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**DETERMINATION OF PARAMETERS FOR CORRELATED DATA
BY THE USE OF A GENERALIZED LEAST-SQUARES
CRITERION INVOLVING LINEARIZED RESIDUALS**

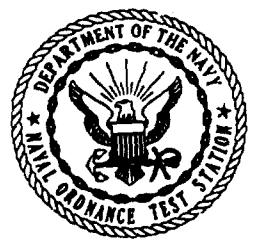
by

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ABSTRACT. This report extends the least-squares methods currently in use at NOTS to cover the case of correlated data. A derivation of the theory is followed by detailed discussions of the applications to the Askania cinetheodolite solution and curve fitting of space-position data. References are given for other local applications, but specific results for these are not included.

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U. S. NAVAL ORDNANCE TEST STATION

China Lake, California
April 1963

INTRODUCTION

This report extends certain least-squares methods currently in use at the Naval Ordnance Test Station (NOTS) to cover the case of correlated data. This extension makes possible, for instance, the use of derived azimuths and elevations in an Askania solution for space position. The general theory of least squares is given in the literature (Ref. 1-3). This report contains independent derivations pertaining to certain cases of special interest at NOTS. A presentation of the theory is followed by detailed discussions of the applications to the Askania cinetheodolite solution and curve fitting of space-position data. References to other local applications are given, but the specific results for these are not presented.

DERIVATION OF THE THEORY

THE COVARIANCE MATRIX OF A LINEAR COMBINATION OF RANDOM VARIABLES

THEOREM 1. Suppose

$U = DV$ where

$$U = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_k \end{pmatrix}, \quad V = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{pmatrix}, \quad D = \begin{pmatrix} d_{11} & d_{12} & \cdots & d_{1n} \\ d_{21} & d_{22} & \cdots & d_{2n} \\ \cdot & \cdot & \cdot & \cdot \\ d_{k1} & d_{k2} & \cdots & d_{kn} \end{pmatrix}$$

the X_i are random variables, and the d_{ij} are constants. Further define

$$S = \begin{pmatrix} \sigma_{X_1}^2 & \sigma_{X_1 X_2} & \cdots & \sigma_{X_1 X_n} \\ \sigma_{X_1 X_2} & \sigma_{X_2}^2 & \cdots & \sigma_{X_2 X_n} \\ \cdot & \cdot & \cdot & \cdot \\ \sigma_{X_1 X_n} & \sigma_{X_2 X_n} & \cdots & \sigma_{X_n}^2 \end{pmatrix}$$

and

$$\bar{\sigma} = \begin{pmatrix} \sigma_{u_1}^2 & \sigma_{u_1 u_2} & \cdots & \sigma_{u_1 u_k} \\ \sigma_{u_1 u_2} & \sigma_{u_2}^2 & \cdots & \sigma_{u_2 u_k} \\ \cdot & \cdot & \cdot & \cdot \\ \sigma_{u_1 u_k} & \cdots & \cdots & \sigma_{u_k}^2 \end{pmatrix}$$

Here $\sigma_{uv} = \text{cov}(u, v)$. Then $\bar{\sigma} = DSD^T$.

Proof. If X_1, X_2, \dots, X_n are random variables and a_i, b_i are constants with

$$T_1 = a_1 X_1 + a_2 X_2 + \cdots + a_n X_n$$

$$T_2 = b_1 X_1 + b_2 X_2 + \cdots + b_n X_n$$

then by taking expected values we obtain

$$E(T_1 T_2) = E \left[\left(\sum_{i=1}^n a_i X_i \right) \left(\sum_{j=1}^n b_j X_j \right) \right] = E \left(\sum_{i,j=1}^n a_i b_j X_i X_j \right) = \sum_{i,j=1}^n a_i b_j E(X_i X_j) \quad (1)$$

$$E(T_1)E(T_2) = E \left(\sum_{i=1}^n a_i X_i \right) E \left(\sum_{j=1}^n b_j X_j \right) = \sum_{i=1}^n a_i E(X_i) \sum_{j=1}^n b_j E(X_j) = \sum_{i,j=1}^n a_i b_j E(X_i) E(X_j) \quad (2)$$

In obtaining Eq. 1 and 2, the linearity of the expected-value operator has been used and the products of sums have been written as double sums. Noting that by definition $\sigma_{uv} = E(uv) - E(u)E(v)$, the subtraction of Eq. 2 from Eq. 1 gives

$$\sigma_{T_1 T_2} = \sum_{i,j=1}^n a_i b_j \sigma_{X_i X_j} \quad (3)$$

and putting $a_i = d_{li}$ and $b_i = d_{pi}$ so that

$$T_1 = u_l = d_{l1}X_1 + d_{l2}X_2 + \dots + d_{ln}X_n$$

$$T_2 = u_p = d_{p1}X_1 + d_{p2}X_2 + \dots + d_{pn}X_n$$

gives, by virtue of Eq. 3,

$$\sigma_{u_l u_p} = \sum_{i,j=1}^n d_{li} d_{pj} \sigma_{X_i X_j} \quad (4)$$

From direct calculation of the lp element of DSD^T , denoted by $(DSD^T)_{lp}$, one obtains

$$(DSD^T)_{lp} = \sum_{i,j=1}^n d_{li} d_{pj} \sigma_{X_i X_j} \quad (5)$$

A comparison of Eq. 4 and 5 gives

$$DSD^T = (\sigma_{u_l u_p})$$

as required.

A FORMULA FOR THE DIFFERENTIATION OF A QUADRATIC FORM

The result obtained here is well known, but is established in a convenient form for use in deriving the normal equations in the following section.

THEOREM 2. *Let*

$$U = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}, \quad C = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}$$

$$P = \begin{pmatrix} p_{11} & p_{12} & \dots & p_{1m} \\ p_{12} & p_{22} & \dots & p_{2m} \\ \cdot & \cdot & \cdot & \cdot \\ p_{1m} & p_{2m} & \dots & p_{mm} \end{pmatrix}, \quad L = \begin{pmatrix} l_{11} & l_{12} & \dots & l_{1n} \\ l_{21} & l_{22} & \dots & l_{2n} \\ \cdot & \cdot & \cdot & \cdot \\ l_{m1} & l_{m2} & \dots & l_{mn} \end{pmatrix}$$

$$F(U) = (LU + C)^T P (LU + C)$$

$$\frac{dF}{dU} = \begin{pmatrix} \frac{\partial F}{\partial u_1} \\ \frac{\partial F}{\partial u_2} \\ \vdots \\ \frac{\partial F}{\partial u_n} \end{pmatrix}$$

Then

$$\frac{dF}{dU} = 2L^T P(LU + C)$$

Proof. It can be verified by expansion and differentiation that

$$\frac{d}{dW} (W^T B W) = 2B W$$

and W is a column vector; also

$$\frac{d}{dW} K W = K^T$$

if K is a row vector.

By the Distributive Law

$$F(U) = (C^T + U^T L^T) P(LU + C) = C^T P C + C^T P L U + U^T L^T P L U + U^T L^T P C$$

Since $C^T P L U$ is a 1×1 matrix and as such is symmetric, it follows that

$$C^T P L U = U^T L^T P^T C = U^T L^T P C$$

Thus,

$$F(U) = C^T P C + 2C^T P L U + U^T (L^T P L) U$$

Hence, by the formulas already derived,

$$\frac{dF}{dU} = 2L^T P L U + 2(C^T P L)^T = 2L^T P(LU + C)$$

as required.

THE GENERALIZED LEAST-SQUARES CRITERION: DERIVATION AND DISCUSSION OF NORMAL EQUATIONS

Let it be required to determine the parameters u_1, u_2, \dots, u_k from measurements m_1, m_2, \dots, m_n with covariance matrix M . Define

$$V = \begin{pmatrix} m_1 - a_1 \\ m_2 - a_2 \\ \dots \\ m_n - a_n \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}, \quad U = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_k \end{pmatrix}$$

$$Q = \begin{pmatrix} q_{11} & q_{21} & \cdots & q_{k1} \\ q_{12} & q_{22} & \cdots & q_{k2} \\ \cdot & \cdot & \cdot & \cdot \\ q_{1n} & q_{2n} & \cdots & q_{kn} \end{pmatrix}, \quad M = \begin{pmatrix} \sigma_{v_1}^2 & \sigma_{v_1 v_2} & \cdots & \sigma_{v_1 v_n} \\ \sigma_{v_1 v_2} & \sigma_{v_2}^2 & \cdots & \sigma_{v_2 v_n} \\ \cdot & \cdot & \cdot & \cdot \\ \sigma_{v_1 v_n} & \sigma_{v_2 v_n} & \cdots & \sigma_{v_n}^2 \end{pmatrix}$$

Here the q_{ij} , q_{ij} and $\sigma_{v_i v_j}$ are constants, M is positive definite, and Q is of rank k . The latter assumption implies that there are sufficient independent data to solve the problem.

It can be shown (Ref. 2 and 3) that the maximum-likelihood estimate of u_1, u_2, \dots, u_k under the assumption of normally distributed errors in the m_i is given by

$$G(U) = (V - QU)^T M^{-1} (V - QU) = \text{minimum} \tag{6}$$

This criterion is taken as the generalized least-squares criterion for correlated data.

By Theorem 2,

$$\frac{dG}{dU} = 2(-Q)^T M^{-1} (V - QU)$$

Equating to zero gives the normal equations

$$AU = Q^T M^{-1} V \tag{7}$$

where

$$A = Q^T M^{-1} Q$$

We show that A is non-singular. Consider the quadratic form $H(X) = X^T M^{-1} X$, which is positive definite. If we perform a linear transformation, $X = QY$, there results

$$H(QY) = Y^T (Q^T M^{-1} Q) Y$$

By a theorem (Ref. 4) from linear algebra,

$$\text{rank } Q + \text{nullity } Q = \text{number of columns of } Q$$

Since $\text{rank } Q = \text{number of columns of } Q = k$, it follows that $\text{nullity } Q = 0$. Thus QY can be zero only if $Y = 0$. Hence $H(QY)$, when regarded as a quadratic form in Y , is positive definite; $Q^T M^{-1} Q$ is a positive-definite matrix and, as such, has only positive eigenvalues. That is to say, $Q^T M^{-1} Q$ is non-singular. (Note that if Q had rank less than k , then A would be singular, since the rank of a product is at most equal to the rank of any factor.)

Equation 7 can therefore be solved uniquely for U as follows:

$$U = A^{-1} Q^T M^{-1} V \tag{8}$$

In order to prove that Eq. 8 actually furnishes a minimum of the expression for $G(U)$, Eq. 6, let U_0 be the solution given by Eq. 8. That is, let $U_0 = A^{-1} Q^T M^{-1} V$ and let U^* be any other real column vector having dimension k . It follows by direct expansion, making use of this expression for U_0 , that

$$G(U^*) - G(U_0) = (U^* - U_0)^T A (U^* - U_0)$$

Since it has already been shown that A is positive definite, it is concluded that U_0 does indeed furnish a minimum of Eq. 6.

If S_U is the variance-covariance matrix of U , we have by a direct application of Theorem 1

$$S_U = (A^{-1} Q^T M^{-1}) M (A^{-1} Q^T M^{-1})^T = A^{-1} (Q^T M^{-1} Q) A^{-1}$$

or

$$S_U = A^{-1} \tag{9}$$

Thus the entire least-squares solution consists of computing S_U by Eq. 9 and U by Eq. 8. The application of this solution to the various specific situations merely consists of properly defining the matrix Q and the quantities a_i . This is done in detail for the Askania cinetheodolite solution and the application to curve fitting of space-position data. References are given for other applications.

APPLICATIONS

APPLICATION TO THE ASKANIA CINETHEODOLITE SOLUTION

For a more detailed explanation of the notation used in this section the reader may consult Ref. 5. Let r be the number of Askania stations. Then, $n = 2r$. It is assumed that the i th Askania station determines azimuth and elevation measurements A_i and E_i with covariance matrix

$$\begin{pmatrix} \sigma_{A_i}^2 & \sigma_{A_i E_i} \\ \sigma_{A_i E_i} & \sigma_{E_i}^2 \end{pmatrix} \quad (i = 1, 2, \dots, r)$$

and that the measurement errors from a given station are independent of those from any other station. Of course, since A_i and E_i are assumed correlated here, it would be permissible to use azimuths and elevations derived from other primary measurements rather than direct Askania readings. Under these conditions,

$$M = \begin{pmatrix} \sigma_{A_1}^2 & 0 & \cdot & 0 & \sigma_{A_1 E_1} & 0 & 0 & 0 \\ 0 & \sigma_{A_2}^2 & 0 & 0 & 0 & \sigma_{A_2 E_2} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \sigma_{A_r}^2 & 0 & 0 & \cdot & \sigma_{A_r E_r} \\ \hline \sigma_{A_1 E_1} & 0 & \cdot & 0 & \sigma_{E_1}^2 & 0 & \cdot & 0 \\ 0 & \sigma_{A_2 E_2} & 0 & 0 & 0 & \sigma_{E_2}^2 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \sigma_{A_r E_r} & 0 & 0 & \cdot & \sigma_{E_r}^2 \end{pmatrix}$$

We have

$$m_i = i\text{th azimuth reading, } i = 1, 2, \dots, r$$

$$m_i = (i - r)\text{th elevation reading, } i = r + 1, \dots, 2r$$

In order to obtain M^{-1} as required for the normal equations, one may follow the analysis¹ of Ref. 6 with the following result, which is easily verified by direct calculation.

¹ The use of this procedure, which finds M^{-1} in terms of submatrices that are diagonal, was suggested by Mrs. D. Saitz of the Test Department, NOTS.

$$M^{-1} = \begin{pmatrix} \frac{\sigma_{E_1}^2}{D_1} & 0 & \cdot & 0 & \frac{-\sigma_{A_1 E_1}}{D_1} & 0 & \cdot & 0 \\ 0 & \frac{\sigma_{E_2}^2}{D_2} & 0 & 0 & 0 & \frac{-\sigma_{A_2 E_2}}{D_2} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \frac{\sigma_{E_r}^2}{D_r} & 0 & \cdot & \cdot & \frac{-\sigma_{A_r E_r}}{D_r} \\ \hline \frac{-\sigma_{A_1 E_1}}{D_1} & 0 & \cdot & 0 & \frac{\sigma_{A_1}^2}{D_1} & 0 & \cdot & 0 \\ 0 & \frac{-\sigma_{A_2 E_2}}{D_2} & 0 & 0 & 0 & \frac{\sigma_{A_2}^2}{D_2} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \frac{-\sigma_{A_r E_r}}{D_r} & 0 & \cdot & 0 & \frac{\sigma_{A_r}^2}{D_r} \end{pmatrix}$$

where $D_i = \sigma_{A_i}^2 \sigma_{E_i}^2 - (\sigma_{A_i E_i})^2$. None of the D_i will be zero, for if $D_i = 0$, then the corresponding covariance matrix

$$\begin{pmatrix} \sigma_{A_i}^2 & \sigma_{A_i E_i} \\ \sigma_{A_i E_i} & \sigma_{E_i}^2 \end{pmatrix}$$

would be singular.

The unknowns are the corrections $u_1 = \Delta x$, $u_2 = \Delta y$, and $u_3 = \Delta z$ to be applied to an initial estimate x_0, y_0, z_0 of space position. Therefore $k = 3$. We define the coordinates of the i th Askania station as X_i, Y_i, Z_i where $i = 1, \dots, r$.

Then

$$a_i = \tan^{-1} \frac{z_0 - Z_i}{x_0 - X_i} \quad (i = 1, 2, \dots, r)$$

$$a_i = \tan^{-1} \frac{y_0 - Y_{i-r}}{[(x_0 - X_{i-r})^2 + (y_0 - Y_{i-r})^2]^{1/2}} \quad (i = r + 1, \dots, n)$$

The q_{ji} are defined as follows:

$$q_{1i} = \frac{Z_i - z_0}{(X_i - x_0)^2 + (Z_i - z_0)^2} \quad (i = 1, 2, \dots, r)$$

$$q_{1i} = \frac{-(X_{i-r} - x_0)(Y_{i-r} - y_0)}{[(X_{i-r} - x_0)^2 + (Y_{i-r} - y_0)^2 + (Z_{i-r} - z_0)^2][(X_{i-r} - x_0)^2 + (Z_{i-r} - z_0)^2]^{1/2}} \quad (i = r + 1, \dots, n)$$

$$q_{2i} = 0 \quad (i = 1, 2, \dots, r)$$

$$q_{2i} = \frac{[(X_{i-r} - x_0)^2 + (Z_{i-r} - z_0)^2]^{1/2}}{[(X_{i-r} - x_0)^2 + (Y_{i-r} - y_0)^2 + (Z_{i-r} - z_0)^2]} \quad (i = r + 1, \dots, n)$$

$$q_{3i} = \frac{-(X_i - x_0)}{(X_i - x_0)^2 + (Z_i - z_0)^2} \quad (i = 1, 2, \dots, r)$$

$$q_{3i} = \frac{-(Y_{i-r} - y_0)(Z_{i-r} - z_0)}{[(X_{i-r} - x_0)^2 + (Y_{i-r} - y_0)^2 + (Z_{i-r} - z_0)^2][(X_{i-r} - x_0)^2 + (Z_{i-r} - z_0)^2]^{1/2}} \quad (i = r + 1, \dots, n)$$

The solution shown here is ordinarily iterated until all the corrections u_i are negligible. For further detail see Ref. 5.

APPLICATION TO CURVE FITTING OF SPACE-POSITION DATA

Suppose that it is required to fit polynomials in the time, t , to space position, x, y, z , in the form

$$x = u_1 + u_2 t + \dots + u_{l_1+1} t^{l_1}$$

$$y = u_{l_1+2} + u_{l_1+3} t + \dots + u_{l_1+l_2+2} t^{l_2}$$

$$z = u_{l_1+l_2+2} + u_{l_1+l_2+3} t + \dots + u_{l_1+l_2+l_3+3} t^{l_3}$$

The quantities required to apply the method of this report are obtained below.

The basic data are x_i, y_i, z_i, M_i, t_i (space positions, variance-covariance matrices, and values of time) for $i = 1, 2, \dots, r$, where

$$M_i = \begin{pmatrix} \sigma_{x_i}^2 & \sigma_{x_i y_i} & \sigma_{x_i z_i} \\ \sigma_{x_i y_i} & \sigma_{y_i}^2 & \sigma_{y_i z_i} \\ \sigma_{x_i z_i} & \sigma_{y_i z_i} & \sigma_{z_i}^2 \end{pmatrix}$$

By definition, $n = 3r$, $a_i = 0$ for $i = 1, 2, \dots, 3r$,

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Determination of Parameters for Correlated Data by the Use of a Generalized Least-Squares Criterion Involving Linearized Residuals, by Otto Neall Strand. China Lake, Calif., NOTS, April 1963. 10 pp. (NAVWEPS Report 7942, NOTS TP 2979), UNCLASSIFIED.

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