Fitting data to nonlinear functions with uncertainties in all measurement variables

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An analytical approach is made to the nonlinear least squares problem having uncertainties in all measurements coordinates. It is shown how the unknown independent coordinates may be eliminated from the sum of the squares, thus reducing it to an ordinary minimisation problem. An algorithm is derived using analytical derivatives, but a simple procedure also allows the use of standard numerical derivatives.

(Received April 1974)

The problem under consideration here is that of using the least square method of curve fitting the function $f(x_i, a_j)$ which may be nonlinear in x_i, the adjusted X_i data coordinate, and nonlinear in the M parameters a_j to the data $Y_i \pm \sigma_{yi}$ and $X_i \pm \sigma_{xi}$ where i goes from 1 to N the number of data points.

A previous paper by the author (Southwell, 1969) presented an iterative solution to the problem and partially demonstrated its use by applying it to a well-known example. Since then, D. R. Powell and J. R. Macdonald (1972) claim that the method would not converge to the least squares solution and often would not converge at all.

The purpose of this paper is to generalise the method and make it more explicit, to show how the central theory allows the use of any nonlinear minimisation algorithm (of which there are several successful ones), to show that it does converge to the least squares solution, to present a simple numerical derivative application of the method that requires no analytical derivatives to be supplied, and finally, to comment on several other claims made by Powell and Macdonald.

Several examples are included that demonstrate various aspects of the application of the theory.

Theory

According to the least squares principle we minimise the quantity $\chi^2/2$, denoted by S,

$$S = \sum_i S_i = \sum_i \tfrac{1}{2}[w_{yi}(Y_i - f(x_i, a_j))^2 + w_{xi}(X_i - x_i)^2] \qquad (1)$$

where the weights are $w_{yi} = 1/\sigma_{yi}^2$ and $w_{xi} = 1/\sigma_{xi}^2$. This is a nonlinear minimisation problem requiring an iterative procedure starting from some initial approximations. The first step in this method is to eliminate the x_i dependence in S by the condition

$$\frac{\partial S}{\partial x_i} = \frac{\partial S_i}{\partial x_i} = d_i = 0 \; . \qquad (2)$$

These are N equations each containing only one x_i, thus simultaneous solution procedures are not necessary. When (2) is solved directly for x_i, substitution in (1) then allows the parameters a to be determined by standard nonlinear minimisation techniques. S will have a new form but will not have any x_i dependence, $S = S(a_j)$.

When (2) does not yield a closed form solution $x_i = x_i(a_j)$, then it must be solved by numerical iteration for x_i (by using Newton's method, for example, although it is not globally convergent) from some initial starting values, usually X_i. Using this numerical value for x_i allows the proper evaluation of S, but will not provide its functional dependence in a_j. What we have is $S = S(x_i(a_j), a_j)$ where the explicit function $x_i = x_i(a_j)$ is not known.

To minimise S we evaluate its derivatives with respect to the a_j. To obtain them we apply the chain rule to the function $S(x_i(a_j), a_j)$

$$\frac{\partial}{\partial a_k} \rightarrow \frac{\partial x_i}{\partial a_k}\frac{\partial}{\partial x_i} + \frac{\partial}{\partial a_k}\bigg|_{x_i = \text{ const.}} \qquad (3)$$

As stated above we do not have the explicit function $x_i(a_j)$, so it would appear we are unable to apply (3). However, by differentiation of (2), which is the equation that determines the x_i, with respect to a_k we obtain an equation linear in $\partial x_i/\partial a_k$. Thus with the numerical value of x_i from a solution to (2), we can always apply (3) no matter what nonlinearity there is in f.

Having the derivatives of S we are now able to apply any nonlinear minimisation technique. Convergence of the chosen technique insures that we have the least squares solution.

Implicit models

The function f represents y_i, the adjusted Y_i coordinate. If y_i is contained implicitly in the model $A = A(y_i, x_i, a_j) = 0$, such that there does not exist a closed form function $f = y_i = f(x_i, a_j)$, then A must be solved iteratively for each y_i whenever f_i is required in applying the above theory. This is done in the same way x_i was determined from d_i in (2). Newton's method may be used, with Y_i usually providing good starting points. The derivatives of f_i are determined by implicit differentiation of A using the chain rule in exactly the same way the derivatives of x_i were determined from d_i. This process was programmed and used successfully with real data on an implicit equation of state model.

Further generalisations

It is straightforward to generalise the above theory to include models having more than one independent variable.

A recent paper by H. I. Britt and R. H. Luecke (1973) presents a solution to the problem, which we discuss further below, in which the problem is formulated to include even further generalisations. Their solution is also applicable to models where f has a different functional dependence at each data point such that $\partial f/\partial x_2$ may be a function of x_1 and x_3, for example, and where data covariances are considered. Such generalisations are possible with our present method, but we have not done so here.

Application of theory

We now proceed to derive the algorithm in terms of the function $f(x_i, a_j)$ and its derivatives.

Equation (2) is solved by Newton's iterative method

$$x_i^{\text{new}} = x_i - d_i \Big/ \frac{\partial d_i}{\partial x_i} \cdot \qquad (4)$$

The right hand side is evaluated at the present values of x_i and a_j. Performing the indicated derivatives we have

$$x_i^{\text{new}} = x_i + \left[w_{yi}(Y_i - f_i)\frac{\partial f_i}{\partial x_i} + w_{xi}(X_i - x_i)\right] D/w_{yi} \; , \qquad (5)$$

where

$$D = w_{yi} \Big/ \left[w_{xi} + w_{yi} \left(\frac{\partial f_i}{\partial x_i} \right)^2 - w_{yi}(Y_i - f_i) \frac{\partial^2 f_i}{\partial x_i^2} \right] . \quad (6)$$

and where $f_i = f(x_i, a_j)$. The first entry will use some initial estimates for x_i (usually X_i). The improved x_i^{new} is tested to determine if $|x_i^{new} - x_i|$ is less than some small quantity, say, 10^{-7}. If not, x_i is set equal to x_i^{new} and another step is taken. After convergence is obtained, the solution could be saved and used as starting points for successive iterations to conserve computer time.

Whenever S or any of its derivatives are evaluated, the solution to (4) provides a numerical value for x_i.

Most of the nonlinear minimisation techniques use only S and its gradient g, the components of which are

$$g_k = \frac{\partial S}{\partial a_k} . \quad (7)$$

Differentiating (1) using (3) we obtain

$$g_k = \sum_i \left[-w_{yi}(Y_i - f_i) \left(\frac{\partial x_i}{\partial a_k} \frac{\partial f_i}{\partial x_i} + \frac{\partial f_i}{\partial a_k} \right) - w_{xi}(X_i - x_i) \frac{\partial x_i}{\partial a_k} \right] . \quad (8)$$

where $\partial x_i / \partial a_k$ is determined by differentiation of (2),

$$\frac{\partial x_i}{\partial a_k} = \left[(Y_i - f_i) \frac{\partial^2 f_i}{\partial a_k \partial x_i} - \frac{\partial f_i}{\partial a_k} \frac{\partial f_i}{\partial x_i} \right] D , \quad (9)$$

where D is given in (6) above.

The question as to which minimisation technique is best probably depends on the function f and the data. Recently Cornwell and Rigler (1972) made a comparison of four successful stable algorithms, conjugate gradient, variable metric, damped least squares, and Grey's orthogonalisation on a variety of problems. Their conclusion was that there was no 'universally best nonlinear optimiser' and that each method was best for at least one problem. All of these methods require only S and $\mathbf{g}$ to be evaluated and all, in theory at least, may be applied to the present problem.

It has been the author's experience that the method outlined in his previous paper (Southwell, 1969), which is a generalised Newton–Raphson approach, has been highly successful. The parameters in this approach are iteratively determined by the relation

$$\mathbf{a}^{new} = \mathbf{a} - \mathbf{R}^{-1} \mathbf{g} \quad (10)$$

where the components of the square matrix $\mathbf{R}$ are

$$\mathbf{R}_{lk} = \frac{\partial^2 S}{\partial a_l \partial a_k} . \quad (11)$$

To obtain $\mathbf{R}$ in terms of f and its derivatives, we differentiate (8) using (3) again. The result is

$$\begin{aligned} \mathbf{R}_{lk} = \sum_i \Bigg\{ & w_{yi} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial f_i}{\partial x_i} + \frac{\partial f_i}{\partial a_l} \right) \left(\frac{\partial x_i}{\partial a_k} \frac{\partial f_i}{\partial x_i} + \frac{\partial f_i}{\partial a_k} \right) \\ & - w_{yi}(Y_i - f_i) \left[\frac{\partial x_i}{\partial a_k} \left(\frac{\partial x_i}{\partial a_l} + \frac{\partial^2 f_i}{\partial x_i^2} + \frac{\partial^2 f_i}{\partial a_l \partial x_i} \right) \right. \\ & \left. + \frac{\partial f_i}{\partial x_i} \frac{\partial^2 x_i}{\partial a_l \partial a_k} + \frac{\partial x_i}{\partial a_l} \frac{\partial^2 f_i}{\partial x_i \partial a_k} + \frac{\partial^2 f_i}{\partial a_l \partial a_k} \right] \\ & - w_{xi}(X_i - x_i) \frac{\partial^2 x_i}{\partial a_l \partial a_k} + w_{xi} \frac{\partial x_i}{\partial a_l} \frac{\partial x_i}{\partial a_k} \Bigg\} . \end{aligned} \quad (12)$$

The partial of x_i with respect to a_j is given in (9). To obtain the necessary second partial, (9) is differentiated using (3) again. This gives

$$\begin{aligned} \frac{\partial^2 x_i}{\partial a_l \partial a_k} = & \left[(Y_i - f_i) \left(\frac{\partial x_i}{\partial a_l} \frac{\partial^3 f_i}{\partial a_k \partial x_i^2} + \frac{\partial^3 f_i}{\partial a_l \partial a_k \partial x_i} \right) \right. \\ & - \frac{\partial^2 f_i}{\partial a_k \partial x_i} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial f_i}{\partial x_i} + \frac{\partial f_i}{\partial a_l} \right) - \frac{\partial f_i}{\partial a_k} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial^2 f_i}{\partial x_i^2} + \frac{\partial^2 f_i}{\partial a_l \partial x_i} \right) \\ & \left. - \frac{\partial f_i}{\partial x_i} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial^2 f_i}{\partial x_i \partial a_k} + \frac{\partial^2 f_i}{\partial a_l \partial a_k} \right) \right] D \\ & - \left[(Y_i - f_i) \frac{\partial^2 f_i}{\partial a_k \partial x_i} - \frac{\partial f_i}{\partial a_k} \frac{\partial f_i}{\partial x_i} \right] \\ & \left[2 \frac{\partial f_i}{\partial x_i} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial^2 f_i}{\partial x_i^2} + \frac{\partial^2 f_i}{\partial a_l \partial x_i} \right) - (Y_i - f_i) \right. \\ & \left(\frac{\partial x_i}{\partial a_l} \frac{\partial^3 f_i}{\partial x_i^3} + \frac{\partial^3 f_i}{\partial a_l \partial x_i^2} \right. \\ & \left. \left. + \frac{\partial^2 f_i}{\partial x_i^2} \left(\frac{\partial x_i}{\partial a_l} \frac{\partial f_i}{\partial x_i} + \frac{\partial f_i}{\partial a_l} \right) \right] D^2 . \end{aligned} \quad (13)$$

Equation (13) with (9) enables the determination of all the components of $\mathbf{g}$ and $\mathbf{R}$ in terms of f and its derivatives. For the present value of x_i and a_j, the quantities that need to be supplied are

$$f_i, \frac{\partial f_i}{\partial x_i}, \frac{\partial^2 f_i}{\partial x_i^2}, \frac{\partial^3 f_i}{\partial x_i^3}, \frac{\partial f_i}{\partial a_k}, \frac{\partial^2 f_i}{\partial a_k \partial x_i}, \frac{\partial^3 f_i}{\partial a_k \partial x_i^2}, \frac{\partial^2 f_i}{\partial a_k \partial a_l},$$

and

$$\frac{\partial^3 f_i}{\partial a_k \partial a_l \partial x_i} . \quad (14)$$

The first four are scalars, the next three are vectors of length M, and the last two are symmetric matrices of size M by M.

The new parameters determined by (10) are checked to determine convergence. One way to do this is to determine if the relative derivatives $|a_k g_k|$ approach zero (less than, say, 10^{-7}). If not, $\mathbf{a}$ is set equal to $\mathbf{a}^{new}$ and (10) is reapplied. In evaluating the components of $\mathbf{g}$ and $\mathbf{R}$, (5) is first applied to obtain a numerical value for the x_i.

Numerical derivatives

There are situations where f is of such a nature that the analytical derivatives are difficult to obtain. Fortunately, it is possible to apply the method in a simple fashion using regular numerical difference approximations for the derivatives. To do this we write (4) in terms S_i,

$$x_i^{new} = x_i - \frac{0{\cdot}5 \Delta_x [S_i(x_i + \Delta_x, a_j) - S_i(x_i - \Delta_x, a_j)]}{[S_i(x_i + \Delta_x, a_j) - 2S_i(x_i, a_j) + S_i(x_i - \Delta_x, a_j]} \quad (15)$$

As an alternative one could use numerical derivatives on f_i alone and use in (5) and (6) with about the same efficiency. Each requires three evaluations of f_i. (One could also rewrite d_i into the form $x_i = F(x_i)$, as done previously (Southwell, 1969.) This requires evaluation of only first derivatives of f_i. However, Newton's method has better convergence properties and is preferred even though convergence with $x_i = F_i(x_i)$ is improved using Aitken or Wegstein interpolation.)

The components of the gradient vector are given by

$$g_k = \frac{0{\cdot}5}{\Delta_{ak}} [S(a_k + \Delta_{ak}) - (S(a_k - \Delta_{ak})] . \quad (16)$$

Each evaluation of S is made first using (15) iteratively to obtain the appropriate x_i.

Likewise, the diagonal components of $\mathbf{R}$ are

$$\mathbf{R}_{kk} = \frac{1}{\Delta_{ak}^2} [S(a_k + \Delta_{ak}) - 2S(a_k) + S(a_k - \Delta_{ak})] \quad (17)$$

and the off-diagonal elements are

$$\begin{aligned} \mathbf{R}_{lk} = \frac{1}{\Delta_{al} \Delta_{ak}} & [S(a_l + \Delta_{al}, a_k + \Delta_{ak}) - S(a_l + \Delta_{al}, a_k) \\ & - S(a_l, a_k + \Delta_{ak}) + S(a_l, a_k)] . \end{aligned} \quad (18)$$

These are approximations to the true derivatives given in (8)

and (12) above since, as discussed in the theory section, we have a proper evaluation of S.

This numerical approach is simple in concept, easy to program —requiring only the analytical evaluation of f_i—and, as it turns out, quite successful in practice. Its limitations are those usually encountered with numerical differentiation. To obtain better accuracy one has to make the Δ increments smaller, but this requires more significant digits to subtract nearly equal numbers.

Parameter variances

The author's previous paper (1969) derived an expression for the 'exact' parameter variances, that is a relationship giving the parameter variances as functions of the data variances involving no approximations. It has since come to the author's attention that the starting point in this derivation

$$\delta a_j = \sum_i \left[\frac{\partial a_j}{\partial Y_i} \delta Y_i + \frac{\partial a_j}{\partial X_i} \delta X_i \right], \qquad (19)$$

relating the deviations in a_j to the deviations in the data, is itself an approximation.

However, it turns out that in all cases the author has treated, the standard deviations so derived were less than 1 per cent different from the square roots of the diagonal elements of $\mathbf{R}^{-1}$, the usual approximation for the variances. Since the $\mathbf{R}^{-1}$ matrix is already being used (using Newton–Raphson iteration) in adjusting the parameters, we suggest using it as the parameter variance-covariance matrix approximation instead of evaluating the more complicated expression given previously. Thus,

$$\text{var}\,(a_j) \simeq \mathbf{R}^{-1}_{jj} \qquad (20)$$

and

$$\text{covariance}\,(a_j, a_k) \simeq \mathbf{R}^{-1}_{jk} \,. \qquad (21)$$

When relative values of the data variances are known but their magnitudes are not, it is common practice to multiply the right side of (20) and (21) by $2S/(N - M)$ which estimates this constant of proportionality. Powell and Macdonald (1972) include this factor even when the data variances are known.

It turns out that the parameter standard deviations derived from (20) are fairly close to the usual approximations using first derivatives as given by Britt and Luecke (1973) and Deming (1943) when properly compared with or without the $2S/(N - M)$ factor. However, Powell and Macdonald (1972) claim about a 40 per cent decrease in the parameter standard deviations from those given by Deming. They attribute this decrease to their particular procedure for calculating $\mathbf{R}$. Actually their claims are invalid and result from a mistake in their formulation, which is the following.

The usual parameter variance-covariance matrix is the second partial derivative of $\chi^2/2$. Powell and Macdonald use the second partials of χ^2. This makes their derivative matrix a factor of 2 too high and their variances a factor of 2 too low. Consequently, their standard deviations are off by a factor of $1/\sqrt{2}$, which is about 40 per cent.

Discussion

Since the earlier paper (Southwell, 1969) was published, two other papers on the subject have appeared (Powell and Macdonald, 1972; and Britt and Luecke, 1973). It is appropriate here to compare these methods with the method of this paper. Both papers have discussed Deming's method and both point out that Deming's method is good, but is only approximate because it does not quite satisfy the *least* squares criteria.

Basically the approach of this paper is to consider the problem of minimising (1) as a function of the M parameters. We do this by eliminating the x_i from (1) by solving (2). Even when x_i has no analytical solution we are able to completely eliminate the x_i by obtaining a numerical value for it and by the fact that we can always obtain an analytical expression for $\partial x_i/\partial a_k$ and thus apply the chain rule for the analytical derivatives.

Both other methods consider the problem of minimising (1) as a function of $M + N$ variables, a_j and x_i. Both methods make one step adjustments on the a_j and x_i at each iteration until convergence is achieved. Powell and Macdonald's algorithm uses a Newton–Raphson type iteration, whereas, Britt and Luecke's method uses a Gauss–Newton type iteration. As correctly stated by Britt and Luecke, convergence on both the a_j and the x_i is necessary to satisfy the least squares criteria.

It has been demonstrated that it is possible to satisfy a convergence criteria on the a_j and still not be at *the* least squares solution because S may not be stationary with respect to the x_i. Since Powell and Macdonald's termination criteria considers only the a_j, their method is not guaranteed to be the least squares solution even when they achieve convergence in the a_j.

Both papers discuss convergence problems when starting parameters are far from the solutions and both suggest using other approximate methods before applying their algorithms. These problems are often overcome using stabilising modifications in the step length and/or direction, as discussed by Britt and Leucke (1973). They observe that it is not possible to modify their algorithm for straightforward application of most of these modifications, such as a one-dimensional search at each iteration. Since we are adjusting only the a_j at each iteration, no such limitation exists for the method of this paper, and a one-directional search using quadratic interpolation has been successfully applied.

Another point of comparison is that both other methods require the storage and inversion of an M by M matrix. When computer storage is a problem, the theory of this method may be applied using the conjugate gradient method (Fletcher and Reeves, 1964), for example, which requires only two vectors, one of length M for $\mathbf{g}$ and one of length $2M$ as a working vector, besides storage for the data and parameters. This procedure was applied; however, convergence was slower than with the generalised Newton–Raphson procedure.

It should be pointed out that with one difference Powell and Macdonald's method is equivalent to the Newton–Raphson, numerical derivative application of this method. The difference is that the x_i adjustment (their Equation (14)) be tested and if necessary repeated until convergence is complete each time it is used. Another minor difference is the form used for the numerical derivatives for the off-diagonal elements of $\mathbf{R}$. The form we use was chosen because it requires one less evaluation of S.

Powell and Macdonald claim their method is successful only with their 'unconventional derivative approximations', which means first adjusting the x_i each time S is evaluated for the numerical derivatives. When using their 'exact analytical derivatives' they obtain very poor convergence, 148 iterations compared to 4 for their numerical approach in the straight line example. This discrepancy results because they did not use the chain rule when taking their analytical derivatives. We show in an example below that when using the correct analytical derivatives, convergence is achieved in three iterations.

Examples

This procedure was programmed for the CDC 6600 and results of several common example problems are given here. Generally $|x_i^{\text{new}} - x_i| < 10^{-7}$ and $|a_k\, g_k| < 10^{-7}$ were used as termination conditions. For each problem a subroutine was written that returns numbers for f_i and its derivatives with an input of x_i and $\mathbf{a}$. In the numerical derivative program only f_i is evaluated. Unless otherwise noted, the numerical derivatives use $\Delta_x = x_i\Delta$ and $\Delta_{aj} = a_j\Delta$, where $\Delta = 10^{-5}$, unless x_i or a_j are zero, in which case Δ_x and Δ_{aj} are set equal to Δ.

Example 1:
$f = a_1 + a_2x$, straight line fit with uncertainties in both Y_i and X_i using data given in **Table 1.** This example was also used by Powell and Macdonald (1972), by Britt and Luecke (1973), and by the author (Southwell, 1969), where it was shown the x_i in (2) may be solved algebraically. The iterative solution for x_i is also used here, for comparison, using both analytical and numerical derivatives. In all three cases we use the same convergence criteria. We start from the same values used by Powell and Macdonald which were the final results of Deming's method. The results are given in **Table 2.**

We note the advantage in convergence speed using an analytical approach as opposed to the numerical approach.

It appears Powell and Macdonald (1972) attempted to apply the method of adjusting the x_i using analytical derivatives as outlined by the author (Southwell, 1969) to this problem. In their effort to program the method, they apparently failed to do two things: (1) check for convergence on the x_i iteration. The scheme $x = F(x)$ converges only when $|\partial F/\partial x| < 1$ unless interpolation methods are employed; (2) use the chain rule when forming the derivatives. Admittedly, these two points were not explicitly stated in the previous paper. It should be noted, however, that the derivatives in **g** and **R** were taken after the x_i were eliminated from S, which is central to the theory presented.

Powell and Macdonald's statement that this problem remains linear in the parameters is incorrect. By observing Equations (32) and (33) of the previous paper (Southwell, 1969) it is seen that the slope a_2 enters nonlinearly. Britt and Luecke also verify this conclusion.

Another (minor) point, Powell and Macdonald also state that $f = a_1 + a_2x$ is the only model for which the x_i may be explicitly eliminated. Actually there are others, for example, a quadratic model and the model $f = ax^{1/2}$ each produces a cubic in x for Equation (2) for which analytic solutions exist.

Example 2:
$f = a_1 + a_2x + a_3x^2 + a_4x^3$, cubic with uncertainties in both Y_i and X_i using the data in Table 1, except using unity relative weights instead of the data variances. Thus we set $w_{yi} = w_{xi} = 1$ for all the data points. Again we use Deming's results as starting points. The results are given in **Table 3.**

In this case we cannot eliminate x_i explicitly so we use numerical determination of x_i and analytical derivatives as described in this paper. Convergence was obtained in two iterations.

For comparison we rewrote (2) into the form $x_i = F(x_i)$,

$$x_i^{\text{new}} = X_i + \frac{w_{yi}}{w_{xi}}(Y_i - f_i)\frac{\partial f_i}{\partial x_i}, \qquad (22)$$

and used it in the iteration scheme instead of (5) and (6). It was successful; the results were identically the same and required two iterations. Next we used (22) as above except we allowed only one adjustment on x_i each time and did not test for final convergence. After six iterations convergence in the parameters was achieved. However, $2S = 0{\cdot}50721328$ and the parameters were a little different. The largest difference was in $a_3 = 0{\cdot}15628790$. This verifies the assertion made above that when adjusting x_i in a single step each time, that convergence in the parameters does not insure the least squares solution.

Next we went back to Newton's iteration on x_i, (5) and (6), except we allowed only one adjustment on x_i each time with no testing on x_i convergence. After two iterations the parameters had all reached convergence, but $2S = 0{\cdot}48516246$, and the parameters were slightly different, for example, $a_3 = 0{\cdot}15247241$. This demonstrates the better convergence of Newton's iteration over (22).

Table 1 Data used in example 1

Y	Weight $= \sigma_y^{-2}$	X	Weight $= \sigma_x^{-2}$
5·9	1·0	0·0	1000·0
5·4	1·8	0·9	1000·0
4·4	4·0	1·8	500·0
4·6	8·0	2·6	800·0
3·5	20·0	3·3	200·0
3·7	20·0	4·4	80·0
2·8	70·0	5·2	60·0
2·8	70·0	6·1	20·0
2·4	100·0	6·5	1·8
1·5	500·0	7·4	1·0

Table 2 Results for example 1

$2S = 11{\cdot}866353$

Starting point	*Final results*
$a_1 =$ 5·3961000	5·4799102
$a_2 =$ −0·46345000	−0·48053341
Method	*No. of iterations*
Eliminating x_i analytically	3
Adjusting x_i, analytical derivatives	3
Adjusting x_i, numerical derivatives	4

Table 3 Results for example 2

$2S = 0{\cdot}48515249$

Starting point	*Final results*
$a_1 =$ 5·9988000	6·0152637
$a_2 =$ −1·0050000	−0·99983535
$a_3 =$ 0·1570600	0·15247160
$a_4 =$ −0·0137200000	−0·013240529

Table 4 Results for example 3

$2S = 0{\cdot}45032567$

Starting point	*Final results*
$a_1 =$ 5·9240000	5·9148260
$a_2 =$ −0·74070000	−0·60316689
$a_3 =$ 0·026880000	−0·080320319
$a_4 = -3{\cdot}3240000 \times 10^{-3}$	$0{\cdot}026322024$
$a_5 = 2{\cdot}6920000 \times 10^{-3}$	$-8{\cdot}2771911 \times 10^{-4}$
$a_6 = -3{\cdot}2080000 \times 10^{-4}$	$-1{\cdot}6750503 \times 10^{-4}$

Example 3:
$f = a_1 + a_2x + a_3x^2 + a_4x^3 + a_5x^4 + a_6x^5$, quintic with uncertainties in both Y_i and X_i using data in Table 1, except using unity relative weights as in Example 2. The results of Deming's approximation are used as starting points. The results are given in **Table 4.** Convergence was obtained in three iterations.

We then attempted to apply our numerical derivative program to this problem on the CDC 6600 with the same standard precision as used in the analytical derivative approach. After trying Δ's of 10^{-4}, 10^{-5}, and 10^{-6}, convergence did not stabilise even after trying Powell and Macdonald's suggestion of separating S_i into $S_{yi} + S_{xi}$. We found that, when compared to the analytical derivatives, $\Delta = 10^{-4}$ gave closer numerical derivatives, but apparently did not have sufficient accuracy. We concluded that double precision on the 6600 would be necessary for the numerical derivative program to work on this example. Powell and Macdonald apparently used double precision with 29 significant digits and required 10 iterations. Also, they arrive at a different solution, for example, their a_5 equals $-8{\cdot}119 \times 10^{-4}$. This time their results are significantly

different from the least squares solution.

We next report the results of applying the analytical derivative approach on an IBM 1130. The parameters were the same as the CDC 6600 results after three iterations to within one part in six digits and the convergence criteria were satisfied in four iterations.

This example demonstrates a limitation of the numerical derivative approach. For this example, the numerical program requires a computer with something well over 16 significant digit accuracy, whereas the analytical derivative program worked well with less than about nine significant digits.

We note that numerical first derivatives were more accurate than second derivatives. Thus, some gradient minimisation methods might be more successful whenever the numerical approach is required in certain problems.

Example 4:
$f = a_1(1 + a_2^{-1}\, a_3 x)^{-1/a_3}$, fit to the data of **Table 5** with unity relative weights on both Y_i and X_i, $w_{yi} = w_{xi} = 1$. This example is taken from Powell and Macdonald (1972). The results are given in **Table 6.** These results were the same as those given by Powell and Macdonald.

We now consider the same problem with no uncertainties in the Y_i, $w_{yi} = 0$ and $w_{xi} = 1$. This may be considered an ordinary least squares problem in a coordinate system with X_i and Y_i interchanged. It would be an implicit model if we were to use the same function; however, we first analytically inverted it,

$$f = a_2 a_3^{-1}[(a_1^{-1}x)^{-a_3} - 1] \ .$$

The results are also given in Table 6. The parameter solution is again slightly different from that given by Powell and Macdonald; for example, they give $a_2 = 32{\cdot}5481$. Their approach to the problem would not allow direct application of $w_{yi} = 0$. What they had to do was apply some nonzero $w_{yi} \ll w_{xi}$.

Table 5 Data used in example 4

Y	X	Y	X
26·38	1·0	23·50	8·0
25·79	2·0	23·24	9·0
25·29	3·0	23·00	10·0
24·86	4·0	22·78	11·0
24·46	5·0	22·58	12·0
24·10	6·0	22·39	13·0
23·78	7·0	22·22	14·0

Table 6 Results for example 4

$w_{yi} = 1$ and $w_{xi} = 1$	$2S = 0{\cdot}0011444195$
Starting point	*Final results*
$a_1 = 27{\cdot}116700$	27·116749
$a_2 = 33{\cdot}644600$	33·642704
$a_3 = 6{\cdot}6209600$	6·6212191
$w_{yi} = 0$ and $w_{xi} = 1$	$2S = 0{\cdot}012683983$
Starting point	*Final results*
$a_1 = 27{\cdot}154600$	27·155198
$a_2 = 32{\cdot}566300$	32·554227
$a_3 = 6{\cdot}8051700$	6·8064817

Conclusions

We have presented a method of solving the generalised least squares problem wherein the adjustable independent coordinates are eliminated and the problem reduced to one of ordinary nonlinear minimisation of a function of the parameters only. The approach adds versatility to the solution of the problem. The availability of first derivative or second derivative methods —either numerical or analytical—allows the application to depend on the particular problem and on the computer size and time available. Convergence acceleration techniques may be applied in the usual fashion. All the above features are distinct advantages over two recently published methods (Powell and Macdonald, 1972; Britt and Luecke, 1973).

We have demonstrated that the generalised Newton–Raphson method used without modification on the parameters and in eliminating the independent coordinates produces a rapidly converging program when the initial parameters are fairly reasonable. We have shown that the use of analytical derivatives in this approach has faster convergence and may be used on computers having fewer significant digits than when using numerical derivatives. Generally, when necessary, numerical first derivatives are more accurate than numerical second derivatives.

Furthermore, we have demonstrated in regard to Powell and Macdonald's paper (1972): (1) that their approach does not invariably converge to the least squares solution; (2) that their 'unconventional numerical approximations for partial derivatives' can indeed be related to analytical derivatives by merely using the chain rule; and (3) that their claim of approximately 40 per cent reduction in parameter standard derivations estimates when compared with ordinary linearised estimates is invalid and results from an oversight in their approach.

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