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ON NONNEGATIVE QUADRATIC UNBIASED ESTIMABILITY OF VARIANCE COMPONENTS

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Under a quadratic subspace condition, Pukelsheim (1981a) has proved that for estimating linear combinations of variance components, either standard methods provide a nonnegative quadratic unbiased estimate or such an estimate does not exist. This result is proved, replacing the quadratic subspace condition by a weaker condition. This answers in the negative a question raised by Pukelsheim (1981b).

1. Introduction. Recently Hartung (1981) and Pukelsheim (1981a) have made significant contributions to the theory of nonnegative estimation of variance components. While Hartung has proposed nonnegative quadratic estimates by dropping unbiasedness, Pukelsheim is concerned with nonnegative quadratic unbiased estimability. The present paper is devoted to nonnegative quadratic unbiased estimability and is inspired by Pukelsheim's work.

Under a quadratic subspace condition, Pukelsheim (1981a) has proved that for a linear combination of variance components, either the standard unbiased estimate (which is the MINQUE given I_n) is nonnegative or a nonnegative quadratic unbiased estimate does not exist. In a subsequent paper, Pukelsheim (1981b) raises the question of whether the quadratic subspace condition is necessary for such a property to hold. The present paper answers this question in the negative and obtains a necessary and sufficient condition for such a property to hold. The reader is referred to Seely (1970) for additional background information.

2. Nonnegative quadratic unbiased estimation. We use the same notations as in Pukelsheim (1981a). Let the random R^n-vector Y have mean vector $X\beta$ and dispersion matrix $\sum_{j=1}^{\ell} \tau_j V_j$, where β is a vector of unknown parameters, $\tau = (\tau_1, \tau_2, \cdots, \tau_\ell)'$ is the unknown vector of variance components, X is a known matrix and $V_1, V_2, \cdots, V_\ell$ are known real symmetric $n \times n$ matrices. The above model is denoted as $Y \sim (X\beta, \sum \tau_j V_j)$. We assume

$$\tau \in \bar{G} = \{t = (t_1, t_2, \cdots, t_\ell)' \mid \sum t_j V_j \text{ is nnd}\}.$$

Let

$$M = I - X(X'X)^- X' \text{ and } S_M = ((\text{tr } MV_i MV_j))(i, j = 1, 2, \cdots, \ell).$$

Then $q'\tau = q_1\tau_1 + q_2\tau_2 + \cdots + q_\ell\tau_\ell$ has a quadratic unbiased estimate iff q lies

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in the range of S_M. Thus if $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_\ell)'$ is such that $S_M\lambda = q$, then a quadratic unbiased estimate of $q'\tau$ is $Y'(\sum \lambda_j MV_jM)Y$. This is the MINQUE (given I_n) of $q'\tau$ and is referred to as the standard unbiased estimate by Pukelsheim (1981a).

We now introduce the following definition.

DEFINITION. Let $\mathscr{B}$ be a subspace of real symmetric $n \times n$ matrices. Let P be the projector onto $\mathscr{B}$ orthogonal with respect to the trace inner product $(A, B) = \operatorname{tr} A'B$. We say that $\mathscr{B}$ preserves nonnegative definiteness if $P(A)$ is nnd whenever A is nnd.

Lemma 2 in Pukelsheim (1981a) states that a quadratic subspace preserves nonnegative definiteness. The author has not been able to obtain a necessary and sufficient condition (in a verifiable form) for a subspace to preserve nonnegative definiteness, other than the following Lemma 1. Lemma 2 proved below gives a sufficient condition which is also necessary in some special cases.

LEMMA 1. *For a real symmetric matrix B, let B_+ and B_- denote the positive and negative parts of B respectively. Then a subspace $\mathscr{B}$ of real symmetric matrices preserves nonnegative definiteness iff $B_+ \in \mathscr{B}$ whenever $B \in \mathscr{B}$.*

PROOF. Let $B_+ \in \mathscr{B}$ whenever $B \in \mathscr{B}$. Then from the proof of Lemma 2 of Pukelsheim (1981a) it follows that $\mathscr{B}$ preserves nonnegative definiteness. Conversely let $\mathscr{B}$ preserve nonnegative definiteness and let $B \in \mathscr{B}$. Then $B_+ - B_- = B = P(B) = P(B_+) - P(B_-)$. Hence $\| B_+ \|^2 + \| B_- \|^2 = \| P(B_+) \|^2 + \| P(B_-) \|^2 - 2 \operatorname{tr} P(B_+)P(B_-) \leq \| P(B_+) \|^2 + \| P(B_-) \|^2$ (since $P(B_+)$ and $P(B_-)$ are nnd). The above inequality implies $B_+ = P(B_+)$ or equivalently $B_+ \in \mathscr{B}$. □

LEMMA 2. *Let $\mathscr{B}$ be a k-dimensional subspace of real symmetric $n \times n$ matrices and let $U_1, U_2, \cdots, U_k$ be an orthonormal basis for $\mathscr{B}$ (with respect to the trace inner product). Let $\sum_{j=1}^k U_j \otimes U_j$ is nnd, then $\mathscr{B}$ preserves nonnegative definiteness. The above condition is also necessary if $\mathscr{B}$ is a commutative subspace or if $k = 2$.*

PROOF. Let A be nnd. We have $P(A) = \sum_{j=1}^k (\operatorname{tr} AU_j)U_j$. Thus $\mathscr{B}$ preserves nonnegative definiteness iff $\sum_{j=1}^k (\operatorname{tr} AU_j)U_j$ is nnd for every A nnd iff $\sum (a'U_ja)U_j$ is nnd for every real vector a iff $\sum (a'U_ja)(b'U_jb) \geq 0$ for all real vectors a and b iff

$$(1) \qquad (a' \otimes b')(\textstyle\sum U_j \otimes U_j)(a \otimes b) \geq 0$$

for all real vectors a and b, which is satisfied if $\sum U_j \otimes U_j$ is nnd. If $\mathscr{B}$ is a commutative subspace, then the U_i's could be reduced to diagonal matrices using the same orthogonal matrix; it then follows that (1) holds for all real vectors a and b iff $\sum U_j \otimes U_j$ is nnd. If $\mathscr{B}$ preserves nonnegative definiteness, then from Lemma 1 it follows that $\mathscr{B}$ has a basis consisting of nnd matrices. When $k = 2$, let B_1 and B_2 form such a basis for $\mathscr{B}$. Then there exists a nonsingular matrix T

such that $T'B_1T$ and $T'B_2T$ are diagonal (see Theorem 6.2.3 in Rao and Mitra, 1971). Hence $T'BT$ is diagonal for every $B \in \mathscr{B}$. Thus when $k = 2$, (1) holds for all a and b iff $\sum_{j=1}^{2} U_j \otimes U_j$ is nnd. □

REMARK. From the proof of Lemma 2, it is clear that if there exists a nonsingular matrix T such that $T'U_iT$ is diagonal for $i = 1, 2, \cdots, k$, then the condition given in Lemma 2 is also necessary. That this is not true in general can be seen from the following example. Let $\mathscr{B}$ be the vector space of all real 2×2 symmetric matrices. Then clearly $\mathscr{B}$ preserves nonnegative definiteness. Consider the orthonormal basis

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad U_3 = \begin{pmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix}.$$

Then (1) holds for all a and b, but $\sum_{j=1}^{3} U_j \otimes U_j$ is not nnd.

For the model $Y \sim (X\beta, \sum \tau_j V_j)$, let $\mathscr{B}_M$ be the linear span of $MV_1M, \cdots, MV_\ell M$ and let $\bar{G}_M = \{t = (t_1, t_2, \cdots, t_\ell)' \mid \sum t_j MV_j M \text{ is nnd}\}$. Let $\mathscr{L}$ be the set of all R^ℓ-vectors q such that $q'\tau$ has a nonnegative quadratic unbiased estimator. Pukelsheim (1981a) has observed that $\mathscr{L} \supset S_M(\bar{G}_M)$ and if $\mathscr{B}_M$ is an ℓ-dimensional quadratic subspace, then $\mathscr{L} = S_M(\bar{G}_M)$, i.e. $q'\tau$ has a nonnegative quadratic unbiased estimate iff its standard unbiased estimate is nonnegative. That this interesting observation is valid in a more general setup is the main result of this paper, proved below.

THEOREM. *$\mathscr{L} = S_M(\bar{G}_M)$ iff $\mathscr{B}_M$ preserves nonnegative definiteness.*

PROOF. Suppose $\mathscr{B}_M$ preserves nonnegative definiteness. Let $q \in \mathscr{L}$. From the proof of Theorem 1 in Pukelsheim (1981a), we get

$$q = (\text{tr } AMV_1M, \cdots, \text{tr } AMV_\ell M)'$$

for some nnd A. Then $P(A) = \sum t_j MV_j M$ is nnd and $\text{tr } AMV_iM = \sum_j t_j \text{tr } MV_iMV_jM$. Hence $q \in S_M(\bar{G}_M)$. Thus $\mathscr{L} \subset S_M(\bar{G}_M)$. Since the other inclusion always holds, we get $\mathscr{L} = S_M(\bar{G}_M)$. Conversely suppose $\mathscr{L} = S_M(\bar{G}_M)$. Hence for any nnd A, there exists $\lambda \in \bar{G}_M$ satisfying $(\text{tr } AMV_1M, \cdots, \text{tr } AMV_\ell M)' = S_M\lambda$, which implies $\text{tr } AMV_iM = \text{tr} V_i \sum_j \lambda_j MV_jM$. Writing $P(A) = \sum t_j MV_jM$, the above equality implies $\text{tr } AMV_iM = \text{tr } P(A)MV_iM = \text{tr } V_i \sum_j t_jMV_jM = \text{tr } V_i \sum_j \lambda_j MV_jM$, which implies $P(A) = \sum t_jMV_jM = \sum_j \lambda_j MV_jM$, which is nnd since $\lambda \in \bar{G}_M$. Thus $\mathscr{B}_M$ preserves nonnegative definiteness. □

The proof of the "if" part of the theorem is also clear from the proof of Theorem 2 in Pukelsheim (1981a) since the only condition used in his proof is that $\mathscr{B}_M$ preserves nonnegative definiteness. Unlike Pukelsheim (1981a), we have not assumed that $\mathscr{B}_M$ is ℓ-dimensional.

In practice (for example when the dispersion matrix is $\sigma^2 V$), there are subspaces which preserve nonnegative definiteness, but may not be quadratic subspaces. Consider the model $Y \sim (0, \sum_{j=1}^{\ell} \sigma_j^2 V_j)$, where $V_j = \text{diag}(0, 0, \cdots, V_{j0}, 0, \cdots, 0)$, i.e. V_j has its jth diagonal block the nnd matrix V_{j0} and zeros elsewhere. Since $V_i V_j$ is the null matrix (for $i \neq j$) the subspace $\mathscr{B}$ spanned by $V_1, V_2, \cdots, V_\ell$ has an orthonormal basis consisting of nnd matrices. From Lemma 2 it follows that $\mathscr{B}$ preserves nonnegative definiteness for any choice of the nnd matrices $V_{j0} (j = 1, 2, \cdots, \ell)$. However, $\mathscr{B}$ need not be a quadratic subspace.

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