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FORTRAN IV PROGRAM FOR NONLINEAR ESTIMATION

By

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in cooperation with the
American Association of Petroleum Geologists
Tulsa, Oklahoma

COMPUTER CONTRIBUTION 34

State Geological Survey
The University of Kansas, Lawrence
1969

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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

$$N = \frac{k}{1 + e^{(a - rt)}}$$

where N is the number of individuals in the population at time t, and a, k, and r are parameters of the population. Clearly, no transformation will make a, k, and r 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

$$f(x) = \frac{\alpha}{\sqrt{2\pi}\,\sigma_1} e^{-\frac{1}{2}\left(\frac{x - \mu_1}{\sigma_1}\right)^2} + \frac{(1 - \alpha)}{\sqrt{2\pi}\,\sigma_2} e^{-\frac{1}{2}\left(\frac{x - \mu_2}{\sigma_2}\right)^2} \qquad 0 \leq \alpha \leq 1$$

where x if the variable of interest, μ_1, μ_2, σ_1, and σ_2 are the respective means and standard deviations of the two populations, and α 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

$$y = f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_p) \qquad (1)$$

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 θ_i 's are nonlinear with respect to y.

We start by considering a set of values $\{\theta_1^\circ, \ldots, \theta_p^\circ\}$ 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 Talyor's series about the values $\theta_1^\circ, \ldots, \theta_p^\circ$, and retain only the terms up to the first partial derivatives. Thus,

$$y \simeq f(x_1, \ldots, x_k; \theta_1^\circ, \ldots, \theta_p^\circ) + \sum_{j=1}^{p} \left[\frac{\partial f}{\partial \theta_j}\right]_{\theta_j = \theta_j^\circ} (\theta_j - \theta_j^\circ). \qquad (2)$$

If we convert this to an equality, we have a linear expression in $\Delta\theta_j = (\theta_j - \theta_j^\circ)$ 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

$$y_i - f_i(x_{1i}, \ldots, x_{ki}; \theta_1^\circ, \ldots, \theta_p^\circ) = \sum_{j=1}^{p} \left[\frac{\partial f_i}{\partial \theta_j}\right]_{\theta_j = \theta_j^\circ} \Delta\theta_j \quad i = 1, \ldots, n \qquad (3)$$

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 $\Delta\theta_j$'s. If we define the following row vectors

$f' = \{(y_1 - f_1), \ldots, (y_n - f_n)\}$ and $(\theta - \theta^\circ)' = \{(\theta_1 - \theta_1^\circ), \ldots, (\theta_p - \theta_p^\circ)\}$ and the matrix $D = \{d_{ij}\} = \{(\frac{\partial f_i}{\theta_j})_{\theta_j = \theta_j^\circ}\}$ we can write as the solution for (3)

$$\theta = \theta^\circ + D^{-1} f \qquad (4)$$

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

$$\theta^k = \theta^{k-1} + D_{k-1}^{-1} f_{k-1}.$$

It is assumed that after a finite number of steps θ^k will converge to θ 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 $f'f$ is a minimum for any choice of θ. 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 θ based on an initial estimate becomes

$$\theta = \theta^\circ + (D'D)^{-1} D'f \qquad (5)$$

using the same vectors and the same matrix as before. For the k^{th} stage of the iterative process

$$\theta^k = \theta^{k-1} + (D_{k-1}' D_{k-1})^{-1} D_{k-1}' f_{k-1} \qquad (6)$$

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

$$\theta^k = \theta^{k-1} + \gamma (D_{k-1}' D_{k-1})^{-1} D_{k-1}' f_{k-1}$$

where γ is a specified constant. Usually, several γ values rather than a single value are used where each value results in a different value for

$$f_k' f_k \qquad (7)$$

which represents the error sum of squares for a particular estimate of θ. At each step, that change in $\Delta\theta$ is chosen for which (7) is a minimum. From past experience, the set of γ 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,

$$\frac{\partial f}{\partial \theta_i} \sim \frac{f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_i + \delta\theta_i, \ldots, \theta_p) - f(x_1, \ldots, x_k; \theta_1, \ldots, \theta_i, \ldots, \theta_p)}{\delta\theta_i}$$

   where δ is a specified constant. The appropriate value for δ depends upon the function, but reasonable value for δ 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

Columns	Name		Description
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	=	{ 1 finite difference quotients used; 0 partial derivatives used
20	ITEST	=	{ 1 test parameter values for validity; 0 do not test parameter values
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 decrease 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	=	{ 1 weighted nonlinear estimation; 0 unweighted nonlinear estimation
39	ISMLT	=	{ 1 exact simultaneous equations; 0 nonexact simultaneous equations
40	NR	=	number of runs
41-60			blank spaces
61-80	IP(J)	=	{ 1 j^{th} parameter to be estimated; 0 j^{th} parameter held constant

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)

UP(J) = name of j^{th} parameter
UP(J), J=1, NCOL
FORMAT (2X, 10A4)

Card 4: (A 4 punched in Column 2)

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

NWGT = 1
(F(I), Y(I), WT(I), (X(I,J), J=1, NIDV), I=1, NUM)

NWGT = 0
(F(I), Y(I), (X(I,J), J=1, NIDV), I=1, NUM)

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

NWGT = 1
(Y(I), WT(I), (X(I,J), J=1, NIDV), I=1, NUM)

NWGT = 0

(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)

FORMAT (2XI3,5(I3,E12.5)/(5XI3,E12.5, I3,E12.5,I3,E12.5,I3,E12.5,I3, E12.5))

(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} observations

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

$$K = \begin{cases} 1 & \text{any parameter value found unacceptable} \\ 0 & \text{otherwise} \end{cases}$$

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

$$f(x) = \frac{\alpha}{\sqrt{2\pi}\sigma_1} e^{-\frac{1}{2}\left(\frac{x-\mu_1}{\sigma_1}\right)^2} + \frac{(1-\alpha)}{\sqrt{2\pi}\sigma_2} e^{-\frac{1}{2}\left(\frac{x-\mu_2}{\sigma_2}\right)^2} \qquad (8)$$

where μ_1, μ_2, σ_1, and σ_2 are the respective means and standard deviations and α represents the degree

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

f (x)	x
0.00	-0.50
0.02	-0.25
0.11	0.00
0.44	0.25
1.35	0.50
3.24	0.75
6.06	1.00
9.02	1.25
12.67	1.50
20.90	1.75
26.00	2.00
15.34	2.25
4.05	2.50
0.66	2.75
0.12	3.00
0.02	3.25
0.00	3.50

of mixing of the two populations. For a given set of data, we wish to estimate values for μ_1, μ_2, σ_1, σ_2, and α. 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

$\mu_1 = 1.5 \qquad \mu_2 = 2.0$
$\sigma_1 = 0.5 \qquad \sigma_2 = 0.25$
$\alpha = .5$

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

$$y = Ndf(x) \tag{9}$$

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.

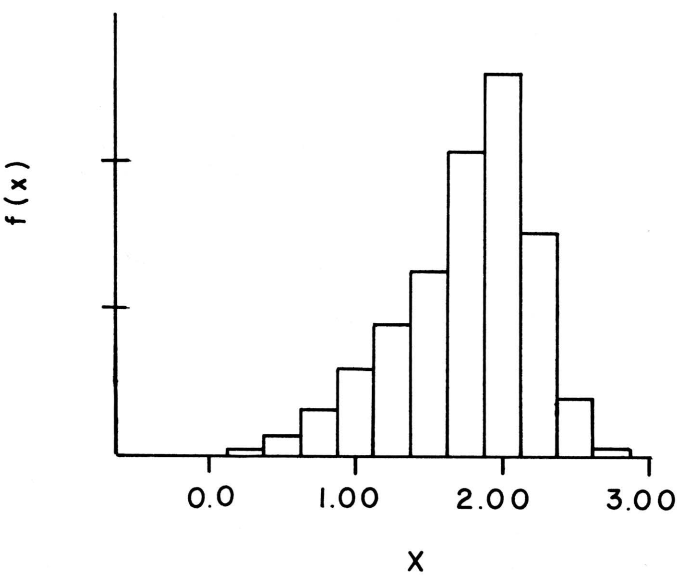

Figure 1. - Histogram constructed from weight frequency data given in Table 1.

In addition to the density function, we need the partial derivatives of (9) with respect to the different parameters. To simplify the following expressions, we first define

$\alpha_1 = \alpha \qquad \alpha_2 = 1 - \alpha$

$$u_1(x) = e^{-\frac{1}{2}\left(\frac{x-\mu_1}{\sigma_1}\right)^2} \qquad u_2(x) = e^{-\frac{1}{2}\left(\frac{x-\mu_2}{\sigma_2}\right)^2}$$

$$C = \frac{Nd}{\sqrt{2\pi}}$$

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

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

with respect to the population standard deviations

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

and with respect to the degree of mixing

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

It follows from the density function that $\sigma_i > 0$ and $\alpha_2 + \alpha_2 = 1$ where $\alpha_i \geq 0$.

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:

$\mu_1^\circ = 1.4 \qquad u_2^\circ = 1.8$
$\sigma_1^\circ = .45 \qquad \sigma_2^\circ = .22$
$\alpha^\circ = .55$

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

$$\Delta t_\sigma = \Delta t_m(1-\phi) + \Delta t_f\phi \tag{10}$$

where Δt_o is the observed transit time in microseconds per foot, Δt_m is the transit time for the given

Table 2. - Input data for mixture of two normal populations

```
00000000011111111112222222222333333333344444444445555555555666666666677777777778
12345678901234567890123456789012345678901234567890123456789012345678901234567890

1DISECT   17 5 6 101200 9 1   3         1                             11111

2DISSECTION OF A FREQUENCY FUNCTION INTO TWO NORMAL COMPONENTS

3  M1  S1  M2  S2  WT   C

4(1H04X20HF(CALC)  F(OBS)     X//(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    .45     3   1.8      4   .22       5   .55

      6 9.9736
```

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

```
STARTING VALUES
     M1 =  0.14000E 01       S1 =  C.45000E 00      M2 =  0.18000E 01      S2 =  0.22000E 00
     WT =  0.550C0E CC        C =  C.99736E 01

          DISSECTION OF A FREQUENCY FUNCTION INTO TWO NORMAL COMPONENTS

                    INITIAL SUM OF SQUARES IS    0.31774E 03

  AFTER     10 ITERATIONS USING  9 REDUCTION FACTORS, THE SUM OF SQUARES IS C.58816E-04

            M1 =  C.14995E C1    S1 =  0.49996E 00    M2 =  0.20000E 01    S2 =  0.25005E 00
            WT =  0.49955E CC
```

F(CALC)	F(OBS)	X
C.00	0.0	-0.5C
0.C2	0.02	-C.25
C.11	0.11	C.C
0.44	C.44	C.25
1.35	1.35	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	26.0C	2.CC
15.34	15.34	2.25
4.05	4.05	2.5C
0.66	0.66	2.75
0.12	0.12	3.CC
0.C2	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).

Δt_o (μ sec/ft)	ϕ
48.9	0.023
48.2	0.040
55.4	0.093
51.9	0.107
53.9	0.107
59.0	0.157

matrix material, Δt_f is the transit time of the contained fluid, and ϕ is the porosity. If porosities of vuggy carbonates calculated from sonic logs are compared with core derived porosities, the log derived porosities are invariably lower. To correct for this difference, the usual procedure is to choose an "apparent" high fluid velocity (low transit time) in order to make the log derived porosities match the core derived porosities.

A different approach is to devise a nonlinear function which allows the use of the correct fluid velocity in order to make the log derived porosities match the core derived porosities.

A different approach is to devise a nonlinear function which allows the use of the correct fluid velocity and which also provides a best fit for an observed set of data. One condition, however, is that the function reduce in the limit to the time average equation when, in fact, the nonlinear effects associated with the irregular acoustic wave path through the rock material are neglible. A nonlinear function which meets these requirements is

$$\Delta t_o = \Delta t_m (1-\phi) e^{-k\phi} + \Delta t_f \phi e^{-\ell(1-\phi)} \qquad (11)$$

where k and ℓ are parameters which characterize the nonlinear portion of the time average equation. Clearly, for $k=\ell=o$, (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.

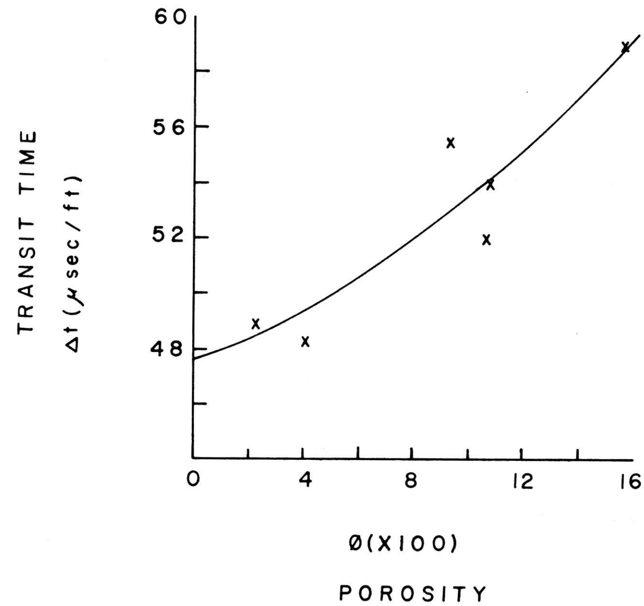

Figure 2. - Plot of Caddo Limestone samples and best fitting curve determined by nonlinear estimation.

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

```
STARTING VALUES
     K =   0.50000E 00        L =   0.50000E 00       TM =   0.45000E 02       TF =   0.19000E 03

          POROSITY CALCULATION FOR CADDC LIPESTCNE

                    INITIAL SUM CF SQLARES IS    0.63570E 02

  AFTER     6 ITERATIONS USING  9 REDLCTION FACTORS, THE SUM CF SCUARES IS 0.12382E 02

          K =   0.2887CE C1      L = -0.13294E 00     TM =   0.47474E 02

   T(CALC)   T(OBS)     P

    48.4      48.9    C.C23
    49.2      48.2    C.04C
    52.9      55.4    C.C93
    54.0      51.9    0.1C7
    54.0      53.9    C.1C7
    58.8      59.0    C.157
```

In order to fit an equation of the type expressed in (11), it is necessary to obtain estimates for k and ℓ using nonlinear methods. In most instances, it is necessary also to estimate Δt_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, ℓ and Δt_m are given by

$$\frac{\partial \Delta t_o}{\Delta k} = -\Delta t_m \, \phi(1-\phi) e^{-k\phi},$$

$$\frac{\partial \Delta t_o}{\partial} = -\Delta t_f \, \phi(1-\phi) e^{-\ell(1-\phi)}, \text{ and}$$

$$\frac{\partial \Delta t_o}{\partial \Delta t} = (1-\phi) e^{-k\phi}.$$

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.

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```
C
C                  NONLINEAR ESTIMATION PROGRAM
C
C
C             A COMPUTER PROGRAM TO OBTAIN ESTIMATES OF PARAMETERS
C      FOR ALGEBRAIC NONLINEAR SIMULTANEOUS EQUATIONS. THE PRESENT
C      PROGRAM ALLOWS FOR UP TO 10 PARAMETERS TO BE ESTIMATED BASED ON
C      A MAXIMUM OF 250 OBSERVATIONS AND 10 INDEPENDENT VARIABLES. THESE
C      LIMITS CAN BE ADJUSTED UPWARDS BY INCREASING THE DIMENSION OF THE
C      APPROPRIATE VARIABLES IN THE PROGRAM.
C
C
C      ORDER OF INPUT CARDS
C        1. PROGRAM CONTROL CARD
C        2. TITLE CARD
C        3. PARAMETER NAME CARD
C        4. OUTPUT FORMAT CARD
C        5. DATA FORMAT CARD
C          ** DATA CARDS **
C        6. INITIAL PARAMETER ESTIMATE CARD
C        7. BLANK CARD
C
C
C      FORMAT OF PROGRAM CONTROL CARD
C
C      COLUMNS
C
C       1 -  2             CARD NUMBER (A 1 PUNCHED IN COLUMN52 )
C       3 -  8        NO   PROBLEM IDENTIFICATION
C       9 - 12       NUM   NUMBER OF OBSERVATIONS
C      15 - 16      NCOL   TOTAL NUMBER OF PARAMETERS
C      17 - 18      NIDV   NUMBER OF INDEPENDENT (CONTROL) VARIABLES
C        19         NOPT   NOPT=1, FINITE DIFFERENCE QUOTIENTS USED
C                          NOPT=0, PARTIAL DERIVATIVES SUPPLIED
C        20        ITEST   ITEST=1, TEST PARAMETER VALUES FOR VALIDITY
C                          ITEST=0, NO VALIDITY TEST FOR PARAMETER VALUES
C      21 - 23      NTIM   MAXIMUM NUMBER OF ITERATIONS
C      24 - 25       NRD   NUMBER OF PROPORTIONAL PARAMETER ADJUSTMENT
C                          CONSTANTS (SUGGESTED NRD=9)
C      26 - 29      FRAC   INITIAL PROPORTIONAL PARAMETER ADJUSTMENT
C                          CONSTANT (SUGGESTED FRAC=1.0)
C      30 - 33       RDC   ORDER OF DECREASE OF PROPORTIONAL PARAMETER
C                          ADJUSTMENT CONSTANTS (SUGGESTED RDC=3.0)
C      34 - 37      DELT   FRACTIONAL INCREMENT OF PARAMETER VALUES FOR
C                          FINITE DIFFERENCE QUOTIENTS IF NOPT=1
C                          (SUGGESTED DELT=.05); OTHERWISE, DELT=0.0
C        38         NWGT   NWGT=1, WEIGHTED NONLINEAR ESTIMATION
C                          NWGT=0, UNWEIGHTED NONLINEAR ESTIMATION
C        39        ISMLT   ISMLT=1, EXACT SIMULTANEOUS EQUATIONS
C                          ISMLT=0, NONEXACT SIMULTANEOUS EQUATIONS
C        40           NR   NUMBER OF RUNS
C      41 - 60             COLUMNS FILLED WITH BLANK SPACES
C      61 - 80        IP   IP(J)=1, JTH PARAMETER TO BE ESTIMATED
C                          IP(J)=0, JTH PARAMETER TO BE HELD CONSTANT
C
C
C       SUBROUTINES REQUIRED
C
C         MATINT   MATRIX INVERSION SUBROUTINE
C
```

```
C         FUNC      FUNCTION EVALUATION SUBROUTINE
C
C         DERIV     PARTIAL DERIVATIVE EVALUATION SUBROUTINE
C                   (IF NOPT=1, THEN A DUMMY DERIV MUST BE SUPPLIED)
C
C         TESPAR    PARAMETER VALIDITY TEST SUBROUTINE (IF ITEST=0, THEN
C                   A DUMMY TESPAR SUBROUTINE MUST BE SUPPLIED)
C
C
C
C     ************
C     MAIN PROGRAM
C     ************
      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
     1M(10),V(10),FMT(18),FML(18),FMO(18),D(10),IP(10),IN(10),UJ(10),KY(
     210),X1(10),UK(10),UL(10),NO(2)
      DATA ZERO/0.E1/
      NINT=5
      NOUT=6
      ISOLV=0
C
C     READ PROGRAM CONTROL CARD
C
    2 READ(NINT,101) NO(1),NO(2),NUM,NP,NCOL,NIDV,NOPT,ITEST,NTIM,NRD,FR
     1AC,RDC,DELT,NWGT,ISMLT,NR,(IP(J),J=1,NCOL)
  101 FORMAT(2XA4,A2,I4,3I2,2I1,I3,I2,3F4.2,3I1,20X20I1)
      IF(NUM.EQ.0) GO TO 99
      K=0
      DO 11 I=1,NCOL
      IF(IP(I))11,11,10
   10 K=K+1
      KY(K)=I
   11 CONTINUE
      RF(1)=FRAC
C
C     CALCULATE PROPORTIONAL PARAMETER ADJUSTMENT CONSTANTS
C
      DO 9 K=2,NRD
    9 RF(K)=RF(K-1)/RDC
C
C     READ TITLE,PARAMETER NAME,AND FORMAT CONTROL CARDS
C
      READ(NINT,102)(FML(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)
C
C     READ INPUT DATA CARDS
C
      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
C
```

```
C     READ INITIAL PARAMETER ESTIMATE CARD
C
      READ(NINT,104) NI,(IN(J),UJ(J),J=1,NI)
  104 FORMAT(2X,I3,5(I3,E12.5)/(5XI3,E12.5,I3,E12.5,I3,E12.5,I3,E12.5,I3
     1,E12.5))
      DO 15 I=1,NI
      J=IN(I)
      UI(J)=UJ(I)
   15 PV(J)=UI(J)
      WRITE(NOUT,200) NO(1),NO(2),(UP(J),UI(J),J=1,NCOL)
  200 FORMAT(1H1/1H0/1H 22X32HNON-LINEAR LEAST SQUARES PROGRAM /1H 31X 7
     1HPROBLEM,2XA4,A2//1H 15HSTARTING VALUES/( 4(4XA4,3H = ,E12.5)))
      WRITE(NOUT,221) (FML(J),J=1,18)
  221 FORMAT(1H010X18A4)
      IF(ISMLT.EQ.0) GO TO 7
      WRITE(NOUT,335)
  335 FORMAT(1H0 5X41HSOLUTION FOR EXACT SIMULTANEOUS EQUATIONS   )
    7 CONTINUE
      DO 8 K=1,NRD
      DO 8 J=1,NP
      I=KY(J)
    8 PR(K,J)=UI(I)
      NC=0
      ITN=0
C
C     TEST FOR NUMBER OF ITERATIONS
C
   17 IF(ITN-NTIM)331,89,89
   89 WRITE(NOUT,334) NTIM
  334 FORMAT(1H 5X33HTHE NUMBER OF ITERATIONS EXCEEDED,I5)
      GO TO 90
  331 CONTINUE
C
C     EVALUATE FUNCTION AND CALCULATE TEST CRITERION FOR INITIAL
C     PARAMETER ESTIMATES
C
   14 DO 20 K=1,NRD
      FX(K)=0.
      DO 21 N=1,NP
      I=KY(N)
   21 PV(I)=PR(K,N)
      IF(ITEST)26,26,27
   27 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
      DO 68 I=1,NIDV
   68 X1(I)=X(J,I)
      CALL FUNC(Y1,X1,PV,NP)
      W(K,J)=Y1
      IF(ISMLT.EQ.0) GO TO 69
      FX(K)=FX(K)+WT(J)*ABS(Y(J)-W(K,J))
      GO TO 67
   69 FX(K)=FX(K)+WT(J)*(Y(J)-W(K,J))**2
   67 CONTINUE
   20 CONTINUE
C
```

```
C     CHOOSE THE SET OF PARAMETER ESTIMATES FOR WHICH THE TEST
C     CRITERION IS A MINIMUM
C
      MIN=1
      FZ=FX(1)
      DO 25 K=2,NRD
      IF(FX(K)-FZ)24,25,25
   24 MIN=K
      FZ=FX(K)
   25 CONTINUE
      IF(NC)53,53,31
   31 IF(FZ-FY)52,90,90
   53 NC=1
      IF(ISMLT.NE.0) GO TO 702
      WRITE(NOUT,701)FZ
  701 FORMAT(1H020X25HINITIAL SUM OF SQUARES IS ,E15.5 )
      GO TO 52
  702 WRITE(NOUT,703) FZ
  703 FORMAT(1H020X34HINITIAL SUM OF ABSOLUTE VALUES IS ,E15.5 )
C
C     CALCULATE THE SET OF PARTIAL DERIVATIVES
C
   52 DO 56 J=1,NP
      I=KY(J)
      UI(I)=PR(MIN,J)
      DO 56 K=1,NRD
   56 PR(K,J)=PR(MIN,J)
      FY=FZ
      DO 70 J=1,NUM
   70 F(J)=W(MIN,J)
      IF(NOPT)62,62,66
   62 DO 63 J=1,NUM
      DO 64 I=1,NIDV
   64 X1(I)=X(J,I)
      CALL DERIV(D,UI,X1,NP)
      DO 61 K=1,NP
      L=KY(K)
   61 DF(J,K)=D(L)
   63 CONTINUE
      GO TO 76
   66 DO 71 I=1,NCOL
   71 UJ(I)=UI(I)
      DO 72 I=1,NP
      J=KY(I)
      UK(J)=(1.+DELT)*UJ(J)
   72 UL(J)=UK(J)-UJ(J)
      DO 73 J=1,NUM
      DO 75 I=1,NIDV
   75 X1(I)=X(J,I)
      DO 74 I=1,NP
      K=KY(I)
      UJ(K)=UK(K)
      CALL FUNC(Y1,X1,UJ,NP)
      D1=(Y1-F(J))/UL(K)
      DF(J,I)=D1
   74 UJ(K)=UI(K)
   73 CONTINUE
   76 CONTINUE
C
C     CALCULATE THE CHANGE REQUIRED TO IMPROVE THE CURRENT SET OF
```

```
C     PARAMETER VALUES
C
   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,ISOLV)
C
C     CALCULATE THE SETS OF FRACTIONALLY INCREASING PARAMETER VALUES
C
      DO 42 I=1,NP
      V(I)=ZERO
      DO 42 J=1,NP
   42 V(I)=V(I)+AM(I,J)*BM(J)
   40 DO 60 K=1,NRD
      DO 60 J=1,NP
   60 PR(K,J)=PR(K,J)+RF(K)*V(J)
      ITN=ITN+1
      GO TO 17
   90 CONTINUE
C
C     PRINT OUT RESULTS
C
      DO 88 J=1,NP
      I=KY(J)
      UK(J)=UP(I)
   88 UJ(J)=UI(I)
      IF(ISMLT.NE.0) GO TO 704
      WRITE(NOUT,500) ITN,NRD,FY,(UK(J),UJ(J),J=1,NP)
  500 FORMAT(1H0/1H 2X5HAFTER,I6,17H ITERATIONS USING,I3,41H 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(1H0/1H 2X5HAFTER,I6,17H ITERATIONS USING,I3,51H REDUCTION F
     1ACTORS, THE SUM OF ABSOLUTE VALUES IS  ,E12.5 //(1H 10XA4,3H = ,E1
     22.5,2XA4,3H = ,E12.5,2XA4,3H = ,E12.5,2XA4,3H = ,E12.5,2X))
  705 CONTINUE
      IF(NWGT)39,39,41
   39 WRITE(NOUT,FMO)(F(I),Y(I),(X(I,J),J=1,NIDV),I=1,NUM)
      GO TO 43
   41 WRITE(NOUT,FMO)(F(I),Y(I),WT(I),(X(I,J),J=1,NIDV),I=1,NUM)
   43 CONTINUE
      GO TO 2
   99 CONTINUE
      STOP
       END
```

```
C
C
C     ************
      SUBROUTINE MATINT (O,B,K,ISOLV)
C     ************
C
      DIMENSION A(10,20),O(10,10),C(10,10),B(10)
      DATA ZERO/0.E1/,ONE/1.E0/
      NTI=5
      NTO=6
      CALL OVERFL(K000FX)
       GO TO(5,5),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 1060 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)) 1058,1060,1058
 1058 BP=A(I,N)
```

```
      B(I)=B(I)-B(N)*BP
      DO 1595 J=N,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 (1H0,21H 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
```

```
C
C
C     ************
      SUBROUTINE FUNC(Y,X,P,N)
C     ************
C
C     SUBROUTINE TO CALCULATE DENSITY FUNCTION FOR A MIXTURE OF TWO
C     NORMAL DISTRIBUTIONS
      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
```

```
C
C
C      ************
       SUBROUTINE DERIV(D,P,X,N)
C      ************
C
C      SUBROUTINE TO EVALUATE PARTIAL DERIVATIVES FOR THE PARAMETERS
C      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     ************
      SUBROUTINE TESPAR(P,N,K)
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).LT.0.) GO TO 4
      IF(P(5)-1.) 6,6,4
    4 K=1
    6 RETURN
      END
```

KANSAS GEOLOGICAL SURVEY COMPUTER PROGRAM
THE UNIVERSITY OF KANSAS, LAWRENCE

PROGRAM ABSTRACT

Title (If subroutine state in title):

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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26. FORTRAN IV computer program for simulation of transgression and regression with continuous-time Markov models, by W.C.Krumbein, 1968.
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