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QUADRATIC UNBIASED ESTIMATION OF NONSTANDARD PARAMETRIC FUNCTIONS

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ABSTRACT. Almost all topics in quadratic estimation deal with linear functions of variance components in a normal linear model. Considering a seminormal linear model we characterize all quadratically estimable parametric functions. Moreover, for such functions, the Uniformly Best Quadratic Unbiased Estimators and their variances are given.

1. Introduction and notation

Almost all topics in quadratic estimation (see, e.g. Rao and Kleffe [4]) restrict to linear functions of variance components in a normal linear model. Several years ago Pázman [2], [3], Štulajter [6], [7], and Volaufová [8] considered unbiased estimation of some nonlinear functions of the mean (cf. Kubáček [1; Sec. 6.4]). Some of the problems reduce to quadratic estimation.

We focus on quadratic unbiased estimation in a seminormal linear model. All quadratically estimable parametric functions are characterized. Moreover, for such functions, the uniformly best quadratic unbiased estimators and their variances are given explicitly. Throughout this paper the usual matrix notation is used. Among others, if $\mathbf{M}$ is a matrix, then by $\mathbf{M}'$, $R(\mathbf{M})$, $r(\mathbf{M})$ and $P_{\mathbf{M}}$ are denoted, respectively, its transpositon, range (column space), rank and the orthogonal projector on $R(\mathbf{M})$.

If $\mathbf{M}$ is quadratic, then $\operatorname{tr}\mathbf{M}$ denotes its trace. Moreover, the symbols $\mathbb{R}^n$ and $\mathcal{S}_n$ stand, respectively, for the space of $n \times 1$ vectors and for the space of $n \times n$ symmetric matrices.

Let $\boldsymbol{X}$ be a normal random vector in $\mathbb{R}^n$ with expectation $\mathbf{A}\beta$ and covariance matrix $\sigma\mathbf{K}$ where $R(\mathbf{A}) \subseteq R(\mathbf{K})$.

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Then there exists a nonsingular linear transformation F such that

$$\mathbf{X} = F \begin{bmatrix} \mathbf{Y}_1 \\ \dots \\ \mathbf{Y}_2 \end{bmatrix},$$

where $\mathbf{Y}_1$ has covariance matrix $\sigma \mathbf{I}_{n_1}$ for some $n_1 \leq n$ and $\mathbf{Y}_2 = \mathbf{O}$ with probability one. Thus without loss of generality one can assume that $\mathbf{K} = \mathbf{I}_n$.

It is well known (cf. Searle [5; p. 57 and 451]) that if $\mathbf{X} \sim N(\mathbf{A}\beta, \sigma\mathbf{I}_n)$ then for arbitrary $\mathbf{Q}, \mathbf{Q}_1, \mathbf{Q}_2 \in \mathcal{S}_n$

$$E(\mathbf{X}'\mathbf{Q}\mathbf{X}) = \sigma \operatorname{tr} \mathbf{Q} + \beta'\mathbf{A}'\mathbf{Q}\mathbf{A}\beta, \tag{1.1}$$

$$\operatorname{var}(\mathbf{X}'\mathbf{Q}\mathbf{X}) = 2\sigma^2 \operatorname{tr} \mathbf{Q}^2 + 4\sigma\beta'\mathbf{A}'\mathbf{Q}^2\mathbf{A}\beta, \tag{1.2}$$

$$\operatorname{cov}(\mathbf{X}'\mathbf{Q}_1\mathbf{X}, \mathbf{X}'\mathbf{Q}_2\mathbf{X}) = 2\sigma^2 \operatorname{tr}(\mathbf{Q}_1\mathbf{Q}_2) + 4\sigma\beta'\mathbf{A}'\mathbf{Q}_1\mathbf{Q}_2\mathbf{A}\beta. \tag{1.3}$$

DEFINITION 1.1. We shall say that a random vector $\mathbf{X} \in \mathbb{R}^n$ is *subject* to a seminormal linear model and write $\mathbf{X} \sim SN(\mathbf{A}\beta, \sigma\mathbf{I}_n)$ if the conditions (1.1) – (1.3) are satisfied.

Some results on quadratic unbiased estimation in a seminormal linear model are presented in the next section.

2. The results

THEOREM 2.1. *Let $\mathbf{X}$ be subject to a seminormal linear model $SN(\mathbf{A}\beta, \sigma\mathbf{I}_n)$, where $\mathbf{A}$ is a given $n \times p$ matrix such that $r(\mathbf{A}) < n$, $\beta \in \mathbb{R}^P$ is unknown, while $\sigma > 0$ can be known or not. Then*

(a) *A parametric function $\psi = \psi(\beta, \sigma)$ is unbiasedly estimable among quadratic forms of $\mathbf{X}$ if and only if*

$$\psi(\beta, \sigma) = c\sigma + \beta'\mathbf{C}\beta, \tag{2.1}$$

where c is a scalar and $\mathbf{C}$ is a symmetric matrix of order p such that $R(\mathbf{C}) \subseteq R(\mathbf{A}')$.

(b) *A quadratic form $\mathbf{X}'\mathbf{Q}\mathbf{X}$ is the Uniformly Best Quadratic Unbiased Estimator (UBQUE) of its expectation if and only if $\mathbf{Q} \in \mathcal{T}$, where*

$$\mathcal{T} = \{\mathbf{T} \in \mathcal{S}_n : \ \mathbf{T} = c\mathbf{I}_n + \mathbf{S}, \ c \in \mathbb{R}, \ R(\mathbf{S}) \subseteq R(\mathbf{A})\}. \tag{2.2}$$

(c) *If $\psi(\beta, \sigma) = c\sigma + \beta'\mathbf{C}\beta$ is unbiasedly estimable and $\mathbf{C} = \sum_{i=1}^{p} \lambda_i \mathbf{v}_i \mathbf{v}_i'$ is the canonical form of $\mathbf{C}$ then the UBQUE of ψ may be presented in the form $\mathbf{X}'\mathbf{Q}\mathbf{X}$, where*

$$\mathbf{Q} = \sum_{i=1}^{p} \lambda_i \mathbf{w}_i \mathbf{w}_i' + c_o(\mathbf{I}_n - \mathbf{P}_A), \tag{2.3}$$

while $\mathbf{w}_i$ *is the unique vector in* $R(\mathbf{A})$ *satisfying the equation*

$$\mathbf{A}'\mathbf{w}_i = \mathbf{v}_i\,, \qquad i = 1, \ldots, p, \tag{2.4}$$

and

$$c_o = \frac{c - \sum \lambda_i \mathbf{w}_i' \mathbf{w}_i}{n - r(\mathbf{A})}\,.$$

Proof.

(a) The necessity of (2.1) follows directly from (1.1). On the other hand, if $R(\mathbf{C}) \subseteq R(\mathbf{A}')$ then the equation (2.4) is consistent. Now one can easily verify that (2.3) satisfies $E(\boldsymbol{X}'\mathbf{Q}\boldsymbol{X}) = \psi(\boldsymbol{\beta}, \sigma)$.

(b) It follows from (1.1) that a quadratic form $\boldsymbol{X}'\mathbf{N}\boldsymbol{X}$ is an unbiased estimator of zero if and only if $\operatorname{tr}\mathbf{N} = 0$ and $\mathbf{A}'\mathbf{N}\mathbf{A} = \mathbf{O}$. These two conditions can be rewritten in the form $\mathbf{N} \in \mathcal{T}^{\perp}$, where $\mathcal{T}^{\perp} = \{\mathbf{Q} \in \mathcal{S}_n :\ \operatorname{tr}(\mathbf{QT}) = 0$ for any $\mathbf{T} \in \mathcal{T}\}$, while $\mathcal{T}$ is defined in (2.2). Thus by Lehmann-Scheffé theorem we only need to show that

$$\operatorname{cov}(\boldsymbol{X}'\mathbf{Q}\boldsymbol{X}, \boldsymbol{X}'\mathbf{N}\boldsymbol{X}) = 0 \qquad \text{for any} \quad \mathbf{N} \in \mathcal{T}^{\perp} \tag{2.5}$$

if and only if $\mathbf{Q} \in \mathcal{T}$.

By formula (1.3) we get

$$\operatorname{cov}(\boldsymbol{X}'\mathbf{Q}\boldsymbol{X}, \boldsymbol{X}'\mathbf{N}\boldsymbol{X}) = \sigma \operatorname{tr}\big[(\mathbf{QB} + \mathbf{BQ})\mathbf{N}\big] = 2\sigma \operatorname{tr}(\mathbf{QBN})\,,$$

where $\mathbf{B} = \sigma\mathbf{I} + 2\mathbf{A}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{A}'$.

Thus the condition (2.5) reduces to

$$\mathbf{QB} + \mathbf{BQ} \in \mathcal{T} \qquad \text{for any} \quad \mathbf{B} \in \mathcal{T}. \tag{2.6}$$

Now the necessity of the condition $\mathbf{Q} \in \mathcal{T}$ follows from putting in (2.6) $\mathbf{B} = \mathbf{I}$, while the sufficiency follows from the fact that the set $\mathcal{T}$ constitutes a Jordan space, that is it satisfies the condition $\mathbf{T}_1\mathbf{T}_2 + \mathbf{T}_2\mathbf{T}_1 \in \mathcal{T}$ for arbitrary $\mathbf{T}_1, \mathbf{T}_2 \in \mathcal{T}$.

(c) By the first and the second part of the proof it remains to note that the matrix $\mathbf{Q}$ defined in (2.3) belongs to the set $\mathcal{T}$ defined in (2.2) and satisfies the condition $E(\boldsymbol{X}'\mathbf{Q}\boldsymbol{X}) = \psi$. □

COROLLARY 2.2. *All UBQUE's constitute a Jordan space.*

Remark 2.1. The matrix $\mathbf{I}_n$ appearing in the formula (2.2) can be replaced by the orthogonal projector $\mathbf{I}_n - \mathbf{P}_{\mathbf{A}}$.

A corresponding result for the case $r(\mathbf{A}) = n$ is given in:

THEOREM 2.3. *Let* $\mathbf{X}$ *be subject to a seminormal linear model* $SN(\mathbf{A}\beta, \sigma\mathbf{I}_n)$, *where* $\mathbf{A}$ *is a given* $n \times p$ *matrix such that* $r(\mathbf{A}) = n$, $\boldsymbol{\beta} \in \mathbb{R}^p$ *is unknown while* $\sigma > 0$ *can be known or not. Then*

(a) *Any quadratic form* $\mathbf{X}'\mathbf{Q}\mathbf{X}$ *is the UBQUE of its expectation.*

(b) *A parametric function* $\psi = \psi(\boldsymbol{\beta}, \sigma)$ *is unbiasedly estimable among quadratic forms of* $\mathbf{X}$ *if and only if*

$$\psi(\boldsymbol{\beta}, \sigma) = c\sigma + \boldsymbol{\beta}'\mathbf{C}\boldsymbol{\beta}, \tag{2.7}$$

where $\mathbf{C}$ *is a symmetric matrix of order* p *such that* $R(\mathbf{C}) \subseteq R(\mathbf{A}')$ *and* $c = \operatorname{tr}[\mathbf{C}(\mathbf{A}'\mathbf{A})^+]$, *where* $^+$ *means the Moore-Penrose generalized inverse.*

(c) *If* $\psi(\boldsymbol{\beta}, \sigma) = c\sigma + \boldsymbol{\beta}'\mathbf{C}\boldsymbol{\beta}$ *is unbiasedly estimable then its UBQUE can be presented in the form* $\mathbf{X}'\mathbf{Q}\mathbf{X}$, *where*

$$\mathbf{Q} = (\mathbf{A}\mathbf{A}')^{-1}\mathbf{A}\mathbf{C}\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}. \tag{2.8}$$

P r o o f. The assertion (a) follows directly from the fact that $\mathbf{X}'\mathbf{Q}\mathbf{X}$ is an unbiased estimator of zero if and only if $\mathbf{Q} = \mathbf{O}$. Hence to prove (b) and (c) we only need to show that

$$E(\mathbf{X}'\mathbf{Q}\mathbf{X}) = c\sigma + \beta'\mathbf{C}\beta \tag{2.9}$$

if and only if $R(\mathbf{C}) \subseteq R(\mathbf{A}')$, $c = \operatorname{tr}[\mathbf{C}(\mathbf{A}'\mathbf{A})^+]$ and $\mathbf{Q}$ satisfies the condition (2.8).

Really, the condition (2.9) by (1.1) implies

$$\mathbf{A}'\mathbf{Q}\mathbf{A} = \mathbf{C} \tag{2.10}$$

and, in consequence, $R(\mathbf{C}) \subseteq R(\mathbf{A}')$. Next, by left-side and right-side multiplication of (2.10) by $(\mathbf{A}\mathbf{A}')^{-1}\mathbf{A}$ and $\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}$, respectively, we get (2.8). Moreover $c = \operatorname{tr}\mathbf{Q} = \operatorname{tr}[\mathbf{C}\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-2}\mathbf{A}]$. One can easily verify that $\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-2}\mathbf{A}$ is just equal to $(\mathbf{A}'\mathbf{A})^+$. On the other hand, if $R(\mathbf{C}) \subseteq R(\mathbf{A}')$ and $c = \operatorname{tr}[\mathbf{C}(\mathbf{A}'\mathbf{A})^+]$, then the matrix (2.8) satisfies the condition $E(\mathbf{X}'\mathbf{Q}\mathbf{X}) = \psi$, completing the proof. □

Remark 2.2. Under additional assumption $p = n$ the condition (2.8) can be replaced by $\mathbf{Q} = (\mathbf{A}^{-1})'\mathbf{C}\mathbf{A}^{-1}$.

A consequence of the Theorems 2.1 and 2.3 is the following theorem:

THEOREM 2.4. *Let* X *be subject to a seminormal linear model* $SN(\mathbf{A}\beta, \sigma\mathbf{I}_n)$, *where* $\mathbf{A}$ *is a given* $n \times p$ *matrix,* $\boldsymbol{\beta} \in \mathbb{R}^p$ *is unknown, while* $\sigma > 0$ *can be known or not. Then*

(a) *The parameter* σ *is estimable by quadratics of* X *if and only if* $r(\mathbf{A}) < n$ *and, if so, the variance of its UBQUE is* $\frac{2\sigma^2}{n - r(\mathbf{A})}$.

(b) *If* $\psi(\boldsymbol{\beta},\sigma) = c\sigma + \boldsymbol{\beta}'\mathbf{C}\boldsymbol{\beta}$ *is estimable and* $\mathbf{C} = \sum_{i=1}^{p} \lambda_i \mathbf{v}_i \mathbf{v}_i'$ *is the canonical form of* $\mathbf{C}$ *then all parametric functions* $\varphi_i = \mathbf{v}_i'\boldsymbol{\beta}$, $i = 1,\dots,p$, *are estimable by linear forms of* $\mathbf{X}$.

(c) *If* $r(\mathbf{A}) < n$ *and* ψ *is estimable then the UBQUE of* ψ *may be presented in the form* $\hat{\psi} = \sum_{i=1}^{p} \lambda_i(\hat{\varphi}_i)^2 + \left[c - \frac{1}{\sigma}\sum_{i=1}^{p} \lambda_i \operatorname{var}(\hat{\varphi}_i)\right]\hat{\sigma}$, *where* $\hat{\varphi}_i$ *is the UBLUE of* φ_i, $\hat{\sigma}$ *is the UBQUE of* σ *and*

$$\operatorname{var}(\hat{\psi}) = 2\sum_i\sum_j \lambda_i\lambda_j\left[\operatorname{cov}(\hat{\varphi}_i,\hat{\varphi}_j)\right]^2 + 2\frac{\left[c\sigma - \sum_i \lambda_i \operatorname{var}(\hat{\varphi}i)\right]^2}{n - r(\mathbf{A})} + 4\sum_i\sum_j \lambda_i\lambda_j\varphi_i\varphi_j \operatorname{cov}(\hat{\varphi}_i,\hat{\varphi}_j)\,.$$

(d) *If* $r(\mathbf{A}) = n$ *and* ψ *is estimable then the UBQUE of* ψ *may be presented in the form* $\hat{\psi} = \sum_{i=1}^{p} \lambda_i(\hat{\varphi}_i)^2$, *where* $\hat{\varphi}_i$ *is the UBLUE of* φ_i *and*

$$\operatorname{var}(\hat{\psi}) = 2\sum_i\sum_j \lambda_i\lambda_j\left[\operatorname{cov}(\hat{\varphi}_i,\hat{\varphi}_j)\right]^2 + 4\sum_i\sum_j \lambda_i\lambda_j\varphi_i\varphi_j \operatorname{cov}(\hat{\varphi}_i,\hat{\varphi}_j)\,.$$

Proof.

(a) follows directly from Theorems 1.1(a) and 2.3(b) while (b) follows from formula (2.4).

(c) and (d): We only need to use (2.3), (2.8) and (1.2) taking into consideration that the UBLUE of $\varphi_i = v_i'\boldsymbol{\beta}$, $i = 1,\dots,p$, is $\hat{\varphi}_i = \mathbf{w}_i'\mathbf{X}$, $\operatorname{var}(\hat{\varphi}_i) = \sigma\mathbf{w}_i'\mathbf{w}_i$ and $\operatorname{cov}(\hat{\varphi}_i,\hat{\varphi}_j) = \sigma\mathbf{w}_i'\mathbf{w}_j'$, for $i,j = 1,\dots,p$ and, moreover, that the matrix $\mathbf{Q}$ defined by (2.8) may be presented in the form $\mathbf{Q} = \sum_i \lambda_i \mathbf{w}_i \mathbf{w}_i'$. □

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