

INVARIANT QUADRATIC UNBIASED ESTIMATION FOR TWO VARIANCE COMPONENTS

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For a normally distributed mixed model with two unknown variance components θ_1 and θ_2 , a tractable characterization is given for the admissible estimators within the class \mathcal{N}_{δ} of invariant quadratic unbiased estimators for $\delta_1\theta_1 + \delta_2\theta_2$. Here the term admissible is used with reference only to the class \mathcal{N}_{δ} . This characterization is based on a result for general linear models which characterizes the admissible estimators within the class of linear unbiased estimators. The admissibility of MINQUE estimators and the usual analysis of variance estimators is considered.

1. Introduction and summary. Unbiased quadratic estimation of variance components has received considerable attention in the literature. For example, see Searle [11] for a review of the literature prior to 1970 and more recently see Rao [7, 8] where the MINQUE (Minimum Norm Quadratic Unbiased Estimation) theory is developed. Although quadratic unbiased estimators can have serious drawbacks such as negative estimates, they are still the most commonly employed variance component estimators. In this paper a class of quadratic unbiased estimators which are invariant under a natural translation group is investigated. For this class of estimators the minimal complete class is characterized for a mixed model having two unknown variance components. We give a very tractable characterization of the minimal complete class; but we have not attempted, except in one special case, to recommend any one particular estimator. However, our results constitute the starting point for any further such investigation. Additionally, our results provide a routine check which any proposed invariant quadratic unbiased estimator should pass, i.e., it should belong to the minimal complete class. In this regard we have found that the MINQUE estimators are in, but do not exhaust, the minimal complete class; whereas in many circumstances the usual analysis of variance (Henderson III) estimator for the random "block" effect variance component is not a member of the minimal complete class.

Our underlying concern is to answer the question of which variance component estimators are admissible when attention is restricted to the class of invariant quadratic unbiased estimators. Our basic theoretical results, however, are not confined to this question and are stated in terms of linear unbiased

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estimators in a very general linear model framework. These results are given in Section 3 (see Proposition 3.3 and Corollary 3.7) and are completely independent of, although motivated by, the development in Sections 2, 4, 5 and 6, which deal specifically with invariant quadratic estimation for two variance components.

The completely random one-way classification model is a special case of the model we consider. For this model the notion of an admissible quadratic unbiased estimator has been explored by Harville [4]; but with the exception of Section 2 our results are of a different flavor. We approach the problem along the lines in [14] as this allows many standard results from linear model theory to be utilized.

In Section 2 we introduce the mixed model with two variance components and via sufficiency reduce the class of invariant quadratic unbiased estimators to a complete class in Theorem 2.2. This theorem allows us to conveniently consider the variance component problem within a standard linear model setup. Using the results of Section 3, we reduce the complete class obtained in Section 2 to a minimal complete class in Section 4. In Section 5 we give a means of calculating the estimators in the minimal complete class via normal equations. And in Section 6 we consider how MINQUE and the usual analysis of variance estimators relate to the minimal complete class.

Some notation we use throughout is $\mathbf{R}(A)$, $\mathbf{N}(A)$, $\mathbf{r}(A)$, A' , and A^- to denote the range, null space, rank, transpose, and g -inverse respectively of a matrix A . Other notation will be introduced as needed.

2. The two variance component model—an initial reduction. We consider a random vector Y distributed according to an n -dimensional normal distribution with mean vector $X\beta$ where X is a known $n \times p$ matrix of rank p and β is a $p \times 1$ vector of unknown parameters. The covariance matrix of Y is taken to be $\Sigma_\theta = \theta_1 I + \theta_2 V$ where V is a known nonnegative definite (n.n.d.) matrix and $\theta = (\theta_1, \theta_2)'$ is a vector of unknown parameters called variance components. More precisely, the parameter space of our model is $R^p \times \Omega$ where $\beta \in R^p$, $\theta \in \Omega$ and $\Omega = \{\theta : \theta_1 > 0, \theta_2 \geq 0\}$.

The problem we consider is invariant quadratic unbiased estimation for linear parametric functions $\delta'\theta$, $\delta \in R^2$. Specifically, we confine attention to the class, say $\tilde{\mathcal{N}}$, of quadratic forms which are invariant under the group of transformations $\mathcal{G} = \{g_x : x \in \mathbf{R}(X)\}$ where $g_x : y \rightarrow y + x$. The class $\tilde{\mathcal{N}}$ is a natural subset of the quadratic forms to consider for estimating $\delta'\theta$ (e.g., see [7] and [13]) and most quadratic estimators which have been proposed in the literature are in $\tilde{\mathcal{N}}$. For estimating a given $\delta'\theta$, we consider as candidates the subset $\tilde{\mathcal{N}}_\delta^*$ of $\tilde{\mathcal{N}}$ consisting of those that are unbiased. We use the variance of an estimator as a comparison criterion; and for this criterion it is well known that only in special cases does a single uniformly best estimator exist. Our goal in this section and in Section 4 is to reduce $\tilde{\mathcal{N}}_\delta^*$ to a minimal complete class.

Let \mathcal{N} denote the set of symmetric matrices B such that $X'B = 0$. Then $\tilde{\mathcal{N}} = \{Y'BY : B \in \mathcal{N}\}$. It is convenient to investigate $\tilde{\mathcal{N}}$ as quadratic forms in $Z = Q'Y$ where Q is an $n \times q$ ($q = n - p$) matrix whose columns form an orthonormal basis for $N(X')$. Because \mathcal{N} may be expressed as $\{QAQ' : A \in \mathcal{A}\}$ where \mathcal{A} denotes the vector space of $q \times q$ symmetric matrices, it follows that $\tilde{\mathcal{N}}$ is simply all quadratic forms in Z . (That this should be the case is suggested by the fact that Z is a maximal invariant with respect to the group of transformations \mathcal{G} , e.g., see [13].) Dealing with Z instead of Y simplifies the problem by eliminating the nuisance parameter β .

The family of distributions induced by Z is $\mathcal{P}_Z = \{N_q(0, \Lambda_\theta) : \theta \in \Omega\}$ where $\Lambda_\theta = \theta_1 I + \theta_2 W$, $W = Q'VQ$. An initial reduction in $\tilde{\mathcal{N}}$ may be made via sufficiency. Let $0 \leq \lambda_1 < \dots < \lambda_m$ denote the m distinct eigenvalues of W with multiplicities r_1, \dots, r_m respectively. And for $k = 1, \dots, m$ let $T_k = Z'E_k Z/r_k$ where E_k denotes the orthogonal projection operator on the subspace of eigenvectors corresponding to λ_k . Some facts concerning the T_k 's are

- (a) $r_k(\theta_1 + \lambda_k \theta_2)^{-1} T_k \sim \chi^2_{(r_k)}$ for $k = 1, \dots, m$.
- (b) T_1, \dots, T_m are statistically independent.
- (c) $T = (T_1, \dots, T_m)'$ is minimal sufficient for \mathcal{P}_Z .
- (d) T is complete and sufficient for \mathcal{P}_Z if and only if $m \leq 2$.

Facts (a)—(c) are straightforward to verify; they also may be obtained by minor modification of the results of Graybill and Hultquist [3]; (d) may be obtained by combining Example 8 in [14] with the main theorem in [13].

REMARK 2.1. The matrix Q is not uniquely determined and so Z and W are not unique. However, it can be shown that λ_i, r_i , and T_i ($i = 1, \dots, m$) do not depend upon the choice of Q .

In the space \mathcal{A} of symmetric matrices define \mathcal{F} to be the subspace spanned by E_1, \dots, E_m and let $\tilde{\mathcal{F}} = \{Z'AZ : A \in \mathcal{F}\}$. Let π denote the orthogonal projection operator on \mathcal{F} with orthogonality defined by means of the trace inner product $(A, B) = \text{tr}(AB)$.

THEOREM 2.2. For each $Z'AZ \in \tilde{\mathcal{N}}$ which is not in $\tilde{\mathcal{F}}$ there exists a $Z'BZ \in \tilde{\mathcal{F}}$ with the same expectation and having smaller variance uniformly over the parameter space Ω . Moreover, one choice for $Z'BZ$ is $h'T$ where $h = (\text{tr}(E_1 A), \dots, \text{tr}(E_m A))'$.

PROOF. Suppose $Z'AZ$ is as stated. Let $B = \pi A$, let $F = (I - \pi)A = A - B$, and let $\theta \in \Omega$ be fixed. Because $F \in \mathcal{F}^\perp$ and $\Lambda_\theta \in \mathcal{F}$, we have $E(Z'FZ|\theta) = (F, \Lambda_\theta) = 0$. Since $A = B + F$,

$$\text{Var}(Z'AZ|\theta) = \text{Var}(Z'BZ|\theta) + 2(F, \Lambda_\theta F \Lambda_\theta) + 4(F, \Lambda_\theta B \Lambda_\theta).$$

Because $\Lambda_\theta B \Lambda_\theta \in \mathcal{F}$, we have $(F, \Lambda_\theta B \Lambda_\theta) = 0$. And because Λ_θ is positive definite and $F \neq 0$, we have $(F, \Lambda_\theta F \Lambda_\theta) > 0$. As $\theta \in \Omega$ was selected arbitrarily, it follows that $Z'BZ$ has the same expectation as $Z'AZ$ and has uniformly smaller variance. To conclude the proof, use the fact that $B \in \mathcal{F}$ and $A - B \in \mathcal{F}^\perp$ to obtain the formula $B = \sum_{i=1}^m r_i^{-1}(A, E_i)E_i$. Hence $Z'BZ = h'T$. \square

REMARK 2.3. The above theorem was originally given by Olsen [6]. When applied to a completely random one-way model, it is essentially the culmination of Theorems 1, 2, and 3 in [4] with attention restricted to μ -invariant (Harville's terminology) quadratic unbiased estimators. A version of the theorem not restricted to two variance components has recently been given by Kleffe and Pincus (see Theorem 8 in [5]).

From Theorem 2.2 it is clear that we need only consider estimators of the form $h'T$. This suggests viewing our problem in a linear model framework. Thus, let

$$G' = \begin{bmatrix} 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \dots & \lambda_m \end{bmatrix}$$

so that $E(T|\theta) = G\theta$ for all $\theta \in \Omega$; and for $a \geq 0$ let

$$V(a) = \text{diag} \{(1 + \lambda_1 a)^2/r_1, \dots, (1 + \lambda_m a)^2/r_m\}$$

so that $\text{Cov}(T|\theta) = 2\theta_1^2 V(\rho)$ where $\rho = \theta_2/\theta_1$. For estimating $\delta'\theta$, $\delta \in \mathbf{R}(G')$, standard linear model results suggest investigating the class of estimators $\{\delta'\hat{\theta}_a : a \geq 0\}$ where $\hat{\theta}_a$ in the Gauss–Markov estimator with respect to the covariance matrix $V(a)$. Unfortunately, this class does not in general constitute a complete class. To further reduce our estimation problem we need the results in the next section.

3. Admissible estimators in linear models. Let U be a $k \times 1$ random vector following the linear model $E(U) = H\psi$ and $\text{Cov}(U) = \Sigma$ where H is a known $k \times l$ matrix and (ψ, Σ) is an element of a known subset Θ in $R^l \times \mathcal{D}$, \mathcal{D} being the set of $k \times k$ nonnegative definite matrices. Note that this linear model formulation allows for a possible relationship between the parameters ψ and Σ . We are interested in functions on the parameter space Θ of the form $g(\psi, \Sigma) = \delta'\psi$. To estimate such a linear parametric function we consider only linear unbiased estimators $b'U$. Let us assume that the parameters ψ in R^l which appear as components of elements of Θ form a spanning set for R^l ; then $b'U$ is unbiased if and only if $H'b = \delta$. Throughout this section let δ be a fixed vector in $\mathbf{R}(H')$ and let $\mathcal{B} = \{b : H'b = \delta\}$ be the set of coefficient vectors of the linear unbiased estimators for $\delta'\psi$. Our concern here is to investigate admissibility within this linear model context.

Let \mathcal{V} be the set of all Σ in \mathcal{D} which appear as components of elements of Θ . We will compare the estimators $b'U$, $b \in \mathcal{B}$, according to their possible variances $b'\Sigma b$, $\Sigma \in \mathcal{V}$. For $b, h \in \mathcal{B}$ we say b is *as good as* h if $b'\Sigma b \leq h'\Sigma h$ for all $\Sigma \in \mathcal{V}$; b is *better than* h if b is as good as h and $b'\Sigma b < h'\Sigma h$ for at least one $\Sigma \in \mathcal{V}$; b is *admissible* if no vector in \mathcal{B} is better than b .

Regard \mathcal{V} as a subset of the vector space \mathcal{S} of symmetric $k \times k$ matrices endowed with the usual Euclidean topology. For any subset \mathcal{U} of \mathcal{S} let $[\mathcal{U}]$ denote the smallest closed convex cone in \mathcal{S} containing \mathcal{U} . We say \mathcal{U} generates $[\mathcal{V}]$ if $[\mathcal{U}] = [\mathcal{V}]$. The definition of the relationship “as good as” remains

the same if \mathcal{V} is replaced by any set \mathcal{U} which generates $[\mathcal{V}]$, in particular, by $[\mathcal{V}]$ itself. This can be verified by noting that $\{\Lambda \in \mathcal{S}: b' \Lambda b \leq h' \Lambda h\}$ is a closed convex cone. Similarly, the definitions of “better than” and “admissible” remain the same. It is this observation that leads one to consider $[\mathcal{V}]$.

We will use the fact that every element of $[\mathcal{V}]$ is an n.n.d. matrix. This holds because \mathcal{D} is a closed convex cone containing \mathcal{V} .

A subset \mathcal{C} of \mathcal{B} is called a *complete class* if for every vector $b \in \mathcal{B}$ which is not in \mathcal{C} there exists a vector in \mathcal{C} which is better than b ; a subset \mathcal{C} is called an *essentially complete class* if for every $b \in \mathcal{B}$ there exists a vector in \mathcal{C} which is as good as b . One can check (see Section 2.1 in [2]) that the following three statements are equivalent: (1) the class \mathcal{B}_a of admissible vectors in \mathcal{B} is an essentially complete class; (2) \mathcal{B}_a is a complete class; (3) \mathcal{B}_a is a minimal complete class. In Proposition 3.3 below we will prove statement (3) by verifying statement (1). First we need two lemmas.

Let \mathcal{F} be the intersection of $\mathbf{N}(H')$ with the intersection of all the null spaces $\mathbf{N}(\Sigma)$, $\Sigma \in [\mathcal{V}]$, and let \mathcal{M} be any subspace of $\mathbf{N}(H')$ such that $\mathbf{N}(H')$ is the direct sum $\mathcal{M} \oplus \mathcal{F}$. For any $b_0 \in \mathcal{B}$, we have $\mathcal{B} = b_0 + \mathbf{N}(H') = b_0 + \mathcal{M} + \mathcal{F}$. Now for each $b \in \mathcal{B}$ write $b = a + f$ where $a \in b_0 + \mathcal{M}$ and $f \in \mathcal{F}$. Since $b' \Sigma b = a' \Sigma a$ for all $\Sigma \in [\mathcal{V}]$, we can conclude:

LEMMA 3.1. *For any $b_0 \in \mathcal{B}$, the set $b_0 + \mathcal{M}$ is an essentially complete class.*

The advantage of $b_0 + \mathcal{M}$ over \mathcal{B} is that it has the following compactness property.

LEMMA 3.2. *Let $b_0 \in \mathcal{B}$ and let K be the set of all vectors \bar{b} in $b_0 + \mathcal{M}$ which are as good as b_0 . Then K is compact.*

PROOF. For each $\Sigma \in [\mathcal{V}]$ the set $K(\Sigma) = \{b \in b_0 + \mathcal{M}: b' \Sigma b \leq b_0' \Sigma b_0\}$ is a closed convex set because $b' \Sigma b$ is a continuous convex function of b . Hence $K = \bigcap_{\Sigma \in [\mathcal{V}]} K(\Sigma)$ is closed and convex. To show K is compact it suffices to show that K has no direction of recession (see Theorem 8.4 in [10]). That is, if $h \in R^k$ is such that $b + \lambda h \in K$ for all $b \in K$ and $\lambda \geq 0$, then we must show $h = 0$. For such an h we have $b_0 + h \in K$, so that $h \in \mathcal{M}$. Moreover, $b_0 + \lambda h \in K(\Sigma)$ for all $\lambda \geq 0$ implies $2\lambda h' \Sigma b_0 + \lambda^2 h' \Sigma h \leq 0$ for all $\lambda \geq 0$, which implies $\Sigma h = 0$. This holds for all $\Sigma \in [\mathcal{V}]$ and so $h \in \mathcal{M} \cap \mathcal{F} = \{0\}$. \square

PROPOSITION 3.3. *In the set \mathcal{B} of coefficient vectors of the linear unbiased estimators for $\delta' \psi$, the set \mathcal{B}_a of admissible vectors is a minimal complete class.*

PROOF. It suffices to show \mathcal{B}_a is essentially complete. Let b_0 be any vector in \mathcal{B} . We must find an admissible vector which is as good as b_0 . If attention is restricted to the compact set K defined in Lemma 3.2, then it is known that the admissible elements of K form a complete class in K (see Theorem 2.22 in Wald [15]). In particular, there exists some element \bar{b} which is admissible in K . For the convenience of the reader, a proof of this fact will be given in the next paragraph.

Define the ordering $<$ on K by defining $b_1 < b_2$ if b_1 is as good as b_2 . For each $b \in K$ let $K(b) = \{h \in K : h < b\}$ and note that $K(b)$ is closed. Consider a chain C of elements in K . For any finite number of elements b_1, \dots, b_m in C we have $b_j \in \bigcap_{i=1}^m K(b_i)$ where b_j is minimal among them. By the finite intersection property of compact sets (see page 223 in [1]), $\bigcap_{b \in C} K(b)$ is nonempty. Any element in this intersection is a lower bound for C . By Zorn's lemma (see page 32 in [1]), there exists a minimal element \bar{b} in K . Then \bar{b} is admissible in K .

It remains to show \bar{b} is admissible in \mathcal{B} . Suppose there is some $b_1 \in \mathcal{B}$ which is better than \bar{b} . By Lemma 3.1 we can suppose $b_1 \in b_0 + \mathcal{M}$. Since \bar{b} is as good as b_0 , so is b_1 ; hence $b_1 \in K$. But this contradicts the admissibility of \bar{b} in K . \square

Now we want to characterize the admissible vectors. For a n.n.d. matrix Σ we say a vector $b \in \mathcal{B}$ is Σ -best if $b' \Sigma b \leq h' \Sigma h$ for all $h \in \mathcal{B}$. In the language of decision theory a Σ -best vector would be called a Bayes rule. (Here, of course, the term Bayes is to be interpreted with reference only to the class of linear unbiased estimators.) Some known properties of Σ -best vectors which we will use are listed in the following lemma (see Theorem 3 in [16] and Corollary 1.2 in [14]).

LEMMA 3.4. *For any given nonnegative definite matrix Σ*

- (i) *There exists a Σ -best vector in \mathcal{B} .*
- (ii) *b is Σ -best if and only if $\Sigma b \in \mathbf{R}(H)$.*
- (iii) *There is only one Σ -best vector in \mathcal{B} if and only if $\mathbf{N}(\Sigma) \cap \mathbf{N}(H') = \{0\}$.*

LEMMA 3.5. *There is a compact convex set \mathcal{W} , not containing the zero matrix, which generates $[\mathcal{V}]$. Every nonzero element of $[\mathcal{V}]$ is a positive multiple of an element of \mathcal{W} .*

PROOF. Let $\|\cdot\|$ be a norm on the Euclidean space \mathcal{S} and let \mathcal{E} be the compact unit sphere $\{\Lambda \in \mathcal{S} : \|\Lambda\| = 1\}$. Choose \mathcal{W} to be the convex hull of $\mathcal{E} \cap [\mathcal{V}]$; by Theorem 17.2 in [10], \mathcal{W} is compact. Since $\mathcal{W} \subset [\mathcal{V}]$, we have $[\mathcal{W}] \subset [\mathcal{V}]$. On the other hand, every nonzero element $\Sigma \in [\mathcal{V}]$ is a positive multiple of the element $\|\Sigma\|^{-1} \Sigma \in \mathcal{W}$, and so $[\mathcal{V}] \subset [\mathcal{W}]$. The zero matrix cannot be in \mathcal{W} because a convex combination of nonzero n.n.d. matrices is nonzero. \square

PROPOSITION 3.6. *If b is admissible in the set \mathcal{B} of coefficient vectors of the linear unbiased estimators for $\delta' \psi$, then b is Σ -best for some nonzero $\Sigma \in [\mathcal{V}]$.*

PROOF. Suppose b is admissible. We will show b is Σ -best for some Σ in the set \mathcal{W} in Lemma 3.5. Suppose not. Then Lemma 3.4(ii) implies $\Sigma b \notin \mathbf{R}(H)$ for all $\Sigma \in \mathcal{W}$. This is equivalent to $F' \Sigma b \neq 0$ for all $\Sigma \in \mathcal{W}$, where F is a $k \times s$ matrix such that $\mathbf{R}(F) = \mathbf{N}(H')$. Define $f: \mathcal{S} \rightarrow R^s$ by $f(\Lambda) = F' \Lambda b$. This is a linear mapping and hence preserves compactness and convexity. Thus the set $W = \{F' \Sigma b : \Sigma \in \mathcal{W}\}$ is compact and convex in R^s . Since $0 \notin W$, the separating hyperplane theorem assures the existence of a vector $a \in R^s$ such that $W \subset \{x : a'x < 0\}$. Note that for each $\Sigma \in \mathcal{W}$ we have $a'F' \Sigma b < 0$, hence also

$a'F'\Sigma Fa > 0$. For $\Sigma \in \mathscr{W}$ and $\gamma \in R^1$ let

$$\pi(\Sigma, \gamma) = (b + \gamma Fa)' \Sigma (b + \gamma Fa) - b' \Sigma b = 2\gamma a' F' \Sigma b + \gamma^2 a' F' \Sigma Fa.$$

Then for arbitrary, but fixed, $\Sigma \in \mathscr{W}$ the quadratic polynomial $\pi(\Sigma, \gamma)$ in γ achieves its minimum value of $-(a' F' \Sigma b)^2 / (a' F' \Sigma Fa) < 0$ when $\gamma = g(\Sigma) = -(a' F' \Sigma b) / (a' F' \Sigma Fa) > 0$. Since g , considered as a mapping from \mathscr{W} to R^1 , is continuous and strictly positive on the compact set \mathscr{W} , there exists $\varepsilon > 0$ such that $g(\Sigma) \geq \varepsilon$ for all $\Sigma \in \mathscr{W}$. We see that $\varepsilon^{-1} \pi(\Sigma, \varepsilon) \leq g(\Sigma)^{-1} \pi(\Sigma, g(\Sigma)) < 0$ for all $\Sigma \in \mathscr{W}$ so that $(b + \varepsilon Fa)' \Sigma (b + \varepsilon Fa) < b' \Sigma b$ for all $\Sigma \in \mathscr{W}$. This contradicts the admissibility of b since $b + \varepsilon Fa \in \mathscr{B}$. \square

COROLLARY 3.7. *Suppose $N(\Sigma) \cap N(H') = \{0\}$ for all nonzero $\Sigma \in [\mathscr{V}]$. Then for $b \in \mathscr{B}$*

- (i) *b is admissible if and only if b is Σ -best for some nonzero $\Sigma \in [\mathscr{V}]$.*
- (ii) *If b is inadmissible, then there is a vector $b_1 \in \mathscr{B}$ which is uniformly better than b in the sense that $b_1' \Sigma b_1 < b' \Sigma b$ for all nonzero $\Sigma \in [\mathscr{V}]$.*

PROOF. Half of (i) follows from Proposition 3.6. Conversely, suppose b is Σ -best and $N(\Sigma) \cap N(H') = \{0\}$. Then Lemma 3.4(iii) says $b' \Sigma b < h' \Sigma h$ for all other $h \in \mathscr{B}$, and so b must be admissible. To prove (ii), suppose b is inadmissible. By (i) b is not Σ -best for any nonzero $\Sigma \in [\mathscr{V}]$. Let \mathscr{W} be as in Lemma 3.5. Then the proof of Proposition 3.6 shows the existence of a vector $b_1 (= b + \varepsilon Fa)$ such that $b_1' \Sigma b_1 < b' \Sigma b$ for all $\Sigma \in \mathscr{W}$. And since any nonzero element of $[\mathscr{V}]$ is a positive multiple of an element of \mathscr{W} , the result follows. \square

REMARK 3.8. (1) Note that Corollary 3.7 holds true if $[\mathscr{V}]$ is replaced by any set \mathscr{W} such as in Lemma 3.5. (2) Under the conditions of Corollary 3.7, the class of admissible vectors is exactly the class of Σ -best vectors for nonzero $\Sigma \in [\mathscr{V}]$. It can be shown that this is also the class of Bayes rules in the wide sense with respect to the parameter space Θ , provided that \mathscr{V} does not contain 0 in its closure.

4. The minimal complete class. In Section 2 the problem of invariant quadratic unbiased estimation was reduced to considering linear combinations of T_1, \dots, T_m . Recall for $\theta \in \Omega$ that $E(T|\theta) = G\theta$ and that $\text{Cov}(T|\theta) = 2\theta_1^2 V(\rho)$ where $\rho = \theta_2/\theta_1$. Let $\delta \in R^2$ be fixed, let $\mathscr{T}_\delta = \{b: G'b = \delta\}$, and let $\tilde{\mathscr{T}}_\delta = \{b'T: b \in \mathscr{T}_\delta\}$ be the set of linear unbiased estimators for $\delta'\theta$. Our terminology here is generally consistent with that introduced in Section 3, except we often use $\tilde{\mathscr{T}}_\delta$ in place of \mathscr{T}_δ . To avoid trivial technicalities we suppose $m \geq 2$. From Proposition 3.3 we conclude that $\tilde{\mathscr{T}}_\delta$ can be reduced to a minimal complete class, say \mathscr{E}_δ . We investigate \mathscr{E}_δ by first showing Corollary 3.7 in applicable and then by examining the relationship between \mathscr{E}_δ and $[\mathscr{V}]$ where $\mathscr{V} = \{\text{Cov}(T|\theta): \theta \in \Omega\}$.

First note that $D \in \mathscr{V}$ may be written as a nonnegative linear combination of diagonal matrices D_1, D_2, D_3 having diagonal elements $r_i^{-1}, \lambda_i r_i^{-1}, \lambda_i^2 r_i^{-1}$

($i = 1, \dots, m$) respectively. Since the cone \mathcal{H} generated by the convex hull of D_1, D_2, D_3 is closed (see Corollary 9.6.1 in [10]), it follows that $[\mathcal{V}] \subset \mathcal{H}$. Let S denote the simplex of vectors $w = (w_1, w_2, w_3)$ having nonnegative components which sum to one and for $w \in S$ let $D_w = \sum_{i=1}^3 w_i D_i$ so that $\mathcal{H} = \{\gamma D_w : \gamma \geq 0, w \in S\}$.

LEMMA 4.1. *If $w \in S$, then $\mathbf{N}(D_w) \cap \mathbf{N}(G') = \{0\}$. Moreover, if D_w is singular (i.e., $w_1 = \lambda_1 = 0$), then $D_w + J$ is positive definite (p.d.) where J is an $m \times m$ matrix of ones.*

PROOF. We suppose $w_1 = \lambda_1 = 0$ since D_w is p.d. otherwise. Now $\mathbf{R}(D_w + J) = \mathbf{R}(D_w) + \mathbf{R}(J)$ because D_w and J are n.n.d. matrices. Thus, $D_w + J$ is p.d. because $\mathbf{R}(D_w) \cap \mathbf{R}(J) = \{0\}$ and $\mathbf{r}(D_w) = m - 1$. To conclude note that $\mathbf{R}(J) \subset \mathbf{R}(G)$ so that $[\mathbf{R}(D_w) + \mathbf{R}(G)]^\perp = (R^m)^\perp$. \square

Because $[\mathcal{V}] \subset \mathcal{H}$, Lemma 4.1 and Corollary 3.7 imply $\tilde{\mathcal{E}}_\delta$ consists of the D -best estimators for $\delta'\theta$ where $D \neq 0$ and $D \in [\mathcal{V}]$. To further investigate $\tilde{\mathcal{E}}_\delta$ let

$$w(a) = (1 + a)^{-2}(1, 2a, a^2), \quad a \geq 0.$$

Note that $w(a) \in S$ and that $V(a) = (1 + a)^2 D_{w(a)}$. Thus, the set of $D_{w(a)}$'s constitute a generating set for $[\mathcal{V}]$; and hence so does $\mathcal{W} = \{D_w : w \in S_C\}$ where S_C is defined as the closure of the convex hull of $\{w(a) : a \geq 0\}$. Because the mapping $w \rightarrow D_w$, $w \in S_C$, may be viewed as a linear map restricted to the compact convex set S_C , the set \mathcal{W} is compact and convex. Hence, because $0 \notin \mathcal{W}$, Corollary 9.6.1 in [10] implies

$$(4.2) \quad [\mathcal{V}] = \{\gamma D_w : \gamma \geq 0, w \in S_C\}.$$

Using this fact and Remark 3.8 we have proved the following:

THEOREM 4.3. *Within the class of invariant unbiased quadratic estimators for $\delta'\theta$, the subset*

$$\tilde{\mathcal{E}}_\delta = \{c_w' T : w \in S_C\}$$

is the minimal complete class where c_w is the unique vector in \mathcal{T}_δ satisfying $D_w c_w \in \mathbf{R}(G)$, i.e., c_w is D_w -best.

In Theorem 4.3 the set $\tilde{\mathcal{E}}_\delta$ is characterized via the weights in S_C . In some cases the entire set S_C is not needed to characterize $\tilde{\mathcal{E}}_\delta$. For example, if $m = 2$ then T is complete so that $\tilde{\mathcal{E}}_\delta$ consists of exactly one estimator, i.e., $c_u = c_w$ for all $u, w \in S_C$. (The case for $m = 1$ is the same, except here only multiples of $\theta_1 + \lambda_1 \theta_2$ are estimable.) In the succeeding two propositions we examine the relationship between $w \in S_C$ and the D_w -best vector c_w for $m \geq 3$. The reader may find it helpful to think of S as an equilateral triangle and to visualize S_C as that portion of S whose boundary consists of the curve $\{w(a) : a \geq 0\}$ and the base of the triangle, i.e., the line segment joining $w = (1, 0, 0)$ and $w = (0, 0, 1)$.

PROPOSITION 4.4. *If $m = 3$, the minimal complete class in $\tilde{\mathcal{F}}_\delta$ may be written as*

$$\tilde{\mathcal{E}}_\delta = \{c'_{w(a)}T : a \geq 0\} \cup \{c'_w T\}$$

where $\bar{w} = (0, 0, 1)$.

PROOF. Let h and $f \neq 0$ be such that $G'h = \delta$ and $G'f = 0$; and define $\gamma(w) = f'D_w h / f'D_w f$ for each $w \in S_C$. Note that f spans $\mathbf{N}(G')$ and that $f'D_w(h - \gamma(w)f) = 0$; hence $c_w = h - \gamma(w)f$. Since γ is a continuous function on S_C which is a compact connected set, the range of γ must be a closed finite interval, say $[M_1, M_2]$. And similarly the range of γ restricted to the compact connected subset $S_1 = \{w(a) : a \geq 0\} \cup \{\bar{w}\}$ of S_C will also be a closed finite interval, say $[m_1, m_2]$. The validity of the proposition will follow if we can establish that $m_i = M_i$ for $i = 1, 2$. Since γ is the ratio of two linear functions on S_C with the denominator always positive, it can be shown that γ is both quasi-concave and quasi-convex on S_C , i.e., if $\alpha \in [0, 1]$ and $u, w \in S_C$, then

$$\min \{\gamma(u), \gamma(w)\} \leq \gamma(\alpha u + (1 - \alpha)w) \leq \max \{\gamma(u), \gamma(w)\}.$$

From this it follows that the range of γ restricted to the boundary of S_C , say S_B , is precisely $[M_1, M_2]$. Now applying the quasi-concavity and quasi-convexity of γ to the line segment S_2 joining $w^* = (1, 0, 0)$ and \bar{w} , and noting that $w^*, \bar{w} \in S_1$ and $S_B = S_1 \cup S_2$, it follows that $m_i = M_i$ for $i = 1, 2$. \square

PROPOSITION 4.5. *Suppose $m \geq 4$ and $\delta \neq 0$. If $u, w \in S_C$ are such that $u \neq w$, then $c_u \neq c_w$.*

PROOF. We may suppose $u \neq (0, 0, 1)$ so that $c_u \in \mathbf{R}(D_u^{-1}G)$. Let $D = D_w + J$ where J is a matrix of ones. Then D is p.d.; see Lemma 4.1 for the only questionable case. Since $\mathbf{R}(J) \subset \mathbf{R}(G)$, it follows that $Dc_w \in \mathbf{R}(G)$ so that $c_w \in \mathbf{R}(D^{-1}G)$. Thus, it is sufficient to show $\mathbf{R}(D_u^{-1}G) \cap \mathbf{R}(D^{-1}G) = \{0\}$; or equivalently, that $\mathbf{r}(D_u^{-1}G, D^{-1}G) = 4$. Now multiply by $D_u D = D_w D_u + D_u J$ to obtain the equivalent condition $\mathbf{r}(D_w G + B, D_u G) = 4$ where $B = D_u J D_u^{-1}G$. But as $\mathbf{R}(B) \subset \mathbf{R}(D_u G)$ we get the equivalent condition $\mathbf{r}(D_w G, D_u G) = 4$. We can write $(D_w G, D_u G) = RLM$, where $R = \text{diag}(r_1^{-1}, \dots, r_m^{-1})$, L is an $m \times 4$ matrix with i th row $(1, \lambda_i, \lambda_i^2, \lambda_i^3)$, and

$$M = \begin{bmatrix} w_1 & 0 & u_1 & 0 \\ w_2 & w_1 & u_2 & u_1 \\ w_3 & w_2 & u_3 & u_2 \\ 0 & w_3 & 0 & u_3 \end{bmatrix}.$$

When $m \geq 4$ we have $\mathbf{r}(RL) = 4$ so that $\mathbf{r}(RLM) = 4$ if and only if $\mathbf{r}(M) = 4$. The determinant of M is

$$\Delta = w_3 d_1^2 + w_2 d_1 d_3 + w_1 d_3^2 = u_3 d_1^2 + u_2 d_1 d_3 + u_1 d_3^2$$

where $d_i = u_i - w_i$ for $i = 1, 3$. This determinant can be regarded as a positive definite quadratic form if either u or w satisfies $w_1 w_3 - 4^{-1} w_2^2 > 0$. Then $\Delta = 0$ would imply $d_1 = d_3 = 0$, which is impossible if $u \neq w$. It can be shown that

the only remaining case is when u and w both satisfy $w_1 w_3 - 4^{-1} w_2^2 = 0$, i.e., $u_2 = 2(u_1 u_3)^{\frac{1}{2}}$ and $w_2 = 2(w_1 w_3)^{\frac{1}{2}}$. These equations together with $\Delta = 0$ lead to the contradictory conclusion $d_1 = d_3 = 0$. Therefore, $\Delta \neq 0$ and so $r(M) = 4$. \square

With respect to Theorem 4.3 and Propositions 4.4 and 4.5 several comments seem appropriate: (1) The conclusion of Theorem 4.3 can be somewhat strengthened by Corollary 3.7(ii) in that if $Z'AZ$ is unbiased for $\delta'\theta$ and is not in \mathcal{E}_{δ} , then there is an estimator in $\tilde{\mathcal{E}}_{\delta}$ which has smaller variance uniformly over the parameter space Ω . (2) The Gauss–Markov estimators $\delta'\hat{\theta}_a$ mentioned at the end of Section 2 are in fact $D_{w(a)}$ -best estimators. (3) The estimator corresponding to the weight $\bar{w} = (0, 0, 1)$ is rather interesting in that it may be viewed as a limiting Gauss–Markov estimator, i.e., $c_{w(a)} \rightarrow c_{\bar{w}}$ as $a \rightarrow \infty$. (4) The restriction to three distinct eigenvalues considered in Proposition 4.4 is not an uninteresting case. For example, a set of data arising from a balanced incomplete block arrangement with treatments fixed, blocks random, and more blocks than treatments falls within this situation (see [12]). (5) When $m \geq 4$, the conclusion of Proposition 4.4 is not true as seen from Proposition 4.5. (6) Proposition 4.5 says that the mapping $w \rightarrow c_w$, $w \in S_C$, is one to one when $m \geq 4$. (7) When $m = 3$ the mapping $w \rightarrow c_w$, even when restricted to S_1 , is not necessarily one to one (see [6]).

5. Computations via normal equations. In the previous section the estimators in the minimal complete class \mathcal{E}_{δ} were described via the D_u -best vectors c_u , $u \in S_C$. To compute the estimators one would probably resort to normal equations. Here we briefly summarize the pertinent equations and present some alternative expressions for the components of the equations.

As in Section 4 suppose $m \geq 2$. Let $u \in S_C$ and for the present suppose D_u is p.d., i.e., either λ_1 is positive or $u \neq (0, 0, 1)$. Define $\hat{\theta}(u)$ to be the random vector satisfying the normal equations $G'D_u^{-1}G\hat{\theta}(u) = G'D_u^{-1}T$. Then we have $c_u'T = \delta'\hat{\theta}(u)$. To construct these normal equations from G and D_u one must first obtain the eigenvalues and multiplicities of W . To avoid computing the λ_i 's and r_i 's let $\Lambda_u = u_1I + u_2W + u_3W^2$ and note that the diagonal elements of D_u are formed from the distinct eigenvalues of Λ_u divided by their multiplicities. Given this fact, it is straightforward to rewrite the previous normal equations as

$$(5.1) \quad \begin{bmatrix} \text{tr}(\Lambda_u^{-1}) & \text{tr}(\Lambda_u^{-1}W) \\ \text{tr}(W\Lambda_u^{-1}) & \text{tr}(W\Lambda_u^{-1}W) \end{bmatrix} \begin{bmatrix} \hat{\theta}_1(u) \\ \hat{\theta}_2(u) \end{bmatrix} = \begin{bmatrix} Z'\Lambda_u^{-1}Z \\ Z'W\Lambda_u^{-1}Z \end{bmatrix}.$$

These equations may also be written in terms of the original quantities of the problem Y , X and V to avoid the necessity of obtaining Q . To see this let $\Sigma_u = u_1I + u_2V + u_3VNV$ where $N = I - X(X'X)^{-1}X'$. Note that $Q'Q = I$, $QQ' = N$, and $\Lambda_u = Q'\Sigma_u Q$. Because Λ_u is p.d., Theorem 4.11.8 in [9] implies $Q\Lambda_u^{-1}Q' = N(N\Sigma_u N)^{-1}N$. And when Σ_u is p.d., we have (see Problem 33, page 77, in [8])

$$Q\Lambda_u^{-1}Q' = \Sigma_u^{-1} - \Sigma_u^{-1}X(X'\Sigma_u^{-1}X)^{-1}X'\Sigma_u^{-1}.$$

These observations allow one to easily rewrite equation (5.1). For example, $\text{tr}(\Lambda_u^{-1}) = \text{tr}(Q\Lambda_u^{-1}Q')$ and $Z'W\Lambda_u^{-1}Z$ may be written as $Y'NV(Q\Lambda_u^{-1}Q')Y$. It is interesting to note that $Z'\Lambda_u^{-1}Z = \min_{\beta} \|Y - X\beta\|_u^2$ where $\|b\|_u^2 = b'\Sigma_u^{-1}b$.

Now let us consider the case when D_u is singular and $u \in S_C$. Then it must be that $\lambda_1 = 0$ and $u = (0, 0, 1)$, so that $D_u = D_3$. Let $\delta = (\delta_1, \delta_2)'$ be in R^2 and let $\hat{\theta}(u)$ be such that $\delta'\hat{\theta}(u)$ is the D_3 -best estimator for $\delta'\theta$. Using the conditions $D_3c_u \in \mathbf{R}(G)$ and $G'c_u = \delta$ it is straightforward to verify that

$$(5.2) \quad \delta'\hat{\theta}(u) = \delta_1 T_1 + \delta_2 [(Z'W^+Z - \text{tr}(W^+)T_1)/r(W)]$$

where W^+ denotes the Moore–Penrose inverse of W . This expression can also be written in terms of Y, X and V by using (iii) and (iv) of problem 5, page 67, in [9] to show that

$$QW^+Q' = NB[(B'NB)^+]^2B'N = (NVN)^+,$$

where B may be any matrix satisfying $V = BB'$. Additionally, with respect to (5.2) see (6.1) in the following section.

6. MINQUE's and Henderson III. For the model we are considering, the MINQUE estimators given by Rao [7] are included in the minimal complete class. This may be seen by comparing equations (4.7) in [7] with equations (5.1) using the weights $w = w(a)$ for $a \geq 0$. In comparing these two sets of equations, G, V_1, V_2 , and H in Rao's notation correspond to Q, I, W , and $I + aW$ respectively. Also, note for $a \geq 0$ that $\Lambda_{w(a)} = (1 + a)^{-2}(I + aW)^2$. Among the MINQUE estimators Rao suggests using $a = 1$ or, if available, using a as an a priori ratio of the two unknown variance components.

A common procedure, when it can be used, for estimating $\delta'\theta$ is Henderson's Method III, e.g., see Searle [11]. The Henderson III estimators are invariant under the group defined in Section 2, and a natural question to consider is their relationship with the corresponding minimal complete classes. To answer this question consider the model as arising from the mixed linear model $Y = X\beta + Bb + e$ where b and e are random having independent $N_s(0, \theta_2 I)$ and $N_n(0, \theta_1 I)$ distributions respectively with B a known $n \times s$ matrix. Thus $V = BB'$. In this notation we have

- (a) The matrices $B'QQ'B = B'(I - X(X'X)^{-1}X')B$ and $W = Q'BB'Q$ have the same positive eigenvalues and multiplicities.
- (b) $r(W) = r(X, B) - r(X)$.
- (6.1) (c) W is singular (i.e., $\lambda_1 = 0$) if and only if $n - r(X, B)$ is positive.
- (d) If W is singular, then $r_1 = n - r(X, B)$ and

$$r_1 T_1 = \min_{\alpha, \beta} \|Y - X\beta - B\alpha\|^2,$$
 where $\|\cdot\|$ denotes the usual norm on R^n .

Statement (a) is a general matrix fact and is often useful computationally,

especially when s is small relative to n . Lemma 1 in [17] implies (b) which in turn implies (c). And assuming W is singular, (d) may be established by showing that QE_1Q' is the orthogonal projection on $\mathbf{R}(X, B)^\perp$.

The Henderson III estimators for θ_1 and θ_2 , say $\tilde{\theta}_1$ and $\tilde{\theta}_2$, depend upon two sums of squares. Thinking of b as a vector of fixed effects in the representation $Y = X\beta + Bb + e$, the two sums of squares are the residual sum of squares and the sum of squares for the b -effects adjusted for the β -effects. Thus, from (6.1.d) the Henderson III procedure is applicable only when W is singular, in which case the two sums of squares are

$$r_1 T_1 \quad \text{and} \quad \sum_{i=2}^m r_i T_i = Z'Z - r_1 T_1.$$

To obtain the Henderson III estimators, these two sums of squares are equated to their expectations and the resulting equations are solved to obtain $\tilde{\theta}_1$ and $\tilde{\theta}_2$. Using the condition $D_2 c \in \mathbf{R}(G)$, it can be verified that $\delta'\tilde{\theta}$ is precisely the D_2 -best estimator for $\delta'\theta$. The relationship between the Henderson III estimators and the admissible estimators is considered in

PROPOSITION 6.2. *Suppose W is singular and assume $m \geq 3$. Then*

- (a) $\tilde{\theta}_1 = \hat{\theta}_1(w)$ for $w = (0, 0, 1) \in S_G$.
- (b) If $m = 3$, then $\tilde{\theta}_2 = \hat{\theta}_2(w(a))$ where

$$a = [(r_1 + r_2 + r_3)/r_1 \lambda_2 \lambda_3]^\frac{1}{2}.$$

- (c) For $m \geq 4$, there does not exist $w \in S_G$ such that $\tilde{\theta}_2 = \hat{\theta}_2(w)$.

PROOF. Since $\tilde{\theta}_1 = T_1$, part (a) follows from (5.2). Let

$$c' = (\sum_{i=2}^m \lambda_i r_i)^{-1} [-(\sum_{i=2}^m r_i), r_2, \dots, r_m].$$

Then $c'T = \tilde{\theta}_2$. Part (b) follows by showing that $D_{w(a)} c \in \mathbf{R}(G)$. For $m \geq 4$, it can be shown that the matrix $(D_1 c, D_3 c, G)$ has rank 4. Suppose there is a $w \in S_G$ such that $D_w c \in \mathbf{R}(G)$. But this implies $w_1 = w_3 = 0$ since $\mathbf{r}(D_1 c, D_3 c, G) = 4$ and this contradicts $w \in S_G$; hence part (c) follows. \square

From the remarks in this section, we mention two points with regard to using invariant quadratic unbiased estimators. First, the MINQUE's, while admissible in $\tilde{\mathcal{N}}$, do not in general constitute a complete class; and without further justification seem too restrictive. For example, when W is singular the usual estimator for θ_1 is T_1 ; and when $m \geq 3$ this estimator cannot be obtained from the MINQUE equations (4.7) in Rao [7]. Moreover, some limited numerical comparisons in Olsen [6] suggest that T_1 will perform in a more satisfactory manner over the entire parameter space than will any of the MINQUE estimators. And second, the usual or Henderson III estimator for θ_2 , except for special cases, can be improved upon uniformly over the parameter space. For example, in a completely random one-way classification model with four groups and observations within groups of 2, 2, 3, 3, respectively, the estimator $\hat{\theta}_2(w(a))$ with $a = .495$ can be shown to have uniformly smaller variance over Ω than $\tilde{\theta}_2$. The

gain in efficiency of the admissible estimator over the Henderson III estimator in this example is, however, extremely small.

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REFERENCES

- [1] DUGUNDJI, J. (1966). *Topology*. Allyn and Bacon, Boston.
- [2] FERGUSON, T. (1967). *Mathematical Statistics*. Academic Press, New York.
- [3] GRAYBILL, F. A. and HULTQUIST, R. A. (1961). Theorems concerning Eisenhart's Model II. *Ann. Math. Statist.* **32** 261-269.
- [4] HARVILLE, D. A. (1969). Quadratic unbiased estimation of variance components for the one-way classification. *Biometrika* **56** 313-326 (Correction (1970). *Biometrika* **57** 226.)
- [5] KLEFFE, J. and PINCUS, R. (1974). Bayes and best quadratic unbiased estimators for parameters of the covariance matrix in a normal linear model. *Math. Operationsforsch. Statist.* **5** 43-67.
- [6] OLSEN, A. R. (1973). Quadratic unbiased estimation for two variance components. Ph. D. thesis, Oregon State Univ.
- [7] RAO, C. R. (1972). Estimating variance and covariance components in linear models. *J. Amer. Statist. Assoc.* **67** 112-115.
- [8] RAO, C. R. (1973). *Linear Statistical Inference and Its Applications*, 2nd ed. Wiley, New York.
- [9] RAO, C. R. and MITRA, S. K. (1971). *Generalized Inverse of Matrices and its Applications*. Wiley, New York.
- [10] ROCKAFELLAR, R. T. (1970). *Convex Analysis*. Princeton Univ. Press.
- [11] SEARLE, S. R. (1971). Topics in variance component estimation. *Biometrics* **27** 1-76.
- [12] SEELY, J. (1971). Quadratic subspaces and completeness. *Ann. Math. Statist.* **42** 710-721.
- [13] SEELY, J. (1972). Completeness for a family of multivariate normal distributions. *Ann. Math. Statist.* **43** 1644-1647.
- [14] SEELY, J. and ZYSKIND, G. (1971). Linear spaces and minimum variance unbiased estimation. *Ann. Math. Statist.* **42** 691-703.
- [15] WALD, A. (1950). *Statistical Decision Functions*. Wiley, New York.
- [16] ZYSKIND, G. (1967). On canonical forms, nonnegative covariance matrices and best and simple least squares linear estimators in linear models. *Ann. Math. Statist.* **38** 1092-1109.
- [17] ZYSKIND, G. and MARTIN, F. (1969). On best linear estimation and a general Gauss-Markov theorem in linear models with arbitrary nonnegative covariance structure. *SIAM J. Appl. Math.* **17** 1190-1202.

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