On the Best Quadratic Minimum Bias Non-Negative Estimator of a Two-Variance Component Model

Research article

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Abstract:

Variance components (VCs) in linear adjustment models are usually successfully computed by unbiased estimators. However, for many unbiased VC techniques estimated variance components might be negative, a result that cannot be tolerated by the user. This is, for example, the case with the simple additive VC model $a\sigma_1^2 + b\sigma_2^2$ with known coefficients a and b, where either of the unbiasedly estimated variance components σ_1^2 and σ_2^2 may frequently come out negative. This fact calls for so-called non-negative VC estimators. Here the Best Quadratic Minimum Bias Non-negative Estimator (BQMBNE) of a two-variance component model is derived. A special case with independent observations is explicitly presented.

Keywords:

Variance Components, Minimum bias, BQMBNE, Non-negative estimation

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Received 2011-05-02; accepted 2011-06-16

1. Introduction

Variance component (VC) estimation by Minimum Norm Quadratic Unbiased Estimation (MINQUE) (Rao 1973) is a well-known technique applied in many fields working with adjustment of discrete data. It is also well known that MINQUE has the bad property that the estimated VCs may be negative, a reality that, of course, is not satisfactory. Typical reasons for such unwanted results could be that the adjustment and/or VC models are bad and or that the redundancy in the adjustment problem is poor (i.e. the number of observations are too few with respect to the number of estimated variance components). Another reason could be that the approximate VCs, used in an iterative procedure to estimate the VCs, are bad. To avoid such a problem special techniques have been designed that warrant non-negative VC estimates. The ideal non-

negative estimator is unbiased and has minimum variance among all non-negative estimators. However, the desires on non-negative and unbiased estimation can seldom be met simultaneously, and La Motte (1973) and Pukelsheim (1981) demonstrated that such "non-negative MINQU estimators" do not generally exist. Hence, in order to search for a practical non-negative estimator, one has to give up the condition on unbiasedness, which implies that the estimator will be biased.

This brings us to the idea of finding the Best Quadratic Non-Negative Estimator (BQNE), which is the non-negative VC estimator that minimizes the mean square error, i.e. the sum of the variance and the bias squared. However, as shown by Sjöberg (1984), it turns out that the BQNE is the same as the Best Quadratic Estimator, which, unfortunately is not a practical one that can be improved, e.g. by iteration, but it is totally based on the a priori estimated variance-covariance matrix of the observations.

Some comments on non-negative VC estimation can be found also in Amiri-Simkooei (2007, Sects. 3.3.6 and 4.8.1).

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A typical situation for non-negative estimation is the case for an observation with an additive two-variance component model for the observation variance (σ_l^2) as follows:

$$\sigma_1^2 = a\sigma_1^2 + b\sigma_2^2,\tag{1}$$

where a and b are given coefficients and σ_1^2 and σ_2^2 are the unknown variance components. This type of VC model is very common for various types of observations, e.g. EDM measurements, angle measurements, GNSS observations, gravity observations to mention a few, and for correlated data it is generalized below to the model of Eq. (7). Frequently, the estimators for σ_1^2 and σ_2^2 come out negative by MINQUE, and in Sect. 3 we illustrate also that these variance components cannot be estimated as unbiased non-negative estimators. That is, we cannot warrant the unbiased estimators to be non-negative. Hence, the BQMBNE is useful for this type of VC models. The BQMBNE for Eq. (1) was derived in Sjöberg (1984). However, as the proof was too short to be appreciated by some geodesists, we will give a more extensive proof of it in Ch. 4. Sect. 2 starts with the general, linear adjustment model condition adjustment with unknowns, which is the general basis for the VC estimation models.

2. Linear adjustments

The Gauss-Helmert adjustment model, or condition adjustment with unknowns, is given by (e.g. Bjerhammar 1973, pp. 278-279)

$$AX + B\varepsilon = W$$
, $E\{\varepsilon\varepsilon^T\} = Q$ and $E\{\varepsilon\} = 0$, (1a)

where **A** and **B** are known design matrices of dimension $(k \times m)$ and $(k \times n)$, respectively, where $n \ge k \ge m$, and

$$W = BL - c$$
; $c = constant$, knownvector; $L = vector of observations$. (1b)

Furthermore, X and ε are the vectors of unknowns and normal distributed errors, and the covariance matrix Q is assumed to be positive definite.

The least squares solution to Eq. (1), minimizing $\boldsymbol{\varepsilon}^T \mathbf{Q}^{-1} \boldsymbol{\varepsilon}$, becomes

$$\hat{\mathbf{X}} = \left(\mathbf{A}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{W} \tag{2a}$$

Journal of Geodetic Science

and

$$\hat{\epsilon} = QB^{T}C^{-1}\left(W - A\hat{X}\right), \tag{2b}$$

281

where

$$C = BQB^{T}$$
 withrank $(C) = k$. (2c)

Note. A may be rank deficient, implying that the inverse of Eq. (2a) is any generalized inverse, \hat{X} is non-unique but $A\hat{X}$ is unique.

Premultiplying each term of Eq. (1a) by $(I - A^0)$, where $A^0 = A(A^TC^{-1}A)^{-1}A^TC^{-1}$, one obtains

$$(I - A^0) B\varepsilon = \bar{W}, \tag{3a}$$

where

$$\bar{\mathbf{W}} = \mathbf{W} - \mathbf{A}\mathbf{X} = (\mathbf{I} - \mathbf{A}^0) \,\mathbf{W}. \tag{3b}$$

Equation (3a) is the basic linear adjustment model for VC component estimation. It includes two important special cases:

Case I (adjustment by elements): B = I and c = 0, implying

$$(\mathbf{I} - \mathbf{A}^0) \, \boldsymbol{\varepsilon} = \bar{\mathbf{W}} = (\mathbf{I} - \mathbf{A}^0) \, \mathbf{L}. \tag{4}$$

Case II (condition adjustment): A = 0, implying

$$B\varepsilon = W. \tag{5}$$

3. Quadratic estimation of variance components

We will be concerned with the two-variance component model for the observation variance $(\sigma_{l_i}^2)$ and covariance $(\sigma_{l_i l_i})$, i.e.

$$\sigma_{l_i}^2 = a_i \sigma_1^2 + b_i \sigma_2^2 \tag{6a}$$

and

$$\left(\sigma_{l_i l_i}\right) = a_{ij}\sigma_1^2 + b_{ij}\sigma_2^2,\tag{6b}$$

where the coefficients are regarded as known parameters and the two variance components σ_1^2 and σ_2^2 are the unknowns to be estimated. Equations (6a) and (6b) applied to the observation vector ${\bf L}$ then yields the error covariance matrix

$$\mathbf{Q} = \sigma_1^2 \mathbf{Q}_1 + \sigma_2^2 \mathbf{Q}_2,\tag{7}$$

where the cofactor matrices Q_1 and Q_2 given by the coefficients of Eqs. (6a) and (6b).

The quadratic estimation of the variance components σ_i^2 , i = 1 and 2, is provided by the general model under *translational invariance*

$$\tilde{\sigma}_i^2 = \bar{\mathbf{W}}^\mathsf{T} \mathbf{M} \bar{\mathbf{W}},\tag{8}$$



where M is an arbitrary matrix. Assuming that \bar{W} is normally distributed, it follows that the expectation and variance of the above VC estimator are

$$E\left\{\tilde{\sigma}_{i}^{2}\right\} = E\left\{\bar{\mathbf{W}}^{\mathsf{T}}\mathbf{M}\bar{\mathbf{W}}\right\} = \operatorname{tr}\left[\mathbf{M}\mathbf{E}\left\{\bar{\mathbf{W}}\bar{\mathbf{W}}^{\mathsf{T}}\right\}\right] = \operatorname{tr}\left[\mathbf{M}\mathbf{K}\right],$$
(9a)

and

$$\operatorname{Var}\left\{\tilde{\sigma}_{i}^{2}\right\} = 2\operatorname{tr}\left[\mathsf{KMKM}\right],\tag{9b}$$

where

$$K = (I - A^{0})C(I - A^{0})^{T} = C(I - A^{0})^{T} = (I - A^{0})C$$
 (9c)

with $C = BQB^T$.

Note. Translation invariant estimability implies here that W is substituted by \bar{W} , which is invariant/independent of the unknown vector X. (See e.g. Rao and Kleffe 1988, p.78.)

Assuming that Eq. (9a) yields an unbiased estimate of σ_i^2 , and introducing a decomposition of K as

$$\begin{split} K &= \sigma_1^2 K_1 + \sigma_2^2 K_2 \text{, with} \quad K_i = (I - A^0) C_i (I - A^0)^T \\ &\quad \text{and} \quad C_i = B Q_i B^T \end{split} \tag{10}$$

one readily obtains from Eq. (9a):

$$\sigma_i^2 = \sigma_1^2 \text{tr}[MK_1] + \sigma_2^2 \text{tr}[MK_2].$$
 (11)

Hence, unbiased estimation of σ_i^2 requires that the two conditions

$$tr[MK_i] = 1 \text{ and } tr[MK_{i\neq i}] = 0$$
 (12)

are satisfied. This type of estimators always exists, and we may derive the Best Quadratic Unbiased Estimator (BQUE) among all the estimators satisfying Eqs. (12). See e.g. Sjöberg (1984).

Now, if we want to warrant *non-negative unbiased estimation* by Eq. (8), it should satisfy the conditions (12) (condition for an unbiased estimation) as well as the following *condition on non-negative estimation:*

$$M = G_i G_i^T; i = 1, 2,$$
 (13)

where G_i are arbitrary (with compatible dimensions). Inserting Eq. (13) into Eq. (12) we readily obtain:

$$\begin{split} &\text{tr}\left[G_i^T(I-A^0)C_i(I-A^0)^TG_i\right]=\ 1\ \text{and}\\ &\text{tr}\left[G_i^T(I-A^0)C_{i\neq i}(I-A^0)^TG_i\right]=\ 0. \end{split} \tag{14}$$

In the standard case, where both C_1 and C_2 are non-singular, the two parts of Eq. (14) has no common solution for G_i . This is

because the only solutions for G_i of the second equation are then those matrices that satisfy $(I-A^0)^TG_i=0$. However, for these choices of G_i the first trace of Eq. (14) cannot be equated to unity. Unfortunately, this negative result is generally valid when applying the variance-covariance model of Eqs. (6a) and (6b). The conditions on having an unbiased \underline{and} non-negative estimator cannot both be met, and this implies that one must make a choice to either go for an unbiased or a non-negative estimator. Below we study the non-negative estimators with minimum bias.

4. The Quadratic Minimum Bias Estimators

As already suggested in Sect. 3 the non-negative estimators of variance components σ_i^2 are given by the formula

$$\tilde{\sigma}_i^2 = \bar{\mathbf{W}}^\mathsf{T} \mathbf{G}_i \mathbf{G}_i^\mathsf{T} \bar{\mathbf{W}},\tag{15}$$

where matrices G_i are arbitrary (but with compatible dimensions). From now on we only study the variance component σ_1^2 (and we drop the index of G_1). Then we obtain:

$$E\left\{\tilde{\sigma}_{1}^{2}\right\} = \sigma_{1}^{2}t_{1} + \sigma_{2}^{2}t_{2},\tag{16}$$

where $t_i = \text{tr} \left[\mathbf{G} \mathbf{G}^\mathsf{T} \mathbf{K}_i \right]$, implying that $\tilde{\sigma}_1^2$ has the bias

$$b = \sigma_1^2 (t_1 - 1) + \sigma_2^2 t_2. \tag{17}$$

If one tries to minimize the bias squared by differentiating it w.r.t. \boldsymbol{G} and equating to zero, it results in the two equations

$$t_1 = -(\sigma_2^2/\sigma_1^2) t_2 \text{ and } t_1 = 1 - (\sigma_2^2/\sigma_1^2) t_2.$$
 (18)

The first equation leads to the bias $-\sigma_1^2$, which corresponds to a maximum for b^2 . The second equation yields b=0, which was discussed above to have no solution for \mathbf{G} . So this way does not lead to a minimum bias solution for the estimator.

As an alternative we start from the target function

$$H = \sigma_1^4 (1 - t_1)^2 + \sigma_2^4 t_2^2, \tag{19}$$

and we define the minimum bias estimator as the one that minimizes H. Assuming that C_2 is non-singular, differentiating H w.r.t. G and equating to zero, one obtains:

$$-(1-t_1)K_1G + v^4t_2K_2G = 0, (20a)$$

or

$$D\left(I - A^{0}\right)^{T}G = 0, \tag{20b}$$



where

$$D = \kappa I - C_2^{-1} C_1 \tag{20c}$$

$$\kappa = v^4 t_2 / (1 - t_1) \tag{20d}$$

and $v=\sigma_2/\sigma_1$. One solution to Eq. (20b) is that $\left(I-A^0\right)^TG=0$, which is the case with no solution for the VC discussed in Sect. 3. On the other hand, if $\left(I-A^0\right)^TG\neq 0$, Eqs. (20b) and (20c) imply that each column vector (χ) of $\left(I-A^0\right)^TG$ must satisfy the equation

$$\left(\kappa \mathbf{I} - \mathbf{C}_2^{-1} \mathbf{C}_1\right) \chi = \mathbf{0},\tag{21}$$

which is nothing but the equation for the eigenvector χ of the matrix $C_2^{-1}C_1$ (see e.g. Bjerhammar 1973, pp. 102 and 145), and the eigen-values κ can be determined from the determinant

$$\left| \kappa \mathbf{I} - \mathbf{C}_2^{-1} \mathbf{C}_1 \right| = 0. \tag{22}$$

Hence, by solving Eq. (22) each solution for κ yields a candidate for matrix \mathbf{D} , useful for computing the minimum bias non-negative VC.

A relevant question is, of course, which κ should be used for the BQMBNE. To answer this question we first return to Eq. (20a), which we post-multiply by G^T . The trace of the new equation becomes

$$-(1-t_1)t_1+v^4t_2^2=0, (23)$$

which, after considering also Eq. (20d), yields

$$t_1 = \kappa t_2 = \kappa^2 / \left(\kappa^2 + \nu^4\right) \tag{24}$$

and, from Eq. (19),

$$H = \sigma_1^4 \left[1 - \kappa^2 / \left(\kappa^2 + v^4 \right) \right]. \tag{25}$$

It is thus obvious that the minimum of H is provided by the largest eigen-value $\kappa=\lambda_{\rm max}$. From Eqs. (17) and (24) one can express the corresponding bias as

$$b = \sigma_1^2 v^2 \frac{\kappa - v^2}{\kappa^2 + v^4},\tag{26}$$

which also shows that that the bias approaches zero when κ goes to large values.

Returning to Eq. (20b), it follows (see Bjerhammar 1973, p.112) that

$$\left(\mathbf{I} - \mathbf{A}^{0}\right)^{\mathsf{T}} \mathbf{G} = \left(\mathbf{I} - \mathbf{D}^{0}\right) \mathbf{N},\tag{27}$$

where $D^0=D^-D$ and N is arbitrary (with compatible dimensions). Here D^- is an arbitrary generalized inverse to D. Inserting Eq. (27) into Eq. (15), the estimator for σ_1^2 becomes:

$$\tilde{\sigma}_1^2 = \mathbf{W}^\mathsf{T} \left(\mathbf{I} - \mathbf{D}^0 \right) \mathbf{U} \left(\mathbf{I} - \mathbf{D}^0 \right)^\mathsf{T} \mathbf{W},\tag{28a}$$

or, as $I - A^0$ is idempotent,

$$\tilde{\sigma}_1^2 = \stackrel{\leftarrow}{\mathbf{W}}^{\mathsf{T}} \left(\mathbf{I} - \mathbf{D}^0 \right) \mathbf{U} \left(\mathbf{I} - \mathbf{D}^0 \right)^{\mathsf{T}} \stackrel{\leftarrow}{\mathbf{W}}, \tag{28b}$$

where $U = NN^T$, which shows that the estimator is not unique.

Assuming that the observation errors are normally distributed, it follows from Eq. (28a) that the variance of the estimator is given by

$$\operatorname{Var}\left\{\tilde{\sigma}_{1}^{2}\right\} = 2\operatorname{tr}\left\{\operatorname{RURU}\right\},\tag{29a}$$

where

$$R = R^{T} = (I - D^{0})^{T} C (I - D^{0}).$$
 (29b)

By considering Eq. (20c) C can be rewritten as

$$C = C_2 \left[\left(\kappa \sigma_1^2 + \sigma_2^2 \right) I - \sigma_1^2 D \right], \tag{30}$$

so that Eq. (29b) reduces to

$$R = R^{T} = (\kappa \sigma_{1}^{2} + \sigma_{2}^{2}) (I - D^{0})^{T} C_{2} (I - D^{0})$$
$$= (\kappa \sigma_{1}^{2} + \sigma_{2}^{2}) P,$$
(31)

and Eq. (29a) becomes

$$\operatorname{Var}\left\{\tilde{\sigma}_{1}^{2}\right\} = 2\left(\kappa\sigma_{1}^{2} + \sigma_{2}^{2}\right)^{2}\operatorname{tr}\left\{\operatorname{PUPU}\right\}. \tag{32}$$

In view of Eq. (27) matrix $U=NN^T$ is not arbitrary, but related with matrix G, which in turn is constrained by Eq. (24). If the latter equation is rewritten in the form

$$t_2 = \operatorname{tr}\left(\mathbf{G}\mathbf{G}^\mathsf{T}\mathbf{K}_2\right) = \lambda_{\max}/\left(\lambda_{\max}^2 + \mathbf{v}^4\right),$$
 (33)

where λ_{max} has been defined as the eigen-value that minimizes the target function ("bias") H, and Eqs. (27) and (31) are considered, Eq. (33) can be written

$$t_2 = \operatorname{tr}\left[\mathsf{U}\left(\mathsf{I} - \mathsf{D}^0\right)^{\mathsf{T}} \mathsf{C}_2\left(\mathsf{I} - \mathsf{D}^0\right)\right] = \operatorname{tr}\left(\mathsf{UP}\right)$$
$$= \lambda_{\max} / \left(\lambda_{\max}^2 + \nu^4\right). \tag{34}$$

Hence, the remaining task is to find the minimum variance of Eq. (32) under the condition of Eq. (33). To solve this problem we define the target function

$$F = \operatorname{Var}\left\{\tilde{\sigma}_{1}^{2}\right\} - 4c\left[t_{2} - \lambda_{\max}/\left(\lambda_{\max}^{2} + \nu^{2}\right)\right], \quad (35)$$

where c is introduced as a Lagrange's multiplicator. The BQMBE is provided by the minimum for F w.r.t. U, which solution is obtained by the matrix equation

$$\frac{\partial F}{\partial U} = 0. {36}$$



UPU - cP = 0, (37)

where c is a constant to be determined below. Hence, we obtain

$$U = cP^{-}, \tag{38}$$

where P^- is any generalized inverse of P.

Now, the constant c is obtained by inserting Eq. (38) into Eq. (34). The result is

$$c = \frac{\lambda_{\text{max}}}{(\lambda_{\text{max}}^2 + \nu^4) t'},\tag{39}$$

where $t = \text{tr}(PP^-) = rank(P)$. Finally, the BQMBNE is obtained from Eqs. (38), (39) and (28a) or (28b):

$$\hat{\sigma}_1^2 = c \mathbf{W}^{\mathsf{T}} (\mathbf{I} - \mathbf{D}^0) \mathbf{P}^{-} (\mathbf{I} - \mathbf{D}^0)^{\mathsf{T}} \mathbf{W}$$
 (40a)

or

$$\hat{\sigma}_1^2 = c \bar{\mathbf{W}}^\mathsf{T} (\mathbf{I} - \mathbf{D}^0) \mathbf{P}^- (\mathbf{I} - \mathbf{D}^0)^\mathsf{T} \bar{\mathbf{W}}. \tag{40b}$$

In a similar way the BQMBNE of σ_2^2 can be estimated.

Note. The estimated variance component $\hat{\sigma}_1^2$ is unique with respect to the choice of inverse P^- . This is because both the trace of t and $(I-D^0)P^-\left(I-D^0\right)^T$ are invariant under a change of this inverse.

For a numerical example, see Sjöberg (2004).

4.1. A special case

Here we follow Sjöberg (1995) to present the explicit solution for the case with two VCs and *n* independent observations, yielding the covariance matrix of the observations:

$$\mathbf{Q} = \sigma_1^2 \mathbf{I} + \sigma_2^2 \mathbf{F},\tag{41a}$$

where

$$F = \text{diag.}(f_1, f_2, ..., f_n).$$
 (41b)

The VCs σ_1^2 and σ_2^2 are estimated for adjustment by elements:

$$AX = E\{L\}, \tag{42}$$

which corresponds to $\it Case 1$ of Sect. 1. It follows that the BQMBNEs can be expressed as

$$\hat{\sigma}_{1}^{2} = \frac{f_{\min}}{1 + v^{4} f_{\min}^{2}} \frac{\hat{\varepsilon}_{i}^{2}}{\sum_{k=1}^{n} (I - A^{0})_{ik}^{2} f_{k}} = d_{1} \hat{\varepsilon}_{i}^{2}$$
 (43a)

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and

$$\hat{\sigma}_{2}^{2} = \frac{f_{\text{max}}}{f_{\text{max}}^{2} + \nu^{-4}} \frac{\hat{\varepsilon}_{j}^{2}}{\sum_{k=1}^{n} (\mathbf{I} - \mathbf{A}^{0})_{ik}^{2} f_{k}} = d_{2}\hat{\varepsilon}_{j}^{2}, \quad (43b)$$

where f_{\min} and f_{\max} are the minimum and maximum elements of F and i and j denote the corresponding rows in the matrix $(I-A^0)$. The variances of these estimators become

$$\operatorname{Var} \left\{ \hat{\sigma}_{m}^{2} \right\} = 2d_{m}^{2} \left[\left(\sigma_{1}^{2} + \sigma_{2}^{2} f_{m} \right) - \mathbf{e}_{m}^{\mathsf{T}} \mathsf{A}^{\mathsf{0}} \mathbf{Q} \mathbf{e}_{m} \right]^{2}$$
$$= 2d_{m}^{2} \left(\sigma_{1}^{2} + \sigma_{2}^{2} f_{m} \right)^{2} \left[1 - \left(\mathsf{A}^{\mathsf{0}} \right)_{mm} \right]^{2}, \quad (44a)$$

where

$$d_1 = \frac{f_{\min}}{1 + v^4 f_{\min}^2} \frac{1}{\sum_{k=1}^{n} (\mathbf{I} - \mathbf{A}^0)_{k}^2 f_k}$$
(44b)

and

$$d_2 = \frac{f_{\text{max}}}{f_{\text{max}}^2 + v^{-4}} \frac{1}{\sum_{k=1}^{n} (\mathbf{I} - \mathbf{A}^0)_{ik}^2 f_k}.$$
 (44c)

Here m=1,2 and ${\bf e}$ is a vector with elements δ_{mi} and δ_{mj} , respectively, δ being Kronecker's delta function.

5. Concluding remark

In general the MINQUE is preferred to the BQMBNE, and this is primarily due to its property of being unbiased in opposite to the latter. However, if the MINQUE of a VC becomes negative, which is frequently a reality in additive VC models, the BQMBNE can solve the problem. A typical example is that the observation errors are the sums of two or more error components, whose variance components are to be estimated. It remains to generalize this approach to more than two VCs.

Acknowlegement

The author thanks Dr. Mehdi Eshagh for several comments and questions on the related chapter of Sjöberg (1984). These discussions inspired the author to formulate the present paper. Also, two reviewers provided a number of helpful suggestions to a first version of the manuscript. All these supports are cordially acknowledged.

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Journal of Geodetic Science

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