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UNITED STATES DEPARTMENT OF THE INTERIOR BUREAU OF MINES HELIUM ACTIVITY HELIUM RESEARCH CENTER

INTERNAL REPORT

NON-LINEAR REGRESSION AND THE PRINCIPLE OF LEAST SQUARES

THE METHOD OF EVALUATING THE CONSTANTS AND THE

CALCULATION OF VARIANCES AND COVARIANCES

BY

Robert E. Barieau

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by

Robert E. Barieau¹ and B. J. Dalton²

ABSTRACT

This report is concerned with the necessary mathematical equations in order to accomplish the following objectives: 1. to evaluate the parameters such that the sum of the weighted squares of the residuals of an experimental observable be a true minimum, regardless of the functional relationship between the variables and these parameters; 2. to evaluate all variances and covariances of the parameters evaluated by means of the law for the propagation of errors; and 3. to insure that a true minimum will always be obtained. The equations presented in this report were developed for a three-parameter problem.

INTRODUCTION

The Helium Research Center, Bureau of Mines, has as one of its long-range objectives the development of an equation of state for

Work on manuscript completed December 1965.

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helium that will reproduce the data to within the accuracy with which the data are known.

The Helium Research Center also has an experimental program for obtaining PVT data on gases and mixtures by the Burnett $(2)^{3/2}$ method.

3/ Underlined numbers in parentheses refer to items in the list of references at the end of this report.

In the Burnett method, one of the constants that must be evaluated is the volume-ratio of two containers. By the theory of the method, this constant is inherently non-linear. It was therefore decided to develop a capability for handling non-linear regression problems. This report gives the principles of the method the Helium Research Center uses in such problems.

Our method differs in several important respects from methods currently in use. In solving non-linear problems, the problem must be linearized and an iteration technique used to obtain the solution. All texts on non-linear regression, of which we are aware, linearize the problem before the normal equations are formed. This method is known as the Gauss-Newton method. In our method, the exact normal equations are formed, and the problem is linearized by expanding the exact normal equations in a Taylor's series expansion retaining the first two terms. This method is known as the Newton-Raphson method (7). The only work that we have been able to locate that uses this method in non-linear least squares problems is that of Strand, Kohl, and Bonham (8).

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These two different methods, as will be shown later, lead to the same least squares solution provided the iteration procedure converges to an answer. We have found that if one starts within the region of convergence, the Newton-Raphson method converges more rapidly than the Gauss-Newton method. This is one advantage of the method we have chosen.

If on applying the Gauss-Newton or the Newton-Raphson method, the problem is diverging after the first iteration, a method must be found that will lead to convergence. One of the methods that may be tried at this stage is the negative gradient or method of steepest descent. If the step in the direction of the negative gradient is small enough, this method must lead to a smaller sum of the squares of the deviations. The problem with this method in the past has been deciding on the size of the step to be taken. If the Newton-Raphson method has been used in developing the normal equations for the first iteration, then the size of the step to be taken in the direction of the negative gradient can be evaluated very simply from the coefficients appearing in the normal equations. This is the second advantage of the method we have chosen.

The third advantage involves the calculation of the variances and covariances of the constants evaluated. As far as we are aware, all authors and all programs available calculate variances and covariances on the assumption that the formulas that apply to linear problems will apply to non-linear problems once the non-linear problems have been linearized. We reject this assumption, preferring to calculate

These two different methods, as will be shown later, lead to the same least squares solution provided the iteration procedure converges to an answer. We have found that if one starts within the region of convergence, the Seviar Separa method converges more aspudic than the convergence of the Seviar Separa method converges more aspudic than the convergence.

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variances and covariances from the fundamental definition of these quantities and the law for the propagation of errors. (1, 5).

Some authors (6) claim that the least squares values of the constants evaluated in a non-linear problem are biased and should be corrected. All the proofs of this, that we have seen, assume the deviations are distributed with zero mean. This, of course, is never true in a non-linear problem unless this condition is imposed as a constraint. Further, the principle of least squares maximizes the probability that the deviations are equal to the true random errors. This is true for both linear and non-linear problems. This being true, we fail to see how any solution can be better than the least squares solution. We therefore take the least squares solution as being non-biased and apply no correction.

We have set the following objectives for our method.

.

1. To evaluate the parameters so that the sum of the weighted squares of the residuals of an experimental observable is a true minimum.

2. Objective 1 is to be accomplished even though the functional relationship between the observables and parameters is such that the observable involved in the minimum of the sum of the weighted squares of the residuals cannot be explicitly expressed as a function of other observables and the parameters.

3. All variances and covariances are to be calculated, with no approximations, by means of the law for the propagation of errors.

4. The method is to be such that a true minimum will always be obtained.

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A. The method is to be such that a true minimum will always be obtained.

This report is concerned with the necessary mathematical equations in order to accomplish the above-named objectives. The equations are developed for a three-parameter problem. The extension to the evaluation of more parameters should be obvious.

EVALUATION OF THE CONSTANTS

Suppose one has experimentally determined a set of n data points x_i , y_i . Let the functional relationship between x and y and the parameters A, B, and C be given by

$$F(y,x,A,B,C) = 0 \tag{1}$$

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We assume that there are no random errors in the x_i 's and that random errors occur in the observed y_i 's.

Now suppose we have evaluated the constants A, B, and C by some means or other. Then, because of random errors in y_i , equation (1) will not be exactly satisfied when the observed y_i and x_i values are substituted in equation (1). We will let F_i be the numerical value of F, when the observed y_i and x_i values are substituted in equation (1). Thus,

$$F_{i} = F(y_{i(0)}, x_{i}, A, B, C)$$
 (2)

Now when x_i is substituted in equation (1), we may solve for y_i so that equation (1) is satisfied exactly. We will designate this y_i as $y_i(calc)$. Thus,

$$F(y_{i(calc)}, x_{i}, A, B, C) = 0$$
(3)

The residual of y_i is given by

This report is connerted atth the accession wolfsenstical equalions is only to secondial the above-samed dejectives. The equations are developed for a chran-parameter problem. The extendence to the evaluation of race parameter about he contour

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Now suppose we have evaluated the constructs of B, and C by some means of other. Then, because of random errors in g, equation (1) will not be exactly subjected whan the concruse of our s, welles are abbeticated to equation (1) we will let P, be the emported wells of F, when the observed T, and s, values are substituted in spatements).

Now when x₁ is substituted in equiction (2), we say solve for y₁ and that equation (1) is catherined exactly. We will designate this y₁ as y₁(cale). Thus,

$$(C) \qquad 0 = (O, B, A, A, A, (a), (a), (b))^{2}$$

The realdual of y. is given by

$$\mathbf{x}_{i} = \mathbf{y}_{i(o)} - \mathbf{y}_{i(calc)} \tag{4}$$

Now Y_i , the residual of y_i , is the difference between the observed and calculated values. This is not the true random error in our observed y_i because we do not know the true value of y_i . However, we can maximize the probability that our Y_i 's are equal to the true random errors, and this is just what the principle of least squares does. The principle of least squares says that we maximize the probability that the Y_i 's represent the true random errors by minimizing the sum of the weighted squares of the residuals.

Thus, the function to be minimized is given by

$$R = \sum_{i=1}^{n} w_{y_{i}(o)} Y_{i}^{2}$$
(5)

where w is the weight assigned to y_{i(o)}. R is a function of y_{i(o)} the constants to be evaluated: A, B, and C. The condition that R be a minimum is determined by

$$\frac{1}{2} \left(\frac{\partial R}{\partial A} \right)_{B,C} = \sum_{i=1}^{n} w_{y_i(o)} Y_i \left(\frac{\partial Y_i}{\partial A} \right) = 0$$
(6)

$$\frac{1}{2} \left(\frac{\partial \mathbf{R}}{\partial \mathbf{B}} \right)_{\mathbf{A},\mathbf{C}} = \sum_{i=1}^{n} w_{y_{i}(o)} Y_{i} \left(\frac{\partial Y_{i}}{\partial \mathbf{B}} \right) = 0$$
(7)

and

$$\frac{1}{2} \left(\frac{\partial R}{\partial C} \right)_{A,B} = \sum_{i=1}^{n} w_{y_i(o)} Y_i \left(\frac{\partial Y_i}{\partial C} \right) = 0$$
(8)

Now Y_1 , the realdual of y_1 , is the difference between the observed and calculated values. This is not the true random struct in our observed y_1 because we do not know the true value of y_1 . However, we can maximize the probability that our Y_1 's are read to the true random structs, and this is just what the principle of least squares dees. The principle of least squares says that we waimize the probability that the Y_1 's represent the true random secore by ministandom structs of the wighted squares only the true random secore by miniprobability that the Y_1 's represent the true random secore by ministandom structs and of the wighted squares of the readom secore by mini-

Thus, the function to be wintaked is given by

where we fit the weight serigned to $y_1(a)$. It is a function of the constants to be evaluated: A, B, and C. The condition that R be a minimum is determined by

(1)
$$0 - \left(\frac{1}{\sqrt{2}}\right)_{x} \left(0\right)_{x} \left(\frac{1}{\sqrt{2}}\right)_{x} = 0 \quad (1)$$

 $\frac{1}{2} \left(\frac{3\pi}{2\pi} \right)_{A,C} = \sum_{l=1}^{N} \frac{\pi}{2} I(c_l)^{T_l} \left(\frac{3Y_l}{2\pi} \right) = 0$ (2)

ban

(a)
$$0 = \left(\frac{1}{2} \frac{x_{0}}{60}\right)_{1} \frac{x_{0}}{1} = \sum_{i=1}^{n} \frac{x_{i}}{x_{i}(0)} \frac{x_{i}}{1} \left(\frac{36}{60}\right) = 0$$
 (a)

In the application of equations (6), (7), and (8), the observed y_i 's and x_i 's are to be held constant in the derivatives: $\left(\frac{\partial R}{\partial A}\right)_{B,C}$, $\left(\frac{\partial R}{\partial B}\right)_{A,C}$, $\left(\frac{\partial R}{\partial C}\right)_{A,B}$. Equations (6), (7), and (8) are the

exact normal equations.

If Y_i is non-linear in the undetermined constants, then the solutions of our normal equations will not be straightforward. It will be necessary to solve them by an iterative technique in which values of the constants are assumed. This is done by expanding Y_i , $\left(\frac{\partial Y_i}{\partial A}\right)$, $\left(\frac{\partial Y_i}{\partial B}\right)$, and $\left(\frac{\partial Y_i}{\partial C}\right)$ in a Taylor's series expansion about an approximate solution, Y_i^0 , retaining only the first two terms. Thus,

$$\mathbf{X}_{\mathbf{i}} = \mathbf{Y}_{\mathbf{i}}^{\mathbf{o}} + \left(\frac{\partial \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{A}}\right)^{\mathbf{o}} \Delta \mathbf{A} + \left(\frac{\partial \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{B}}\right)^{\mathbf{o}} \Delta \mathbf{B} + \left(\frac{\partial \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C}}\right)^{\mathbf{o}} \Delta \mathbf{C}$$
(9)

$$\left(\frac{\partial Y_{i}}{\partial A}\right) = \left(\frac{\partial Y_{i}}{\partial A}\right)^{\circ} + \left(\frac{\partial^{2} Y_{i}}{\partial A^{2}}\right)^{\circ} \Delta A + \left(\frac{\partial^{2} Y_{i}}{\partial A \partial B}\right)^{\circ} \Delta B + \left(\frac{\partial^{2} Y_{i}}{\partial A \partial C}\right)^{\circ} \Delta C \quad (10)$$

$$\left(\frac{\partial Y_{i}}{\partial B}\right) = \left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ} + \left(\frac{\partial^{2} Y_{i}}{\partial B \partial A}\right)^{\circ} \Delta A + \left(\frac{\partial^{2} Y_{i}}{\partial B^{2}}\right)^{\circ} \Delta B + \left(\frac{\partial^{2} Y_{i}}{\partial B \partial C}\right)^{\circ} \Delta C \quad (11)$$

$$\left(\frac{\partial \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C}}\right) = \left(\frac{\partial \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C}}\right)^{\circ} + \left(\frac{\partial^{2} \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C} \partial \mathbf{A}}\right)^{\circ} \Delta \mathbf{A} + \left(\frac{\partial^{2} \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C} \partial \mathbf{B}}\right)^{\circ} \Delta \mathbf{B} + \left(\frac{\partial^{2} \mathbf{Y}_{\mathbf{i}}}{\partial \mathbf{C}^{2}}\right)^{\circ} \Delta \mathbf{C} \quad (12)$$

where the quantities $\triangle A$, $\triangle B$, and $\triangle C$ are defined as

$$\Delta A = A - A_{o}$$
$$\Delta B = B - B_{o}$$
$$\Delta C = C - C_{o}$$

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In the application of equations (5), (7), and (8), the observed y_1 's and x_1 's are to be held constant in the derivatives: $\begin{pmatrix} 33\\ 24\\ 34\end{pmatrix}$, $\begin{pmatrix} 38\\ 24\\ 34\end{pmatrix}$, $\begin{pmatrix} 38\\ 26\\ 3$

If V_{1} is non-linear in the underentered constants, then the same time of our nermal equations will not be attaightforward it will be marrasury to solve them by an inerative rechnique in which values of the constants are assumed. This is done by as match values of the constants are assumed. This is done by as match values of the constants are assumed. This is done by as a match values of the constants are assumed. This is done by an endities t_{1} , $\left(\frac{3^{V}}{2A}\right)$, $\left(\frac{3^{V}}{3\pi}\right)$, and $\left(\frac{3^{V}}{4c}\right)$ is a Taylor's sories expansion the strate terms. Thus the tire tires are assumed to the terms. Thus we have the tires are assumed to the solution of the tires are assumed to the terms.

where the quantitrice (A, 65, and M are decimed as

$$\Delta A = A - A_0$$

$$\Delta B = B - B_0$$

$$\Delta G = G - G_0$$

where A, B, and C are our undetermined constants, and A_0 , B_0 , and C_0 are approximate values for these quantities. Then to first order in the Δ 's

$$Y_{i}^{o}\left(\frac{\partial Y_{i}}{\partial A}\right)^{o} + \left[\left(\frac{\partial Y_{i}}{\partial A}\right)^{o^{2}} + Y_{i}^{o}\left(\frac{\partial^{2} Y_{i}}{\partial A^{2}}\right)^{o}\right] \Delta A$$

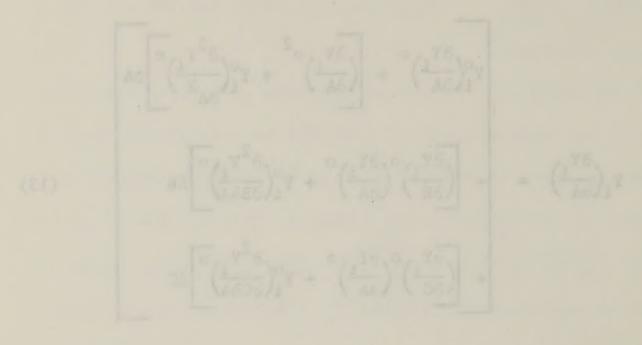
$$Y_{i}\left(\frac{\partial Y_{i}}{\partial A}\right) = + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{o}\left(\frac{\partial Y_{i}}{\partial A}\right)^{o} + Y_{i}^{o}\left(\frac{\partial^{2} Y_{i}}{\partial B \partial A}\right)^{o}\right] \Delta B$$

$$+ \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{o}\left(\frac{\partial Y_{i}}{\partial A}\right)^{o} + Y_{i}^{o}\left(\frac{\partial^{2} Y_{i}}{\partial C \partial A}\right)^{o}\right] \Delta C$$

$$(13)$$

$$Y_{i}\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ} + \left[\left(\frac{\partial Y_{i}}{\partial A}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial A\partial B}\right)^{\circ}\right] \Delta A + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}^{2} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B^{2}}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta A + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta A + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial B}\right)^{\circ}\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ} + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial B\partial C}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right)^{\circ}\right] \Delta B + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right]^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right] \right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] + Y_{i}^{\circ}\left(\frac{\partial^{2} Y_{i}}{\partial C^{2}}\right)^{\circ}\right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] \right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] \right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right)^{\circ}\right] \right] \Delta C + \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right] \right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right] \right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] + \left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left(\frac{\partial Y_{i}}{\partial C}\right] \right] \left[\left($$

where A, B, and C are our undetermined constants, and A₀. B₀, and C₀ are appreximate values for these quantities. Then to first ender in the A's



 $\sum_{i=1}^{n} \left(\frac{1}{16\pi \epsilon} \right)_{i}^{n} Y + \left(\frac{1}{36} \right) \left(\frac{1}{36} \right)_{i}^{n} + \frac{1}{2}$

$$a_1 \Delta A + b_1 \Delta B + c_1 \Delta C = m_1$$
 (16)

$$a_2 \Delta A + b_2 \Delta B + c_2 \Delta C = m_2$$
 (17)

$$a_{3} \triangle A + b_{3} \triangle B + c_{3} \triangle C = m_{3}$$
 (18)

where

$$a_{1} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial A} \right)^{o^{2}} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial A^{2}} \right)^{o} \right]$$
(19)

$$a_{2} = b_{1} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial B} \right)^{o} \left(\frac{\partial Y_{i}}{\partial A} \right)^{o} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial A \partial B} \right)^{o} \right]$$
(20)

$$a_{3} = c_{1} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial A} \right)^{o} \left(\frac{\partial Y_{i}}{\partial C} \right)^{o} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial A \partial C} \right)^{o} \right]$$
(21)

$$\mathbf{b}_{2} = \sum_{i=1}^{n} \mathbf{w}_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial B} \right)^{o^{2}} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial B^{2}} \right)^{o} \right]$$
(22)

$$b_{3} = c_{2} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial B} \right)^{o} \left(\frac{\partial Y_{i}}{\partial C} \right)^{o} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial B \partial C} \right)^{o} \right]$$
(23)

$$c_{3} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial C} \right)^{o^{2}} + Y_{i}^{o} \left(\frac{\partial^{2} Y_{i}}{\partial C^{2}} \right)^{o} \right]$$
(24)

Subseitenting equations (1), (14), and (15) into our cornel

$$a_2\Delta A + b_2\Delta B + c_2\Delta C = m_2$$
 (17)

(21)
$$\left[\left(\frac{1}{2} \frac$$

(05)
$$\left[\left(\frac{1}{4} \frac{x^{2}}{5} \right) \left(\frac{x^{2}}{6} \right) \left(\frac{x^{2}}{6} \right) \left(\frac{x^{2}}{6} \right) \right]_{(5)} \left(\frac{x^{2}}{6} \right) \right]_{(5)} \left(\frac{x^{2}}{6} \right) \left(\frac{x^{2}}{$$

$$(15). \left[\left(\frac{\gamma^{2} \sigma}{(2 \sigma A \sigma)} \right)^{2} + \left(\frac{\gamma \varepsilon}{2 \sigma} \right)^{2} \left(\frac{\gamma \sigma}{A \sigma} \right) \right]_{(0)x} \left(\frac{\gamma}{2} - \frac{\gamma}{2} - \frac{\gamma}{2} - \frac{\gamma}{2} \right)^{2} = \frac{\gamma}{2}$$

$$\mathbf{s}_{2} = \sum_{i=1}^{n} \mathbf{v}_{2i(o)} \left[\left(\frac{\partial \mathbf{x}_{i}}{\partial \mathbf{n}} \right)^{2} + \mathbf{v}_{1}^{2} \left(\frac{\partial^{2} \mathbf{y}_{i}}{\partial \mathbf{n}} \right)^{2} \right] . \qquad (22)$$

$$(2.2) = \frac{1}{2} = \frac{1}{1-1} = \frac{1}{2} \left[\left(\frac{1}{20} \right)^{0} \left(\frac{1}{20} \right)^{0} \left(\frac{1}{20} \right)^{0} \left(\frac{1}{20} \right)^{0} + \frac{1}{2} \left(\frac{1}{20000} \right)^{0} \right]$$

$$(2.2)$$

$$c_{3} = \sum_{j=1}^{n} u_{2j}(\alpha) \left[\left(\frac{\delta T}{\delta c} \right)^{\alpha} + T_{1} \left(\frac{\delta T}{\delta c^{2}} \right)^{\alpha} \right]$$
(24)

$$m_{1} = -\sum_{i=1}^{n} w_{y_{i}(o)} Y_{i}^{o} \left(\frac{\partial Y_{i}}{\partial A}\right)^{o}$$
(25)

$$m_{2} = -\sum_{i=1}^{n} w_{y_{i}(o)} Y_{i}^{o} \left(\frac{\partial Y_{i}}{\partial B}\right)^{o}$$
(26)

$$m_{3} = -\sum_{i=1}^{n} w_{y_{i}(o)} Y_{i}^{o} \left(\frac{\partial Y_{i}}{\partial C}\right)^{o}$$
(27)

The solutions to equations (16), (17), and (18) are

$$D_0 \Delta A = D_1 m_1 + D_2 m_2 + D_3 m_3$$
 (28)

$$D_{O} \Delta B = D_{4} m_{1} + D_{5} m_{2} + D_{6} m_{3}$$
(29)

$$D_0 \Delta C = D_7 m_1 + D_8 m_2 + D_9 m_3$$
 (30)

where

$$D_1 = b_2 c_3 - b_3 c_2 \tag{31}$$

$$D_2 = b_3 c_1 - b_1 c_3 \tag{32}$$

$$D_3 = b_1 c_2 - b_2 c_1 \tag{33}$$

$$D_4 = a_3 c_2 - a_2 c_3 \tag{34}$$

$$D_5 = a_1 c_3 - a_3 c_1 \tag{35}$$

$$D_6 = a_2 c_1 - a_1 c_2 \tag{36}$$

$$D_7 = a_2 b_3 - a_3 b_2$$
 (37)

$$D_8 = a_3 b_1 - a_1 b_3 \tag{38}$$

$$D_9 = a_1 b_2 - a_2 b_1 \tag{39}$$

$$= -\sum_{i=1}^{n} v_{1(0)} Y_{i}^{0} \left(\frac{\partial Y_{i}}{\partial A}\right)^{0}$$
(25)

$$m_{3} = -\sum_{l=1}^{n} v_{2}(a) \frac{v_{1}^{2}}{i} \left(\frac{ac}{ac}\right)^{a}$$
(27)

he solutions to equations (16), (17), and (18) are

 $D_{0}^{EA} = D_{1}^{m_{1}} + D_{2}^{m_{2}} + D_{3}^{m_{3}}$ (28)

$$D_{a}\Delta B = D_{a}m_{1} + D_{5}m_{2} + D_{6}m_{3}$$
 (29)

$$\sum_{n=0}^{\infty} \int C = D_{n} m_{1} + D_{0} m_{2} + D_{0} m_{3}$$
 (30)

whe re

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$$D_{0} = a_{1}D_{1} + a_{2}D_{2} + a_{3}D_{3}$$
(40)

The solutions of equations (28), (29), and (30) give the corrections to be applied to the assumed values of our undetermined constants.

In the Gauss-Newton method of linearization, the second term in the summations of the a's, b's, and c's of equations (19)-(24) is neglected; this does not lead to an error as long as the method converges because the exact solutions of equations (16), (17), and (18) are: $\Delta A = \Delta B = \Delta C = 0$.

When the functional relationship between the observables is such that $y_{i(calc)}$ cannot be solved for explicitly, it will be necessary to solve equation (3) for $y_{i(calc)}$ by a series of approximations. Let us expand F in a truncated Taylor's series expansion about the point x_i , $y_{i(o)}$:

$$F = F_{i} + \left(\frac{\partial F}{\partial y}\right)_{\substack{x,A,B,C \\ y=y_{i}(o) \\ x=x_{i}}} \left(y_{i(calc)} - y_{i(o)}\right) = 0 \quad (41)$$

or

$$y_{i(o)} - y_{i(calc)} = \frac{F_{i}}{\left(\frac{\partial F}{\partial y}\right)_{x,A,B,C}}$$
(42)
$$y_{i(o)} = \frac{F_{i}}{\left(\frac{\partial F}{\partial y}\right)_{x,A,B,C}}$$
(42)

where in equations (41) and (42) the symbol $\begin{pmatrix} \partial F \\ \partial y \end{pmatrix}$ means that x,A,B,C $y=y_i(o)$ $x=x_i$

$$D_{0} = a_{1}D_{1} + a_{2}D_{2} + a_{3}D_{3}$$
 (40)

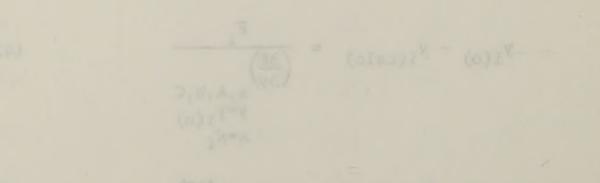
The solutions of equations (28), (29), and (30) give the corrections to be applied to the sesumed values of our undetermined constants.

In the summariant of the s's, b's, and c's of equations (19)-(24) is neglected; this does not lead to an error as long as the method converges because the exact solutions of equations (10), (17), and (18) are: $\Delta A = \Delta A = \Delta F = 0$.

When the functional relationship between the observables is such that $y_{1}(calc)$ cannot be solved for explicitly. It will be necessary to solve equation (3) for $y_{1}(calc)$ by a series of approximations. Let us expand F in a truncated Taylor's series expansion about the point x_1 . $y_{1}(c_{0})$:

$$(10) \quad 0 = (00)^{1/2} (00)^{1/2} (00)^{1/2} (00)^{1/2} (0)^{1/2}$$

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Amere in equations (61) and (62) the symbol (57) sides.

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the derivative of F with regard to y, keeping x, A, B, and C constant, is to be evaluated at the point

 $y = y_{i(0)}$ $x = x_{i}$

The solution of equation (42) gives the first approximation for $y_{i(calc)}$. We designate this value as $y_{i(calc)_{1}}$. This value is then substituted into equation (3), and if $y_{i(calc)_{1}}$ is not the exact answer, equation (3) will not be satisfied exactly. We designate this value of F as $F_{i(calc)_{1}}$. Thus,

$$F_{i(calc)_{1}} = F(x_{i}, y_{i(calc)_{1}}, A, B, C)$$
(43)

Then the second approximation, $y_{i(calc)_2}$, of $y_{i(calc)}$ is obtained from the expression

$$y_{i(calc)_{1}} - y_{i(calc)_{2}} = \frac{F_{i(calc)_{1}}}{\left(\frac{\partial F}{\partial y}\right)_{\substack{x,A,B,C\\y=y_{i}(calc)_{1}\\x=x_{i}}}}$$
(44)

This iteration is repeated until equation (3) is satisfied to within any amount we wish to specify.

Once we have $y_{i(calc)}$ and $y_{i(o)}$, then $Y_{i} = y_{i(o)} - y_{i(calc)}$, and Y_{i}^{2} can be calculated. Then if $w_{i(o)}$ is known or has been assigned, $y_{i(o)}$ R may be calculated by means of equation (4). the derivative of F with regard to y, keeping x, A, D, and C constant, is to be evaluated at the point

The solution of equation (42) gives the livet approximation for Y(calc). We designate this value as vi(calc); This value is then substituted into equation (3), and if vi(calc); is not the exact answer, equation (3) will not be satisfied exactly. We designate this value of F as F, reals). Thus,

Then the second approximation, y((alc), of y((alc) is obtained from the expression

$$\frac{1}{2(calcl)_1} = \frac{1}{2(colcl)_2} = \frac{1}{2(colcl)_1}$$

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This theration is reputed multi equation (3) is satisfied to within any amount we wish to specify.

Once we have $y_1(calc)$ and $y_1(c)$, then $Y_1 = y_1(c) - y_1(calc)$, and $Y_1 = and be calculated. Then if a micro or has been assigned, is may be calculated by means of equation (4).$

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If the $y_{i(0)}$'s all have the same precision index, they will all have the same weight and w = 1. If the $y_{i(0)}$'s do not all have the same precision index, then

$$w_{y_{i(0)}} = \frac{L^2}{s_{y_{i(0)}}^2}$$
 (45)

where L is a constant and $S_{y_{i(0)}}^2$ is the variance of $y_{i(0)}$. In a particular problem, it may be necessary to assume that $w_{i(0)} = 1$ in the beginning. However, if this is done, the residuals, $\left[y_{i(0)} - y_{i(calc)}\right]$, should be examined to see if there is any statistical evidence for the residuals squared being a function of y. Any assumption as to the variance, $S_{y_{i(0)}}^2$, being a function of y can always be checked by examining the residuals. In any event, $w_{y_{i(0)}}$ is not a function of the constants to be evaluated.

We now proceed to develop the equations needed to calculate the coefficients of our normal equations. Differentiating equation (4) with regard to A, keeping $x_i^{}$, $y_{i(o)}^{}$, B, and C constant, we have

$$\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C} = -\left(\frac{\partial y_{i}(calc)}{\partial A}\right)_{x_{i},B,C}$$
(46)

Differentiating equation (3) with regard to A, keeping x_i , B, and C constant, we have

$$\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}\left(\frac{\partial y_{i}(calc)}{\partial A}\right)_{x_{i},B,C} + \left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)} = 0 \quad (47)$$

If the $y_1(\alpha)$'s all have the same precision index, they will all have the same weight and w = 1. If the $y_1(\alpha)$'s do not all have the same precision index, then

$$u_{\mathcal{F}_{1}(\alpha)}^{\mathcal{F}_{2}} = \frac{u^{2}}{u^{2}}$$
(45)

where L is a constant and $3_{1(0)}^{2}$ is the variance of $y_{1(0)}$. In a particular problem, it may be necessary to assume that $w_{1(0)} = 1$ in the beginning. However, if this is done, the residuals, $y_{1(0)} = 1$, $y_{1(0)} = y_{1(0)}$] should be assamined to see if there is any arotistical evidence for the residuals squared being a function of y. Any assumption as to the variance, $8_{1(0)}^{2}$, being a function of y can always be checked by examining the residuals. In any avent, $w_{1(0)}^{2}$ is not a function of the residuals. In any avent, $w_{1(0)}^{2}$

Mg now proceed to develop the equations needed to calculate the coefficients of our normal equations. Differentiating equation (6) view regard to A, keeping x, yito, B, and C constant, we have

$$(ab) = -\left(\frac{(1+1)}{2\pi}\right)_{x_1,y_2} = -\left(\frac{(1+1)}{2\pi}\right)_{x_1,y_2}$$

Differentiation equation (3) with regard to A. keeping x1. D.

$$\left(\frac{\partial F}{\partial y_{t}(colo)}\right)_{x_{1}, A, B, C}\left(\frac{\frac{\partial y_{1}(colo)}{\partial A}}{\partial A}\right)_{x_{1}, B, C}+\left(\frac{\partial F}{\partial A}\right)_{x_{1}, Y_{1}(colo)}b_{s}c = 0 \quad (4.7)$$

$$\begin{pmatrix} \frac{\partial y_{i(calc)}}{\partial A} \end{pmatrix}_{x_{i},B,C} = - \frac{\begin{pmatrix} \frac{\partial F}{\partial A} \end{pmatrix}_{x_{i},y_{i(calc)},B,C}}{\begin{pmatrix} \frac{\partial F}{\partial y_{i(calc)}} \end{pmatrix}_{x_{i},A,B,C}}$$
(48)

and if we substitute equation (48) in equation (46), we have

$$\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C} = \frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}}$$
(49)

Similarly, it can be shown that

$$\begin{pmatrix} \frac{\partial Y_{i}}{\partial B} \end{pmatrix}_{x_{i}, y_{i}(o), A, C} = \frac{\begin{pmatrix} \frac{\partial F}{\partial B} \end{pmatrix}_{x_{i}, y_{i}(calc), A, C}}{\begin{pmatrix} \frac{\partial F}{\partial y_{i}(calc)} \end{pmatrix}_{x_{i}, A, B, C}}$$
(50)

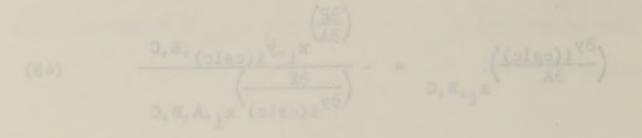
and that

$$\begin{pmatrix} \frac{\partial Y_{i}}{\partial C} \end{pmatrix}_{x_{i}, y_{i}(o), A, B} = \frac{\begin{pmatrix} \frac{\partial F}{\partial C} \end{pmatrix}_{x_{i}, y_{i}(calc), A, B}}{\begin{pmatrix} \frac{\partial F}{\partial Y_{i}(calc)} \end{pmatrix}_{x_{i}, A, B, C}}$$
(51)

Differentiating equation (49) with regard to A, keeping x_i , $y_i(o)$, B, and C constant, we have.

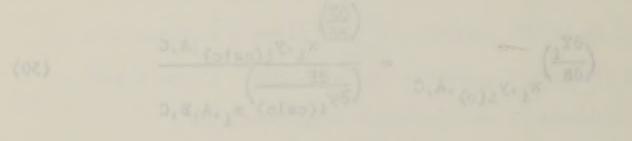
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or



and if we substitute squation (48) in squation (45), we have

Similarly, it can be shown that



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Differentiating equation (49) with regard to A, hosping vi 'i(a)' B, and C constant, we have.

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$$\frac{\left[\frac{\partial}{\partial A}\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C^{-}x_{i},B,C}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}} (52)$$

$$\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,c^{\left[\frac{\partial}{\partial A}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C},X_{i},B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}} (52)$$

 $\left(\frac{\partial^2 Y_i}{\partial A^2}\right)_{x_i,y_{i(o)},B,C}$

$$\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C} = G(y_{i}(calc),A,B,C)$$

$$\begin{bmatrix} d \left(\frac{\partial F}{\partial A}\right)_{x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, B, C} = \begin{bmatrix} \frac{\partial}{\partial A} \left(\frac{\partial F}{\partial A}\right)_{x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, y_{i}(\text{calc})} & dA \\ & & & & \\ & & & \\ & & & & \\$$

and

$$\left(\frac{\partial F}{\partial A} \right)_{x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, B, C} = \left\{ \begin{array}{c} \left[\frac{\partial}{\partial A} \left(\frac{\partial F}{\partial A} \right)_{x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, y_{i}(\text{calc})} \right]_{x_{i}, y_{i}(\text{calc})} \left[\frac{\partial}{\partial A} \left(\frac{\partial F}{\partial A} \right)_{x_{i}, y_{i}(\text{calc})}, B, C^{-}x_{i}, A, B, C^{-}x_{i}, B, C^{-}x_{i}, A, B, C^{$$

Also,

$$\left(\frac{\partial F}{\partial y_{i(calc)}}\right)_{x_{i},A,B,C} = g\left(y_{i(calc)},A,B,C\right)$$

$$\left[d\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},B,C}\right] = \left[\frac{\partial}{\partial y_{i}(calc)}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},A,B,C}x_{i},A,B,C\right] dA + \left[\frac{\partial}{\partial A}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},y_{i}(calc),B,C\right] dA$$
(55)

and

$$\frac{\partial}{\partial A} \left(\frac{\partial F}{\partial y_{i}(calc)} \right)_{x_{i},A,B,C} x_{i},B,C = \begin{bmatrix} \frac{\partial}{\partial A} \left(\frac{\partial F}{\partial y_{i}(calc)} \right)_{x_{i},A,B,C} x_{i},y_{i}(calc),B,C \\ + \begin{bmatrix} \frac{\partial}{\partial A} \left(\frac{\partial F}{\partial y_{i}(calc)} \right)_{x_{i},A,B,C} \right]_{x_{i},A,B,C} x_{i},A,B,C \end{bmatrix} (56)$$

When we substitute equations (54) and (56) into equation (52), we find

$$-\frac{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}\left(\frac{\partial^{2}F}{\partial A^{2}}\right)_{x_{i},y_{i}(calc)},B,C}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}^{2}}$$

$$+\frac{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}\left(\frac{\partial^{2}F}{\partial y_{i}(calc)}\right)_{x_{i},B,C}\left(\frac{\partial Y_{i}(calc)}{\partial A}\right)_{x_{i},B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}^{2}}$$

$$-\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C\left(\frac{\partial^{2}F}{\partial A\partial y_{i}(calc)}\right)_{x_{i},A,B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}^{2}}$$

$$-\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C\left(\frac{\partial^{2}F}{\partial y_{i}^{2}(calc)}\right)_{x_{i},A,B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}^{2}}$$

But from equation (48)

 $\left(\frac{\partial^2 Y}{\partial Y}\right)$

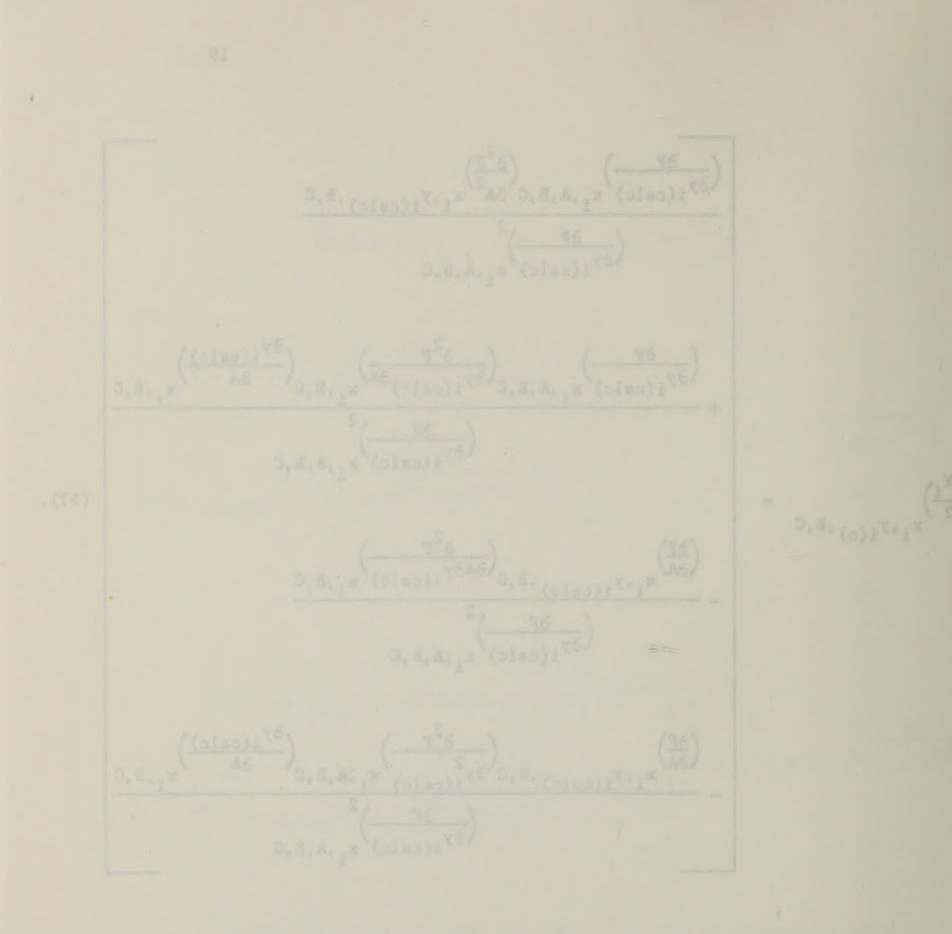
·∂A²

^xi,^yi(o),^B,C

$$\left(\frac{\partial y_{i(calc)}}{\partial A}\right)_{x_{i},B,C} = -\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i(calc)},B,C}}{\left(\frac{\partial F}{\partial y_{i(calc)}}\right)}$$
(48)

19

(57)



But from equation (44)

$$\frac{\partial_{x} g_{1}(aste)}{\partial_{x}} = \frac{\left(\frac{\partial F}{\partial a_{1}}\right)}{\left(\frac{\partial F}{\partial a_{1}}\right)} = \frac{\partial F}{\partial a_{1}} = \frac{\left(\frac{\partial F}{\partial a_{2}}\right)}{\left(\frac{\partial F}{\partial a_{2}}\right)}$$

When we substitute equation (48) in equation (57), we see that

$$B,C = \begin{pmatrix} \left(\frac{\partial^{2}F}{\partial A^{2}}\right)_{x_{i},y_{i}(calc)},B,C} \\ \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\ \left(\frac{\partial F}{\partial A^{2}}\right)_{x_{i},y_{i}(calc)},B,C} \\ \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\ \left(\frac{\partial F}{\partial A^{2}}\right)_{x_{i},y_{i}(calc)},B,C} \\ \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\ \left($$

Similarly,

 $(\partial^2 Y_i)$

ba²

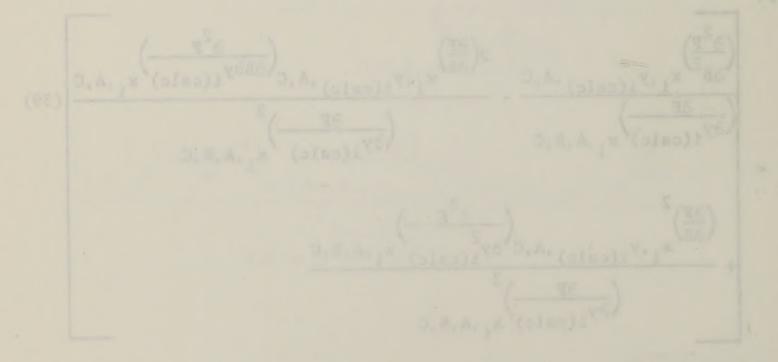
x_i,y_{i(o)}

and

When we substitute equation (48) in equation (57); we use that

Similarly,

-



forms.

$$\frac{\partial^{2} Y_{i}}{\partial c^{2}} \Big|_{x_{i}, y_{i}(o)}, A, B} = \begin{pmatrix} \frac{\partial^{2} F}{\partial c^{2}} \\ \frac{\partial F}{\partial y_{i}(calc)} \\ \frac{\partial F}{\partial y_{i}(calc)}$$

Differentiating equation (49) with regard to B, keeping $x_i, y_i(o)$, A,C fixed, we have

 $\begin{bmatrix} \frac{\partial}{\partial B} \begin{pmatrix} \frac{\partial Y_{i}}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(o)}, B, C \\ x_{i}, y_{i}(o) \end{pmatrix}^{A, C}$

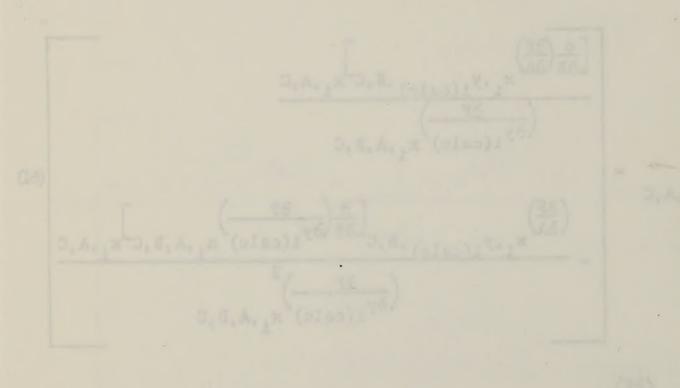
$$\begin{bmatrix}
\frac{\partial}{\partial B} \begin{pmatrix} \partial F \\ \partial A \end{pmatrix} \\
x_{i}, y_{i}(calc), B, C^{-}x_{i}, A, C \\
\hline
\begin{pmatrix}
\frac{\partial F}{\partial y_{i}(calc)} \end{pmatrix} \\
\frac{\partial F}{\partial x_{i}, y_{i}(calc)} \\
x_{i}, A, B, C
\end{bmatrix}$$
(61)
$$\begin{pmatrix}
\frac{\partial F}{\partial A} \\
x_{i}, y_{i}(calc), B, C^{-} \\
\frac{\partial F}{\partial y_{i}(calc)} \end{pmatrix} \\
\frac{\partial F}{\partial y_{i}(calc)} \\
\frac{\partial F}{\partial y_{i$$

Let us differentiate $\begin{pmatrix} \partial F \\ \partial A \end{pmatrix}_{x_i, y_i(calc)}$, with regard to B, keeping x_i , i, $y_i(calc)$, B,C A, and C constant. When we do this, we get

$$\frac{\partial}{\partial B}\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C^{-}x_{i},A,C} = \begin{bmatrix} \frac{\partial}{\partial B}\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C^{-}x_{i},y_{i}(calc)},A,C \\ + \begin{bmatrix} \frac{\partial}{\partial B}\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C^{-}x_{i},A,B,C \end{bmatrix}_{x_{i},A,B,C} \begin{pmatrix} \frac{\partial y_{i}(calc)}{\partial B} \end{pmatrix}_{x_{i},A,C}$$
(62)

Differentiating suistion (49) with regard to N, heaping 21,91(0) 14,C

Svad an , Louis



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But

$$\left(\frac{\partial y_{i(calc)}}{\partial B}\right)_{x_{i},A,C} = -\frac{\left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i(calc)},A,C}}{\left(\frac{\partial F}{\partial y_{i(calc)}}\right)_{x_{i},A,B,C}}$$
(63)

and if we substitute equation (63) in equation (62), we see that

$$\begin{bmatrix} \frac{\partial}{\partial B} \begin{pmatrix} \frac{\partial F}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(\text{calc}), B, C^{-}x_{i}, A, C} = \begin{pmatrix} \frac{\partial^{2}F}{\partial A\partial B} \end{pmatrix}_{x_{i}, y_{i}(\text{calc}), C} \\ - \begin{pmatrix} \frac{\partial^{2}F}{\partial A\partial y_{i}(\text{calc})} \end{pmatrix}_{x_{i}, B, C} \begin{pmatrix} \frac{\partial F}{\partial B} \end{pmatrix}_{x_{i}, y_{i}(\text{calc}), A, C} \\ \frac{\partial^{2}F}{\partial A\partial y_{i}(\text{calc})} \end{pmatrix}_{x_{i}, B, C} \begin{pmatrix} \frac{\partial F}{\partial B} \end{pmatrix}_{y_{i}(\text{calc}), A, C} \end{pmatrix}$$
(64)

Now if we differentiate $\left(\frac{\partial F}{\partial y_i(calc)}\right)_{x_i,A,B,C}$ with regard to B, holding x_i , A, and C constant, we get

$$\frac{\partial}{\partial B}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},A,C = \begin{bmatrix} \frac{\partial}{\partial B}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},y_{i}(calc),A,C \\ + \begin{bmatrix} \frac{\partial}{\partial B}\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}x_{i},A,B,C \end{bmatrix}_{x_{i},A,B,C} \begin{pmatrix} \frac{\partial y_{i}(calc)}{\partial B}\right)_{x_{i},A,C}$$
(65)

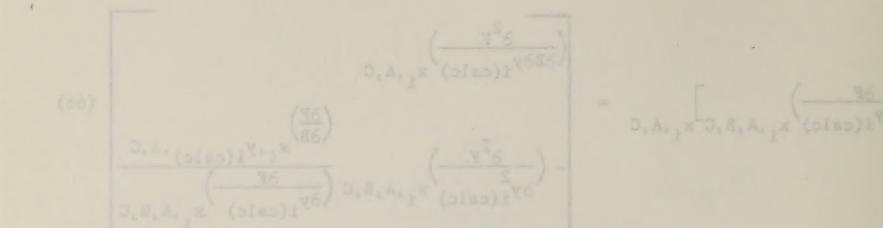
or, substituting equation (63) in equation (65),

$$\begin{bmatrix} \frac{\partial}{\partial B} \left(\frac{\partial F}{\partial y_{i}(calc)} \right)_{x_{i},A,B,C} \\ = \begin{bmatrix} \left(\frac{\partial^{2}F}{\partial B\partial y_{i}(calc)} \right)_{x_{i},A,C} \\ - \left(\frac{\partial^{2}F}{\partial y_{i}(calc)} \right)_{x_{i},A,B,C} \\ \frac{\partial^{2}F}{\partial y_{i}(calc)} \\ \frac{\partial^{2}F}{\partial y_{i}(calc)}$$

Therefore, if we substitute equations (64) and (66) in equation (61), equation (61) is expressible as

 $\left(\frac{\partial^2 Y_i}{\partial A \partial B}\right)_{x_i, y_i(o)}, C$

$$\begin{pmatrix} \left(\frac{\partial^{2}F}{\partial A\partial B}\right)_{x_{i},y_{i}(calc)}, C} & \left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i}(calc)}, A, C} \left(\frac{\partial^{2}F}{\partial A\partial y_{i}(calc)}\right)_{x_{i},B,C} \\
\begin{pmatrix} \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} & \left(\frac{\partial^{2}F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
- & \left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)}, B, C \left(\frac{\partial^{2}F}{\partial B\partial y_{i}(calc)}\right)_{x_{i},A,C} \\
\begin{pmatrix} \left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)}, B, C \left(\frac{\partial F}{\partial B\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
\begin{pmatrix} \left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)}, B, C \left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i}(calc)}, A, C \left(\frac{\partial^{2}F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
+ & \left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)}, B, C \left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i}(calc)}, A, C \left(\frac{\partial^{2}F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
+ & \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
\end{pmatrix}^{3} \\
\begin{pmatrix} \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C} \\
\end{pmatrix}^{3} \\$$



Therefore, if we substitute equations (64) and (66) in equation (61), equation (61) and (66) in equation (61).

We can derive expressions for $\left(\frac{\partial^2 Y_i}{\partial A \partial C}\right)_{x_i, y_i(o)}$, B and

 $\left(\frac{\partial^2 Y_i}{\partial B \partial C}\right)_{x_i, y_i(o)}, A$

24

 $\frac{\begin{pmatrix} \frac{\partial^2 F}{\partial A \partial C} \end{pmatrix}_{x_i, y_i(calc)}, B}{\begin{pmatrix} \frac{\partial F}{\partial C} \end{pmatrix}_{x_i, y_i(calc)}, A, B} \begin{pmatrix} \frac{\partial^2 F}{\partial A \partial y_i(calc)} \end{pmatrix}_{i(calc)} x_i, B, C}{\begin{pmatrix} \frac{\partial F}{\partial C} \end{pmatrix}_{i(calc)} x_i, A, B, C}$ $\left(\frac{\partial^{2} Y_{i}}{\partial A \partial C}\right)_{x_{i}, y_{i}(o), B} = -\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i}, y_{i}(calc)}, B, C} \left(\frac{\partial^{2} F}{\partial C \partial y_{i}(calc)}\right)_{x_{i}, A, B}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)^{2}} \left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i}, A, B, C}}$ $+\frac{\left(\frac{\partial F}{\partial A}\right)_{x_{i},y_{i}(calc)},B,C}\left(\frac{\partial F}{\partial C}\right)_{x_{i},y_{i}(calc)},A,B}\left(\frac{\partial^{2}F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)^{3}}$ $\frac{\left(\frac{\partial^{2}F}{\partial B\partial C}\right)_{x_{i},y_{i}(calc),A}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}} - \frac{\left(\frac{\partial F}{\partial C}\right)_{x_{i},y_{i}(calc),A,B}}{\left(\frac{\partial F}{\partial J_{i}(calc)}\right)_{x_{i},A,B,C}} \left(\frac{\partial^{2}F}{\partial B\partial y_{i}(calc)}\right)_{x_{i},A,B,C}$ $\frac{\left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i}(calc)},A,C}\left(\frac{\partial^{2}F}{\partial C\partial y_{i}(calc)}\right)_{x_{i},A,B}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)^{2}}$ 1,^y1(0),^A $\frac{\left(\frac{\partial F}{\partial B}\right)_{x_{i},y_{i}(calc)},A,C\left(\frac{\partial F}{\partial C}\right)_{x_{i},y_{i}(calc)},A,B\left(\frac{\partial^{2}F}{\partial y_{i}^{2}(calc)}\right)_{x_{i},A,B,C}}{\left(\frac{\partial F}{\partial y_{i}(calc)}\right)_{x_{i},A,B,C}^{3}}$

similar to equation (67). The results are

(68)

(69)

We can devive expressions for

similar to equation (67). The results are

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E.A., x (2122)1 (EDE) 3. A. (0120)2 (.) x (EEE D.E.A., x (2122)1 (EDE) (36) (36) (36) (36)

(24)

The method of obtaining a least squares solution for the constants A, B, and C is as follows.

We have n pairs of the observed quantities, x and y i(o).

1. We assume values for A, B, and C.

2. We then calculate the n values of F_i , using equation (2).

3. We next calculate the n values of y_i(calc)^{using an iterative method involving equations (42), (43), and (44).}

4. We next calculate the n values of Y, from equation (4).

5. We next calculate the n values of Y_i^2 .

6. Using designated values for w, we next calculate R, $y_{i(o)}$ the sum of the weighted squares of the residuals, using equation (5).

7. We next calculate the n values of (∂F/∂y_i(calc)) by differentiation of the analytical expression for F, keeping x_i, A,
 B, and C constant.

8. We next calculate the n values of $(\partial F/\partial A)$, evaluated at $y_{i(calc)}$, by differentiation of the analytical expression for F, keeping x_{i} , $y_{i(calc)}$, B, and C constant.

9. We next calculate the n values of (dF/dB), evaluated at y_{i(calc)}, by differentiating the analytical expression for F, keeping x_i, y_{i(calc)}, A, and C constant.

10. We next calculate the n values of $(\partial F/\partial C)$, evaluated at $y_{i(calc)}$, by differentiation of the analytical expression for F, keeping x_{i} , $y_{i(calc)}$, A, and B constant.

11. We next calculate the n values of $(\partial^2 F/\partial A^2)$, evaluated at $y_i(calc)$, by differentiating the analytical expression for F twice.

The method of obtaining a least squares solution for the con-

We have n pairs of the observed quantities, x, and yster-

I. We assume volues for A. D. and C.

2. We then calculate the n values of F ,, using equation (2)

3. We mant calculate the a values of y_t(calc)^{using an itera-}

4. We next calculate the n values of Y_1 from equation (4). 5. We next calculate the n values of Y_2^2 .

6. Using designated values for w , we make calculate X , ²1(o)

 We must calculate the a values of (37/391(calc)) by differentiation of the analytical expression for F, keeping x₁, A.
 and C constant.

3. We nont calculate the n values of (3F/3A), evaluated at Y1(calc)' by differentiation of the analytical expression for F, keeping x., y., ..., B; and C constant.

9. We next calculate the n values of (35/38), evaluated at /(calc) ' by differentiating the analytical axpression for F,

10. We next calculate the n values of (37/30), svaluated at vi(calc), by differentiation of the enalytical expression for F, keeping x., y.c., A. and B constant.

11. We rest calculate the a values of (6"F/6A"), evaluated at "I(calc)" by differentiating the analytical expression for F twice.

12. We next calculate the n values of $(\partial^2 F/\partial B^2)$, evaluated at ^yi(calc), by differentiation of the analytical expression for F twice.

13. We next calculate the n values of $(\partial^2 F/\partial C^2)$, evaluated at $y_{i(calc)}$, by differentiating the analytical expression for F twice.

14. We next calculate the n values of $(\partial^2 F/\partial y_{i(calc)}^2)$ by differentiating the analytical expression for F twice.

15. We next calculate the n values of $(\partial^2 F/\partial A\partial B)$, evaluated at y_{i(calc)}, which is obtained from the analytical expression for F.

16. We next calculate the n values of $(\partial^2 F/\partial A\partial C)$, evaluated at y_i(calc), which is obtained from the analytical expression for F.

17. We next calculate the n values of $(\partial^2 F/\partial B\partial C)$, evaluated at $y_{i(calc)}$, which is obtained from the analytical expression for F.

18. We next calculate the n values of $(\partial^2 F/\partial y_{i(calc)} \partial A)$ which is obtained from the analytical expression for F.

19. We next calculate the n values of $(\partial^2 F/\partial y_i(calc)\partial B)$ which is obtained from the analytical expression for F.

20. We next calculate the n values of $(\partial^2 F/\partial y_i(calc)^{\partial C})$ which is obtained from the analytical expression for F.

21. We next calculate the n values of $(\partial Y_i/\partial A)$ using equation (49).

22. We next calculate the n values of $(\partial Y_i/\partial B)$ using equation (50).

23. We next calculate the n values of $(\partial Y_i/\partial C)$ using equation (51).

14. We news colculate the n values of (6 7/67 1(oals)) by differentiating the analytical expression for 7 totes.

11 We next calculate the o values of (3'7/3438), evaluated at y₁(cald) which is obtained from the analytical expression for F. 16. We next calculate the n values of (3²2/3430), evaluated at Y₁(cald), this obtained from the solytical expression for F.

17. We next calculate the to values of (5 F/383C), evaluated at Vi(calc), which is contained from the analytical expression for F.

id. We neve calculate the o values of (3 7/3) (calc) 50 which is obtained from the analytical expression for F.

19. We maxt calculate the n values of (5"F/6v (calc) 63) which is obtained from the anglution terpression for F.

20. We mean valoriant the a values of (3 2/3y ((ualc) 30) which is obtained from the analytical aspresaton for F.

21. We taxt fulculate the n values of (3Y,/3A) wing squation (49).

22. We naxt calculate the z values of (31/33) using equation:

23. We next-televiste the n values of (37,/30) using equation

24. We next calculate the n values of $(\partial^2 Y_i / \partial A^2)$ using equation (58).

25. We next calculate the n values of $(\partial^2 Y_i / \partial B^2)$ using equation (59).

26. We next calculate the n values of $(\partial^2 Y_i / \partial C^2)$ using equation (60).

27. We next calculate the n values of $(\partial^2 Y_i / \partial A \partial B)$ using equation (67).

28. We next calculate the n values of $(\partial^2 Y_i / \partial A \partial C)$ using equation (68).

29. We next calculate the n values of $(\partial^2 Y_i / \partial B \partial C)$ using equation (69).

30. We next calculate a_1 from equation (19).

31. We next calculate $a_2 = b_1$ from equation (20).

32. We next calculate $a_3 = c_1$ from equation (21).

33. We next calculate b, from equation (22).

34. We next calculate $b_3 = c_2$ from equation (23).

35. We next calculate c₃ from equation (24).

36. We next calculate m₁ from equation (25).

37. We next calculate m₂ from equation (26).

38. We next calculate m₃ from equation (27).

39. We next calculate D₁ from equation (31).

40. We next calculate D₂ from equation (32).

41. We next calculate D_3 from equation (33).

42. We next calculate D_4 from equation (34).

43. We next calculate D_5 from equation (35).

44. We next calculate D_6 from equation (36).

45. We next calculate D_7 from equation (37).

46. We next calculate D_8 from equation (38).

47. We next calculate D_9 from equation (39).

48. We next calculate D from equation (40).

49. We next calculate AA from equation (28).

50. We next calculate $\triangle B$ from equation (29).

51. We next calculate $\triangle C$ from equation (30).

52. We now return to step 1 and calculate $A_0 + \Delta A$, where A_0 is the value originally assumed in step 1.

53. We next calculate $B_0 + \Delta B$, where B_0 is the value originally assumed in step 1.

54. We next calculate $C_0 + \Delta C$, where C_0 is the value originally assumed in step 1.

55. Using $(A_0 + \Delta A)$, $(B_0 + \Delta B)$, and $(C_0 + \Delta C)$ as new values of A, B, and C, we proceed to step 2 and repeat steps 2 through 6.

56. At this point, we compare the value of R, the sum of the weighted squares of the residuals, with the initially calculated value of R. If it is smaller, we proceed to step 7 and repeat steps 7 through 55. We continue to repeat the iteration until $m_1 = m_2 = m_3 = 0$ within some predetermined small quantity. Our final values of A, B, and C are our least squares solution for these quantities.

	mal saupa			

52. We now return to step 1 and calculate $A_0 + \Delta A_1$ where A_0 is the value originally assumed in step 1

53. We next calculate B + 48, where B is the value originally

54. We next celculate C + 55, where C is the value originally assumed in army 1.

55. Saints ($A_0 + \Delta A$), ($B_0 + \Delta B$), and ($C_0 + \Delta C$) as new values of A, B, and C, we proceed to step 2 and repeat steps 2 through b.

35. At this point, we compare the value of X, the sum of the ealghted squeres of the residuals, with the initially calculated value of R. If it is muller, we proteed to acep 7 and repeat stape 7 through 55. We continue to repeat the iteration until $m_1 = m_2 = m_3 = 0$ within some predetermined small quantity. Our final values of A, B, and C are our issue squares solution for these quanticles. If in step 56 the sum of the weighted squares of the residuals, R, is larger than the initial value of R, the problem is diverging, and at this point, a technique must be used that will lead to convergence. One method that will lead to a smaller sum of R is the negative gradient or the method of steepest descent. The components of a vector in the direction of the negative gradient are given by

$$-\left(\frac{\partial R}{\partial A}\right)^{\circ}$$
; $-\left(\frac{\partial R}{\partial B}\right)^{\circ}$; and $-\left(\frac{\partial R}{\partial C}\right)^{\circ}$

Thus, if we take

$$\Delta A = -k \left(\frac{\partial R}{\partial A}\right)^{\circ}$$
(70)

$$\Delta B = -k \left(\frac{\partial R}{\partial B}\right)^{\circ}$$
(71)

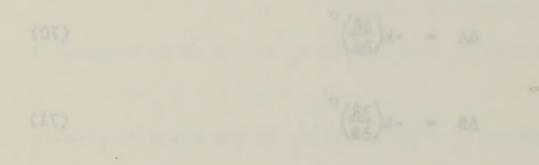
$$\Delta C = -k \left(\frac{\partial R}{\partial C}\right)^{\circ}$$
(72)

where k is a positive constant, we will move in the direction of the negative gradient; k has been called the size of the step. We determine the size of the step in the following way. We expand R in a Taylor's series expansion, retaining terms through the second derivatives. Thus,

If in step 55 the sam of the weighted squares of the residuals, R, is larger than the initial value of R, the problem is diverging. and at this point, a rechnique sust be used that will lead to convergence. One mathod that will lead to a smaller sum of R is the negative gradient or the method of stappent descent. The components of a vector in the direction of the negative gradient are given by

$$\binom{46}{56}$$
 - bas $\binom{66}{56}$ - $\binom{66}{56}$ - $\binom{46}{56}$ -

Thus, if we cake



$$\Delta C = -16 \left(\frac{26}{3C} \right) = -26$$

where k is a positive constant, we will nove in the direction of the megative gradiant; k has been called the size of the step. We determine the size of the step in the following way. We expand 2 in a laylor's suries expansion, retaining terms through the second derivatives. Thus,

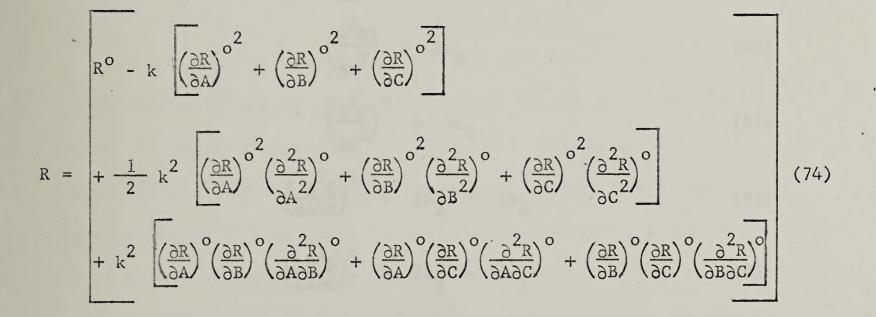
$$R = \left(\frac{\partial R}{\partial A}\right)^{\circ} \Delta A + \left(\frac{\partial R}{\partial B}\right)^{\circ} \Delta B + \left(\frac{\partial R}{\partial C}\right)^{\circ} \Delta C$$

$$R = \left(\frac{1}{2}\left(\frac{\partial^{2} R}{\partial A^{2}}\right)^{\circ} (\Delta A)^{2} + \left(\frac{\partial^{2} R}{\partial B^{2}}\right)^{\circ} (\Delta B)^{2} + \left(\frac{\partial^{2} R}{\partial C^{2}}\right)^{\circ} (\Delta C)^{2}\right)$$

$$\left(\frac{\partial^{2} R}{\partial A \partial B}\right)^{\circ} \Delta A \Delta B + \left(\frac{\partial^{2} R}{\partial A \partial C}\right)^{\circ} \Delta A \Delta C + \left(\frac{\partial^{2} R}{\partial B \partial C}\right)^{\circ} \Delta B \Delta C$$

$$(73)$$

We now substitute in equation (73) for ΔA , ΔB , and ΔC from equations (70), (71), and (72). The result is



We now differentiate equation (74) with regard to k, set the derivative equal to zero, and solve for k. The result is

$$k = \frac{\left(\frac{\partial R}{\partial A}\right)^{o^{2}} + \left(\frac{\partial R}{\partial B}\right)^{o^{2}} + \left(\frac{\partial R}{\partial C}\right)^{o^{2}} + \left(\frac{\partial R}{\partial C}\right)^{o^{2}}}{\left(\frac{\partial R}{\partial A}\right)^{o}\left(\frac{\partial^{2} R}{\partial A^{2}}\right)^{o} + \left(\frac{\partial R}{\partial B}\right)^{o^{2}}\left(\frac{\partial^{2} R}{\partial C^{2}}\right)^{o} + \left(\frac{\partial R}{\partial C}\right)^{o^{2}}\left(\frac{\partial^{2} R}{\partial C^{2}}\right)^{o}} + 2\left(\frac{\partial R}{\partial A}\right)^{o}\left(\frac{\partial R}{\partial C}\right)^{o}\left(\frac{\partial^{2} R}{\partial A \partial C}\right)^{o} + 2\left(\frac{\partial R}{\partial B}\right)^{o}\left(\frac{\partial R}{\partial C}\right)^{o}\left(\frac{\partial^{2} R}{\partial A \partial C}\right)^{o} + 2\left(\frac{\partial R}{\partial B}\right)^{o}\left(\frac{\partial R}{\partial C}\right)^{o}\left(\frac{\partial R}{\partial C}\right)^{o}\left(\frac{\partial$$

We good subjectivity is separations (23) ins in. As, and in tree aquetions

he are collerentiate equation (24) with repart to by and the

From equation (5) and equations (19) - (27), it is possible to show that

$$\left(\frac{\partial R}{\partial A}\right)^{O} = -2m_{1} \tag{76}$$

$$\left(\frac{\partial R}{\partial B}\right)^{\circ} = -2m_2 \tag{77}$$

$$\left(\frac{\partial R}{\partial C}\right)^{\circ} = -2m_{3}$$
(78)

$$\left(\frac{\partial^2 R}{\partial A^2}\right)^{\circ} = 2a_1 \tag{79}$$

$$\left(\frac{\partial^2 R}{\partial B^2}\right) = 2b_2 \tag{80}$$

$$\left(\frac{\partial^2 R}{\partial C^2}\right)^{\circ} = 2c_3 \tag{81}$$

$$\left(\frac{\partial^2 R}{\partial A \partial B}\right)^{\circ} = 2a_2 = 2b_1$$
 (82)

$$\left(\frac{\partial^2 R}{\partial A \partial C}\right)^{\circ} = 2a_3 = 2c_1$$
(83)

$$\left(\frac{\partial^2 R}{\partial B \partial C}\right)^{\circ} = 2b_3 = 2c_2$$
(84)

Substituting equations (76) - (84) into equation (75), we have

bridd sublation is In-

$$k = \frac{m_1^2 + m_2^2 + m_3^2}{\left[2a_1m_1^2 + 2b_2m_2^2 + 2c_3m_3^2 + 4a_2m_1m_2 + 4a_3m_1m_3 + 4b_3m_2m_3\right]}$$
(85)

From equation (5) and equations (19) - (27), it is possible

to show that

$$\left(\frac{2\pi}{2\lambda}\right)^{\circ} = -2m_{1} \tag{76}$$

$$\left(\frac{\partial R}{\partial B}\right) = -2m_2 \tag{77}$$

$$\left(\frac{2\pi}{3\pi}\right)^{0} = -2\pi_{3} \tag{78}$$

$$\left(\frac{3^{\frac{5}{2}}}{3a^2}\right)^{\circ} = 2a_1$$
 (29)

$$\left(\frac{3\frac{2\pi}{3}}{38}\right) = 2b_2$$
 (80)

$$\binom{9.16}{30^2} = \frac{2c_3}{2c_3}$$
 (81)

$$\left(\frac{3^{+}R}{3A3R}\right)^{\circ} = 2^{+}2^{-} = 2^{\circ}1$$
 (82)

$$\left(\frac{3^{2} \pi}{3 A B C}\right)^{\circ} = 2a_{3} = 2a_{1} - ... (83)$$

$$\left(\frac{3^{2} \pi}{3 B B C}\right)^{\circ} = 2b_{2} = 2a_{3} ... (84)$$

Substituting equations (76) - (84) into equation (75), we have

$$= \frac{m_1^2 + m_2^2 + m_3^2}{2a_1m_1^2 + 2b_2m_2^2 + 2c_3m_3^2}$$
(85)
$$= \frac{44a_2m_1m_2 + 4a_3m_1m_3 + 4b_3m_2m_3}{4b_3m_2m_3}$$

3.2

We see, therefore, that if the Newton-Raphson method is used in setting up the normal equations, the size of the step to be taken in the direction of the negative gradient can be evaluated very simply from the coefficients appearing in the normal equations, provided the calculation of k leads to a positive quantity. If equation (85) leads to a negative quantity, this means that the curvature of the surface is such that the trial solution is near a maximum and not a minimum. Under these conditions, the negative value of k must be ignored and positive values of k explored on a trial basis.

Of course, the same formal calculation can be made if the Gauss-Newton method is used to set up the normal equations. However, if one is in a region of divergence, this means that the trial solution is far from the true answer. Under these conditions, the residuals will be large and the second summation in the a's, b's, and c's, involving the second derivative terms, will be of importance compared to the first term in the summation. We therefore believe that if it is necessary to use the negative gradient method, it is better to use the Newton-Raphson method in setting up the normal equations and in calculating the size of the step.

If our problem is diverging after the first iteration, we calculate ΔA , ΔB , and ΔC from

ΔA	=	2km1	(86)
∆B	=	2km2	(87)
∆C	=	2km ₂	(88)

We see, therefore, that if the Newton-Haphson method is used in satting up the normal equations, the size of the step to be taken in the direction of the negative gradient can be evaluated very simply from the coefficients appoaring in the normal equations, provided the calculation of k leads to a positive quantity. If equation (85) leads to a negative quantity, this means that the aurvature of the surface is such that the trial solution is near a maximum and not a minimum. Under these conditions, the negative value of k must be ignored and positive values of k explored on a trial basis.

Of course, the same formal calculation can be made if the Gauss-Rewton mathod is used to set up the normal equations. Nowever, if one is in a region of divergence, this means that the trial colution is far from the true answer. Under these conditions, the residuals will be large and the second summation in the a's, b's, and o's, involving the second darivative terms, will be of importance compared to the first term in the summation. We therenethed, it is better to use the Newton-Raphson method in setting of the normal equations and in calculating the size of the setting

If our problem is diverging siler the first iteration, we calculate 24, 23, and 20 from

SE.

with k calculated from equation (85). Using $A_0 + \Delta A$, $B_0 + \Delta B$, and $C_0 + \Delta C$ as new values of our undetermined constants, A, B, and C, we then return to step 2 of the iteration. For each new value of A, B, and C, we solve the normal equations and calculate a new value of R. If we are diverging, we continue with the negative gradient method until the region of convergence is reached. As soon as this happens, we drop the negative gradient method and iterate by solving the normal equations for ΔA , ΔB , and ΔC . A scheme such as this should always lead to convergence.

Although the above scheme should always lead to convergence, the negative gradient method may be tediously slow in entering the region of convergence for the solution of the normal equations. Under these conditions, other schemes can be tried which may enter the region of convergence more rapidly than the negative gradient method.

Some of these methods are: (1) the Hartley (3) method; (2) a modification of the Hartley method due to Strand, Kohl, and Bonham (8); and (3) the method of Marquardt (4).

We do not have enough experience to judge the relative merits of these various methods. In our applications so far, we have not been troubled by lack of convergence.

CALCULATION OF VARIANCES AND COVARIANCES

With the value of our constants determined, the remaining questions to be answered are: (1) What are the variances and covariances of the constants evaluated? (2) What are the variances which a control the sequences of our understand constants, A, B, and C, + M, as now values of our understanted constants, A, B, and C, we then return to stap 2 of the literation. For each per value of A, D, and C, we solve the normal equations and calculate a one value of B. If we are alverging, we contribute and calculate the scale as raise hereads and if the return sectors are as a second as the start for a solve the second and such the regstart for a solve of the return stations and calculate a second as the bapping, we contribute state the second bas second as the bapping, we contribute stations and and istance of a solve of the return stations and a bas acces as the bapping, we constitue stations would be accessed by solve of a second squartened to a solve of a statement of a sheet state access appreciate to a solve be a solve of the second state of the second and the solve of a statement would be a sheet state accessed of the constants and the second state and a sheet state access and the second statement of the second state access a state of the second statement of the second state access a state of the second statement of the second state accessed of the second statement of the

the angustes produce another to the second and be recipied with a to the enceting the regard of convergence for the solution of the cornel equalions. Under these conditients, where schedel can be tried which any enter the region of corners are more republy than the month of the product

Star of annue esthods are: (2) the vesslay (2) settod((2) a southing on at the Barting method dwe to Schami, Kuhi. and Bonhan (2); and (3) the method of Marquerds (8).

We do not have enough experience to judge the relative merica of these various marneds. In our applications so far, we have not here troubled by lack of convergence.

CALCULATION OF VARIATION AND OUVAILANCES

With the value of our constants determined, the remaining securions to be answered are: (1) what are the variances and coversances of the constants evaluated; (2) What are the variances

of the calculated y_i's and of any other calculated y that reduces F to zero?

To answer these questions, we apply the law for the propagation of errors. This law states that if we have a quantity or function, Q, that is a function of the independent quantities, y_1 , y_2 , y_3 , ..., then the variance of Q is given by

$$s_{\mathbf{Q}}^{2} = \sum_{i=1}^{n} \left(\frac{\partial Q}{\partial y_{i}(o)}\right)^{2} s_{y_{i}(o)}^{2}$$
(89)

where S_Q^2 is the variance of Q, and $S_{y_i(o)}^2$ is the variance of $y_{i(o)}$.

The value of the constant A that we have evaluated is a function of all of the observed x_i 's and of all of the observed y_i 's. Since we have assumed there are no random errors in the x_i 's, the variances of the x_i 's are zero. Then the expression for the variance of A is given by the equation

$$s_{A}^{2} = \sum_{i=1}^{n} \left(\frac{\partial A}{\partial y_{i}(o)}\right)^{2} s_{y_{i}(o)}^{2}$$
(90)

and there will be an equation similar to equation (90) for evaluating the variance of B and of C.

To evaluate equation (90), we must evaluate $(\partial A/\partial y_{i(0)})$ for each $y_{i(0)}$, multiply this quantity by S , square the product, $y_{i(0)}$ and then sum the product over all of the observed y_i 's.

Now we have a total of n pairs of the observed quantities x_i , y_i . Then our constants to be evaluated are determined by the

of the salculated y's and of any other calcolated y that reduces

To ensure these questions, we apply the las for the propagation of errors. Into low status that it we have a quanticy or function, Q. that is a function of the independent quanticles, Y. Fy. Sy. ... then the variance of Q is given by

$$s_{q}^{2} = \sum_{1=1}^{7} \left(\frac{20}{3y_{1}(0)} \right)^{2} s_{y_{1}(0)}^{2}$$
 (83)

where S_0^2 is the variance of 0, and S_{-1}^2 is the variance of $Y_1(a)$. The value of the constant A that we have evaluated is a function of all of the observed x_1^2 's and of all of the observed $Y_1's$. Since we have essented there are no random errors in the $x_1's$, the variances of the $x_1's$ are zero. Then the expression for the variance of A is given by the equation

$$\sum_{AA}^{A} = \sum_{i=1}^{n} \left(\frac{3A}{(a)} \right)^2 \sum_{i=1}^{n} \left(\frac{3A}{(a)} \right)^2 \sum_{i=1}^{n} \left(\frac{3A}{(a)} \right)^2 \left(\frac{3A}{(a)} \right)^2$$

and Linere will be an equation similar to equation (90) for eval-

To dvaluate equation (90), we must evaluate (64/891(0)) for each fi(s), multiply shis quantity by 8, , square the product and then sum the product over all of the shastwed y,'s.

Now we have a total of n pairs of the observed quantities N

solutions of equations (6), (7), and (8). Now suppose we change one of the y_i 's, $y_{2(o)}$ say, to $y_{2(o)} + \Delta y_2$. Then on solving equations (6), (7), and (8), we would get new values of (A + Δ A), (B + Δ B), and (C + Δ C) for our constants. Then we can calculate

$$\frac{\partial A}{\partial y_2(o)} = \frac{\Delta A}{\Delta y_2}$$
(91)

$$\frac{\partial B}{\partial y_{2(0)}} = \frac{\Delta B}{\Delta y_{2}}$$
(92)

$$\frac{\partial C}{\partial y_2(o)} = \frac{\Delta C}{\Delta y_2}$$
(93)

This means that when $y_{2(o)}$ is changed by a small amount, equations (6), (7), and (8) must still hold exactly. Mathematically, this means that

$$\frac{\partial}{\partial y_{i(0)}} \left(\frac{\partial R}{\partial A} \right)_{x_{i}, y_{i(0)}, B, C} = 0$$
(94)

$$\frac{\partial}{\partial y_{i(0)}} \left(\frac{\partial R}{\partial B} \right)_{x_{i}, y_{i(0)}, A, C} = 0$$
(95)

$$\frac{\partial}{\partial y_{i(0)}} \left(\frac{\partial R}{\partial C} \right)_{x_{i}, y_{i(0)}, A, B} = 0$$
(96)

All of the Y_i 's are explicit functions of the $y_{i(0)}$'s, the x_i 's, and the constants A, B, and C. In the application of equations (94),

and at the string the sales of the sales and (d). (T), and (d). The suppose at change and at the string the sales and sale at sales at the sale attend (d), (T), and (R), an would get an estimates the the sale (R, + 45), and (C + 45) for our sounds sales at the test of the

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All of the "," a are explicit to pretime of the Face, " a, the Face and the managements of the second (94).

(95), and (96), the derivatives $(\partial R/\partial A)_{x_i,y_i(o)}, B, C'$ $(\partial R/\partial B)_{x_i,y_i(o)}, A, C, and (\partial R/\partial C)_{x_i,y_i(o)}, A, B are to be considered$ $functions of all of the <math>y_{i(o)}$'s and of the constants evaluated, with A, B, and C being functions of all of the $y_{i(o)}$'s. Under these conditions,

 $\frac{\partial}{\partial y_{i(0)}} \left(\frac{\partial R}{\partial A} \right)_{x_{i}, y_{i(0)}, B, C} x_{i}, y_{j \neq i}$

 $\left(\frac{\partial^2 R}{\partial A^2}\right)_{x_i,y_i(o)},B,C}\left(\frac{\partial A}{\partial y_i(o)}\right)_{y_i\neq i}$ $+ \left(\frac{\partial^{2} R}{\partial B \partial A}\right)_{x_{i}, y_{i(0)}, C} \left(\frac{\partial B}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + \left(\frac{\partial^{2} R}{\partial C \partial A}\right)_{x_{i}, y_{i(0)}, B} \left(\frac{\partial C}{\partial y_{i(0)}}\right)_{y_{j\neq i}}$ (97)+ $\left[\frac{\partial \left(\frac{\partial R}{\partial A}\right)_{x_{i}, y_{i(0)}, B, C}}{\partial y_{i(0)}}\right]_{x_{i}, y_{j \neq i}, A, B, C}$ $\left(\frac{\partial^2 R}{\partial B^2}\right)_{x_i, y_i(0)}, A, C\left(\frac{\partial B}{\partial y_i(0)}\right)_{j \neq i}$ $+ \left(\frac{\partial^{2} R}{\partial A \partial B}\right)_{x_{i}, y_{i}(o)}, C\left(\frac{\partial A}{\partial y_{i}(o)}\right)_{i \neq i}$ $= + \left(\frac{\partial^{2} R}{\partial C \partial B}\right)_{x_{i}, y_{i}(o)}, A \left(\frac{\partial C}{\partial y_{i}(o)}\right)_{y_{j\neq i}}$ $+ \left[\frac{\partial \left(\frac{\partial R}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C}{\partial y_{i}(o)}\right]_{x_{i}, y_{j\neq i}, A, B, C}$ (98)

$$\frac{\partial}{\partial y_{i(o)}} \left(\frac{\partial R}{\partial B} \right)_{x_{i}, y_{i(o)}, A, C}_{x_{i}, y_{j \neq i}}$$

(35), and (30), the derivatives $(3R/2A)_{x_1,y_1(q)}$. B,C' (3R/3N) $(3R/3N)_{x_1,y_1(q)}$, A,C' and $(3R/3C)_{x_1,y_1(q)}$, A,B are to be considered functions of all of the $y_1(q)$'s and of the constants evaluated, with A, S, and C being functions of all of the $y_1(q)$'s. Under these

- (<u>-26</u>) 142 (<u>0)1 (6</u>) A (0)1 (<u>1)</u> (<u>65)</u> (<u>65)</u>

 $\left(\frac{\partial^{2} R}{\partial C^{2}}\right)_{x_{i}, y_{i(o)}, A, B} \left(\frac{\partial C}{\partial y_{i(o)}}\right)_{y_{j \neq i}}$ $+ \left(\frac{\partial^{2} R}{\partial A \partial C}\right)_{x_{i}, y_{i}(o)}, B^{\left(\frac{\partial A}{\partial y_{i}(o)}\right)}_{y_{j \neq i}}$ $\frac{\partial}{\partial y_{i(0)}} \left(\frac{\partial R}{\partial C} \right)_{x_{i}, y_{i(0)}, A, B}$ + $\left(\frac{\partial^2 R}{\partial B \partial C}\right)_{x_i, y_i(0)}, \left(\frac{\partial B}{\partial y_i(0)}\right)_{j \neq i}$ (99)= 0 $+ \frac{\partial \left(\frac{\partial R}{\partial C}\right)_{x_{i}, y_{i(0)}, A, B}}{\partial y_{i(0)}}_{x_{i}, y_{i\neq i}, A, B, C}$

Equations (97), (98), and (99) contain terms involving the derivative of each constant with respect to $y_{i(0)}$ and can be solved by elementary algebra for the derivatives of the constants with respect to $y_{i(0)}$. These derivatives are then to be multiplied by $s_{j(0)}$, the product squared, and then the squared product is to be summed over all of the observed $y_{i(0)}$'s. These sums give us the variance of each constant evaluated.

Differentiating R, given by equation (5), by the constants A, B, and C keeping x_i and $y_{i(o)}$ constant, we have

$$\left(\frac{\partial R}{\partial A}\right)_{x_{i},y_{i}(o)},B,C = 2\sum_{i=1}^{n} w_{y_{i}(o)} Y_{i}\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C$$
(100)

Equations (37), (38), and (39) contain terms involving the derivatives of each constant with respect to $y_{1(0)}$ and can be solved by elementary sigebra for the derivatives of the constants with respect to $y_{1(0)}$. These derivatives are then to be miltiplied by $\frac{2}{3}$, the product equared, and then the squared product is to be summed over all of the observed $y_{1(0)}$'s. These sum give us the squared product is to be summed over all of the observed $y_{1(0)}$'s.

Differentiating R. given by equation (3), by the constants A.

$$\left(\frac{\partial R}{\partial B}\right)_{x_{i},y_{i(0)},A,C} = 2 \sum_{i=1}^{n} w_{y_{i(0)}} Y_{i} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i(0)},A,C}$$
(101)

$$\left(\frac{\partial R}{\partial C}\right)_{x_{i},y_{i}(o),A,B} = 2 \sum_{i=1}^{n} w_{y_{i}(o)} Y_{i} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o),A,B}$$
(102)

Differentiating equation (100) with regard to each constant, we have

$$\left(\frac{\partial^{2} R}{\partial A^{2}}\right)_{x_{i},y_{i}(o)},B,C = 2 \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial A}\right)^{2}_{x_{i},y_{i}(o)},B,C + Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial A^{2}}\right)_{x_{i},y_{i}(o)},B,C \right]$$
(103)

$$\begin{bmatrix} \frac{\partial}{\partial B} \begin{pmatrix} \frac{\partial R}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(0)}, B, C \\ x_{i}, y_{i}(0) \end{pmatrix}_{x_{i}, y_{i}(0)}, A, C = \begin{bmatrix} 2 \sum_{i=1}^{n} w_{y_{i}(0)} \begin{pmatrix} \frac{\partial Y_{i}}{\partial B} \end{pmatrix}_{x_{i}, y_{i}(0)}, A, C \begin{pmatrix} \frac{\partial Y_{i}}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(0)}, B, C \\ + 2 \sum_{i=1}^{n} w_{y_{i}(0)} Y_{i} \begin{bmatrix} \frac{\partial}{\partial B} \begin{pmatrix} \frac{\partial Y_{i}}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(0)}, B, C \\ \frac{\partial}{\partial B} \begin{pmatrix} \frac{\partial Y_{i}}{\partial A} \end{pmatrix}_{x_{i}, y_{i}(0)}, B, C \end{bmatrix}$$
(104)

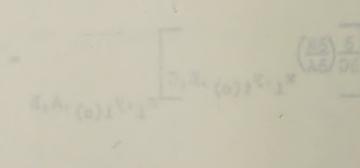
$$\begin{bmatrix}
\frac{\partial}{\partial C} \left(\frac{\partial R}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \\
x_{i}, y_{i}(o), B, C \\
x_{i}, y_{i}(o), A, B
\end{bmatrix} = \begin{cases}
2 \sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, A, B \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \\
+ 2 \sum_{i=1}^{n} w_{y_{i}(o)} Y_{i} \left[\frac{\partial}{\partial C} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \\
+ 2 \sum_{i=1}^{n} w_{y_{i}(o)} Y_{i} \left[\frac{\partial}{\partial C} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \\
x_{i}, y_{i}(o), A, B
\end{bmatrix} (105)$$

$$\frac{36}{26} \left| x_{1} \cdot x_{1}(o) \cdot A_{1} \right|^{2} = \sum_{l=1}^{n} \left| x_{2}(o) \cdot x_{l} \right|^{2} \left(\frac{37}{38} \right) \left| x_{2} \cdot x_{1} \cdot x_{1}(o) \cdot A_{1} \right|^{2}$$
(101)

Differenciating equation (100) with tegard to each constant, we have

$$\left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} + \left[\left(\frac{1}{2}\right)^{2}\right]^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2}\right]^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left(\frac{1}{2}\right)^{2} = \left[\left(\frac{1}{2}\right)^{2} = \left(\frac{1}{2}\right)^{2} = \left(\frac{1}{2}\right)^{2}$$

$$= \sum_{i=1}^{n} x_{i(0)} (a_{i}^{2})_{a_{i}} ($$



Differentiating equation (100) with regard to a single $y_{i(o)}$, keeping A, B, and C constant, we have

$$\frac{\partial \left(\frac{\partial R}{\partial A}\right)_{x_{i},y_{i}(o)},B,C}{\partial y_{i}(o)} = 2 + w_{y_{i}(o)} Y_{i}\left(\frac{\partial Y_{i}}{\partial y_{i}(o)}\right)_{x_{i},y_{j\neq i},A,B,C} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C + w_{y_{i}(o)} Y_{i}\left(\frac{\partial Y_{i}}{\partial y_{i}(o)}\right)_{x_{i},y_{i}(o)},B,C + w_{y_{i}(o)} Y_{i}\left(\frac{\partial Y_{i}}{\partial y_{i}(o)}\right)_{x_{i}(o)},B,C + w_{y_{i}(o)} Y_{i}\left(\frac{\partial Y_{i}}{\partial y_{i}(o)}\right$$

The right-hand side of equation (106) reduces to a single term, since a single y_{i(o)} only appears in one term in the summation. Now from equation (4)

$$Y_{i} = y_{i(0)} - y_{i(calc)}$$
(4)

so that

$$\left(\frac{\partial Y_{i}}{\partial y_{i(0)}}\right)_{x_{i}, y_{j \neq i}, A, B, C} = 1$$
(107)

and it follows that

$$\frac{\partial}{\partial A} \left(\frac{\partial Y_{i}}{\partial y_{i(0)}} \right)_{x_{i}, y_{j \neq i}, A, B, C} = 0$$
(108)

Substituting equations (107) and (108) into equation (106), we have

Differentiating equation (100) with regard to a single fi(c) /

Resping A, B. and C constant, We have

 $= \frac{1}{2} \left[\frac{1}{2$

The right-hard side of equation (104) reduces to a single term, since a single yi(a) caly appears in one term in the summation. New from equation (4)

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substituting equations (107) and (106) into equation (106), we have

$$\frac{\partial \left(\frac{\partial R}{\partial A}\right)_{x_{i}, y_{i(0)}, B, C}}{\partial y_{i(0)}} = 2w_{y_{i(0)}} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i(0)}, B, C}$$
(109)

Substituting equations (103), (104), (105), and (109) in equation (97), we get

$$\left(\frac{\partial A}{\partial y_{i}(o)}\right)_{y_{j\neq i}} \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial A}\right)^{2}_{x_{i},y_{i}(o)}, B, C + Y_{i}\left(\frac{\partial^{2}Y_{i}}{\partial A^{2}}\right)_{x_{i},y_{i}(o)}, B, C\right] + \left(\frac{\partial^{2}Y_{i}}{\partial A^{2}}\right)_{x_{i},y_{i}(o)}, B, C\right] + \left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{y_{j\neq i}} \left[\sum_{i=1}^{n} w_{y_{i}(o)}\left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(o)}, A, C\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right] + \sum_{i=1}^{n} w_{y_{i}(o)}Y_{i}\left[\frac{\partial}{\partial B}\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right]_{x_{i},y_{i}(o)}, A, C\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right] + \left(\frac{\partial^{2}Y_{i}}{\partial y_{i}(o)}\right)_{y_{j\neq i}} \left[\sum_{i=1}^{n} w_{y_{i}(o)}\left(\frac{\partial^{2}Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}, A, B\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right]_{x_{i},y_{i}(o)}, B, C\right] + w_{y_{i}(o)}\left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right]_{x_{i},y_{i}(o)}, A, B\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, A, B\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right] + w_{y_{i}(o)}\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, B, C\right]_{x_{i},y_{i}(o)}, A, B\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}, A, B\left(\frac{\partial^{2}Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}$$

.10)

Subscituting squations (103), (104), (103), and (109) in squation

2. A. (0) 2 K. 1 2. B. (0) 2 K. 2 (AS) - Elix (0) 2 K. 3 + 242 (0) 2 KS)

(011)

Upon differentiating equations (101) and (102) with regard to a single $y_{i(0)}^{}$, we obtain two expressions similar to equation (110). We will write equation (110) and the two other equations as

$$a_{1}\left(\frac{\partial A}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + b_{1}\left(\frac{\partial B}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + c_{1}\left(\frac{\partial C}{\partial y_{i(0)}}\right)_{y_{j\neq i}} = n_{1} \quad (111)$$

$$a_{2}\left(\frac{\partial A}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + b_{2}\left(\frac{\partial B}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + c_{2}\left(\frac{\partial C}{\partial y_{i(0)}}\right)_{y_{j\neq i}} = n_{2} \quad (112)$$

$$a_{3}\left(\frac{\partial A}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + b_{3}\left(\frac{\partial B}{\partial y_{i(0)}}\right)_{y_{j\neq i}} + c_{3}\left(\frac{\partial C}{\partial y_{i(0)}}\right)_{y_{j\neq i}} = n_{3} \quad (113)$$

where

$$a_{1} = \sum_{i=1}^{n} w_{y_{i}(o)} \left[\left(\frac{\partial Y_{i}}{\partial A} \right)^{2}_{x_{i}, y_{i}(o)}, B, C} + Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial A^{2}} \right)_{x_{i}, y_{i}(o)}, B, C} \right]$$
(114)

$$a_{2} = b_{1} = \begin{vmatrix} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i}, y_{i}(0)}, A, C \left(\frac{\partial Y_{i}}{\partial A} \right)_{x_{i}, y_{i}(0)}, B, C \\ + \sum_{i=1}^{n} w_{y_{i}(0)} Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial B \partial A} \right)_{x_{i}, y_{i}(0)}, C \end{vmatrix}$$
(115)

$$\mathbf{A}_{3} = \mathbf{c}_{1} = \begin{bmatrix} \sum_{i=1}^{n} \mathbf{w}_{y_{i}(o)} \begin{pmatrix} \frac{\partial Y_{i}}{\partial C} \end{pmatrix}_{x_{i}, y_{i}(o)}, \mathbf{A}, \mathbf{B}^{\left(\frac{\partial Y_{i}}{\partial A}\right)}_{x_{i}, y_{i}(o)}, \mathbf{B}, \mathbf{C} \\ + \sum_{i=1}^{n} \mathbf{w}_{y_{i}(o)} Y_{i} \begin{pmatrix} \frac{\partial^{2} Y_{i}}{\partial C \partial A} \end{pmatrix}_{x_{i}, y_{i}(o)}, \mathbf{B} \end{bmatrix}$$
(116)

Upon differentiating equations (101) and (102) with regard to a single Ti(o), we obtain two expressions similar to equation (110). We will write equation (110) and the two other equations as

$$(111) 1^{\alpha} = \left(\frac{36}{10^{3}}\right)_{1^{\alpha}} + \frac{1}{10}\left(\frac{36}{10^{3}}\right)_{1^{\alpha}} + \frac{1}{10}\left(\frac{36}{10^{3}}\right)_{1^{\alpha}} + \frac{1}{10}\left(\frac{16}{10^{3}}\right)_{1^{\alpha}} + \frac{1}{10}\left(\frac{16}{10^{3}$$

$$= \frac{1}{12} = \frac{1}{1$$

$$b_{2} = \sum_{i=1}^{n} w_{y_{i}(0)} \left[\left(\frac{\partial Y_{i}}{\partial B} \right)^{2}_{x_{i}, y_{i}(0), A, C} + Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial B^{2}} \right)_{x_{i}, y_{i}(0), A, C} \right] (117)$$

$$b_{3} = c_{2} = \left[\sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i}, y_{i}(0), A, C} \left(\frac{\partial Y_{i}}{\partial C} \right)_{x_{i}, y_{i}(0), A, B} \right] (118)$$

$$+ \sum_{i=1}^{n} w_{y_{i}(0)} Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial C \partial B} \right)_{x_{i}, y_{i}(0), A}$$

$$e_{3} = \sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C} \right)_{x_{i}, y_{i}(o), A, B}^{2} + Y_{i} \left(\frac{\partial^{2} Y_{i}}{\partial C^{2}} \right)_{x_{i}, y_{i}(o), A, B}$$
(119)

$$n_{1} = -w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C$$
(120)

$$n_{2} = -w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i}, y_{i}(o)}, A, C$$
(121)

$$n_{3} = -w_{y_{i(o)}} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i(o)}, A, B}$$
(122)

Notice that the a's, b's, and c's defined by equations (114) - (119) are of the same form as the a's, b's, and c's defined by

(120)

2 = -w 1(0) (38) 311 (0) A.C

(122)

 $I_{A}A_{1}(o), I_{1,2}^{R} = \left(\frac{1}{26}\right)_{(o),2}^{R} e^{-\frac{1}{2}} e^{2}$

1 . .

Matter that the a's, b's, and d's defined by equations (114). (119) are of the same form as the s's, b's, and c's defined by equations (19) - (24) which appear in our normal equations. The difference between these two definitions is that equations (114) -(119) apply when the least squares solution is obtained while equations (19) - (24) apply to trial solutions. The a's, b's, and c's given by equations (114) - (119) can be considered as the values of the coefficients in the normal equations for the final iteration.

Solving equations (111), (112), and (113) simultaneously for $(\partial A/\partial y_{i(0)})$, $(\partial B/\partial y_{i(0)})$, and $(\partial C/\partial y_{i(0)})$, we get

$$D_{0}\left(\frac{\partial A}{\partial y_{i(0)}}\right) = D_{1}n_{1} + D_{2}n_{2} + D_{3}n_{3}$$
(123)

$$D_{o}\left(\frac{\partial B}{\partial y_{i(o)}}\right) = D_{4}n_{1} + D_{5}n_{2} + D_{6}n_{3}$$
(124)

$$D_{o}\left(\frac{\partial C}{\partial y_{i(o)}}\right) = D_{7}n_{1} + D_{8}n_{2} + D_{9}n_{3}$$
 (125)

where

$$D_1 = b_2 c_3 - b_3 c_2 \tag{126}$$

$$D_2 = b_3 c_1 - b_1 c_3 \tag{127}$$

$$D_3 = b_1 c_2 - b_2 c_1 \tag{128}$$

$$D_4 = a_3 c_2 - a_2 c_3 \qquad (129)$$

$$D_5 = a_1 c_3 - a_3 c_1 \tag{130}$$

aquations (10) - (24) Which appear is out doubt equitions. The definitions between these two dolinitions is that equitions (114) -(114) apply when the laint equates solution is obtained while squations (13) - (24) apply to trial colutions. The s's, b's, and t's press of equitions (114) - (110) of he commidated as the rest and the second fictors is the normal equiviors for the first breast com

(allowing equilibria (iii). (iii), and (iii) similaringe allowing the (allowing), the set

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$$D_6 = a_2 c_1 - a_1 c_2 \tag{131}$$

$$D_7 = a_2 b_3 - a_3 b_2 \tag{132}$$

$$D_8 = a_3 b_1 - a_1 b_3 \tag{133}$$

$$D_9 = a_1 b_2 - a_2 b_1 \tag{134}$$

$$D_{o} = a_{1}D_{1} + a_{2}D_{2} + a_{3}D_{3}$$
(135)

Notice that the D's defined by equations (126) - (135) are of the same form as the D's defined by equations (31) - (40) and, for the last iteration, when the least squares solution is obtained, they will be identical.

Squaring equation (123) and multiplying by $S_{y_i(0)}^2$, we have

$$D_{o}^{2}\left(\frac{\partial A}{\partial y_{i}(o)}\right)^{2} s_{y_{i}(o)}^{2} = \frac{D_{1}^{2} n_{1}^{2} s_{y_{i}(o)}^{2} + D_{2}^{2} n_{2}^{2} s_{y_{i}(o)}^{2} + D_{3}^{2} n_{3}^{2} s_{y_{i}(o)}^{2}}{+ 2 D_{1} D_{2} n_{1} n_{2} s_{y_{i}(o)}^{2} + 2 D_{1} D_{3} n_{1} n_{3} s_{y_{i}(o)}^{2}}$$
(136)
$$+ 2 D_{2} D_{3} n_{2} n_{3} s_{y_{i}(o)}^{2}$$

But from equation (120)

$$n_{1}^{2}s_{y_{i}(0)}^{2} = w_{y_{i}(0)}^{2} \left(\frac{\frac{\partial Y_{i}}{\partial A}}{x_{i},y_{i}(0)}\right)_{x_{i},y_{i}(0)}^{2} s_{y_{i}(0)}^{2}$$
(137)

$$D_{7} = a_{2}b_{3} - a_{3}b_{2}$$
 (132)

$$D_9 = a_1 b_2 - a_2 b_1$$
 (124)

$$D_{0} = a_{1}D_{1} + a_{2}D_{2} + a_{3}D_{3}$$
(135)

Motice that the D's defined by equations (126) - (135) are of the same form as the D's defined by equations (31) - (40) and, for the lest iteration, when the least equares solution is obtained, they will be identical.

Equations equation (123) and multiplying by
$$S_{y(q)}^{2}$$
, we have

$$D_{0}^{2}\left(\frac{\partial L}{\partial \gamma_{L}(\alpha)}\right)^{2} e^{\gamma}_{L}(\alpha) = \frac{D_{1}^{2} D_{1}^{2} e^{\gamma}_{L}^{2}}{D_{1}^{2} D_{1}^{2} P_{1}^{2}} + \frac{D_{2}^{2} D_{2}^{2} e^{\gamma}_{L}^{2}}{D_{1}^{2} D_{2}^{2} B_{1}^{2}} + \frac{D_{2}^{2} D_{2}^{2} B_{2}^{2}}{D_{2}^{2} B_{2}^{2}} + \frac{D_{2}^{2} D_{2}^{2} B_{2}^{2}}{D_{2}^{2}} + \frac{D_{2}^{2} D_{2}^{2} + \frac{D_{2}^{2} D_{2}^{2}}{D_{2}} + \frac{D_{2}^{2} D_{2}^{2}}{D_{2}^{2}} + \frac{D_{2}^{2} D_{2}^{2}}{D_{2}^{2}} + \frac{D_{$$

But from aquation (120)

$$a_{1}^{2}a_{2}^{2}$$
 = $w_{1(0)}^{2}$ = $w_{1(0)}^{2}$ $\left(\frac{\delta Y_{1}}{\delta A}\right)_{g_{1}Y_{1}(0)}^{2}$, B_{1}^{2} (437)

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Now

$$S_{y_{i(0)}}^{2} = \frac{L^{2}}{w_{y_{i(0)}}}$$
 (138)

where L is a constant. Substituting equation (138) in equation (137), we find that

$$n_{1}^{2}S_{y_{i}(o)}^{2} = L^{2} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}^{2},y_{i}(o)}^{2} (139)$$

Similarly, we find that

$$n_{2}^{2}S_{y_{i(0)}}^{2} = L^{2} w_{y_{i(0)}} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i(0)},A,C}^{2}$$
(140)

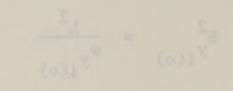
$$n_{3}^{2} S_{y_{i}(o)}^{2} = L^{2} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}^{2} (141)$$

$$n_{1}n_{2}S_{y_{i}(o)}^{2} = L^{2} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(o)},A,C$$
(142)

$$n_{1}n_{3}S_{y_{i}(o)}^{2} = L^{2} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)},B,C} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)},A,B}$$
(143)

$$n_{2}n_{3}S_{y_{i(0)}}^{2} = L^{2} w_{y_{i(0)}} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i(0)},A,C} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i(0)},A,B}$$
(144)

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where L is a constant. Substituting equicion (138) in equation (137). we find that

$$(221)^{2} = L^{2} = \sum_{1 \le i \le 1} (\frac{3x_{i}}{3A})^{2} = \frac{1}{1 \le i \le 1} = \frac{1}{1 \le i \le 1} (139)$$

R

Similarly, we find chat

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$$\frac{32}{2} \frac{3}{2} \frac{3}{2} \frac{3}{2} \chi_{1(0)} = L^{2} \frac{3}{2} \frac{3}{2} \frac{1}{2} \frac{3}{2} \frac{1}{2} \frac{3}{2} \frac{1}{2} \frac{$$

$$a_{3}^{2} g_{11(0)}^{2} = L^{2} u_{11(0)} \left(\frac{\delta Y_{1}}{\delta c}\right)_{X_{1},Y_{1}(0)}^{2} A_{A} D$$
 (141)

$$(161) = L^{2} \psi_{1}(u) \left(\frac{3\chi}{3\chi}\right)_{\pi_{1},\psi_{1}(u)} \left(\frac{3\chi$$

$$(14.1)^{n} = L^{2} = V_{1(0)}^{2} \begin{pmatrix} \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \end{pmatrix}_{\chi_{1}, \gamma_{1}(0)} \begin{pmatrix} \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \end{pmatrix}_{\chi_{1}, \gamma_{1}(0)} \begin{pmatrix} \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \\ \frac{3^{n}}{6^{n}} \end{pmatrix}_{\chi_{1}, \gamma_{1}(0)} \begin{pmatrix} \frac{3^{n}}{6^{n}} \\ \frac{$$

Substituting equations (139), (140), (141), (142), (143), and (144) into equation (136) and then summing over all of the observed y_{i(o)}'s, we have

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$$\begin{cases} D_{1}^{2} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(0)}^{2}, B, C \\ + D_{2}^{2} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, A, C \\ + D_{3}^{2} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ + 2D_{1}D_{2} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(0)}^{2}, B, C \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ + 2D_{1}D_{3} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(0)}^{2}, B, C \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ + 2D_{2}D_{3} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(0)}^{2}, B, C \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ + 2D_{2}D_{3} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, B, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ + 2D_{2}D_{3} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(0)}^{2}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(0)}^{2}, A, B \\ \end{cases}$$

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(145)

(144) into equation (136) and then summing over all of the observed $Y_1(o)$'s, we have

Squaring equation (124), multiplying by $S^2_{y_{i(0)}}$ and then summing, we find that

$$\sum_{i=1}^{n} \left(\frac{\partial B}{\partial y_{i(0)}}\right)^{2} s_{y_{i(0)}}^{2} = s_{B}^{2} = \frac{L^{2}}{D_{0}^{2}} \left(\frac{\partial Y_{i}}{\partial A}\right)^{2} s_{y_{i(0)}} \left(\frac{\partial Y_{i}}{\partial B}\right)^{2} s_{y_{i(0)}} \left(\frac{\partial Y_{i}}{\partial A}\right)^{2} s_{y_{$$

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 $\sum_{i=1}^{n} \left(\frac{1}{2} \left(\frac{1}{2} \left(\frac{1}{2} \right) \right)_{i} \left(\frac{1}{2} \left(\frac{1}{2} \left(\frac{1}{2} \right) \right)_{i} \left(\frac{1}{2} \left(\frac{1}{2} \left(\frac{1}{2} \right) \right)_{i} \left(\frac{1}{2} \left(\frac$

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$${}^{2}s_{y_{i}(o)}^{2} = s_{c}^{2} = \frac{L^{2}}{D_{o}^{2}} \left(\frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{o}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^{2}}{b_{o}^{2}} + \frac{b_{i}^{2}}{b_{o}^{2}} + \frac{b_{i}^{2}}{b_{i}^{2}} + \frac{b_{i}^$$

Similarly, from equation (125), we find that

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T

 $\sum_{i=1}^{n} ($

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 $\left(\frac{\partial y}{\partial y}\right)$ i(o)

(1) x (1) D. B. (0) X 1 x (2X6) (0) x Z PORES +

For the covariances, we find from equations (123), (124), and (125)

n

i=1

 $\frac{\partial A}{\partial y_{i(o)}}$

dy_i

(0)

$$S_{y_{i}(o)}^{2} = S_{AB}^{2} = \frac{L^{2}}{D_{o}^{2}} + \frac{D_{2}D_{5}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)^{2}}{\sum_{i=1}^{n} w_{j_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)^{2}} + \frac{D_{2}D_{5}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)^{2}}{\sum_{i,j}^{n} y_{i(o)}, A, C} + \frac{D_{3}D_{6}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C}\right)^{2}}{\sum_{i=1}^{n} y_{i(o)}, A, B} + (D_{2}D_{4}+D_{1}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C} + (D_{1}D_{6}+D_{3}D_{4})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i}, y_{i}(o)}, B, C \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, B} + (D_{2}D_{6}+D_{3}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, A, B} + (D_{2}D_{6}+D_{3}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, A, B} + (D_{2}D_{6}+D_{3}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, A, B} + (D_{2}D_{6}+D_{3}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, A, B} + (D_{2}D_{6}+D_{3}D_{5})\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i}, y_{i}(o)}, A, C \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i}, y_{i}(o)}, C \left(\frac{\partial Y$$

for the covertances, we find from equations (123); (124), and

(125)

$$= \frac{\left[\sum_{i=1}^{n} \sum_{j=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \frac{D_{2}D_{8} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \frac{D_{3}D_{9} \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial C} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{1}D_{8} + D_{2}D_{7} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{1}D_{9} + D_{3}D_{7} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial A} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \right]_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},y_{i}(0)}^{2} \\ + \left(D_{2}D_{9} + D_{3}D_{8} \right) \sum_{i=1}^{n} w_{y_{i}(0)} \left(\frac{\partial Y_{i}}{\partial B} \right)_{x_{i},$$

 $\sum_{j=1}^{n} \left(\frac{\partial A}{\partial y_{i(0)}}\right) \left(\frac{\partial C}{\partial y_{i(0)}}\right) s_{y_{i(0)}}^{2} = s_{AC}^{2} = \frac{L}{D}$

and finally,

n

 $\sum_{i=1}^{n} \left(\frac{\partial B}{\partial y_{i(o)}} \right)$

$$\frac{\partial C}{\partial y_{i}(o)} s_{y_{i}(o)}^{2} = s_{BC}^{2} = \frac{L^{2}}{D_{o}^{2}} + \frac{D_{5}D_{8}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}^{2} , A, C}{(\partial Y_{i}(o))^{2}} + \frac{D_{6}D_{9}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(o)}^{2} , A, C}{(\partial Y_{i}(o))^{2}} + \frac{D_{6}D_{9}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}^{2} , A, B}{(\partial Q_{a}^{2})_{x_{i},y_{i}(o)}^{2} , B, C} + \frac{D_{6}D_{9}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}^{2} , A, B} + \frac{D_{6}D_{9}\sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}^{2} , B, C} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(o)}^{2} , A, C} + \frac{D_{6}D_{9} + D_{6}D_{7}}{(D_{4}^{2}D_{9} + D_{6}D_{7})} \sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial A}\right)_{x_{i},y_{i}(o)}^{2} , B, C} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}^{2} , A, B} + \frac{D_{5}D_{9} + D_{6}D_{7}}{(D_{5}D_{9} + D_{6}D_{7})} \sum_{i=1}^{n} w_{y_{i}(o)} \left(\frac{\partial Y_{i}}{\partial B}\right)_{x_{i},y_{i}(o)}^{2} , A, C} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}^{2} , A, C} \left(\frac{\partial Y_{i}}{\partial C}\right)_{x_{i},y_{i}(o)}^{2} , A, C} \right)$$

$$(150)$$

and finally,

Equations (145), (146), (147), (148), (149), and (150) allow us to calculate the variances and covariances of the constants evaluated.

Now D_{o} is the value of the determinate of the coefficients that appear in the final normal equations. In a linear problem, it is found that D_{o} may be factored from the right-hand side of equations (145) - (150) so that the expressions for the variances and covariances only involve D_{o} to the first power in the denominator. This is not true for a non-linear problem as can be shown from the exact derivation given above. The present method in use in calculating variances and covariances is therefore only an approximation. How good this approximation is can only be decided by testing it against the mathematically exact calculation given above. Since this is true, we prefer to calculate variances and covariances using the mathematically exact equations given above.

We now answer the question, how do we calculate the variance of a calculated y which reduces the function F to zero for a given x? The answer to this question is obtained as follows: y is a function of x, and through the constants evaluated, is a function of all of the observed $y_{i(0)}$'s and x_i 's. When we apply the law for the propagation of errors, we have

$$s_{y}^{2} = \sum_{i=1}^{n} \left(\frac{\partial y}{\partial y_{i(0)}}\right)^{2} s_{y_{i(0)}}^{2}$$
(151)

Equations (145), (146), (147), (148), (149), and (150) allow us to calculate the veriances and covariances of the constants evalveted.

New D_o is the value of the determinate of the constituients that annear in the final vormal equations to a linear problem, it is fough that D_o may be factored from the right-hand side of equations (145) - (150) so that the expressions for the variances and coverlances only involve D_o to the first power in the denominator. This is not true for a non-linear problem as can be shown from the exact derivation given above. The present method in use in calculating yariances and covariances is therefore only an approximation. How the methematically gract calculation given above, Since this is true, we prefer to calculate variances and covariants in constituted by testing the constituted by each solar the second the second covariances using the second solar provides the second the second the second state of the second the second solar the methematically gract calculation given above. Since this is

We now answer the question, how do we calculate the variance of a calculated y which reduces the function F to zero for a given x? The answer to this question is obtained as follows: y is a function of x, and through the constants evaluated, is a function of all of the elserved $y_{1(0)}$'s and x_1 's. When we apply the law for the groupszelog of errors, we have

We calculate $\left(\frac{\partial y}{\partial y_{i(0)}}\right)_{\substack{y \neq i, x, x \\ j \neq i}}$ from equation (1). Differentiating equation (1), we have

$$\begin{pmatrix} \frac{\partial F}{\partial A} \end{pmatrix}_{x,y,B,C} \begin{pmatrix} \frac{\partial A}{\partial y_{i(0)}} \end{pmatrix}_{j\neq i} , x_{i}^{x} + \begin{pmatrix} \frac{\partial F}{\partial B} \end{pmatrix}_{x,y,A,C} \begin{pmatrix} \frac{\partial B}{\partial y_{i(0)}} \end{pmatrix}_{j\neq i} , x_{i}^{x}$$

$$= 0 \quad (152)$$

$$+ \begin{pmatrix} \frac{\partial F}{\partial C} \end{pmatrix}_{x,y,A,B} \begin{pmatrix} \frac{\partial C}{\partial y_{i(0)}} \end{pmatrix}_{j\neq i} , x_{i}^{x} + \begin{pmatrix} \frac{\partial F}{\partial y} \end{pmatrix}_{x,A,B,C} \begin{pmatrix} \frac{\partial y}{\partial y_{i(0)}} \end{pmatrix}_{j\neq i} , x_{i}^{x} , x$$

Solving equation (152) for $\left(\frac{\partial y}{\partial y_{i(0)}}\right)_{\substack{y_{j\neq i}, x_{i}, x}}$, we get

$$\left(\frac{\partial y}{\partial y_{i(0)}}\right)_{y_{j\neq i},x_{i},x} = -\frac{1}{\left(\frac{\partial F}{\partial y}\right)_{x,A,B,C}} + \left(\frac{\partial F}{\partial B}\right)_{x,y,A,C} \left(\frac{\partial B}{\partial y_{i(0)}}\right)_{y_{j\neq i},x_{i}} + \left(\frac{\partial F}{\partial C}\right)_{x,y,A,B,C} \left(\frac{\partial C}{\partial C}\right)_{x_{i},x_{i}} + \left(\frac{\partial F}{\partial C}\right)_{x_{i},x_{i}} + \left(\frac{\partial F}{$$

Squaring equation (153), multiplying by $S_{y_{i(0)}}^{2}$, and then summing over all the observed $y_{i(0)}$'s, we obtain

$$s_{A}^{2} \left(\frac{\partial F}{\partial A}\right)_{x,y,B,C}^{2} + s_{B}^{2} \left(\frac{\partial F}{\partial B}\right)_{x,y,A,C}^{2}$$

$$+ s_{C}^{2} \left(\frac{\partial F}{\partial C}\right)_{x,y,A,B}^{2} + 2s_{AB}^{2} \left(\frac{\partial F}{\partial A}\right)_{x,y,B,C} \left(\frac{\partial F}{\partial B}\right)_{x,y,A,C}$$

$$+ 2s_{AC}^{2} \left(\frac{\partial F}{\partial A}\right)_{x,y,B,C} \left(\frac{\partial F}{\partial C}\right)_{x,y,A,B}$$

$$+ 2s_{BC}^{2} \left(\frac{\partial F}{\partial B}\right)_{x,y,A,C} \left(\frac{\partial F}{\partial C}\right)_{x,y,A,B}$$

(154)

where the variances and covariances in equation (154) are to be calculated from equations (145), (146), (147), (148), (149), and (150). Equation (154) is the general formula for calculating the variance of a calculated y, regardless of the functional relationship between y and x and the parameters, A, B, and C.

This concludes the derivations of the formulas used by us in the solution of general non-linear least squares problems.

In a later paper, we will apply these general formulas to the reduction of PVT data obtained by the Burnett method.

Squaring equation (153), multiplying by S' , and then summing , aver all the observed v. . 's. we obtain

•

(134)

where the variances and covariances in equation (154) are to be calculared from equations (145), (146), (147), (148), (149), and (150), Equation (154) is the general formula for calculating the variance of a cajculated y, regardless of the fumerional relationship between y and x and the parameters, A, B, and C.

This concludes the derivations of the formulas used by us in the solution of general non-linear least squares problems

In a latar papar, we will apply these general formulas to the reduction of FVT data obtained by the Burnett method.

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