Invariance of the BLUE under the linear fixed and mixed effects models

JARKKO ISOTALO, MÄRT MÖLS, AND SIMO PUNTANEN

ABSTRACT. We consider the estimation of the parametric function \( X_1 \beta_1 \) under the partitioned linear fixed effects model \( y = X_1 \beta_1 + X_2 \beta_2 + \epsilon \) and the linear mixed effects model \( y = X_1 \beta_1 + X_2 \gamma_2 + \epsilon \), where \( \gamma_2 \) is considered to be a random vector. Particularly, we consider when the best linear unbiased estimator, BLUE, of \( X_1 \beta_1 \) under the linear fixed effects model equals the corresponding BLUE under the linear mixed effects model.

1. Introduction

We begin by introducing the notation. We will denote \( \mathbb{R}^{m,n} \) the set of \( m \times n \) real matrices and \( \mathbb{R}^m = \mathbb{R}^{m,1} \). The symbols \( A' \), \( A^- \), \( A^+ \), \( \mathcal{C}(A) \), \( \mathcal{C}(A)^\perp \), \( \mathcal{N}(A) \), and \( r(A) \) will stand for the transpose, a generalized inverse, the Moore–Penrose inverse, the column space, the orthogonal complement of the column space, the null space, and the rank, respectively, of \( A \in \mathbb{R}^{m,n} \). By \( A^\perp \) we denote any matrix satisfying \( \mathcal{C}(A^\perp) = \mathcal{N}(A') = \mathcal{C}(A)^\perp \). Further we will write \( P_A = AA^+ = A(A'A)^-A' \) to denote the orthogonal projector (with respect to the standard inner product) onto \( \mathcal{C}(A) \), and \( M_A = I - P_A \) to denote the orthogonal projector onto \( \mathcal{C}(A)^\perp \), where \( I \) denotes the identity matrix. Particularly,

\[
P_i = P_{X_i}, \quad M_i = I - P_i, \quad i = 1, 2.
\]

Moreover, by \( (A : B) \) we denote the partitioned matrix with \( A \in \mathbb{R}^{m,n} \) and \( B \in \mathbb{R}^{m,k} \) as submatrices.

In this paper we consider the partitioned linear fixed effects model

\[
y = X_1 \beta_1 + X_2 \beta_2 + \epsilon, \quad (1.1)
\]

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or in another notation,
\[ \mathcal{F} = \{ y, X\beta, R \} = \{ y, X_1\beta_1 + X_2\beta_2, R \}, \]  
with
\[ E(y) = X\beta, \quad E(\varepsilon) = 0, \quad \text{cov}(y) = \text{cov}(\varepsilon) = R, \]
where \( E(\cdot) \) denotes expectation (or expected value) and \( \text{cov}(\cdot) \) the covariance (or dispersion) matrix. The vector \( y \) is an \( n \times 1 \) observable random vector, \( \varepsilon \) is an \( n \times 1 \) unobservable random error vector, and \( \beta = (\beta_1', \beta_2')' \) is a \( p \times 1 \) vector of unknown fixed effects with \( p = p_1 + p_2 \), and \( \beta_1 (p_1 \times 1) \) and \( \beta_2 (p_2 \times 1) \). The model (or design) matrix \( X \) is \( n \times p \) and partitioned columnwise as \( X = (X_1 : X_2) \) with \( p = p_1 + p_2 \), and \( X_1 (n \times p_1) \) and \( X_2 (n \times p_2) \). Both the model matrix \( X \) and the covariance matrix \( R \) are known but can be of arbitrary rank.

However, in many practical situations it can be difficult to determine whether some of the fixed parameters in the model equation (1.1) should actually be treated as random variables; see, e.g., Searle et al. (1992, Section 1.4). For example, if the fixed parameters \( \beta_2 \) in (1.1) are alternatively considered to be random (and denoted as \( \gamma_2 \) with expected value \( E(\gamma_2) = 0 \)), then we have the linear mixed effects model
\[ y = X_1\beta_1 + X_2\gamma_2 + \varepsilon, \]
or in another notation,
\[ \mathcal{M} = \{ y, X_1\beta_1, V \} = \{ y, X_1\beta_1, X_2G X'_2 + R \}, \]  
with
\[ E(y) = X_1\beta_1, \quad E(\gamma_2) = 0, \quad E(\varepsilon) = 0, \quad \text{cov}(\gamma_2) = G, \quad \text{cov}(\varepsilon) = R, \quad \text{cov}(\gamma_2, \varepsilon) = 0, \quad \text{cov}(y) = V = X_2G X'_2 + R, \]
where the covariance matrix \( G \) is also assumed to be known but again can be of arbitrary rank.

Let us now consider the estimation of the linear parametric function \( K_1\beta_1 \), \( K_1 \in \mathbb{R}^{k_1 \times p_1} \), of the fixed effects \( \beta_1 \) under both models \( \mathcal{F} \) and \( \mathcal{M} \). The parametric function \( K_1\beta_1 \) is said to be estimable under the fixed effects model \( \mathcal{F} \) if there exists a linear unbiased estimator for \( K_1\beta_1 \), i.e., if there exists a matrix \( A \) such that \( A(X_1 : X_2) = (K_1 : 0) \), or in other words, \( \mathcal{G}(K_1, 0) \subset \mathcal{G}(X_1', X_2') \).

Equivalently, the parametric function \( K_1\beta_1 \) is estimable under the mixed effects model \( \mathcal{M} \) if \( \mathcal{G}(K_1) \subset \mathcal{G}(X_1') \). Hence if \( K_1\beta_1 \) is estimable under the model \( \mathcal{F} \), then it is also estimable under the model \( \mathcal{M} \) but not necessarily other way round. Moreover, if we consider the estimation of all estimable linear parametric functions of the fixed effects \( \beta_1 \) under the model \( \mathcal{F} \), then
it is equivalent just to consider the estimation of the parametric function $M_2X_1\beta_1$; see Groß and Puntaen (2000, Lemma 1).

Under the fixed effects model $\mathcal{F}$, a linear statistic $LY$ is the best linear unbiased estimator, BLUE, for the parametric function $M_2X_1\beta_1$ if the covariance matrix $\text{cov}(LY)$ is minimal, in the Löwner sense, among all covariance matrices $\text{cov}(FY)$ such that $FY$ is unbiased for $M_2X_1\beta_1$. It is well known that $LY$ is the BLUE of $M_2X_1\beta_1$ under the model $\mathcal{F}$ if and only if $L$ satisfies the fundamental equation of the BLUE:

$$L(X_1 : X_2 : RX^\perp) = (M_2X_1 : 0 : 0).$$

Similarly, a linear statistic $LY$ is the BLUE of $M_2X_1\beta_1$ under the mixed effects model $\mathcal{M}$ if and only if $L$ satisfies the equation:

$$L(X_1 : VX_1^\perp) = (M_2X_1 : 0).$$

For a proof of (1.4a) and (1.4b), see, e.g., Drygas (1970, p. 50), Rao (1973, p. 282), and recently, Baksalary (2004). Also, explicit representations for the BLUES of $M_2X_1\beta_1$ are obtainable from the equations (1.4a) and (1.4b).

For example, the BLUES of $M_2X_1\beta_1$ under the models $\mathcal{F}$ and $\mathcal{M}$ can, respectively, be written as

$$\text{BLUE}(M_2X_1\beta_1 | \mathcal{F}) = M_2X_1[X'(R + XX')^{-1}X']^{-1}X'(R + XX')^{-1}y,$n$$

$$\text{BLUE}(M_2X_1\beta_1 | \mathcal{M}) = M_2X_1[X_1'(V + X_1X_1')^{-1}X_1]^{-1}X_1'(V + X_1X_1')^{-1}y.$$n

In this paper, roughly speaking, we consider when the BLUE of $M_2X_1\beta_1$ under the fixed effects model $\mathcal{F}$ equals the BLUE of $M_2X_1\beta_1$ under the mixed effects model $\mathcal{M}$. The parameters associated to the model matrix $X_2$ are considered to be nuisance parameters, and we are interested in characterizing the invariance of the BLUE of $M_2X_1\beta_1$ with respect to the choice of $\mathcal{F}$ or $\mathcal{M}$. However, since the covariance matrices $R$ and $G$ can be singular, the fundamental equations (1.4a) and (1.4b) do not necessarily have unique solutions. Thus, if $L_1y$ and $L_2y$ are two different representations of the BLUE$(M_2X_1\beta_1)$ under the model $\mathcal{F}$, then it is possible that even if $L_1y$ is also the BLUE$(M_2X_1\beta_1)$ under the model $\mathcal{M}$, $L_2y$ is not. Hence, in view of Mitra and Moore (1973), we can further specify the problem of the invariance of the BLUE to the following three problems:

1. When does there exist at least one linear transformation $L$ such that $LY$ is the BLUE of $M_2X_1\beta_1$ simultaneously under the models $\mathcal{F}$ and $\mathcal{M}$?
2. When is every representation of the BLUE of $M_2X_1\beta_1$ under the model $\mathcal{F}$ also the BLUE of $M_2X_1\beta_1$ under the model $\mathcal{M}$?
3. When is every representation of the BLUE of $M_2X_1\beta_1$ under the model $\mathcal{M}$ also the BLUE of $M_2X_1\beta_1$ under the model $\mathcal{F}$?
2. Main results

Before proceeding any further, let us define the following matrices:

\[
\begin{align*}
W &= R + UXU', & U \text{ arbitrary with } \mathcal{C}(W) &= \mathcal{C}(X : R), \\
W_f &= R + X_1 U_f X_1', & U_f \text{ arbitrary with } \mathcal{C}(W_f) &= \mathcal{C}(X_1 : R), \\
W_m &= V + X_1 U_m X_1', & U_m \text{ arbitrary with } \mathcal{C}(W_m) &= \mathcal{C}(X_1 : V),
\end{align*}
\]

and

\[
\hat{M}_2 = M_2 (M_2 W_f M_2)^+ M_2.
\]

We can now state the following lemma.

**Lemma.** Consider the models $\mathcal{F}$ and $\mathcal{M}$ defined in (1.2) and (1.3), respectively. Then

(a) $\mathcal{C}(X_2 : RX^\perp)^\perp = \mathcal{C}((\hat{M}_2 X_1 : M_2 - \hat{M}_2 W_f M_2))$

(b) $\mathcal{C}(VX^\perp_1)^\perp = \mathcal{C}(W_m X_1 : M_{W_m})$.

**Proof.** By using Lemma 1 in Isotalo and Puntanen (2006), it is easy to establish the following identity:

\[
\mathcal{C}(X_2 : RX^\perp)^\perp = \mathcal{C}(\hat{M}_2 X_1 : M_2 - \hat{M}_2 W_f M_2).
\]

But since also

\[
M_W = I - p_{(X_2 : W_f)} = I - (P_{X_2} + P_{M_2 W_f M_2})
\]

\[
= M_2 - M_2 W_f M_2 (M_2 W_f M_2)^+
\]

\[
= M_2 - \hat{M}_2 W_f M_2,
\]

part (a) of lemma is proved.

Proof of part (b) is given by, e.g., Rao (1973, Section 2). \hfill \Box

Consider Problem 1. There exists a matrix $L$ such that $Ly$ is the BLUE of $M_2 X_1 \beta_1$ under the both models $\mathcal{F}$ and $\mathcal{M}$ if and only if $L$ satisfies the fundamental equations (1.4a) and (1.4b) simultaneously. The following theorem gives characterization for this to hold.

**Theorem 1.** Consider the models $\mathcal{F}$ and $\mathcal{M}$ defined in (1.2) and (1.3), respectively. There exists a linear transformation $L$ such that $Ly$ is the BLUE of $M_2 X_1 \beta_1$ under the models $\mathcal{F}$ and $\mathcal{M}$ if and only if

\[
\mathcal{N}(X_1 : X_2 : RX^\perp_1) \subset \mathcal{N}(M_2 X_1 : 0 : 0).
\]

**Proof.** There exists a matrix $L$ such that $Ly$ is the BLUE of $M_2 X_1 \beta_1$ under the both models $\mathcal{F}$ and $\mathcal{M}$ if and only if the following equation has a solution with respect to $L$:

\[
L(X_1 : X_2 : RX^\perp_1 : VX^\perp_1) = (M_2 X_1 : 0 : 0 : 0).
\]
When \( L \mathbf{X}_2 = 0 \), then \( L \mathbf{V} \mathbf{X}_1^+ = L \mathbf{R} \mathbf{X}_1^+ \), and because \( \mathcal{C}(\mathbf{X}_1^+) \subset \mathcal{C}(\mathbf{X}_1^+) \), equation (2.2) has a solution if and only if
\[
L(\mathbf{X}_1 : \mathbf{X}_2 : \mathbf{R} \mathbf{X}_1^+) = (\mathbf{M}_2 \mathbf{X}_1 : \mathbf{0} : \mathbf{0})
\]
has a solution, which is clearly equivalent to (2.1).

Let us now consider Problem 2. Note that one representation of the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{F} \) is
\[
\text{BLUE}(\mathbf{M}_2 \mathbf{X}_1 \beta_1 | \mathcal{F}) = \mathbf{M}_2 \mathbf{X}_1 (\mathbf{X}_1' \hat{\mathbf{M}}_2 \mathbf{X}_1')^{-1} \mathbf{X}_1' \hat{\mathbf{M}}_2 \mathbf{y} + \mathbf{M} \mathbf{w} \mathbf{y}. \tag{2.3}
\]
To show that (2.3) holds, verify that the matrix
\[
L = \mathbf{M}_2 \mathbf{X}_1 (\mathbf{X}_1' \hat{\mathbf{M}}_2 \mathbf{X}_1')^{-1} \mathbf{X}_1' \hat{\mathbf{M}}_2 + \mathbf{M} \mathbf{w}
\]
satisfies the fundamental BLUE equation (1.4a).

**Theorem 2.** Consider the models \( \mathcal{F} \) and \( \mathcal{M} \) defined in (1.2) and (1.3), respectively. Then every representation of the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{F} \) is also the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{M} \) if and only if
\[
\mathcal{C}(\mathbf{X}_2 : \mathbf{R} \mathbf{X}_1^+) \subset \mathcal{C}(\mathbf{V} \mathbf{X}_1^+). \tag{2.5}
\]

**Proof.** Let every representation of the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{F} \) be also the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{M} \). Then the representation given in (2.3) must also be the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{M} \). That is, the matrix \( \mathbf{L} \) given in (2.4) must satisfy the equation \( L \mathbf{V} \mathbf{X}_1^+ = 0 \), which is equivalent to the inclusion \( \mathcal{C}(\mathbf{L}') \subset \mathcal{C}(\mathbf{V} \mathbf{X}_1^+) \). However, because
\[
\mathbf{L}'(\hat{\mathbf{M}}_2 \mathbf{X}_1 : \mathbf{M} \mathbf{w}) = (\hat{\mathbf{M}}_2 \mathbf{X}_1 : \mathbf{M} \mathbf{w}),
\]
and obviously \( \mathcal{C}(\mathbf{L}') \subset \mathcal{C}(\hat{\mathbf{M}}_2 \mathbf{X}_1 : \mathbf{M} \mathbf{w}) \), we have that \( \mathcal{C}(\mathbf{L}') = \mathcal{C}(\hat{\mathbf{M}}_2 \mathbf{X}_1 : \mathbf{M} \mathbf{w}) \). Thus, in view of part (a) in Lemma, the inclusion (2.5) follows.

Converse is obvious, and thus the proof is completed.

Problem 3 can be solved as Problem 2. Thus we only state the following theorem.

**Theorem 3.** Consider the models \( \mathcal{F} \) and \( \mathcal{M} \) defined in (1.2) and (1.3), respectively. Then every representation of the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{M} \) is also the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under the model \( \mathcal{F} \) if and only if
\[
\mathcal{C}(\mathbf{X}_1 : \mathbf{X}_2 \mathbf{G} : \mathbf{R}) \subset \mathcal{C}(\mathbf{V} \mathbf{X}_1^+).
\]

If the column space property \( \mathcal{C}(\mathbf{X}_1 : \mathbf{X}_2 \mathbf{G} : \mathbf{R}) = \mathbb{R}^n \) holds, then obviously \( \mathcal{C}(\mathbf{X}_1 : \mathbf{X}_2 : \mathbf{R}) = \mathbb{R}^n \) holds too, and the BLUE of \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) has unique representation under both models \( \mathcal{F} \) and \( \mathcal{M} \). That is, if \( L_1 \mathbf{y} \) and \( L_2 \mathbf{y} \) are two arbitrary BLUEs for \( \mathbf{M}_2 \mathbf{X}_1 \beta_1 \) under either of the models \( \mathcal{F} \) or \( \mathcal{M} \), then \( L_1 = L_2 \); see Groß (2004, Section 2). Thus, under property \( \mathcal{C}(\mathbf{X}_1 : \mathbf{X}_2 \mathbf{G} : \mathbf{R}) = \mathbb{R}^n \), all three considered problems become the same,
and it is obvious from Theorems 2 and 3 that the BLUEs of $M_2X_1\beta_1$ under the models $F$ and $M$ equal if and only if
\[ \mathcal{E}(X_2 : RX^\perp) = \mathcal{E}(VX_1^\perp). \] (2.6)

In the following corollary we give equivalent characterization to (2.6), and consider the equality of BLUEs under particular condition $\mathcal{E}(R) = \mathbb{R}^n$.

**Corollary.** Consider the models $F$ and $M$ defined in (1.2) and (1.3), respectively.

(a) If $\mathcal{E}(X_1 : X_2G : R) = \mathbb{R}^n$, then the BLUEs of $M_2X_1\beta_1$ under the models $F$ and $M$ equal if and only if
\[ \mathcal{E}(X_1) \subset \mathcal{E}(WX_2^\perp). \] (2.7)

(b) If $\mathcal{E}(R) = \mathbb{R}^n$, then the BLUEs of $M_2X_1\beta_1$ under the models $F$ and $M$ equal if and only if
\[ \mathcal{E}(X_1) \subset \mathcal{E}(RX_2^\perp). \] (2.8)

**Proof.** If $\mathcal{E}(X_1 : X_2G : R) = \mathbb{R}^n$, then the column space equality (2.6) is equivalent to the equality
\[ \mathcal{E}(\tilde{M}_2X_1 : MW) = \mathcal{E}(W_m^{-1}X_1), \] (2.9)
since $\mathcal{E}(VX_1^\perp)^\perp = \mathcal{E}(W_mX_1^\perp)^\perp = \mathcal{E}(W_m^{-1}X_1)$. The equality (2.9) is further equivalent to the equalities
\[ \mathcal{E}(W_f\tilde{M}_2X_1) = \mathcal{E}(X_1), \] (2.10)
\[ \mathcal{E}(\tilde{M}_2X_1) = \mathcal{E}(W_m^{-1}X_1). \] (2.11)
The equality (2.11) implies that $X_2^TW_m^{-1}X_1 = 0$, i.e., $\mathcal{E}(X_1) \subset \mathcal{E}(W_mX_2^\perp) = \mathcal{E}(W_fX_2^\perp)$.

Conversely, if (2.7) holds, then $W_f\tilde{M}_2X_1 = X_1$, i.e., the column space equality (2.10) holds, and hence part (a) is proved.

If $\mathcal{E}(R) = \mathbb{R}^n$, then the matrix $\tilde{M}_2$ can be chosen to have a representation
\[ \tilde{M}_2 = M_2(M_2RM_2)^+M_2. \]
Furthermore, if $\mathcal{E}(R) = \mathbb{R}^n$, the column space equality (2.6) is equivalent to the equality
\[ \mathcal{E}(RM_2X_1) = \mathcal{E}(X_1). \] (2.12)
It is now straightforward to show the equivalence between (2.12) and (2.8). \qed
3. Example

A sensitive measuring device is calibrated to work properly at a specific temperature, \( T_{\text{calibrated}} \). However, it is useful to know how small deviations from the specified temperature can affect the measurements. An experiment can be conducted to investigate the relationship between the measurement bias and temperature. The measurement error, \( y := \text{Measurement} - \text{True Value} \), takes the role of the dependent variable and the error in working temperature, \( x_1 := T_{\text{actual}} - T_{\text{calibrated}} \), is used as explanatory variable.

The relationship between \( y \) and \( x_1 \) can be assumed to be linear for small absolute values of \( x_1 \). If the measuring devices are properly calibrated the intercept term should be zero, but usually one might be willing to add an additional factor (device) to the model to account for the calibration error. Hence the final model matrix for an experiment done using two measurement devices can be

\[
X = (x_1 : X_2) = \begin{pmatrix}
-2 & -1 & 0 & 1 & 2 & -2 & -1 & 0 & 1 & 2 \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}'.
\]

The model error terms are independent and one can assume constant variance if the absolute value of \( x_1 \) remains small: \( R = \sigma^2 I \).

The factor corresponding to the measuring device can be fixed (no more than two such measurement devices exist in the world, hence this can not be considered as a sample from an population) or random (in future more devices like these might be available). If the factor corresponding to the measuring device is considered to be random, then one can assume the corresponding random effects to have expectation equal to zero — the calibration process should not be systematically biased.

The regression slope, \( \beta_1 \), is estimable under both models — fixed or mixed. Fortunately \( X'_2 R^{-1} x_1 = 0 \) and from part (b) in Corollary it follows that BLUEs under the models \( F \) and \( M \) are equal. Hence the estimate of regression slope \( \beta_1 \) will remain the same regardless of which model, \( F \) or \( M \), one might favor.

References


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DEPARTMENT OF MATHEMATICS, STATISTICS & PHILOSOPHY, FI-33014 UNIVERSITY OF TAMPERE, FINLAND

*E-mail address: jarkko.isotalo@uta.fi*

INSTITUTE OF MATHEMATICAL STATISTICS, UNIVERSITY OF TARTU, J. LHVII 2, 50409 TARTU, ESTONIA

*E-mail address: martm@kodu.ee*

DEPARTMENT OF MATHEMATICS, STATISTICS & PHILOSOPHY, FI-33014 UNIVERSITY OF TAMPERE, FINLAND

*E-mail address: simo.puntanen@uta.fi*