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NONLIN: A Computer Program for Least Squares Estimation of Nonlinear Parameters and Applications

BDX-613-813

December, 1972

Project Leader:
B. J. Neal
Department 416

Project Team:
W. E. Krueger

Prepared for the U. S. Atomic Energy Commission
Albuquerque Operations Office under Contract
Number AT(29-1)-613 USAEC.

**Kansas City
Division**

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PARAMETERS AND APPLICATIONS

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NONLIN: A COMPUTER PROGRAM FOR LEAST SQUARES ESTIMATION OF NONLINEAR PARAMETERS AND APPLICATIONS

BDX-613-813, UNCLASSIFIED, Distributed December 1972

Prepared by B. J. Neal, D/416

A computer program, NONLIN, which determines the least squares estimates of the unknown parameters in a nonlinear model was developed. The mathematical basis of Marquardt's compromise algorithm, which is the computing procedure used in NONLIN is described in detail. Applications of NONLIN are given.

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THE BENDIX CORPORATION

KANSAS CITY DIVISION

KANSAS CITY, MISSOURI

A prime contractor for the
Atomic Energy Commission

Contract Number AT(29-1)-613 USAEC

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SUMMARY

Fitting experimental data to a mathematical model is useful in data analysis. Mathematical models provide prediction equations to determine the levels of process variables which provide an optimum response. The models also establish experimental regions for future investigations. In many situations the proposed model is nonlinear with respect to the unknown parameters.

A computer program, NONLIN, was written to estimate the unknown parameters. NONLIN uses Marquardt's compromise algorithm and is efficient in fitting a variety of functions. Good initial estimates are required for convergence. Applications of the program are included. A printout of the computer program and requirements for its use are also given.

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DISCUSSION

SCOPE AND PURPOSE

A commonly used statistical technique in analyzing experimental data is the fitting of a linear model to the data by the method of least squares. A linear model is one which is linear with respect to the parameters of interest. A linear model takes the form

$$E(Y) = B_0 + B_1 Z_1 + B_2 Z_2 + \dots + B_p Z_p \quad (1)$$

where the Z_i can represent any function of the independent variables.

Although this model has wide application, there are some situations for which the linear model is not adequate. Technical knowledge of the experimental situation being investigated might dictate that an appropriate model is nonlinear with respect to the unknown parameters. Any model which is not of the form given in Equation 1 is nonlinear in its parameters.

ACTIVITY

Several investigations at Bendix Kansas City have led to the frequent use of the three nonlinear models shown in the examples below. These models were used to provide prediction equations for response variables, to determine the levels of process variables which provide an optimum response, and to establish experimental regions for future investigations. A computer program, NONLIN, was developed to estimate the unknown parameters in nonlinear models.

Example 1: Moisture Pickup of Desiccant Material

The purpose of this study was to determine the moisture pickup of a molded desiccant material in order to include an estimate of the moisture pickup versus time curve in a larger study. Percent moisture pickup was defined as a change in weight compared with the initial weight as follows:

$$\text{percent moisture pickup} = \frac{W_t - W_0}{W_0} \times 100, \quad (2)$$

where W_i is the weight at time $t = i$.

The physical properties of the part indicated that some form of exponential model would be appropriate. The chosen model resulted from previous studies with desiccant material and is given by

$$Y = A - A e^{B(t)^C}, \quad (3)$$

where

t = time in hours,

Y = percent moisture pickup at time t , and

A , B , and C are parameters to be estimated (A is the saturation level).

This exponential model provided a good equation for predicting the percent moisture pickup. The model also proved useful for estimating the saturation level. The time derivative gives an expression which can be used to estimate the efficiency of moisture pickup at any given time.

Example 2: Effect of Catalysts on Compressive Strength

One-inch core specimens of polyurethane rigid foam were used as test specimens to determine the effect of two catalysts on compressive strength. The density and compressive strength are related by the formula

$$\text{Compressive strength} = K \rho^\alpha, \quad (4)$$

where ρ is the core density.

The parameters K and α were estimated for each catalyst to compare the compressive strengths generated by the catalysts. The fitted equations showed that the added catalysts did not significantly alter the average compressive properties of the core specimen.

Example 3: Determination of Profile Milling Conditions

Combinations of feed rate, and axial and radial depths of cuts that provide zero lateral deflection in profile milling were investigated using the model

$$Y = 2wf^{(1-\lambda)} (A_0 + A_1 x + A_2 x^2 + A_3 x^3 + A_4 x^4), \quad (5)$$

where

λ and A_i , $i = 0, \dots, 4$ are the parameters to be estimated,

Y = normal force (lb),

f = feed rate (inch per revolution per tooth),

d = radial depth (inch),

D = cutter diameter (inch),

w = axial depth (inch), and

$x = d/D$.

This model provided a useful means of defining an experimental region of the variables where lateral deflection is minimized. The computer printouts for the examples are shown in Appendix B.

The Problem of Nonlinear Estimation

Suppose the model to be fitted to the data is given by

$$E(Y) = f(X_1, X_2, \dots, X_m, \theta_1, \dots, \theta_p), \quad (6)$$

$$E(Y) = f(\underline{X}, \underline{\theta}) \quad (6a)$$

where X_k , $k = 1, \dots, m$ are independent variables, and θ_i , $i = 1, \dots, p$ are the unknown population parameters, and $E(Y)$ is the expected value of the dependent variable Y . Let

$$(Y_i, X_{i1}, X_{i2}, \dots, X_{im}), i = 1, 2, \dots, n$$

denote the data points. The problem is to determine a set of estimates of the parameters which will minimize the sums of squares function

$$\Phi = \sum_{i=1}^n \left(Y_i - f(\underline{X}_i, \underline{\theta}) \right)^2 = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 \quad (7)$$

where $\hat{Y}_i$ is the value of Y_i predicted by Equation 6 at the i -th data point. Most methods for least squares estimation of nonlinear parameters are variations

of either of two techniques, the linearization method or the steepest descent (gradient) method.

The linearization method expands the function $f(\underline{X}, \underline{\theta})$ in a Taylor series through its linear terms about some trial parameter vector, such as $\underline{\theta}_0$.

$$\langle Y_i \rangle = f(\underline{X}_i, \underline{\theta}_0 + \underline{\delta}_t) = f(\underline{X}_i, \underline{\theta}_0) + \sum_{j=1}^p \frac{\partial f_i}{\partial \theta_j} (\theta_j - \theta_{0j}) \quad (8)$$

$$\langle Y_i \rangle = f(\underline{X}_i, \underline{\theta}_0) + \sum_{j=1}^p \frac{\partial f_i}{\partial \theta_j} \delta_{tj} \quad (8a)$$

$$\langle \underline{Y} \rangle = \underline{f}_0 + \underline{P} \underline{\delta}_t \quad (8b)$$

where $\underline{\theta}_0$ is an estimate of $\underline{\theta}$, $\underline{\delta}_t$ is a small correction vector to $\underline{\theta}_0$, and $\langle \underline{Y} \rangle$ is the predicted value of $\underline{Y}$ determined from the linearized model. Since $\underline{\delta}_t$ appears linearly, its components can be found by standard least squares. Thus, $\underline{\delta}_t$ is found by solving

$$\underline{A} \underline{\delta}_t = \underline{g} \quad (9)$$

where

$$\underline{P}^{(n \times p)} = \left(\frac{\partial f_i}{\partial \theta_j} \right), \quad i=1, 2, \dots, n, j=1, 2, \dots, p \quad (10)$$

$$\underline{A}^{(p \times p)} = \underline{P}' \underline{P} \quad (11)$$

$$\underline{g}^{(p \times 1)} = \left(\sum_{i=1}^n (Y_i - f_i) \frac{\partial f_i}{\partial \theta_j} \right) \quad j=1, 2, \dots, p \quad (12)$$

$$\underline{g}^{(p \times 1)} = \underline{P}' (\underline{Y} - \underline{f}_0). \quad (12a)$$

The gradient methods step off from the current trial vector $\underline{\theta}_0$ in the direction of the negative gradient of Φ . Thus,

$$\underline{\delta}_g = - \left(\frac{\partial \Phi}{\partial \theta_1}, \frac{\partial \Phi}{\partial \theta_2}, \dots, \frac{\partial \Phi}{\partial \theta_p} \right) \quad (13)$$

Both methods have drawbacks for certain problems, in that

- Convergence may be slow, and
- It is necessary to control the step size carefully, once the direction of the correction vector has been developed.

D. W. Marquardt developed an algorithm called Marquardt's compromise. This compromise method interpolates between the linearization method and the gradient method. The method determines the maximum neighborhood in which the Taylor series expansion of the function through its linear terms gives an adequate representation of the model.¹ This compromise procedure eliminates some serious drawbacks of both previously stated methods in that it determines simultaneously the direction of the correction vector and the step size. It is this compromise algorithm which is programmed in NONLIN.

The Compromise Algorithm

The mathematical basis of the algorithm is contained in three theorems which can be found in Marquardt.¹ At the r -th step define the scaled matrix $\underline{A}^*$ and a scaled vector $\underline{g}^*$

$$\underline{A}_r^* = (a_{jj}^*) = \left(\frac{a_{jj}'}{\sqrt{a_{jj} a_{jj}'}} \right) \quad \begin{matrix} j = 1, 2, \dots, p \\ j' = 1, 2, \dots, p \end{matrix} \quad (14)$$

where

$$\begin{aligned} a_{jj}' &= \sum_{i=1}^n \left(\frac{\partial f(\underline{X}_i, \underline{\theta})}{\partial \theta_j} \right) \left(\frac{\partial f(\underline{X}_i, \underline{\theta})}{\partial \theta_{j'}} \right) \quad \underline{\theta} = \underline{\theta}_r \\ \underline{g}_r^* &= (\underline{g}_j^*) = \frac{\sum_{i=1}^n (Y_i - f(\underline{X}_i, \underline{\theta})) \left(\frac{\partial f(\underline{X}_i, \underline{\theta})}{\partial \theta_j} \right)}{\sqrt{a_{jj}}} \quad \underline{\theta} = \underline{\theta}_r \end{aligned} \quad (15)$$

Construct the equation

$$(\underline{A}_r^* + \lambda_r \underline{I}) \underline{\delta}_r^* = \underline{g}_r^* \quad (16)$$

Note that when $\lambda_r = 0$, Equation 16 reduces to $\underline{A}_r \underline{\delta}_r^* = \underline{g}_r^*$. This means that for $\lambda_r = 0$, $\underline{\delta}_r^*$ equals $\underline{\delta}_t$ in equation 9 except for a scaling factor.

Solve this equation for $\underline{\delta}_r^*$, then determine the correction vector $\underline{\delta}_r$ from the relationship

$$(\delta_j)_r = \frac{(\delta_j^*)_r}{\sqrt{a_{jj}}} \quad (17)$$

The new trial vector

$$\underline{\theta}_{(r+1)} = \underline{\theta}_r + K_r \underline{\delta}_r \quad (18)$$

will lead to a new sum of squares Φ_{r+1} , where K_r is a suitable constant. It is essential to select λ_r such that

$$\Phi_{(r+1)} < \Phi_r \quad (19)$$

To determine such a λ_r , the following strategy is applied.

- (1) Choose $\nu > 1$. In NONLIN $\nu = 10$.
- (2) Let λ_{r-1} denote the value λ from the previous iteration. The initial value of λ was chosen as 0.01.
- (3) Compute $\Phi(\lambda_{r-1})$ and $\Phi(\lambda_{r-1}/\nu)$. If λ_{r-1}/ν is already negligible by comparison with 1.0 to the number of significant digits carried, then only $\Phi(\lambda_{r-1})$ is computed.
 - (a) If $\Phi(\lambda_{r-1}/\nu) \leq \Phi_r$, let $\lambda_r = \lambda_{r-1}/\nu$.
 - (b) If $\Phi(\lambda_{r-1}/\nu) > \Phi_r$, and $\Phi(\lambda_{r-1}) \leq \Phi_r$, let $\lambda_r = \lambda_{r-1}$.

(c) If $\Phi(\lambda_{r-1}/v) > \Phi_r$, and $\Phi(\lambda_{r-1}) > \Phi_r$, increase λ by successive multiplication by v until for some smallest w ,
 $\Phi(\lambda_{r-1}v^w) \leq \Phi_r$. Let $\lambda_r = \lambda_{r-1}v^w$. To prevent the value of λ from becoming unreasonably large, K_r in Equation 18 is 1, if $\gamma_r \geq \gamma_0$, where γ_r is the angle between $\underline{\delta}_r^*$ and $\underline{g}_r^*$ and γ_0 is a criterion angle $< \pi/2$. In NONLIN, $\gamma_0 = \pi/4$. If test (c) is not passed and $\gamma < \gamma_0$, make K_r sufficiently small so that $\Phi_{r+1} < \Phi_r$.

Repetition of these steps leads to a feasible neighborhood in which the Taylor series gives an adequate representation of the function. The iterations have converged when

$$\frac{|(\delta_j)_r|}{\tau + |\theta_j|} < \epsilon, \text{ for all } j$$

for some suitably small $\epsilon > 0$ and some suitable τ .

Computer Program NONLIN

The computer program, NONLIN, written in FORTRAN IV, computes the least squares estimates of the nonlinear parameters using Marquardt's compromise algorithm previously discussed. The program was written for use on the Bendix in-house time-sharing system, INTERCOM. However, for problems with a large amount of data, the program can be run as a batch job on the CDC 6600. The program is dimensioned to allow a maximum of 200 data points, 15 unknown parameters, and 15 independent variables. NONLIN provides the option of evaluating the functional derivatives analytically or numerically. NONLIN requires two subroutines, DIFF1 and EF. The data points and current parameter values are passed from the main program to the subprograms through a COMMON block.

Subroutine DIFF1.

This subroutine provides the main program with values of the analytical derivatives of the function. The number of the parameter for which the derivative is taken, the number of the observation at which it is evaluated and the computed value appear as arguments of DIFF1.

Subroutine EF

This subroutine provides the main program with values of the theoretical function corresponding to each data point for the current trial parameter vector. The number of the data point at which the function is evaluated and the resulting value are arguments of EF.

ACCOMPLISHMENTS

As stated earlier, NONLIN has been used frequently to estimate the parameters of the three models. Equations 3, 4, and 5. NONLIN is also efficient in fitting models which involve logarithmic and trigonometric functions, in addition to polynomials. Experience in using the program indicates that good initial values of the parameters are needed, and that the analytical derivatives should be used whenever possible.

REFERENCE

- ¹D. W. Marquardt, "An Algorithm for Least Squares Estimation of Nonlinear Parameters," Journal of the Society For Industrial and Applied Mathematics, Vol. 2, (1963), pp 431-441.

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Appendix A

NONLIN

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Appendix A

NONLIN

DATA INPUT

The user must supply NONLIN with the following data input:

- (1) Format specifications for reading in the observations and initial parameter values;
- (2) Indicator denoting the use of analytical or estimated derivatives;
- (3) Number of parameters, number of observations, number of independent variables, and an indicator if all calculation steps are to be printed;
- (4) An epsilon value denoting the desired accuracy of the convergence;
- (5) An indicator as to how the data will be read into the computer (data file or punch cards);
- (6) The data matrix whose rows are the observation vector, i.e., the values of the independent variables and the corresponding response; and
- (7) The initial values of the parameters.

DATA OUTPUT

The printed output from NONLIN is as follows.

- (1) All intermediate calculations at the option of the user.
- (2) At each step (optional)
 - (a) Value of parameters tried at each iteration within a given step.
 - (b) Number of iterations within each step and the number of the step.
 - (c) The sum of squares function using current parameter values and corrected parameter values which are used at the next step.
- (3) The value of the final sum of squares function and standard error of the estimate.

- (4) The final parameter estimates.
- (5) Observed response, predicted response and difference between the two.

OTHER FEATURES OF NONLIN

I. There are three ways of stopping the program.

A. Convergence to the desired set of parameter estimates: there are three convergence criteria.

- (1) Epsilon Test: This test is passed if

$$\frac{|\delta_j|}{\tau + |\theta_j|} < \epsilon \quad \text{for all } j.$$

If this test is passed, no message is printed.

- (2) Gamma Lambda Test: This test is passed if λ becomes greater than 1.0 when γ is greater than 90 degrees. When convergence is due to this test, the message "Convergence by Gamma Lambda test" is printed.
- (3) Gamma Epsilon Test: This test is passed if all parameter increments become small enough to pass the "Epsilon Test" as a result of successive halving of the increments when $\gamma < \gamma_0$. When this test is passed the message, "Convergence by alternate test successive halving," is printed.

B. The maximum number of steps allowed has been exceeded. In NONLIN 500 steps are allowed. The message, "Convergence doesn't occur in the number of iterations allowed," is printed.

C. Irregularities in calculations.

- 1. A singular matrix is encountered
- 2. Division by zero

If one of these irregularities occurs, the message, "The iterations take a divergent path for initial values," is printed. At this point the user has the option of stopping the program or starting again with a new set of initial estimates.

- II. The user can run as many problems as desired using the same model without recalling the program.

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Appendix B

COMPUTER PRINTOUTS AND PLOTS FOR EXAMPLES

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ENTER FORMAT FOR READING IN OBSERVATIONS
 (10F5.4)
 ENTER NO. OF PARAMETERS, NO. OF OBS., NO. OF INDEP. VARIABLES,
 AND THE NO. 1 IF ALL STEPS ARE PRINTED, OTHERWISE ENTER 0.
 FORMAT FOR THIS INPUT IS 514
 3 54 1 0
 ENTER ACCURACY NEEDED, USE FORMAT(F8.6)
 .00001
 ENTER VALUE OF INDEP. VAR. ROW-WISE, VALUES OF DEP. VAR.,
 1.00 2.08 3.05 4.07 4.95 6.20 7.17 8.18 10.20 11.18
 12.22 13.18 14.22 15.23 16.23 17.23 18.22 19.22 20.23 21.20
 22.07 22.95 24.28 26.30 28.12 30.15 32.17 34.15 36.12 38.18
 40.17 42.20 44.18 46.18 48.28 50.08 52.10 54.17 56.12 58.08
 60.12 62.18 64.17 66.15 68.15 70.18 72.08 74.13 76.30 80.18
 84.15 88.18 92.15 96.27 2.05 3.48 4.66 5.73 6.55 7.47
 8.23 9.02 10.28 10.85 11.55 11.97 12.50 12.90 13.23 13.66
 13.96 14.27 14.55 14.98 15.12 15.37 15.71 16.18 16.77 16.91
 17.22 17.59 17.84 18.24 18.38 18.52 18.66 18.74 18.77 18.74
 18.71 18.74 18.80 18.77 18.77 18.85 18.83 18.91 18.85 18.88
 18.85 18.77 18.83 18.80 18.85 18.85 18.91 18.91
 ENTER INITIAL VALUES OF PARAMETERS, USE DATA FTM
 18.9 -.1 .9

EXAMPLE 1. MOISTURE PICKUP OF DESICCANT MATERIAL

NONLINEAR ESTIMATION

THE INITIAL PARAMETER MATRIX IS

18.90000	-.10000	.90000
19.16470	-.09264	.91925

FOR ITERATION 1 IN STEP 1

SS(1)= 4.54523 SS(.00100)= 2.33194 DIFF.= -2.21329

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

19.16470	-.09264	.91925
19.15841	-.09230	.92192

FOR ITERATION 1 IN STEP 2

SS(2)= 2.33194 SS(.00010)= 2.32126 DIFF.= -.01068

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

19.15841	-.09230	.92192
19.15982	-.09234	.92167

FOR ITERATION 1 IN STEP 3

SS(3)= 2.32126 SS(.00001)= 2.32124 DIFF.= -.00003

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

19.15982	-.09234	.92167
19.15972	-.09234	.92169

FOR ITERATION 1 IN STEP 4

SS(4)= 2.32124 SS(.00000)= 2.32124 DIFF.= -.00000

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

19.15972	-.09234	.92169
19.15973	-.09234	.92168

EXAMPLE 1 CONTINUED

NONLINEAR REGRESSION

UNEXPLAINED VARIATION= 2.32124 S. E. OF ESTIMATE= .21334

THE FINAL PARAMETER ESTIMATES ARE:

19.15973	-.09234	.92168
----------	---------	--------

ACTUAL VS PREDICTED RESULTS

ACTUAL	PREDICTED	RESIDUAL
.205000000E+01	.168996869E+01	.360031313E+00
.348000000E+01	.317791817E+01	.302081831E+00
.466000000E+01	.435822551E+01	.301774492E+00
.573000000E+01	.547728613E+01	.252713875E+00
.655000000E+01	.635846663E+01	.191533366E+00
.747000000E+01	.749537485E+01	-.253748506E-01
.823000000E+01	.829641862E+01	-.664186151E-01
.902000000E+01	.906403853E+01	-.440385255E-01
.102800000E+02	.104226039E+02	-.142603858E+00
.108500000E+02	.110074375E+02	-.157437480E+00
.115500000E+02	.115813958E+02	-.313957913E-01
.119700000E+02	.120722103E+02	-.102210290E+00
.125000000E+02	.125652895E+02	-.652895078E-01
.129000000E+02	.130088612E+02	-.108861215E+00
.132300000E+02	.134165969E+02	-.186596882E+00
.136600000E+02	.137955321E+02	-.135532145E+00
.139600000E+02	.141445137E+02	-.184513731E+00
.142700000E+02	.144726170E+02	-.202616993E+00
.145500000E+02	.147809950E+02	-.230994992E+00
.149800000E+02	.150570167E+02	-.770167009E-01
.151200000E+02	.152889802E+02	-.168980222E+00
.153700000E+02	.155096048E+02	-.139604756E+00
.157100000E+02	.158183088E+02	-.108308830E+00
.161800000E+02	.162358715E+02	-.558714883E-01
.167700000E+02	.165654287E+02	.204571300E+00
.169100000E+02	.168877680E+02	.222320462E-01
.172200000E+02	.171673754E+02	.526245908E-01
.175900000E+02	.174069257E+02	.183074275E+00
.178400000E+02	.176157862E+02	.224213833E+00
.182400000E+02	.178068374E+02	.433162641E+00
.183800000E+02	.179682835E+02	.411716511E+00
.185200000E+02	.181126095E+02	.407390471E+00
.186600000E+02	.182360888E+02	.423911179E+00
.187400000E+02	.183456757E+02	.394324263E+00
.187700000E+02	.184464489E+02	.323551114E+00
.187400000E+02	.185226077E+02	.217392257E+00
.187100000E+02	.185982229E+02	.111777069E+00

EXAMPLE 1 CONTINUED

Actual VS Predicted

Actual	Predicted	Residual
.187400000E+02	.186662130E+02	.737870208E-01
.188000000E+02	.187225585E+02	.774415319E-01
.187700000E+02	.187725831E+02	-.258307454E-02
.187700000E+02	.188184636E+02	-.484635992E-01
.188500000E+02	.188591766E+02	-.917655214E-02
.188300000E+02	.188938042E+02	-.638041799E-01
.189100000E+02	.189242281E+02	-.142280772E-01
.188500000E+02	.189513669E+02	-.101366880E+00
.188800000E+02	.189756636E+02	-.956636190E-01
.188500000E+02	.189957893E+02	-.145789269E+00
.187700000E+02	.190150044E+02	-.245004378E+00
.188300000E+02	.190328590E+02	-.202859020E+00
.188000000E+02	.190593996E+02	-.259399615E+00
.188500000E+02	.190807463E+02	-.230746310E+00
.188500000E+02	.190977197E+02	-.247719658E+00
.189100000E+02	.191108285E+02	-.200828462E+00
.189100000E+02	.191214783E+02	-.211478262E+00

STOP

COMMAND= REWIND.CER3.

Figure B-1. Example 1: Desiccant Moisture Pickup at 2000 psi Mold Pressure

EXAMPLE 2. EFFECT OF CATALYSTS ON COMPRESSIVE STRENGTH

```

CORE MAP 10.30.19. NORMAL CONTROL
---TIME---LOAD MODE---L1---L2---TYPE-----USER---♦---C
FWA LOADER 033771 FWA TABLES 031657
-PROGRAM---ADDRESS- --LAELED---COMMON--
NONLIN 000100
MINV 016431
TPRD 017027
GMPRD 017203
DCPY 017304
LOC 017354
DIFF1 017423
EF 017454
GETBA 017505
SI05 017524
SYSTEM$ 021100
ACG0ER$ 022062
INPUTC$ 022075
KODER$ 022213
KRAKER$ 023606
OUTPIC$ 025277
ALNLOGE 025373
ASNCUSE 025432
LEGVAR$ 025546
SQRT 025553
EXPE 025575
----UNSATISFIED EXTERNALS----- REFER

```

ENTER FORMAT FOR READING IN OBSERVATIONS

ENTER NO. OF PARAMETERS, NO. OF OHS., NO. OF INDEP. VARIABLES,
AND THE NO. 1 IF ALL STEPS ARE PRINTED, OTHERWISE ENTER 0.
FORMAT FOR THIS INPUT IS SI4

ENTER ACCURACY NEEDED, USE FORMAT(F8.6)

ENTER VALUE OF INDEP. VAR., VALUE OF DEP. VAR. ROW-WISE.,

ENTER INITIAL VALUES OF PARAMETERS, USE DATA FIM

NONLINEAR ESTIMATION

THE INITIAL PARAMETER MATRIX IS

7.00000 1.50000

FOR ITERATION 1 IN STEP 1

SS(1)=*06554.81634 SS(.00100)=*68721.47365 DIFF.=*37833.34273

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

4.71717 1.91567

FOR ITERATION 1 IN STEP 2

SS(2)=*68721.47365 SS(.00010)= 46094.59037 DIFF.=*22626.88329

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

5.28592 1.81659

FOR ITERATION 1 IN STEP 3

SS(3)= 46094.59037 SS(.00001)= 40706.08200 DIFF.= -5388.50836

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

5.61053 1.79231

FOR ITERATION 1 IN STEP 4

SS(4)= 40706.08200 SS(.00000)= 40566.69307 DIFF.= -139.38893

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

5.63682 1.79131
FOR ITERATION 1 IN STEP 5
SS(5) = 40566.69307 SS(.00000) = 40566.68728 DIFF. = -.00579

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

5.63739 1.79128
NONLINEAR REGRESSION

UNEXPLAINED VARIATION = 40566.68728 S. E. OF ESTIMATE = 26.44666

THE FINAL PARAMETER ESTIMATES ARE:

5.63740 1.79128

ACTUAL VS PREDICTED RESULTS

ACTUAL	PREDICTED	RESIDUAL
.370000000E+03	.377874330E+03	-.787433047E+01
.345000000E+03	.340550143E+03	.444985723E+01
.338000000E+03	.332557324E+03	.544267574E+01
.324000000E+03	.325253863E+03	-.125386349E+01
.335000000E+03	.324043589E+03	.109564108E+02
.330000000E+03	.324043589E+03	.595641078E+01
.315000000E+03	.281240066E+03	.337599345E+02
.314000000E+03	.280105160E+03	.338948401E+02
.318000000E+03	.284086194E+03	.339138058E+02
.320000000E+03	.282376998E+03	.376230022E+02
.303000000E+03	.276712613E+03	.262813873E+02
.316000000E+03	.281808278E+03	.341917216E+02
.102000000E+04	.105143149E+04	-.314314937E+02
.106000000E+04	.106673475E+04	-.673474665E+01
.107000000E+04	.108625896E+04	-.162589552E+02
.105500000E+04	.106571149E+04	-.107114916E+02
.105800000E+04	.105244867E+04	.555132918E+01
.103000000E+04	.108419641E+04	-.541964110E+02
.107500000E+04	.108316579E+04	-.816578837E+01
.118000000E+04	.110178320E+04	.162168009E+02
.104200000E+04	.106571149E+04	-.237114916E+02
.109600000E+04	.109970768E+04	-.370767857E+01
.105000000E+04	.107185753E+04	-.218575277E+02
.101800000E+04	.106162281E+04	-.436228099E+02
.320000000E+03	.312645533E+03	.735446742E+01
.319000000E+03	.315627536E+03	.337246398E+01
.341000000E+03	.313240933E+03	.277590672E+02
.345000000E+03	.316225437E+03	.287745631E+02
.352000000E+03	.323439200E+03	.285608004E+02
.358000000E+03	.318622037E+03	.393779629E+02
.350000000E+03	.333781529E+03	.162184711E+02
.332000000E+03	.328288265E+03	.371173495E+01
.351000000E+03	.324043589E+03	.269564108E+02
.343000000E+03	.330724744E+03	.122752559E+02
.335000000E+03	.318022138E+03	.169778623E+02
.328000000E+03	.320424731E+03	.757526913E+01
.692000000E+03	.705338954E+03	-.133389538E+02
.676000000E+03	.703634789E+03	-.276347892E+02
.670000000E+03	.696836349E+03	-.268363489E+02
.656000000E+03	.695141296E+03	-.391412960E+02
.668000000E+03	.703634789E+03	-.356347892E+02
.688000000E+03	.707898614E+03	-.198986144E+02
.696000000E+03	.712173815E+03	-.161738147E+02
.684000000E+03	.725930803E+03	-.419308031E+02

.722000000E+03	.734587914E+03	-.125879144E+02
.676000000E+03	.711317865E+03	-.353178650E+02
.698000000E+03	.725930803E+03	-.279308031E+02
.702000000E+03	.717319059E+03	-.153190588E+02
.137200000E+04	.134509402E+04	.269059767E+02
.140000000E+04	.135328972E+04	.367102808E+02
.138000000E+04	.135531581E+04	.246841866E+02
.139600000E+04	.135417837E+04	.418216289E+02
.135000000E+04	.135190475E+04	-.190475204E+01
.130600000E+04	.134509402E+04	-.390940233E+02
.136400000E+04	.136899801E+04	-.499801345E+01
.140000000E+04	.138618608E+04	.138139223E+02
.141800000E+04	.140115898E+04	.168410216E+02
.144100000E+04	.141852364E+04	.224763597E+02
.142800000E+04	.136785551E+04	.601444883E+02
.139600000E+04	.137357223E+04	.224277667E+02

Figure B-2. Example 2: Effect of Catalysts on Compressive Strength

```

..
MINV      UPDATED
TPRD      UPDATED
GMPRD     UPDATED
DCPY      UPDATED
LOC       UPDATED
COPYL DONE
..TT,DATA1.
ENTER FORMAT FOR READING IN OBSERVATIONS AND FTM FOR
READING PARAMETER VALUES
      (4(IX,E16.7))
(6F10.5)
DO YOU WISH ESTIMATED DERIVATIVES? ANS. YES OR NO NO
ENTER NO. OF PARAMETERS, NO. OF DBVS., NO. OF INDEP. VARIABLES,
AND THE NO. 1 IF ALL STEPS ARE PRINTED, OTHERWISE ENTER 0.
FORMAT FOR THIS INPUT IS 514
      6  94  3  0
ENTER ACCURACY NEEDED,USE FORMAT(F8.6)
      .00001
DO YOU WISH DATA INPUT FROM A FILE? ANS. YES OR NO Y
ENTER INITIAL VALUES OF PARAMETERS, USE DATA FTM
.4654      -609.0      160.0      21.92      328.0      1541.0
DO YOU WISH A STEP BY STEP SUMMARY? ANS. YES OR NO Y

```

EXAMPLE 3. DETERMINATION OF PROFILE MILLING CONDITIONS

NONLINEAR ESTIMATION

THE INITIAL PARAMETER MATRIX IS

```

.46540      -609.00000      160.00000      21.92000      328.00000
1541.00000

```

FOR ITERATION 1 IN STEP 1

```

SS( 1)= 55.41880 SS( .00100)= 24.57886 DIFF.= -30.83994

```

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

```

.509252634E+00      -.305162307E+03      .612730312E+03      .376334939E+03
.724580285E+03      -.433019881E+03

```

FOR ITERATION 1 IN STEP 2

```

SS( 2)= 24.57886 SS( .00010)= 14.82551 DIFF.= -9.75335

```

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

```

.514814637E+00      -.368929366E+03      .202893680E+03      .878561159E+03
.769415336E+03      -.494087493E+03

```

FOR ITERATION 1 IN STEP 3

```

SS( 3)= 14.82551 SS( .00001)= 14.80047 DIFF.= -.02504

```

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

```

.534297348E+00      -.299395520E+03      .174263122E+03      .718695354E+03
.648063445E+03      -.423887882E+03

```

FOR ITERATION 1 IN STEP 4

```

SS( 4)= 14.80047 SS( .00000)= 14.78992 DIFF.= -.01055

```


THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

.532862557E+00 -.311116978E+03 .176265448E+03 .763601681E+03
 .666934018E+03 -.453830102E+03

FOR ITERATION 1 IN STEP 5

SS(5)= 14.78992 SS(.00000)= 14.78991 DIFF.= -.00001

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

.533344118E+00 -.309737342E+03 .175718931E+03 .758823801E+03
 .664141666E+03 -.450409781E+03

FOR ITERATION 1 IN STEP 6

SS(6)= 14.78991 SS(.00000)= 14.78991 DIFF.= -.00000

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

.533327596E+00 -.309828204E+03 .175684104E+03 .759514789E+03
 .664297762E+03 -.451001609E+03

FOR ITERATION 1 IN STEP 7

SS(7)= 14.78991 SS(.00000)= 14.78991 DIFF.= -.00000

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

.533334490E+00 -.309807019E+03 .175675796E+03 .759443246E+03
 .664255589E+03 -.450951451E+03

FOR ITERATION 1 IN STEP 8

SS(8)= 14.78991 SS(.00000)= 14.78991 DIFF.= -.00000

THE PARAMETER MATRIX FOR THE NEXT ITERATION IS

.533334223E+00 -.309808365E+03 .175675333E+03 .759453185E+03
 .664257922E+03 -.450959923E+03

NONLINEAR REGRESSION

UNEXPLAINED VARIATION= 14.78991 S. E. OF ESTIMATE= .40996

THE FINAL PARAMETER ESTIMATES ARE:

.533334320E+00 -.309808061E+03 .175675219E+03 .759452131E+03
 .664257320E+03 -.450959177E+03

ACTUAL VS PREDICTED RESULTS

ACTUAL	PREDICTED	RESIDUAL
.312500000E+00	.687083911E-03	.311812916E+00
.587500000E+00	.246673138E+00	.340826862E+00
.500000000E+00	.284991234E+00	.215008766E+00
.125000000E+01	.522084822E+00	.727915178E+00
.953125000E+00	.763968239E+00	.189156761E+00

.906250000E+00	.101543110E+01	-.109181099E+00
.103125000E+01	.731335588E+00	.299914412E+00
.543750000E+00	.626367451E+00	-.826174508E-01
-.362500000E+00	-.212125356E+00	-.150374644E+00
.543750000E+00	.596960528E+00	-.532105282E-01
.450000000E+00	.776181546E+00	-.326181546E+00
.906250000E+00	.100094242E+01	-.946924207E-01
.118750000E+01	.110911713E+01	.783828697E-01
.168750000E+01	.123084130E+01	.456658699E+00
.156250000E+01	.134014892E+01	.222351079E+00
.162500000E+01	.165880669E+01	-.338066854E-01
.268750000E+00	.693471576E-01	.199402842E+00
.137500000E+01	.184277593E+01	-.467775930E+00
.234375000E+01	.242098209E+01	-.772320946E-01
.906250000E+00	.422630049E+00	.483619951E+00
.112500000E+01	.189751203E+00	.935248797E+00
.875000000E+00	.178664990E+00	.696335010E+00
-.275000000E+00	.696256924E-01	-.344625692E+00
.225000000E+01	.290355080E+00	.195964492E+01
.162500000E+01	.109469389E+00	.151553061E+01
-.437500000E-01	-.177020522E+00	.133270522E+00
-.937500000E-01	-.168072639E+00	.743226394E-01
-.937500000E-01	-.171938606E+00	.781886057E-01
.437500000E-01	-.169690418E+00	.213440418E+00
.875000000E-01	-.183648683E+00	.271148683E+00
-.362500000E+00	-.217001966E+00	-.145498034E+00
-.453125000E+00	-.220651846E+00	-.232473154E+00
-.656250000E+00	-.419721463E+00	-.236528537E+00
-.875000000E-01	-.108380333E+00	.208803326E-01
.875000000E-01	.146148669E+00	-.586486685E-01
.875000000E-01	.692073590E-01	.182926410E-01
.718750000E+00	.454236075E+00	.264513925E+00
.718750000E+00	.430074607E+00	.288675393E+00
.125000000E+00	.344737405E-01	.905262595E-01
.218750000E+00	.167127671E+00	.516223291E-01
.453125000E+00	.608499463E+00	-.155374463E+00
-.106250000E+01	-.100746929E+00	-.961753071E+00
-.187500000E+00	-.123593699E+00	-.639063013E-01
-.156250000E+00	-.753128151E-01	-.809371849E-01
-.125000000E+00	-.106072448E+00	-.189275522E-01
-.312500000E+00	-.285250312E+00	-.272496881E-01
-.231250000E+00	-.189436770E+00	-.418132298E-01
-.468750000E+00	-.301162504E+00	-.167587496E+00
-.268750000E+00	-.505955943E+00	.237205943E+00
-.234375000E+00	-.116003043E+00	-.118371957E+00
-.187500000E+00	-.874234391E-01	-.100076561E+00
-.187500000E+00	-.173204974E+00	-.142950256E-01
.562500000E+00	.524506204E+00	.379937965E-01
.312500000E+00	.573384112E+00	-.260884112E+00
.362500000E+00	.767364573E+00	-.404864573E+00
.450000000E+00	.913265645E+00	-.463265645E+00
.109375000E+01	.597043255E+00	.496706745E+00
.593750000E+00	.548333349E+00	.454166511E-01
-.312500000E+00	-.170569012E+00	-.141930988E+00
-.281250000E+00	-.936377223E-01	-.187612278E+00
.687500000E+00	.878922741E+00	-.191422741E+00
.937500000E+00	.107334315E+01	-.135843151E+00
.500000000E-01	.200423035E+00	-.150423035E+00
.750000000E-01	.200423035E+00	-.125423035E+00
.131250000E+00	.398145555E+00	-.266895555E+00
.350000000E+00	.864336311E+00	-.514336311E+00
-.125000000E+00	-.494622351E+00	.369622351E+00
-.587500000E+00	-.247446796E+00	-.340053204E+00
-.500000000E+00	-.285885072E+00	-.214114928E+00
-.125000000E+01	-.523722272E+00	-.726277728E+00
-.953125000E+00	-.766364325E+00	-.186760675E+00

-.906250000E+00	-.101861587E+01	.112365865E+00
-.103125000E+01	-.733629326E+00	-.297620674E+00
-.543750000E+00	-.628331970E+00	.845819703E-01
-.543750000E+00	-.598832817E+00	.550828168E-01
-.450000000E+00	-.778615937E+00	.328615937E+00
-.906250000E+00	-.100408175E+01	.978317456E-01
-.118750000E+01	-.111259573E+01	-.749042690E-01
-.168750000E+01	-.123470167E+01	-.452798327E+00
-.156250000E+01	-.134435212E+01	-.218147878E+00
-.162500000E+01	-.166400932E+01	.390093155E-01
-.234375000E+01	-.242857519E+01	.848251881E-01
-.718750000E+00	-.456890385E+00	-.261859615E+00
-.718750000E+00	-.432587731E+00	-.286162269E+00
-.312500000E+00	-.575182456E+00	.262682456E+00
-.362500000E+00	-.769771311E+00	.407271311E+00
-.450000000E+00	-.916129983E+00	.466129983E+00
-.109375000E+01	-.598915803E+00	-.494834197E+00
-.593750000E+00	-.550053125E+00	-.436968753E-01
-.687500000E+00	-.881679367E+00	.194179367E+00
-.500000000E-01	-.203795953E+00	.153795953E+00
-.750000000E-01	-.203795953E+00	.128795953E+00
-.131250000E+00	-.403878176E+00	.272628176E+00
-.350000000E+00	-.876781290E+00	.526781290E+00

$$Y = 2wf^{0.4667} (-309.81 + 175.68X + 759.45X^2 + 664.25X^3 - 450.96X^4)$$

STANDARD ERROR OF ESTIMATE = 0.40996

Figure B-3. Example 3: Determination of Profile Milling Conditions: $X = -1$

$$Y = 2wf^{0.4667} (-309.81 + 175.68X + 759.45X^2 + 664.26X^3 - 450.96X^4)$$

STANDARD ERROR OF ESTIMATE = 0.40996

$X = +1$

$X = d/D$

$C = 2wf$

$B = f^{-1}$

Figure B-4. Example 4: Determination of Profile Milling Conditions: $X = +1$

Appendix C

PRINTOUT OF COMPUTER PROGRAM NONLIN

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WAS INTENTIONALLY
LEFT BLANK

```

$$$$$$$$$  $$$$$$  $$  $$  $$  $$$$$$$$$$  $$  $$  $$
  $$  $$  $$  $$$$  $$  $$  $$  $$$$  $$  $$  $$
  $$  $$  $$  $$  $$  $$  $$  $$  $$$$  $$  $$  $$
  $$  $$$$$$  $$  $$  $$  $$  $$$$$$  $$  $$  $$$$$$$$$$
  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$
  $$  $$  $$$$  $$$$$$$$$$  $$  $$  $$  $$$$$$$$$$  $$  $$
  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$  $$
  $$  $$  $$  $$  $$  $$  $$$$  $$  $$  $$  $$  $$
  $$$$$$$$$$  $$$$$$  $$  $$  $$  $$$$$$$$$$  $$  $$  $$
PROGRAM NONLIN(TAPE2,INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT) 000100
DIMENSION DELTA1(15),DELTA(15),Y(200),Z(3000),A(225) 000110
1,A0(225),CW(225),G(15),WX(200),SZ(225),CLW(15),L1(15), 000120
IM1(15),FTM(18),FV(200),TP(15),FTM1(18) 000130
COMMON XT(200,15),PRAM(15) 000135
DATA CONST/.01/,NU,NCOUNT/10,0/,GR0/.7853981634/,IA/2HNO/ 000140
317 WRITE(6,200) 000150
200 FORMAT(1X,*ENTER FORMAT FOR READING IN OBSERVATIONS AND FTM FOR*/ 000160
1,* READING PARAMETER VALUES*/ ) 000170
13 FORMAT(4(2X,E16.9)) 000180
READ(5,2) FTM 000190
READ(5,2) FTM1 000200
WRITE(6,1106) 000210
1106 FORMAT(1X,*DO YOU WISH ESTIMATED DERIVATIVES\ ANS. YES OR NO *) 000220
READ(5,6) IAS 000230
IF(IAS.EQ.IA) GO TO 888 000240
WRITE(6,438) 000242
438 FORMAT(1X,*DO YOU WISH TO INPUT ACCURACT FOR THE ESTIMATE\*/ 000244
1* ANSWER YES OR NO* ) 000245
READ(5,6) IA1 000250
IF(IA1.EQ.IA) GO TO 887 000260
WRITE(6,890) 000270
READ(5,23) H 000280
GO TO 888 000290
887 H=1.0E-05 000300
890 FORMAT(1X,*ENTER DELTA VALUE, FTM IS F8.6*) 000310
2 FORMAT(18A4) 000320
888 WRITE(6,201) 000330
889 FORMAT(1X,*DO YOU WISH TO INPUT THE DELTA VALUE FOR ESTIMATING THE 000340
1 DERIVATIVE\ ANS. YES OR NO. *) 000350
201 FORMAT(1X,*ENTER NO. OF PARAMETERS, NO. OF OBVS., NO. OF INDEP. VA 000360
1RIABLES,*/ AND THE NO. 1 IF ALL STEPS ARE PRINTED, OTHERWISE ENTE 000370
2R 0.*/ * FORMAT FOR THIS INPUT IS 514*/ ) 000380
READ(5,3) NP,N0,NK,NM 000390
WRITE(6,133) 000400
133 FORMAT(1X,*ENTER ACCURACY NEEDED,USE FORMAT(F8.6)*,/) 000410
READ(5,23) ESP 000420
23 FORMAT(F8.6) 000430
3 FORMAT(8I4) 000440
WRITE(6,33) 000450
READ(5,6) IIA 000460
IF(IIA.EQ.IA) GO TO 1200 000470
DO 436 J=1,N0 000472
436 READ(2,FTM)(XT(J,I),I=1,NK),Y(J) 000480
GO TO 101 000490
33 FORMAT(1X,*DO YOU WISH DATA INPUT FROM A FILE\ ANS. YES OR NO *) 000500
6 FORMAT(1A2) 000510
1200 WRITE(6,202) 000520
202 FORMAT(1X,*ENTER VALUE OF INDEP. VAR. ROW-WISF. VALUES OF DEP.VAR. 000530
1,*/ ) 000540
DO 478 J=1,N0 000545
478 READ(5,FTM)(XT(J,I),I=1,NK),Y(J) 000550
101 IF(NCOUNT.NE.0) NCOUNT=0 000560
1201 WRITE(6,102) 000570
READ(5,FTM1)(PRAM(I),I=1,NP) 000580

```


102	FORMAT(1X,*ENTER INITIAL VALUES OF PARAMETERS*/)	000590
	NT=NP*NO	000600
	NST=NP*NP	000610
	SS1=0.0	000620
	WRITE(6,312)	000630
312	FORMAT(1X,*DO YOU WISH A STEP BY STEP SUMMARY\ ANS. YES OR NO*)	000640
	READ(5,6) I2A	000650
	WRITE(6,65)	000660
	WRITE(6,1000) (PRAM(I),I=1,NP)	000670
65	FORMAT(1H=,27X,*NONLINEAR ESTIMATION*/)	000680
660	FORMAT(1H=)	000690
30	NCOUNT=NCOUNT+1	000700
	ID=NC=0	000710
	CONST=CONST/NU	000720
	IF(CONST.LT.1.0E-8) CONST=CONST*NU	000730
	CALCULATE MATRIX OF PARTIAL DERIVATIVES	000732
	DO 10 I=1,NP	000740
	DO 10 J=1,NO	000750
	NC=NC+1	000760
	IF(IAS.EQ.1A) GO TO 1108	000770
	CALL DIFFA(I,J,H,TEM)	000780
	GO TO 1109	000790
1108	CALL DIFF1(I,J,TEM)	000800
1109	Z(NC)=TEM	000810
	L=LEGVAR(Z(NC))	000820
	IF(L)32,10,32	000830
10	CONTINUE	000840
	IF(NM.EQ.0) GO TO 300	000850
	WRITE(6,57) NCOUNT	000860
	KK=1	000870
	KK1=NO	000880
	DO 500 I=1,NP	000890
	WRITE(6,13) (Z(J),J=KK,KK1)	000900
	KK=KK1+1	000910
	WRITE(6,11)	000920
11	FORMAT(1H())	000930
500	KK1=KK1+NO	000940
	CALCULATE SCALED A-MATRIX AND SCALED GRADIENT VECTOR	000942
300	CALL TPRD(Z,Z,SZ,NO,NP,0,0,NP)	000950
	CALL DCPY(SZ,C1W,NP,0)	000960
	DO 1100 I=1,NP	000970
	J=LEGVAR(C1W(I))	000980
	IF(J)32,1100,32	000990
1100	CONTINUE	001000
1101	NC=0	001010
	DO 12 I=1,NP	001020
	DO 12 J=1,NP	001030
	NC=NC+1	001040
	CW(NC)=0.0	001050
	IF(I.EQ.J) CW(NC)=1.0/SQRT(C1W(I))	001060
	J1=LEGVAR(CW(NC))	001062
	IF(J1)32,12,32	001064
12	CONTINUE	001070
	CALL TPRD(CW,SZ,AO,NP,NP,0,0,NP)	001080
	DO 1900 KI=1,NST	001082
	J1=LEGVAR(AO(KI))	001084
	IF(J1)32,1900,32	001086
1900	CONTINUE	001088
	CALL GMPRD(AO,CW,A,NP,NP,NP)	001090
	DO 1901 KI=1,NST	001092
	J1=LEGVAR(A(KI))	001094
	IF(J1)32,1901,32	001096
1901	CONTINUE	001098
	CALCULATE RESIDUAL SUM OF SQUARES	001099
20	SS=0.0	001100
316	FORMAT(1X,*ANOTHER PROBLEM\ ANS. YES OR NO *)	001110

DO 14 I=1,NO	001120
CALL EF(I,F)	001130
WX(I)=Y(I)-F	001140
FV(I)=F	001150
14 SS=SS+WX(I)*WX(I)	001160
55 FORMAT(7(2X,E16.7))	001163
IF(ID.NE.0) GO TO 22	001170
SS1=SS	001180
CALL TPRD(Z,WX,G,NO,NP,0,0,1)	001190
DO 15 I=1,NP	001200
G(I)=G(I)/SQRT(C1W(I))	001210
JJ=LEGVAR(G(I))	001212
IF(JJ)32,15,32	001214
15 CONTINUE	001216
26 ID=ID+1	001220
CONST=CONST*NU	001230
IF(ID.EQ.1) CONST=CONST/NU	001240
NC=0	001250
DG=GV=D=0.0	001260
DO 16 I=1,NP	001270
DO 16 J=1,NP	001280
NC=NC+1	001290
AO(NC)=A(NC)	001300
IF(I.EQ.J) AO(NC)=A(NC)+CONST	001310
16 CONTINUE	001320
CALCULATE CORRECTION VECTOR	001322
CALL MINV(AO,NP,DM,L1,M1)	001330
IF(DM)333,32,333	001335
333 CALL GMPD(AO,G,DELTA1,NP,NP,1)	001340
DO 1903 KI=1,NP	001342
JJ=LEGVAR(DELTA1(KI))	001344
IF(JJ)32,1903,32	001346
1903 CONTINUE	001348
DO 18 I=1,NP	001350
DELTA(I)=DELTA1(I)/SQRT(C1W(I))	001360
JJ=LEGVAR(DELTA(I))	001362
IF(JJ)32,189,32	001364
189 DG=DELTA1(I)*G(I)+DG	001370
D=DELTA1(I)*DELTA1(I)+D	001380
GV=G(I)*G(I)+GV	001390
J1=LEGVAR(DG)	001392
J2=LEGVAR(D)	001393
J3=LEGVAR(GV)	001394
IF((J1.OR.J2.OR.J3).NE.0) GO TO 32	001395
18 CONTINUE	001400
SIG=DG/(SQRT(GV)*SQRT(D))	001410
GAMR=ACOS(SIG)	001420
TK=1	001430
LK=0	001440
GO TO 44	001450
HALVING ROUTINE FOR CUTTING STEP SIZE	001452
35 TK=TK/2.0	001460
LK=LK+1	001470
DO 97 I=1,NP	001480
DELTA(I)=DELTA(I)*TK	001490
97 PRAM(I)=TP(I)+DELTA(I)	001500
GO TO 80	001510
CALCULATE NEW PARAMETER VECTOR	001512
44 DO 96 I=1,NP	001520
IF(ID.EQ.1) TP(I)=PRAM(I)	001530
96 PRAM(I)=PRAM(I)+TK*DELTA(I)	001540
80 CONTINUE	001550
GO TO 20	001560
TEST FOR CONVERGENCE	001562
22 DIFF=SS-SS1	001570
IF(NM.EQ.0) GO TO 27	001590

WRITE(6,60) ID,NCOUNT,NCOUNT,SS1,CONST,SS,DIFF	001600
27 IF (DIFF)28,28,24	001610
24 IF (((GAMR-GRO).LT.0.0).AND.(DIFF.GT.0.0)) GO TO 35	001620
GO TO 26	001630
28 DO 93 I=1,NP	001680
TRY=ABS(DELTA(I))/(.001+ABS(PRAM(I)))	001690
IF (TRY.GT.ESP) GO TO 3011	001700
93 CONTINUE	001710
GO TO 344	001712
3011 IF (GAMR.LE.1.57079633.OR.CONST.LE.1.0) GO TO 301	001715
WRITE(6,993)	001716
GO TO 34	001717
344 IF (LK.NE.0)WRITE(6,103)	001720
103 FORMAT(1X,*CONVERGENCE BY ALTERNATE TEST - SUCCESSIVE HALVING*/)	001730
GO TO 34	001740
301 IF (NM.EQ.1) GO TO 501	001750
IF (I2A.EQ.1A) GO TO 313	001760
WRITE(6,60) ID,NCOUNT,NCOUNT,SS1,CONST,SS,DIFF	001770
WRITE(6,61)	001780
WRITE(6,13) (PRAM(I),I=1,NP)	001790
501 CONTINUE	001800
313 IF (NCOUNT.LE.500) GO TO 994	001810
WRITE(6,64)	001820
GO TO 991	001830
994 GO TO 30	001840
32 WRITE(6,203)	001850
203 FORMAT(1H\$,1X,*THE ITERATIONS TAKE A DIVERGENT PATH FOR THE*/1X,	001860
1*INITIAL VALUES. IF OTHER STARTING VALUES ARE TRIED ENTER 1,*/	001870
1*OTHERWISE ENTER 0.*/)	001880
READ(5,104) LL	001890
IF (LL.EQ.1) CONST=.01	001892
IF (LL.EQ.1) GO TO 101	001900
104 FORMAT(11)	001910
WRITE(6,60) ID,NCOUNT,NCOUNT,SS1,CONST,SS,DIFF	001920
GO TO 46	001930
34 SE=SS/(NO-NP)	001940
SE=SQRT(SE)	001950
WRITE(6,89)	001960
WRITE(6,82) SS,SE	001970
WRITE(6,62)	001980
WRITE(6,13) (PRAM(I),I=1,NP)	001990
WRITE(6,63)	002000
DO 84 I=1,NO	002010
84 WRITE(6,83) Y(I),FV(I),WX(I)	002020
46 WRITE(6,75)	002030
WRITE(6,316)	002040
READ(5,6) I4A	002050
IF (I4A.NE.1A) GO TO 317	002060
60 FORMAT(1H),2X,* FOR ITERATION *,I2,* IN STEP *,I2/	002070
12X,*SS(*,I2,*)=*,F12.5,2X,*SS(*,F10.5,*)=*,F12.5,2X,*DIFF.=*,F12.5	002080
1/,F12.5/)	002090
61 FORMAT(1H),2X,*THE PARAMETER MATRIX FOR THE NEXT ITERATION IS*/)	002100
1000 FORMAT(1H),2X,*THE INITIAL PARAMETER MATRIX IS*/5(2X,F12.5))	002110
89 FORMAT(1H=,25X,*NONLINEAR REGRESSION*/)	002120
82 FORMAT(5X,*UNEXPLAINED VARIATION=*F12.5,2X,*S. E. OF ESTIMATE=*,	002130
1F10.5//)	002140
62 FORMAT(2X,*THE FINAL PARAMETER ESTIMATES ARE:*/)	002150
64 FORMAT(1H),1X,*CONVERGENCE DOESN'T OCCUR IN THE NO. OF ITERATIONS	002160
1 ALLOWED*/)	002170
993 FORMAT(1H),*CONVERGENCE BY GAMMA LAMBDA TEST*/)	002180
63 FORMAT(1H\$,22X,*ACTUAL VS PREDICTED RESULTS*/	002190
18X,*ACTUAL*,12X,*PREDICTED*,12X,*RESIDUAL*/)	002200
83 FORMAT(3X,E16.9,4X,E16.9,3X,E16.9)	002210
991 STOP	002220
57 FORMAT(1H\$,2X,*FOR STEP *,I2,* THE Z"-MATRIX IS AS FOLLOWS*/)	002230
75 FORMAT(1H=)	002240

END	002250
SUBROUTINE MINV	002260
RETURN	002270
END	002280
SUBROUTINE TPRD	002290
RETURN	002300
END	002310
SUBROUTINE GMPRD	002320
RETURN	002330
END	002340
SUBROUTINE DCPY	002350
RETURN	002360
END	002370
SUBROUTINE LOC	002380
RETURN	002390
END	002400
SUBROUTINE DIFFA(I,J,H,TEM)	002410
COMMON XT(200,15),PRAM(15)	002415
TB=PRAM(I)	002420
CALL EF(J,F)	002430
T1=F	002440
PRAM(I)=PRAM(I)+H*PRAM(I)	002450
CALL EF(J,F)	002460
T2=F	002470
PRAM(I)=PRAM(I)-TB	002480
CALL EF(J,F)	002490
TEM=(T2-T1)/PRAM(I)	002500
PRAM(I)=TB	002510
RETURN	002520
END	002530
SUBROUTINE DIFF1(I,J,TEM)	002540
COMMON XT(200,15),PRAM(15)	002550
TEM1=(119.0-XT(J,1))*PRAM(4)	002560
TEM2=(151.0-XT(J,1))*PRAM(6)	002562
GO TO (1,2,3,4,5,6)I	002580
1 TEM=1.0	002590
GO TO 500	002610
2 TEM=XT(J,1)	002620
GO TO 500	002630
3 TEM=EXP(-1.0*TEM1**2)	002640
GO TO 500	002650
4 TEM=-2.0*PRAM(3)*EXP(-1.0*TEM1**2)*TEM1*(119.0-XT(J,1))	002660
GO TO 500	002662
5 TEM=EXP(-1.0*TEM2**2)	002663
GO TO 500	002664
6 TEM=-2.0*(151.0-XT(J,1))*PRAM(5)*EXP(-1.0*TEM2**2)*TEM2	002665
55 FORMAT(7(2X,E16.7))	002667
500 RETURN	002710
END	002720
SUBROUTINE EF(I,F)	002730
COMMON XT(200,15),PRAM(15)	002740
TEM1=(119.0-XT(I,1))*PRAM(4)	002750
TEM2=(151.0-XT(I,1))*PRAM(6)	002752
F=PRAM(1)+PRAM(2)*XT(I,1)+PRAM(3)*EXP(-1.0*TEM1**2)	002760
1+PRAM(5)*EXP(-1.0*TEM2**2)	002761
55 FORMAT(7(2X,E16.7))	002763
RETURN	002780
END	002790