)

NOREJ rejection of data
NOREJ = 1 no rejection of data
NOREJ = 2 rejection of data with subsequent second least squares fit
3.7 PROGRAM LISTING
PROGRAM MULTI (INPUT, TAPE1=INPUT, OUTPUT, TAPE2=OUTPUT)

REGRESSION ANALYSIS OF DATA WITH THREE INDEPENDENT VARIABLES

COMMON/TRID/STR(140, 40), DAT(140, 40), RES(140, 40), AGE(140), AG(140), 1X(41), Y(41), F(2, 140), G(8, 40), H(8, 40), KT(8), KX(8), KY(8), SNOM, NSE

DIMENSION A(50, 50)

IN=1
IO=2
NOREJ=2

READ(IN, 400) NP, NR, NSE, PRO

DO 100 I=1, NR
    READ(IN, 401) (STR(I, N), N=1, NP)
  100 CONTINUE

READ(IN, 401) (AGE(I), I=1, NR)

READ(IN, 401) (X(I), I=1, NP)

READ(IN, 401) (Y(I), I=1, NP)

READ(IN, 402) NF, NG, NH

IF(NF, EQ., 0) GO TO 150

READ(IN, 402) (KT(I), I=1, NF)

READ(IN, 402) (KX(I), I=1, NG)

READ(IN, 402) (KY(I), I=1, NH)

READ(IN, 402) (STR(I, N), N=1, NP)

WRITE(IO, 300)

CALL OUTXX(STR, AGE, NP, NR)

WRITE(IO, 301)

WRITE(IO, 302)

P=NP

NPH=P/2.0+0.6

NFH=NF*NG*NH

X(NP+1)=Y(NP+1)=0.0

DO 102 I=1, NPH
    J=1+NPH

WRITE(IO, 303) I, X(I), Y(I), J, X(J), Y(J)

102 CONTINUE

CALL REGRESSION ROUTINES

DO 103 I=1, NR
    DO 103 N=1, NP
    RES(I, N)=0.0
  103 CONTINUE

WRITE(IO, 304)

CALL REGRES(NP, NR, NF, NG, NH, NFH, A)

GO TO (150, 104) NOREJ

104 WRITE(IO, 305)

CALL REJECT(NP, NR)
WRITE(10,306)
CALL REGRES(NP, NR, NF, NG, NH, NFH, A)

300 FORMAT(1HI, ///, 10X,*ORIGINAL DATA /*, //)
301 FORMAT(///, 10X, *COORDINATES */, //)
302 FORMAT(10X,2(*POINT#, I1X, *Y#, 15X, *Z#, 20X)*/)
303 FORMAT(10X,2(I3,8X,E11.4,8X,F11.4,15X))
304 FORMAT(1HI, ///, 10X,*FIRST LEAST SQUARES FIT*, //)
305 FORMAT(1HI, ///, 10X,*DATA REJECTION*, //)
306 FORMAT(1HI, ///, 10X,*SECOND LEAST SQUARES FIT*, //)
400 FORMAT(1HI, ///, 10X,*SECOND LEAST SQUARES FIT*, //)
401 FORMAT(10FH*0)
402 FORMAT(B(I,J)*X))
150 CALL EXIT
END
SUBROUTINE OUTXX(S, AGE, NP, NR)

DIMENSION S(140,40), AGE(140)

10 = 2

DO 100 L = 1, NP, 8

NA = L

NE = L + 7

IF (NE.GT.NP) NE = NP

WRITE(10, 300) (N, N = NA, NE)

WRITE(10, 301)

DO 100 I = 1, NR

WRITE(10, 302) AGE(I), (S(I,N), N = NA, NE)

100 CONTINUE


301 FORMAT(/)

302 FORMAT(5X, E12.4, 5X, E14.4)

RETURN

END
SUBROUTINE SOLVE(C,B,X,N)

DIMENSION C(N,N),B(N),X(N),A(50,51),IROW(50)

M=N+1
DO 100 I=1,N
IROW(I)=I
A(I,M)=B(I)
DO 100 J=1,N
A(I,J)=C(I,J)
100 CONTINUE

DET=1.
DO 106 I=1,M
BIG=0.0
DO 101 II=1,N
IF(BIG.GE.ABS(A(II,I))) GO TO 101
BIG=ABS(A(II,I))
K=II
101 CONTINUE
IF(BIG.EQ.0) GO TO 102
WRITE(10,*) 000
CALL EXIT
102 IF(K.EQ.1) GO TO 104
L=IROW(I)
IROW(I)=IROW(K)
IROW(K)=L
DO 103 J=1,M
Z=A(I,J)
A(I,J)=A(K,J)
A(K,J)=Z
103 CONTINUE

104 Z=A(I,I)
DET=Z*DET
DO 105 J=1,M
A(I,J)=A(I,J)/Z
105 CONTINUE
IF(I.EQ.N) GO TO 107
II=I+1
DO 106 K=II,N
Z=A(K,I)
DO 106 J=1,M
A(K,J)=A(K,J)-Z*A(I,J)
106 CONTINUE
107 X(N)=A(N,M)
I=N
108 Z=0.0
DO 109 J=I,N
Z=Z+A(I-1+J)*X(J)
109 CONTINUE
IF(1.0.1) GO TO 108
Z=Z-A(I+M)-Z
RETURN
END
SUBROUTINE REJECT(NP, NR)
  COMMON/TH(I)/STR(140, 40) • DAT(140, 40) • RES(140, 40) • AGE(140) • AG(140), 1X(41), Y(41) • F(8, 140), G(8, 40), H(8, 40), KT(8), KX(8), KY(8), SNOM, NSE, 2PRO
  10 = 2
  WRITE(10, 300)  CALL OUTXX(RES, AGE, NP, NR)

  C. COMPUTE SUM OF SQUARES AND STANDARD ERROR
  SUM = 0.0
  DO 100 I = 1, NR
    DO 100 L = 1, NP
      SUM = RES(I, L) • RES(I, L) • SUM
    100 CONTINUE
    WRITE(10, 301) SNOM
    WRITE(10, 302) SUM
    STD = SQRT(SUM / SNOM)
    WRITE(10, 303) STD, PRO

  C. REJECT DATA, COMPUTE NEW SUM OF SQUARES AND STANDARD ERROR
  STD = PRO • STD
  WRITE(10, 304)
  DO 101 I = 1, NR
    DO 101 L = 1, NP
      IF (ABS(RES(I, L)) • LE • STD) GO TO 101
      SNOM = SNOM - 1.0
      SUM = SUM - RES(I, L) • RES(I, L)
      RES(I, L) = 2.0E+300
    101 CONTINUE
    WRITE(10, 305) AGE(I), L
    CALL OUTXX(RES, AGE, NP, NR)
    WRITE(10, 306) SUM
    STD = SQRT(SUM / SNOM)
    WRITE(10, 307) STD, PRO
    WRITE(10, 308) SNOM

  300 FORMAT(/, *10X • "RESIDUALS BEFORE REJECTION")
  301 FORMAT(/, *10X • "TOTAL NO. OF DATA BEFORE REJECTION", 14X, F7.0)
  302 FORMAT(/, *10X • "SUM OF SQUARES BEFORE REJECTION", 13X, E11.4)
  303 FORMAT(/, *10X • "STANDARD ERROR BEFORE REJECTION", 13X, E11.4, *10X, *BAND)

  304 FORMAT(/, *10X • "REJECTED DATA", 18X, E11.4, *9X, 12X, *POINT, 7)
  305 FORMAT(30X, E11.4, *9X, 12X, *POINT, 7)
  306 FORMAT(/, *10X • "RESIDUALS AFTER REJECTION")
  307 FORMAT(/, *10X • "TOTAL NO. OF DATA AFTER REJECTION", 14X, F7.0)
  308 FORMAT(/, *10X • "SUM OF SQUARES AFTER REJECTION", 13X, E11.4)

  1 WIDTH FACTOR, 5X, F6.3)
  RETURN
END
SUBROUTINE PEGRESCNP(NP,NR,NF,NG,NH,NFH,A)  

COMMON/TRID/STRH(140,40),DAT(140,40),RES(140,40),AGE(140),AG(140),
X(41),Y(41),F(E,140),G(B,40),H(B,40),KT(B),KX(B),KY(B),SNUM,NSE,

2PRO
DIMENSION A(NFH,NFH),R(50),B(50)

IO=2
WRITE(IO,300)
WRITE(IO,301)
WRITE(IO,302) (KT(L),L=1,NF)
WRITE(IO,303)
WRITE(IO,304)
WRITE(IO,305) (KX(L),L=1,NG)
WRITE(IO,306)
WRITE(IO,307)
WRITE(IO,308) (KY(L),L=1,NH)

C  LOG, OR NON-LOG, SCALE FOR VARIABLE X

C  GO TO (100,102) NSE

100 DO 101 I=1,NR
AG(I)=AGE(I)
101 CONTINUE
WRITE(IO,309)
GO TO 104

102 DO 103 I=1,NR
AG(I)=0.0
IF(AGE(I),GT,0.0) AG(I)=ALOG10(AGE(I))
103 CONTINUE
WRITE(IO,310)

C  COMPUTE VALUES OF REGRESSION SUBFUNCTIONS F, G, AND H

C  DO 107 I=1,NR

F(1,I)=1.0
F(2,I)=AG(I)
F(5,I)=AG(I)*AG(I)
F(6,I)=AG(I)*F(5,I)

IF(AG(I),LE,0.0) 105,106
105 F(3,I)=F(4,I)=F(7,I)=F(8,I)=0.0
GO TO 107

106 F(3,I)=SQRT(AG(I))
F(4,I)=1.0/AG(I)
F(7,I)=ALOG10(AG(I))
F(8,I)=SQRT(F(3,I))

107 CONTINUE

DO 110 L=1,NP
G(1,L)=1.0
G(2,L)=X(L)
G(5,L)=X(L)*X(L)
G(6,L)=X(L)*G(5,L)

IF(X(L),LE,0.0) 108,109
108 G(3,L)=G(4,L)L*G(7,L)=G(8,L)=0.0
GO TO 110

109 G(3,L)=SQRT(X(L))
G(4,L)=1.0/X(L)
G(7,L)=ALOG10(X(L))
G(8,L)=SQRT(G(3,L))

C  LOG, OR NON-LOG, SCALE FOR VARIABLE X

C  GO TO (100,102) NSE

104 DO 107 I=1,NR

F(1,I)=1.0
F(2,I)=AG(I)
F(5,I)=AG(I)*AG(I)
F(6,I)=AG(I)*F(5,I)

IF(AG(I),LE,0.0) 105,106
105 F(3,I)=F(4,I)=F(7,I)=F(8,I)=0.0
GO TO 107

106 F(3,I)=SQRT(AG(I))
F(4,I)=1.0/AG(I)
F(7,I)=ALOG10(AG(I))
F(8,I)=SQRT(F(3,I))

107 CONTINUE

DO 110 L=1,NP
G(1,L)=1.0
G(2,L)=X(L)
G(5,L)=X(L)*X(L)
G(6,L)=X(L)*G(5,L)

IF(X(L),LE,0.0) 108,109
108 G(3,L)=G(4,L)L*G(7,L)=G(8,L)=0.0
GO TO 110

109 G(3,L)=SQRT(X(L))
G(4,L)=1.0/X(L)
G(7,L)=ALOG10(X(L))
G(8,L)=SQRT(G(3,L))
110 CONTINUE
DO 113 L=1,NP
H(I,L)=1.0
H(2,L)=Y(L)
H(5,L)=Y(L)*Y(L)
H(6,L)=Y(L)*H(5,L)
IF(Y(L).LE.0.0) 111,112
111 H(3,L)=H(4,L)=H(7,L)=H(8,L)=0.0
GO TO 113
112 H(3,L)=SQRT(Y(L))
H(4,L)=1.0/Y(L)
H(7,L)=ALOG10(Y(L))
H(8,L)=SQRT(H(3,L))
113 CONTINUE
DO 115 J=1,NF
KK=KT(J)
IF(J.EQ.KK) GO TO 115
DO 114 I=1,NR
F(J,I)=F(KK,I)
114 CONTINUE
115 CONTINUE
DO 117 J=1,NG
KK=KX(J)
IF(J.EQ.KK) GO TO 117
DO 116 L=1,LP
G(J,L)=G(KK,L)
116 CONTINUE
117 CONTINUE
DO 119 J=1,NH
KK=KY(J)
IF(J.EQ.KK) GO TO 119
DO 118 L=1,LP
H(J,L)=H(KK,L)
118 CONTINUE
119 CONTINUE
C GENERATE SYSTEM OF SIMULTANEOUS EQUATIONS
C
DO 120 J=1,NFH
R(J)=0.0
DO 120 K=1,NFH
A(J,K)=0.0
120 CONTINUE
SNOM=0.0
NGH=NG*NH
DO 122 I=1,NR
DO 122 N=1,MP
IF(FR(I,N).GE.0.0) GO TO 122
IF(RE(S,T,N).GT.1.0E+300) GO TO 122
SNOM=SNOM+1.0
122 CONTINUE
DO 121 J=1,NF
DO 121 K=1,NF
DO 121 L=1,NH
NV=(J-1)*NGH+(K-1)*NH+L
U(NV)=FR(S,T,N)+F(J,T,N)+G(K,N)*H(L,N)+H(NV)
DO 121 JH=1,NF
DO 121 KN=1,NH
DO 121 LH=1,NH
121 CONTINUE
\[ \begin{align*}
121 \text{ CONTINUE} \\
122 \text{ CONTINUE} \\
\end{align*} \]

\textbf{C \ S O L V E \ S I M U L T A N E O U S \ E Q U A T I O N S}

\begin{align*}
\text{CALL SOLVE}(A,R,NF) \\
\text{WRITE}(10,311) \\
J I = (J I - 1) * N G H \\
\text{WRITE}(10,312) \\
D O 123 K = 1 * N G \\
J A = J I + (K - 1) * N H + 1 \\
J E = J A + N H - 1 \\
\text{WRITE}(10,313) \; J,K,(R(M),M=J A,J E) \\
123 \text{ CONTINUE} \\
\end{align*}

\textbf{C \ C O M P U T E \ F I T T E D \ D A T A}

\begin{align*}
D O 124 I = 1 * N P \\
D O 124 N = 1 * N P \\
D A T(I,N) = 0,0 \\
D O 124 J = 1 * N F \\
D O 124 K = 1 * N G \\
D O 124 L = 1 * N H \\
N V = (J I - 1) * N G H + (K I - 1) * N H + L \\
124 \text{ CONTINUE} \\
\end{align*}

\textbf{C \ C O M P U T E \ R E S I D U A L S}

\begin{align*}
D O 125 I = 1 * N P \\
D O 125 N = 1 * N P \\
R E S(I,N) = 0,0 \\
I F(S T R(I,N) \neq 0,0) \; R E S(I,N) = S T R(I,N) - D A T(I,N) \\
125 \text{ CONTINUE} \\
\end{align*}

\textbf{F O R M A T}(/)
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