DANIEL F. MERRIAM, Editor

FORTRAN IV PROGRAM FOR NONLINEAR ESTIMATION

By

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FORTRAN IV Program For Nonlinear Estimation

by

Richard B. McCammon

ABSTRACT

NONLIN is a FORTRAN IV computer program for estimating parameters in algebraic nonlinear simultaneous equations. The program is designed for problems in which the number of observations equals or exceeds the number of parameters to be estimated. Starting from initial estimates, a modified Gauss-Newton procedure is used to obtain an improved set of parameter values. The process is continued until a set of best estimates has been obtained. A number of options in the program offer wide flexibility in handling a variety of nonlinear problems. Numerical examples are given for dissecting a bimodal distribution into normal components and estimating the porosity in vuggy carbonates.

INTRODUCTION

Discrete linear methods have attained a foremost position in the numerical processing of geologic data. The reasons for this are clear: simplicity and ease of computation. In developing mathematical models that describe geologic processes, linear models are the first that come to mind. For the linear model, the nature and properties of the solution are well known. With advent of computers, the algorithms have been made highly efficient and require small amounts of computer time.

In many instances, however, the linear model is inadequate in describing a particular process (James, 1967). Consider, for example, the growth in numbers of a population described by the logistic function

\[ N = \frac{k}{1 + e^{-\left(\frac{x - \mu_1}{\sigma_1} + \frac{x - \mu_2}{\sigma_2}\right)}} \]

where \( N \) is the number of individuals in the population at time \( t \), and \( \alpha, k, \mu_1, \mu_2, \sigma_1, \text{ and } \sigma_2 \) are parameters of the population. Clearly, no transformation will make \( \alpha, k, \mu_1, \text{ and } \mu_2 \) linear with respect to \( N \) and \( t \) simultaneously. Or consider a mixture of two normally distributed populations where the problem is to estimate the parameters in each population. The equation for such a mixture is

\[ f(x) = \frac{\alpha}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x - \mu_1)^2}{2\sigma_1^2}} + \frac{(1 - \alpha)}{\sqrt{2\pi}\sigma_2} e^{-\frac{(x - \mu_2)^2}{2\sigma_2^2}} \]

where \( x \) is the variable of interest, \( \mu_1, \mu_2, \sigma_1, \text{ and } \sigma_2 \) are the respective means and standard deviations of the two populations, and \( \alpha \) is a degree of mixing. The variable might represent particle size of a sediment, for instance, which would describe the mixing of two different modes of transport. The problem would be to identify and determine the textural characteristics of each mode given the observed particle size frequency distribution.

In both examples, the parameters enter into the equations in a nonlinear fashion. It may be possible by a suitable transformation to transform a nonlinear equation into one which is linear. For instance, the logarithm

\[ y = ax^n \]

becomes

\[ \log y = \log a + n \log x \]

where \( \log a \) and \( n \) are linear in terms of \( \log y \) and \( \log x \). In the two examples, however, no single transformation will convert each function into a linear form, and hence, such functions are considered to be intrinsically nonlinear (Draper and Smith, 1967, p. 132). Clearly, special methods are needed to solve these types of equations.

The algorithm described here is designed for nonlinear equations. It is intended for use where the number of observations exceeds or is equal to the number of parameters. The algorithm provides the best local estimates of the parameters with respect to the given estimates. For this reason, the initial estimates or what are called starting values assume considerable importance in the solution to most nonlinear type problems. In this respect, nonlinear methods differ markedly from linear techniques which are independent of initial values.

Acknowledgments - The program was written during my employment with Gulf Research and Development Company. I wish to thank Chester Pelto whose early version of the program led to the development of this program and Dr. Thomas Elkins for suggesting the application of nonlinear estimation to the dissection of bimodal distributions.

MATHEMATICAL DEVELOPMENT
Consider that we have a function of the form
\[ y = f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_p) \]  
and that we wish to estimate the values of the parameters \( \theta_1, \ldots, \theta_p \) given a set of observations on \( y \) and \( \{x_1, \ldots, x_k\} \). \( y \) is considered to be the dependent variable and the set of \( x_i \)'s the independent variables. Let us assume that one or more of the \( \theta_i \)'s are nonlinear with respect to \( y \).

We start by considering a set of values \( \{\theta_1^0, \ldots, \theta_p^0\} \) which are sufficiently close to the true values of the parameters \( \{\theta_1, \ldots, \theta_p\} \). As a first approximation to \( y \), we expand (1) into a Taylor's series about the values \( \theta_1^0, \ldots, \theta_p^0 \) and retain only the terms up to the first partial derivatives. Thus,
\[
y = f(x_1, \ldots, x_k; \theta_1^0, \ldots, \theta_p^0) + \sum_{i=1}^{p} \left[ \frac{\partial f}{\partial \theta_i} \right]_i (\theta_i - \theta_i^0). \tag{2}\]

If we convert this to an equality, we have a linear expression in \( \Delta \theta_i = (\theta_i - \theta_i^0) \) with respect to \( y \). If there are at least \( p \) observations on \( y \) with the corresponding values for \( \{x_1, \ldots, x_k\} \), we can express (2) as a set of simultaneous linear equations
\[
y_i = f_i(x_1, \ldots, x_k; \theta_1^0, \ldots, \theta_p^0) = \sum_{i=1}^{p} \left[ \frac{\partial f_i}{\partial \theta_i} \right]_i \theta_i = \theta_i^0 \Delta \theta_i \quad i = 1, \ldots, n \tag{3}\]
where \( n \) is the number of observations.

We first consider the situation where \( n = p \). We have a set of exact simultaneous linear equations which we can solve for the \( \Delta \theta_i \)'s. If we define the following row vectors
\[
f^i = \{ (y_1 - f_1), \ldots, (y_n - f_n) \} \quad \text{and} \quad (\theta - \theta^0)^i = \{ (\theta_1 - \theta_1^0), \ldots, (\theta_p - \theta_p^0) \} \]
and the matrix \( D = [d_{ij}] = \left\{ \left[ \frac{\partial f_i}{\partial \theta_j} \right]_{i,j} \theta_j = \theta_j^0 \right\} \) we can write as the solution for (3)
\[
\theta = \theta^0 + D^{-1}f \tag{4}\]
where \( D^{-1} \) is the inverse of \( D \). The expression in (4) gives a set of values which are, as a rule, closer to the true values of the unknown parameters than the initial values. We now repeat the process replacing the initial estimates with the improved set of values.

If we continue the process, we can write for the \( k \)'th step
\[
\theta^k = \theta^{k-1} + D_{k-1}^{-1}f_{k-1}. \tag{5}\]

It is assumed that after a finite number of steps \( \theta^k \) will converge to \( \theta \) which represents the vector bearing the true parameter values. Only in a few limited instances, however, can convergence be guaranteed. Usually, it is necessary to have a fair idea of how the function behaves so that the initial estimates will approximate closely the true values. This method for finding the roots of simultaneous nonlinear equations is known as the Newton-Raphson method. A more complete description can be found in Scarborough (1966).

For \( n > p \), we no longer have a set of exact simultaneous equations; thus, we must choose a criterion for obtaining the "best" solution. The one most used is that for which \( f^i \) is a minimum for any choice of \( \theta \). This is the least-squares criterion for which the solution to the system of equations given in (3) is well known. The expression for the improved least squares estimate of \( \theta \) based on an initial estimate becomes
\[
\theta = \theta^0 + (D^iD)^{-1}D^if \tag{5}\]
using the same vectors and the same matrix as before.

For the \( k \)'th stage of the iterative process
\[
\theta^k = \theta^{k-1} + (D_{k-1}^iD_{k-1})^{-1}D_{k-1}^if_{k-1} \tag{6}\]
This is known as the Gauss-Newton method of nonlinear regression and is described more fully in Draper and Smith (1967). Again it is essential to use reasonably accurate initial estimates of the parameters.

**MODIFIED GAUSS-NEWTON PROCEDURE**

Past experience with nonlinear regression methods has shown that it is necessary to modify slightly the iterative process described in (6). The best known of these modifications is described in Draper and Smith (1967). In the program described here, however, a simpler procedure is used. This is justified on the basis that if reasonably accurate initial estimates are provided, the process converges rapidly to the local minimum value. The procedure is defined by modifying equation (6) to read
\[
\theta^k = \theta^{k-1} + \gamma(D_{k-1}^iD_{k-1})^{-1}D_{k-1}^if_{k-1} \tag{7}\]
where \( \gamma \) is a specified constant. Usually, several \( \gamma \) values rather than a single value are used where each value results in a different value for
\[
\theta^k \quad \text{for} \quad f_{k-1}^i \quad \tag{7}\]
which represents the error sum of squares for a particular estimate of \( \theta \). At each step, that change in \( \Delta \theta \) is chosen for which (7) is a minimum. From past experience, the set of \( \gamma \) values that has provided consistently improved parameter values and faster rates of convergence is \([1, 1/3, (1/3)^2, \ldots, (1/3)^n]\) where \( n \) is an arbitrary number depending on the desired accuracy of the final parameter estimates.

**PROGRAM OPERATION**

**Program Dimensions**

The program is dimensioned so that estimates are obtainable for up to 10 parameters based on a maximum of 250 observations and up to 10 independent (control) variables. These numbers are arbitrary, however, and may be made larger by increasing the dimensions for the appropriate program variables. No other changes in the program are necessary.

**Special Options**

A number of options are available which make the program highly flexible in handling a wide variety of problems. The options available to the user are as follows:

1. **Exact Versus Nonexact Equations** - If the number of observations, \( n \), equals the number of parameters, \( p \), to be estimated, use the algorithm specified in equation (4) where there are \( p \) exact simultaneous equations; if \( n \) exceeds \( p \), use the algorithm given by equation (5) of an overdetermined system of equations; in either situation, the iterations are performed until there is no further improvement in the performance criterion.

2. **Weighted Observations** - Some of the observations may receive greater weight than other observations in determining the best choice of parameter values; in such instances, separate weights are entered along with each observation and the estimation procedure is modified to give a weighted best fit.

3. **Finite difference approximation for partial derivatives** - It may not be possible to obtain closed form expressions of the partial derivatives. Therefore an option may be used in which the partial derivatives are approximated by finite difference quotients.

Thus, for the \( i^{th} \) partial derivative,

\[
\frac{\Delta f}{\Delta \theta_i} = \frac{f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_i + \delta \theta_i, \ldots, \theta_p) - f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_i, \ldots, \theta_p)}{\delta \theta_i}
\]

where \( \delta \) is a specified constant. The appropriate value for \( \delta \) depends upon the function, but reasonable value for \( \delta \) is 0.05.

4. **Test for parameter validity** - In many problems, the solution to the set of simultaneous equations during the iterative process will yield values of the parameters which are either unacceptable or for which the function cannot be evaluated. For instance, a negative value may result for a parameter which takes on only positive values in a function. To avoid this difficulty, an option is available in which the user can supply a subroutine to test any or all of the parameters. This procedure does not result in a constrained solution to a problem, it merely avoids evaluating the function for improper values of the parameters.

5. **Multiple Runs** - It may be difficult, if not impossible, to obtain reasonable initial estimates for part or all of the parameters. In such situations, it is desirable to perform a pattern search where certain parameters are held fixed while solving for the remaining ones. The search is conducted on a grid in which the values of the performance criterion are mapped for different fixed values of the parameters. In conducting a search, it is necessary, therefore, to make multiple runs. For each run, the values of the parameters held fixed are changed accordingly. The final values of the parameters to be estimated are retained from the previous run so that a more rapid convergence is obtained with the new set of values. The option allows the user to perform any number of runs using the same set of observations. A further advantage to the multiple run option is that in cases where it is thought that values corresponding to a highly local minima for the performance criterion have been found, different sets of initial estimates can be tried to see whether the process converges to a different set of values.

**ORDER OF INPUT CARDS**

1. Program control card
2. Title card
3. Parameter name card
4. Output format card
5. Data format card
   Data cards
6. Initial parameter estimate card
7. Blank card

PROGRAM USAGE

Card 1:

Columns

1-2   card number (a 1 punched in column 2)
3-8   NO = problem identification
9-12  NUM = number of observations
13-14 NP = number of parameters to be estimated
15-16 NCOL = total number of parameters
17-18 NIDV = number of independent (control) variables
19    NOPT =
       \begin{align*}
         &1 \text{ finite difference quotients used} \\
         &0 \text{ partial derivatives used}
       \end{align*}
20    ITEST =
       \begin{align*}
         &1 \text{ test parameter values for validity} \\
         &0 \text{ do not test parameter values}
       \end{align*}
21-23 NTIM = maximum number of iterations
24-25 NRD = number of proportional constants (suggested NRD = 9; NRD must not exceed 10).
26-29 FRAC = initial proportional constant (suggested FRAC = 1.0).
30-33 RDC = order of geometric rate decay for proportional constants (suggested RDC = 3.0).
34-37 DELT = fractional increment of parameter values for finite difference quotients if NOPT = 1 (suggested DELT = .05); otherwise, DELT = 0.0.
38    NWGT =
       \begin{align*}
         &1 \text{ weighted nonlinear estimation} \\
         &0 \text{ unweighted nonlinear estimation}
       \end{align*}
39    ISMLT = \begin{align*}
         &1 \text{ exact simultaneous equations} \\
         &0 \text{ nonexact simultaneous equations}
       \end{align*}
40    NR = number of runs
41-60 blank spaces

61-80 IP(J) =
       \begin{align*}
         &1 \text{ th parameter to be estimated} \\
         &0 \text{ th parameter held constant}
       \end{align*}

IP(J), J=1, NCOL

Card 2: (A 2 punched in Column 2)

Columns 3-74 may be used for the title.

Card 3: (A 3 punched in Column 2)

\begin{align*}
UP(J) = \text{name of } &J\text{ th parameter} \\
\text{UP(J), J=1, NCOL} \\
\text{FORMAT (2X, 10A4)}
\end{align*}

Card 4: (A 4 punched in Column 2)

Columns 3-74 may be used to specify output format which has either of two forms:

\begin{align*}
\text{NWGT = 1} \\
(F(I), Y(I), WT(I), (X(I,J), J=1, NIDV), I=1, NUM)
\end{align*}

\begin{align*}
\text{NWGT = 0} \\
(F(I), Y(I), (X(I,J), J=1, NIDV), I=1, NUM)
\end{align*}

where \( F(I) = \text{calculated value of } i\text{ th observation} \)
\( Y(I) = \text{value of } i\text{ th observation} \)
\( WT(I) = \text{weight on } i\text{ th observation} \)
\( X(I,J) = \text{value of } i\text{ th independent variable for } J\text{ th observation} \)

Card 5: (A 5 punched in Column 2)

Columns 3-74 may be used to specify the input format for the data in either of two forms:

\begin{align*}
\text{NWGT = 1} \\
(Y(I), WT(I), (X(I,J), J=1, NIDV), I=1, NUM)
\end{align*}

\begin{align*}
\text{NWGT = 0}
\end{align*}
(Y(I), (X(I,J), J=1, NIDV), I=1, NUM)

Data Cards:
Data cards according to format specified in Card 5.

Card 6: (A'6 punched in Column 2)
NI = total number of parameter values to be read
IN(I) = i

th parameter
UJ(I) = value of i

th parameter
NI, (IN(I), UJ(I), I=1, NI)

(a total of NR Card 6's)
(if a new set of data is to be read, go to Card 1)
(a blank card follows the last data card)

SUBROUTINES REQUIRED
MATINT = subroutine to invert a matrix
FUNC = subroutine to evaluate the function. The subroutine is entered by the statement
CALL FUNC (Y, X, P, N)
where
Y = value of i

th observation
X = vector of independent (control) variables of i

th observation
P = parameter vector
N = number of parameters to be estimated.
The user must supply this subroutine.

DERIV = subroutine to evaluate partial derivations. The subroutine is entered by the statement
CALL DERIV (D, P, X, N)
where
D = partial derivative vector of i

th observation and P, X, and N are defined as in subroutine FUNC.
The user must supply this subroutine. If NOPT = 1, a dummy DERIV must then be supplied.

TESPAR = subroutine to test parameter values for validity. The subroutine is entered by the statement
CALL TESPAR (P, N, K)
where
K = 1 any parameter value found unacceptable
= 0 otherwise
and P and N have the same meaning as in subroutine FUNC. The user must supply this subroutine. If ITEST=0, a dummy TESPAR then must be supplied.

GEOLOGICAL EXAMPLES

Bimodal Distributions

In sampling from geological populations, it is not uncommon to find the values of a particular variable characterized by a bimodal distribution. In such situations, it is reasonable to suppose that the observed distribution represents a mixture of two parent populations. The problem becomes one of estimating the parameters of each population. Consider, for example, a bimodal distribution of grain diameters of particles making up a sediment sample in which the diameters of particles making up the sample are expressed in phi units. Assuming the observed distribution to represent a mixture of two normal populations, the density function is written as

\[ f(x) = \alpha \frac{-\frac{1}{2} \left( \frac{x - \mu_1}{\sigma_1} \right)^2}{\sqrt{2\pi} \sigma_1} + (1-\alpha) \frac{-\frac{1}{2} \left( \frac{x - \mu_2}{\sigma_2} \right)^2}{\sqrt{2\pi} \sigma_2} \]

(8)

where \(\mu_1, \mu_2, \sigma_1, \) and \(\sigma_2\) are the respective means and standard deviations and \(\alpha\) represents the degree of

Table 1. - Calculated frequencies at one-quarter phi unit intervals for mixed normal distribution having parameter values given in text.

<table>
<thead>
<tr>
<th>x</th>
<th>f(x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.50</td>
<td>0.00</td>
</tr>
<tr>
<td>-0.25</td>
<td>0.02</td>
</tr>
<tr>
<td>0.00</td>
<td>0.11</td>
</tr>
<tr>
<td>0.25</td>
<td>0.44</td>
</tr>
<tr>
<td>0.50</td>
<td>1.35</td>
</tr>
<tr>
<td>0.75</td>
<td>3.24</td>
</tr>
<tr>
<td>1.00</td>
<td>6.06</td>
</tr>
<tr>
<td>1.25</td>
<td>9.02</td>
</tr>
<tr>
<td>1.50</td>
<td>12.67</td>
</tr>
<tr>
<td>1.75</td>
<td>20.90</td>
</tr>
<tr>
<td>2.00</td>
<td>26.00</td>
</tr>
<tr>
<td>2.25</td>
<td>15.34</td>
</tr>
<tr>
<td>2.50</td>
<td>4.05</td>
</tr>
<tr>
<td>2.75</td>
<td>0.66</td>
</tr>
<tr>
<td>3.00</td>
<td>0.12</td>
</tr>
<tr>
<td>3.25</td>
<td>0.02</td>
</tr>
<tr>
<td>3.50</td>
<td>0.00</td>
</tr>
</tbody>
</table>
of mixing of the two populations. For a given set of data, we wish to estimate values for \( \mu_1, \mu_2, \sigma_1, \sigma_2, \) and \( \alpha. \) Clearly, it is not possible to convert (8) into a linear expression by any transformation. Thus we must employ nonlinear methods.

Taking a numerical example, Table 1 lists the weight percentage of particles at one-quarter phi unit intervals generated from a mixture of two normal populations characterized by the parameter values

\[
\begin{align*}
\mu_1 &= 1.5 \\
\mu_2 &= 2.0 \\
\sigma_1 &= 0.5 \\
\sigma_2 &= 0.25 \\
\alpha &= .5
\end{align*}
\]

The histogram for the resulting mixture is shown in Figure 1. If we did not know the true values of the parameters, the problem would be to estimate these values from the given frequency data.

For estimates based on interval data, it is necessary to modify (8) slightly by introducing

\[
y = N d f(x) \tag{9}
\]

as a nonlinear function where \( N \) represents the total sample weight and \( d \) represents the class interval. For this example, \( N = 100 \) and \( d = 0.25. \)

\[
C = \frac{N d}{\sqrt{2\pi}}
\]

so that

\[
y = C \left[ \frac{\alpha_1}{\sigma_1} u_1(x) + \frac{\alpha_2}{\sigma_2} u_2(x) \right]
\]

The partial derivatives with respect to the population means become

\[
\frac{\partial y}{\partial \mu_i} = C \frac{\alpha_i}{\sigma_i} \left( \frac{x - \mu_i}{\sigma_i} \right) u_i(x), \quad i = 1, 2
\]

with respect to the population standard deviations

\[
\frac{\partial y}{\partial \sigma_i} = C \frac{\alpha_i}{\sigma_i} \left( \frac{(x - \mu_i)^2 - 1}{\sigma_i} \right) u_i(x), \quad i = 1, 2
\]

and with respect to the degree of mixing

\[
\frac{\partial y}{\partial \alpha_i} = C \left[ \frac{1}{\sigma_1} u_1(x) - \frac{1}{\sigma_2} u_2(x) \right].
\]

It follows from the density function that \( \alpha_i > 0 \) and \( \alpha_1 + \alpha_2 = 1 \) where \( \alpha_i \approx 0. \)

To illustrate the use of the program, the true values of the parameters were perturbed slightly and the following values used as the initial or starting values:

\[
\begin{align*}
\mu_1^0 &= 1.4 \\
\sigma_1^0 &= .45 \\
\mu_2^0 &= 1.8 \\
\sigma_2^0 &= .22 \\
\alpha^0 &= .55
\end{align*}
\]

The subroutines FUNC, DERIV, and TESPAR for this function are included in the program listing. Remember that these subroutines are different for each problem. The input data are listed in Table 2 and the results are given in Table 3. The program converged to the solution after 10 iterations resulting in a near perfect fit of the relative frequency data. For actual data, the fit would not be as exact. This example, however, provides a test set of data which can be used to check the program on a computer at a different installation.

Porosity Determination

Another example in which nonlinear functions prove useful is in the determination of porosity in vuggy carbonates based on the travel times observed on sonic logs. It is recognized widely that the Wyllie time average equation for this type of rock material results in anomalously high fluid velocities. The equation for the porosity for a single rock type based on the observed travel time is

\[
\Delta t_o = \Delta t_m (1-\phi) + \Delta t_f \phi \tag{10}
\]

where \( \Delta t_o \) is the observed transit time in microseconds per foot, \( \Delta t_m \) is the transit time for the given
Table 2. - Input data for mixture of two normal populations

<table>
<thead>
<tr>
<th>1DISECT</th>
<th>17</th>
<th>5</th>
<th>6</th>
<th>101200</th>
<th>9</th>
<th>1</th>
<th>3</th>
<th>1</th>
<th>11111</th>
</tr>
</thead>
</table>

2 DISSECTION OF A FREQUENCY FUNCTION INTO TWO NORMAL COMPONENTS

3 M1 S1 M2 S2 WT C

4 \[1H04X20HG(CALC)\] F(OBS) \[\times/\{1H 4XF5.2,4XF5.2,3XF5.2\}\]

5 (16F5.2)

\[
00 -50 02 -25 11 00 44 25 135 50 324 75 606 100 902 125
\]

\[
1267 150 2090 175 2600 200 1534 225 405 250 66 275 12 300 02 325
\]

\[
00 350
\]

6 6 1 1.4 2 0.45 3 1.8 4 0.22 5 0.55

6 9.9736

---

Table 3. - Results of dissecting mixture of two normal populations into separate components.

<table>
<thead>
<tr>
<th>STARTING VALUES</th>
<th>M1 = 0.14000E 01</th>
<th>S1 = 0.45000E 00</th>
<th>M2 = 0.13000E 01</th>
<th>S2 = 0.22000E 00</th>
</tr>
</thead>
<tbody>
<tr>
<td>WT = 0.55000E CC</td>
<td>C = 0.95736E 01</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

DISSECTION OF A FREQUENCY FUNCTION INTO THE NORMAL COMPONENTS

INITIAL SUM OF SQUARES IS 0.31774E 03

AFTER 10 ITERATIONS USING 5 REALCT FACTORS, THE SUM OF SQUARES IS 0.58816E-04

<table>
<thead>
<tr>
<th>M1 = 0.14455E E1</th>
<th>S1 = 0.45996E 00</th>
<th>M2 = 0.20000E 01</th>
<th>S2 = 0.25005E 00</th>
</tr>
</thead>
<tbody>
<tr>
<td>WT = 0.45555E CC</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

F(CALC) F(OBS) X

| 0.00 | 0.0 | -0.5C |
| 0.02 | 0.02 | -0.25 |
| 0.11 | 0.11 | C.C  |
| 0.44 | 0.44 | C.25 |
| 1.35 | 1.25 | C.5C |
| 3.24 | 3.24 | C.75 |
| 6.06 | 6.06 | 1.CC |
| 9.02 | 9.02 | 1.25 |
| 12.67 | 12.67 | 1.5C |
| 20.90 | 20.90 | 1.75 |
| 26.00 | 26.00 | 2.CC |
| 15.34 | 15.24 | 2.25 |
| 4.05 | 4.05 | 2.5C |
| 0.66 | 0.66 | 2.75 |
| 0.12 | 0.12 | 3.CC |
| 0.02 | 0.02 | 3.25 |
| 0.00 | 0.0 | 3.5C |
Table 4.- Observed transit time versus core porosity for Caddo Limestone samples (Data from Meese and Walther, 1967).

<table>
<thead>
<tr>
<th>$\Delta t_o$ (µsec/ft)</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>48.9</td>
<td>0.023</td>
</tr>
<tr>
<td>48.2</td>
<td>0.040</td>
</tr>
<tr>
<td>55.4</td>
<td>0.093</td>
</tr>
<tr>
<td>51.9</td>
<td>0.107</td>
</tr>
<tr>
<td>53.9</td>
<td>0.107</td>
</tr>
<tr>
<td>59.0</td>
<td>0.157</td>
</tr>
</tbody>
</table>

\[ \Delta t_f = \Delta t_m (1-\phi)e^{-k\phi} + \Delta t_f e^{-\ell (1-\phi)} \]  \hspace{1cm} (11)

where $k$ and $\ell$ are parameters which characterize the nonlinear portion of the time average equation. Clearly, for $k=\ell=0$, (11) is the same as (10).

As an example, Table 4 lists data taken from Meese and Walther (1967) relating log derived transit times with measured core porosities for six samples of the Caddo Limestone.

![Graph](image)

Figure 2.- Plot of Caddo Limestone samples and best fitting curve determined by nonlinear estimation.

Table 5.- Results of fitting nonlinear function given by equation (11) for six samples of Caddo Limestone.

<table>
<thead>
<tr>
<th>Starting Values</th>
<th>$k = 0.50000E\ 00$</th>
<th>$L = 0.50000E\ 00$</th>
<th>$T_m = 0.45000E\ 02$</th>
<th>$T_f = 0.19000E\ 03$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Sum of Squares is</td>
<td>0.63570E\ 02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>After 6 iterations using 9 reduction factors, the sum of squares is</td>
<td>0.12382E\ 02</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$T_{(calc)}$</th>
<th>$T_{(obs)}$</th>
<th>$P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>48.9</td>
<td>48.9</td>
<td>0.223</td>
</tr>
<tr>
<td>48.2</td>
<td>48.2</td>
<td>0.044</td>
</tr>
<tr>
<td>52.9</td>
<td>55.4</td>
<td>0.053</td>
</tr>
<tr>
<td>54.0</td>
<td>51.9</td>
<td>0.107</td>
</tr>
<tr>
<td>54.0</td>
<td>52.9</td>
<td>0.107</td>
</tr>
<tr>
<td>58.8</td>
<td>59.0</td>
<td>0.157</td>
</tr>
</tbody>
</table>
In order to fit an equation of the type expressed in (11), it is necessary to obtain estimates for \( k \) and \( \ell \) using nonlinear methods. In most instances, it is necessary also to estimate \( \Delta t_m \), the matrix transit time. The latter stems from the lack of knowledge of the exact mineral composition.

The partial derivatives with respect to the unknown parameters \( k \), \( \ell \) and \( \Delta t_m \) are given by

\[
\frac{\partial \Delta t_c}{\partial k} = -\Delta t_m \phi (1 - \phi) e^{-k\phi}, \\
\frac{\partial \Delta t_c}{\partial \ell} = -\Delta t_f \phi (1 - \phi) e^{-\ell(1-\phi)}, \quad \text{and} \quad \\
\frac{\partial \Delta t_c}{\partial \Delta t} = (1 - \phi) e^{-k\phi}.
\]

With this information, we may proceed to estimate the values of the parameters.

Table 5 lists the results obtained for the data in the Caddo Limestone. The curve drawn in Figure 2 represents the relationship that exists between log transit time and porosity. Consequently, more reliable estimates of porosity are now made possible from sonic logs.

REFERENCES


NONLINEAR ESTIMATION PROGRAM

A COMPUTER PROGRAM TO OBTAIN ESTIMATES OF PARAMETERS FOR ALGEBRAIC NONLINEAR SIMULTANEOUS EQUATIONS. THE PRESENT PROGRAM ALLOWS FOR UP TO 10 PARAMETERS TO BE ESTIMATED BASED ON A MAXIMUM OF 250 OBSERVATIONS AND 10 INDEPENDENT VARIABLES. THESE LIMITS CAN BE ADJUSTED UPWARDS BY INCREASING THE DIMENSION OF THE APPROPRIATE VARIABLES IN THE PROGRAM.

ORDER OF INPUT CARDS
1. PROGRAM CONTROL CARD
2. TITLE CARD
3. PARAMETER NAME CARD
4. OUTPUT FORMAT CARD
5. DATA FORMAT CARD
** DATA CARDS **
6. INITIAL PARAMETER ESTIMATE CARD
7. BLANK CARD

FORMAT OF PROGRAM CONTROL CARD

COLUMNS

1 - 2 CARD NUMBER (A 1 PUNCHED IN COLUMN 52)
3 - 8 NO PROBLEM IDENTIFICATION
9 - 12 NUM NUMBER OF OBSERVATIONS
15 - 16 NGOL TOTAL NUMBER OF PARAMETERS
17 - 18 NIDV NUMBER OF INDEPENDENT (CONTROL) VARIABLES
19 NOPT NOPT=1, FINITE DIFFERENCE QUOTIENTS USED
       NOPT=0, PARTIAL DERIVATIVES SUPPLIED
20 ITEST ITEST=1, TEST PARAMETER VALUES FOR VALIDITY
       ITEST=0, NO VALIDITY TEST FOR PARAMETER VALUES
21 - 25 NTIM MAXIMUM NUMBER OF ITERATIONS
24 - 25 NRD NUMBER OF PROPORTIONAL PARAMETER ADJUSTMENT
       CONSTANTS (SUGGESTED NRD=9)
26 - 29 FRAC INITIAL PROPORTIONAL PARAMETER ADJUSTMENT
       CONSTANT (SUGGESTED FRAC=1.0)
30 - 33 RDC ORDER OF DECREASE OF PROPORTIONAL PARAMETER
       ADJUSTMENT CONSTANTS (SUGGESTED RDC=3.0)
34 - 37 DFLT FRACTIONAL INCREMENT OF PARAMETER VALUES FOR
       FINITE DIFFERENCE QUOTIENTS IF NOPT=1
       (SUGGESTED DFLT=.05); OTHERWISE, DFLT=0.0
38 NWGT NWGT=1, WEIGHTED NONLINEAR ESTIMATION
       NWGT=0, UNWEIGHTED NONLINEAR ESTIMATION
39 ISMLT ISMLT=1, EXACT SIMULTANEOUS EQUATIONS
       ISMLT=0, NONEXACT SIMULTANEOUS EQUATIONS
40 NR NUMBER OF RUNS
41 - 60 COLUMNS FILLED WITH BLANK SPACES
61 - 80 IP IP(J)=1, JTH PARAMETER TO BE ESTIMATED
       IP(J)=0, JTH PARAMETER TO BE HELD CONSTANT

SUBROUTINES REQUIRED
MATINT MATRIX INVERSION SUBROUTINE
FUN E  FUNCTION EVALUATION SUBROUTINE
DERIV  PARTIAL DERIVATIVE EVALUATION SUBROUTINE
        (IF NOPT=1, THEN A DUMMY DERIV MUST BE SUPPLIED)
TESPAR  PARAMETER VALIDITY TEST SUBROUTINE (IF ITEST=0, THEN
        A DUMMY TESPAR SUBROUTINE MUST BE SUPPLIED)

***************
MAIN PROGRAM
***************
DIMENSION Y(250),F(250),X(250,10),W(10,250),DF(250,10),WT(250)
DIMENSION PV(10),FX(10),PR(10,10),UP(10),UI(10),RF(10),AM(10,10),B
IM(10),V(I),FMT(I8),FML(I8),FMO(I8),D(I),IP(I),IN(I),UJ(10),KY(I)
210,X(I),UK(I),UL(I),NO(2)
DATA ZER0/0,1/0
NINT=5
NOUT=6
ISOLV=0

READ PROGRAM CONTROL CARD

2 READ(NINT,101) NO(I),NO(2),NUM,NP,NCOL,NIDV,NOPT,ITEST,NTIM,NVR,FR
1AC,RDC,DELT,NWGT,ISMLT,NR,(IP(J),J=1,NCOL)
101 FORMAT(2X,A2,4,F15.6,2X,I2,1X,A2,1X,A2,1X,A2,1X,A2,1X,A2)
       IF(NUM.EQ.0) GO TO 99
       K=0
       DU 11 I=1,NCOL
       IF(IP(I)) 11,11,10
10  K=K+1
     KY(K)=1
11 CONTINUE
     RF(I)=FRAC

CALCULATE PROPORTIONAL PARAMETER ADJUSTMENT CONSTANTS

DO 9 K=2,NRC
9 RF(K)=RF(K-1)/RDC

READ TITLE,PARAMETER NAME,AND FORMAT CONTROL CARDS

READ(NINT,102) (FMT(I),I=1,18)
102 FORMAT(2X,18A4)
      READ(NINT,103) (UP(J),J=1,NCOL)
103 FORMAT(2X,18A4)
      READ(NINT,102) (FMO(I),I=1,18)
      READ(NINT,102) (FMT(I),I=1,18)

READ INPUT DATA CARDS

IF(NWGT)35,35,37
35 DO 36 I=1,NUM
36 WT(I)=1.
       READ(NINT,FMT) (Y(I),X(I,J),J=1,NIDV),I=1,NUM
       GO TO 13
37 READ(NINT,FMT) (Y(I),WT(I),X(I,J),J=1,NIDV),I=1,NUM
13 DO 43 INR=1,NR

11
READ INITIAL PARAMETER ESTIMATE CARD

READ(NINT,104) NI,(IN(J),0J(J),J=1,NI)
DO 15 I=1,NI
15 UI(J)=UJ(I)
WRITE(NOUT,200) NO(1),NO(2),(UP(J),UI(J),J=1,NCOL)
200 FORMAT(1H1/1HO/1H22X32HNON-LINEAR LEAST SQUARES PROGRAM / 1H 31X 7
1HPROBLEM,2X4A4,A2//1H 15HSTARTING VALUES / ( 4(4X4A4,3H = ,E12.5) )
WRITE(NOUT,221) (FML(J),J=1,18)
221 FORMAT(1HO10X18A4)
IF(ISMLT.EQ.0) GO TO 7
WRITE(NOUT,335)
335 FORMAT(1HO 5X41H SOLUTION FOR EXACT SIMULTANEOUS EQUATIONS )
7 CONTINUE
DO 8 K=1,NRD
8 DO 9 J=1,NP
I=KY(J)
9 PR(K,I)=UI(I)
NC=0
ITN=0

TEST FOR NUMBER OF ITERATIONS

17 IF(ITN-NTI4)331,89,89
89 WRITE(NOUT,334) NTIM
334 FORMAT(1H 5X33H THE NUMBER OF ITERATIONS EXCEEDED,15)
GO TO 90
331 CONTINUE

EVALUATE FUNCTION AND CALCULATE TEST CRITERION FOR INITIAL
PARAMETER ESTIMATES

14 DO 20 K=1,NRD
FX(K)=0
20 DO 21 N=1,NP
I=KY(N)
21 PV(I)=PR(K,N)
IF(ITEST)26,26,27
26 NPASS=0
CALL TESPAR(PV,NP,NPASS)
IF(NPASS)26,26,29
29 FX(K)=FY
GO TO 20
26 CONTINUE
65 DO 67 J=1,NUM
67 DO 68 I=1,NIDV
63 XI(I)=X(J,I)
CALL FUNC(Y1,XI,PV,NP)
WK(K,J)=Y1
IF(ISMLT.EQ.0) GO TO 69
FX(K)=FX(K)+WT(J)*ABS(Y(J)-WK(K,J))
GO TO 67
69 FX(K)=FX(K)+WT(J)*(Y(J)-WK(K,J))*2
67 CONTINUE
20 CONTINUE
CHOOSE THE SET OF PARAMETER ESTIMATES FOR WHICH THE TEST CRITERION IS A MINIMUM

\[ \text{MIN}=1 \]
\[ FZ=FX(1) \]
\[ \text{DO 25 K}=2, \text{NKD} \]
\[ \text{IF}(FX(K)-FZ)24,25,25 \]
24 \[ \text{MIN}=K \]
\[ FZ=FX(K) \]
25 \[ \text{CONTINUE} \]
\[ \text{IF}(NC)53,53,31 \]
31 \[ \text{IF}(FZ-FY)52,90,90 \]
53 \[ NC=1 \]
\[ \text{IF}(ISMLT, NE, 0) \text{GO TO 702} \]
\[ \text{WRITE}(NOUT,701)FZ \]
701 \[ \text{FORMAT}(1H020X25HINITIAL SUM OF SQUARES IS } ,E15.5 \]
702 \[ \text{GO TO 52} \]
703 \[ \text{WRITE}(NOUT,703)FZ \]

CALCULATE THE SET OF PARTIAL DERIVATIVES

\[ \text{DO 56 J}=1, \text{NP} \]
\[ I=KY(J) \]
\[ UI(I)=PR(MIN,J) \]
\[ \text{DO 56 K}=1, \text{NKD} \]
56 \[ P(K,J)=PR(MIN,J) \]
\[ FY=FZ \]
\[ \text{DO 70 J}=1, \text{NUM} \]
70 \[ F(J)=W(MIN,J) \]
\[ \text{IF}(NOPT)62,62,66 \]
62 \[ \text{DO 63 J}=1, \text{NUM} \]
\[ \text{DO 64 I}=1, \text{NIDV} \]
64 \[ X(I)=X(J,I) \]
\[ \text{CALL DERIV0, UI, X1, NP} \]
\[ \text{DO 61 K}=1, \text{NP} \]
\[ L=KY(K) \]
61 \[ DF(J,K)=D(L) \]
63 \[ \text{CONTINUE} \]
\[ \text{GO TO 76} \]
66 \[ \text{DO 71 I}=1, \text{NCOL} \]
71 \[ UJ(I)=UI(I) \]
\[ \text{DO 72 I}=1, \text{NP} \]
\[ J=KY(I) \]
\[ UK(J)=(1,+DELTL)*UJ(J) \]
72 \[ UL(J)=UK(J)-UJ(J) \]
\[ \text{DO 73 J}=1, \text{NUM} \]
\[ \text{DO 75 I}=1, \text{NIDV} \]
75 \[ X(I)=X(J,I) \]
\[ \text{DO 74 I}=1, \text{NP} \]
\[ K=KY(I) \]
\[ UJ(K)=UK(K) \]
\[ \text{CALL FUNC(Y1,X1,UJ, NP)} \]
\[ D1=(Y1-F(J))/UL(K) \]
\[ DF(J,I)=D1 \]
74 \[ UJ(K)=UI(K) \]
73 \[ \text{CONTINUE} \]
76 \[ \text{CONTINUE} \]

CALCULATE THE CHANGE REQUIRED TO IMPROVE THE CURRENT SET OF
PARAMETER VALUES

59 IF(ISMLT.NE.0) GO TO 45
DO 34 I=1,NP
DO 33 J=1,NP
AM(I,J)=ZERO
DO 33 K=1,NUM
33 AM(I,J)=AM(I,J)+WT(K)*DF(K,I)*DF(K,J)
BM(I)=ZERO
DO 34 K=1,NUM
34 BM(I)=BM(I)+WT(K)*DF(K,I)*(Y(K)-W(MIN,K))
GO TO 44
45 DO 46 I=1,NP
BM(I)=WT(I)*(Y(I)-W(MIN,I))
DO 46 J=1,NP
46 AM(I,J)=WT(I)*DF(I,J)
44 CALL MATINT(AM,V,NP,ISDLV)

CALCULATE THE SETS OF FRACTIONALLY INCREASING PARAMETER VALUES

DO 42 I=1,NP
VI(I)=ZERO
DO 42 J=1,NP
42 VI(I)=VI(I)+AM(I,J)*BM(J)
DO 60 K=1,NRD
DO 60 J=1,NP
60 PK(K,J)=PK(K,J)+RF(K)*V(J)
ITN=ITN+1
GO TO 17
90 CONTINUE

PRINT OUT RESULTS

DO 88 J=1,NP
I=KY(J)
UK(J)=UP(I)
88 UJ(J)=UJ(I)
IF(ISMLT.NE.0) GO TO 704
WRITE(NOUT,500) ITN,NRD,FY,(UK(J),UJ(J),J=1,NP)
500 FORMAT(140,I1H,2X) HEADER,16,17H ITERATIONS USING,13,51H REDUCTION F
1ACTORS, THE SUM OF SQUARES IS ,E12,5 // (1H 10XA4,3H = ,E12,5,2XA4
2,3H = ,E12,5,2XA4,3H = ,E12,5,2XA4,3H = ,E12,5,2X)
GO TO 705
704 WRITE(NOUT,501) ITN,NRD,FY,(UK(J),UJ(J),J=1,NP)
501 FORMAT(140,I1H,2X) HEADER,16,17H ITERATIONS USING,13,51H REDUCTION F
1ACTORS, THE SUM OF ABSOLUTE VALUES IS ,E12,5 // (1H 10XA4,3H = ,E1
2,5,2XA4,3H = ,E12,5,2XA4,3H = ,E12,5,2XA4,3H = ,E12,5,2X)
705 CONTINUE

END
C
C  **************
C  SUBROUTINE MATINT (O,B,K,ISOLV)
C  **************
C
DIMENSION A(10,20),B(10),C(10,10),O(10,10)
DATA ZERO/0.0,E1/,ONE/1.0,E0/
NTI=5
NTO=6
CALL OVERFL(K000FX)
GO TO(15,5),K000FX
5 CONTINUE
DO 115 I=1,K
B(I)=ZERO
DO 115 J=1,K
C(I,J)=ZERO
115 A(I,J)=O(I,J)
M=2*K
KPO=K+1
DO 20 I=1,K
DO 20 J=KPO,M
IF(J-K-I)19,12,19
12 A(I,J)=ONE
GO TO 20
19 A(I,J)=ZERO
20 CONTINUE
DO 350 N=1,K
NPO=N+1
DMAX=ABS(A(N,N))
KEEP=N
IF (N-K)346,362,362
346 DO 350 I=NPO,K
X=ABS(A(I,N))
IF (X-DMAX)350,350,348
348 DMAX=X
KEEP=I
350 CONTINUE
IF (KEEP-N)353,362,353
353 TEMP=B(N)
B(N)=B(KEEP)
B(KEEP)=TEMP
DO 360 J=1,M
TEMP = A(N,J)
A(N,J)=A(KEEP,J)
360 A(KEEP,J) =TEMP
362 IF (A(N,N))1012,30,1012
1012 AP=A(N,N)
B(N)=B(N)/AP
DO 1050 I=N,M
1050 A(N,I)=A(N,I)/AP
CALL OVERFL(K000FX)
GO TO(1051,1053),K000FX
1051 WRITE (NTO,1052)
1052 FORMAT (1H0,12H MQ OVERFLOW)
GO TO 200
1053 DO 1060 I=1,K
IF (I-N)1056,1060,1056
1056 IF (A(I,N))1065,1060,1056
1065 IF (A(I,N))1058,1060,1058
1058 BP=A(I,N)
B(I)=B(I)-B(N)*BP
DO 1595 J=4,M
1595 A(I,J)=A(I,J)-A(N,J)*BP
1060 CONTINUE
   CALL OVERFL(K000FX)
   GO TO(1061,34),K000FX
1061 WRITE (NTO,1062)
1062 FORMAT (1AH,21H ACCUMULATOR OVERFLOW)
   GO TO 200
30 WRITE (NTO,31)
   GO TO 200
31 FORMAT(///19H MATRIX SINGULAR )
34 CONTINUE
   DO 36 I=1,K
   DO 36 J=1,K
      J1=J+K
36 D(I,J)=A(I,J1)
200 RETURN
END
**SUBROUTINE** TO CALCULATE DENSITY FUNCTION FOR A MIXTURE OF TWO NORMAL DISTRIBUTIONS

```c
DIMENSION P(1),X(1)
Y=P(6)*(P(5)*EXP(-((X(1)-P(1))/P(2))**2/2.))/P(2)+(1.-P(5))*EXP(-1.((X(1)-P(3))/P(4))**2/2.))/P(4))
RETURN
END
```
***************
SUBROUTINE DERIV(D,P,X,N)
***************
SUBROUTINE TO EVALUATE PARTIAL DERIVATIVES FOR THE PARAMETERS
OF A MIXED NORMAL DISTRIBUTION
DIMENSION D(1),P(1),X(1)
U1=EXP(-((X(1)-P(1))/P(2))**2/2.)
U2=EXP(-((X(1)-P(3))/P(4))**2/2.)
U3=(X(1)-P(1))/P(2)
U4=(X(1)-P(3))/P(4)
D(1)=P(6)*P(5)*U3*U1/P(2)**2
D(2)=P(6)*P(5)*(U3**2-1.)*U1/P(2)**2
D(3)=P(6)*(1.-P(5))*U4*U2/P(4)**2
D(4)=P(6)*(1.-P(5))*(U4**2-1.)*U2/P(4)**2
D(5)=P(6)*(U1/P(2)-U2/P(4))
RETURN
END
C
C
C
C
***************
SUBROUTINE TE$
C
C
C
C
SUBROUTINE TO TEST PARAMETER VALUES OF A MIXED NORMAL DISTRIBUTION
DIMENSION P(1)
K=0
IF(P(2).LE.0.) GO TO 4
IF(P(4).LE.0.) GO TO 4
IF(P(5).LE.0.) GO TO 4
IF(P(5)-1.) 6,6,4
4 K=1
6 RETURN
END
FORTRAN IV PROGRAM FOR NONLINEAR ESTIMATION

Date: February, 1969

Author, organization: Richard B. McCammon
Department of Geological Sciences, University of Illinois at Chicago

Direct inquiries to: ______________________________________________________

Name: Richard B. McCammon Address: Department of Geological Sciences
University of Illinois at Chicago

Purpose/description: To estimate the parameters in nonlinear algebraic simultaneous
equations.

Mathematical method: A modified Gauss-Newton procedure

Restrictions, range: The program is currently dimensioned for estimating up to 10 parameters
based on up to 250 observations and 10 independent (control) variables.

Computer manufacturer: IBM Model: 360/50

Programming language: FORTRAN IV
Memory required: 10 K Approximate running time: ____________________________

Special peripheral equipment required: ____________________________

Remarks (special compilers or operating systems, required word lengths, number of successful runs, other machine versions, additional information useful for operation or modification of program): ____________________________

__________________________________________________

__________________________________________________

__________________________________________________
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