WANL-TME-756
April 27, 1964

SUBMITTED BY:

Westinghouse Electric Corporation
Astronuclear Laboratory
Pittsburgh 36, Pennsylvania

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

INFORMATION CATEGORY

unclassified
DW Drawbaugh 4/24/64
Authorized Classifier - Date

PREPARED BY:

C. P. Saalbach
C. P. Saalbach

APPROVED BY:

DW Drawbaugh
D. W. Drawbaugh

A GENERALIZED

LEAST SQUARES PROGRAM

(Title Unclassified)

MASTER

DISTRIBUTION OF THIS REPORT

500

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

I. SUMMARY

This report contains descriptions and directions for use of the following routines:

1. Subroutine LSTSQR - a generalized least squares routine for fitting functions of the type
$$y = c_1 \phi_1(x) + c_2 \phi_2(x) + \dots + c_N \phi_N(x)$$
to a set of data points. The variable x may represent one or more independent variables.
2. Subroutine POLY - a routine for use with the LSTSQR subroutine when the ϕ_i are polynomial terms in one or more variables.
3. Subroutine PLYTPE - a routine for use with LSTSQR subroutine when the ϕ_i are polynomial type terms in one or more variables with non-integral exponents.
4. Program FIT1 - a complete program (which uses LSTSQR and POLY) for fitting polynomial functions to a set of data. Input to this program is described in Appendix I.
5. Program FIT2 - a complete program (which uses LSTSQR and PLYTPE) for fitting polynomial type functions with non-integral exponents to a set of data. Input to this program is described in Appendix I.

The program is currently being used by Safeguards Engineering to find a function $\lambda = f(v, \alpha)$ which fits a set of points (v, α, λ) which have been obtained from various programs. The variables λ , v , and α are:

v = velocity of a particle in orbit

α = angle of reentry into the earth's atmosphere of the orbital particle

λ = distance travelled by the particle before touching the surface of the earth.

II. METHOD

Consider the generalized least squares problem where given a set of points $\{(x_j, y_j^E), j = 1, M\}$ and a set of functions $\{\phi_i(x), i = 1, N\}$ with $N \leq M$, it is desired to find the $\{c_i, i = 1, N\}$ such that the function $y(x)$ where

$$(1) y(x) = c_1 \phi_1(x) + c_2 \phi_2(x) + \dots + c_N \phi_N(x)$$

best fits the set of given points in the least squares sense. This is defined to mean that the function $S(c_1, c_2, \dots, c_N)$ where

$$\begin{aligned} (2) S(c_1, c_2, \dots, c_N) &= \sum_{j=1}^M w_j \left[y_j^E - y(x_j) \right]^2 \\ &= \sum_{j=1}^M w_j \left[y_j^E - c_1 \phi_1(x_j) - c_2 \phi_2(x_j) - \dots - c_N \phi_N(x_j) \right]^2 \end{aligned}$$

and w_j is a weight associated with each point j , must be a minimum with respect to the variables $\{c_i, i=1, N\}$. In the most general problem the independent variable x may represent a set of independent variables. (Ref. 1)

Examples

1. Suppose it is desired to fit a polynomial of degree 3 to a set of data points $\{(x_j, y_j^E), j=1, M\}$. This is an example of the

generalized least squares problem with $\phi_1(x) = 1$, $\phi_2(x) = x$, $\phi_3(x) = x^2$, and $\phi_4(x) = x^3$. The problem is to find c_1 , c_2 , c_3 , and c_4 such that

$$y(x) = c_1 + c_2 x + c_3 x^2 + c_4 x^3$$

best fits the given data points in the least squares sense.

2. Suppose it is desired to fit the most general polynomial of degree 2 in two independent variables r and θ to a set of data $\{(r_j, \theta_j, y_j^E), j=1, M\}$. This is an example of the generalized least squares problem with $x = (r, \theta)$ and $\phi_1(x) = \phi_1(r, \theta) = 1$, $\phi_2(r, \theta) = r$, $\phi_3(r, \theta) = \theta$, $\phi_4(r, \theta) = r^2$, $\phi_5(r, \theta) = \theta^2$, and $\phi_6(r, \theta) = r\theta$. The problem is to find $\{c_i, i=1, 6\}$ such that

$$w(x) = w(r, \theta) = c_1 + c_2 r + c_3 \theta + c_4 r^2 + c_5 \theta^2 + c_6 r\theta$$

best fits the given data points in the least squares sense.

3. Suppose it is desired to fit a finite FOURIER type series of cosine functions to a set of data points $\{(x_j, y_j^E), j=1, M\}$. Here $\phi_i(x) = \cos(i-1)x$ and it is necessary to find $\{c_i, i=1, N\}$ such that

$$w(x) = c_1 + c_2 \cos x + c_3 \cos 2x + \dots + c_N \cos (N-1) x$$

best fits the given data points in the least squares sense.

Returning to the generalized problem, necessary and sufficient conditions that $S(c_1, c_2, \dots, c_N)$ described by (2) have a minimum is that

$$(3) \quad \frac{\partial S(c_1, c_2, \dots, c_N)}{\partial c_i} = 0$$

for all $c_i, i=1, N$. Differentiating (2) with respect to c_i and setting the result to zero we have

$$(4) \quad \frac{\partial S}{\partial c_i} = \sum_{j=1}^M 2w_j \phi_i(x_j) \left[y_j^E - c_1 \phi_1(x_j) - c_2 \phi_2(x_j) - \dots - c_N \phi_N(x_j) \right] = 0$$

or after multiplication and transposition

$$(5) \quad c_1 \sum_{j=1}^M \phi_i(x_j) w_j \phi_1(x_j) + c_2 \sum_{j=1}^M \phi_i(x_j) w_j \phi_2(x_j) + \dots + c_N \sum_{j=1}^M \phi_i(x_j) w_j \phi_N(x_j) = \sum_{j=1}^M y_j^E w_j \phi_i(x_j)$$

Since there is an equation for each i from 1 to N , we may solve for the c_i by solving the following set of simultaneous linear equations:

$$(6) \quad c_1 \sum_{j=1}^M \phi_1(x_j) w_j \phi_1(x_j) + c_2 \sum_{j=1}^M \phi_1(x_j) w_j \phi_2(x_j) + \dots + c_N \sum_{j=1}^M \phi_1(x_j) w_j \phi_N(x_j) = \sum_{j=1}^M y_j^E w_j \phi_1(x_j)$$

$$\begin{aligned} c_1 \sum_{j=1}^M \phi_2(x_j) w_j \phi_1(x_j) + c_2 \sum_{j=1}^M \phi_2(x_j) w_j \phi_2(x_j) + \dots \\ + c_N \sum_{j=1}^M \phi_2(x_j) w_j \phi_N(x_j) = \sum_{j=1}^M y_j^E w_j \phi_2(x_j) \\ \vdots \end{aligned}$$

$$c_1 \sum_{j=1}^M \phi_N(x_j) w_j \phi_1(x_j) + c_2 \sum_{j=1}^M \phi_N(x_j) w_j \phi_2(x_j) + \dots$$

$$+ c_N \sum_{j=1}^M \phi_N(x_j) w_j \phi_N(x_j) = \sum_{j=1}^M y_j^E w_j \phi_N(x_j)$$

Consider now the following matrices.

$$A = \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \dots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \dots & \phi_N(x_2) \\ \phi_1(x_3) & \phi_2(x_3) & \dots & \phi_N(x_3) \\ \vdots & \vdots & & \vdots \\ \phi_1(x_M) & \phi_2(x_M) & \dots & \phi_N(x_M) \end{pmatrix}$$

$$W = \begin{pmatrix} w_1 & 0 & 0 & \dots & 0 \\ 0 & w_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & 0 \\ 0 & 0 & \dots & 0 & w_M \end{pmatrix}$$

$$C = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \quad D = \begin{pmatrix} \sum_{j=1}^M y_j^E w_j \phi_1(x_j) \\ \sum_{j=1}^M y_j^E w_j \phi_2(x_j) \\ \vdots \\ \sum_{j=1}^M y_j^E w_j \phi_N(x_j) \end{pmatrix}$$

It may be verified by matrix multiplication (Ref. 2) that the equations (6) may be represented by the following matrix equation

$$(7) \quad (A^T W A)C = D$$

where A^T is the transpose of A (i.e. the matrix A with the rows and columns interchanged). The element $d_{m,n}$ in the m th row and n th column of the matrix $A^T W A$ is precisely the coefficient of c_n in row m of equations (6), i.e., $A^T W A$ is the matrix of the coefficients of the c_i in equations (6).

The least squares subroutine requires as input the matrices A and W and the values $\{y_j^E, j=1, M\}$. It calculates the matrix $A^T W A$ and the vector D , and solves equation (7) for the vector c using the ISIMEQ subroutine for solving simultaneous linear equations.

III. THE PROGRAM

The purpose of writing the LSTSQR subroutine was to supply the user with a routine which is completely independent of the functions $\phi_i(x)$ in equation (1). The burden of choosing these functions and the evaluation

of the matrix A is placed upon the user. However, since polynomial type functions are so widely used for fitting curves, two other routines, POLY and PLYTPE, are supplied for the evaluation of the matrix A when the $\phi_i(x)$ are polynomial type terms. The subroutine POLY uses fixed point exponentiation and can be used when the functions ϕ_i are products of any number of variables with integral (positive or negative) exponents. Examples of such ϕ_i are x^3 , x^2y^{-3} , $xy^{-5}z^4$, etc. Subroutine PLYTPE is used when the ϕ_i are products of any number of independent variables, and any of the variables have non-integral (positive or negative) exponents. Examples of such functions are $x^{\frac{1}{2}}$, $x^2y^{.56}$, $x^{.27}y^{-1.7}z^3$, etc. The subroutine PLYTPE will, of course, solve any problem which can be solved with the POLY routine. The POLY routine is supplied for those cases where there may be concern for the computer time used in floating point exponentiation.

Output of the LSTSQR subroutine consists of y_j and y_j^E for the given data points and the percentage error $(y_j^E - y_j)/y_j^E$. Also calculated is the standard error $SIGMA = \frac{1}{M} \sum_{j=1}^M (y_j^E - y_j)^2$. The coefficients c_i are also available for use.

Considerable effort was expended to make LSTSQR a general, fast, and small subroutine. In addition, the routine is very conservative of storage in that only $N*(N+1)$ temporary storage locations are required.

IV. USAGE

A. Subroutine LSTSQR

1. Calling sequence with A as a one dimensional variable

CALL LSTSQR (A, Y, W, NCOF, NPTS, IADIM, NMBRA)

where

NCOF = number of functions $\phi_1(x)$ in equation (1). (Same as N)

NPTS = number of given data points. (Same as M)

IADIM must be zero. This the control which tells LSTSQR that A is a one dimensional array.

NMBRA is the dimension of A. This must be at least as large as $NCOF*(NPTS + NCOF + 1)$.

A = a one dimensional array where the matrix A is stored.
The following rules apply:

- a. $\phi_1(x_1), \phi_1(x_2), \dots, \phi_1(x_M)$ must be stored in A(1) through A(NPTS) followed by $\phi_2(x_1), \phi_2(x_2), \dots, \phi_2(x_M)$ in A(NPTS+1) through A(2*NPTS), etc.
- b. The coefficients c_i are stored in A(NCOF*NPTS+1) through A(NCOF*NPTS+NCOF) upon return from the subroutine.
- c. LSTSQR destroys A(NCOF*NPTS+1) through A(NCOF*(NPTS+NCOF+1)).

Y is a one dimensional array containing $y_1^E, y_2^E, \dots, y_M^E$ in Y(1) through Y(NPTS).

W is a one dimensional array containing the weights $w_1, w_2, \dots, w_M$ in W(1) through W(NPTS).

2. Calling sequence with A as a two dimensional variable

CALL LSTSQR (A, Y, W, NCOF, NPTS, IADIM, NMBRA)

where

NCOF is same as in 1.

NPTS is same as in 1.

IADIM = first dimension of A in the DIMENSION statement

NMBRA = total storage allocated to A. This must be at least $NCCF \times (IADIM + NCOF + 1)$ or c_i will not be calculated.

A is a two dimensional variable where the matrix A is stored. $\phi_j(x_i)$ is stored in $A(I, J)$. The c_i are returned in $(A(I, NCOF + 1), I = 1, NCOF)$

Y is the same as in 1.

W is the same as in 1.

B. Subroutine POLY

1. General Description

The purpose of the POLY subroutine is to construct the A matrix needed in the LSTSQR routine when the functions $\phi_i(x)$ are polynomial type terms with positive or negative integral exponents. Examples of such ϕ_i are x^2 , xy^{-3} , $x^2y z^{-5}$, etc. The routine requires the values of the independent variables where the y_j^E are known, and the exponents of the independent variables in the individual polynomial type terms.

2. Calling Sequence

CALL POLY (NVAR, NPTS, NCOF, IPWR, A, X)

NVAR = total number of independent variables in the ϕ_i

NPTS = number of points where y^E is known

NCOF = number of polynomial type terms in the fitted function. The constant term, if present, is counted as one of these terms.

IPWR is a singly dimensioned variable containing the exponents for each of the polynomial type terms. They are arranged in the following manner:

```

IPWR(1) to IPWR(NVAR) - exponents for 1st polynomial term
IPWR(NVAR+1) to IPWR(2*NVAR) " " 2nd " "
.
.
.
IPWR(NVAR *(NCOF-1)+1) to IPWR (NVAR*NCOF) - exponents
for the last polynomial term

```

IPWR may contain positive, negative or zero values. The zero value designates the absence of the corresponding independent variable in that term. The constant term is described by all zero exponents.

A is a singly dimensioned output argument which will contain the matrix A which is needed in the LSTSQR routine.

X is a singly dimensioned variable containing values of the independent variables for NPTS points. They are arranged in the following manner:

```

X(1) to X(NVAR) - values of independent variables for 1st
point
X(NVAR+1) to X(2*NVAR) - values of independent variables
for 2nd point
.
.
.
X((NPTS-1)*NVAR+1) to X(NPTS*NVAR) - values of independent
variables for the last point

```

Arrangement of the variables in this array must be the same as in IPWR.

3. Example

Construct the matrix A for the polynomial

$$y = c_1 + c_2 r^2 + c_3 \theta^2 + c_4 r\theta$$

when the following 12 points are given:

r	θ	y^E
0	1	2
0	2	5
0	3	10
0	4	17
1	1	4
1	2	8
1	3	14
1	4	22
2	1	8
2	2	13
2	3	20
2	4	29

For this problem $NVAR = 2$, $NPTS = 12$, $NCOF = 4$. The IPWR are:

$IPWR(1) = 0$ $IPWR(2) = 0$ for the exponents for the constant term
 $IPWR(3) = 2$ $IPWR(4) = 0$ for the exponents for the r^2 term
 $IPWR(5) = 0$ $IPWR(6) = 2$ for the exponents for the θ^2 term
 $IPWR(7) = 1$ $IPWR(8) = 1$ for the exponents for the $r\theta$ term

The X are

$X(1) = 0$ $X(2) = 1$ are r, θ values for first point
 $X(3) = 0$ $X(4) = 2$ are r, θ values for second point
 $\vdots$
 $X(23) = 2$ $X(24) = 4$ are r, θ values for last point

The subroutine will construct the matrix A

$$A = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 4 & 0 \\ 1 & 0 & 9 & 0 \\ 1 & 0 & 16 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 4 & 2 \\ 1 & 1 & 9 & 3 \\ 1 & 1 & 16 & 4 \\ 1 & 4 & 1 & 2 \\ 1 & 4 & 4 & 4 \\ 1 & 4 & 9 & 6 \\ 1 & 4 & 16 & 8 \end{pmatrix}$$

C. Subroutine PLYTPE

1. General Description

The purpose of the PLYTPE routine is exactly that of the POLY routine except that the exponents may be non-integral.

2. Calling Sequence

CALL PLYTPE (NVAR, NPTS, NCOF, XPWR, A, X)

The description of the arguments is exactly the same as the POLY routine except for XPWR. The XPWR variable description is the same as for IPWR, except that XPWR contains floating point exponents.

V. ACKNOWLEDGMENT

The author wishes to express his thanks to T. Manning of IBM for his help with this program.

Nomenclature

y	= calculated value of the dependent variable.
x	= a vector of the independent variables.
y^E	= given (experimental) value of the dependent variable.
$\phi_i(x)$	= given functions of the independent variable.
w_j	= the weight associated with point j . The w_j should be a function of the reliability of point j . If all points are equally reliable, w_j will be 1 for all j .
c_i	= coefficients in the fitted function.
M	= number of given data points.
N	= number of coefficients c_i in the fitted function.
$S(c_1, c_2, \dots, c_N)$	= function which must be minimized in least squares sense in order to solve for the c_i .
A	= a rectangular matrix whose terms a_{ij} are the functional values $\phi_j(x_i)$. The term a_{ij} is the element in the i th row and j th column of A while $\phi_j(x_i)$ is the value of the j th function at point i .
W	= a diagonal matrix whose terms are the weights.
A^T	= the transpose of the matrix A .
C	= the column vector of the c_i .
D	= the column vector of the constant terms in the set of simultaneous linear equations to be solved.

References

1. F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill Company, 258-262, (1956).
2. G. Birkhoff and S. MacLane, A Survey of Modern Algebra, Macmillan Company, 209-213, (1954).

APPENDIX I

A. FITL Program

1. Purpose

The FITL program fits polynomials in any number of independent variables to a given set of data points. The exponents in the polynomial may be positive or negative integers or zero. It should be cautioned that when negative exponents are used, the domain of the independent variables should not include a pole of the fitted function.

2. The Program

The FITL program consists of a main program and the subroutines LSTSQR and POLY. The ISIMEQ routine, which solves a set of simultaneous linear equations, is also required. This is a regular library routine on the Westinghouse Astronuclear System Tape.

3. Input

- a. Card 1 FORMAT (13A6, A2)

This is a card of title information.

- b. Card 2 FORMAT (3I5)

Contains NVAR, NCOF, and NPTS where

NVAR = number of independent variables

NCOF = number of coefficients in the polynomial including
the constant term

NPTS = number of given data points

- c. Next Cards FORMAT (⁶12.5)

Punch the values of the independent variables followed by the value y^E followed by the weight for that point. Use as many cards as are necessary for each point but begin each new point on a new card. Cards must be supplied for NPTS points.

If the weight field is left blank (this field may not be omitted), the weight for this point will be set equal to 1.

d. Next cards FORMAT (14I5)

Punch the values of the exponents of the independent variables in each of the polynomial terms. Begin each new term on a new card and supply cards for NCOF terms. A zero exponent is used to indicate the absence of the corresponding variable in that term, and the constant term is described by all zeros.

e. Example

Fit the polynomial

$$y = c_1 + c_2 r^2 + c_3 \theta^2 + c_4 r \theta$$

in the two independent variables r and θ to the following

12 data points:

<u>r</u>	<u>θ</u>	<u>y^E</u>
0	1	2
0	2	5
0	3	10
0	4	17
1	1	4
1	2	8
1	3	14
1	4	22
2	1	8
2	2	13
2	3	20
2	4	29

The following page gives the input for this problem. The computer solution is given in Appendix II.

Westinghouse Electric Corporation

CODING FORM FOR IBM TYPE 7090 COMPUTER
FORTRAN - FAP

TITLE										ANALYST										PHONE										DATE										PROGRAM NO.										DECK NO.										L.S. NO.										SHEET									
FORTRAN										STAT. NO. #										FORTRAN STATEMENT										DECK NO.										SEQ. NO.																																							
FAP										SYMBOL										OPERATION										ADDRESS, TAG, DECREMENT										REMARKS																																							
REF.										1 2 3 4 5 6 7										8 9 10 11 12 13 14										15 16 17 18 19 20 21 22 23 24 25 26 27 28 29										30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49										50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72										73 74 75 76 77 78 79 80																			
										2										4										12										NVAR, NCDF, and NPTS.																																							
0.																				1.										2.										1.										n, θ , γ^E , and W for point										1																			
0.																				2.										5.										1.										"										2																			
0.																				3.										10.										1.										"										3																			
0.																				4.										17.										1.										"										4																			
1.																				1.										4.										1.										"										5																			
1.																				2.										8.										1.										"										6																			
1.																				3.										14.										1.										"										7																			
1.																				4.										22.										1.										"										8																			
2.																				1.										8.										1.										"										9																			
2.																				2.										13.										1.										"										10																			
2.																				3.										20.										1.										"										11																			
2.																				4.										29.										1.										"										12																			
0										0																				n, θ exponents in first term																																																	
2										0																				" second "																																																	
0										2																				" third "																																																	
1										1																				" fourth "																																																	

B. FIT2 Program

1. Purpose

The FIT2 program fits polynomial type functions in any number of independent variables to a given set of data points. The exponents may be any real numbers. It should be cautioned that when negative exponents are used, the domain of the independent variables should not include a pole of the fitted function.

2. The Program

The FIT2 program consists of a main program and the subroutines LSTSQ and PLYTPE. The ISIMEQ routine, which solves a set of simultaneous linear equations, is also required. This is a regular library routine on the Westinghouse Astronuclear System Tape.

3. Input

Input is identical with the FIT1 program except for the cards containing the exponents. The description of these cards is the same except for the format, which for floating point exponents is now FORMAT (6E12.5).

APPENDIX II

PROGRAM AND SAMPLE PROBLEMS

```
C MAIN PROGRAM FOR FIT1 PROGRAM. MAY BE USED FOR FITTING POLYNOMIAL
C FUNCTIONS IN ANY NUMBER OF VARIABLES TO A GIVEN SET OF POINTS.
C
C     COMMON A,Y,W,X,IPWR
C     DIMENSION A(15000),Y(1000),W(1000),X(8000),IPWR(500)
C     DIMENSION TITLE(14)
C
C READ AND PRINT TITLE.
C
C     5 READ INPUT TAPE 5,103,(TITLE(I),I=1,14)
C     WRITE OUTPUT TAPE 6,104,(TITLE(I),I=1,14)
C
C READ NO. OF VARIABLES, NO. OF COEFFICIENTS, AND NO. OF POINTS.
C
C     READ INPUT TAPE 5,100,NVAR,NCOF,NPTS
C     N1= 1
C     N2= NVAR
C
C READ DATA POINTS AND WEIGHTS.
C
C     DO 1 I=1,NPTS
C     READ INPUT TAPE 5,101,(X(J),J=N1,N2),Y(I),W(I)
C     N1= N1+NVAR
C     1 N2= N2+NVAR
C
C READ POWERS.
C
C     N1= 1
C     N2= NVAR
C     DO 2 I=1,NCOF
C     READ INPUT TAPE 5,102,(IPWR(J),J=N1,N2)
C     N1= N1+NVAR
C     2 N2= N2+NVAR
C
C SET ALL ZERO WEIGHTS TO 1.0
C
C     DO 3 I=1,NPTS
C     IF(W(I)) 3,4,3
C     4 W(I)= 1.0
C     3 CONTINUE
C
C POLY CALCULATES A MATRIX.
```

```
C      CALL POLY(INVAR,NPTS,NCOF,IPWR,3,X)
C
C      LSTSQR CALCULATES COEFFICIENTS.
C
C      CALL LSTSQR(A,Y,W,NCOF,NPTS,0,15000)
      GO TO 5
100  FORMAT(3I5)
101  FORMAT(6E12.5)
102  FORMAT(14I5)
103  FORMAT(13A6,A2)
104  FORMAT(1H1 13A6,A2)
      END
```


SUBROUTINE POLY(NVAR,NPTS,NCOF,IPWR,A,X)

4/24/64

PAGE 1

SUBROUTINE POLY(NVAR,NPTS,NCOF,IPWR,A,X)

C
C SUBROUTINE POLY CALCULATES THE MATRIX A NEEDED BY THE LSTSQR ROUTINE.
C THE ARGUMENTS ARE
C NVAR= NUMBER OF INDEPENDENT VARIABLES IN POLYNOMIAL.
C NPTS= NUMBER OF GIVEN DATA POINTS.
C NCOF= NUMBER OF TERMS IN THE POLYNOMIAL.
C IPWR IS THE ARRAY WHERE THE EXPONENTS ARE STORED.
C X IS THE ARRAY WHERE VALUES OF THE INDEPENDENT VARIABLES
C ARE STORED.
C A IS THE ARRAY WHERE POLY STORES THE MATRIX A.
C

DIMENSION IPWR(2),A(2),X(2)
NVR1= NVAR
NPT1= NPTS
NCF1= NCOF
I1= 1
N1= 1
DO 1 I2=1,NCF1
N2= 1
N3= NVR1
DO 2 I3=1,NPT1
I4= N1
A(I1)= 1.0
DO 3 I5=N2,N3
IF(IPWR(I4)) 4,3,4
4 A(I1)= A(I1)*(X(I5)**IPWR(I4))
3 I4= I4+1
N2= N2+NVR1
N3= N3+NVR1
2 I1= I1+1
1 N1= N1+NVR1
RETURN
END

SUBROUTINE LSTSQR(A,Y,W,NCOF,NPTS,IADIM,NMBRA)

4/24/64

PAGE

SUBROUTINE LSTSQR(A,Y,W,NCOF,NPTS,IADIM,NMBRA)

```
C
C SUBROUTINE LSTSQR CALCULATES TPL MATRICES (AT*W*A) AND D AND SOLVES
C THE MATRIX EQUATION (AT*W*A)*C= D FOR C USING THE ISIMEQ
C SUBROUTINE. THE ARGUMENTS OF LSTSQR ARE
C   A      IS A ONE OR TWO DIMENSIONAL ARRAY WHERE THE MATRIX A
C           IS STORED.
C   Y      IS A ONE DIMENSIONAL ARRAY WHERE YE IS STORED.
C   W      IS AN ARRAY WHERE THE WEIGHTS ARE STORED.
C   NCOF= NUMBER OF UNKNOWN COEFFICIENTS IN THE FITTED FUNCTION.
C   NPTS= NUMBER OF GIVEN DATA POINTS. ALSO NUMBER OF Y AND W.
C   IADIM= 0 IF A IS ONE DIMENSIONAL.
C   IADIM= FIRST DIMENSION OF A IF A IS TWO DIMENSIONAL.
C   NMBRA= TOTAL NUMBER OF STORAGE SPACES ALLOCATED TO A.
C
C   DIMENSION A(2),Y(2),W(2)
C   NCF1= NCOF
C   NPT1= NPTS
C   IA1= IADIM
C   I1D= 0
C   IF(IA1) 12,13,12
C
C   INITIALIZE I1D AND N1 IF A IS TWO DIMENSIONAL.
C
C   12 I1D= IA1-NPT1
C      N1= NCF1*IA1
C      GO TO 14
C
C   CALCULATE N1 IF A IS ONE DIMENSIONAL.
C
C   13 N1= NCF1*NPT1
C   14 N2= N1+1
C      N3= N1+NCF1
C      N4= N1+NCF1*NCF1+1
C      N5= N4+NCF1-1
C
C   TEST IF A IS TOO SMALL.
C
C      IF(NMBRA-N5) 1,2,2
C   1 WRITE OUTPUT TAPE 6,100
C   CALL EXIT
C
C   CALCULATE THE SYMMETRIC MATRIX AT*W*A. THE UPPER HALF ONLY
```

C IS CALCULATED. AT*W*A IS STORED BY COLUMNS IN CONSECUTIVE
C LOCATIONS BEGINNING IN A(NCOF*NPTS+1) IF A IS ONE DIMENSIONAL,
C AND BEGINNING IN A(1,NCOF+1) IF A IS TWO DIMENSIONAL.

C

```
2 DO 3 I=N2,N5
3 A(I)= 0.
  I1= 1
  DO 4 I2=1,NCF1
  DO 5 I3=1,NPT1
  Z= A(I1)*W(I3)
  I4= I1
  DO 6 I5=N2,N3
  A(I5)= A(I5)+A(I4)*Z
6 I4= I4+NPT1+I1D
5 I1= I1+1
  I1= I1+I1D
  I6= N2
```

C

C SET LOWER HALF OF A EQUAL TO UPPER HALF.

C

```
DO 7 I7=N2,N3
A(I6)= A(I7)
7 I6= I6+NCF1
  N2= N2+NCF1+1
4 N3= N3+NCF1
```

C

C CALCULATE THE MATRIX D.

C

```
  I1= 1
  DO 11 I2=N4,N5
  DO 8 I3=1,NPT1
  A(I2)= A(I2)+W(I3)*A(I1)*Y(I3)
8 I1= I1+1
11 I1= I1+I1D
  N6= N1+1
```

C

C SOLVE FOR C.

C

```
CALL ISIMEQ(A(N6),NCF1,NCF1,1)
WRITE OUTPUT TAPE 6,101,(A(I),I=N4,N5)
I1= N1+1
DO 15 I=N4,N5
A(I1)= A(I)
```

```
15 I1= I1+1
   WRITE OUTPUT TAPE 6,102
   SIGMA= 0.
```

C
C
C
C

```
C CALCULATE Y FROM FITTED FUNCTION. CALCULATE PERCENTAGE DIFFERENCE
C OF Y AND YE. ALSO CALCULATE STANDARD ERROR.
```

```
   DO 9 J=1,NPT1
   Z= 0.
   I1= J
   DO 10 I2=N4,N5
   Z= Z+A(I1)*A(I2)
10 I1= I1+NPT1+I1D
   DEL= Y(J)-Z
   SIGMA= SIGMA+DEL*DEL
   DEL= DEL/Y(J)
9 WRITE OUTPUT TAPE 6,103,Y(J),Z,DEL
   FN= NPT1
   SIGMA= SQRTF(SIGMA/FN)
   WRITE OUTPUT TAPE 6,104,SIGMA
   RETURN
100 FORMAT(52H1 DIMENSION OF A MUST BE AT LEAST NCOF*(NPTS+NCOF+1)
101 FORMAT(22H0 THE COEFFICIENTS ARE/1H /(6E16.6))
102 FORMAT(1H1 8X,1HY 15X,2HYC 12X,5HDELTA/1H )
103 FORMAT(3E16.6)
104 FORMAT(12H0 SIGMA IS E14.6)
END
```

FITTING (C1 + C2*R**2 + C3*TH**2 + C4*R*TH) TO (1 + R**2 + TH**2 + R*TH)

THE COEFFICIENTS ARE

0.100000E 01 1.000000E 00 1.000000E 00 0.100000E 01

Y		YC		DELTA
0.200000E	01	0.200000E	01	0.
0.500000E	01	0.500000E	01	0.
0.100000E	02	1.000000E	01	0.119209E-07
0.170000E	02	0.170000E	02	0.140246E-07
0.400000E	01	0.400000E	01	0.
0.800000E	01	0.800000E	01	0.
0.140000E	02	0.140000E	02	0.
0.220000E	02	0.220000E	02	0.108372E-07
0.800000E	01	0.800000E	01	0.149012E-07
0.130000E	02	0.130000E	02	0.916995E-08
0.200000E	02	0.200000E	02	0.
0.290000E	02	0.290000E	02	0.

SIGMA IS 0.114134E-06

C MAIN PROGRAM FOR FIT 2 PROGRAM. MAY BE USED FOR FITTING POLYNOMIAL
C TYPE FUNCTIONS WITH INTEGRAL OR NON-INTEGRAL POWERS TO A GIVEN SET
C OF DATA POINTS. FUNCTIONS MAY HAVE ANY NUMBER OF VARIABLES.

C
COMMON A,Y,W,X,XPWR
DIMENSION A(15000),Y(1000),W(1000),X(8000),XPWR(500)
DIMENSION TITLE(14)

C
C READ AND PRINT TITLE.

C
5 READ INPUT TAPE 5,103,(TITLE(I),I=1,14)
WRITE OUTPUT TAPE 6,104,(TITLE(I),I=1,14)

C
C READ NO. OF VARIABLES, NO. OF COEFFICIENTS, AND NO. OF POINTS.

C
READ INPUT TAPE 5,100,NVAR,NCOF,NPTS
N1= 1
N2= NVAR

C
C READ DATA POINTS AND WEIGHTS.

C
DO 1 I=1,NPTS
READ INPUT TAPE 5,101,(X(J),J=N1,N2),Y(I),W(I)
N1= N1+NVAR
1 N2= N2+NVAR

C
C READ POWERS.

C
N1= 1
N2= NVAR
DO 2 I=1,NCOF
READ INPUT TAPE 5,101,(XPWR(J),J=N1,N2)
N1= N1+NVAR
2 N2= N2+NVAR

C
C SET ALL ZERO WEIGHTS TO 1.0

C
DO 3 I=1,NPTS
IF(W(I)) 3,4,3
4 W(I)= 1.0
3 CONTINUE

4/24/64

0318

```
C POLY CALCULATES A MATRIX.
C
C   CALL PLYTPE(NVAR,NPTS,NCOF,XPWR,A,X)
C
C LSTSQR CALCULATES COEFFICIENTS.
C
C   CALL LSTSQR(A,Y,W,NCOF,NPTS,0,15000)
C   GO TO 5
100 FORMAT(3I5)
101 FORMAT(6E12.5)
103 FORMAT(13A6,A2)
104 FORMAT(1H1 13A6,A2)
END
```


SUBROUTINE PLYTPE(NVAR,NPTS,NCOF,XPWR,A,X)

4/24/64

PAGE 1

SUBROUTINE PLYTPE(NVAR,NPTS,NCOF,XPWR,A,X)

C SUBROUTINE PLYTPE CALCULATES THE MATRIX A NEEDED BY LSTSQR.

C THE ARGUMENTS ARE

C NVAR= NUMBER OF INDEPENDENT VARIABLES IN POLYNOMIAL.

C NPTS= NUMBER OF GIVEN DATA POINTS.

C NCOF= NUMBER OF TERMS IN THE POLYNOMIAL.

C XPWR IS THE ARRAY WHERE THE EXPONENTS ARE STORED.

C X IS THE ARRAY WHERE VALUES OF THE INDEPENDENT VARIABLES
C ARE STORED.

C A IS THE ARRAY WHERE POLY STORES THE MATRIX A.

C
C DIMENSION XPWR(2),A(2),X(2)

NVR1= NVAR

NPT1= NPTS

NCF1= NCOF

I1= 1

N1= 1

DO 1 I2=1,NCF1

N2= 1

N3= NVR1

DO 2 I3=1,NPT1

I4= N1

A(I1)= 1.0

DO 3 I5=N2,N3

IF(XPWR(I4)) 4,3,4

4 A(I1)= A(I1)*(X(I5)**XPWR(I4))

3 I4= I4+1

N2= N2+NVR1

N3= N3+NVR1

2 I1= I1+1

1 N1= N1+NVR1

RETURN

END