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The Covariance Matrix for the Solution Vector of an Equality-Constrained Least-Squares Problem

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PREFACE

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THE COVARIANCE MATRIX FOR THE SOLUTION VECTOR OF AN EQUALITY-CONSTRAINED LEAST SQUARES PROBLEM

1. INTRODUCTION

Consider the linear least squares problem

$$Ex \cong f$$

subject to the linear equality constraints

$$Cx = d$$

We refer to this as Problem LSE denoting Lease Squares with Equality constraints.

Methods for solving Problem LSE are described in Chapters 20 - 22 of Ref. (1).

In this note we describe methods for computing the covariance matrix V for the solution vector x. Different methods of computing V will be discussed which are convenient for use with each of the different solution algorithms given in Ref. (1). Any reference to a Chapter, Section, or Page without further qualification is to be understood to refer to Ref. (1).

We assume throughout that the covariance matrix of f is the identity matrix. If the covariance matrix of f is known to be something other than the identity matrix then a preliminary left multiplication of E and f by an appropriate matrix will produce the desired standard situation. (See Chapter 25, Section 2.)

We assume that E, C, and d are known exactly, or at least that their errors are very small relative to those of f.

Let C be an $m_1 \times n$ matrix and let E be $m_2 \times n$. We assume that

$$m_1 < n$$

$$m_1 + m_2 \geq n$$

$$\text{Rank }(C) = m_1$$

$$\text{Rank }\left(\begin{bmatrix} C \\ E \end{bmatrix}\right) = n$$

With these assumptions Problem LSE has a unique solution vector and all of the solution methods to be discussed apply without the need to consider unusual special cases.

As a small numerical example to illustrate the computational methods to be presented we use the same problem that was used in Chapters 20 - 22. (See p. 140).

$$C = \begin{bmatrix} 0.4087 & 0.1593 \end{bmatrix} \qquad d = 0.1376$$

$$E = \begin{bmatrix} 0.4302 & 0.3516 \\ 0.6246 & 0.3384 \end{bmatrix} \qquad f = \begin{bmatrix} 0.6593 \\ 0.9666 \end{bmatrix}$$

The computations described in Chapters 20 - 22 were done using a relative precision of 10^{-8} whereas intermediate and final results were rounded to about four decimal places for publication. In this note we begin with the published intermediate results when applicable and compute using a pocket calculator.

2. SOLUTION METHOD USING A BASIS OF THE NULL SPACE

This solution method is described in Chapter 20, pages 134-141. It may be summarized as follows.

Apply Householder orthogonal transformations to C from the right to reduce C to lower triangular form. Apply these same transformations to E from the right. Denoting the product of these orthogonal transformations by the $n \times n$ orthogonal matrix K these operations may be represented by the equation:

$$\begin{bmatrix} C \\ E \end{bmatrix} K = \begin{array}{c} \left[\begin{array}{cc} \tilde{C}_1 & O \\ \tilde{E}_1 & \tilde{E}_2 \end{array}\right] \begin{array}{l} \}m_1 \\ \}m_2 \end{array} \\ \begin{array}{cc} \underbrace{\quad}_{m_1} & \underbrace{\quad}_{n-m_1} \end{array} \end{array} \tag{1}$$

Solve the following lower triangular system for y_1:

$$\tilde{C}_1 \, y_1 = d$$

Compute:

$$\tilde{f} = f - \tilde{E}_1 \, y_1$$

Solve the least squares problem:

$$\tilde{E}_2 \, y_2 \cong \tilde{f} \tag{2}$$

Compute:

$$x = K \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

To compute the covariance matrix, V, for x, first compute the covariance matrix S for y_2:

$$S = (\tilde{E}_2^T \, \tilde{E}_2)^{-1} \tag{3}$$

Then the covariance matrix for

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

is

$$U = \begin{bmatrix} 0 & 0 \\ 0 & S \end{bmatrix} \tag{4}$$

and the covariance matrix for x is

$$V = KUK^T \tag{5}$$

Consider the numerical example given on pp 140-141.

In this example

$$\tilde{E}_2 = \begin{bmatrix} 0.1714 \\ 0.0885 \end{bmatrix}$$

and

$$K = \begin{bmatrix} -0.9317 & -0.3632 \\ -0.3632 & 0.9317 \end{bmatrix}$$

Thus using Eq. (3) - (5) we obtain

$$S = (0.037210)^{-1} = 26.874$$

and

$$V = \begin{bmatrix} 3.545 & -9.094 \\ -9.094 & 23.33 \end{bmatrix} \tag{6}$$

Note that although Eq. (3) is a valid mathematical definition of S it does not represent the most stable way to compute S. If Problem (2) is solved using Householder transformations, then one would have an upper triangular matrix R such that

$$Q\tilde{E}_2 = \begin{bmatrix} R \\ 0 \end{bmatrix} \tag{7}$$

where Q is $m_2 \times m_2$ orthogonal.

Then, as is described in Chapter 12, one could compute S as

$$S = R^{-1} (R^{-1})^T \tag{8}$$

3. SOLUTION METHOD USING DIRECT ELIMINATION

This solution method is described in Chapter 21, pp 144-147. It may be summarized as follows.

Assume column interchanges have been done in the augmented matrix

$$\begin{bmatrix} C \\ E \end{bmatrix},$$

if necessary, to assure that the first m_1 columns of C are linearly independent.

Use Gaussian elimination to zero all elements below the diagonal in the first m_1 columns of

$$\begin{bmatrix} C \\ E \end{bmatrix},$$

$$G \begin{bmatrix} C & d \\ E & f \end{bmatrix} = \begin{array}{l} \left.\begin{bmatrix} \tilde{C}_1 & \tilde{C}_2 & \tilde{d} \\ 0 & \tilde{E}_2 & \tilde{f} \end{bmatrix}\begin{matrix} \}\, m_1 \\ \}\, m_2 \end{matrix}\right. \\ \quad \underbrace{}_{m_1} \; \underbrace{}_{n-m_1} \; \underbrace{}_{1} \end{array}$$

Solve the least squares problem:

$$\tilde{E}_2 x_2 \cong \tilde{f} \tag{9}$$

Solve for x_1 in

$$\tilde{C}_1 x_1 = \tilde{d} - \tilde{C}_2 x_2 \tag{10}$$

Then the solution vector is

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

To compute the covariance matrix of x introduce the $m_1 \times (n - m_1)$ matrix H, obtained by solving

$$\tilde{C}_1 H = \tilde{C}_2$$

Then from Eq. (10) we may write

$$x_1 = \tilde{C}_1^{-1} \tilde{d} - H x_2 \tag{11}$$

Let $\mathcal{E}$ denote the expected value operator. Introduce the mean values

$$\bar{x}_1 = \mathcal{E}(x_1)$$

and

$$\bar{x}_2 = \mathcal{E}(x_2)$$

These mean values satisfy Eq. (11), i.e.,

$$\bar{x}_1 = \tilde{C}_1^{-1} \tilde{d} - H \bar{x}_2 \tag{12}$$

Subtract Eq. (12) from Eq. (11) obtaining

$$(x_1 - \bar{x}_1) = -H(x_2 - \bar{x}_2) \tag{13}$$

from which we may write

$$x - \bar{x} = \begin{bmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \end{bmatrix} = \begin{bmatrix} -H \\ I \end{bmatrix} \cdot (x_2 - \bar{x}_2) \tag{14}$$

Let W denote the $(n - m_1) \times (n - m_1)$ covariance matrix of x_2, which from Eq. (9) may be defined as

$$W = (\tilde{E}_2^T \tilde{E}_2)^{-1} \tag{15}$$

Then using Eq. (14) the covariance matrix V of x can be written as

$$V = \begin{bmatrix} -H \\ \\ I \end{bmatrix} W \begin{bmatrix} -H^T & I \end{bmatrix} = \begin{bmatrix} HWH^T & -HW \\ \\ -WH^T & W \end{bmatrix}$$

Consider the same numerical example as before, solved by this method. (See p. 147). We have

$$\tilde{E}_2 = \begin{bmatrix} 0.1839 \\ \\ 0.0949 \end{bmatrix}$$

and

$$H = \tilde{C}_1^{-1} \tilde{C}_2 = (0.4087)^{-1}(0.1593) = 0.38977$$

We compute

$$W = (\tilde{E}_2^T \tilde{E}_2)^{-1} = (0.042825)^{-1} = 23.351$$

and

$$V = \begin{bmatrix} 3.548 & -9.101 \\ \\ -9.101 & 23.351 \end{bmatrix}$$

Note that Eq. (15) is a valid mathematical definition of W but not a recommended computational formula. See the remark at the end of Sec. 2 for suggestions for a more stable way of computing W.

4. SOLUTION BY WEIGHTING

This solution method is described in Chapter 22. It may be summarized as follows:

Suppose the data are scaled so that the elements of largest magnitude in the matrices C and E are approximately the same size. Introduce a scale factor, ϵ, such that ϵ^2 is smaller than the working precision. For instance set $\epsilon < 10^{-4}$ for Univac single precision arithmetic and $\epsilon < 10^{-9}$ for Univac double precision.

Solve the least squares problem

$$\begin{bmatrix} C \\ \epsilon E \end{bmatrix} x \cong \begin{bmatrix} d \\ \epsilon f \end{bmatrix} \tag{16}$$

using Householder or Givens orthogonal transformations.

Solving the problem by either of these methods involves triangularization by left multiplication by an orthogonal matrix Q:

$$Q \begin{bmatrix} C & d \\ \epsilon E & \epsilon f \end{bmatrix} = \begin{array}{c} \begin{bmatrix} \tilde{C} & \tilde{d} \\ \epsilon \tilde{E}_1 & \epsilon \tilde{f}_1 \\ 0 & \epsilon \tilde{f}_2 \end{bmatrix} \\ \begin{array}{cc} \underbrace{\hphantom{\epsilon\tilde{E}_1}}_{n} & \underbrace{\hphantom{\epsilon\tilde{f}_1}}_{1} \end{array} \end{array} \begin{array}{l} \}\, m_1 \\ \}\, n - m_1 \\ \}\, m_1 + m_2 - n \\ \\ \end{array}$$

Then x is obtained by solving the upper triangular system

$$\begin{bmatrix} \tilde{C} \\ \epsilon \tilde{E}_1 \end{bmatrix} x = \begin{bmatrix} \tilde{d} \\ \epsilon \tilde{f}_1 \end{bmatrix}$$

The condition number of this problem is very large (about ϵ^{-1}) however this does not affect the accuracy of the solution because of the special structure of the matrix and right-side vector.

The covariance matrix, V, of x is

$$V = \epsilon^2 \begin{bmatrix} \tilde{C} \\ \\ \epsilon\tilde{E}_1 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \tilde{C} \\ \\ \epsilon\tilde{E}_1 \end{bmatrix}^{-1^T} \tag{17}$$

Even though the triangular matrix $\begin{bmatrix} \tilde{C} \\ \epsilon\tilde{E}_1 \end{bmatrix}$ has a large condition number its inverse can be computed without numerical difficulty.

Consider the example used before. The weighted problem to be solved (see p. 156) is

$$\begin{bmatrix} 0.4087 & 0.1593 \\ \\ 0.4302\epsilon & 0.3516\epsilon \\ \\ 0.6246\epsilon & 0.3384\epsilon \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \\ x_2 \end{bmatrix} \cong \begin{bmatrix} 0.1376 \\ \\ 0.6593\epsilon \\ \\ 0.9666\epsilon \end{bmatrix} \tag{18}$$

Since we will be using 4 or 5 place decimal arithmetic we could choose any value of $\epsilon < 10^{-3}$. The point is that for any two numbers, a and b, of comparable magnitude ϵ should be small enough relative to the computational precision so that the computed value of $a^2 + (\epsilon b)^2$ will just be a^2. For our numerical example we will not assign a specific value to ϵ but will use the computational rule that the computed value of an expression of the form $a^2 + (\epsilon b)^2$ is a^2 when a and b are of the same order of magnitude.

The data arrays of Eq. (18) can be triangularized by Householder transformations to obtain the equivalent problem

$$\begin{bmatrix} -0.4087 & -0.15930 \\ \\ 0 & -0.20698\epsilon \\ \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \\ x_2 \end{bmatrix} \cong \begin{bmatrix} -0.13760 \\ \\ -0.80403\epsilon \\ \\ 0.43606\epsilon \end{bmatrix} \tag{19}$$

Solving the nonsingular system represented by the first two rows of Eq. (19) given the solution vector

$$x = \begin{bmatrix} -1.1774 \\ \\ 3.8846 \end{bmatrix}$$

Let R denote the leading 2 × 2 triangular matrix in Eq. (19). We compute

$$R^{-1} = \begin{bmatrix} -2.4468 & 1.8831\epsilon^{-1} \\ \\ 0 & -4.8314\epsilon^{-1} \end{bmatrix}$$

Then using Eq. (17) we compute the covariance matrix V of x as

$$V = \epsilon^2 R^{-1}(R^{-1})^T = \begin{bmatrix} 3.5461 & -9.0980 \\ \\ -9.0980 & 23.342 \end{bmatrix}$$

This computational procedure looks peculiar in some ways but it is valid. For example the upper left element of R^{-1}, namely -2.4468, is entirely lost in the roundoff error when the product $R^{-1}(R^{-1})^T$ is computed and this results in the computed V being singular whereas R^{-1} was clearly nonsingular.

This is exactly the right thing to happen, however, since the covariance matrix V for problem LSE should be singular and should not be influenced by the upper left element of R^{-1}.

Close analysis of this weighted method (See Exercise 22.40, p. 157) shows that with sufficiently small ϵ this is just a sneaky way of performing the direct elimination algorithm treated in Sec. 3 of this note (Chap. 21 of the book).

5. ONE MORE APPROACH

Still another way of looking at Problem LSE is presented on pp. 141-143. As is noted there we expect that this approach may not have practical value but may be of theoretical interest.

Let K be the $n \times n$ orthogonal matrix defined in Sec. 2 of this note (Chapter 20 of the book). Let K be partitioned as

$$K = \left.\begin{bmatrix} \underbrace{K_1}_{m_1} & \underbrace{K_2}_{n-m_1} \end{bmatrix}\right\} n$$

Define

$$\hat{E} = (EK_2)(EK_2)^+ E$$

where the superscript "+" denotes pseudoinverse. Define

$$\hat{A} = \begin{bmatrix} C \\ \hat{E} \end{bmatrix}$$

Then, as is proved in Chapter 20, the least squares solution of

$$\hat{A}x \cong \begin{bmatrix} d \\ f \end{bmatrix} \tag{20}$$

is the same as the solution of problem LSE:

$$\begin{cases} Cx = d \\ Ex \cong f \end{cases}$$

To compute the covariance matrix of x, regarding x as the solution of Eq. (20), we first write

$$x = \hat{A}^+ \begin{bmatrix} d \\ f \end{bmatrix}$$

Assuming the covariance matrix of $\begin{bmatrix} d \\ f \end{bmatrix}$ is

$$\begin{array}{c} \begin{array}{cc} \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix}}_{\hphantom{0}m_1 \quad m_2} & \begin{array}{l} \}\, m_1 \\ \}\, m_2 \end{array} \end{array} \end{array}$$

it follows that the covariance matrix, V, of x is

$$V = \hat{A}^{+} \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} \hat{A}^{+T} \tag{21}$$

From Eq. (20.30) on p. 141 we know that $\hat{A}^{+}$ can be written as

$$\hat{A}^{+} = \Big[\underbrace{C^{+} - K_2(EK_2)^{+}\, EC^{+}}_{m_1},\ \underbrace{K_2(EK_2)^{+}}_{m_2}\Big]\Big\}\, n \tag{22}$$

Substituting Eq. (22) into Eq. (21) gives

$$V = K_2(EK_2)^{+}\,(EK_2)^{+T}\, K_2^T \tag{23}$$

From Eq. (1) we have

$$EK_2 = \tilde{E}_2$$

and thus Eq. (23) can be written as

$$V = K_2\, \tilde{E}_2^{+}\, \tilde{E}_2^{+T}\, K_2^T$$

$$= K_2(\tilde{E}_2^T\, E_2)^{-1}\, K_2^T$$

This last expression is identical to the right-side of Eq. (5). Thus we obtain the same representation of V as in Sec. 2.

REFERENCES

1. C. L. Lawson, and R. J. Hanson, "Solving Least Squares Problems", Prentice-Hall, 1974.