UNBIASED NONNEGATIVE-DEFINITE QUADRATIC ESTIMATION OF A SINGLE VARIANCE COMPONENT

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Abstract

Unbiased quadratic estimation of an individual variance component is considered under the additional requirement of nonnegative-definiteness. It is shown that this procedure automatically entails a reduction from the original model with k variance components to a submodel where the variance component that is to be estimated is the only remaining parameter.

1. Introduction

By definition, let a <u>variance component model</u> for a random $\mathbb{R}^n$-vector y be specified by linear decompositions of both the mean vector and the dispersion matrix:

$$y \sim (X\beta; \sum_{i=1}^{k} \sigma_i^2 V_i) , \tag{1.1}$$

where X is a known rectangular matrix, and $V_1, \cdots, V_k$ are known NND (symmetric and nonnegative-definite) matrices, while the parameters β, and $\sigma_1^2, \cdots, \sigma_k^2$ are to be estimated.

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For example, a general linear model $y = X\beta + \sum_{i=1}^{k} Z_i u_i$ with its standard assumptions for the random effects u_i leads to (1.1), with $V_i = Z_i Z_i'$.

We shall be concerned with estimating a single σ_j^2 by a quadratic form $y'Ay$ which is to be unbiased and NND. Negative estimates of variance components form a major problem in linear model theory; see the discussion in Searle (1971, pp. 406-408). Unbiased quadratic estimation under the additional constraint of nonnegative-definiteness was first investigated by LaMotte (1973). P. S. R. S. Rao and Chaubey (1977) proved our Theorem 1 for the particular model with heteroscedastic variances. Further results will be found in Pukelsheim (1976, 1977, 1978).

Theorem 1 below shows that unbiasedness and nonnegative-definiteness automatically imply a reduction from the original model (1.1) to the smaller model

$$Q_j y \sim (0;\ \sigma_j^2 Q_j V_j Q_j)\ , \tag{1.2}$$

where Q_j is an appropriately constructed projector (idempotent and symmetric matrix). In the Q_j-reduced model (1.2), σ_j^2 is the only surviving parameter; if $Q_j V_j Q_j \neq 0$ then

$$\frac{1}{\operatorname{trace} Q_j V_j Q_j V_j}\ y' Q_j V_j Q_j y \tag{1.3}$$

is an unbiased NND quadratic estimator for σ_j^2, and otherwise no such estimator exists.

2. Nonnegative Estimation of σ_j^2

An often accepted restriction in variance component estimation is that of considering the class of unbiased quadratic estimates which depend on y only through the residuals My, where

$$M := I_n - XX^+ . \tag{2.1}$$

This is not, however, a genuine restriction in the present context, since it is a consequence of unbiasedness and nonnegative-definiteness holding simultaneously:

Lemma 1. *If* $y'Ay$ *is* NND *and unbiased for* σ_j^2, *then* $y'Ay = (My)'A(My)$.

Proof. [2, p. 324], [3, p. 9]. In model (1.1), unbiasedness of $y'Ay$ for σ_j^2 implies $X'AX = 0$. Writing $A = B'B$, one obtains $BX = 0$, and $AX = B'BX = 0$. Hence $MAM = [I_n - X(X'X)^-X']A[I_n - X(X'X)^-X'] = A$. $\_/$

Lemma 1 states that for the present estimation procedure it suffices to investigate the M-reduced model

$$My \sim (0; \Sigma\sigma_i^2 MV_iM) , \tag{2.2}$$

rather than the original model (1.1). A similar argument now leads to the Q_j-reduced model (1.2). Define

$$\begin{aligned} V &:= \Sigma V_i , \\ Q_j &:= M - M(V - V_j)M[M(V - V_j)M]^+ , \end{aligned} \tag{2.3}$$

i.e., Q_j projects onto the orthogonal complement of the nullspace of $M(V - V_j)M$ in the range of M.

Lemma 2. *If* $y'Ay$ *is* NND *and unbiased for* σ_j^2, *then* $y'Ay = (Q_jy)'A(Q_jy)$.

Proof. [4, p. 14]. In model (2.2), unbiasedness of $y'Ay$ for σ_j^2 implies $0 = \text{trace } AMV_iM$ for $i \neq j$, and summation yields $0 = \text{trace } AM(V - V_j)M$. Writing $A = B'B$, and $M(V - V_j)M = \sum_{i \neq j} MV_iM = CC'$, one obtains $0 = \text{trace } B'BCC' = \|BC\|^2$, and $AC = B'BC = 0$. Because of $Q_j = I_n - XX^+ - CC^+$, this entails $Q_jAQ_j = A$. $\_/$

The projector Q_j is such that $Q_j X = 0$, and $Q_j M V_i M = 0$ for $i \neq j$. [Sketch of proof: It suffices to show that

$$M \sum_{\ell \neq j} V_\ell M [M \sum_{\ell \neq j} V_\ell M]^+ M V_i M = M V_i M$$

for $i \neq j$. For a fixed $i \neq j$, this may be identified with the general case $(DD' + EE')(DD' + EE')^+ D = D$. The latter equation is proved as follows:

(i) $(DD' + EE')(DD' + EE')^+$ projects onto the range (column space) of $DD' + EE'$.

(ii) But because of $DD' + EE' = [D : E][D : E]'$, the range of $DD' + EE'$ coincides with that of $[D : E]$, and hence contains the range of D.]

Thus Lemma 2 means a restriction to the Q_j-reduced model (1.2). Up to now we worked under the assumption that an unbiased NND quadratic estimator for σ_j^2 exists, but Q_j also allows us to ascertain such existence.

Lemma 3. <u>There exists an unbiased NND quadratic estimator for σ_j^2 if and only if</u> $Q_j V_j Q_j \neq 0$.

Proof. Direct part. The proof of Theorem 4.1 in [3, p. 11] yields a vector x such that $M(V - V_j)Mx = 0 \neq MV_j Mx$. For this x one obtains $x'Q_j V_j Q_j x = x'MV_j Mx \neq 0$, hence $Q_j V_j Q_j \neq 0$.

Converse part. Since trace $Q_j V_j Q_j V_j = \|Q_j V_j Q_j\|^2 \neq 0$, the assertion is satisfied by the estimator in (1.3). _/

In summary, unbiased NND estimation of a single variance component always reduces to the trivial case (1.2) with one and only one variance component:

Theorem 1. In model (1.1) there exists an unbiased NND quadratic estimator for any individual variance component σ_j^2 if and only if $Q_j V_j Q_j \neq 0$. In this case every such estimator depends on y only through $Q_j y$, i.e., attention may be restricted to the Q_j-reduced model (1.2) with standard estimate (1.3). _/

Note that one may reformulate the present setup so that Lemma 2 precedes Lemma 1, with necessary changes. That is, $0 = \text{trace } A(V - V_j)$ implies a reduction to $\bar{Q}Y \sim (\bar{Q}X\beta;\ \sigma_j^2 \bar{Q}V_j Q)$, where $\bar{Q} := I_n - (V - V_j)(V - V_j)^+$; and an equivalent of Lemma 1 leads to $\bar{M}\bar{Q}Y \sim (0;\ \sigma_j^2 \bar{M}\bar{Q}V_j \bar{Q}\bar{M})$, where $\bar{M} = I_n - \bar{Q}X(\bar{Q}X)^+$. This approach was chosen by P. S. R. S. Rao and Chaubey (1977, pp. 7-8).

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