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ON THE METHOD OF LEAST SQUARES

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ABSTRACT

A method for fitting models to observed data by least squares when the data appear nonlinearly in the equations of condition, where there are nonlinear constraints among model parameters, and where the observations may be correlated, is described. The method is independent of the form in which the equations of condition are expressed, and is a generalization of the classical technique. The method is nearly as simple to apply in practice as the classical method of least squares.

I. INTRODUCTION

The method of least squares, first used by Gauss to calculate definitive orbits of solar system bodies, remains one of the most important tools for the reduction of observations in all fields, not only in astronomy. The standard method of least squares, however, has not always been adequate, as assumptions are made which are not always valid in practice (see Deeming 1964 for an example in stellar spectral classification).

The method of least squares, as it is usually given in standard references (see e.g., Meyer 1975) considers primarily the case where (1) the equations of condition are linear in the parameters, (2) there are no exact constraints among the parameters, (3) each equation of condition involves only one observation subject to error, and the observed quantity has been explicitly solved for, and (4) the errors in the observations are uncorrelated. It is not difficult to generalize the method so as to eliminate some of the conditions; Meyer, for example, treats the case of correlated observations, the case where there are *linear* constraints involving only parameters, and the case where the equations of condition are nonlinear in the parameters but no constraints are given.

A more general treatment (called HDB in the following) was given by Helmert (1872) and by Deming (1938), and was expanded by Brown (1955) to exclude all of the restrictions given above; in particular, their technique is capable of treating the case where more than one observation appears in an equation of condition, or where the observations are not explicitly solved for. Their technique, however, has several shortcomings. As was pointed out by Eichhorn and Clary (1974), it will fail if the observations appear nonlinearly in the equations of condition and the observational errors (residuals) are large. It even fails for much simpler cases. Consider, for example, the problem of fitting a straight line through the origin. The model is

$$y = ax, \text{ or } y - ax = 0. \tag{1}$$

A straightforward linear regression yields the solution

$$a \cong \hat{a}_1 = \Sigma\, xy/\Sigma\, x^2 \tag{2}$$

(assuming equal weights), which is the solution also given by the method of HDB. However, it is well known that if the observations are the x's, and the y's are without error, then the correct solution is obtained by solving Eqs. (1) for x and then performing the regression of x on y. This yields

$$a \cong \hat{a}_2 = \Sigma\, y^2/\Sigma\, xy, \tag{3}$$

which is quite different. The method of HDB, however, would in this case give the same result as Eqs. (2) if applied to Eqs. (1) as they stand, even though the errors are explicitly assumed to be in x rather than y. Thus this method does not distinguish between a regression of x on y and a regression of y on x; another way to put it is that the results of this method depend on the *form* in which the equations are expressed, hardly a satisfactory situation. Deming, in fact, was aware of this (see Exercise 8 on p. 185 of his book).

The distinction between formulas (2) and (3) as estimators of a is not trivial. When the errors occur in x, rather than y, it is easy to show that formula (2) provides a *biased estimator* of a. In fact, formula (2) has as its expectation value for large n

$$\langle \hat{a}_1 \rangle = a[1 - (\sigma/\bar{x})^2], \tag{4}$$

where σ is the standard deviation of the observations x, and $\bar{x}$ is the mean of the observations of x. The bias of Eq. (4) is *constant*; it does not go to zero as the number of observations becomes arbitrarily large. This is a serious shortcoming of the method of HDB.

While often in practice the practical results of these differences may be of little consequence, it would be desirable to have a generally useful technique that avoids these shortcomings. Eichhorn and Clary went a step further than HDB by explicitly including quadratic terms in the residuals and parameter corrections in their solution. As Deming remarks, the principal difference between a regression of y on x and one of x on y is due to the neglect of quadratic terms; however, Eichhorn and

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Clary appear to have been the first to attempt to take them into account.

In the present paper we shall develop a simple modification of the standard (e.g., Helmert-Deming-Brown) technique of least squares that accomplishes all of the above aims and more. The equations of condition are assumed nonlinear in both parameters and observations; nonlinear constraints among the parameters are allowed; observations may be correlated, and more than one observation may appear in an equation of condition; the solution is independent of the form of expression of the condition equations; and full account is taken of the nonlinearities of the equations of condition. The method is also simpler than that of Eichhorn and Clary as it does not require calculation of derivatives higher than the first.

II. STATEMENT OF THE PROBLEM

Let the vector $\mathring{\mathbf{x}}$ of observations be given whose covariance matrix σ is assumed known (at least up to a constant factor). The observations are assumed to satisfy a set of *equations of condition*

$$\mathbf{f}(\mathring{\mathbf{x}} + \mathbf{v},\mathbf{a}) = \mathbf{0}, \tag{5}$$

where $\mathbf{f}$ is a vector function of its arguments, $\mathbf{v}$ is the vector of the actual residuals (i.e., $\mathbf{x} = \mathring{\mathbf{x}} + \mathbf{v}$ would have been the actual observations if there were no errors), and $\mathbf{a}$ is a vector of parameters. In addition, we assume that a set of constraints on the parameters

$$\mathbf{g}(\mathbf{a}) = \mathbf{0} \tag{6}$$

may be given, where $\mathbf{g}$ is another vector function.

Following Brown, the principle of least squares can be stated as follows: Find estimates $\hat{\mathbf{v}}$ and $\hat{\mathbf{a}}$ of $\mathbf{v}$ and $\mathbf{a}$ such that

$$\mathbf{f}(\mathring{\mathbf{x}} + \hat{\mathbf{v}},\hat{\mathbf{a}}) = \mathbf{0},$$
$$\mathbf{g}(\hat{\mathbf{a}}) = \mathbf{0} \tag{7}$$

are satisfied while simultaneously minimizing the quadratic form

$$S_0 = \frac{1}{2}\hat{\mathbf{v}}^t\,\sigma^{-1}\hat{\mathbf{v}}, \tag{8}$$

where the superscript "t" indicates transpose.

As is well known, the solution of the posed problem is most readily obtained by the method of Lagrange multipliers. If $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ are vectors of Lagrange multipliers, then we can restate the problem as follows: Find estimates $\hat{\mathbf{v}}$ and $\hat{\mathbf{a}}$ of $\mathbf{v}$ and $\mathbf{a}$, and vectors $\hat{\boldsymbol{\lambda}}$ and $\hat{\boldsymbol{\mu}}$ which minimize the function

$$S = \frac{1}{2}\hat{\mathbf{v}}^t\sigma^{-1}\hat{\mathbf{v}} + \mathbf{f}^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\,\hat{\boldsymbol{\mu}} + \mathbf{g}^t(\hat{\mathbf{a}})\,\hat{\boldsymbol{\lambda}}, \tag{9}$$

where we have defined $\hat{\mathbf{x}} = \mathring{\mathbf{x}} + \hat{\mathbf{v}}$ for convenience. Denoting the matrix of partial derivatives with respect to a variable by a subscript, this is equivalent to solving the following normal equations:

$$\sigma^{-1}\hat{\mathbf{v}} + \mathbf{f}_{\hat{\mathbf{x}}}{}^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\,\hat{\boldsymbol{\mu}} = \mathbf{0}, \tag{10a}$$
$$\mathbf{f}_{\hat{\mathbf{a}}}{}^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\hat{\boldsymbol{\mu}} + \mathbf{g}_{\hat{\mathbf{a}}}{}^t(\hat{\mathbf{a}})\,\hat{\boldsymbol{\lambda}} = \mathbf{0}, \tag{10b}$$
$$\mathbf{f}(\hat{\mathbf{x}},\hat{\mathbf{a}}) = \mathbf{0}, \tag{10c}$$
$$\mathbf{g}(\hat{\mathbf{a}}) = \mathbf{0}. \tag{10d}$$

These equations are exact; they involve no approximations. This is the key that distinguishes the present method from those of HDB and of Eichhorn and Clary, all of whom used approximate equations of condition in forming S. It should be evident that the solution of Eqs. (10) will give the solution of the posed problem, regardless of the form in which $\mathbf{f}$ is expressed, and regardless of nonlinearities (provided the solution exists at all).

III. SOLUTION OF THE NORMAL EQUATIONS

Equations (10) are in general nonlinear and must be solved by successive approximations. Assume that an approximate solution of Eqs. (10) has been obtained somehow. One effective method of improving this solution is to use Newton's method, i.e., linearize about the approximate solution and determine corrections to it.

With a slight abuse of the notation, let the approximate solution be given by $(\hat{\mathbf{x}},\hat{\mathbf{a}})$ and let the corrections be denoted by $(\hat{\boldsymbol{\epsilon}},\hat{\boldsymbol{\delta}})$, respectively. Then Eqs. (10) become (where $\hat{\mathbf{v}} = \hat{\mathbf{x}} - \mathring{\mathbf{x}}$).

$$\sigma^{-1}(\hat{\mathbf{v}} + \hat{\boldsymbol{\epsilon}}) + \mathbf{f}_{\hat{\mathbf{x}}}{}^t\,\hat{\boldsymbol{\mu}} = \mathbf{0}, \tag{11a}$$
$$\mathbf{f}_{\hat{\mathbf{a}}}{}^t\hat{\boldsymbol{\mu}} + \mathbf{g}_{\hat{\mathbf{a}}}{}^t\,\hat{\boldsymbol{\lambda}} = \mathbf{0}, \tag{11b}$$
$$\hat{\mathbf{f}} + \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\boldsymbol{\epsilon}} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}} = \mathbf{0}, \tag{11c}$$
$$\hat{\mathbf{g}} + \mathbf{g}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}} = \mathbf{0}, \tag{11d}$$

where we have ignored products of $\hat{\boldsymbol{\epsilon}}$ and $\hat{\boldsymbol{\delta}}$ with Lagrange multipliers, which does not affect the final result; a caret means evaluation at $(\hat{\mathbf{x}},\hat{\mathbf{a}})$.

Solving Eq (11a) for $\hat{\boldsymbol{\epsilon}}$ we obtain

$$\hat{\boldsymbol{\epsilon}} = -\hat{\mathbf{v}} - \sigma\,\mathbf{f}_{\hat{\mathbf{x}}}{}^t\,\hat{\boldsymbol{\mu}}. \tag{12}$$

Substituting this into Eq. (11c) we obtain

$$\hat{\mathbf{f}} - \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\mathbf{v}} - \mathbf{f}_{\hat{\mathbf{x}}}\,\sigma\,\mathbf{f}_{\hat{\mathbf{x}}}{}^t\,\hat{\boldsymbol{\mu}} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}} = \mathbf{0}, \tag{13}$$

so that

$$\hat{\boldsymbol{\mu}} = \mathbf{W}\,(\hat{\mathbf{f}} - \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\mathbf{v}} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}}), \tag{14}$$

where the "weight matrix" $\mathbf{W}$ is given by

$$\mathbf{W} = (\mathbf{f}_{\hat{\mathbf{x}}}\,\sigma\,\mathbf{f}_{\hat{\mathbf{x}}}{}^t)^{-1}. \tag{15}$$

Substituting this into Eq. (11b) we obtain

$$\mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}(\hat{\mathbf{f}} - \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\mathbf{v}} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}}) + \mathbf{g}_{\hat{\mathbf{a}}}{}^t\,\hat{\boldsymbol{\lambda}} = \mathbf{0}. \tag{16}$$

Equations (16) and (11d) may be put together in matrix form to yield the *reduced normal Eqs.* (17):

$$\begin{bmatrix} \mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} & \mathbf{g}_{\hat{\mathbf{a}}}{}^t \\ \mathbf{g}_{\hat{\mathbf{a}}} & \mathbf{0} \end{bmatrix}\begin{bmatrix} \hat{\boldsymbol{\delta}} \\ \hat{\boldsymbol{\lambda}} \end{bmatrix} = -\begin{bmatrix} \mathbf{f}_{\hat{\mathbf{a}}}{}^t\,\mathbf{W}\,\hat{\boldsymbol{\phi}} \\ \hat{\mathbf{g}} \end{bmatrix}, \tag{17}$$

where we have defined

$$\hat{\phi} = \hat{\mathbf{f}} - \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\mathbf{v}}. \tag{18}$$

With this solution, one computes the improved residuals from

$$\hat{\mathbf{v}}_{\text{new}} = -\,\sigma\,\mathbf{f}_{\hat{\mathbf{x}}}{}^{t}\,\mathbf{W}\,(\hat{\phi} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\delta}), \tag{19}$$

which follows from Eqs. (10a), (14), and (18). Then

$$\begin{aligned} \hat{\mathbf{a}}_{\text{new}} &= \hat{\mathbf{a}} + \hat{\delta}, \\ \hat{\mathbf{x}}_{\text{new}} &= \mathring{\mathbf{x}} + \hat{\mathbf{v}}_{\text{new}} \end{aligned} \tag{20}$$

define the improved solution. If the improved solution is insufficiently accurate, the process should be repeated until satisfactory convergence is attained.

The natural starting point for this scheme is to set $\hat{\mathbf{x}} = \mathring{\mathbf{x}}$ as the initial approximation, so that $\hat{\mathbf{v}} = \mathbf{0}$, and to use a vector $\mathring{\mathbf{a}}$ of initial approximations of $\mathbf{a}$ for $\hat{\mathbf{a}}$. Obtaining a suitable $\mathring{\mathbf{a}}$ is a difficult question that is outside the scope of this paper; it must be close enough to the solution that the process given by Eqs. (11)–(20) converges. The result of the first iteration from this starting point is identical to that obtained by the method of HDB; subsequent iterations, of course, give differing results.

It is instructive to examine the reduced normal Eqs. (17) closely, for they are remarkably similar to those obtained from the classical solution. The matrix $\mathbf{f}_{\hat{\mathbf{a}}}{}^{t}\,\mathbf{W} \times \mathbf{f}_{\hat{\mathbf{a}}}$ on the left-hand side corresponds closely to the usual product-sum matrix of the classical least-squares problem; the only difference is that it is to be evaluated at the best estimate of the *actual* solution $\hat{\mathbf{x}}$, rather than on the observation vector $\mathring{\mathbf{x}}$. This means that the product-sum matrix must be recomputed from scratch for *each iteration*, in contrast to the usual method in which only the right-hand side is reevaluated.

The term $-\mathbf{f}_{\hat{\mathbf{a}}}{}^{t}\,\mathbf{W}\,\hat{\phi}$ on the right-hand side is analogous to the term which appears on the right-hand side of the classical problem; the latter would be $-\mathbf{f}_{\hat{\mathbf{a}}}{}^{t}\,(\mathring{\mathbf{x}},\hat{\mathbf{a}})\,\mathbf{W} \times \mathbf{f}(\mathring{\mathbf{x}},\hat{\mathbf{a}})$, where $\hat{\mathbf{a}}$ is the best value of $\mathbf{a}$, but the functions are again evaluated on the observation vector $\mathring{\mathbf{x}}$. Note that

$$\begin{aligned} \hat{\phi} &= \mathbf{f}(\hat{\mathbf{x}},\hat{\mathbf{a}}) - \mathbf{f}_{\hat{\mathbf{x}}}\,\hat{\mathbf{v}} \\ &= \mathbf{f}(\hat{\mathbf{x}},\hat{\mathbf{a}}) - \mathbf{f}_{\hat{\mathbf{x}}}(\hat{\mathbf{x}} - \mathring{\mathbf{x}}) \cong \mathbf{f}(\mathring{\mathbf{x}},\hat{\mathbf{a}}), \end{aligned} \tag{21}$$

so that the right-hand sides of the classical normal equations differ only by terms of order higher than the first from those of the present method. Eichhorn and Clary's method includes the next higher order (quadratic) terms only. In any case, if $\hat{\mathbf{a}}$ is the solution of the classical problem, then $\mathbf{f}_{\hat{\mathbf{a}}}{}^{t}(\mathring{\mathbf{x}},\hat{\mathbf{a}})\,\mathbf{W}\,\mathbf{f}(\mathring{\mathbf{x}},\hat{\mathbf{a}}) = \mathbf{0}$, and Eq. (21) shows that $\mathbf{f}_{\hat{\mathbf{a}}}{}^{t}\,\mathbf{W}\,\hat{\phi} \cong \mathbf{0}$ also. The classical solution evidently differs from the present solution in the omission of terms of order higher than the first in $\hat{\mathbf{v}}$.

IV. AN EXAMPLE

As an example of an application of this method, we consider the fitting of a straight line $y = \alpha + \beta t$ to data points (y_i, t_i), $i = 1, \ldots, n$, where both y_i and t_i may have errors. There are n equations of condition:

$$y_i - \alpha - \beta t_i = 0. \tag{22}$$

To consider all observations on an equal footing, we relabel (y_i, t_i) as follows:

$$\begin{aligned} y_i &= x_{2i-1}, \\ t_i &= x_{2i}, \; i = 1, \ldots, n, \end{aligned}$$

so that the vector of observations is $(x_1, x_2, \ldots, x_{2n})^t = (y_1, t_1, y_2, t_2, \ldots, y_n, t_n)^t$.

In a similar fashion we let the vector of parameters $\mathbf{a}$ have the components $a_1 = \alpha$, $a_2 = \beta$.

The equations of condition, written in vector form, now take the form

$$\mathbf{f}(\mathbf{x},\mathbf{a}) = \begin{bmatrix} x_1 - a_1 - a_2 x_2 \\ x_3 - a_1 - a_2 x_4 \\ \vdots \\ x_{2n-1} - a_1 - a_2 x_{2n} \end{bmatrix} = 0. \tag{23}$$

There are no exact constraints among the parameters. Inspection of Eqs. (11) reveals that the required matrices are

$$\mathbf{f}_{\hat{\mathbf{x}}} = \begin{bmatrix} 1 & -\hat{a}_2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -\hat{a}_2 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\hat{a}_2 \end{bmatrix}, \tag{24}$$

$$\mathbf{f}_{\hat{\mathbf{a}}} = \begin{bmatrix} -1 & -\hat{x}_2 \\ -1 & -\hat{x}_4 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ -1 & -\hat{x}_{2n} \end{bmatrix} = \begin{bmatrix} -1 & -\hat{t}_1 \\ -1 & -\hat{t}_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ -1 & -\hat{t}_n \end{bmatrix}. \tag{25}$$

For simplicity, we let the covariance matrix of the observations, σ, take the form

$$\sigma = \text{diag}\,(\sigma_0, \sigma_0, \ldots, \sigma_0), \tag{26}$$

where

$$\sigma_0 = \begin{bmatrix} \sigma_{yy} & \sigma_{yt} \\ \sigma_{ty} & \sigma_{tt} \end{bmatrix}, \; \sigma_{yt} = \sigma_{ty}, \tag{27}$$

i.e., we allow each pair of numbers in an observation (y_i,t_i) to be correlated, but allow no correlation between different observations.

Then

$$\mathbf{f}_{\hat{\mathbf{x}}}\sigma\mathbf{f}_{\hat{\mathbf{x}}}{}^{t} = \bar{\sigma}\,\mathbf{I}, \tag{28}$$

where $\mathbf{I}$ is a unit matrix, and

$$\bar{\sigma} = \sigma_{yy} - 2\sigma_{yt}\hat{a}_2 + \sigma_{tt}\hat{a}_2^2. \tag{29}$$

Thus,

$$\mathbf{W} = \mathbf{I}/\bar{\sigma}. \tag{30}$$

From Eqs. (18), (23), and (24), using $\hat{\mathbf{v}} = \hat{\mathbf{x}} - \mathring{\mathbf{x}}$, we obtain

$$\hat{\boldsymbol{\phi}} = \begin{bmatrix} \mathring{y}_1 - \hat{a}_1 - \hat{a}_2\mathring{t}_1 \\ \mathring{y}_2 - \hat{a}_1 - \hat{a}_2\mathring{t}_2 \\ \vdots \\ \mathring{y}_n - \hat{a}_1 - \hat{a}_2\mathring{t}_n \end{bmatrix} = \begin{bmatrix} \hat{\phi}_1 \\ \hat{\phi}_2 \\ \vdots \\ \hat{\phi}_n \end{bmatrix}. \tag{31}$$

The normal equations (17), after cancelling the common factor $1/\bar{\sigma}$, therefore become

$$\begin{bmatrix} n & \Sigma\hat{t} \\ \Sigma\hat{t} & \Sigma\hat{t}^2 \end{bmatrix} \begin{bmatrix} \hat{\delta}_1 \\ \hat{\delta}_2 \end{bmatrix} = \begin{bmatrix} \Sigma\hat{\phi} \\ \Sigma\hat{\phi}\hat{t} \end{bmatrix}. \tag{32}$$

Notice how similar in form these are to the usual normal equations for this problem. There are two major differences: (1) The normal equations are calculated using the *best current estimate* of the observation vector $\hat{\mathbf{x}} = \mathring{\mathbf{x}} + \hat{\mathbf{v}}$, rather than $\mathring{\mathbf{x}}$; and (2) the right-hand side is computed using $\hat{\boldsymbol{\phi}}$ as defined, rather than $\hat{\mathbf{f}}$ as might be expected (although here by chance, $\hat{\boldsymbol{\phi}} = \hat{\mathbf{f}}$).

After solving Eqs. (32) for $\hat{\boldsymbol{\delta}}$, we compute

$$\hat{\mathbf{v}}_{\text{new}} = -\sigma\mathbf{f}_{\hat{\mathbf{x}}}{}^t\,\mathbf{W}\,(\hat{\boldsymbol{\phi}} + \mathbf{f}_{\hat{\mathbf{a}}}\,\hat{\boldsymbol{\delta}})_{\text{old}} \tag{33}$$

and iterate to convergence. In this example, we obtain

$$\hat{y}_k - \mathring{y}_k = -\frac{\sigma_{yy} - \hat{a}_2\sigma_{yt}}{\sigma_{yy} - 2\hat{a}_2\sigma_{yt} + \hat{a}_2^2\sigma_{tt}}(\mathring{y}_k - \hat{a}_1 - \hat{a}_2\mathring{t}_k),$$

$$\hat{t}_k - \mathring{t}_k = -\frac{\sigma_{yt} - \hat{a}_2\sigma_{tt}}{\sigma_{yy} - 2\hat{a}_2\sigma_{yt} + \hat{a}_2^2\sigma_{tt}}(\mathring{y}_k - \hat{a}_1 - \hat{a}_2\mathring{t}_k). \tag{34}$$

Two cases of particular interest are (1) all error in y and (2) all error in t. In case (1), Eqs. (34) imply that

$$\hat{t}_k - \mathring{t}_k = 0,$$

$$\hat{y}_k - \mathring{y}_k = -(\mathring{y}_k - \hat{a}_1 - \hat{a}_2\mathring{t}_k) \quad \text{or}$$

$$\hat{y}_k = \hat{a}_1 + \hat{a}_2\hat{t}_k,$$

as expected from the classical problem. On the other hand, in case (2) we have

$$\hat{y}_k - \mathring{y}_k = 0,$$

$$\hat{t}_k - \mathring{t}_k = \frac{1}{\hat{a}_2}(\mathring{y}_k - \hat{a}_1 - \hat{a}_2\mathring{t}_k) \quad \text{so}$$

$$\hat{t}_k = \frac{1}{\hat{a}_2}(\hat{y}_k - \hat{a}_1),$$

which is to be expected for a regression of t on y. In intermediate cases (where both y and t are in error, and where there may be correlations), the factors involving the covariances in Eqs. (34) apportion the total errors $\hat{\boldsymbol{\phi}}$ among both $\hat{\mathbf{y}}$ and $\hat{\mathbf{t}}$ in a way which reflects the relative precision of each. Note that the quantity $\hat{\boldsymbol{\phi}}$ is (with the exception of quadratic terms in $\hat{\mathbf{v}}$, which do not appear in this example) just the amount by which the equations of condition fail to be satisfied when the *actual observations* are substituted in them.

V. THE COVARIANCE MATRIX OF THE ADJUSTMENT

The calculation of the covariance matrix of the adjustment is quite easy and presents no surprises. Let the matrix of Eq. (17) be

$$\mathbf{Q} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^t & \mathbf{0} \end{bmatrix}, \tag{35}$$

and let its inverse be

$$\mathbf{Q}^{-1} = \begin{bmatrix} \alpha & \beta \\ \beta^t & \gamma \end{bmatrix}. \tag{36}$$

Then the covariance matrix of $\hat{\boldsymbol{\delta}}$ and $\hat{\boldsymbol{\lambda}}$ is

$$\sigma_{\hat{\delta}\hat{\lambda}} = \left\langle \begin{bmatrix} \hat{\delta} \\ \hat{\lambda} \end{bmatrix} \begin{bmatrix} \hat{\delta} \\ \hat{\lambda} \end{bmatrix}^t \right\rangle = \begin{bmatrix} \alpha & \beta \\ \beta^t & \gamma \end{bmatrix} \begin{bmatrix} \mathbf{f}_{\hat{\mathbf{a}}}{}^t\,\mathbf{W}\mathbf{f}_{\hat{\mathbf{x}}}\langle\hat{\mathbf{v}}\hat{\mathbf{v}}^t\rangle\mathbf{f}_{\hat{\mathbf{x}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \alpha & \beta \\ \beta^t & \gamma \end{bmatrix}, \tag{37}$$

since on the solution, $\hat{\mathbf{f}} = \mathbf{0}$ and $\hat{\mathbf{g}} = \mathbf{0}$. But

$$\begin{aligned} \mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{x}}}\langle\hat{\mathbf{v}}\hat{\mathbf{v}}^t\rangle\mathbf{f}_{\hat{\mathbf{x}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} &= \mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{x}}}\sigma\mathbf{f}_{\hat{\mathbf{x}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} \\ &= \mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}\mathbf{W}^{-1}\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} \\ &= \mathbf{f}_{\hat{\mathbf{a}}}{}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{a}}} \\ &= \mathbf{A}, \end{aligned} \tag{38}$$

by Eqs. (15) and (17). Performing the matrix product and retaining the upper left-hand component, we find that

$$\sigma_{\hat{\delta}\hat{\delta}} = \langle\hat{\boldsymbol{\delta}}\,\hat{\boldsymbol{\delta}}^t\rangle = \alpha\,\mathbf{A}\,\alpha. \tag{39}$$

On the other hand, the upper left-hand component of the product $\mathbf{Q}^{-1} = \mathbf{Q}^{-1}\,\mathbf{Q}\,\mathbf{Q}^{-1}$ is just

$$\alpha = \alpha\,\mathbf{A}\,\alpha + \beta\mathbf{B}^t\,\alpha + \alpha\mathbf{B}\,\beta^t, \tag{40}$$

while the upper left-hand component of the product

$$\mathbf{I} = \mathbf{Q}^{-1}\,\mathbf{Q} \quad \text{is}$$

$$\mathbf{I} = \alpha\mathbf{A} + \beta\mathbf{B}^t. \tag{41}$$

Postmultiplying (41) by α yields

$$\alpha = \alpha\mathbf{A}\alpha + \beta\mathbf{B}^t\alpha. \tag{42}$$

Equations (40) and (42) together imply that $\alpha\mathbf{B}\beta^t = \mathbf{0} = (\beta\mathbf{B}^t\alpha)^t$ so that finally we have

$$\sigma_{\hat{\delta}\hat{\delta}} = \alpha\mathbf{A}\alpha = \alpha. \tag{43}$$

It follows that the covariance matrix of the parameters is obtained, as usual, by striking these rows and columns of the inverse matrix of the reduced normal equations which correspond to the constraints (Jefferys 1979). (Note that in the general case where there are constraints, $\alpha \neq \mathbf{A}^{-1}$, and the relation $\alpha\mathbf{A}\alpha = \alpha$ implies that α is in fact singular. This is, of course, to be expected

since the constraints mean that there must be linear relationships between the parameters.)

It should also be noted in this connection that $\mathbf{A}^{-1}$ need not exist for the method to work. It may be, for example, that several of the constraints have been introduced for the purpose of making the matrix of the reduced normal Eqs. (17) nonsingular (See Eichhorn and Russell 1976; Jefferys 1979). It was for this reason that the proof of this section does not involve inverting $\mathbf{A}$ explicitly. (Note that Meyer's solution of the case where linear constraints exist assumes the existence of $\mathbf{A}^{-1}$; his method, while very instructive and elegant, is therefore not always applicable.)

In many, if not most cases, one employs instead of σ a matrix Σ which is proportional to it:

$$\sigma = \sigma\Sigma. \tag{44}$$

In order to estimate the covariance matrix of the parameters in such a case, one must estimate σ. If one uses the familiar fact that

$$S_0 = \hat{\mathbf{v}}^t\, \sigma^{-1}\hat{\mathbf{v}} \tag{45}$$

should have a χ^2 distribution with $n - k + r$ degrees of freedom (where n is the number of observations, i.e., the dimension of $\hat{\mathbf{v}}$; k the number of parameters, i.e., the dimension of $\hat{\boldsymbol{\delta}}$; and r the number of constraints, i.e., the dimension of $\hat{\boldsymbol{\lambda}}$), then an unbiased estimator of S_0 is

$$\langle S_0 \rangle = n - k + r,$$

so that

$$\langle \sigma \rangle = \frac{\hat{\mathbf{v}}^t\Sigma^{-1}\hat{\mathbf{v}}}{n - k + r}. \tag{46}$$

A more convenient estimate of S_0 can be obtained by noting that when convergence is obtained, $\hat{\boldsymbol{\delta}} = \mathbf{0}$ so that

$$\hat{\mathbf{v}} = -\sigma\mathbf{f}_{\hat{\mathbf{x}}}{}^t\mathbf{W}\hat{\boldsymbol{\phi}}$$

and

$$\begin{aligned} S_0 &= \hat{\boldsymbol{\phi}}^t\mathbf{W}\mathbf{f}_{\hat{\mathbf{x}}}\sigma\,\sigma^{-1}\sigma\mathbf{f}_{\hat{\mathbf{x}}}{}^t\mathbf{W}\hat{\boldsymbol{\phi}} \\ &= \hat{\boldsymbol{\phi}}^t\mathbf{W}\hat{\boldsymbol{\phi}}. \end{aligned} \tag{47}$$

If we now define

$$\begin{aligned} \tilde{\mathbf{W}} &= (\mathbf{f}_{\hat{\mathbf{x}}}\boldsymbol{\Sigma}\mathbf{f}_{\hat{\mathbf{x}}}{}^t)^{-1} \\ &= \sigma\mathbf{W}, \end{aligned} \tag{48}$$

we have

$$S_0 = \frac{1}{\sigma}\hat{\boldsymbol{\phi}}^t\tilde{\mathbf{W}}\hat{\boldsymbol{\phi}},$$

so that our estimator for σ becomes

$$\hat{\sigma} = \frac{\hat{\boldsymbol{\phi}}^t\tilde{\mathbf{W}}\hat{\boldsymbol{\phi}}}{n - k + r}. \tag{49}$$

Thus, if $\boldsymbol{\Sigma}$ is used instead of $\boldsymbol{\sigma}$, a convenient estimator $\hat{\sigma}$ for σ exists and is given by Eq. (49).

VI. CONCLUDING REMARKS

The scheme for solving the nonlinear equations of condition by Newton's method is a reasonable one, but as Eichhorn and Clary remark in their paper, it need not converge if the residuals are very large. In such a case it may become necessary to take quadratic terms explicitly into account, at least until the vector $\hat{\mathbf{v}}$ has been estimated with sufficient accuracy, or to use another method (e.g., the method of steepest descent) to obtain a solution. Nevertheless, Newton's method should suffice for the great majority of problems.

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