NON-LINEAR ESTIMATIONS

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INTRODUCTION TO NON-LINEAR ESTIMATIONS

Fundamental to the field of curve fitting in which estimation of non-linear parameters is involved is the idea of a "best fit." To obtain the "best fit", the principle of least squares is many times used. This principle underlies the research in this paper.

However, three other methods of curve fitting are mentioned in this report. The first is the obvious one of merely plotting the points on a graph, but this method fails when the number of dimensions is greater than two.

A method of grouping data into n groups and then using the average of each group as one of the n observations will result in n equations in n variables and, in general, a unique solution. This method is called averaging. Personal judgment can influence decisions. Thus, the division of ten observations into three groups involves some arbitrariness.

A third method is the principle of selected points, which is exactly what the name implies. One chooses n representative points and solves a resulting set of n equations to determine the n constants or parameters. The results obtained using this method would seem to be primarily a function of the points chosen, and this is actually the case. Regardless of this shortcoming, one would gain some idea of the values of the parameters if he is careful in the selection of the points. This idea of a starting value or a reasonably good estimate is basic to the Gauss-Newton iteration procedure of estimating non-linear parameters.

Basic to Regression Analysis is the idea of knowing what family of curves to attempt to fit to a given set of data. In

other words, the form of the equation and the parameters must be known before there can be an attempt to estimate the parameters.

Of first importance are the polynomial equations. If the observations are such that the x steps or changes, Δx, are equal, and the i^{th} difference ($\Delta^i y$) of y is approximately constant, then an i^{th} degree polynomial would be a good choice for a curve to which to fit the data. For example, if the Δx's are equal and $\Delta^2 y \doteq$ constant, then one should attempt to fit the data to the family of the form $y = Ax^2 + Bx + C$.

One should note the delusion involved in increasing i, the degree of the polynomial. As i approaches n, the error sum of squares will decrease, since for i = n, the error sum of squares equals 0, because n points will determine the n parameters or variables. As one increases the degree of the polynomial, the number of parameters being estimated increases, and, hence, the degrees of freedom decrease. Comparisons in curve fittings are made only when the degrees of freedom in the respective fittings are the same. Of importance also is the idea that one is fitting to a curve an approximation that fluctuates everytime there is an error in the measurement or the recording of the measurement or a malfunction in the experimental apparatus.

There are at least three basic families of curves which are of importance to industry and science that involve non-linear parameters. The three are based on the exponential, the power, and the hyperbolic functions.

To help one decide whether to attempt to fit a given set of data to an exponential function of the form $y = ab^x$, one can make a simple check which is derived from the properties of this family

of curves. When x is increased by one, y is multiplied by b. Therefore, if the x's are in an arithmetic progression and the corresponding y's form a geometric progression, the data is such that it could be closely approximated by means of an exponential function. For the modified exponential $y = a + bc^x$, where the x's are in an arithmetic progression, the changes in y (Δy) form a geometric progression although the y's themselves do not.

For the power function $y = ax^b$ where the x's are in a geometric progression, the y's will also form a geometric progression. For the case of the modified power function $y = a + bx^c$ where the x's are in a geometric progression, the y's will form a geometric progression although the y's themselves do not (10, p. 324).

For the hyperbolic equation of the form $y = a + b/x$, the expression $\Delta y/\Delta(1/x)$ is a constant because in the space with axes of $1/x$ and y, the equation is linear with slope $\Delta y/\Delta(1/x)$. For a hyperbolic equation of the form $y = x/(a + bx)$, one can deduce that $\Delta(x/y) / \Delta x$ is equal to a constant, by reasoning similar to the above.

One could find requirements for many different families of equations; however, those that are given seem to be the ones most commonly used and should serve as examples in case others are needed.

THE GAUSS-NEWTON METHOD

Seemingly the idea of least squares was first formulated by Legendre about 1806 (12, p. 210). He said that the most satisfactory solution to a set of m linear equations in n variables, with m greater than n, was the one giving a minimum to the sum of squares of error. If the i^{th} equation is of the form (2.1),

$$(2.1) \quad y_i \doteq a_1 x_{1i} + a_2 x_{2i} + \cdots + a_n x_{ni} \qquad (i = 1, 2, \ldots, m)$$

then the function to be minimized is $F(a_k;\ k = 1, 2, \ldots, n) = \sum_{i=1}^{m} E_i^2$, where E_i is given by

$$E_i = a_1 x_{1i} + a_2 x_{2i} + \cdots + a_n x_{ni} - y_i \qquad (i = 1, 2, \ldots, m).$$

The minimization can be done by setting the n first order partial derivatives with respect to the a_k of $F(a_k;\ k = 1, 2, \ldots, n)$ equal to zero. A system of n equations in n variables is obtained. The equations are called the normal equations. Since it can be shown that the coefficient matrix obtained in this manner has rank n when the x's are linearly independent, there is a unique solution of the system.

The development of the normal equations is given in part A of the appendix. One can form the first normal equation for a set of m equations in the following way: Multiply the first equation by the coefficient of the first variable of the first equation, multiply the second equation by the coefficient of the first variable in the second equation, and so on for all m equations; then add together the computed multiples of the original set of equations, and the result is the first normal equation (see part B

in the appendix). By using the coefficients of the second variable, one can obtain the second normal equation and, in similar manner, form all n normal equations. One should note that the coefficient matrix of equations obtained in this way will be symmetric. This simplifies considerably the amount of work involved in setting up the system and enables one to use results from the theory of symmetric matrices.

The method of least squares is easily used whenever all the parameters one wishes to estimate are involved linearly as the coefficients of terms in a function. Whenever a parameter is involved as an exponent, such as the parameter b in the function $y = ax^b$, the method thus illustrated leads to a system of equations for which the solution is very difficult to find. Most statisticians are well acquainted with a transformation which will change the above power function into a form such that the regular method of least squares can be easily used; but an important aspect of the situation is that few users of this technique realize its shortcomings.

The technique of changing the form to one which involves a function of a and a function of b linearly, is that of taking the logarithm of both sides. The resulting equation, $\log y = \log a + b \log x$ ($Y = A + bX$), is then linear in log a and b and can be fitted by the regular least squares method. In fact, in the space with distance measured by log y and log x, one is guaranteed a minimum for the error sum of squares.

Consider now an example of fitting the data given in Table 1 to a curve of the family $y = ax^b$ by this technique.

Table 1. Data for Power Function Fitting

x	y	X=log x	Y=log y	X^2	XY
1	2.5	0.	.3979	.0	.0
2	8.	.3010	.9031	.0906	.2718
3	19.	.4771	1.2788	.2276	.6101
4	50.	.6021	1.6990	.3625	1.0230
		$\sum X$=1.3802	$\sum Y$=4.2788	$\sum X^2$=.6807	$\sum XY$=1.9049

The normal equations are as follows:

$$4.0000\ A + 1.3802\ b = 4.2788$$

$$1.3802\ A + 0.6807\ b = 1.9049$$

The solution is that b = 2.096 and A = 0.3472, hence, a = 2.224. The required equation is then $y = 2.224x^{2.096}$. Table 2 shows the error sum of squares to be equal to 100.202.

Table 2. Calculations to find the Error Sum of Squares

x	y(calculated)	y(observed)	E	E^2
1	2.224	2.5	.276	.076
2	9.510	8.	-1.510	2.280
3	22.243	19.	-3.243	10.517
4	40.655	50.	9.345	87.329
				$\sum E^2$=100.202

Now for contrast, consider what happens if one selects the member of this family which passes through the last two points. This requires that $19 = a3^b$ and $50 = a4^b$. Then solving for b gives b = (log 50 - log 19) $\div$ (log 4 - log 3) = 3.36 and, therefore, a = 0.474. When one evaluates the error sum of squares, one finds a somewhat surprising value of only 13.93. This is considerably smaller than the "minimum!"

One needs to examine more closely what happens when one uses the logarithmic transformation. After using the transformation, one is then minimizing the error sum of squares of the logarithms of the deviations and not the error sum of squares of the deviations themselves. Logarithms are such that if the logarithms of two small numbers differ by 0.1, then the numbers can still be close together; whereas, the same difference in the logarithms of larger numbers may correspond to a much larger difference in the numbers. Since for the error sum of squares one is interested in the differences of the numbers, one would need to weight the logarithmic values to obtain the desired results. If one evaluates the error sum of squares of the logarithms of deviations in the first least squares fitting, one finds a value of 0.02098 while the corresponding number for the selected points fit is considerably higher at 0.56838.

A challenging problem has now arisen. By selecting two points through which to force the two parameter family of curves, one has obtained a better fit by the least squares criterion than one obtained by using a logarithmic transformation followed by a fitting of the transformed variables by least squares. Since one could have picked any combination of two points from the given set, this solution would have only a small probability of being the one that would give a minimum to the error sum of squares.

It seems that no simple one-step method exists that will guarantee the desired minimum; however, there are iterative procedures that will guarantee a reduction in the error sum of squares such that repetition of the process will enable the error sum of squares to approach a minimum, since the error sum of

squares is bounded from below. The method used in general practice to estimate non-linear parameters is now outlined. It is known as the Gauss-Newton Method.

Assume that the system to be satisfied, as nearly as possible,

$$(2.2) \qquad E_1(x,y;a) = 0, \quad E_2(x,y;a) = 0, \ldots, \quad E_n(x,y;a) = 0$$

is the system of equations (2.2); where x represents the independent variables, y represents the response variables, and $\underline{a}$ represents the parameters. Assume also that an approximate solution of the system is known. This last assumption is not unreasonable because an approximate solution can be obtained by determining the values of the parameters for the curve through a particular set of n points by the selected points method as was done earlier.

For any particular set of values of x_{ki} $(k = 1, 2, \ldots, n)$ and the corresponding value of y_i, the value of E_i is a function of the parameters. For the purpose of illustration, consider the case with two parameters. Represent these parameters by $\underline{a}$ and b with the beginning approximations of them by a_o and b_o.

If E is a function which can be represented by a Taylor series, then the system represented by (2.3) can be obtained. Each partial derivative is evaluated at the starting values; $a = a_o$, $b = b_o$.

$$(2.3) \quad E_i(a,b) = E_i(a_o,b_o) + (a - a_o)\frac{\partial E_i}{\partial a} + (b - b_o)\frac{\partial E_i}{\partial b} +$$

$$\frac{1}{2}\left[(a - a_o)^2\frac{\partial^2 E_i}{\partial a^2} + 2(a - a_o)(b - b_o)\frac{\partial^2 E_i}{\partial a \partial b} + (b - b_o)^2\frac{\partial^2 E_i}{\partial b^2}\right] + \ldots$$

Now, the equations of the system (2.4) are linear in the unknown corrections $(a - a_o)$ and $(b - b_o)$ of the parameters. One

is able them to use the method of least squares previously developed to estimate the adjustments to the starting values in place of estimating the true values themselves. The solution of the normal equations formed from (2.4) can be thought of as follows,

$$f = B_0 + B_1 Z_1 + B_2 Z_2$$

where Z_i is the partial derivative of f with respect to the i^{th} variable, and the B's are the estimates of the adjustments. Since B_1 is estimating the quantity $(a - a_0)$, or $B_1 \doteq a - a_0$, then $\underline{a} \doteq a_0 + B_1$. From this, one obtains a new starting value of the parameter $\underline{a}$. Similarly, one obtains new starting values for the other parameters. How close one actually gets to the true value of the parameters depends on the original starting values themselves for, if they are too much in error, neglect of higher order terms of the adjustments is not justified. Hence, an interpretation of the solution could definitely be misleading.

Continue now the work with the previous example to see if an improvement in fitting the data of Table 1 to the family of curves $y = ax^b$ can be made by using the Gauss-Newton method of estimating non-linear parameters. By using the starting values of $\underline{a}$ and b obtained when passing the curve exactly through the third and fourth points, the following equations and first order expansions are obtained. For simplification in writing let $u = (a - a_0) = (a - .474)$ and $v = (b - b_0) = (b - 3.36)$.

$f_1 = a - 2.5$	$f_1 \doteq -2.026 + u$	$= 0$
$f_2 = a2^b - 8.0$	$f_2 \doteq -3.135 + 10.267u + 3.372v$	$= 0$
$f_3 = a3^b - 19.0$	$f_3 \doteq 40.098u + 20.874v$	$= 0$
$f_4 = a4^b - 50.0$	$f_4 \doteq 105.411u + 69.314v$	$= 0$

The resulting normal equations are:

$$12{,}825.740\ u + 8{,}179.084\ v = 34.213$$
$$8{,}179.084\ u + 5{,}251.525\ v = 10.571$$

The corresponding solution is $u = 0.197$ and $v = -0.305$. Consequently, the revised estimates of a and b are as follows:

$$a = 0.474 + 0.197 = 0.671$$
$$b = 3.36 - 0.305 = 3.055$$

For the function $y = 0.671x^{3.055}$, the error sum of squares is 22.628 which is better than that obtained by the logarithmic fit but still is not as good as the fit obtained by the selected points methods. Remember, this is an iterative procedure with the results a function of the starting values. A second iteration where the functions are expanded about the adjusted values of the parameters gives the following results: $a = 0.733$, $b = 3.039$, and an error sum of squares equal to 10.052. This is smaller than any previously obtained error sum of squares. There is no reason to stop here if one wishes to obtain the minimum. One should continue until the improvement in the error sum of squares between successive fittings is sufficiently small. However, this suffices to show the improved results and how to use the technique.

MODIFICATIONS

An extension of the standard method of estimating non-linear parameters was developed by Kenneth Levenberg (8, p. 164) of the Frankford Arsenal. His method insures an improvement of the initial solution. One might appropriately ask why this is necessary. The reason is that the usual procedure has produced new values of the parameters which are not sufficiently close to the initial ones and has given rise to larger values of the sum of squares of the residuals (the error sum of squares) than that corresponding to the initial solution.

Let $h(x,y,z,\ldots;\alpha,\beta,\gamma,\ldots)$ be the function to be approximated or the actual true function in nature and $H(x,y,z,\ldots;a,b,c,\ldots)$ be the approximating function, where a, b, c,... are the least squares estimates of the unknown parameters α, β, γ,... and x, y, z,... are the observed variables. Then the residuals at the points $(x_1,y_1,z_1,\ldots)$ $i = 1,2,\ldots m$ are

$$f_i(\alpha,\beta,\gamma,\ldots) =$$

$$H(x_1,y_1,z_1,\ldots;a,b,c,\ldots) - h(x_1,y_1,z_1,\ldots;\alpha,\beta,\gamma,\ldots).$$

The least squares criterion requires minimization of the expression in (3.1).

$$(3.1) \qquad s(a,b,c,\ldots) = \sum_{i=1}^{m} f_i^2$$

Choosing an initial solution, $p_0 = (a_0,b_0,c_0,\ldots)$, at which it is assumed s does not have a stationary value, the first order Taylor expansion of the residuals taken about p_0 gives a set of linear approximations (3.2) to the residuals, where $\Delta a = a - a_0$,

$\Delta b = b - b_0, \ldots$, and the partial derivatives are evaluated at p_0.

$$(3.2)\quad f_i(\alpha,\beta,\gamma,\ldots) \doteq F_i(a,b,c,\ldots) = f_i(p_0) + \frac{\partial f_i}{\partial a}\Delta a + \frac{\partial f_i}{\partial b}\Delta b + \ldots$$

The Gauss-Newton method then requires the minimizing of S given in (3.3) by setting the partial derivatives of S with respect to the various parameters equal to zero.

$$(3.3)\quad S(a,b,c,\ldots) = \sum_{i=1}^{m} F_i^2$$

The system (3.4) is obtained where the bracket [ ] symbol stands for summation of the partial derivatives e.g. $[aa] = \sum_{i=1}^{m}\left(\frac{\partial F_i}{\partial a}\right)^2$, $[ab] = \sum_{i=1}^{m}\left(\frac{\partial F_i}{\partial a}\cdot\frac{\partial F_i}{\partial b}\right)$, $[aO] = \sum_{i=1}^{m}\left(\frac{\partial F_i}{\partial a}\cdot F_i\right)$. It is understood that these partial derivatives are evaluated at the starting point of each iteration.

$$(3.4)\quad \begin{aligned}
\tfrac{1}{2}\frac{\partial S}{\partial a} &= [aa]\Delta a + [ab]\Delta b + \ldots + [an]\Delta n + [aO] = 0\\
\tfrac{1}{2}\frac{\partial S}{\partial b} &= [ba]\Delta a + [bb]\Delta b + \ldots + [bn]\Delta n + [bO] = 0\\
&\vdots\\
\tfrac{1}{2}\frac{\partial S}{\partial n} &= [na]\Delta a + [nb]\Delta b + \ldots + [nn]\Delta n + [nO] = 0
\end{aligned}$$

One should note that large values of the increments Δa, $\Delta b, \ldots$ obtained by solving the above normal equations (3.4) may introduce a large error into the first order Taylor approximation of the next cycle such that a decrease in S, defined in equation (3.3), may not correspond to a decrease in s (3.1). In such cases, it would seem advisable to limit or damp the absolute values of the

increments of the parameters in order to improve on the first order Taylor approximation and to minimize simultaneously, if possible, the sum of the squares of the approximating residuals under these damped conditions. In order to make the increments and the residuals small in absolute value, one can apply the idea of least squares to the expression (3.5) where A, B, C,... is a set of positive constants or weighting factors expressing the relative importance of damping the different increments, and w is a positive quantity indicating the relative importance of the residuals and increments in the minimizing process.

$$(3.5)\quad \bar{S}(a,b,c,\ldots) = wS(a,b,c,\ldots) + A(\Delta a)^2 + B(\Delta b)^2 + C(\Delta c)^2 + \ldots$$

Denote the point at which $\bar{S}$ takes its minimum, for a given positive value of w, by $p_w = (a_w, b_w, c_w, \ldots)$ and set $Q(a,b,c,\ldots) = A(\Delta a)^2 + B(\Delta b)^2 + C(\Delta c)^2 + \ldots$.

Under the assumption that s is not stationary at p_o, one can obtain the following inequality:

$$wS(p_w) < wS(p_w) + Q(p_w) = \bar{S}(p_w) < \bar{S}(p_o) = wS(p_o) + Q(p_o) = wS(p_o).$$

It follows then that $S(p_w)$ is less than $S(p_o)$, and this shows that the minimization of (3.5) will diminish the sum of squares of the approximating residuals S.

By denoting the standard least squares solution to (3.4) by p_∞, the following inequality can be obtained:

$$wS(p_w) + Q(p_w) = \bar{S}(p_w) < \bar{S}(p_\infty) = wS(p_\infty) + Q(p_\infty) < wS(p_w) + Q(p_\infty).$$

It follows then that $Q(p_w)$ is less than $Q(p_\infty)$ which shows that the

increments given by the standard least squares solution of (3.4) will be improved in the sense that the weighted sum of their squares, Q, will be reduced.

The normal equations resulting in minimizing (3.5) are nearly the same as the system (3.4). The partial derivatives are as follows: $\frac{\partial \overline{S}}{\partial a} = w \frac{\partial S}{\partial a} + 2A\,\Delta a$, $\frac{\partial \overline{S}}{\partial b} = w \frac{\partial S}{\partial b} + 2B\,\Delta b$, ...

After dividing these partial derivatives by 2w, the resulting system can be simplified to the following:

$$\begin{aligned}
&([aa] + \tfrac{A}{w})\Delta a + [ab]\,\Delta b + \cdots + [an]\,\Delta n + [aC] = 0 \\
&[ba]\,\Delta a + ([bb] + \tfrac{B}{w})\Delta b + \cdots + [bn]\,\Delta n + [bC] = 0 \\
&\quad\vdots \\
&[na]\,\Delta a + [nb]\,\Delta b + \cdots + ([nn] + \tfrac{N}{w})\Delta n + [nC] = 0
\end{aligned}$$

This system is the same as (3.4), except for the coefficients of the principle diagonal elements, which are increased by quantities proportional to the weighting factors A, B, C,..., respectively. One is now able to see that by letting w become infinite, one obtains the regular normal equations and, hence, the reason for the notation, p_∞, as the ordinary least squares solution. This method will be referred to as "damped least squares."

It has been proven above that the sum of squares of the approximating residuals can be reduced by this technique; however, it remains to be shown that the sum of squares of the true residuals, s, can be diminished. This is done by showing that the derivative of s with respect to w is negative at some point. It can be shown (8, p. 167) that

$$\left(\frac{ds}{dw}\right)_{w=0} = -2\left\{\left[\frac{aO}{A}\right]^2 + \left[\frac{bO}{B}\right]^2 + \ldots + \left[\frac{nO}{N}\right]^2\right\}$$

which shows that the derivative of s with respect to w is negative at w = 0, since the fact that not all the partial derivatives are zero follows from the assumption that s is not stationary at the point p_o, and that A, B, C,... are positive constants. All this assures one that there is a value of w which can be found for which the sum of squares of the true residuals will be reduced.

The best value of w to use may be determined in theory by solving the following equation:

$$\frac{d\ S(p_w)}{dw} = 0.$$

However, due to the generally complicated nature of this equation, a first order Taylor expansion is generally substituted, giving the following:

$$S(p_w) \doteq S(p_o) + (w - 0)\left(\frac{dS}{dw}\right)_{w=0}.$$

By assuming that p_o was chosen so that the decreased value $S(p_w)$ is small, one can obtain the following equation for w.

$$w \doteq -\frac{S(p_o)}{\left(\frac{dS}{dw}\right)_{w=0}}$$

Levenberg (8, p. 167) says that this value of w may be improved upon by calculating $S(p_w)$ for several different trial values of w, so that the approximate minimum may be located graphically. One with a little experience will usually be able to get a good idea of the general order of magnitude of the best value of w,

especially in connection with fitting a particular function H, after graphing only a few points.

One should note that the coefficients of the weighting system A, B, C,... have been left arbitrary, the only restriction being that the weighting factors be positive. If the criterion that the directional derivatives of s, taken at w = 0 along the curve $a = a_0$, $b = b_0$,..., should have their minimum value, namely, the negative gradient, then the result is that the factors A, B, C,... are all equal. One can see by equation (3.5) that no generality is lost by letting them all equal unity. For this weighting system, the formation of the damped normal equations may be thought of as being accomplished simply by the addition of a positive constant, 1/w, to the coefficients of the principal diagonal of the standard normal equations. Another weighting system which has been used successfully is $A = [aa]$, $B = [bb]$,..., $N = [nn]$; in this case the damped normal equations are formed by multiplying the coefficients of the principal diagonal of the standard normal equations by a constant factor greater than unity, namely, $1 + 1/w$.

Since there is generally a tendency to go beyond the desired adjustment (6, p. 227), there has been introduced in practice the idea of damping the adjustments, say to seventy-five per cent of the least squares estimates. This is done to every parameter which one is estimating. The results of this technique are sometimes improved in that the speed of convergence is faster, but in other cases the opposite is true. Such a process, then, would not be recommended for a multi-purpose high speed digital computer program.

In this method of damped least squares, one is not required to decide on an arbitrary pre-assigned procedure restricting all the variables to the same extent. It seems that it is the greater degree of freedom given by this method to the individual variables that accounts for the fact that this method has solved (8, p. 168) types of problems which are of much greater complexity than those to which the principle of least squares is ordinarily applied. The rate of convergence has been sufficiently fast.

Almost simultaneous with Levenberg's publication was one (3) published by Haskell B. Curry, also of Frankford Arsenal, concerning non-linear estimations by using the method of steepest descent. His method has a much more theoretical basis but yields approximately the same results and, therefore, only brief reference is made to it in this report. There has been, however, a more recent development in the field of estimating non-linear parameters, and the intuitive notion that the adjustments tend to over-correct seems to be included.

Dr. H. O. Hartley, a professor at Iowa State University, has developed (6, p. 269) another modification of the standard Gauss-Newton method for estimating non-linear parameters by using the principle of least squares. This modification follows the standard method until one finds a first solution to the normal equations. At this point in the process, one can define a function of v as follows:

$$S(v) = S(x, \theta_0 + vD), \qquad 0 \leq v \leq 1.$$

The x represents the observed variables, θ_0 represents the

parametric variables evaluated at the starting point, and D represents the least squares solutions just obtained from the normal equations. Hence, $\theta_0 + vD$, where v is a scalar, represents the parametric variables evaluated at their starting values plus a part of the adjustment indicated by the least squares solution. If one then denotes by v' the value of v for which S(v) is a minimum on the unit interval of v and defines $\theta_1 = \theta_0 + v'D$, one can conclude that $S(x,\theta_1) \leq S(x,\theta_0)$. One can then repeat the process by starting with a Taylor expansion about θ_1 and will be assured convergence to the minimum under the assumption that θ_0 is not a stationary in S. The process up to this point seems to be quite similar to the one developed by Levenberg.

Hartley proves (6, p. 272) that under the given set of conditions; first, the functions are continuous; second, the coefficient matrix has full rank; and third, there exists a starting vector θ_0 in the interior of a bounded convex set T such that $S(x,\theta_0) < \square$ where $\square$ equals the lim inf $S(x,\theta)$ on $\overline{T}$, the compliment of T; then by using S(v'), one will obtain in the limit a unique minimum. However, the worth of this modification and a significant difference from the previous methods seem to lie in the fact that one need not find this v' exactly but can use a relatively easily obtained approximation to it, say v_p, as given in (3.6).

$$(3.6) \qquad v_p = \tfrac{1}{2} + \tfrac{1}{4}\left\{[S(0) - S(1)] \;/\; [S(1) - 2S(\tfrac{1}{2}) + S(0)]\right\}$$

This is nothing more than finding the sum of squares of residuals at $(\theta_0 + \tfrac{1}{2}D)$ which is equal to $S(\tfrac{1}{2})$ and then finding the v coordinate of the horizontal tangent to a "parabola" fitted through

the three points $[0, S(0)]$, $[\frac{1}{2}, S(\frac{1}{2})]$, and $[1, S(1)]$ in a $[v, S(v)]$ space. Then one is ready to repeat the process using $\theta_1 = \theta_0 + v_p D$ as the starting vector.

Consider now a numerical example of the modified Gauss-Newton method. The data of Table 3 has been taken from a fertilizer

Table 3. Data from Fertilizer Experiment

x	y
-5	127
-3	151
-1	379
1	421
3	460
5	426

experiment in which there were six responses representing the yields of wheat corresponding to six rates of application of fertilizer which, on a coded scale, are given the values in the table.

It is intended to fit this data to a curve representing the exponential law of the following form.

$$y = L + Be^{Kx}$$

This equation is sometimes called Mitcherlisch's Law of Diminishing Returns in which x is the only input variable. L is the asymptotic yield for large rates of fertilizer application, K is the exponential rate of the response decrease, and B defines the mid-point response at x = 0 by giving it the value L + B. For this example, choose the following starting values.

$$L_0 = 580 \qquad B_0 = -180 \qquad K_0 = -.160$$

The partial derivatives needed for (2.4) are:

$$\frac{\partial Y}{\partial L} = 1 \qquad \frac{\partial Y}{\partial B} = e^{Kx} \qquad \frac{\partial Y}{\partial K} = Bxe^{Kx}$$

The normal equations are exhibited in Table 4 where $D_1 = L - L_0$, $D_2 = B - B_0$, and $D_3 = K - K_0$.

Table 4. The formulas for the coefficients in the normal equations of Nitcherlisch's law.

D_1	D_2	D_3	
n	$\sum e^{K_0x}$	$B_0\sum xe^{K_0x}$	$\sum(y-y_0)$
$\sum e^{K_0x}$	$\sum e^{2K_0x}$	$B_0\sum xe^{2K_0x}$	$\sum(y-y_0)e^{K_0x}$
$\sum xe^{K_0x}$	$B_0\sum xe^{2K_0x}$	$B_0^2\sum x^2e^{2K_0x}$	$B_0\sum(y-y_0)xe^{K_0x}$

The evaluation of the entries of Table 4 is given in Table 5, and the solution of the normal equations is:

$$D_1 = -89.68 \qquad D_2 = 58.89 \qquad D_3 = -.06312$$

Table 5. Coefficients in the normal equations for cycle 1

D_1	D_2	D_3/B_0	
6.	6.935	-12.194	-267.634
6.935	10.253	-31.093	-370.782
-12.194	-31.093	157.927	1055.627

The next stage is to find the minimum of S(v) on the unit interval of v. One can use the approximating parabola corresponding to (3.6) to find the minimum. The error sums of squares are

$$S(0) = 27376.8 \qquad S(\tfrac{1}{2}) = 17400.7 \qquad S(1) = 14586.0,$$

and it follows that $v_p = .9965$. To find the next trial values of

the parameters, one replaces L by $L_0 + v_p D_1$ and the other parameters by similar expressions. The following values are obtained.

$$L_1 = 495.2 \qquad B_1 = -124.3 \qquad K_1 = -.2197$$

These and further results are listed in Table 6.

Table 6. Convergence of least squares estimates in four cycles.

	L	B	K	S(0)
Cycle 1	580.00	-180.00	-.16000	27376.
2	495.21	-124.26	-.21974	14590.
3	524.96	-159.27	-.19065	13639.
4	519.42	-152.49	-.20354	13394.
	523.3	-157.0	-.1994	

For further examples, see (6, p. 277).

FURTHER MODIFICATIONS

The modified Gauss-Newton method as developed by Hartley and at least hinted at earlier by G. E. P. Box (6, p. 280) is one method of estimating non-linear parameters in regression analysis that is particularly well suited for application on the high speed digital computers. In fact, Mr. Carlton Hassell and Dr. Dale Cooper, both of the Mathematical Research Section of Continental Oil Company, have worked for some time in this area and plan to publish their results soon. Their program, called NONLN, was written for the International Business Machines' 7090 and is capable of solving a great number of the conceivable practical problems. It uses the modification given by Hartley.

Presented now are some additional ideas of interest in estimating non-linear parameters with the majority of the results being applicable to computers. One can modify even more the Hartley modification of the Gauss-Newton method. One of the best changes in technique is to eliminate the need for having a starting value of any of the linear parameters. One could fit a curve for various values of the non-linear parameters, with each find the corresponding least squares estimate of the linear parameters and then, by graphing the results, find the value of the non-linear parameters where one should hope to find a smaller error sum of squares. Next will be given a method of finding the adjustment of the non-linear parameters without having to estimate any linear parameters and also not relying as much on a trial and error procedure as the graphing procedure just described.

Hartley considers (6, p. 274) an equation of the form (4.1) where y is the response variable and x is the independent variable,

$$y = r + se^{tx} = f(x). \tag{4.1}$$

The letters r, s, and t, therefore, stand for parameters to be estimated but only r and s are involved linearly. Hence this is a non-linear estimation problem. Consider then the first order Taylor expansion of (4.1) given in (4.2) and simplified in (4.3).

$$y = f_0 + (r - r_0)\frac{\partial f}{\partial r} + (s - s_0)\frac{\partial f}{\partial s} + (t - t_0)\frac{\partial f}{\partial t} \tag{4.2}$$

$$y = f_0 + (r - r_0) + (s - s_0)e^{t_0 x} + (t - t_0)s_0 x e^{t_0 x} \tag{4.3}$$

Since the partial derivative of f with respect to r does not involve the variable x, one can consider (4.3) in the form (4.4) where B_0, B_1, and B_2 are parametric constants being solved for by the general method of least squares.

$$y = B_0 + B_1 e^{t_0 x} + B_2 x e^{t_0 x} \tag{4.4}$$

When comparing (4.3) and (4.4), the estimations (4.5) follow.

$$B_0 \doteq y_0 + (r - r_0) \qquad B_1 \doteq s - s_0 \qquad B_2 \doteq (t - t_0)s_0 \tag{4.5}$$

If one will now delete the last term of (4.3), the equation is of the form (4.6) which is the same as (4.1).

$$y = b_0 + b_1 e^{t_0 x} \tag{4.6}$$

If one then fits the same data to (4.6) as fitted to (4.4), the estimations (4.7) follow.

$$b_0 \doteq r_0 \qquad b_1 \doteq s_0 \tag{4.7}$$

By combining the last approximations in (4.5) and (4.7), one obtains the estimate given by (4.8).

$$\frac{B_2}{b_1} = t - t_0 \qquad \text{or} \qquad t = t_0 + \frac{B_2}{b_1} \tag{4.8}$$

This adjustment to t_0 to obtain a better approximation of the true value of the non-linear parameter t has been done without assuming any particular value for any of the linear parameters. The corresponding values of $b_0 = r_0$ and $b_1 = s_0$ are the least squares estimates of those parameters r and s which go with the particular value t_0 of t which has been used.

The generalization of the above example is rather straightforward. A constant term in f causes no difficulty because in the Taylor expansion it can be incorporated into B_0 of (4.4), and it is estimated by a regular least squares method in (4.6). The coefficient of a term is taken care of when it is estimated in (4.6). The adjusted value of a non-linear parameter is obtained as in (4.8).

If two non-linear parameters are assumed as in the following equation,

$$y = r + s_1 e^{t_1 x} + s_2 e^{t_2 x^2},$$

then one needs only to add the corresponding partial derivatives to (4.3) and the corresponding term to (4.6) before making the fittings. However, if two non-linear parameters are involved in one term in such a way that they cannot be combined into one non-linear parameter, then this technique breaks down due to the

interaction of the two non-linear parameters and the need to estimate functions of the observed variables.

The step of deleting a term, as was done in going from (4.4) to (4.6), can be included in a computer program very easily. One can use a first matrix to store the elements of the normal equations of all the terms formed and then use a second matrix in solving the normal set where one transfers to the second matrix only the terms of present interest. Since all terms are still stored in the first matrix, one can obtain all combinations that might be desired.

If one examines the v_p (3.6), he can find some interesting ideas that should be considered if he is to program a high speed computer to solve non-linear estimation problems. Even if one is attacking this lengthy problem by hand, an aid here and there will help. Since one is considering how much of the suggested least squares adjustment should really be taken, one is interested in the error sum of squares as v ranges from zero to one. Since the approximating curve generally used is a parabola through $S(0)$, $S(\frac{1}{2})$, and $S(1)$ where $S(0)$, the sum of squares of residuals at the starting point, and $S(1)$, correspondingly the sum at the full adjustments, are already evaluated. $S(\frac{1}{2})$ is then computed. For the minimum of $S(v)$ to be on the unit interval of v, and where $\Delta S = S(1) - S(0)$, the value of $S(\frac{1}{2})$ must satisfy inequality (4.10).

$$S(\tfrac{1}{2}) \leq \tfrac{1}{2}\left[S(0) + S(1)\right] - \tfrac{1}{4}\left|\Delta S\right| \tag{4.10}$$

The inequality (4.10) implies that

$$\left|S(\tfrac{1}{2}) - S(0)\right| \leq \tfrac{1}{2}\left|\Delta S\right| \qquad \text{or} \qquad S(\tfrac{1}{2}) < S(0).$$

This leads to an answer to the question of why this evaluation should be included in a multipurpose non-linear program. Since equation (3.6) furnishes merely a formula for finding the abscissa of the horizontal tangent, the graph of the equation may have a maximum at v_p; and if the following inequality is satisfied,

$$S(\tfrac{1}{2}) > \tfrac{1}{2}\left[S(0) + S(1)\right] + \tfrac{1}{4}\left|\Delta S\right|,$$

then the value of v obtained will be in the unit interval of v and will correspond to a maximum for the error sum of squares. If one is attempting to find a minimum, then any further evaluation would be a waste of time. Also, if $S(\frac{1}{2})$ is below the average of S(0) and S(1) but does not satisfy (4.10), then the horizontal tangent found by using (3.6) will correspond to a minimum; it will be located outside the unit interval of v and, hence, outside of the domain of definitions of S(v).

One might appropriately ask if all of this is really relevant to the problem or whether these situations actually occur. The answer is yes; they happen often and in two particular places--the beginning and the end. The occurrence at the beginning is usually due to very poor starting values resulting in divergence. A quick check of this tendency would allow one to relinquish the computer and examine this particular problem more closely.

After running only a few iterations of this modified Gauss-Newton method, one will generally be converging upon an answer. Usually within only four or five iterations, even the accuracy of the machine begins to play a part. On one fitting which was run for nine cycles, one could see that a step function had been obtained for the error sum of squares. This was attributed to

the round off error resulting from doing the computation with only eight significant digits. Such errors are the cause of trouble at the end of the converging process; but since one does want the best fit available, it is worthwhile to continue as long as the sum of squares of residuals is decreasing. When the process does give a larger value at S(1) than at S(0), and S($\frac{1}{2}$) is computed, then by examining inequality (4.10), one can tell whether to continue or to be satisfied with the acquired approximation.

Thus far in this section, consideration has been given to techniques useful to computers in estimating the value of non-linear parameters by the modified Gauss-Newton method as developed by Hartley (6, p. 263). There is one aid for non-linear estimation that is applicable to the general Gauss-Newton method and not to the modified method.

If the regular Gauss-Newton method gives a first adjustment to a non-linear parameter to be "add 1.00" and on the second iteration gives an adjustment of "subtract 0.40," the percentage that the second adjustment is of the first, disregarding the sign, is 40. In practice it is found that this percentage which the $(n + 1)^{th}$ adjustment is of the n^{th} is approximately constant. Assuming that the ratio is constant leads one to an infinite geometric series which has an easily calculated sum given by the following, (4.11).

(4.11) $$\text{Sum} = \frac{a}{(1 - r)}$$

The letter a stands for the value of the first adjustment and r for the common ratio. From this, one is able to find after only

two iterations the value of parameters which ordinarily would have taken eight or ten cycles to find. It would be advisable, however, at least until more theory or research is done on this technique, to check the value of the error sum of squares at this new point. This is not added work since one is generally seeking the value of the error sum of squares at this point. This is a simple aid to help find a better approximation faster than the standard Gauss-Newton methods would find it.

In practice, r is usually negative, which means, as illustrated in the accompanying graph, that the tendency is to "over-adjust."

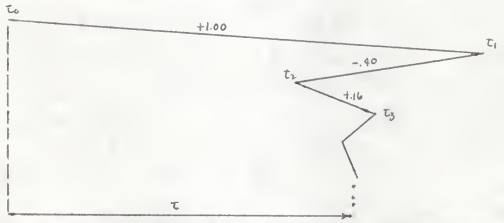

DIAGRAM OF ADJUSTMENTS ON THE NON-LINEAR PARAMETER t

This characteristic of over-correction corresponds with Hartley's principle of finding the minimum of S(v) on the unit interval of v. If the expected value of the sought for non-linear parameter were outside this unit interval, then one would need to extend the domain of S(v) to the whole real line; and this is just exactly the opposite of what has been sought. Most of the difficulties that have occurred in non-linear estimation by the standard

Gauss-Newton method have been associated with too great an adjustment on the parameters thus ruining the first order approximation obtained by Taylor series and resulting in an increase in the error sum of squares.

Mentioned earlier was the fact that this geometric series (4.11) is not formed by the modified Gauss-Newton method. The reason is that the process of finding the minimum on the unit interval of v does not retain the seemingly inherent property of the Taylor series expansion allowing the ratio of successive adjustments to the parameters to remain constant. If a geometric series were formed, this would mean that the minimum is always the same percentage of the distance from the starting value to the adjusted value.

The application of this process to a computer is not of too much value for two reasons. The first is that the modified method is not too much more difficult to program, and it speeds up the convergence from requiring ten cycles down to as few as four. Second, one iteration of NONLN on the I.B.M. 7090 requires approximately four seconds.

APPENDIX

Part A: Development of the Normal Equations

Let y_i be the observed ordinate and Y_i be the calculated approximation to y_i. Therefore,

$$y_i \doteq Y_i = \sum_{j=1}^{n} a_j x_{ij}; \qquad (i = 1,2,\ldots,m).$$

Let the residuals, E_i, be defined as follows:

$$E_i = \sum_{j=1}^{n} a_j x_{ij} - y_i; \qquad (i = 1,2,\ldots,m).$$

Hence,

$$E_i^2 = \sum_{j=1}^{n} a_j^2 x_{ij}^2 + 2 \sum_{j=1}^{n} \sum_{\substack{k=1 \\ j \neq k}}^{n} a_j a_k x_{ij} x_{ik} - 2 \sum_{j=1}^{n} a_j x_{ij} y_i + y_i^2$$

for $i = 1,2,\ldots,m$; and

$$F = \sum_{i=1}^{m} E_i^2.$$

Considering the first partial derivative of F with respect to a_1, one finds

$$\frac{\partial F}{\partial a_1} = 2 \sum_{i=1}^{m} a_1 x_{i1}^2 + 2 \sum_{i=1}^{m} \sum_{k=1}^{n} a_k x_{i1} x_{ik} - 2 \sum_{i=1}^{m} x_{i1} y_i,$$

which simplifies to

$$\frac{\partial F}{\partial a_1} = 2 \sum_{i=1}^{m} \sum_{k=1}^{n} a_k x_{i1} x_{ik} - 2 \sum_{i=1}^{m} x_{i1} y_i.$$

One finds that by setting the n first order partial derivatives--$\frac{\partial F}{\partial a_j}$, $j = 1,2,\ldots,n$--to zero, the following system of equations must be satisfied:

$$\sum_{i=1}^{m}\sum_{k=1}^{n} a_k x_{ij} x_{ik} = \sum_{i=1}^{m} x_{ij} y_i; \qquad (j = 1,2,\ldots,n).$$

This system of equations is called the system of normal equations. For a review of what is necessary to make certain that the solution of the above system is a minimum of F, one can read in Brand's "Advanced Calculus" on page 188.

Part B: A method used on computers for forming the Normal Equations.

Consider the two parameter family of straight lines $y = c + bx$ for which five observations have been made, but, where co-ordinates do not actually lie on a straight line. Assume the resulting equations from the observations to be

(1) $c + 1.0b \doteq .9$

(2) $c + 1.9b \doteq 3.0$

(3) $c + 2.6b \doteq 4.0$

(4) $c + 3.2b \doteq 5.5$

(5) $c + 4.0b \doteq 6.9.$

Form the two normal equations in the following manner. Add the five equations to form the first normal equation. It would be $5c + 12.7b = 20.3$. The first normal equation can be formed in this way only when there is a constant term involved, as c is in this example. If there is not a constant term, one forms the first normal equation in a manner similar to the others. The second normal equation can be formed by first multiplying (1) by 1.0, (2) by 1.9, and so on, multiplying each equation by the coefficient of b in that equation and then adding together these computed multiples of the original equations. The result is $12.7c + 37.61b = 62.2$.

If there were more parameters, the corresponding normal equations would be formed in a manner similar to that of forming the second.

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NON-LINEAR ESTIMATIONS

by

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AN ABSTRACT OF A MASTER'S REPORT

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The purpose of this report has been to collect and organize some of the better methods of dealing with problems in regression analysis that are related to non-linear parameters, including some of the techniques that are used in industry which have not yet found their way into publications.

Since the least squares method of estimation is basic to the methods given in this report, its detailed development has been included in the appendix. This makes it available as needed without breaking the continuity of the report.

Due to the extensive length of non-linear estimation problems and the increasing availability of the high speed digital computers, the majority of techniques that are included in this report are those which have applications suitable to programs for digital computers and require fairly simple programing. It should be noted that regression analysis in general is no easy problem.

The procedure has been to illustrate the need for and the development of the basic method of estimating non-linear parameters called the Gauss-Newton Method. The theory of two of the modifications that have proven their worth in applications are given. Some examples have been included to illustrate the processes in action.

The first of the methods considered is called "damped least squares" and was developed by Mr. K. Levenberg of the Frankford Arsenal and published in 1944. This method has solved some of the more complicated problems in non-linear estimation and has a relatively fast rate of convergence. It seems that one needs considerable experience in order to set up the problem.

The second method is attributed to Dr. H. O. Hartley of Iowa State University and was published in 1961 under the name of the Modified Gauss-Newton Method. The applications of this method, when considered in the light of some numerical short cuts, seem to be usable on the digital computers.

With the help of a technique used by Dr. Dale Cooper, of the Continental Oil Company, this second method is simplified even more to the point where a starting estimate of the linear parameters is not required. This, in a sense, reduces the number of approximations that are used in the equations.