A Diagnostic for Bias in Linear Mixed Model Estimators Induced by Dependence Between the Random Effects and the Corresponding Model Matrix

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Abstract

We explore how violations of the often-overlooked standard assumption that the random-effects model matrix in a linear mixed model is fixed (and thus independent of the random effects vector) can lead to bias in estimators of estimable functions of the fixed effects. However, if the random effects of the original mixed model are instead also treated as fixed effects, or if the fixed and random effects model matrices are orthogonal with respect to the inverse of the error covariance matrix (with probability one), or if the random effects and the corresponding model matrix are independent, then these estimators are unbiased. The bias in the general case is quantified and compared to a randomized permutation distribution of the predicted random effects, producing an informative summary graphic for each estimator of interest. This is demonstrated through the examination of sporting outcomes used to estimate a home field advantage.

Keywords: Hausman test, misspecification, randomized permutation test, stochastic model matrix
1 Introduction

Standard linear mixed models are built conditional on the model matrices for the fixed and random effects, meaning that these matrices are assumed to be fixed and constructed without reference to the anticipated errors or random effects. However, this assumption is occasionally not satisfied in practice, such as when the experimenter (or generating process) has some knowledge of the anticipated realizations of the random factor effects and then builds the model matrices with this knowledge in mind. Unless the model matrices for the fixed and random effects are orthogonal with respect to the error covariance matrix, the dependence between the random effects and their corresponding model matrix will induce bias in the estimators of estimable functions of the fixed effects. This paper develops graphical and numeric diagnostics for the bias of estimators of estimable functions of fixed effects in mixed models that are constructed under the assumption that the model matrices are fixed when in fact the random effects model matrix is stochastic. This is a known problem (Allison 1994, Lockwood & McCaffrey 2007), but not well-known enough by users of linear mixed models.

Consider a linear mixed model with fixed model matrices:

\[ Y = X\beta + Z\eta + \epsilon \] \hspace{1cm} (1)

for a continuous response, \( Y \), where \( \eta \) and \( \epsilon \) are independent with \( \eta \sim N_m(0, \sigma^2 G) \) and \( \epsilon \sim N_n(0, \sigma^2 R) \). Although we assume normality for these vectors in order to match the most common applications, the main result on bias does not depend on this assumption. The matrices \( G \) and \( R \) are assumed to be positive definite, \( \sigma^2 \) is assumed to be positive, and neither \( X \) nor \( Z \) are required to be full rank. If \( k'\beta \) is estimable under this model and \( V \equiv (1/\sigma^2)\text{var}(Y) = ZGZ' + R \) is known, then the best linear unbiased estimator (BLUE) of \( k'\beta \) is \( k'\hat{\beta} \) where \( \hat{\beta} = (X'V^{-1}X)^{-}X'V^{-1}Y \). (Here and throughout, for any matrix \( M \), \( M^{-} \) represents an arbitrary generalized inverse of \( M \).)
In many important applications of the linear mixed model, $R$ is known (often, in fact, $R = I$) but $G$ is unknown; more precisely, the elements of $G$ are known functions of an unknown parameter $\theta$, i.e., $G = G(\theta)$. For inference on $k'\beta$ to proceed in such settings it is necessary to first obtain an estimate $\hat{\theta}$ which can be substituted for the unknown $\theta$ to obtain an estimate $\hat{G} = G(\hat{\theta})$ and a corresponding estimate $\hat{V} = Z\hat{G}Z' + R$ of $V$; after that, an empirical BLUE (E-BLUE) of $k'\beta$ may be calculated as $k'\hat{\beta}$ where $\hat{\beta} = \left(X'\hat{V}^{-1}X\right)^{-}X'\hat{V}^{-1}Y$. Though the E-BLUE generally is not linear or best in any sense, it is unbiased provided that $\hat{\theta}$ is an even and translation-invariant estimator [Kackar & Harville 1981]. (An estimator $\hat{\theta} = \hat{\theta}(Y)$ of $\theta$ is even and translation invariant if $\hat{\theta}(\cdot - Y) = \hat{\theta}(Y)$ and $\hat{\theta}(\cdot + Xc) = \hat{\theta}(Y)$ for all $Y$ and all $c$.)

As an alternative to a mixed effects model, a fixed effects model could be fit:

$$Y = X_*\beta_* + \epsilon$$

where $\epsilon \sim N_\eta(0, \sigma^2R)$, $\beta_* = [\beta' \eta']$, $X_* = [X \ Z]$, and $\eta$ is fixed. If $k_*\beta_*$ is estimable under this model and $R$ is known, then the BLUE of $k_*\beta_*$ is $k_*\tilde{\beta}_*$ where $\tilde{\beta}_* = [\tilde{\beta}' \tilde{\eta}']' = (X_*'R^{-1}X_*)^{-}X_*'R^{-1}Y$. In order to consider only estimable functions of effects that are treated as fixed in the mixed effects model [1], we will restrict attention to $k_*$ that satisfy $k_*' = [k' \ 0']$, where the length of the zero vector is equal to $m$, meaning that the BLUE of $k_*\beta_*$ is $k_*\tilde{\beta}$. The decision to treat effects as fixed or random has been widely explored previously [Robinson 1991, Stroup 2012].

The E-BLUE $k'\hat{\beta}$ and BLUE $k'\tilde{\beta}$ of, respectively, estimable functions $k'\beta$ and $k_*\beta_*$ under the mixed and fixed effects models [1] and [2] are potentially biased under more general versions of these models in which $Z$ is stochastic. Henceforth we refer to these more general versions as stochastic-$Z$ mixed and fixed effects models. This issue seems to have received more attention in the economics literature [Wu 1973, Hausman 1978, Hausman & Taylor 1981, Allison 1994, Wooldridge 2001, Lockwood & McCaffrey 2007] than in standard statistics textbooks on linear mixed models [Verbeke & Molenberghs 2000, Littell et al. 2006, Stroup 2012, Demidenko].
Our aim is to increase this awareness by discussing an application with clear visual evidence and by proposing computationally-light diagnostics and graphics that statistical software could produce in order to help quickly detect this bias on an application-by-application basis.

Section 2 provides a practical motivation for considering this problem by comparing the fixed and mixed effects model estimates of home field scoring advantage for several sports. Section 3 derives sampling properties, including bias, of the E-BLUE and BLUE of estimable functions under the stochastic-Z mixed and fixed effects models, and proposes the use of a randomized permutation distribution of predicted random effects to assess the magnitude of the bias. Section 5 applies these results to the home field advantage problem. Section 6 simulates the home field advantage problem in order to illustrate the findings of Section 3 by manipulating the team schedules, Z.

2 Estimating Home Field Advantage

There has long been observed a “home-field advantage” across a variety of sports (Lopez et al. 2018). We define home field scoring advantage (HFA) as the difference in the expected scores of the home and away teams within a game, after the strength of each team has been accounted for. It is possible to account for the team strengths with either fixed or random effects. This section presents both a fixed effects model and a mixed effects model for the home team margins of victory, $Y_i = y_{H_i} - y_{A_i}$, where $y_{H_i}$ and $y_{A_i}$ are the home and away team scores, respectively, for game $i = 1, ..., n$. With $m$ teams in a data set, the pattern of game opponents and locations (the schedule) is recorded in an $n \times m$ matrix $Z$ as follows: if team $T_H$ hosted team $T_A$ in game $i$, then the $i$-th row of $Z$ consists of all zeros except for a 1 in the column corresponding to $T_H$ and a $-1$ in the column corresponding to $T_A$. To simplify the discussion, neutral site games are not considered.
2.1 Fixed Effects Model

The first plausible model we consider for HFA includes a fixed effect $\lambda$ for the HFA and a vector of fixed team strength effects $\bm{\beta} = (\beta_1, \ldots, \beta_m)'$, where the difference between any two team strength effects represents the expected difference in score in a game between the two teams on a neutral field. For each game $i$, this model assumes

$$Y_i \sim N(\lambda + \beta_{H_i} - \beta_{A_i}, \sigma^2)$$

where $H_i$ and $A_i$ are the indices for the home and away teams, respectively, in game $i$. The residuals are assumed to be independent, leading to an overall model

$$\bm{Y} = 1\lambda + \bm{Z}\bm{\beta} + \bm{\epsilon}$$

(3)

where $\bm{Y} = (Y_1, \ldots, Y_n)'$, $\bm{Z}$ is fixed, and $\bm{\epsilon} \sim N(\bm{0}, \sigma^2 \bm{I})$. This model appears previously as Model 2 of Harville & Smith (1994) and Model 1 of Harville (2003). The model matrix $\bm{X}_* = [1, \bm{Z}]$ is not full rank and the individual team strength effects $\beta_i$ are not estimable. However, $\lambda$ is estimable, as are the pairwise differences between team strength effects, provided there is sufficient mixing of the teams. For example, in a sport of three teams $\{A, B, C\}$, $\lambda$ will be estimable if each pair of teams have a home and home series, or if, for example, team B plays at team A, team A plays at team C, and team C plays at team B. Stroup (2012, Section 5.2.1) provides a good summary of the estimability of fixed effects.

2.2 Mixed Effects Model

Alternatively, the team strengths may be modeled as random effects $\bm{\eta} = (\eta_1, \ldots, \eta_m)'$ that are assumed to be independent of the residuals. Then, $Y_i$ is modeled conditional on the random effects as

$$Y_i|\bm{\eta} \sim N(\lambda + \eta_{H_i} - \eta_{A_i}, \sigma^2)$$
producing an overall model

\[ Y|\eta \sim N(1\lambda + Z\eta, \sigma^2 I) \]  
\[ \eta \sim N(0, \sigma^2_g I) \]  

As in the fixed effects model, \( Z \) is assumed to be fixed and \( \lambda \) is estimable. Harville (1977, Equation 2.1) considers a generalization of this model for ranking teams. An advantage of placing a distributional assumption on the team strength effects is that it provides a form of regularization for the model and avoids the aforementioned estimability concern. A disadvantage is that another parameter (\( \sigma^2_g \)) is introduced that must be estimated before inference on \( \lambda \) can proceed. Here \( V = \theta ZZ' + I \) where \( \theta = \sigma^2_g / \sigma^2 \), so there is a single variance component ratio, \( \theta \), to estimate. Commonly, \( \theta \) is estimated by the methods of maximum likelihood or residual maximum likelihood (REML); both methods yield even, translation-invariant estimators (Kackar & Harville 1981).

### 2.3 Results

Scores from the 2000-2017 seasons for each of the six sports of Men’s and Women’s NCAA Division I basketball, NCAA Football Bowl Subdivision (FBS), the National Football League (NFL), the Women’s National Basketball Association (WNBA), and the National Basketball Association (NBA) are furnished by the website of Massey (2017), with some missing WNBA results obtained from WNBA.com. In all cases, neutral site games are excluded in order to simplify the discussion of the application. The supplementary material contains code for downloading the scores from Massey (2017) and for obtaining the REML estimates of the models in Equations 3 and 4 with the R package mvglmmRank (Broatch & Karl 2018).

Generally, professional teams play balanced schedules with an equal number of home and away games and a representative selection of teams from the league. In the regular season, the NBA games are perfectly balanced in the sense that every
Figure 1: EBLUPs of the team ratings from the mixed model for the 2017 men’s college basketball season plotted by proportion of games played at home by the team, along with a LOESS smoother.

team plays 41 home and 41 away games. By contrast, college sports tend to have unbalanced schedules, with the better and more influential teams able to schedule more home than away games. For example, 10% of Division I men’s college basketball teams played no more than 38% of their games at home, while another 10% of teams played no fewer than 62% of their games at home. Furthermore, there is a tendency for influential college teams to intentionally schedule weaker opponents for their surplus home games. Athletic directors of better teams accomplish this by building their schedules ($Z$) for future years using historical knowledge of the quality of their potential opponents and the general tendency for team quality to be (positively) correlated over years. This results in a violation of the assumption in the mixed model (4) that $Z$ is fixed. In fact, not only is $Z$ stochastic, but $Z$ and $\eta$ are dependent. To illustrate, Figure 1 plots the empirical best linear unbiased predictors (EBLUPs) of the 2017 men’s college basketball team ratings ($\hat{\eta}$) from the mixed model against the proportion of games played at home (a function of $Z$).

Figure 2 shows the HFA estimates from the fixed and mixed effects models for each year in each season, including downward trends in the college HFAs that have been
Figure 2: BLUEs of the HFA under the fixed effects model (3) (solid line) are plotted with the corresponding E-BLUEs under the mixed effects model (4) (dashed line) across seasons of college sports (left) and professional sports (right). The lines in the professional plots nearly coincide.
noted by sports journalists (Chatelain 2016, Davis 2017). Estimates of $\lambda$ from the two models are mostly identical in the professional sports, but are cleanly separated in the college sports where the mixed-model estimates (the E-BLUEs) are uniformly larger than the fixed effect estimates (the BLUEs). Interestingly, the separation between the fixed and mixed model estimates of HFA is relatively constant across years within the sports. Section 3 demonstrates that when $Z$ is stochastic, the E-BLUE obtained by fitting the mixed effects model is generally biased but the BLUE obtained by fitting the fixed effects model is unbiased.

3 Sampling Properties of $k'\hat{\beta}$ and $k'\tilde{\beta}$ under Stochastic-Z Models

Throughout this section, let $k'\beta$ be a linear function of $\beta$ that is estimable under the standard (fixed-Z) mixed effects model (1), and suppose that $k'\beta$ is also estimable with probability one under the stochastic-Z version of the fixed effects model (2). (The HFA described in the previous section is such a function.) Furthermore, let $k'\hat{\beta}$ and $k'\tilde{\beta}$ be the E-BLUE and BLUE of $k'\beta$, respectively, obtained by fitting standard versions of those models, where the estimator $\hat{\theta}$ used to obtain $k'\hat{\beta}$ is even and translation-invariant. In this section, we investigate sampling properties, specifically the bias and the variance, of the E-BLUE and BLUE under stochastic-Z versions of the models.

3.1 Bias

Lemma 1. Let $M$ be a generalized inverse of $A'A$ where $A$ is any matrix. Then $MA'$ is a generalized inverse of $A$, so that $AMA'A = A$.

The proof of Lemma 1 can be found in many linear algebra texts, including Harville (2008).
Theorem 2. Let \( \hat{\nu}_k' = k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}X'\hat{\mathbf{V}}^{-1}Z \). If \( Z \) is stochastic in the mixed effects model but \( \epsilon \) and \( Z \) are independent, then the bias of \( k'\hat{\beta} \) is equal to \( E[\hat{\nu}_k'\eta] \).

Proof. Since \( k'\beta \) is estimable under model (1), there exists a vector \( t \) such that \( k' = t'X \). And since \( \hat{\mathbf{V}} \) is positive definite (with probability one) with Cholesky decomposition \( \hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}' \) (where \( \hat{\mathbf{L}} \) is lower triangular and positive definite), there also exists (with probability one) a vector \( t_L = \hat{\mathbf{L}}'t \) such that \( k' = t_L'\hat{\mathbf{L}}^{-1}X \). Then

\[
E[k'\hat{\beta}] = E[E[k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}X'\hat{\mathbf{V}}^{-1}Y|\eta, Z)] \\
= E[E[k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}(X\beta + Z\eta + \epsilon)|\eta, Z]] \\
= E[k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}(X\beta + Z\eta)] \\
= E[t_L'\hat{\mathbf{L}}^{-1}X(X\hat{\mathbf{L}}'^{-1}\hat{\mathbf{L}}^{-1}X)^{-1}X'\hat{\mathbf{L}}'^{-1}\hat{\mathbf{L}}^{-1}(X\beta + Z\eta)] \\
= k'\beta + E[\hat{\nu}_k'\eta]
\]

where Equation 5 uses the main result of Kackar & Harville (1981) and Equation 6 uses Lemma 1 with \( A = \hat{\mathbf{L}}^{-1}X \).

Our first corollary to Theorem 2 reveals that bias in \( k'\hat{\beta} \) occurs because of dependence between \( \hat{\nu}_k \) and \( \eta \), not merely because \( Z \) is stochastic.

Corollary 3. If \( Z \) is stochastic in the mixed effects model but \( \epsilon, \eta, \) and \( Z \) are independent, then \( k'\hat{\beta} \) is unbiased.

Proof.

\[
E[\hat{\nu}_k'\eta] = E[k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}X'\hat{\mathbf{V}}^{-1}Z\eta] \\
= E(E[k'(X'\hat{\mathbf{V}}^{-1}X)^{-1}X'\hat{\mathbf{V}}^{-1}Z\eta|Z]) \\
= E(0) \\
= 0.
\]

where Equation 7 uses the main result of Kackar & Harville (1981) once again. The result follows by Theorem 2. \( \square \)
Our second corollary to Theorem 2 shows that $k' \hat{\beta}$ can be unbiased even when $Z$ and $\eta$ are dependent, provided that a certain orthogonality condition holds.

**Corollary 4.** If $Z$ is stochastic in the mixed effects model but $\epsilon$ and $Z$ are independent and $Z$ is orthogonal to $X$ with respect to $R^{-1}$ (with probability one), then $k' \hat{\beta}$ is unbiased.

**Proof.** By Theorem 18.2.8 of [Harville (2008)](#), $X' \hat{V}^{-1} Z = X' R^{-1} Z - X' R^{-1} Z \hat{T}' \hat{Z}' R^{-1} Z$ where $\hat{T} = (Z' R^{-1} Z + \hat{G}^{-1})^{-1}$. Since $X' R^{-1} Z = 0$ except on a set of probability zero, $X' \hat{V}^{-1} Z = 0 - 0 \hat{T}' \hat{Z}' R^{-1} Z = 0$, which implies that $\hat{\nu}_k = 0$ with probability 1.

Thus, $E[\hat{\nu}_k' \eta] = 0$. The result follows by Theorem 2.

By contrast with the E-BLUE obtained by fitting a mixed effects model with stochastic $Z$, the next theorem reveals that the BLUE $k' \hat{\beta}$ obtained by fitting the fixed effects model is unbiased when $Z$ is stochastic without any conditions on $\eta$ (other than it being fixed).

**Theorem 5.** If $Z$ is stochastic in the fixed effects model but $\epsilon$ and $Z$ are independent, then $k' \hat{\beta}$ is unbiased.

**Proof.** Since, by assumption, $k' \beta$ is estimable with probability one under the fixed effects model with stochastic $Z$, for every $Z$ on a set of probability one there exists a vector $t_Z$ such that $k' = t'_Z (I - P_{Z\|}) X_{\|}$, where $P_{Z\|} = Z_{\|} (Z'_{\|} Z_{\|})^{-1} Z'_{\|}$, $Z_{\|} = R^{-1/2} Z$, and $X_{\|} = R^{-1/2} X$. Thus, upon defining $\epsilon_{\|} = R^{-1/2} \epsilon$, we find that

$$E(k' \hat{\beta}) = E\{E[k'[X'_{\|} (I - P_{Z\|}) X_{\|}]^{-1} X'_{\|} (I - P_{Z\|}) (X_{\|} \beta + Z_{\|} \eta + \epsilon_{\|}) | Z]\}$$

$$= k' \beta + E\{E[k'[X'_{\|} (I - P_{Z\|}) X_{\|}]^{-1} X'_{\|} (I - P_{Z\|}) \epsilon_{\|} | Z]\}$$

$$= k' \beta + E\{E[k'[X'_{\|} (I - P_{Z\|}) X_{\|}]^{-1} X'_{\|} (I - P_{Z\|})] \epsilon_{\|}\} E(\epsilon_{\|})$$

$$= k' \beta$$
3.2 Variance

The variances of $k'\hat{\beta}$ and $k'\tilde{\beta}$ are also affected by the stochasticity of $Z$ in the mixed and fixed effects models. However, the variance of $k'\hat{\beta}$, unlike the bias, is also affected by the estimation of $\theta$; in fact, if $\hat{\theta}$ is even and translation-invariant, then $\text{var}(k'\hat{\beta})$ is larger than if $\theta$ were known (Kackar & Harville 1984). In order to focus exclusively on the effect of a stochastic $Z$ on this variance, in this section we assume that $\theta$ is known. Results comparing the variances of the E-BLUEs of $k'\beta$ under the fixed-$Z$ and stochastic-$Z$ models when $\theta$ is known should shed some light on how those variances compare when $\theta$ is unknown.

**Theorem 6.** If $Z$ is stochastic in the mixed effects model but the conditions of Theorem 2 hold and $\theta$ is known, the variance of the BLUE, $k'\hat{\beta}$, is $\sigma^2E[k'(X'V^{-1}X)^{-}k] + \text{var}(\nu_k'\eta) - \sigma^2E(\nu_k'G\nu_k)$.

**Proof.**

\[
\text{var}(k'\hat{\beta}) = \text{var}\{E[k'(X'V^{-1}X)^{-}X'V^{-1}Y|\eta, Z]\} + \text{var}(k'(X'V^{-1}X)^{-}X'V^{-1}\epsilon|\eta, Z]\}
\]

\[
=\text{var}(k'(X'V^{-1}X)^{-}X'V^{-1}(X\beta + Z\eta)] + \text{var}(k'(X'V^{-1}X)^{-}X'V^{-1}\epsilon|\eta, Z]\}
\]

\[
=\text{var}(k'\beta + \nu_k'\eta) + E\{k'(X'V^{-1}X)^{-}X'V^{-1}\sigma^2[V - ZGZ']V^{-1}X[(X'V^{-1}X)^{-}]|k}\}
\]

\[
=\sigma^2E[k'(X'V^{-1}X)^{-}k] + \text{var}(\nu_k'\eta) - \sigma^2E(\nu_k'G\nu_k)
\]

**Corollary 7.** If $Z$ is stochastic in the mixed effects model but $\epsilon$, $\eta$, and $Z$ are independent, then $\text{var}(k'\hat{\beta}) = \sigma^2E[k'(X'V^{-1}X)^{-}k]$.

**Proof.**

\[
\text{var}(\nu_k'\eta) = E[\nu_k'\eta\eta'\nu_k] - (E[\nu_k'\eta])^2
\]

\[
= E[\text{tr}(\nu_k\nu_k'\eta\eta')]
\]

\[
= \text{tr}(E[\nu_k\nu_k']\sigma^2G)
\]

\[
= \sigma^2E[\nu_k'G\nu_k]
\]
which implies that \( \text{var}(k'\hat{\beta}) = \sigma^2 \text{E}[k'(X'V^{-1}X)^{-}k] \) by Theorem 6.

**Corollary 8.** If \( Z \) is stochastic in the mixed effects model, but \( \epsilon \) and \( Z \) are independent and \( Z \) is orthogonal to \( X \) with respect to \( R^{-1} \) (with probability one), then \( \text{var}(k'\hat{\beta}) = \text{E}[k'(X'V^{-1}X)^{-}k] - \sigma^2 \text{E}(\nu_k'G\nu_k) \).

**Proof.** The same argument that established that \( \text{E}(\hat{\nu}_k'\eta) = 0 \) in the proof of Corollary 5 also yields \( \text{var}(\nu_k'\eta) = 0 \). Thus, by Theorem 6,

\[
\text{var}(k'\hat{\beta}) = \sigma^2 \text{E}[k'(X'V^{-1}X)^{-}k] - \sigma^2 \text{E}(\nu_k'G\nu_k)
\]

Since \( \sigma^2 \text{E}(\nu_k'G\nu_k) \geq 0 \), the variance of \( k'\hat{\beta} \) is generally smaller under the conditions of Corollary 8 than it is under the conditions of Corollary 7.

**Theorem 9.** If \( Z \) is stochastic in the fixed effects model but \( \epsilon \) and \( Z \) are independent, then \( \text{var}(k'\hat{\beta}) = \sigma^2 \text{E}\{k'[X'R^{-1}X - X'R^{-1}Z(Z'R^{-1}Z)^{-}Z'R^{-1}X]^{-}k\} \).

**Proof.** Using the same notation as in the proof of Theorem 5,

\[
\text{var}(k'\hat{\beta}) = \text{E}\{\text{E}\{k'[X'_\alpha(I - P_{Z_\alpha})X_{\alpha}][X'_\alpha(I - P_{Z_\alpha})X_{\alpha}]^{-}k|Z\}\} + 0
\]

\[
= \sigma^2 \text{E}\{k'[X'_\alpha(I - P_{Z_\alpha})X_{\alpha}]^{-}k\}
\]

\[
= \sigma^2 \text{E}\{k[X'R^{-1/2}[I - R^{-1/2}Z(Z'R^{-1}Z)^{-}Z'R^{-1/2}]R^{-1/2}X]^{-}k\}
\]

\[
= \sigma^2 \text{E}\{k[X'R^{-1}X - X'R^{-1}Z(Z'R^{-1}Z)^{-}Z'R^{-1}X]^{-}k\}
\]

By Theorem 9, the variance of \( k'\hat{\beta} \) is equal to \( \sigma^2 k'(X'R^{-1}X)^{-}k \) when \( X'R^{-1}Z = 0 \) (with probability 1). In the disallowed case where \( Z = X \) (with probability 1), the expression inside of the generalized inverse is \( 0 \).
4 Bias Diagnostics

In situations where the mixed effects model E-BLUE \((k'\hat{\beta})\) is estimable (with probability one) and biased, but the fixed effects model BLUE \((k'\hat{\beta})\) is estimable and unbiased under stochastic-\(Z\) versions of the models, the magnitude of the difference \(k'\hat{\beta} - k'\hat{\beta}\) provides an estimate of the bias. [Hausman, 1978] uses this difference to formulate a specification test for the consistency of the generalized least squares estimators in a random intercept model.

Alternatively, the EBLUP of \(\eta\) from the fitted mixed effects model can be substituted into \(E(\hat{\nu}_k'\eta)\) to produce a diagnostic value \(\hat{\nu}_k'\hat{\eta}\) that can serve as an internal estimate of the bias of \(k'\hat{\beta}\). And although it is not pursued further here, the plug-in estimate \(\hat{\nu}_k\) of \(\nu_k\) might benefit from using the bias-corrected precision estimator of [Kenward & Roger, 2009] in place of \((X'\hat{V}^{-1}X)^{-}\).

4.1 Randomization Test for Independence of \(\nu_k\) and \(\eta\)

Even when \(X\) and \(Z\) are not orthogonal with respect to \(R^{-1}\) (Corollary 4), \(k'\hat{\beta}\) is still unbiased if \(\eta\) is sampled independently of \(\nu_k\) (Corollary 3). Under the null hypothesis of independence of \(\eta\) and \(\nu_k\), the observed value \(\hat{\nu}_k'\hat{\eta}\) could be compared to the randomized permutation distribution (Edgington & Onghena, 2007) of

\[\hat{\nu}_k'\pi(\hat{\eta})\]

where \(\pi()\) is a permutation function and \(\hat{\nu}_k\) is held fixed at the value obtained during the original model fit. For a diagonal \(G\), the permutations performed by \(\pi(\hat{\eta})\) are stratified within each random factor present in \(\eta\) (corresponding to unique diagonal entries of \(G\)). More generally, when \(G\) has nonnull off-diagonal entries, the permutation function \(\pi(\hat{\eta})\) can be constructed as follows.

1. Simulate a vector, \(w_0\), from \(N(0, \hat{G})\).
2. Let \(w = w_0\).
3. For each random factor (corresponding to the unique diagonal elements of $G$), replace the smallest element of $w$ with the smallest element of the corresponding factor from $\hat{\eta}$.

4. Repeat Step 3 for the component of $w$ corresponding to the second smallest entry in the original $w_0$ for each factor, the third smallest, etc.

5. Return $w$.

This function $\pi(\hat{\eta})$ shuffles $\hat{\eta}$ within each factor according to the correlation structure assumed by $G$, provided that $G$ has equicorrelation within factors (meaning that random effects within a factor are exchangeable).

The permutation distribution provides an estimate of the distribution of the observed $\hat{\nu}_k' \hat{\eta}$ that would be expected under random sampling of $\eta$ (prior to the generation of $Y$), and the mean of this distribution provides an estimate of $E[\hat{\nu}_k' \hat{\eta}]$ under random sampling of the random effects, a value that should equal 0 if the other conditions of Corollary 3 hold. The percentile of the observed value within the distribution of permuted values can be used to detect inconsistency with the hypothesis of independence of $\eta$ and $\nu_k$. Small percentiles (say, < 0.005), corresponding to negative bias, or large percentiles (say, > 0.995), corresponding to positive bias, indicate that $\eta$ and $\nu_k$ may not be independent. As demonstrated in the next section, a plot of the randomized permutation distribution along with a vertical line at $\hat{\nu}_k' \hat{\eta}$ provides a useful graphical summary for each estimable effect $k'\beta$ of interest.

While the predictions $\hat{\eta}$ from many common mixed models sum to 0 within each random factor (Searle 1997), this may not be true in all cases. If this sum is different from zero, then the randomization distribution of $\hat{\nu}_k' \pi(\hat{\eta})$ may have mean different from zero, indicating the presence of bias in $k'\hat{\beta}$ regardless of the randomization of $\eta$. This would represent some other departure from modeling assumptions, perhaps due to dependence between the model matrices and $\epsilon$, or due to the presence of a nonignorable missingness process.
4.2 Simulation Based Estimate of Bias

While Equation 6 suggests that $\hat{\nu} \hat{\eta}'$ can serve as an internal estimate of the bias for the associated estimator of the estimable function using only a single model fit, it is also possible to estimate the bias via simulation by using the model matrices and estimates from the original fit and repeatedly replacing the residual vector with a random vector drawn from $N(0, \hat{\sigma}^2 R)$. Specifically,

1. Fit $Y|\eta \sim N(X\beta + Z\eta, \sigma^2 R)$ where $\eta \sim N(0, \sigma^2 G)$ in order to obtain solutions $\hat{\beta}$, $\hat{\eta}$, and $\hat{\sigma}^2 R$. The estimated random effects covariance matrix, $\hat{\sigma}^2 \hat{G}$, is not used in the rest of the simulation.

2. Repeatedly simulate a new response vector $Y_s = X\hat{\beta} + Z\hat{\eta} + e_s$, where $e_s$ is a random deviate from $N(0, \hat{\sigma}^2 R)$. Then fit $Y_s$ using the same mixed model as Step 1 and record the estimate $k'\hat{\beta}_s$.

3. Compare the mean of the sampling distribution of $k'\hat{\beta}_s$ to the target of $k'\hat{\beta}$ (the original estimate from $Y$ in Step 1). The difference between $\text{mean}_s(k'\hat{\beta}_s)$ and $k'\hat{\beta}$ provides an estimate of the bias in the E-BLUE of $k'\beta$ for this particular data set.

The advantage of the internal estimate of bias, $\hat{\nu} \hat{\eta}'$, over the estimate obtained by simulation is that the model does not need to be fit repeatedly and it can be calculated using matrices that have already been produced by the original model fit.

5 Bias in the Mixed Model HFA Estimator

Table 1 contains the estimated bias $\hat{\nu} \hat{\eta}'$ for each sport in 2017 from the application of Section 2 (where $k = 1$ and the estimable effect of interest is simply the intercept). These represent an internal estimate of the bias in the HFA E-BLUE. They are strongly correlated ($\rho = 0.989$) with the difference between the mixed and fixed
Table 1: 2017 HFA estimates (in points) from the mixed and fixed effect models, along with the standard error of the mixed model estimates (calculated under the fixed-$Z$ assumption), the difference between the mixed and fixed HFA estimates, the internal estimates of bias, and the percentile of the observed bias in the randomized permutation distribution. The final two columns present the simulation results described in Section 4.2.

| Sport              | Fixed ($\hat{\lambda}$) | Mixed ($\tilde{\lambda}$) | Mixed S.E | Mixed - Fixed | $\nu_k' \tilde{\eta}$ | Percentile in $\nu_k' \pi(\tilde{\eta})$ | 1k Sim Mean | 1k Sim Bias |
|--------------------|--------------------------|----------------------------|-----------|---------------|------------------------|------------------------------------------|-------------|-------------|
| NCAA Football      | 2.47                     | 3.00                       | 0.55      | 0.54          | 0.38                   | $> 0.999999$                           | 3.47        | 0.46        |
| NCAA Basketball (M) | 2.84                     | 3.16                       | 0.32      | 0.32          | 0.28                   | $> 0.999999$                           | 3.49        | 0.32        |
| NCAA Basketball (W) | 2.85                     | 3.00                       | 0.16      | 0.16          | 0.14                   | $> 0.999999$                           | 3.15        | 0.15        |
| NFL                | 2.33                     | 2.43                       | 0.78      | 0.10          | 0.06                   | 0.995                                   | 2.49        | 0.07        |
| NBA                | 3.05                     | 3.05                       | 0.35      | 0.00          | 0.00                   | 0.903                                   | 3.05        | -0.01       |
| WNBA               | 3.16                     | 3.18                       | 0.82      | 0.01          | 0.01                   | 0.945                                   | 3.18        | -0.00       |

effects model estimates of HFA, and with the simulation estimates ($\rho = 0.994$), which represent external estimates of the mixed model bias. The percentile of the observed value $\nu_k' \tilde{\eta}$ in the distribution of a sample of one million permutations $\nu_k' \pi(\tilde{\eta})$ is also reported, and is displayed for the 2017 seasons of the sports in Figure 3. The college sports produce observed values that are larger than all of the other sampled permutations of $\tilde{\eta}$, providing strong evidence that $\nu_k$ and $\eta$ are not independent in these applications. Combined with the fact that none of the means of the sampling distributions differ substantially from zero (see the supplementary data tables), we can conclude that the mixed effects model E-BLUEs of HFA in Table 1 pertaining to the college sports are significantly biased upward. It is worth noting that the percentiles for $\nu_k' \tilde{\eta}$ in their permutation distributions from the professional sports (available in the supplementary material) are not always as large (i.e. $> 0.9$) in other seasons. Additionally, the sum of the team ratings $\tilde{\eta}$ in each year is equal to 0, as expected (Searle, 1997).

If every team in a sport plays the same number of home games as they play away games, then under model (4), $X'IZ = 0$ and the conditions of Corollaries 4 and 8...
hold. The NBA schedule is only slightly unbalanced in this sense due to post-season games. This is reflected in Table 1 by the rounded-to-zero NBA estimate for $\hat{\nu} k \hat{\eta}$ and by the relatively small variability in the NBA permutation distribution in Figure 3.

To assess the practical significance of the observed bias, the magnitude of $\hat{\nu} k \hat{\eta}$ could be compared to the standard error of the corresponding point estimate. The standard errors reported in Table 1 are those produced by the software under the fixed-$Z$ assumption, rather than those that would be produced by Corollary 6. For college men’s and women’s basketball, the bias is equal to about 90% of the standard error, while for college football the estimated bias is equal to about 70% of the standard error. In the professional sports, the bias estimates are negligible compared to the standard errors.

6 Simulating the Sports Scheduling Problem

Since the bias of $k'\hat{\beta}$ depends on the expected value of $\hat{\nu} k \hat{\eta}$ where $Z$ and $\eta$ are dependent, an experimenter with (approximate) knowledge of $\eta$ could induce positive (or negative) bias in $k'\hat{\beta}$ by selecting $Z$ such that $E[\hat{\nu} k \hat{\eta}] > 0$ (or $E[\hat{\nu} k \hat{\eta}] < 0$).

Figure 3 shows that the observed values of $\hat{\nu} k \hat{\eta}$ for the college sports are larger than any of the million sampled permutations $\hat{\nu} k \pi(\hat{\eta})$, suggesting that the nonrandom mechanism by which college sports schedules are built produces larger values of $\hat{\nu} k \hat{\eta}$ than would be expected under random scheduling. Using this knowledge, it is possible to reproduce the bias in the home field advantage estimator from the mixed model via simulation by selecting the schedule $Z$ (after $\eta$ as been generated) that maximizes $\nu k \pi(\eta)$, replicating the behavior of the real schedules observed in Figure 3. R code to reproduce the results of this section is available in the supplementary material.

In order to simulate the biasing behavior seen in Figure 2, 5000 candidate schedules ($Z$) with 12 games per team are generated after the vector of 50 team strength
Figure 3: Randomized permutation distributions (one million permutations) of $\hat{\nu}_k'\pi(\hat{\eta})$ for the 2017 schedules for each sport. The solid line indicates the observed bias, $\hat{\nu}_k'\hat{\eta}$. The dashed line is placed at zero to show that the sampling distributions have mean 0 for this application.
Figure 4: Box plots of 1000 simulations of home field advantage estimates from both models when $Z_s$ has been selected in order to maximize $\nu_k'\eta$. The true value for the HFA in the simulation was 0. The third column contains the box plot for the matched pair differences between intercept estimates from each simulation: E-BLUE minus the BLUE.

effects, $\eta_s \sim N_{50}(0, 225I)$, has been generated. The only restriction on the teams during the game assignments is that teams are not allowed to play themselves. As a result, the teams do not necessarily play the same number of home games.

The schedule, $Z_s$, that maximizes $\nu_k'\eta_s$ is selected, and then game outcomes, $Y_s = 0 + Z_s\eta_s + e_s$, are simulated, where $e_s \sim N_{300}(0, 529I)$. The variances were chosen to represent typical values observed from historical data. Note that $\nu_k$ (with $k = 1$ in this application) depends on $G$ and $R$; in practice, estimates of these matrices are available from previous seasons. $Y_s$ is fit with the fixed effects model (Equation 3) and with the mixed effects model (Equation 4), and the estimates for the intercept are recorded. 1000 such simulations are run in this example, all using the same schedule ($Z_s$) and teams ($\eta_s$).

Figure 4 shows how the mixed effects model produces biased E-BLUEs of the intercept in the presence of this carefully chosen $Z_s$, while the BLUE from fitting the fixed effects model remains unbiased. The HFA E-BLUEs from the 1000 simulations have a mean of 0.7892 and a 95% confidence interval of (0.7014, 0.8771). This confi-
The confidence interval contains the true simulated bias of $\nu_k' \eta = 0.7108$. The corresponding BLUES of HFA from fitting the fixed effects model have a mean of $-0.1065$ and a 95% confidence interval of $(-0.1350, 0.0469)$, which contains the simulated HFA of 0. Figure 4 also shows the matched pair differences between the HFA estimates from the two models: the E-BLUE is uniformly larger than the BLUE from the fixed effects model for the same data set. These differences show a correlation of 0.97 with the observed values of $\nu_k' \hat{\eta}$.

7 Conclusion

We have seen how dependence between the random effects vector $\eta$ and the random effects model matrix $Z$ violates an important assumption of the mixed effects model (Equation 1) that $Z$ is fixed, and can potentially lead to bias in the standard estimators of $k' \beta$ that are derived under the misspecified assumption. More specifically, Corollary 3 illustrates that the source of this bias is the dependence between $Z$ and $\eta$, and not the mere fact that $Z$ is stochastic. In these situations, it may be more appropriate to model $\eta$ as a fixed effects vector, or to build the fixed effects model matrix in the mixed model such that $X' R^{-1} Z = 0$ (with probability one). The later option may involve finding important covariates to include as fixed effects that were previously omitted from the model.

The behavior of the predicted random effects themselves could also be studied. However, this situation is not as straightforward because these individual effects are not always estimable when converted to fixed effects (as with the HFA example) and because of the shrinkage properties of the random effects. For a predictor $\hat{\eta}$ of the random effects, unbiasedness requires $E[\hat{\eta}] = E[\eta] = 0$, and not that $E[\hat{\eta}| \eta] = \eta$ for all $\eta$ (Robinson 1991).

There are also implications for experimental design (DOE) software when generating split-plot designs: correlations between columns of $Z$ and $X$ (with respect to
leave open the potential for bias in \( \mathbf{k}' \hat{\mathbf{\beta}} \) depending on the direction of the sampled \( \mathbf{\eta} \) vector. As such, these correlations are potentially more damaging than those that appear strictly between columns of \( \mathbf{X} \) or between columns of \( \mathbf{Z} \), and should perhaps receive greater attention in an optimality criterion.

The primary recommendations resulting from this study are

1. Mixed model estimation software could print the estimated bias, \( \hat{\nu}_k' \hat{\mathbf{\eta}} \), next to the parameter estimates (or estimates of user-specified estimators) and their standard errors (potentially also including the standard errors calculated under the stochastic-\( \mathbf{Z} \) model in Section 3.2), along with the percentile of this value from within the randomization distribution \( \hat{\nu}_k' \pi(\hat{\mathbf{\eta}}) \), and the graphs shown in Figure 3. In addition to being useful for detecting bias that would otherwise go undetected, this would raise awareness of the issues discussed in this paper.

2. When designing an experiment, choose \( \mathbf{Z} \) and \( \mathbf{X} \) such that \( \mathbf{X}' \mathbf{R}^{-1} \mathbf{Z} = 0 \), for an anticipated error covariance matrix \( \mathbf{R} \), in order to obtain an unbiased estimator \( \mathbf{k}' \hat{\mathbf{\beta}} \) and in order to minimize both \( \text{var}(\mathbf{k}' \hat{\mathbf{\beta}}) \) and \( \text{var}(\hat{\nu}_k' \mathbf{\eta}) \). For observational data analysis, it may be possible to include fixed effects such that this orthogonality condition holds.

3. Be alert that, given an anticipated random effects vector \( \mathbf{\eta} \), selecting \( \mathbf{X} \) and/or \( \mathbf{Z} \) such that \( \text{E}[\hat{\nu}_k' \mathbf{\eta}] \neq 0 \) will lead to bias in the mixed model estimator of the estimable function \( \mathbf{k}' \hat{\mathbf{\beta}} \). This is, of course, not a recommended practice; however, there is a potential for this property to be exploited by a malicious party.

A similar biasing process also likely exists for (single- or multi-response) generalized linear mixed models (GLMMs). The study is more difficult in that setting owing to a lack of closed form estimators of estimable functions of \( \mathbf{\beta} \) (Karl et al. 2014). However, given a set of maximum likelihood estimates for the GLMM, the linearization technique of Wolfinger & O’Connell (1993) – the default estimation routine in
SAS PROC GLIMMIX – could be used in order to apply the methods of this paper to a pseudo-response of the linearized GLMM likelihood function in order to obtain an approximation of the bias.

SUPPLEMENTARY MATERIAL

Supplement: Directory of folders containing code and data sets that are needed to replicate the analyses in the paper. (ZIP compressed file)

README: File containing descriptions of each of the folders contained in Supplement.zip. (TXT file)

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