

NON-LINEAR ESTIMATION BY PARABOLIC APPROXIMATION

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1. INTRODUCTION AND REVIEW OF LITERATURE

1.1 Introduction

The least squares solutions for the constants, θ , in a model, $g(X, \theta)$, are those values $\theta = \beta$ which minimize the function,

$$F(\theta) = (Y - \hat{Y}^*)' (Y - \hat{Y}^*) ,$$

where the vector Y represents the n observations collected during the experiment, and $\hat{Y}^* = g(X, \theta)$, the corresponding values predicted by the model. The symbol \hat{Y} will replace \hat{Y}^* when $\theta = \beta$. That is, $\hat{Y} = g(X, \beta)$. The symbol X represents a known design matrix or vector.

Non-linear models are those for which the elements of \hat{Y}^* are non-linear functions of θ . Much biological modelling, including component compartments in system models, involves non-linearly arranged parameters. It is also a characteristic of biological investigations, as opposed to engineering or physical investigations, to involve, at least in their early stages, some evaluations among different models. For example, investigation into the selection and arrangement of possible control variables can result in the inclusion of some redundant information, which may or may not be suspected by the investigator, but which may figure prominently in the biological assessment and comparison of the models. Such "instructive abuse" of regression analyses is not uncommon in many biological investigations employing multiple linear regressions.

The widely used techniques for estimating these parameters and their variances, developed for the most part since 1960, in some respects do not meet the often less restrictive requirements of the

biologist. Most require the evaluation of the derivatives $\partial f(\theta)/\partial\theta$ or $\partial g(X,\theta)/\partial\theta$. Unless finite difference approximations are used, which have a tendency to become unstable near the minimum, the arithmetic for the evaluation of the derivatives is model dependent. This usually involves considerable additional computer programming.

The methods reviewed in this chapter can be classified as linearization methods, gradient methods, and variable metric methods. The use of the term gradient, in this chapter, differs from much of the literature. For example, Bard (1970), classifies any method involving evaluation of the gradient $\partial f(\theta)/\partial\theta$, as a gradient method. This grouping would apply to most of the methods of this chapter. Remmler et al. (1966) propose a classification into gradient methods and direct and random search methods. Gradient, in this chapter, includes some of the methods called search methods by Remmler, and excludes some methods, called gradient methods by Bard, to form the linearization group. Linearization, in this chapter, is similar to the use of the term by Marquardt (1963).

Another grouping, for example that of Powell (1962), differentiates between methods with second order convergence, and those not having this property. Membership in these groups depends upon whether or not the method would converge from an arbitrary value of β in one cycle, if $f(\theta)$ were in fact quadratic.

1.2 Linearization Methods

Linearization methods are based on expansion of the model in a Taylor's series through the linear terms. This basis is frequently referred to by some permutation of the names Gauss, Raphson, and

Newton. In the series, the known values are $\theta_k \neq \beta$ in general. That is,

$$g(X, \beta) = g(X, \theta_k) + \frac{\partial g(X, \theta_k)'}{\partial \theta_k} (\beta - \theta_k) ,$$

or,

$$\hat{Y} = Y^* + \frac{\partial g(X, \theta_k)'}{\partial \theta_k} (\beta - \theta_k) .$$

Now \hat{Y} differs from Y only by the addition of an error term.

Hence the series can be re-written,

$$Y + \epsilon = Y^* + \frac{\partial g(X, \theta)'}{\partial \theta_k} (\beta - \theta_k) ,$$

which has the least squares solution,

$$\beta = \theta_k + \left[\frac{\partial g(X, \theta)}{\partial \theta_k} \frac{\partial g(X, \theta)'}{\partial \theta_k} \right]^{-1} \frac{\partial g(X, \theta)'}{\partial \theta_k} (Y^* - Y) .$$

If $g(X, \theta)$ is a linear function of θ , then

$$\frac{\partial g(X, \theta)'}{\partial \theta_k} = X ,$$

and β is the least squares solution. In the non-linear case, $\beta = \theta_{k+1}$, the trial value for the next iteration.

In practice, the adjustment made to θ_k may extrapolate beyond the region where the series adequately represents the function, resulting in divergence of the iterates from β . Marquardt (1963) cites papers by Booth et al. (1959), Hartley (1961), and Marquardt et al. (1961), concerned with selecting a value m , between zero and one, to scale the step size so that $f(\theta_{k+1}) < f(\theta_k)$ is ensured.

Bard (1970), in a paper comparing several non-linear estimation algorithms, associates convergence difficulties with conditioning of the matrix

$$\frac{\partial g(X, \theta)}{\partial \theta_k} \frac{\partial g(X, \theta)'}{\partial \theta_k} ,$$

or, equivalently, the failure of the matrix

$$\frac{\partial^2 f(\theta)}{\partial \theta^2}$$

to be positive definite in the area of the search. He cites papers by Greenstadt (1967) and Fariss and Law¹ (1967), in which small, or for the latter matrix, even negative eigenvalues are replaced by reasonable positive values.

In this method, the matrix

$$B = C^{-1} \frac{\partial g(X, \theta)}{\partial \theta_k} \frac{\partial g(X, \theta)'}{\partial \theta_k} C^{-1}$$

is formed, where C is a diagonal matrix with elements equal to the square root of the absolute values of the diagonal elements of the matrix of derivatives. If λ_i represents the i-th root of B, and α_i the corresponding vector, then,

$$B^{-1} = \sum_{i=1}^r \frac{\alpha_i \alpha_i'}{\lambda_i} .$$

Note that

$$\left[\frac{\partial g(X, \theta)}{\partial \theta_k} \frac{\partial g(X, \theta)'}{\partial \theta_k} \right]^{-1} = C^{-1} B^{-1} C^{-1} .$$

Instead, replace this inverse with

¹Fariss, R. H., and V. J. Law. 1967. Practical tactics for overcoming difficulties in non-linear regression and equation solving. American Institute of Chemical Engineers Meeting, Houston, Texas.

$$R = C^{-1} A^{-1} C^{-1},$$

where

$$A^{-1} = \sum_{i=1}^r \frac{\alpha_i \alpha_i'}{\pi_i}.$$

In this expression,

$$\begin{aligned} \pi_i &= |\lambda_i| \quad \text{if} \quad |\lambda_i| > 10^{-6} \\ &= 1 \quad \text{otherwise.} \end{aligned}$$

Bard (1970) states that R is guaranteed positive semidefinite; since zero roots are eliminated as well, it would appear that R is positive definite, except if inexactness of the calculations exceeds 10^{-6} .

Marquardt (1963, p. 138) uses the matrix

$$\begin{aligned} R &= C^{-1} (B + mI)^{-1} C^{-1} \\ &= \left[\frac{\partial g(X, \theta)}{\partial \theta_k} \frac{\partial g(X, \theta)'}{\partial \theta_k} + mC^2 \right]^{-1}. \end{aligned}$$

The constant m is selected such that $f(\theta_{k+1}) < f(\theta_k)$, being small ". . . whenever conditions are such that the unmodified Taylor's series would converge nicely." Marquardt outlines a series of steps to compute trial values of m sufficiently large so that the deviation sum of squares is reduced. As pointed out by Bard (1970), computing R in a manner analogous with the Greenstadt - Fariss, Law procedure can be computationally more efficient, and yields a minimum value for m.

The problem of singularities or near singularities in the matrix is handled by Jennrich and Sampson (1968) by inverting the matrix in a manner analagous with step-wise regression, using a pivotal inversion procedure. This allows an assessment of the contribution of each variable in turn, and the offending variable can be identified, at least in those stages of the iteration where the iterates are approaching the minimum.

1.3 Gradient Methods

Gradient methods simply move the current trial value θ_k in the direction of the negative gradient of the deviation sum of squares. In its simplest form,

$$\theta_{k+1} = \theta_k - \frac{\partial f(\theta)}{\partial \theta_k} .$$

It is necessary to test that $f(\theta_{k+1}) < f(\theta_k)$, and procedures are available (see for example Rosenbrock (1960)) for either shortening the step length when $f(\theta_{k+1}) > f(\theta_k)$, or lengthening the step when the reverse is true.

Even when the model is linear, several iterations are required. Then, as the value $\theta_{k+1} - \theta_k$ approaches zero,

$$-\frac{\partial f(\theta)}{\partial \theta_k} = 2X'Y - 2X'X\theta_k \rightarrow 0 ,$$

implying

$$\theta_k \rightarrow (X'X)^{-1} X'Y ,$$

the usual (linear) least squares estimate.

A gradient method not involving evaluation of derivatives is that proposed by Nelder and Mead (1965), based on earlier work by Spendley et al. (1962). For a model in r dimensions, that is,

$$= \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_r \end{bmatrix}$$

the simplex

$$i = (\theta_{1,i}, \theta_{2,i}, \dots, \theta_{r,i}), \quad i = 1, 2, \dots, r+1$$

is formed, and the corresponding values of $f(\theta_i)$ computed. The vertex corresponding to $f(\theta_h) = \max_i (f(\theta_i))$ is omitted, and the centroid, $\bar{\theta}$, is computed.

A new point θ^* is computed, on the line joining θ_h and $\bar{\theta}$, but on the opposite side of $\bar{\theta}$ from θ_h . The authors found taking the distance $||\theta^* \bar{\theta}|| = ||\theta_h \bar{\theta}||$ to be "best". That is,

$$\theta^* = 2\bar{\theta} - \theta_h .$$

Then, if

$$f(\theta_l) < f(\theta^*) < f(\theta_h),$$

where $f(\theta_l) = \min_i (f(\theta_i))$, a new simplex with $f(\theta^*)$ replacing $f(\theta_h)$ is

defined, and the procedure repeated.

If, on the other hand,

$$f(\theta^*) < f(\theta_l) ,$$

indicating that the reflection operation has produced a vertex whose corresponding sum of squares is less than all of the others, a point $\bar{\theta}^{**}$ further along the line is computed. In this case, the authors recommend making the distance $||\bar{\theta}^{**} - \bar{\theta}|| = 2 ||\bar{\theta}^* - \bar{\theta}||$, implying,

$$\begin{aligned}\bar{\theta}^{**} &= 2 \bar{\theta}^* - \bar{\theta} \\ &= 3 \bar{\theta} - 2 \theta_h .\end{aligned}$$

If it turns out that

$$f(\bar{\theta}^{**}) > f(\theta_h) ,$$

the expansion operation has failed, and $\bar{\theta}^*$ replaces θ_h in the simplex as before.

Finally, if

$$f(\theta_i) < f(\bar{\theta}^*) < f(\theta_h) , \quad i \neq h ,$$

a contraction rather than expansion operation is performed, and $\bar{\theta}^{**}$ between θ_h and $\bar{\theta}$ is computed. In this case the authors suggest taking $2 ||\bar{\theta}^{**} - \bar{\theta}|| = ||\theta_h - \bar{\theta}||$, making

$$\bar{\theta}^{**} = \frac{1}{2} \theta_h + \frac{1}{2} \bar{\theta} .$$

If contraction fails, that is, if $f(\bar{\theta}^{**}) > \min(f(\theta_h), f(\bar{\theta}^*))$, then all the values θ_i are replaced by $(\theta_i + \bar{\theta}) / 2$, and the process is re-started.

Several gradient methods are available which, by making use of the properties of quadratic functions, can considerably improve the rate of convergence when compared with the classical gradient, or

steepest descent methods. These methods include the method of parallel tangents, by Shah et al. (1964), and a method due to Powell (1962).

1.4 Variable Metric Method

This method was originated by Davidon (1959) and subsequently modified by Fletcher and Powell (1963). The method utilizes the linear mapping of changes in position, $\theta_{k+1} - \theta_k$, onto changes in the gradient, $\partial f(\theta) / \partial \theta_{k+1} - \partial f(\theta) / \partial \theta_k$, specified by the matrix $\partial^2 f(\theta) / \partial \theta^2$ in the relation,

$$\frac{\partial f(\theta)}{\partial \theta_{k+1}} - \frac{\partial f(\theta)}{\partial \theta_k} = \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) .$$

The squared length of the difference in the gradient can be measured with respect to the matrix of second order derivatives. In this sense, the matrix of second derivatives provides the metric for measuring the (squared) length of the gradient vector. This length is,

$$\left[\frac{\partial f(\theta)}{\partial \theta_{k+1}} - \frac{\partial f(\theta)}{\partial \theta_k} \right]' \left[\frac{\partial^2 f(\theta)}{\partial \theta^2} \right]^{-1} \left[\frac{\partial f(\theta)}{\partial \theta_{k+1}} - \frac{\partial f(\theta)}{\partial \theta_k} \right] .$$

Note that, taking $\theta_{k+1} = \beta$, implying $\partial f(\theta) / \partial \beta = 0$, the inverse mapping is,

$$\beta - \theta_k = - \left[\frac{\partial^2 f(\theta)}{\partial \theta^2} \right]^{-1} \frac{\partial f(\theta)}{\partial \theta_k} ,$$

and,

$$D = \frac{1}{2} \frac{\partial f(\theta)}{\partial \theta_k}' \left[\frac{\partial^2 f(\theta)}{\partial \theta^2} \right]^{-1} \frac{\partial f(\theta)}{\partial \theta_k}$$

is the distance $f(\theta_k) - f(\beta)$, or the distance to the minimum sum of squares.

In the variable metric method, $[\partial^2 f(\theta) / \partial \theta^2]^{-1}$ is replaced initially by a positive definite, symmetric, but otherwise arbitrary matrix R . The length of the gradient vectors are measured with respect to R , and values of the gradient at each step are used to improve R such that its final value will be $[\partial^2 f(\theta) / \partial \theta^2]^{-1}$. Since R changes at each step, Davidon coined the term "variable metric."

The improvement which suggests itself is to move to the indicated minimum at each step, which implies making,

$$D_k = \frac{1}{2} \frac{\partial f(\theta)'}{\partial \theta_{k+1}} R_k \frac{\partial f(\theta)}{\partial \theta_k} = 0 .$$

From the inverse mapping,

$$\frac{\partial f(\theta)'}{\partial \theta_{k+1}} (\theta_{k+1} - \theta_k) = \frac{\partial f(\theta)'}{\partial \theta_{k+1}} (-R_k) \frac{\partial f(\theta)}{\partial \theta_k} = -2D_k .$$

Hence D_k can be made to be zero by making $\partial f(\theta) / \partial \theta_{k+1}$ orthogonal to $\theta_{k+1} - \theta_k$.

The procedure is to take

$$\theta_{k+1} = \theta_k + \lambda_m (-R_k) \frac{\partial f(\theta)}{\partial \theta_k} ,$$

where λ_m is the value of λ which minimizes

$$f(\theta^*) = f(\theta_k + \lambda (-R_k) \frac{\partial f(\theta)}{\partial \theta_k}) .$$

By taking the co-ordinates of θ_{k+1} as a (continuous) function of λ , the total derivative

$$\frac{\partial f(\theta^*)}{\partial \lambda} = \frac{\partial f(\theta^*)}{\partial \theta^*} \frac{\partial \theta^*}{\partial \lambda} .$$

Then at $\lambda = \lambda_m$, $f(\theta^*) = f(\theta_{k+1})$, and,

$$\begin{aligned} \frac{\partial f(\theta^*)}{\partial \lambda_m} &= 0 \\ &= \frac{\partial f(\theta)}{\partial \theta_{k+1}} \frac{\partial \theta_{k+1}}{\partial \lambda_m} \\ &= \frac{\partial f(\theta)}{\partial \theta_{k+1}} (-R_k) \frac{\partial f(\theta)}{\partial \theta_k} \\ &= \frac{\partial f(\theta)}{\partial \theta_{k+1}} (\theta_{k+1} - \theta_k) . \end{aligned}$$

That is, the tangent line at θ_{k+1} has direction cosines proportional to $\partial \theta_{k+1} / \partial \lambda$ and is perpendicular to a line whose direction cosines are proportional to $\partial f(\theta) / \partial \theta_{k+1}$ (see, for example, Smail (1949) sections 385, 391, 393).

The value of R_{k+1} is obtained by adding to R_k , two matrices A_k and B_k , such that,

$$\begin{aligned} R_{k+1} \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) &= (R_k + A_k + B_k) \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) \\ &= (\theta_{k+1} - \theta_k) . \end{aligned}$$

Consider first the relation

$$\begin{aligned} \theta_{k+1} - \theta_k &= A_k \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) \\ &= A_k \left[\frac{\partial f(\theta)}{\partial \theta_{k+1}} - \frac{\partial f(\theta)}{\partial \theta_k} \right] \end{aligned}$$

notationally altered to

$$(\Delta\theta) = A_k (\Delta G) .$$

Then if A_k is taken to be symmetric, and of rank one,

$$A_k = \begin{bmatrix} a_{1,1} & a_{1,1}K' \\ K a_{1,1} & K a_{1,1}K' \end{bmatrix}$$

$$= \begin{bmatrix} a_{1,1} \\ k_1 a_{1,1} \\ \vdots \\ k_{r-1} a_{1,1} \end{bmatrix} (1 \quad k_1 \quad \dots \quad k_{r-1}) ,$$

and the above relation becomes,

$$\begin{bmatrix} a_{1,1} \\ k_1 a_{1,1} \\ \vdots \\ k_{r-1} a_{1,1} \end{bmatrix} (1 \quad k_1 \quad \dots \quad k_{r-1}) \begin{bmatrix} (\Delta g_1) \\ (\Delta g_2) \\ \vdots \\ (\Delta g_r) \end{bmatrix} = \begin{bmatrix} (\Delta\theta_1) \\ (\Delta\theta_2) \\ \vdots \\ (\Delta\theta_r) \end{bmatrix} .$$

Multiplying out this expression gives a set of equations in $a_{1,1}$ and k_i , $i = 1, 2, \dots, r-1$ which give the solutions,

$$a_{1,1} = (\Delta\theta_1)^2 / \sum_{j=1}^r (\Delta\theta_j) (\Delta g_j)$$

$$k_i = (\Delta\theta_{i+1}) / (\Delta\theta) , \quad i = 1, 2, \dots, r-1 ,$$

implying,

$$A_k = \frac{(\Delta\theta) (\Delta\theta)'}{(\Delta\theta)' (\Delta G)} .$$

With this solution for A_k , it follows that

$$B_k \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) = (-R_k) \frac{\partial^2 f(\theta)}{\partial \theta^2} (\theta_{k+1} - \theta_k) .$$

Solving this relation in a manner analagous to that used for A_k , where,

$$b_{1,1} = \left(\sum_{j=1}^r r_{1,j}^k (\Delta g_j) \right)^2 / \left(\sum_{j=1}^r (\Delta g_j) \sum_{\ell=1}^r r_{j,\ell}^k (\Delta g_j) \right)$$

$$k_i = \left(\sum_{j=1}^r r_{i+1,j}^k (\Delta g_j) \right) / \left(\sum_{j=1}^r r_{1,j}^k (\Delta g_j) \right)$$

gives,

$$B_k = - \frac{(R_k (\Delta G)) (R_k (\Delta G))'}{(\Delta G)' R_k (\Delta G)} .$$

In the non-linear case, the above relations are approximations, and the procedure can be terminated when the predicted distance to the minimum is less than some required amount, rather than after r steps. Fletcher and Powell (1963) suggest testing $\theta_{k+1} - \theta_k$ as well, and working through at least r steps, where r is the number of elements in θ .

Davidon outlines a method of cubic interpolation over a variable range of $f(\theta^*)$ to locate the value λ_m at the minimum.

1.5 Methods for Selected Models

Before the coincident widespread availability of computers and high level programming languages to facilitate their use, the arithmetic involved in any of the methods reviewed would be prohibitive in all but the simplest models. Numerous methods, not reviewed here, were developed to reduce the labour involved.

These methods, for the most part, were model specific, and many depended upon peculiar linearizing transformations, often without regard for the nature of the error term. Indeed, the estimation procedures were often not based on any discernible criterion, such as least squares or maximum likelihood, and properties of the estimates were largely unknown and unquestioned.

To quote Stevens (1951, p. 247),

The arithmetic labour of making a least-squares adjustment has proved so great that few research-workers appear to have attempted it, with a consequence that unsatisfactory and very inefficient methods have generally been adopted instead.

Many of the methods formerly used for estimating the constants in biological growth models are of this type.

On the other hand, some very efficient and esoteric methods were also developed under this same impetus. Included are those by Stevens (1951), and as generalized by Turner et al. (1961), which apply to whole families of models, including most of the common growth models. Although no attempt has been made to review this literature, other examples include methods by Pimentel-Gomez (1953) and Nelder (1961).

1.6 Resume of Chapter 1

In this chapter, the problem posed by least squares estimation applied to non-linear models is explored and illustrated by several different estimation methods. Basically, the problem differs from the linear case in that solutions cannot, in general, be expressed in closed form. The least squares criterion, that is, obtaining parameter estimates such that the sum of squared deviations between observed and predicted values is minimized, remains the same in either case.

In the linear case, the problem is equivalent to finding those values of the parameters which occur at the minimum of a multi-dimensional paraboloid surface. The regular properties of the paraboloid permit expression of the solution in closed form. The most important of these properties might be summarized as follows. The paraboloid surface is everywhere convex. The slopes of the surface, measured with respect to the parameter axes, are zero at the solutions for the parameters. The rates of change of the slopes, also measured with respect to the parameter axes, are constant, regardless of where along the axes they are measured.

Convexity in the mathematical sense implies that a line connecting any two points which are members of a convex set is itself wholly contained in the set. The statement applies to all points in the set. With respect to the paraboloid surface, equivalently, any tangent drawn to a point on the surface will not intersect or touch the surface at any other point.

If the surface is not convex, least squares solutions do not exist. By knowing the slopes at any point, since these change at a constant rate, the distance from that point to the point at which the slopes are all zero can be computed analytically.

In the non-linear case, the surface is not likely to be convex everywhere, although it must be in the vicinity of the solutions, if these are to exist. Again, the slopes will be zero at the point which defines the solutions, but the rates of change of the slopes vary, depending upon where along the parameter axes they are measured. Hence, the distance between an arbitrary point and the point at which the slopes are zero cannot be determined analytically. Indeed, unlike the linear case, there is no a priori guarantee that the point exists at which the slopes are all zero, or that there may not be several such points.

Estimation of the variances associated with the parameter estimates is also complicated by a non-linear model. In the linear case, the variances involve the rates of change of the slopes. In the non-linear case, the rates of change of the slopes, measured at the point defining the solutions, provide only a minimum estimate of the variances. That is, it is known that the variances are not smaller than those computed from these quantities. If the sample size is small, the real variances can be much larger. This lends some difficulty to using standard t or F statistics to test hypotheses about values of the parameters.

Generally speaking, the methods reviewed in this chapter which simply follow the direction of decreasing slopes towards a minimum,

over distances determined by the rates of change of the slopes, are inefficient, and are likely to fail when the surface is not locally convex. The more reliable methods take into account the fact that convexity cannot be guaranteed. Efficiency is frequently considerably improved by imposing the regular properties of a paraboloid surface onto the real surface, as approximations to this surface. Many of the methods require analytical solutions to the slopes, or their rates of change. This in itself may be so difficult as to result in the use of approximations. Two of the more popular and reliable of the methods reviewed are the linearization method of Marquardt, and the variable metric method of Davidon-Fletcher-Powell.

2. A METHOD OF HIERARCHICAL PARABOLAS

2.1 Introduction

This method utilizes the linear mapping described for the variable metric method. The method assumes the surface to be quadratic, thereby negating the necessity for the evaluation of any derivatives, or explicitly inverting any matrices. Each parameter is considered in turn, holding the remaining parameters constant at their current values. This feature allows the contribution of each parameter to be individually assessed, at least in the vicinity of the minimum, and facilitates adjustments for the covariance among the parameters, or non-orthogonality among the parameter axes.

The method has second order convergence, as defined earlier, and provides estimates of the variance covariance matrix as an integral part of the procedure.

2.2 The Linear Analogue

Consider a (linear) model in r dimensions, for which least squares estimates of the parameters exist, and a set of arbitrary values, θ , of the parameters. Evaluate the sum of squares, $f(\theta)$, for this point, and for two more points which differ from the first in that different arbitrary values are used for one of the parameters. Without loss of generality, assume this is the first parameter. That is,

$$\begin{aligned} f(\theta_1) &= f(\theta_{1,1}, \theta_{2,1}, \dots, \theta_{r,1}) \\ f(\theta_2) &= f(\theta_{1,2}, \theta_{2,1}, \dots, \theta_{r,1}) \\ f(\theta_3) &= f(\theta_{1,3}, \theta_{2,1}, \dots, \theta_{r,1}) \end{aligned} .$$

Then the conditional least squares estimate,

$$\begin{aligned}\theta_{1,1,1} &= \beta_1 | (\theta_{2,1}, \theta_{3,1}, \dots, \theta_{r,1}) \\ &= \frac{(\nabla\theta_1)}{2} - \frac{1}{2a_{1,1}} \frac{(\Delta f(\theta))}{(\Delta\theta_1)},\end{aligned}$$

where,

$(\nabla\theta_1)$ is the sum of any two $\theta_{1,j}$, $j = 1, 2, 3$,

$(\Delta\theta_1)$ is the difference between the same two $\theta_{1,j}$,

$(\Delta f(\theta))$ is the difference between the corresponding sums of squares,

and,

$$\frac{1}{a_{1,1}} = \frac{(\Delta_{1,2}\theta_1) (\Delta_{1,3}\theta_1) (\Delta_{2,3}\theta_1)}{(\Delta_{2,3}\theta_1) (\Delta_{1,2}f(\theta)) - (\Delta_{1,2}\theta_1) (\Delta_{2,3}f(\theta))}.$$

The symbols $(\Delta_{m,n}\theta_1)$ and $(\Delta_{m,n}f(\theta))$ imply differences taken in the order $\theta_{1,m} - \theta_{1,n}$, and $f(\theta_m) - f(\theta_n)$. The subscripting $\theta_{i,k,j}$ implies the j -th conditional estimate of the i -th parameter at the k -th step, where $j = 1, 2, 3$; $i = 1, 2, \dots, k$; and $k = 1, 2, \dots, r$.

If $r = 1$, then $\theta_{1,1,1}$ is the least squares estimate β_1 , and its estimated variance is $\hat{\sigma}^2 / a_{1,1}$.

If $r > 1$, the process is repeated for values $\theta_{2,2}$ and $\theta_{2,3}$, holding the remaining parameters constant. This produces the conditional estimates

$$\begin{aligned}\theta_{1,1,2} &= \beta_1 | (\theta_{2,2}, \theta_{3,1}, \dots, \theta_{r,1}) \\ \theta_{1,1,3} &= \beta_1 | (\theta_{2,3}, \theta_{3,1}, \dots, \theta_{r,1}) .\end{aligned}$$

Since the value of $a_{1,1}$ does not change in these calculations, only two additional sums of squares are required for each additional conditional estimate.

Then compute

$$f(\theta_j) = f(\theta_{1,1,j}, \theta_{2,j}, \theta_{3,1}, \dots, \theta_{r,1}), \quad j = 1, 2, 3$$

and the corresponding conditional estimates for $k = 2$, and $i = 1, 2$.

That is,

$$\begin{aligned} \theta_{i,k,1} &= \beta_i | (\theta_{3,1}, \dots, \theta_{r,1}) \\ &= \frac{(\nabla \theta_i)}{2} - \frac{1}{2a_{i,k}} \frac{(\Delta f(\theta))}{(\Delta \theta_i)}, \end{aligned}$$

where,

$$\frac{1}{a_{i,k}} = \frac{(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)}{(\Delta_{2,3} \theta_i) (\Delta_{1,2} f(\theta)) - (\Delta_{1,2} \theta_i) (\Delta_{2,3} f(\theta))}.$$

If $r = 2$, then $\theta_{1,2,1} = \beta_1$, and $\theta_{2,2,1} = \beta_2$. The estimated variance covariance matrix is,

$$\begin{aligned} & \begin{bmatrix} \text{Var}(\beta_1) & \text{Var}(\beta_1, \beta_2) \\ & \text{Var}(\beta_2) \end{bmatrix} \\ &= \hat{\sigma}^2 \begin{bmatrix} \frac{1}{a_{1,1}} + \frac{1}{a_{1,2}} & \left(\frac{1}{a_{1,2}}\right)^{\frac{1}{2}} \left(\frac{1}{a_{2,2}}\right)^{\frac{1}{2}} \\ & \frac{1}{a_{2,2}} \end{bmatrix}. \end{aligned}$$

For the covariance term, whether the negative or positive square root is extracted depends upon the sign of the product of the arbitrary values, $(\Delta_{1,2}\theta_k) (\Delta_{1,3}\theta_k) (\Delta_{2,3}\theta_k)$. In general, for values $i = 1, 2, \dots, k$, if the sign associated with this product is taken to be positive, then the sign of $(1 / a_{i,k})^{\frac{1}{2}}$ is the same as the sign of the product $(\Delta_{1,2}\theta_i) (\Delta_{1,3}\theta_i) (\Delta_{2,3}\theta_i)$. Conversely, if $(\Delta_{1,2}\theta_k) (\Delta_{1,3}\theta_k) (\Delta_{2,3}\theta_k)$ is negative, the sign of $(1 / a_{i,k})^{\frac{1}{2}}$ is opposite to the sign of $(\Delta_{1,2}\theta_i) (\Delta_{1,3}\theta_i) (\Delta_{2,3}\theta_i)$.

If $r \geq 3$, the process is repeated for $k = 3, 4, \dots, r$. The general computing formulas for the conditional estimates at each step, and the values of $a_{i,k}$ are given above. Note that the values of $a_{i,k}$ do not change, and three points $(f(\theta_j), \theta_j)$ are required only when the final subscript of the conditional estimate is one.

The general variance formula is,

$$\text{Var}(\beta_i, \beta_j) = \hat{\sigma}^2 \sum_{k=j}^r (a_{i,k})^{-\frac{1}{2}} (a_{j,k})^{-\frac{1}{2}},$$

where the positive or negative root is extracted as described above.

Particular arrangements of orthogonal axes can result in $(\Delta\theta_i) = 0$. If $(\Delta\theta_i) = 0$, then the computing formulas become

$$\begin{aligned} \theta_{i,k,j} &= \frac{(\nabla\theta_i)}{2} \\ &= \theta_{i,k-1} \quad \text{for all } j, \end{aligned}$$

and,

$$\frac{1}{a_{i,k}} = 0, \quad i = 1, 2, \dots, k-1.$$

The relations in this section are proved in Appendix 5.2.

2.3 Application to Non-linear Models

In the linear case, the interval along any parameter axis implied by the co-ordinates $\theta_{i,j}$ (or $\theta_{i,k,j}$), $j = 1, 2, 3$ is theoretically not critical, since, for the family of parabolas along the i -th axis, the value of $a_{i,k}$ is constant for any selection of points corresponding to the subscript j . In practice, however, the finite arithmetic capabilities of a computer produce an effective minimum interval width.

This consideration is important in the non-linear case. In this case, the procedure described in the previous section is completed for all r dimensions. The estimates produced are used as starting values for the next iteration, and the intervals about these values are shortened so that the quadratic approximation will become more precise. In the limit, an infinitely small interval will approximate the real surface, at a point, infinitely well.

At present, no theoretical basis for judging the size of the interval along each axis, θ_k , or the effective interval about the point θ , is available, beyond the intuitive requirement of a "short" interval whenever the real surface departs "strongly" from a quadratic surface. Consequently, the procedure used is based on practical considerations arising from experience with the method.

The value of $a_{k,k}$ provides a measure of how quickly the rate of change of the surface is itself changing with respect to the k -th axis. In the linear case, the measure is exact and constant, and in the non-linear case it is some average measure applicable to the interval.

If the value of $a_{k,k}$ is large, the rate of change of the surface is changing rapidly with respect to the k-th axis in the vicinity of the search. The k-th axis can be considered to be important to the determination of the surface, although in early stages of the iteration, the importance may be transitory, as the position along this axis, and the angles it makes with other axes may be only poorly determined. In order to improve the precision of the quadratic approximation, a "smaller" interval along an important axis, than along one whose corresponding a-value was small, would appear desirable.

At first glance, the intervals associated with any subset of the parameters entering the model linearly would appear unimportant, since, the surface measured with respect to these axes, with the others held constant, is parabolic, as in a linear model. However, "large" intervals about important linear parameters (those with large a-values) can cause problems such as boundary violations in the non-linearly arranged parameters. In some models, for example, allowing a non-linear parameter to assume unrealistic values, even temporarily, at an intermediate stage in the calculations, can result in attempting to compute predicted values which are mathematically undefined. Hence, some shortening of intervals along linear axes is required, as well as for non-linear axes.

A formulation which appears to work well is to set up the interval along the k-th axis,

$$\theta_{k,1} < \theta_{k,2} < \theta_{k,3} \quad ,$$

where $\theta_{k,2}$ is the estimate produced by the previous iteration, and $\theta_{k,1}$ and $\theta_{k,3}$ are given by,

$$\theta_{k,2} \pm \min \left[\frac{\text{abs}(\theta_{k,2})}{32}, \frac{\text{abs}(\theta_{k,2})}{2^t}, \frac{(\text{Var}(\theta_{k,2}))^{\frac{1}{2}}}{2^{t-1}} \right] .$$

In this formulation, t is the number of the current iteration. Since $\text{Var}(\theta_{k,2})$ is not estimated until completion of the first iteration, the initial interval is given by $\theta_{k,2} \pm \text{abs}(\theta_{k,2}) / 32$. If the value of $\theta_{k,2} = 0$, the numerator $\text{abs}(\theta_{k,2})$ is replaced by unity. Intervals are decreased in size by powers of two in deference to a hexadecimal computer. For applications such as function minimization only, where the number of observations is zero, or solving simultaneous equations, where the number of observations equals the number of parameters, the formulation is reduced to,

$$\theta_{k,2} \pm \min \left[\frac{\text{abs}(\theta_{k,2})}{32}, \frac{\text{abs}(\theta_{k,2})}{2^t} \right] .$$

Some assurance is required that the interval along an axis does not become so small that the computing facility cannot discriminate among the corresponding changes in the objective function. The problem is not encountered unless the number of iterations becomes excessively large, perhaps twelve or more, in the presence of an axis with an unusually small variance compared with the others, or when the minimum value along an axis is actually zero.

It has been found useful, starting with the tenth iteration, to check each difference $\theta_{k,1} - \theta_{k,2}$, in turn for $k = 1, 2, \dots, r$, to determine if the corresponding change $f(\theta_1) - f(\theta_2)$ exceeds some

value. For a sixteen digit objective function, it is required that,

$$\frac{f(\theta)_h}{f(\theta)_l} - 1 > 10^{-10},$$

where $f(\theta)_h$ is the higher, and $f(\theta)_l$ the lower of $f(\theta_1)$ and $f(\theta_2)$.

When this condition is not met, values of $\theta_{k,1}$ and $\theta_{k,3}$ are computed, based on the range used for the last iteration which produced an acceptable interval.

2.4 Failure of the Algorithm along the k-th Axis

If the surface implied by $f(\theta_j)$, $j = 1, 2, 3$ is not convex in the area of search, the algorithm will fail. Symptomatic of the failure is the calculation of values of $1 / a_{k,k}$ which are negative.

Following the definitions in corollary 1.2.1, Appendix 5.1, and from theorem 2.1, Appendix 5.2, the analytic formula for $1 / a_{k,k}$ is,

$$\frac{1}{a_{k,k}} = \frac{2|A^{(k-1)}|}{|A^{(k)}|}.$$

Hence the determinant of the k-dimensional matrix of second derivatives is,

$$|A^{(k)}| = \left[\begin{array}{cccc} 1 & & & \\ a_{1,1} & & & \\ & 1 & & \\ & a_{2,2} & & \\ & & \dots & \\ & & & 1 \\ & & & a_{k,k} \end{array} \right]^{-1}.$$

It is seen that the negative value of $1 / a_{k,k}$ corresponds to the negative eigenvalue problem described in Chapter 1, with the difference that k may not equal r.

Attempts to adjust to the situation in a manner similar to Marquardt's method, that is, by increasing the values $1 / a_{i,i}$,

$i = 1, 2, \dots, k$ by some amount, m , which would make $1 / a_{k,k} + m > 0$, gave inconsistent results. This was presumably because, if $k < r$, no adjustment can be made to the diagonal a -values for axes $k+1, k+2, \dots, r$.

Reflecting the interval along each axis, from $\min(f(\theta_j))$ in a direction opposite from $\max(f(\theta_j))$, also gave inconsistent results, presumably for the same reason. That is, the new choice of the coordinates θ_i^* , $i = 1, 2, \dots, k$, in the direction of the decreasing gradient, could not be relied upon to generate a smaller value of $f(\theta^*)$ when the current values of θ_i , $i = k+1, k+2, \dots, r$ made up the rest of the vector θ^* . Since, if a solution exists, the set will be convex in the vicinity of the minimum, it seems advisable to devise a method which will ensure a move toward the minimum.

An adjustment procedure which has given consistent results is patterned after the method of Nelder and Mead. The centroid $\bar{\theta}$, of the points

$$\theta_j = (\theta_{1,k-1,j}, \theta_{2,k-1,j}, \dots, \theta_{k-1,k-1,j}, \theta_{k,j}, \theta_{k+1,j}, \dots, \theta_{r,j}), \quad j = 1, 2, 3$$

is computed, and the vector θ_ℓ corresponding to $\min(f(\theta_j))$ determined. The new vector θ^* is computed, where,

$$\theta^* = (1 + \alpha) \theta_\ell - \alpha \bar{\theta}.$$

That is, θ^* is on the line joining θ_ℓ and $\bar{\theta}$, but on the opposite side of θ_ℓ from $\bar{\theta}$. The value of α is taken successively to be 2, 1,

$1/2, 1/4, 1/8, 0$, the process being terminated whenever $f(\theta^*) \leq f(\theta_i)$.

The vector θ^* is then used to start the next iteration. Also, if $\alpha = 0$, the iteration number is incremented, and the interval is shortened as described in the previous section.

2.5 Failure of the Algorithm along a Previous Axis

At the k -th step, the value of an off diagonal $1/a_{i,k}$, $i < k$, can also become negative. The problem in this case is somewhat more obscure than that of the previous section.

The analytic formulation for the off diagonal a -value is,

$$\frac{1}{a_{i,k}} = \frac{2|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|}, \quad i < k.$$

Hence $1/a_{i,k}$ can be negative when $|A^{(k)}| < 0$ as in the previous section. However, $1/a_{i,k}$ can also become negative when $|A^{(k)}| > 0$. Since $|A^{(k-1)}| > 0$ always (or the procedure would have failed on the $(k-1)$ -th step rather than the k -th), the value $|A_{i,k}^{(k)}|^2$ must be negative under these circumstances. This implies imaginary roots for the matrix $A_{i,k}^{(k)}$.

An explanation of this phenomenon will not be found here, beyond the suggestion that, given the current intervals along the i -th and k -th axes, the real surface indicates that the angle between these axes, measured by the quadratic approximation, is not the same when proceeding from i to k as when proceeding from k to i .

As in section 2.4, the problem arises from the joint action of the current effective interval width about θ and the current area of

the search. The solution taken to the problem is that presented in section 2.4.

2.6 Other Considerations

Three possible terminating criteria are suggested. The first is to terminate when $f(\theta)_t - f(\theta)_{t-1}$ is less than some prechosen amount α . This criterion may not work well for some functions, since the values of the objective function at successive iterations can change slowly at locations other than the minimum. If the minimal value of $f(\theta)$ is known, a more satisfactory criterion would be to terminate whenever $f(\theta)_t - f(\theta)_m < \alpha$, where $f(\theta)_m$ is the known minimal value of the objective function. In least squares applications, the value $f(\theta)_m$ would seldom be known.

A second criterion is to terminate when the difference $\theta_{k,t} - \theta_{k,t-1} < \alpha$, for $k = 1, 2, \dots, r$. This criterion was used satisfactorily throughout most of the developmental work on the algorithm. By insisting that every axis be stable by an amount less than α , premature termination because of one or two locally unresponsive axes is negligible. If α is made too small, relative to the computing facility, the problem of minimal interval widths (section 2.3) will become apparent. Variations of this criterion would include a separate value of α for each axis, or using α to represent some prechosen number of digits rather than a prechosen value.

A third criterion is to stabilize the values of $a_{k,k}$ or $\text{Var}(\beta_k)$, rather than θ_k . These values, involving second moments, do not stabilize as quickly as the estimates themselves, making this

criterion the most stringent. It also increases the tendency to solicit more precision than the computing facility can supply.

The imposition of boundary values, in one or both directions, along one or more axes, can frequently improve the efficiency of the algorithm in locating the minimum. To impose boundary values on an axis is to limit the search for the minimum along that axis to within some specified range. This may even be necessary in some cases for the evaluation of $f(\theta)$. In the case of biological applications, there are nearly always biological restrictions which are important in defining the solutions. The imposition of boundary values also has some utility in initiating the procedure, when the investigator may be hard put to supply a reasonable initial value for a parameter, but can easily specify a range within which he expects the final value to lie.

Boundaries which are attained only in the limit (rather than by finite computer calculations) can be approximated by using artificially large or small finite boundaries.

The problem of highly correlated or redundant parameters, sometimes encountered in least squares regression problems, is signalled in two ways. The algorithm will consistently fail for those reasons discussed in section 2.5. That is, no adjustment can be made along the i -th axis, for some $i < k$, after addition of the k -th axis; or, the change produced in the minimum along the i -th axis due to the interval along the k -th axis cannot be assessed. Along with this consistent failure, the value of the determinant of the approximating quadratic form will approach zero. The response to these signals is to rewrite the model omitting the redundant k -th axis.

Weighted least squares analysis, which is important when fitting biological growth models, is accomplished by minimizing,

$$f(\theta) = (Y - \hat{Y}^*)' W(Y - \hat{Y}^*) ,$$

where the weight matrix W is supplied a priori, or computed at each stage of the iterative process.

2.7 Resume of Chapter 2

This chapter develops a method of determining the minimum of a parabola from any three points on its surface. For a one dimensional linear model, the location of the minimum is the least squares estimate of the single parameter involved, and the value of the parabola at the minimum is the deviation sum of squares. An expression for the estimated variance of the parameter as a function of the three points on the surface is also developed.

For a multidimensional linear model, additional parabolas are incorporated in a hierarchical manner, to build up the paraboloid surface specified by the model. Changes in the minima of these parabolas, as new points in different dimensions are added, provide the information necessary to locate the least squares estimates. Formulations for locating the minima, and for computing the variances, are given in this chapter, and are developed in Appendix 5.2.

The method is applied to the non-linear case by evaluating the points on the real surface, and computing the solutions that would be obtained if this surface were paraboloid. A new set of points, restricted to a narrower interval around these solutions, are then

evaluated on the correspondingly restricted region on the real surface, and a new set of solutions computed. The process is repeated until the solutions, or their associated variance estimates, or the value of the deviation sum of squares, change by less than some predetermined amount, or predetermined number of digits.

If the surface is not convex in the area of the search, the solutions produced at that iteration are of no use in locating a new set of points, and may even result in movement away from the least squares solutions. Variance estimates become nonsensical. When this happens, the method reverts to moving an arbitrary distance along the direction of an average decreasing slope. Since the rate of change of the slope is itself non instructive under circumstances of non convexity, an arbitrary distance is moved, subject only to the restriction that the point decided upon is to produce a smaller value of the deviation sum of squares.

Additional considerations in this chapter include the selection of a terminating criterion, the imposition of boundary values along one or more of the parameter axes by substantive considerations of the particular problem, the location of redundant parameters in the model, and weighted least squares analysis.

3. NUMERICAL RESULTS AND COMPARISON WITH OTHER METHODS

3.1 Introduction

Informative comparisons across algorithms are hard to make, because of the difficulty in selecting an unambiguous measure on which to base a comparison. A frequently employed measure is the size of the objective function at a given number of iterations, or vice versa. The difficulty lies in attempting to determine equivalent iterations across algorithms.

For example, for the variable metric method, Fletcher and Powell (1963) count one iteration each time new elements for the vector θ are produced, coincidentally with the improvement of the matrix R . The method has second order convergence, and they count r iterations when $f(\theta)$ is quadratic. The hierarchical parabola method also has the property of second order convergence, and uses the same definition of an iteration, but completes the quadratic case in one iteration. However there is a major difference in the quantity of calculation leading up to the production of a new θ vector and R matrix, with that for the variable metric method being much less.

Bard (1970) counts an iteration every time the objective function and its derivatives are evaluated. Clearly this definition, by itself, presents some difficulty when methods not involving the evaluation of derivatives are considered.

Bard uses this definition in a relative cost type of function, which he calls "the number of equivalent function evaluations," n_e , where,

$$n_e = (r + 1) n_d + n_f ,$$

n_d being the number of times the objective function and its derivatives are evaluated (iterations), and n_f , the number of times the objective function alone was evaluated. On the basis of relative values of n_e , Bard concludes that the linearization methods were best for a variety of problems, when compared with the variable metric and some related methods. However, the quantity of calculation leading up to an equivalent evaluation can also be quite variable. An equivalent evaluation, for example, fails to account for any cost in computing supplemental quantities, such as characteristic roots, when the linearization methods fail. Indeed, no cost penalty is imposed for failure of any of the methods.

Remmler et al. (1966) apparently count an iteration every time a new θ vector is computed. Their comparisons are based on the number of iterations, and computing time to the nearest second, which were required for θ to reasonably approach a known vector. While computing time does provide a measure of the quantity of calculation required for an iteration, it is also specific for a given computer installation, programming language, and includes the optimization ability of the computer programmer. They conclude that the variable metric method was best when compared to linearization, for a variety of problems.

Because of these problems, the data presented in the following sections are intended mainly to test the hierarchical parabola method under a variety of conditions. Numeric comparisons made with other methods are regarded as tenuous and inexact. The presentation of the

data in separate sections for function minimization, solving simultaneous equations, and least squares, is artificial, and has been done only to facilitate the use of published material. Most of the problems have been taken directly from the literature.

3.2 Function Minimization

Several authors, for example, Rosenbrock (1960), Powell (1962), Fletcher and Powell (1963), and Nelder and Mead (1965), have employed one or all of the following objective functions in algorithm tests.

(1) Rosenbrock's Parabolic Valley:

$$f(\theta) = 100 (\theta_2 - \theta_1^2)^2 + (1 - \theta_1)^2 ,$$

starting at (-1.2, 1.0).

(2) Powell's Quartic Function:

$$f(\theta) = (\theta_1 + 10 \theta_2)^2 + 5 (\theta_3 - \theta_4)^2 + (\theta_2 - 2 \theta_3)^4 \\ + 10 (\theta_1 - \theta_4)^4 ,$$

starting at (3, -1, 0, 1).

(3) Fletcher and Powell's Helical Valley:

$$f(\theta) = 100((\theta_3 - 10 h(\theta_1, \theta_2))^2 + ((\theta_1^2 + \theta_2^2)^{\frac{1}{2}} - 1)^2) + \theta_3^2 ,$$

where,

$$2 \pi h(\theta_1, \theta_2) = \tan^{-1}(\theta_2 / \theta_1) \quad , \quad \theta_1 > 0 \\ = \pi + \tan^{-1}(\theta_2 / \theta_1) \quad , \quad \theta_1 < 0 ,$$

starting at $(-1, 0, 0)$. If $-2.5 < \theta < 7.5$, this function attains a minimum at $(1, 0, 0)$.

(4) Fletcher and Powell's Simple Quadratic:

$$f(\theta) = \theta_1^2 - 2 \theta_1 \theta_2 + 2 \theta_2^2 .$$

The entries for the tables in this section have been taken directly from Fletcher and Powell's paper, augmented with the results obtained for this algorithm.

The quadratic function (4) was used to demonstrate the second order convergence property of the variable metric method. That the hierarchical parabola method also has this property is demonstrated in Table 3.1. Table 3.1 also demonstrates the difference in the application of the same definition of an iteration between the two methods, as discussed in section 3.1. The fact that the variable metric method requires less computing per iteration than does the hierarchical parabola method should be kept in mind when examining Table 3.1 and other tables.

Table 3.2 shows the results obtained for the parabolic valley function (1), using a steepest descent method, Powell's method (section 1.3), variable metric and hierarchical parabola methods. According to Fletcher and Powell, "This function is difficult to minimize on account of its having a steep sided valley following the curve $\theta_1^2 = \theta_2$ " (p. 165).

Table 3.3 compares the variable metric and hierarchical parabola methods for the helical valley function (3), showing the progress of the parameter values as well as values of the objective

Table 3.1 Comparison using quadratic function (4)

Item	Iteration	Variable Metric		Hierarchical Parabola	
θ	0	-4	2	-4	2
	1	-1.69	-1.08	0	0
	2	0	0	-	-
$f(\theta)$	0		40	-	-
	1		1.54	0	0
	2		10^{-15}	-	-
Elements of ^a R matrix	0	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$		-	-
	1	$\begin{bmatrix} 0.781 & 0.361 \\ 0.361 & 0.411 \end{bmatrix}$		$\begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}$	
	2	$\begin{bmatrix} 1 & \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$		-	-

^aThe variable metric matrix R_V converges to,

$$R_V = \left[\frac{\partial^2 f(\theta)}{\partial \theta^2} \right]^{-1},$$

while for the hierarchical parabola method, the corresponding matrix is,

$$R_P = \left[\frac{1}{2} \frac{\partial^2 f(\theta)}{\partial \theta^2} \right]^{-1}$$

$$= 2 R_V.$$

Table 3.2 Comparison using parabolic valley function (1)

Iterations	Values of Objective Function			
	Steepest Descents	Powell's Method	Variable Metric	Hierarchical Parabola
0	24.200	24.200	24.200	-
3	3.704	3.643	3.687	2×10^{-4}
6	3.339	2.898	1.605	2×10^{-6}
9	3.077	2.195	0.745	5×10^{-10}
12	2.869	1.412	0.196	-
15	2.689	0.831	0.012	-
18	2.529	0.432	1×10^{-8}	-
21	2.383	0.182	-	-
24	2.247	0.052	-	-
27	2.118	0.004	-	-
30	1.994	5×10^{-5}	-	-
33	1.873	8×10^{-9}	-	-

Table 3.3 Comparison using helical valley function (3)

Iteration	Variable Metric Method				Hierarchical Parabola Method			
	θ_1	θ_2	θ_3	$f(\theta)$	θ_1	θ_2	θ_3	$f(\theta)$
0	-1.000	0.000	0.000	2.5×10^4	-1.000	0.000	0.000	-
1	-1.000	2.278	1.431	5.2×10^3	-0.765	-0.379	0.774	2.900
2	-0.023	2.004	2.649	1.1×10^3	-0.902	-0.262	0.374	1.104
3	-0.856	1.559	3.429	74.080	-0.979	-0.049	0.104	0.112
4	-0.372	1.127	3.319	24.190	-0.998	0.022	-0.032	1.0×10^4
5	-0.499	0.908	3.285	10.942	0.150	0.023	0.115	73.569
6	-0.314	0.900	3.075	9.841	1.000	-9×10^{-4}	-1×10^{-3}	1×10^{-5}
7	0.059	1.069	2.408	6.304	1.000	-4×10^{-6}	-1×10^{-6}	4×10^{-9}
:								
18	1.000	1×10^{-5}	1×10^{-5}	7×10^{-8}				

function. No change, in terms of number of iterations, has been made against the hierarchical parabola method for the adjustment described in section 2.4. Several adjustments were required during the first, third, and sixth iterations. However, by the eleventh iteration, the hierarchical parabola method had reduced the objective function to a value of 1.9×10^{-50} . At this point, θ_1 was one to at least six digits, and θ_2 and θ_3 had values of 8.8×10^{-27} and -5.1×10^{-30} respectively. Corresponding values for the variable metric method at the eleventh iteration were 0.762, 0.894, 0.496, and 0.772 respectively.

At this iteration, the objective function became insensitive to intervals along the θ_2 and θ_3 axes (section 2.3). Further iterations produced machine underflows when attempts were made to compute values of $1 / a$.

The property of stability, in that the objective function is decreased at each iteration, has been proved for the variable metric method by Fletcher and Powell. This property is characteristic of descent methods, in which the direction of search is confined to those directions producing a smaller value of the objective function. Table 3.3 demonstrates this property for the variable metric method, and proves that the hierarchical parabola method is not stable in general. The objective function increases in value at iteration four, accompanying the change in the sign of two of the parameters at this iteration.

The stability property would seem to imply that, if a local minimum occurs between (in an r -dimensioned sense) the area of search

and the true minimum, the method must find the local minimum. That is, there is no opportunity for the objective function to increase in value in order to climb up and out of a local minimum. Whether or not the hierarchical parabola method finds the local minimum would seem to depend upon the effective interval width about θ . If the intervals along all axes were jointly contained in the valley of the local minimum, this minimum would be found. If, however, the interval along one axis included a point outside of the local valley, and the three values of $f(\theta)$ formed a convex set, the hierarchical parabola method can climb out of the local valley. The adjustment, when the values of $f(\theta)$ are not members of a convex set, limits the direction of search to those directions producing a smaller value of the objective function, and hence is stable.

A contour map across $\theta_1 = -0.99$ reveals a narrow valley extending across $-0.015 \leq \theta_3 \leq 0.07$ and $-0.03 \leq \theta_2 < 0.0$. For values $\theta_2 > 0$, the objective function immediately climbed to 1×10^4 , even for values as near zero as $\theta_2 = 5 \times 10^{-7}$. The minimum value obtained in the mapping was $f(\theta) = 0.01$ at $\theta_1 = -0.99$, $\theta_2 = -0.01$, $\theta_3 = 0.015$.

The quartic function (2) provides an example of the behaviour of the algorithm when the matrix of second order derivatives is singular. Also, for this function, as the vector θ approaches zero, the influence of the quartic terms essentially disappears, and in the vicinity of $\theta = 0$, the function tends to

$$f(\theta) = (\theta_1 + 10 \theta_2)^2 + 5 (\theta_3 - \theta_4)^2 ,$$

with solutions,

$$\theta_1 = -10 \theta_2$$

$$\theta_3 = \theta_4 .$$

For this function, after the second iteration, the algorithm failed when attempting to compute $1 / a_{1,4}$; that is, when attempting to adjust θ_1 for its covariance with θ_4 . At this point, the value of the determinant of the approximating quadratic form was 1.9×10^4 . After 124 applications of the adjustment described in section 2.4, the value of the determinant on the third iteration was 1.7×10^{-18} . At this point also, the contribution of the quartic terms was essentially nil, and the solutions,

$$\theta_1 = -0.149209 \times 10^{-5}$$

$$\theta_2 = 0.149199 \times 10^{-6}$$

$$\theta_3 = 0.324555 \times 10^{-6}$$

$$\theta_4 = 0.324554 \times 10^{-6} ,$$

corresponding to,

$$f(\theta) = 9.4 \times 10^{-21}$$

were found. For the next 22 iterations, after which processing was terminated, the value of the objective function remained at about 2×10^{-25} , and, at least to the six digits used on output, $\theta_1 = -10 \theta_2$, and $\theta_3 = \theta_4$. Values obtained varied within narrow ranges about -1.7×10^{-7} and 2.0×10^{-7} respectively.

Although no basis for a comparison with the variable metric method seems available, Fletcher and Powell report that this method

had reduced the objective function to 2.5×10^{-8} in six iterations. They also report that Powell's method produced a value of 9×10^{-3} , and steepest descent, 6.36, both in seven iterations.

Values of the parameters for this function are reported as follows by Remmler et al. (1966).

Variable metric, 50 iterations:

$$\begin{aligned}\theta_1 &= -0.49447 \times 10^{-2} \\ \theta_2 &= 0.48519 \times 10^{-3} \\ \theta_3 &= -0.25346 \times 10^{-2} \\ \theta_4 &= -0.25342 \times 10^{-2} .\end{aligned}$$

Newton-Raphson, 28 iterations:

$$\begin{aligned}\theta_1 &= 0.14646 \times 10^{-3} \\ \theta_2 &= -0.14646 \times 10^{-4} \\ \theta_3 &= 0.38937 \times 10^{-4} \\ \theta_4 &= 0.38937 \times 10^{-4} .\end{aligned}$$

Simplex, 141 iterations:

$$\begin{aligned}\theta_1 &= 0 \\ \theta_2 &= 0.14160 \times 10^{-5} \\ \theta_3 &= 0.89613 \times 10^{-8} \\ \theta_4 &= 0.10964 \times 10^{-14} .\end{aligned}$$

How Remmler et al. (1966) counted iterations for the simplex method is not clear. Since this method is similar to the adjustment operation of section 2.4, these results may compare with the 124 adjustments required in the third iteration of the hierarchical parabola method. For their simplex method, Nelder and Mead (1965) report an average of 219 "evaluations" to satisfy the relation,

$$\left[\frac{\sum (f(\theta) - \overline{f(\theta)})^2}{r} \right]^{\frac{1}{2}} < 10^{-8} ,$$

where summation and averaging are over the points of the simplex.

However, for least squares applications, comparisons of this type may be academic, since interest is in the fact that redundant information has been included, rather than in the minimum value of the objective function under this circumstance.

3.3 Simultaneous Equations

Remmler et al. (1966) include in their report a number of simultaneous equations which they used to compare an unmodified linearization method, the variable metric and simplex methods. For each set of equations, the authors include a set of known solutions. A change in the parameter values of less than 0.0001 was used by Remmler et al., and has been used as well to terminate the following hierarchical parabola tests. In these tests, the fifth decimal place is used for rounding the results given below.

The easiest set of solutions to obtain, in terms of number of iterations and computing time, as measured by Remmler et al. and also here, were the solutions to,

$$(5) \quad g_1(\theta) = \theta_1 + \theta_2 + \theta_3 - 1$$

$$g_2(\theta) = 3\theta_1 + \theta_2 - 3\theta_3 - 5$$

$$g_3(\theta) = \theta_1 - 2\theta_2 - 5\theta_3 - 10 .$$

These solutions are:

$$\theta_1 = 6.0000$$

$$\theta_2 = -7.0000$$

$$\theta_3 = 2.0000 .$$

At this point, the value of the objective function was,

$$f(\theta) = 8 \times 10^{-12} .$$

Also easily solved were,

$$(6) \quad g_1(\theta) = \theta_1^2 + \theta_2^2 + \theta_3^2 - 1$$

$$g_2(\theta) = 2\theta_1^2 + \theta_2^2 - 4\theta_3$$

$$g_3(\theta) = 3\theta_1^2 - 4\theta_2 + \theta_3^2 ,$$

giving,

$$\theta_1 = 0.7852$$

$$\theta_2 = 0.4966$$

$$\theta_3 = 0.3699 ,$$

with,

$$f(\theta) = 5 \times 10^{-11} .$$

The set of equations,

$$(7) \quad g_1(\theta) = \theta_1^2 + \theta_2 - 11$$

$$g_2(\theta) = \theta_1 + \theta_2^2 - 7 \quad ,$$

demonstrate the use of realistic boundary values in defining the solutions (section 2.6). Starting at the point (1, 1), with no imposition of boundaries, the obvious solutions

$$\theta_1 = 3.0000$$

$$\theta_2 = 2.0000$$

were found, rather than the less obvious solutions given by Remmler et al. (1966) of,

$$\theta_1 = 3.5844$$

$$\theta_2 = -1.8481 \quad .$$

In order to find the second solutions, an upper boundary of zero was imposed on the θ_2 axis. Values of the objective function were, respectively,

$$f(\theta) = 5 \times 10^{-10}$$

$$f(\theta) = 5 \times 10^{-8} \quad .$$

A similar problem, but with both solutions positive, is posed by,

$$(8) \quad g_1(\theta) = \theta_1^3 - 3 \theta_1^2 \theta_2 + \theta_2^2 - 7$$

$$g_2(\theta) = \theta_1^2 - 4 \theta_1 + \theta_2^2 - 4 \theta_2 + 4 \quad .$$

The solutions found by Remmler et al. (1966),

$$\theta_1 = 1.9148$$

$$\theta_2 = 0.00182 \quad ,$$

were found by starting at (0, 0). Another set of solutions,

$$\theta_1 = 0.1138$$

$$\theta_2 = 2.6650 \quad ,$$

were found by starting at (1, 1). No boundaries were imposed in either case, and, in the above order,

$$f(\theta) = 5 \times 10^{-11}$$

$$f(\theta) = 8 \times 10^{-11} \quad .$$

The two sets of solutions to equations (7) and (8) might also be interpreted as representing a true solution, and a solution at a local minimum, the distinction being the relative sizes of the objective function. In both of these cases, the values of the objective functions are sufficiently close to zero that double solutions seem more reasonable. The problem is less easily resolved for the next two sets of equations.

$$(9) \quad g_1(\theta) = \theta_1^2 + 12 \theta_2^2 - 1$$

$$g_2(\theta) = 49 \theta_1^2 + 49 \theta_2^2 + 84 \theta_1 + 2324 \theta_2 - 681$$

$$(10) \quad g_1(\theta) = 121 \theta_1^2 - 32 \theta_2^2 - 121$$

$$g_2(\theta) = 7 \theta_1^2 + 7 \theta_1 \theta_2 + 7 \theta_2^2 + 70 \theta_1 - 63 \theta_2 - 34 \quad .$$

Both equations (9) and (10) were hard to solve with the hierarchical parabola method. Remmler et al. (1966) report that the variable metric method failed on equations (9). Also, the solutions found by the linearization method, and by the variable metric method for equations (10), did not agree well with Remmler's known solutions. Disagreement on the third digit, for one or other of the members of each set of solutions, occurred in each case. In all other cases, except one, agreement was to at least six digits, and usually more. For the one exception, equations (6), the variable metric method, linearization, and hierarchical parabola methods agreed with each other to at least six digits, but disagreed with the known solution to θ_1 on the fourth digit.

The problem with equations (9) and (10) involves closely spaced minima, as evidenced by the excessive number of times values of $f(\theta)$ increased at successive iterations.

For equations (9), three increases were obtained in the sixteen iterations required to satisfy the terminating criterion. The progress of the iterates, and the corresponding values of the objective function are shown in Table 3.4, for iterations 10 through 16, covering two of the increases. Also shown is the known solution given by Remmler et al. (1966). Table 3.4 indicates that the solutions obtained by the hierarchical parabola method are somewhat better than the known solutions, based on the values of the objective function. Since values of θ_1 decrease, and those for θ_2 increase, over the length of the table, a parallel valley, comparable to that at iteration 11, is suggested as the location of the known solutions, with a

Table 3.4 Progress of iterates for equations (9)

Iteration	θ_1	θ_2	$f(\theta)$
10	0.222921	0.282244	3.50×10^{-5}
11	0.216551	0.282530	2.28×10^{-5}
12	0.204626	0.283063	3.68×10^{-5}
13	0.188628	0.283769	1.94×10^{-4}
14	0.172997	0.284441	7.74×10^{-6}
15	0.169291	0.284598	3.58×10^{-7}
16	0.169290	0.284598	3.81×10^{-7}
** ^a	0.14285	0.28571	1.2×10^{-4}

^a ** These values are the known solutions provided by Remmler et al. (1966); $f(\theta)$ was evaluated using these values of θ . Since only five digits were provided for the known solutions, a comparable evaluation for the solutions at iteration 16 gave $f(\theta) = 1.57 \times 10^{-5}$.

ridge, comparable to iteration 13, separating these from the solutions obtained here. Figure 3.1 is a contour map, showing values of $f(\theta)$ for selected intervals along the θ_1 and θ_2 axes. A narrow valley is seen to extend across the region of the solutions.

In Figure 3.1, both the ordinate and the abscissa have been scaled into 49 equally spaced intervals; ordinate values are $0.14 \leq \theta_1 \leq 0.22$, and abscissa values, $0.280 \leq \theta_2 \leq 0.289$. The objective function was evaluated at each of the 49×49 points, and deviations from the minimum value are plotted on the following scale:

Symbol	Value of the Deviation
*	$d \geq 2^{10}$
9	$2^8 \leq d < 2^{10} = 1024$
8	$2^6 \leq d < 2^8 = 256$
7	$2^4 \leq d < 2^6 = 64$
6	$2^2 \leq d < 2^4 = 16$
5	$2^0 \leq d < 2^2 = 4$
4	$2^{-2} \leq d < 2^0 = 1$
3	$2^{-4} \leq d < 2^{-2} = 0.25$
2	$2^{-6} \leq d < 2^{-4} = 0.0625$
1	$2^{-8} \leq d < 2^{-6} = 0.015625$
0	$2^{-10} \leq d < 2^{-8} = 0.00390625$
blank	$0 \leq d < 2^{-10} = 0.0009765625$

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Figure 3.1 Contours for equations (9)

A similar, but less severe problem occurs in equations (10). Progress of the iterates and values of the objective function are shown in Table 3.5. Figure 3.2 shows the contours over the ranges,

$$1.274 \leq \theta_1 \leq 1.28625$$

$$1.540 \leq \theta_2 \leq 1.57375 \quad .$$

Equations

$$(11) \quad g_1(\theta) = 2 \theta_1 - 3.18309886 \ln((1 - \theta_3) / (1 + \theta_3)) - 1$$

$$g_2(\theta) = 1.57079632 \theta_1 (1 - \theta_2^2 \theta_3^2) ((\theta_3^2 - \theta_2^2) / (\theta_3 \theta_2^2 (1 + \theta_3^2))) - 5$$

$$g_3(\theta) = \theta_3 - 0.14271816$$

were the most difficult to solve, in terms of finding suitable boundary restrictions along each axis. Figure 3.3 indicates the problem. In Figure 3.3, ordinate and abscissa values are scaled $-0.5 \leq \theta_1 \leq 0.5$ and $0 < \theta_2 < 2.0$, respectively, with $\theta_3 = 0.142718$. The surface is flat, falling away to the lower right hand corner, in a direction away from the minimum at the scaled point (27, 2). The boxed region in Figure 3.3 is enlarged in Figure 3.4, taking $0 \leq \theta_1 \leq 0.35$ and $0.01 \leq \theta_2 \leq 0.17$. The known solutions for equations (11) are,

$$\theta_1 = 0.042591338$$

$$\theta_2 = 0.041400152$$

$$\theta_3 = 0.14271816 \quad .$$

Table 3.5 Progress of iterates for equations (10)

Iteration	θ_1	θ_2	$f(\theta)$
8	1.27591	1.54112	4.87×10^{-4}
9	1.27922	1.55131	6.51×10^{-5}
10	1.28126	1.55757	2.77×10^{-5}
11	1.28360	1.56518	1.00×10^{-3}
12	1.28406	1.56633	4.01×10^{-6}
13	1.28420	1.56674	1.19×10^{-7}
14	1.28273	1.56693	2.49×10^{-1}
15	1.28438	1.56729	6.95×10^{-8}
16	1.28438	1.56730	1.83×10^{-7}
** ^a	1.2857	1.5710	1.64×10^{-2}

^a ** These values are the known solutions provided by Remmler et al. (1966); $f(\theta)$ was evaluated using these values of θ . Since only five digits were provided for the known solutions, a comparable evaluation for the solutions at iteration 15 gave $f(\theta) = 4.01 \times 10^{-5}$.

The equations were solved by imposing the following boundary values:

$$-0.5 \leq \theta_1 \leq 0.5$$

$$0.0 < \theta_2 \leq 0.2$$

$$0.0 < \theta_3 < 1.0 .$$

The solutions obtained were poorer than the known solutions, as judged by the relative sizes of the objective function.

Since $g_3(\theta) = 0$ only when $\theta_3 = 0.14271816$, a reasonable procedure for solving this system of equations would be to set θ_3 at this value, and solve for θ_1 and θ_2 . When this was done, keeping the same boundary values along θ_1 and θ_2 , the known values were obtained.

Another set of equations given by Remmler et al. (1966) produces the same objective function as the quartic function (2), discussed in section 3.2.

3.4 Least Squares

To examine some small sample properties of the estimates, 1000 values, E , were drawn from the set $\{ \epsilon ; \epsilon = -3.0, -2.9, \dots, 0.0, 0.1, \dots, 3.0 \}$. Except for $\epsilon_i = -3.0, 0.0, 3.0$, the probabilities associated with each draw were,

$$P(E = \epsilon_i) = \int_{\epsilon_{i-1}}^{\epsilon_i} n(\mu, \sigma) d\mu , \quad \epsilon_i < 0$$

$$= \int_{\epsilon_i}^{\epsilon_{i+1}} n(\mu, \sigma) d\mu , \quad \epsilon_i > 0 ,$$

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2 86456666777
1 77

Figure 3.4 Enlargement of designated area on Figure 3.3

where $n(\mu, \sigma)$ is a normal density function, having mean zero and variance one.

$$P(E = -3.0) = \int_{-\infty}^{-3.0} n(\mu, \sigma) d\mu$$

$$P(E = 3.0) = \int_{3.0}^{\infty} n(\mu, \sigma) d\mu$$

and

$$P(E = 0.0) = \int_{-0.1}^{0.1} n(\mu, \sigma) d\mu .$$

Hence, E is approximately $N(0, 1)$.

Values of

$$Y = 200 + (150) (0.9)^X$$

were computed for $X = 0, 1, \dots, 9$, and added to the values of E , to form 100 samples each of size 10. The model,

$$(12) \quad Y = \theta_1 + \theta_2 \theta_3^X + E ,$$

was fitted to each of the 100 samples. This model was chosen because it frequently appears in biological growth problems.

If E is distributed $N(0, 1)$, then the deviation sum of squares is distributed as chi square. The parameter associated with this chi square has been taken at seven degrees of freedom, and the frequencies of the observed and expected values of chi square are shown in Table 3.6.

Table 3.6 Comparison of observed sums of squares with chi square^a

Value of Chi Square	Expected Frequency in 100 Observations	Observed Frequency
≤ 1.239	1	0
1.564	1	1
2.167	3	3
2.833	5	5
3.822	10	12
4.671	10	9
6.346	20	25
8.383	20	19
9.803	10	7
12.017	10	11
14.067	5	4
16.622	3	3
18.475	1	0
> 18.475	1	1

^a $\chi^2 = 5.0$.

$\chi^2 = 22.4$ with 13 degrees of freedom, probability 0.95.

Also, if E is distributed $N(0, 1)$, then,

$$t_1 = \frac{\beta_1 - 200}{s_1}$$

$$t_2 = \frac{\beta_2 - 150}{s_2}$$

$$t_3 = \frac{\beta_3 - 0.9}{s_3}$$

are distributed as Student's t , again taken at seven degrees of freedom. The frequencies of the observed and expected values of t are shown in Table 3.7. The values s_i , $i = 1, 2, 3$, are the square roots of the estimated variances of the parameter estimates obtained from each sample, and β_i are the least squares estimates of θ_i . These values are tabulated in Appendix 5.4, and the values of β_i , along with those of $f(\beta)$ used in Table 3.6 are tabulated in Appendix 5.4.

For all 100 samples, the estimates obtained are,

$$\beta_1 = 200.5666$$

$$\beta_2 = 150.6027$$

$$\beta_3 = 0.8998$$

$$\text{Var}(\beta_1) = 69.1429$$

$$\text{Var}(\beta_2) = 63.0760$$

$$\text{Var}(\beta_3) = 0.6493 \times 10^{-4}$$

Table 3.7 Comparison of observed and expected values of t^a

Value of t	Expected Frequency in 100 Observations	Observed Frequencies		
		t_1	t_2	t_3
< 0.130	10	8	7	10
0.130	10	11	10	11
0.236	10	11	12	5
0.402	10	9	7	12
0.549	10	10	13	13
0.711	10	9	9	6
0.896	10	11	12	9
1.119	10	11	9	13
1.415	10	10	11	11
1.895	5	3	2	3
2.365	3	3	4	3
2.998	1	1	1	3
> 3.499	1	3	3	1

$$^a \chi_1^2 = 5.80.$$

$$\chi_2^2 = 9.93.$$

$$\chi_3^2 = 11.40.$$

$$\chi^2 = 21.0 \text{ with 12 degrees of freedom, probability 0.95.}$$

$$\text{Var}(\beta_1, \beta_2) = 65.8503$$

$$\text{Var}(\beta_1, \beta_3) = 0.6617 \times 10^{-1}$$

$$\text{Var}(\beta_2, \beta_3) = 0.6254 \times 10^{-1} .$$

Tables 3.6 and 3.7 indicate that the estimates of σ^2 , β_i and s_i are quite reasonable, even for samples of size 10, using this three parameter model.

The small sample performance for other least squares models has not been studied, although other models have been fitted for numerical testing of the algorithm. These include a least squares model used by Bard (1970) as follows:

$$(13) \quad Y = \theta_1 + \frac{X_1}{\theta_2 X_2 + \theta_3 X_3} + E .$$

For this example, Bard synthesized values of X and Y. Using his data set, his least squares estimates of θ , namely,

$$\beta_1 = 0.08241$$

$$\beta_2 = 1.13303$$

$$\beta_3 = 2.34370 ,$$

were obtained.

An example of a weighted least squares analysis is provided by data presented by Hill (1966). These data are weights, in milligrams, of the eye lens of the cottontail, Sylvilagus floridanus, for 89 known aged individuals. The model is,

$$(14) \quad Y = \theta_1 \exp_{10}(\theta_2 / (X + \theta_3)) + E ,$$

²Hill, E. P., III. 1966. A cottontail rabbit lens growth curve from Alabama. Annual Meeting Southeast Association of Game and Fish Commissioners, Asheville, N. C.

where \exp_{10} implies 10 to the power in parentheses. Since the variance of the lens weight tends to increase with the age of the cottontail (or weight of the lens), a weighted least squares analysis is appropriate. Initial weights were chosen to be reciprocals of the observed lens weights. Starting with the third iteration, the weights were re-estimated at each iteration. Initial parameter values and boundary values imposed along each axis were

$$\begin{aligned}\theta_1 &= 300 ; & \theta_1 &\geq 0 \\ \theta_2 &= -60 ; & \theta_2 &\leq 0 \\ \theta_3 &= 41 ; & \theta_3 &\geq 0 .\end{aligned}$$

The initializing value of θ_1 was chosen to be larger than the largest observed lens weight. Values for θ_2 and θ_3 were taken from Dudzinski and Mykytowycz (1961), where they were determined from a set of comparable data for the European rabbit, Oryctolagus cuniculus, in Australia.

Table 3.8 lists the values of the parameter estimates, residual sum of squares, and estimated variances of the estimates, along with a corresponding set of values obtained by an unweighted least squares analysis of the same data.

3.5 Conclusions

Comparisons with other algorithms indicate that no method is uniformly better than another. The relative performances depend to some extent on the form of the objective function, and, in any event, are difficult to assess due to the lack of a suitable measure of performance.

Table 3.8 Comparison of weighted and unweighted estimates from eye lens data

Item	Weighted Estimate	Unweighted Estimate
β_1	290.07	287.56
β_2	-57.98	-56.16
β_3	34.92	32.76
$f(\beta)$	23.37	3,142.64
$\text{Var}(\beta_1)$	8.92	6.54
$\text{Var}(\beta_2)$	1.70	2.64
$\text{Var}(\beta_3)$	1.24	4.59
$\text{Var}(\beta_1, \beta_2)$	-3.32	-3.62
$\text{Var}(\beta_1, \beta_3)$	2.31	3.61
$\text{Var}(\beta_2, \beta_3)$	-1.32	-3.04

The hierarchical parabola method has some advantages, as follow.

- (1) It can be successfully applied to a wide range of objective functions.
- (2) It is relatively easy to use, since no evaluations of derivatives, or explicit matrix inversions are required.
- (3) It has the property of second order convergence, which considerably reduces the number of iterations required to stabilize the parameter estimates.
- (4) The method has the ability to climb out of local minima, since it is based on an interval across the surface generated by the objective function, rather than a point on this surface.
- (5) The small sample properties of the estimates of the parameters and their estimated variances appear desirable.
- (6) The relative contributions of the parameters can be assessed in a step-wise manner, and redundant axes are easily identified.
- (7) Boundary values are easily imposed along any or all axes.

The main disadvantage to the method is the necessity to incorporate a procedure to be followed when the set of values of the objective function, produced by the intervals along each axis, is not convex.

Further work, to tabulate the small sample properties for a variety of models, and to discover a theoretical basis for controlling the effective interval width in the area of search at each iteration would appear desirable.

3.6 Resume of Chapter 3

To increase the number of functional forms available for numerical testing of the hierarchical parabola method, problems of function minimization as such, and solving sets of non-linear simultaneous equations, as well as least squares applications are considered in Chapter 3. The problems are taken from the literature.

In no case, for the large variety of functional forms considered, was the method unsuccessful in obtaining solutions at least as satisfactory as those appearing in the literature. This is not to imply that the method solved each of the problems with equal facility, however. In the case of equations (11), the area of search had to be restricted more closely than might be considered desirable, in order to obtain satisfactory solutions. The surface generated by equations (11) is deceptive with respect to the location of the minimum.

The ability of this method to climb out of local minima is demonstrated in equation (3), and others. This unique feature of the method is due to the fact that a region over the surface, rather than a point on it, is involved in the minimization process. If the region is, in some sense, wholly contained in the valley of the local minimum, this will be the minimum found. However, local minima which occur at locations remote from that of the global minimum, that is, at some distance away from the solutions, are likely to be encountered early in the iterative process, when the region over the surface is still relatively large, and, therefore, not likely to be contained in the local valley. Hence, while this method does not

guarantee that a local minimum will not be found, it considerably reduces the chances of this occurring.

By constructing the approximating paraboloid surface in a hierarchical manner, redundancies in the model, that is, in a sense, over specification of the model, can be located. This feature is demonstrated in equation (2).

Weighted least squares analysis, used when the variance of the observations changes in a known way over the range of the observations, is demonstrated by equation (14). In this case, the variance of the eye lens weights of cottontails over age increases with the weight of the lens.

Also in Chapter 3, some small sample properties are numerically documented, employing a familiar, three parameter non-linear biological growth equation (12). Results indicate, at least for the model employed, that the estimates of the parameters and their associated variances computed by this method can be used satisfactorily in tests based on the usual t-statistic for samples as small as ten observations.

4. LIST OF REFERENCES

- Bard, Y. 1970. Comparison of gradient methods for the solution of nonlinear parameter estimation problems. Society for Industrial and Applied Mathematics. Journal on Numerical Analysis 7:157-186.
- Booth, G. W., G. E. P. Box, M. E. Muller, and T. I. Peterson. 1959. Forecasting by generalized regression methods, nonlinear estimation. International Business Machines Corporation, Share Program Number 687 WL N11, New York, New York.
- Browne, E. T. 1958. Introduction to the Theory of Determinants and Matrices. University of North Carolina Press, Chapel Hill, N. C.
- Davidon, W. C. 1959. Variable metric method for minimization. Argonne National Laboratory, Atomic Energy Commission Research and Development Report ANL - 5990 Rev., Lemont, Illinois.
- Dudzinski, M. L., and R. Mykytowycz. 1961. The eye lens as an indicator of age in the wild rabbit in Australia. Commonwealth Scientific and Industrial Research Organization 6:156-159.
- Fletcher, R., and M. J. D. Powell. 1963. A rapidly convergent descent method for minimization. The Computer Journal 6: 163-168.
- Greenstadt, J. 1967. On the relative efficiencies of gradient methods. Mathematical Computations 21:360-367.
- Hartley, H. O. 1961. The modified Gauss-Newton method for fitting of nonlinear regression functions by least squares. Technometrics 3:269-280.
- Jennrich, R. I., and P. F. Sampson. 1968. Application of stepwise regression to non-linear estimation. Technometrics 10:63-72.
- Marquardt, D. W. 1963. An algorithm for least-squares estimation on non-linear parameters. Journal of the Society for Industrial and Applied Mathematics 11:431-441.

- Marquardt, D. W., R. G. Bennett, and E. J. Burrell. 1961. Least squares analysis of electron paramagnetic resonance spectra. *Journal of Molecular Spectroscopy* 7:269-279.
- Nelder, J. A. 1961. The fitting of a generalization of the logistic curve. *Biometrics* 17:89-110.
- Nelder, J. A., and R. Mead. 1965. A simplex method for function minimization. *The Computer Journal* 7:308-313.
- Pimentel-Gomez, F. 1953. The use of Mitscherlich's regression law in the analysis of experiments with fertilizers. *Biometrics* 9:498-516.
- Powell, M. J. D. 1962. An iterative method for finding stationary values of a function of several variables. *The Computer Journal* 5:147-151.
- Remmler, K. L., D. W. Cawood, J. A. Stanton, and R. Hill. 1966. Solutions of systems of nonlinear equations. Lockheed Missiles and Space Company, Final Report, Contract NAS8 - 20178, Huntsville, Alabama.
- Rosenbrock, H. H. 1960. An automatic method for finding the greatest or least value of a function. *The Computer Journal* 3:175-184.
- Shah, B. V., R. J. Buehler, and O. Kempthorne. 1964. Some algorithms for minimizing a function of several variables. *Statistical Laboratory, Iowa State University, Iowa City, Iowa, Reprint Series Number 146.*
- Smail, L. L. 1949. *Calculus*. Appleton - Century - Crofts, New York, New York.
- Spendley, W., G. R. Hext, and F. R. Himsworth. 1962. Sequential application of simplex designs in optimization and evolutionary operation. *Technometrics* 4:441-461.
- Stevens, W. L. 1951. Asymptotic regression. *Biometrics* 7:247-267.
- Turner, M. E., R. J. Monroe, and H. L. Lucas, Jr. 1961. Generalized asymptotic regression and non-linear path analysis. *Biometrics* 17:120-143.

5. APPENDICES

5.1 Determinantal Algebra

Theorem 1.1 (Browne, 1958, p. 16)

If A is a square matrix, the determinant of A is equal to the determinant of the transpose of A .

Corollary 1.1.1

If A is symmetric, then $A_{i,j} = A_{j,i}$, where $A_{i,j}$ is the first minor of A .

Proof:

Since A is symmetric, the matrix obtained by striking the i -th row and j -th column is the transpose of the matrix obtained by striking the j -th row and i -th column. Since A is square, the resulting matrices are also square.

Hence

$$(A_{i,j})' = (A_{j,i}) ,$$

and

$$\begin{aligned} |A_{i,j}| &= |(A_{i,j})'| \\ &= |A_{j,i}| . \end{aligned}$$

Theorem 1.2 (Browne, 1958, p. 18)

The value of the determinant $|A|$ is equal to the sum of the products of the elements of any row, or column, of A , each by its own cofactor.

Corollary 1.2.1

$$\sum_{i=1}^k (-1)^{i+k} f_{i,h}^2 |A_{i,k}^{(k)}| = |A_{k,h}^{(k+1)}|, \quad k = 1, 2, \dots, r,$$

where $|A^{(k)}|$ is the principle minor of the matrix

$$A = \begin{bmatrix} f_1^2 & f_{1,2}^2 & \dots & f_{1,r}^2 \\ f_{1,2}^2 & f_2^2 & \dots & f_{2,r}^2 \\ \vdots & \vdots & & \vdots \\ f_{1,r}^2 & f_{2,r}^2 & \dots & f_r^2 \end{bmatrix}$$

obtained by deleting all the rows and columns beyond the k -th, $k = 1, 2, \dots, r$; $|A_{i,k}^{(k)}|$ is the first minor of the corresponding matrix; $|A_{k,h}^{(k+1)}|$ is the first minor of the matrix obtained from $|A^{(k)}|$ by adding as the $k+1$ -th row and column, the elements $f_{1,h}^2, f_{2,h}^2, \dots, f_h^2$, where $h = k+1, k+2, \dots, r$.

Proof:

For the case where $k = 1$, define $|A^0| = 1$, and $|A_{1,1}^{(1)}| = |A^0|$. Then both sides of the equation reduce to $f_{1,h}^2$.

Otherwise,

$$|A_{k,h}^{(k+1)}| = \begin{vmatrix} f_1^2 & f_{1,2}^2 & \dots & f_{1,k}^2 \\ f_{1,2}^2 & f_2^2 & & f_{2,k}^2 \\ \vdots & \vdots & & \vdots \\ f_{1,k-1}^2 & f_{2,k-1}^2 & & f_{k-1,k}^2 \\ f_{1,h}^2 & f_{2,h}^2 & & f_{k,h}^2 \end{vmatrix}.$$

Expanding by the last row gives,

$$\begin{aligned}
 |A_{k,h}^{(k+1)}| &= (-1)^{1+k} f_{1,h}^2 \begin{vmatrix} f_{1,2}^2 & f_{1,3}^2 & \cdots & f_{1,k}^2 \\ f_2^2 & f_{2,3}^2 & \cdots & f_{2,k}^2 \\ \vdots & \vdots & & \vdots \\ f_{2,k-1}^2 & f_{3,k-1}^2 & \cdots & f_{k-1,k}^2 \end{vmatrix} \\
 &+ (-1)^{2+k} f_{2,h}^2 \begin{vmatrix} f_1^2 & f_{1,3}^2 & \cdots & f_{1,k}^2 \\ f_{1,2}^2 & f_{1,3}^2 & \cdots & f_{2,k}^2 \\ \vdots & \vdots & & \vdots \\ f_{1,k-1}^2 & f_{3,k-1}^2 & \cdots & f_{k-1,k}^2 \end{vmatrix} \\
 &+ \dots + (-1)^{2k} f_{k,h}^2 \begin{vmatrix} f_1^2 & f_{1,2}^2 & \cdots & f_{1,k-1}^2 \\ f_{1,2}^2 & f_2^2 & \cdots & f_{2,k-1}^2 \\ \vdots & \vdots & & \vdots \\ f_{1,k-1}^2 & f_{2,k-1}^2 & \cdots & f_{k-1}^2 \end{vmatrix} \\
 &= (-1)^{1+k} f_{1,h}^2 |A_{k,1}^{(k)}| + (-1)^{2+k} f_{2,h}^2 |A_{k,2}^{(k)}| \\
 &\quad + \dots + (-1)^{2k} f_{k,h}^2 |A_{k,k}^{(k)}|.
 \end{aligned}$$

Since the matrix corresponding to $|A^{(k)}|$ is symmetric, by corollary 1.1.1 the above becomes,

$$|A_{k,h}^{(k+1)}| = \sum_{i=1}^k (-1)^{i+k} f_{i,h}^2 |A_{i,k}^{(k)}|.$$

Theorem 1.3 (Browne, 1958, p. 20)

The sum of the products of the elements of any row, or column, by the corresponding cofactors of the elements of another row, or column, is zero.

Corollary 1.3.1 (Browne, 1958, p. 37)

Let the square matrix A be non singular, and consider the matrix

$$A^{-1} = \frac{1}{|A|} \begin{bmatrix} |A_{1,1}| & -|A_{2,1}| & \dots & (-1)^{r+1}|A_{r,1}| \\ -|A_{1,2}| & |A_{2,2}| & \dots & (-1)^{r+2}|A_{r,2}| \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{1+r}|A_{1,r}| & (-1)^{2+r}|A_{2,r}| & \dots & |A_{r,r}| \end{bmatrix} .$$

Then by theorems 1.2 and 1.3,

$$A A^{-1} = A^{-1} A = I ,$$

with an element from A^{-1} equal to,

$$(-1)^{i+j} \frac{|A_{j,i}|}{|A|} .$$

Theorem 1.4

Following the definitions of corollary 1.2.1,

$$|A^{(k-1)}| |A_{i,h}^{(k+1)}| = |A_{i,k}^{(k)}| |A_{k,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| ,$$

$$i \leq k-1 = 1, 2, \dots, r-1 \text{ and } h = k+1, k+2, \dots, r.$$

Proof:

Note that $|A_{k,h}^{(k+1)}| = \sum_{j=1}^k (-1)^{j+k} f_{j,h}^2 |A_{k,j}^{(k)}|$. Hence

$$\begin{aligned} & |A_{i,k}^{(k)}| |A_{k,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\ &= |A_{i,k}^{(k)}| \sum_{j=1}^k (-1)^{j+k} f_{j,h}^2 |A_{k,j}^{(k)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\ &= (-1)^{2k} f_{k,h}^2 |A_{k,k}^{(k)}| |A_{i,k}^{(k)}| + |A_{i,k}^{(k)}| \sum_{j=1}^{k-1} (-1)^{j+k} f_{j,h}^2 |A_{k,j}^{(k)}| \\ &\quad - |A_{i,h}^{(k)}| |A^{(k)}|. \end{aligned}$$

Note that the first term in the above expression is $|A_{k,k}^{(k)}|$ times the last term of $|A_{i,h}^{(k+1)}|$, expanded by its last row. Adding and subtracting the other terms in this expansion gives,

$$\begin{aligned} & |A_{k,k}^{(k)}| \sum_{j=1}^k (-1)^{j+k} f_{j,h}^2 |A_{i,j}^{(k)}| - |A_{k,k}^{(k)}| \sum_{j=1}^{k-1} (-1)^{j+k} f_{j,h}^2 |A_{i,j}^{(k)}| \\ &+ |A_{i,k}^{(k)}| \sum_{j=1}^{k-1} (-1)^{j+k} f_{j,h}^2 |A_{k,j}^{(k)}| - |A_{i,h}^{(k)}| |A^{(k)}|. \end{aligned}$$

In the first term, note that $|A_{k,k}^{(k)}| = |A^{(k-1)}|$. In the second term, expand $|A_{k,k}^{(k)}|$ successively by column 1, 2, ..., k-1, accordingly as the index to the summation assumes these values. That is,

$$\begin{aligned}
|A_{k,k}^{(k)}| &= \sum_{j=1}^{k-1} (-1)^{1+j} f_{1,j}^2 |A_{j,1}^{(k-1)}| \\
&= \sum_{j=1}^{k-1} (-1)^{2+j} f_{2,j}^2 |A_{j,2}^{(k-1)}| \\
&= \dots = \sum_{j=1}^{k-1} (-1)^{j+k-1} f_{j,k-1}^2 |A_{j,k-1}^{(k-1)}|.
\end{aligned}$$

For the third term, expand $|A_{k,j}^{(k)}|$ by the k -th column. Since the index to the summation extends only to $k-1$, the k -th column occurs in all elements of the sum. Substituting these gives,

$$\begin{aligned}
&|A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\
&+ \sum_{j=1}^{k-1} (-1)^{j+k-1} f_{j,h}^2 |A_{i,j}^{(k)}| \sum_{g=1}^{k-1} (-1)^{g+j} f_{g,j}^2 |A_{g,j}^{(k-1)}| \\
&+ \sum_{j=1}^{k-1} (-1)^{j+k} f_{j,h}^2 |A_{i,k}^{(k)}| \sum_{g=1}^{k-1} (-1)^{g+k-1} f_{g,k}^2 |A_{g,j}^{(k-1)}|.
\end{aligned}$$

The elements of the third and fourth terms are multiplied out, and regrouped to make the expression

$$\begin{aligned}
& |A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\
& + \sum_{g=1}^{k-1} \sum_{j=1}^{k-1} (-1)^{g+j} f_{j,h}^2 |A_{g,j}^{(k-1)}| \{ (-1)^{j+k-1} f_{g,j}^2 |A_{i,j}^{(k)}| \\
& + (-1)^{2k-1} f_{g,k}^2 |A_{i,k}^{(k)}| \} \\
& = |A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\
& + \sum_{g=1}^{k-1} \sum_{j=1}^{k-1} (-1)^{g+j} f_{j,h}^2 |A_{g,j}^{(k-1)}| \{ (-1)^{i+j} f_{g,j}^2 |A_{i,j}^{(k)}| \\
& + (-1)^{i+k} f_{g,k}^2 |A_{i,k}^{(k)}| \} (-1)^{k-i-1} .
\end{aligned}$$

Note that $|A^{(k)}|$, expanded by the i -th row is

$$\sum_{j=1}^k (-1)^{i+j} f_{i,j}^2 |A_{i,j}^{(k)}| ,$$

and that the two terms in the braces of the above summation supply the j -th and k -th (last) cofactor in the expansion of $|A^{(k)}|$. When $g = i$, the values $f_{i,j}^2$ and $f_{i,k}^2$ become elements from the appropriate row (the i -th), while for values of $g \neq i$, $f_{g,j}^2$ and $f_{g,k}^2$ are elements from some other row. Hence by adding the missing terms from $|A^{(k)}|$ to each term in the double summation, all terms except that for $g = i$ will be zero by theorem 1.3. The missing terms are also subtracted to preserve equality. That is, on adding and subtracting the missing terms, the expression becomes,

$$\begin{aligned}
& |A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| \\
& + \sum_{g=1}^{k-1} \sum_{j=1}^{k-1} (-1)^{g+j} f_{j,h}^2 |A_{g,j}^{(k-1)}| \sum_{m=1}^k (-1)^{m+i} f_{g,m}^2 |A_{i,m}^{(k)}| (-1)^{k-i-1} \\
& - \sum_{g=1}^{k-1} \sum_{j=1}^{k-1} (-1)^{g+j} f_{j,h}^2 |A_{g,j}^{(k-1)}| \sum_{m \neq j} (-1)^{m+i} f_{g,m}^2 |A_{i,m}^{(k)}| (-1)^{k-i-1} \\
& = |A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| + |A^{(k)}| \sum_{j=1}^{k-1} (-1)^{i+j} f_{j,h}^2 |A_{i,j}^{(k-1)}| (-1)^{k-i-1} \\
& - \sum_{g=1}^{k-1} \sum_{j=1}^{k-1} (-1)^{g+j} f_{j,h}^2 |A_{g,j}^{(k-1)}| \sum_{m \neq j} (-1)^{m+i} f_{g,m}^2 |A_{i,m}^{(k)}| (-1)^{k-i-1} .
\end{aligned}$$

Note that

$$\begin{aligned}
& \sum_{j=1}^{k-1} (-1)^{i+j} f_{j,h}^2 |A_{i,j}^{(k-1)}| (-1)^{k-i-1} \\
& = \sum_{j=1}^{k-1} (-1)^{j+k-1} f_{j,h}^2 |A_{i,j}^{(k-1)}| = |A_{i,h}^{(k)}|
\end{aligned}$$

(expanded by the last row). Multiplying out and re-arranging the elements in the last summation makes the expression,

$$\begin{aligned}
& |A^{(k-1)}| |A_{i,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| + |A^{(k)}| |A_{i,h}^{(k)}| \\
& - \sum_{j=1}^{k-1} \sum_{m \neq j} (-1)^{m+i} f_{j,h}^2 |A_{i,m}^{(k)}| \sum_{g=1}^{k-1} (-1)^{g+j} f_{g,m}^2 |A_{g,j}^{(k-1)}| (-1)^{k-i-1} .
\end{aligned}$$

Note that $|A^{(k-1)}|$ expanded by the j -th column is

$$\sum_{g=1}^{k-1} (-1)^{g+j} f_{g,j}^2 |A_{g,j}^{(k-1)}| .$$

In the above summation, m assumes all values $1, 2, \dots, k-1$, except the value of j , and therefore these terms are again all zero. The above expression becomes, finally,

$$|A^{(k-1)}| |A_{i,h}^{(k+1)}| .$$

Theorem 1.5

Following the definitions of corollary 1.2.1,

$$\frac{|A_{i,j}^{(k)}|}{|A^{(k)}|} = \frac{|A_{i,j}^{(k-1)}|}{|A^{(k-1)}|} + \frac{|A_{i,k}^{(k)}| |A_{j,k}^{(k)}|}{|A^{(k-1)}| |A^{(k)}|} , \quad i \leq j < k = 2, 3, \dots, r,$$

implying,

$$|A^{(k-1)}| |A_{i,j}^{(k)}| = |A^{(k)}| |A_{i,j}^{(k-1)}| + |A_{i,k}^{(k)}| |A_{j,k}^{(k)}| .$$

Proof:

$$|A^{(k-1)}| \text{ expanded by the } i\text{-th row is } \sum_{g=1}^{k-1} (-1)^{i+g} f_{i,g}^2 |A_{i,g}^{(k-1)}| .$$

$$\text{Hence } |A^{(k-1)}| |A_{i,j}^{(k)}| = |A_{i,j}^{(k)}| \sum_{g=1}^{k-1} (-1)^{i+g} f_{i,g}^2 |A_{i,g}^{(k-1)}| . \text{ Note that}$$

$$|A^{(k)}| \text{ expanded by the } j\text{-th column is } \sum_{m=1}^k (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}| ; \text{ at } m = i,$$

the corresponding term in the summation is $(-1)^{i+j} f_{i,j}^2 |A_{i,j}^{(k)}|$, which,

multiplying by $|A_{i,j}^{(k-1)}|$ is the term for which $g = j$. Adding and

subtracting the missing terms gives,

$$\begin{aligned}
|A^{(k-1)}| |A_{i,j}^{(k)}| &= |A_{i,j}^{(k-1)}| \sum_{m=1}^k (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}| \\
&\quad - |A_{i,j}^{(k-1)}| \sum_{m \neq i} (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}| \\
&\quad + |A_{i,j}^{(k)}| \sum_{g \neq j} (-1)^{i+g} f_{i,g}^2 |A_{i,g}^{(k-1)}|.
\end{aligned}$$

Note that the maximum value g can attain is $k-1$, which it will attain when $j \neq k-1$. The maximum value for m is k , which value can always be attained since $\max(i) = k-1$.

Hence the above becomes,

$$\begin{aligned}
|A_{i,j}^{(k-1)}| |A_{i,j}^{(k)}| &- (-1)^{k+j} f_{k,j}^2 |A_{k,j}^{(k)}| |A_{i,j}^{(k-1)}| \\
&- |A_{i,j}^{(k-1)}| \sum_{m \neq i} (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}| \\
&+ |A_{i,j}^{(k)}| \sum_{g \neq j} (-1)^{i+g} f_{i,g}^2 |A_{i,g}^{(k-1)}|,
\end{aligned}$$

for which $\max(m) = \max(g) = k-1$. Note that $|A_{i,k}^{(k)}|$ expanded by the

last row is $\sum_{n=1}^{k-1} (-1)^{n+k-1} f_{n,k}^2 |A_{i,n}^{(k-1)}|$ and that for $n = j$, the term has the value $(-1)^{j+k-1} f_{j,k}^2 |A_{i,j}^{(k-1)}|$, which, upon multiplying by $|A_{k,j}^{(k)}|$ is

the term split off above, when $m = k$. Again adding and subtracting the missing terms gives,

$$\begin{aligned}
& |A_{i,j}^{(k-1)}| |A^{(k)}| + |A_{k,j}^{(k)}| \sum_{n=1}^{k-1} (-1)^{n+k-1} f_{n,k}^2 |A_{i,n}^{(k-1)}| \\
& - |A_{k,j}^{(k)}| \sum_{n \neq j} (-1)^{n+k-1} f_{n,k}^2 |A_{i,n}^{(k-1)}| \\
& - |A_{i,j}^{(k-1)}| \sum_{m \neq i} (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}| \\
& + |A_{i,j}^{(k)}| \sum_{g \neq j} (-1)^{i+g} f_{i,g}^2 |A_{i,g}^{(k-1)}|.
\end{aligned}$$

Note that the first minors in the summations of the third and fifth terms are equal for every value of n and g . Factoring out this common element makes the above,

$$\begin{aligned}
& |A_{i,j}^{(k-1)}| |A^{(k)}| + |A_{k,j}^{(k)}| |A_{i,k}^{(k)}| + \sum_{g \neq j} |A_{i,g}^{(k-1)}| \{ (-1)^{g+i} f_{i,g}^2 |A_{i,j}^{(k)}| \\
& - (-1)^{g+k-1} f_{g,k}^2 |A_{k,j}^{(k)}| \} - |A_{i,j}^{(k-1)}| \sum_{m \neq i} (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}|.
\end{aligned}$$

Recall that $|A^{(k)}|$ expanded by the j -th column is,

$$\sum_{n=1}^k (-1)^{n+j} f_{n,j}^2 |A_{n,j}^{(k)}|;$$

by factoring $(-1)^{g-j}$ from the terms in braces, the first minors become the cofactors in this expansion for $n = i$ and $n = k$. Since $g \neq j$, adding the missing terms in the expansion will make these terms all zero. That is, adding and subtracting the required terms gives,

$$\begin{aligned}
& |A_{i,j}^{(k-1)}| |A^{(k)}| + |A_{k,j}^{(k)}| |A_{i,k}^{(k)}| \\
& + \sum_{g \neq j} |A_{i,g}^{(k-1)}| (-1)^{g-j} \sum_{n=1}^k (-1)^{n+j} f_{n,g}^2 |A_{n,j}^{(k)}| \\
& - \sum_{g \neq j} |A_{i,g}^{(k-1)}| (-1)^{g-j} \sum_{n \neq i} (-1)^{n+j} f_{n,g}^2 |A_{n,j}^{(k)}| \\
& - |A_{i,j}^{(k-1)}| \sum_{m \neq i} (-1)^{m+j} f_{m,j}^2 |A_{m,j}^{(k)}|.
\end{aligned}$$

Now $|A^{(k-1)}|$ expanded by the i -th row is

$$\sum_{g=1}^{k-1} (-1)^{g+i} f_{i,g}^2 |A_{i,g}^{(k-1)}|.$$

Multiplying out and regrouping the last two terms, noting that the last term supplies $|A_{i,j}^{(k-1)}|$ which is missing from the index of summation g , and also that both $n \neq i$ and $m \neq i$, makes the resulting sum zero by theorem 1.3. That is, the expression becomes,

$$\begin{aligned}
& |A_{i,j}^{(k-1)}| |A^{(k)}| + |A_{k,j}^{(k)}| |A_{i,k}^{(k)}| \\
& - \sum_{n \neq i} |A_{n,j}^{(k)}| (-1)^{n-i} \sum_{g=1}^{k-1} (-1)^{g+i} f_{n,g}^2 |A_{i,g}^{(k-1)}|.
\end{aligned}$$

By corollary 1.1.1, $|A_{k,j}^{(k)}| = |A_{j,k}^{(k)}|$, and the above is,

$$|A_{i,j}^{(k-1)}| |A^{(k)}| + |A_{k,j}^{(k)}| |A_{i,k}^{(k)}|.$$

5.2 The Linear AnalogueTheorem 2.1

Given,

- (1) a linear model in r dimensions for which the least squares estimates β_i , $i = 1, 2, \dots, r$, exist;
- (2) sets of points $(f(\theta_m), \theta_m)$, $m = 1, 2, 3$, where the vector θ_m has elements $\theta_{1,m}, \theta_{2,m}, \dots, \theta_{r,m}$ which are arbitrary values assigned to the corresponding β_i , and $f(\theta_m)$ is the sum of squares measured as deviations from θ_m .

Then, by equating $\theta_{h,m} = \theta_{h,n}$, $h = k+1, k+2, \dots, r$, with k assuming the values $1, 2, \dots, r$, estimates β_i^* of the i -th parameter at the k -th step are given by,

$$\beta_i^* = \frac{(\nabla \theta_i)}{2} - \frac{1}{2 a_{i,k}} \left[\frac{(\Delta \text{SSD})}{(\Delta \theta_i)} \right], \quad i = 1, 2, \dots, k,$$

where,

$$(\Delta \text{SSD}) = f(\theta_m) - f(\theta_n)$$

$$(\Delta \theta_i) = \theta_{i,m} - \theta_{i,n}$$

$$(\nabla \theta_i) = \theta_{i,m} + \theta_{i,n},$$

and,

$$\begin{aligned} \frac{1}{a_{i,k}} &= \frac{2 |A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|}, & i < k \\ &= \frac{2 |A^{(k-1)}|}{|A^{(k)}|}, & i = k, \end{aligned}$$

following the notation defined in corollary 1.2.1.

Proof:

Expanding $f(\theta)$ about the vector B gives,

$$f(\theta) = f(B) + \sum_{i=1}^r (\theta_i - \beta_i) f_i + \frac{1}{2} \left[\sum_{i=1}^r (\theta_i - \beta_i) f_i \right]^2,$$

where f_i represents the partial derivative

$$\frac{\partial f(\theta)}{\partial \theta_i},$$

and $f_{i,j}^2$, the partial derivative

$$\frac{\partial^2 f(\theta)}{\partial \theta_i \partial \theta_j},$$

for all i and $j = 1, 2, \dots, r$.

For the least squares solutions, interest lies only in those points for which $f_i = 0$. In the linear model, $f_{i,j}^2$ is constant, and all higher order derivatives vanish.

The difference $f(\theta_m) - f(\theta_n)$ is given by,

$$\begin{aligned} (\Delta \text{SSD}) &= f(\theta_m) - f(\theta_n) \\ &= \frac{1}{2} \sum_{i=1}^r (\Delta \theta_i^2) f_i^2 - \sum_{i=1}^r (\Delta \theta_i) \beta_i f_i^2 \\ &\quad + \sum_{i < j} (\Delta \theta_i \theta_j) f_{i,j}^2 - \sum_{i < j} (\Delta \theta_i) \beta_j f_{i,j}^2 \\ &\quad - \sum_{i < j} \beta_i (\Delta \theta_j) f_{i,j}^2. \end{aligned}$$

The symbol $(\Delta \theta_i)$ is defined in the statement of the theorem; the remaining quantities are,

$$(\Delta \theta_i^2) = \theta_{i,m}^2 - \theta_{i,n}^2$$

$$(\Delta \theta_i \theta_j) = \theta_{i,m} \theta_{j,m} - \theta_{i,n} \theta_{j,n}, \quad i \neq j.$$

Consider now vectors θ_m and θ_n which have some number of elements, $r - k$, equal. Without loss of generality, assume $\theta_{h,m} = \theta_{h,n}$, $h = k+1, k+2, \dots, r$, since the parameters in the model can be rearranged so that the k unequal values are grouped at the first. Hence the θ_i can be taken in the natural order.

Under this situation, note that,

$$(\Delta \theta_h) = 0$$

$$(\Delta \theta_h^2) = 0$$

$$(\Delta \theta_h \theta_j) = 0, \quad j > h$$

$$(\Delta \theta_h \theta_j) = \theta_h (\Delta \theta_j), \quad j < h.$$

In particular, for $k = 1$,

$$(\Delta \text{SSD}) = \frac{1}{2} (\Delta \theta_1^2) f_1^2 - (\Delta \theta_1) \beta_1 f_1^2 + (\Delta \theta_1) \sum_{h=2}^r (\theta_h - \beta_h) f_{1,h}^2,$$

from which,

$$\beta_1^* = \beta_1 - \frac{\sum_{h=2}^r (\theta_h - \beta_h) \frac{f_{1,h}^2}{f_1^2}}{\frac{(\nabla \theta_1)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_1)}} \frac{1}{f_1^2}.$$

If $r = 1$, none of the terms in the summation over h exists, and β_1^* is the least squares estimate β_1 . Also, if $r > 1$, and the axis along which β_1 is measured is perpendicular to the j -th axis, then $f_{1,j}^2 = 0$, and the term in the summation for $h = j$ disappears. The

above expression can be re-written in terms of the matrix A, following the definitions in corollary 1.2.1, as,

$$\beta_1^* = \beta_1 - \frac{r}{\sum_{h=2}^r (\theta_h - \beta_h)} \frac{|A_{1,h}^{(2)}|}{|A^{(1)}|} = \frac{(\nabla \theta_1)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_1)} \frac{1}{|A^{(1)}|} .$$

This value β_1^* may be thought of as the value of β_1 conditional on the arbitrary values θ_h , $h = 2, 3, \dots, r$, and, for $m = 1$, written $\beta_1 \mid \theta_{2,1}, \theta_{3,1}, \dots, \theta_{r,1}$. Similar estimates are obtained only for $\beta_1 \mid \theta_{2,2}, \theta_{3,2}, \dots, \theta_{r,2}$ and $\beta_1 \mid \theta_{2,3}, \theta_{3,3}, \dots, \theta_{r,3}$, where the values of $\theta_{h,m}$ are equal for $h = 3, 4, \dots, r$. When it becomes necessary to specify the value of m , the notation $\beta_{i,m}^*$ will be used. Similarly the symbol $(\Delta_{m,n} \theta_i)$ will signify the difference $\theta_{i,m} - \theta_{i,n}$ with corresponding notation for the remaining quantities.

The generalized relations may be more easily followed after following the development through for $k = 2$. For $k = 2$,

$$\begin{aligned} (\Delta \text{SSD}) &= \frac{1}{2} (\Delta \theta_1^2) f_1^2 + \frac{1}{2} (\Delta \theta_2^2) f_2^2 - (\Delta \theta_1) \beta_1 f_1^2 - (\Delta \theta_2) \beta_2 f_2^2 \\ &+ (\Delta \theta_1 \theta_2) f_{1,2}^2 + (\Delta \theta_1) \sum_{h=3}^r (\theta_h - \beta_h) f_{1,h}^2 \\ &+ (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) f_{2,h}^2 - (\Delta \theta_1) \beta_2 f_{1,2}^2 \\ &- \beta_1 (\Delta \theta_2) f_{1,2}^2 . \end{aligned}$$

But (ΔSSD) can be defined in terms of $(\Delta \theta_2)$ alone, by noting that,

$$\begin{aligned}
(\Delta \theta_1) &= \beta_{1,m}^* - \beta_{1,n}^* \\
&= \beta_1 - \sum_{h=2}^r (\theta_{h,m} - \beta_h) \frac{|A_{1,h}^{(2)}|}{|A^{(1)}|} - \beta_1 \\
&\quad + \sum_{h=2}^r (\theta_{h,n} - \beta_h) \frac{|A_{1,h}^{(2)}|}{|A^{(1)}|} \\
&= -(\Delta \theta_2) \frac{|A_{1,2}^{(2)}|}{|A^{(1)}|} .
\end{aligned}$$

Similarly,

$$\begin{aligned}
(\Delta \theta_1^2) &= \beta_{1,m}^{*2} - \beta_{1,n}^{*2} \\
&= (\Delta \theta_2^2) \frac{|A_{1,2}^{(2)}|^2}{|A^{(1)}|^2} - 2(\Delta \theta_2) \beta_2 \frac{|A_{1,2}^{(2)}|^2}{|A^{(1)}|^2} \\
&\quad + 2 (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{1,2}^{(2)}| |A_{1,h}^{(2)}|}{|A^{(1)}|^2} \\
&\quad - 2 \beta_1 (\Delta \theta_2) \frac{|A_{1,2}^{(2)}|}{|A^{(1)}|} ,
\end{aligned}$$

and

$$\begin{aligned}
(\Delta \theta_1 \theta_2) &= \beta_{1,m}^* \theta_{2,m} - \beta_{1,n}^* \theta_{2,n} \\
&= \beta_1 (\Delta \theta_2) - (\Delta \theta_2) \frac{|A_{1,2}^{(2)}|}{|A^{(1)}|} + (\Delta \theta_2) \beta_2 \frac{|A_{1,2}^{(2)}|}{|A^{(1)}|} \\
&\quad - (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{1,h}^{(2)}|}{|A^{(1)}|} .
\end{aligned}$$

Substituting these into the expression for (ΔSSD) gives, after some algebra,

$$\begin{aligned}
(\Delta \text{SSD}) &= \left\{ \frac{1}{2} (\Delta \theta_2) - (\Delta \theta_2) \beta_2 \right\} \left\{ -|A_{1,2}^{(2)}| (-|A_{1,2}^{(2)}| f_1^2 \right. \\
&\quad \left. + |A^{(1)}| f_{1,2}^2) + |A^{(1)}| (-|A_{1,2}^{(2)}| f_{1,2}^2 \right. \\
&\quad \left. + |A^{(1)}| f_2^2) \right\} \frac{1}{|A^{(1)}|^2} \\
&\quad + (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) \left\{ -|A_{1,h}^{(2)}| (-|A_{1,2}^{(2)}| f_1^2 + |A^{(1)}| f_{1,2}^2) \right. \\
&\quad \left. + |A^{(1)}| (-|A_{1,2}^{(2)}| f_{1,h}^2 + |A^{(1)}| f_{2,h}^2) \right\} \frac{1}{|A^{(1)}|^2} .
\end{aligned}$$

Note that,

$$|A^{(1)}| = f_1^2 = |A_{2,2}^{(2)}| .$$

Then, by theorem 1.3,

$$-|A_{1,2}^{(2)}| f_1^2 + |A^{(1)}| f_{1,2}^2 = 0 ,$$

by theorem 1.1,

$$-|A_{1,2}^{(2)}| f_{1,2}^2 + |A^{(1)}| f_2^2 = |A^{(2)}| ,$$

and by corollary 1.2.1,

$$-|A_{1,2}^{(2)}| f_{1,h}^2 + |A^{(1)}| f_{2,h}^2 = |A_{2,h}^{(3)}| .$$

Hence,

$$\begin{aligned} (\Delta \text{ SSD}) &= \frac{1}{2} (\Delta \theta_2^2) \frac{|A^{(2)}|}{|A^{(1)}|} - (\Delta \theta_2) \beta_2 \frac{|A^{(2)}|}{|A^{(1)}|} \\ &\quad + (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{2,h}^{(3)}|}{|A^{(1)}|} , \end{aligned}$$

from which,

$$\beta_2^* = \beta_2 - \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{2,h}^{(3)}|}{|A^{(2)}|} = \frac{(\nabla \theta_2)}{2} - \frac{(\Delta \text{ SSD})}{(\Delta \theta_2)} \frac{|A^{(1)}|}{|A^{(2)}|} .$$

Similarly, $(\Delta \text{ SSD})$ can be expressed in terms of $(\Delta \theta_1)$, by taking the inverse definitions (from page 85),

$$(\Delta \theta_2) = -(\Delta \theta_1) \frac{|A^{(1)}|}{|A_{1,2}^{(2)}|} ,$$

and,

$$\begin{aligned}
(\Delta \theta_2^2) &= (\Delta \theta_1^2) \frac{|A^{(1)}|^2}{|A_{1,2}^{(2)}|^2} - 2 (\Delta \theta_1) \beta_2 \frac{|A^{(1)}|}{|A_{1,2}^{(2)}|} \\
&\quad + 2 (\Delta \theta_1) \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A^{(1)}| |A_{1,h}^{(2)}|}{|A_{1,2}^{(2)}|^2} \\
&\quad - 2 (\Delta \theta_1) \beta_1 \frac{|A^{(1)}|^2}{|A_{1,2}^{(2)}|^2} ,
\end{aligned}$$

and substituting these into the above expression. Using theorems 1.1, 1.3, and 1.4,

$$\begin{aligned}
(\Delta \text{SSD}) &= \frac{1}{2} (\Delta \theta_1^2) \frac{|A^{(1)}| |A^{(2)}|}{|A_{1,2}^{(2)}|^2} - (\Delta \theta_1) \beta_1 \frac{|A^{(1)}| |A^{(2)}|}{|A_{1,2}^{(2)}|^2} \\
&\quad + (\Delta \theta_1) \sum_{h=3}^r (\theta_h - \beta_h) \frac{-|A^{(1)}| |A_{1,h}^{(3)}|}{|A_{1,2}^{(2)}|^2} ,
\end{aligned}$$

from which, for $k = 2$,

$$\beta_1^* = \beta_1 + \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{1,h}^{(3)}|}{|A^{(2)}|} = \frac{(\nabla \theta_1)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_1)} \frac{|A_{1,2}^{(2)}|^2}{|A^{(1)}| |A^{(2)}|} .$$

If the axes corresponding to the subscripts 1 and 2 are perpendicular, then $|A_{1,2}^{(2)}| = 0$, implying that $(\Delta \theta_1) = 0$, and (ΔSSD) at $k = 2$ becomes,

$$(\Delta \text{SSD}) = \frac{1}{2} (\Delta \theta_2^2) f_2^2 - (\Delta \theta_2) \beta_2 f_2^2 + (\Delta \theta_2) \sum_{h=3}^r (\theta_h - \beta_h) f_{2,h}^2 ,$$

implying that,

$$\beta_2^* = \beta_2 - \sum_{h=3}^r (\theta_h - \beta_h) \frac{f_{2,h}^2}{f_2^2} = \frac{(\nabla \theta_2)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_2)} \frac{1}{f_2^2} .$$

However, under these circumstances, note that,

$$|A_{2,h}^{(3)}| = f_1^2 f_{2,h}^2 ,$$

and

$$|A^{(2)}| = f_1^2 f_2^2 .$$

Hence the above expression is identical to the earlier expression for β_2^* .

Since $|A_{1,2}^{(2)}| = 0$, the inverse relations are undefined. However the expression for β_1^* at $k = 2$ still holds, since, at $k = 1$, the term entering the summation indexed on h is zero for $h = 2$, making the value of β_1^* at $k = 1$ equal to,

$$\beta_1 - \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{1,h}^{(2)}|}{|A^{(1)}|} ,$$

which, since

$$|A_{1,h}^{(3)}| = -f_{1,h}^2 f_2^2 ,$$

is equal to

$$\beta_1 - \sum_{h=3}^r (\theta_h - \beta_h) \frac{|A_{1,h}^{(3)}|}{|A^{(2)}|} .$$

That is, since the two axes are perpendicular, no adjustment is required with the introduction of the second axis, and values of β_1^*

at $k = 1$ and $k = 2$ are equal. The appropriate elements in $|A_{1,h}^{(3)}|$ and $|A_{2,h}^{(3)}|$ for $h = j$ will be zero. The determinant itself will be zero at $h = j$ if both β_1 and β_2 are perpendicular to β_j .

In general, for the k -th step,

$$\begin{aligned}
(\Delta \text{SSD}) &= \frac{1}{2} \sum_{i=1}^{k-1} (\Delta \theta_i^2) f_i^2 + \frac{1}{2} (\Delta \theta_k^2) f_k^2 - \sum_{i=1}^{k-1} (\Delta \theta_i) \beta_i f_i^2 \\
&\quad - (\Delta \theta_k) \beta_k f_k^2 + \sum_{i=1 < j}^{k-1} (\Delta \theta_i \theta_j) f_{i,j}^2 + \sum_{i=1}^{k-1} (\Delta \theta_i \theta_k) f_{i,k}^2 \\
&\quad + \sum_{i=1}^{k-1} (\Delta \theta_i) \sum_{h=k+1}^r (\theta_h - \beta_h) f_{i,h}^2 \\
&\quad + (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) f_{k,h}^2 \\
&\quad - \sum_{i=1 < j}^{k-1} (\Delta \theta_i) \beta_j f_{i,j}^2 - \sum_{i=1}^{k-1} (\Delta \theta_i) \beta_k f_{i,k}^2 \\
&\quad - \sum_{i=1 < j}^{k-1} \beta_i (\Delta \theta_j) f_{i,j}^2 - \sum_{i=1}^{k-1} \beta_i (\Delta \theta_k) f_{i,k}^2 .
\end{aligned}$$

The expression for (ΔSSD) can be expressed in terms of $(\Delta \theta_k)$ by noting that, for $i = 1, 2, \dots, k-1$,

$$(\Delta \theta_i) = (-1)^{i+k} (\Delta \theta_k) \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} ,$$

$$\begin{aligned}
(\Delta \theta_i^2) &= (\Delta \theta_k^2) \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}|^2} - 2 (\Delta \theta_k) \beta_k \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}|^2} \\
&\quad + 2 (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{i,k}^{(k)}| |A_{i,h}^{(k)}|}{|A^{(k-1)}|^2} \\
&\quad + (-1)^{i+k} 2 (\Delta \theta_k) \beta_i \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} ,
\end{aligned}$$

$$\begin{aligned}
(\Delta \theta_i \theta_k) &= (\Delta \theta_k) \beta_i + (-1)^{i+k} (\Delta \theta_k) \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} \\
&\quad - (-1)^{i+k} (\Delta \theta_k) \beta_k \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} \\
&\quad + (-1)^{i+k} (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{i,h}^{(k)}|}{|A^{(k-1)}|} ,
\end{aligned}$$

and for values of $j > i$ through $k-1$,

$$\begin{aligned}
(\Delta \theta_i \theta_j) &= (-1)^{j+k} (\Delta \theta_k) \beta_i \frac{|A_{j,k}^{(k)}|}{|A^{(k-1)}|} + (-1)^{i+k} (\Delta \theta_k) \beta_j \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} \\
&+ (\Delta \theta_k^2) (-1)^{i+k} \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} (-1)^{j+k} \frac{|A_{j,k}^{(k)}|}{|A^{(k-1)}|} \\
&- 2 (\Delta \theta_k) \beta_k (-1)^{i+k} \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} (-1)^{j+k} \frac{|A_{j,k}^{(k)}|}{|A^{(k-1)}|} \\
&+ (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) (-1)^{i+k} \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} (-1)^{j+k} \frac{|A_{j,h}^{(k)}|}{|A^{(k-1)}|} \\
&+ (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) (-1)^{j+k} \frac{|A_{j,k}^{(k)}|}{|A^{(k-1)}|} (-1)^{i+k} \frac{|A_{i,h}^{(k)}|}{|A^{(k-1)}|}.
\end{aligned}$$

Substituting these into the expression for (ΔSSD) gives,

$$\begin{aligned}
(\Delta \text{SSD}) &= \left\{ \frac{1}{2} (\Delta \theta_k^2) - (\Delta \theta_k) \beta_k \right\} \left\{ \sum_{j=1}^{k-1} (-1)^{j+k} |A_{j,k}^{(k)}| \sum_{i=1}^k (-1)^{i+k} f_{i,j}^2 |A_{i,k}^{(k)}| \right. \\
&+ |A^{(k-1)}| \left. \sum_{i=1}^k (-1)^{i+k} f_{i,k}^2 |A_{i,k}^{(k)}| \right\} \frac{1}{|A^{(k-1)}|^2} \\
&+ (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) \left\{ \sum_{j=1}^{k-1} (-1)^{j+k} |A_{j,h}^{(k)}| \sum_{i=1}^k (-1)^{i+k} \right. \\
&\quad \left. f_{i,j}^2 |A_{i,k}^{(k)}| \right. \\
&+ |A^{(k-1)}| \left. \sum_{i=1}^k (-1)^{i+k} f_{i,h}^2 |A_{i,k}^{(k)}| \right\} \frac{1}{|A^{(k-1)}|^2}.
\end{aligned}$$

Note that $\sum_{i=1}^k (-1)^{i+k} f_{i,j}^2 |A_{i,k}^{(k)}| = 0$ for $j = 1, 2, \dots, k-1$, by

theorem 1.3. Also,

$$\sum_{i=1}^k (-1)^{i+k} f_{i,k}^2 |A_{i,k}^{(k)}| = |A^{(k)}|$$

by theorem 1.2. Finally, by corollary 1.2.1,

$$\sum_{i=1}^k (-1)^{i+k} f_{i,h}^2 |A_{i,k}^{(k)}| = |A_{k,h}^{(k+1)}| .$$

Hence,

$$\begin{aligned} (\Delta \text{SSD}) &= \frac{1}{2} (\Delta \theta_k^2) \frac{|A^{(k)}|}{|A^{(k-1)}|} - (\Delta \theta_k) \beta_k \frac{|A^{(k)}|}{|A^{(k-1)}|} \\ &\quad + (\Delta \theta_k) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{k,h}^{(k+1)}|}{|A^{(k-1)}|} , \end{aligned}$$

implying,

$$\beta_k^* = \beta_k - \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{k,h}^{(k+1)}|}{|A^{(k)}|} = \frac{(\nabla \theta_k)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_k)} \frac{|A^{(k-1)}|}{|A^{(k)}|} .$$

The inverse relations required to express (ΔSSD) in terms of $(\Delta \theta_i)$ $i = 1, 2, \dots, k-1$, are,

$$(\Delta \theta_k) = (-1)^{i+k} (\Delta \theta_i) \frac{|A^{(k-1)}|}{|A_{i,k}^{(k)}|} ,$$

$$\begin{aligned}
(\Delta \theta_k^2) &= (\Delta \theta_i^2) \frac{|A^{(k-1)}|^2}{|A_{i,k}^{(k)}|^2} + (-1)^{i+k} (\Delta \theta_i) \beta_k \frac{|A^{(k-1)}|}{|A_{i,k}^{(k)}|} \\
&\quad - (-1)^{i+k} 2 (\Delta \theta_i) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{i,h}^{(k)}| |A^{(k-1)}|}{|A_{i,k}^{(k)}|^2} \\
&\quad - 2 (\Delta \theta_i) \beta_i \frac{|A^{(k-1)}|^2}{|A_{i,k}^{(k)}|^2} .
\end{aligned}$$

Substituting these gives,

$$\begin{aligned}
(\Delta \text{SSD}) &= \frac{1}{2} (\Delta \theta_i^2) \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} - (\Delta \theta_i) \beta_i \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} \\
&\quad + (-1)^{i+k} (\Delta \theta_i) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{k,h}^{(k+1)}|}{|A_{i,k}^{(k)}|} - \frac{|A_{i,h}^{(k)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} .
\end{aligned}$$

By theorem 1.4

$$|A_{i,k}^{(k)}| |A_{k,h}^{(k+1)}| - |A_{i,h}^{(k)}| |A^{(k)}| = |A^{(k-1)}| |A_{i,h}^{(k+1)}| .$$

Hence,

$$\begin{aligned}
(\Delta \text{SSD}) &= \frac{1}{2} (\Delta \theta_i^2) \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} - (\Delta \theta_i) \beta_i \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} \\
&\quad + (-1)^{i+k} (\Delta \theta_i) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A^{(k-1)}| |A_{i,h}^{(k+1)}|}{|A_{i,k}^{(k)}|^2} ,
\end{aligned}$$

implying that,

$$\beta_i^* = \beta_i - (-1)^{i+k} \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A_{i,h}^{(k+1)}|}{|A^{(k)}|}$$

$$= \frac{(\nabla \theta_i)}{2} - \frac{(\Delta \text{SSD})}{(\Delta \theta_i)} \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} .$$

When $k = r$, none of the terms in the summation indexed on h exist, and $\beta_i^* = \beta_i$, the least squares estimate.

If $(\Delta \theta_i) = 0$ for some particular value of $i < k$, say $i = i'$, then none of the terms in the expression for (ΔSSD) , page 90, involving the product of $(\Delta \theta_i)$ with other terms exist when the index of summation $i = i'$. That is, none of the difference (ΔSSD) can be due to the difference $(\Delta \theta_{i'})$. Hence under this circumstance,

$$\beta_{i'}^* = \frac{(\nabla \theta_{i'})}{2} = \theta_{i'} .$$

Corollary 2.1.1

Given the conditions of theorem 2.1, and

$$\frac{1}{a_{i,k}} = 2 \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} ,$$

for $k = 1, 2, \dots, r$, and $i = 1, 2, \dots, k$, then,

$$\frac{1}{a_{i,k}} = \frac{(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)}{(\Delta_{2,3} \theta_i) (\Delta_{1,2}^{\text{SSD}}) - (\Delta_{1,2} \theta_i) (\Delta_{2,3}^{\text{SSD}})}$$

if $(\Delta_{m,n} \theta_i) \neq 0$
 $= 0$ otherwise,

following the definitions in theorem 2.1, page 84.

Proof:

First, note that when $i = k$,

$$\frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} = \frac{|A^{(k-1)}|}{|A^{(k)}|},$$

since $|A_{k,k}^{(k)}| = |A^{(k-1)}|$.

Also note, from definition of $(\Delta \theta_i)$ on page 90, that $(\Delta_{m,n} \theta_i) = 0$ if and only if $|A_{i,k}^{(k)}| = 0$. In all other circumstances $|A_{i,k}^{(k)}| \neq 0$, and $a_{i,k}$ is defined. Then,

$$a_{i,k} = \frac{(\Delta_{2,3} \theta_i) (\Delta_{1,2}^{SSD}) - (\Delta_{1,2} \theta_i) (\Delta_{2,3}^{SSD})}{(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)}.$$

From theorem 2.1, at the k -th step,

$$\begin{aligned} (\Delta_{m,n}^{SSD}) &= \frac{1}{2} (\Delta_{m,n} \theta_i^2) \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} \\ &\quad - (\Delta_{m,n} \theta_i) \beta_i \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} \\ &\quad + (-1)^{i+k} (\Delta_{m,n} \theta_i) \sum_{h=k+1}^r (\theta_h - \beta_h) \frac{|A^{(k-1)}| |A_{i,h}^{(k+1)}|}{|A_{i,k}^{(k)}|^2}. \end{aligned}$$

Substituting this expression into the numerator of $a_{i,k}$ gives,

$$\frac{1}{2} \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} (\Delta_{1,2} \theta_i) (\Delta_{2,3} \theta_i) ((\nabla_{1,2} \theta_i) - (\nabla_{2,3} \theta_i)).$$

Note that,

$$\begin{aligned}
 (\nabla_{1,2} \theta_i) - (\nabla_{2,3} \theta_i) &= \theta_{i,1} + \theta_{i,2} - \theta_{i,2} - \theta_{i,3} \\
 &= (\Delta_{1,3} \theta_i) .
 \end{aligned}$$

Hence,

$$a_{i,k} = \frac{1}{2} \frac{|A^{(k-1)}| |A^{(k)}|}{|A_{i,k}^{(k)}|^2} .$$

Corollary 2.1.2

Given that

$$\text{Var}[\beta \beta'] = \sigma^2 (X' X)^{-1} ,$$

then,

$$\text{Var}[\beta_i, \beta_j] = \sigma^2 \sum_{k=j}^r (a_{i,k})^{-\frac{1}{2}} (a_{j,k})^{-\frac{1}{2}}$$

for values of i and $j = 1, 2, \dots, r$, where the sign of the root of $a_{i,k}$ (and $a_{j,k}$) is determined from the sign of the product

$$(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)$$

(θ_j replacing θ_i for $a_{j,k}$).

Proof:

First, note that an element from $(X' X)$,

$$x_{i,j} = \frac{1}{2} \frac{\partial^2 f(\theta)}{\partial \theta_i \partial \theta_j} = \frac{1}{2} f_{i,j}^2 .$$

Hence,

$$(X' X)^{-1} = 2 A^{-1} ,$$

and,

$$\text{Var}[\beta \beta'] = \sigma^2 2 A^{-1}.$$

An element from A^{-1} , $f^{i,j}$ can be written,

$$f^{i,j} = (-1)^{i+j} \frac{|A_{j,i}|}{|A|} \quad (\text{corollary 1.3.1}),$$

implying

$$\text{Var}[\beta_i, \beta_j] = (-1)^{i+j} \sigma^2 2 \frac{|A_{j,i}|}{|A|},$$

for i and j from 1 through r . Now,

$$\begin{aligned} & \sum_{k=j}^r (a_{i,k})^{-\frac{1}{2}} (a_{j,k})^{-\frac{1}{2}} \\ &= \sum_{k=j}^r \left\{ 2 \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} \right\}^{\frac{1}{2}} \left\{ 2 \frac{|A_{j,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} \right\}^{\frac{1}{2}} \\ &= 2 \sum_{k=j}^r \frac{|A_{i,k}^{(k)}| |A_{j,k}^{(k)}|}{|A^{(k-1)}| |A^{(k)}|} \\ &= 2 \frac{|A_{i,j}^{(j)}| |A_{j,j}^{(j)}|}{|A^{(j-1)}| |A^{(j)}|} + 2 \frac{|A_{i,j+1}^{(j+1)}| |A_{j,j+1}^{(j+1)}|}{|A^{(j)}| |A^{(j+1)}|} + 2 \frac{|A_{i,j+2}^{(j+2)}| |A_{j,j+2}^{(j+2)}|}{|A^{(j+1)}| |A^{(j+2)}|} \\ &\quad + \dots + 2 \frac{|A_{i,r}^{(r)}| |A_{j,r}^{(r)}|}{|A^{(r-1)}| |A^{(r)}|}. \end{aligned}$$

Note that,

$$\frac{|A_{i,j}^{(j)}| |A_{j,j}^{(j)}|}{|A^{(j-1)}| |A^{(j)}|} = \frac{|A_{i,j}^{(j)}|}{|A^{(j)}|},$$

and, setting $j + 1 = k$ in theorem 1.5, and applying this theorem to the first two terms in the summation, gives,

$$2 \frac{|A_{i,j}^{(j)}|}{|A^{(j)}|} + 2 \frac{|A_{i,j+1}^{(j+1)}| |A_{j,j+1}^{(j+1)}|}{|A^{(j)}| |A^{(j+1)}|} = 2 \frac{|A_{i,j}^{(j+1)}|}{|A^{(j+1)}|} ,$$

making the sum,

$$2 \frac{|A_{i,j}^{(j+1)}|}{|A^{(j+1)}|} + 2 \frac{|A_{i,j+2}^{(j+2)}| |A_{j,j+2}^{(j+2)}|}{|A^{(j+1)}| |A^{(j+2)}|} + \dots + 2 \frac{|A_{i,r}^{(r)}| |A_{j,r}^{(r)}|}{|A^{(r-1)}| |A^{(r)}|} .$$

Applying theorem 1.5 to the first two terms in this summation gives,

$$2 \frac{|A_{i,j}^{(j+1)}|}{|A^{(j+1)}|} + 2 \frac{|A_{i,j+2}^{(j+2)}| |A_{j,j+2}^{(j+2)}|}{|A^{(j+1)}| |A^{(j+2)}|} = 2 \frac{|A_{i,j}^{(j+2)}|}{|A^{(j+2)}|} .$$

Repeating this process for $k = j+3, j+4, \dots, r$, at $k = r$, the summation becomes,

$$2 \frac{|A_{i,r}^{(r-1)}|}{|A^{(r-1)}|} + 2 \frac{|A_{i,r}^{(r)}| |A_{j,r}^{(r)}|}{|A^{(r-1)}| |A^{(r)}|} = 2 \frac{|A_{i,j}^{(r)}|}{|A^{(r)}|} .$$

Since $|A^{(r)}| = |A|$ is based on a symmetric matrix, by corollary 1.1.1

$$|A_{i,j}^{(r)}| = |A_{j,i}^{(r)}| .$$

Now $|A_{j,i}^{(r)}|$ is the unsigned cofactor corresponding to $f^{i,j}$. The sign $(-1)^{i+j}$ can be determined, but whether or not the corresponding first minor is itself positive or negative is not immediately apparent, since,

$$\frac{1}{a_{i,k}} = 2 \frac{|A_{i,k}^{(k)}|^2}{|A^{(k-1)}| |A^{(k)}|} \geq 0.$$

Note, however, that,

$$(\Delta_{m,n} \theta_i) = (-1)^{i+k} (\Delta_{m,n} \theta_k) \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|}.$$

Hence,

$$\begin{aligned} & (\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i) \\ &= (-1)^{3(i+k)} (\Delta_{1,2} \theta_k) (\Delta_{1,3} \theta_k) (\Delta_{2,3} \theta_k) \frac{|A_{i,k}^{(k)}|^3}{|A^{(k-1)}|^3}, \end{aligned}$$

implying,

$$\frac{(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)}{(\Delta_{1,2} \theta_k) (\Delta_{1,3} \theta_k) (\Delta_{2,3} \theta_k)} = \left\{ (-1)^{i+k} \frac{|A_{i,k}^{(k)}|}{|A^{(k-1)}|} \right\}^3.$$

The sign of the right hand side depends solely on the value of $(-1)^{i+k} |A_{i,k}^{(k)}|$ and is positive or negative accordingly as this value is positive or negative.

The values in the denominator of the left hand side are completely arbitrary, as therefore is the sign associated with their product. If this sign is taken to be positive, then sign of $(-1)^{i+k} |A_{i,k}^{(k)}|$ is the same as the sign of the product $(\Delta_{1,2} \theta_i) (\Delta_{1,3} \theta_i) (\Delta_{2,3} \theta_i)$. Conversely, if the sign in the denominator is taken to be negative, then the sign in question is opposite to the sign of the product.

Hence, the proper sign for $(-1)^{i+k} |A_{i,k}^{(k)}|$ can be associated with each term in the summation.

Finally, multiplying by σ^2 gives,

$$(-1)^{i+j} \sigma^2 \frac{|A_{j,i}|}{|A|} = \text{Var} [\beta_i, \beta_j] .$$

5.3 Parameter Estimates and Values of Objective Function
for 100 Samples of Size 10

Table 5.1 Parameter estimates and values of objective function for 100 samples of size 10

Sample Number	β_1	β_2	β_3	$f(\beta)$
1	211.495	160.432	0.911097	5.87278
2	205.810	155.911	0.904632	5.21489
3	201.595	151.077	0.902376	2.51931
4	194.473	144.683	0.895402	7.51356
5	189.879	141.363	0.887546	7.70395
6	202.594	152.668	0.902138	2.32314
7	209.533	157.884	0.909632	5.79939
8	207.881	158.025	0.905932	5.97303
9	202.020	152.794	0.900866	7.21184
10	200.396	149.763	0.900228	4.56645
11	201.554	150.936	0.900887	3.43321
12	195.242	146.490	0.892636	10.10424
13	188.232	139.704	0.884774	3.55463
14	187.621	139.037	0.885769	8.21312
15	188.905	139.722	0.888737	14.60881
16	209.616	159.243	0.908414	15.19604
17	190.365	141.651	0.889246	5.10350
18	208.738	157.388	0.908118	7.79203
19	209.518	159.053	0.907957	4.81288
20	196.906	146.553	0.896506	7.50117

continued

Table 5.1 (continued)

Sample Number	β_1	β_2	β_3	$f(\beta)$
21	207.637	157.175	0.907454	12.93935
22	217.539	167.248	0.913978	4.81818
23	199.473	149.472	0.898898	4.10874
24	210.007	159.744	0.908601	7.15043
25	189.835	140.224	0.888558	7.99723
26	207.177	157.125	0.906042	3.40245
27	202.700	153.556	0.902266	6.27390
28	195.741	145.764	0.896853	5.76378
29	204.923	154.570	0.905214	6.43289
30	197.381	147.231	0.896609	6.88055
31	192.631	143.926	0.890986	7.17307
32	200.766	151.973	0.899627	3.76955
33	200.387	149.711	0.899530	13.24891
34	209.043	158.027	0.908221	5.87820
35	199.095	148.393	0.899620	11.36636
36	190.822	141.016	0.890615	6.14817
37	219.905	170.264	0.914857	9.50333
38	205.192	155.574	0.903860	8.84367
39	191.309	142.101	0.890466	10.83520
40	183.555	135.161	0.879867	4.08331
41	202.840	152.174	0.903049	12.02395
42	207.980	158.054	0.905931	9.32155

continued

Table 5.1 (continued)

Sample Number	β_1	β_2	β_3	$f(\beta)$
43	213.657	162.909	0.911524	11.58774
44	207.832	156.634	0.907541	8.42334
45	202.080	151.710	0.902545	10.16988
46	219.154	168.453	0.915732	10.63823
47	205.944	156.416	0.904487	1.69501
48	192.053	142.771	0.891229	2.89680
49	202.006	151.632	0.903621	3.68210
50	198.781	148.682	0.897898	3.20175
51	205.191	155.484	0.903999	9.67224
52	197.555	148.215	0.895832	6.15343
53	219.707	168.640	0.916379	14.53005
54	204.716	155.157	0.903717	8.35041
55	184.685	135.601	0.883457	7.14456
56	196.715	147.242	0.896130	4.02971
57	207.344	157.227	0.907296	5.69726
58	193.171	142.966	0.893755	11.31144
59	198.895	148.581	0.899667	3.25649
60	196.817	146.091	0.898207	6.84318
61	192.696	142.631	0.893254	1.53253
62	183.131	134.023	0.881713	5.58531
63	196.555	146.499	0.897592	4.64180
64	184.254	134.714	0.883090	3.43455

continued

Table 5.1 (continued)

Sample Number	β_1	β_2	β_3	$f(\beta)$
65	200.181	150.860	0.900354	4.08920
66	202.072	152.180	0.900973	10.71924
67	204.727	154.631	0.903930	6.63653
68	197.645	148.382	0.898200	6.14757
69	193.648	143.521	0.893357	11.52996
70	189.556	139.867	0.890145	6.01344
71	205.100	154.585	0.904370	8.92650
72	187.395	137.072	0.885571	2.37967
73	194.612	144.387	0.894888	4.06740
74	191.669	142.006	0.891534	5.01868
75	199.904	149.673	0.899052	3.95590
76	200.244	150.267	0.901506	12.46497
77	203.352	153.281	0.903465	7.12205
78	197.200	146.559	0.898681	11.07815
79	201.679	151.614	0.900644	7.99504
80	213.451	164.333	0.909237	2.10388
81	193.489	144.113	0.893508	7.39190
82	191.277	142.382	0.889263	5.27965
83	197.065	146.830	0.898627	3.72614
84	210.312	161.249	0.908219	5.04503
85	194.575	143.696	0.896353	3.70535
86	205.385	154.582	0.905745	9.91151

continued

Table 5.1 (continued)

Sample Number	β_1	β_2	β_3	$f(\beta)$
87	198.825	149.235	0.899064	4.78980
88	197.787	147.433	0.897016	5.75559
89	206.505	155.804	0.905853	7.83025
90	192.290	143.859	0.891347	5.95741
91	219.228	168.569	0.915595	4.78170
92	204.098	154.292	0.903677	1.72276
93	204.278	154.038	0.904803	3.09918
94	194.482	144.321	0.894892	2.86609
95	207.441	156.086	0.907768	2.78524
96	213.054	161.877	0.912581	8.80364
97	203.218	152.819	0.903445	5.37536
98	201.652	151.927	0.901062	4.42862
99	197.542	148.245	0.895721	24.88006
100	200.468	150.557	0.900616	4.67904

5.4 Variance Estimates for 100 Samples of Size 10

Table 5.2 Variance estimates for 100 samples of size 10

Sample Number	$\text{Var}(\beta_1)$	$\text{Var}(\beta_2)$	$\text{Var}(\beta_3) \times 10^6$
1	85.7359	78.5060	52.5737
2	57.8572	52.3714	45.2720
3	25.6145	23.0705	22.7377
4	56.6445	50.3736	66.1938
5	44.2267	38.7138	66.2629
6	23.6059	21.2485	20.6627
7	82.5372	75.3280	54.6289
8	72.3661	65.5905	53.0979
9	68.6783	61.6836	62.1566
10	42.5864	38.2315	40.8455
11	33.0492	29.6811	30.6332
12	71.5277	63.1864	87.7871
13	18.4561	16.0661	30.3368
14	43.2087	37.7127	69.9046
15	86.8428	76.1789	129.285
16	198.662	181.045	133.649
17	31.5130	27.6573	45.0990
18	101.365	92.2584	70.3530
19	61.5000	55.9701	42.0172
20	59.6746	53.1836	66.0470

continued

Table 5.2 (continued)

Sample Number	$\text{Var}(\beta_1)$	$\text{Var}(\beta_2)$	$\text{Var}(\beta_3) \times 10^6$
21	159.566	145.174	113.254
22	84.3007	77.5431	43.5471
23	35.9652	32.1801	35.8784
24	94.7649	86.3748	62.9777
25	48.7081	42.6478	72.3075
26	40.0483	36.3196	29.6233
27	65.6991	59.0953	56.6514
28	45.8345	40.8849	50.7728
29	75.0130	67.8929	58.7209
30	55.3279	49.2739	60.4581
31	47.6266	41.9456	63.1407
32	33.7487	30.2526	31.9269
33	122.303	109.510	119.619
34	77.9524	70.9599	53.5021
35	103.257	92.5218	102.496
36	39.5502	34.8140	55.0796
37	171.134	157.682	83.0416
38	95.1328	85.9419	76.3486
39	68.4258	60.2484	94.2187
40	17.7641	15.3167	35.1067
41	126.156	113.755	108.292
42	108.198	98.1475	79.5641

continued

Table 5.2 (continued)

Sample Number	$\text{Var}(\beta_1)$	$\text{Var}(\beta_2)$	$\text{Var}(\beta_3) \times 10^6$
43	177.855	162.868	104.198
44	106.461	96.8247	76.1155
45	109.174	98.2643	95.7411
46	192.375	177.632	92.7771
47	18.9111	17.1032	14.7530
48	19.2629	16.9714	25.7953
49	39.8638	35.9909	33.9429
50	27.2816	24.3667	28.2714
51	108.551	98.0136	86.9702
52	48.8557	43.4420	53.8148
53	279.515	258.278	131.739
54	88.9675	80.3912	72.1320
55	35.4322	30.7597	63.7961
56	31.3317	27.8967	34.6875
57	72.1085	65.5496	51.3888
58	83.2437	73.7163	104.156
59	29.9904	26.8698	29.6738
60	59.4144	53.0871	63.2305
61	10.8714	9.6187	13.8375
62	26.6211	23.0278	51.2743
63	38.1462	34.0633	41.0265
64	16.5573	14.3772	30.4861

continued

Table 5.2 (continued)

Sample Number	$\text{Var}(\beta_1)$	$\text{Var}(\beta_2)$	$\text{Var}(\beta_3) \times 10^6$
65	38.6094	34.6317	36.3485
66	103.956	93.3937	94.5923
67	73.2636	66.1688	59.4685
68	53.0188	47.3329	54.6500
69	81.7580	72.3793	102.495
70	38.9408	34.2228	55.8489
71	101.151	91.3687	81.1240
72	12.6103	11.0043	21.1199
73	30.3353	26.9428	36.1020
74	33.4377	29.5001	44.8439
75	36.0742	32.2615	35.7428
76	118.151	106.317	108.525
77	76.4897	68.9990	63.9420
78	94.1523	84.2908	98.2352
79	75.1052	67.4127	69.3990
80	28.9418	26.4083	17.8320
81	54.2427	47.9693	67.1908
82	31.9941	28.0954	45.2510
83	32.7358	29.2613	34.0974
84	65.8536	59.9779	43.4194
85	29.3195	26.1100	33.8906
86	118.698	107.524	91.5312

continued

Table 5.2 (continued)

Sample Number	$\text{Var}(\beta_1)$	$\text{Var}(\beta_2)$	$\text{Var}(\beta_3) \times 10^6$
87	42.6121	38.1398	42.4267
88	47.2976	42.1718	51.0374
89	93.5228	84.8021	70.7891
90	38.5020	33.9951	50.5913
91	89.5781	82.6301	43.3128
92	18.4242	16.6415	15.1124
93	35.4250	32.0342	28.2518
94	21.8031	19.3478	25.9665
95	36.2677	32.9936	25.8804
96	140.794	129.219	80.9275
97	58.6435	52.9118	49.3940
98	43.1788	38.7790	39.3184
99	190.377	169.332	209.995
100	44.2598	39.7397	41.5511