Best Linear Unbiased Prediction and Related Inference in the Mixed Model

In the usual mixed model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}$$

with

$$\mathrm{E}\begin{pmatrix} \mathbf{u} \\ \boldsymbol{\epsilon} \end{pmatrix} = \mathbf{0} \text{ and } \mathrm{Var}\begin{pmatrix} \mathbf{u} \\ \boldsymbol{\epsilon} \end{pmatrix} = \begin{pmatrix} \mathbf{G} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} \end{pmatrix}$$

and using the notation

$$\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$$

we consider problems of prediction related to the random effects contained in $\mathbf{u}$. Under the MVN assumption

$$\mathrm{E}\left[\mathbf{u}|\mathbf{Y}\right] = \mathbf{G}\mathbf{Z}'\mathbf{V}^{-1}\left(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\right) \tag{1}$$

which, obviously, depends on the fixed effect vector $\boldsymbol{\beta}$. (For what it is worth,

$$\mathrm{Var}\begin{pmatrix} \mathbf{u} \\ \mathbf{Y} \end{pmatrix} = \begin{pmatrix} \mathbf{G} & \mathbf{G}\mathbf{Z}' \\ \mathbf{Z}\mathbf{G} & \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R} \end{pmatrix}$$

and the $\mathbf{G}\mathbf{Z}'$ appearing in (1) is the covariance between $\mathbf{u}$ and $\mathbf{Y}$.) Something that is close to the conditional mean (1), but that does not depend on fixed effects is

$$\widehat{\mathbf{u}} = \mathbf{G}\mathbf{Z}'\mathbf{V}^{-1}\left(\mathbf{Y} - \widehat{\mathbf{Y}}^*\right) \tag{2}$$

where $\widehat{\mathbf{Y}}^*$ is the generalized least squares (best linear unbiased) estimate of the mean of $\mathbf{Y}$,

$$\widehat{\mathbf{Y}}^* = \mathbf{X}\left(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\right)^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Y}$$

The predictor (2) turns out to be the Best Linear Unbiased Predictor of $\mathbf{u}$, and if we temporarily abbreviate

$$\mathbf{B} = \mathbf{X}\left(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\right)^{-}\mathbf{X}'\mathbf{V}^{-1} \text{ and } \mathbf{P} = \mathbf{V}^{-1}\left(\mathbf{I} - \mathbf{B}\right) \tag{3}$$

this can be written as

$$\widehat{\mathbf{u}} = \mathbf{G}\mathbf{Z}'\mathbf{V}^{-1}\left(\mathbf{Y} - \mathbf{B}\mathbf{Y}\right) = \mathbf{G}\mathbf{Z}'\mathbf{V}^{-1}\left(\mathbf{I} - \mathbf{B}\right)\mathbf{Y} = \mathbf{G}\mathbf{Z}'\mathbf{P}\mathbf{Y} \tag{4}$$

We consider here predictions based on $\widehat{\mathbf{u}}$ and the problems of quoting appropriate "precision" measures for them.

To begin with the $\mathbf{u}$ vector itself, $\widehat{\mathbf{u}}$ is an obvious approximation and a precision of prediction should be related to the variability in the difference

$$\mathbf{u} - \widehat{\mathbf{u}} = \mathbf{u} - \mathbf{B}\mathbf{Y} = \mathbf{u} - \mathbf{B}\left(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}\right) = \mathbf{u} - \mathbf{B}\mathbf{X}\boldsymbol{\beta} - \mathbf{B}\mathbf{Z}\mathbf{u} - \mathbf{B}\boldsymbol{\epsilon}$$

This random vector has mean $\mathbf{0}$ and covariance matrix

$$\mathrm{Var}\left(\mathbf{u} - \widehat{\mathbf{u}}\right) = \left(\mathbf{I} - \mathbf{B}\mathbf{Z}\right)\mathbf{G}\left(\mathbf{I} - \mathbf{B}\mathbf{Z}\right)' + \mathbf{B}\mathbf{R}\mathbf{B}' = \mathbf{G} - \mathbf{G}\mathbf{Z}'\mathbf{P}\mathbf{Z}\mathbf{G} \tag{5}$$

(This last inequality is not obvious to me, but is what McCulloch and Searle promise on page 170 of their book.)

Now $\widehat{\mathbf{u}}$ in (4) is not available unless one knows the covariance matrices $\mathbf{G}$ and $\mathbf{V}$. If one has estimated variance components and hence has estimates of $\mathbf{G}$ and $\mathbf{V}$ (and for that matter, $\mathbf{R}, \mathbf{B}$, and $\mathbf{P}$) the approximate BLUP

$$\widehat{\widehat{\mathbf{u}}} = \widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{P}}\mathbf{Y}$$

may be used. A way of making a crude approximation to a measure of precision of the approximate BLUP (as a predictor $\mathbf{u}$) is to plug estimates into the relationship (5) to produce

$$\widehat{\mathrm{Var}\left(\mathbf{u}-\widehat{\widehat{\mathbf{u}}}\right)} = \widehat{\mathbf{G}}-\widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{P}}\mathbf{Z}\widehat{\mathbf{G}}$$

Consider now the prediction of a quantity

$$l = \mathbf{c}'\boldsymbol{\beta} + \mathbf{s}'\mathbf{u}$$

for an estimable $\mathbf{c}'\boldsymbol{\beta}$ (estimability has nothing to do with the covariance structure of $\mathbf{Y}$ and so "estimability" means here what it always does). As it turns out, if $\mathbf{c}' = \mathbf{a}'\mathbf{X}$, the BLUP of l is

$$\widehat{l} = \mathbf{a}'\widehat{\mathbf{Y}}^* + \mathbf{s}'\widehat{\mathbf{u}} = \mathbf{a}'\mathbf{B}\mathbf{Y} + \mathbf{s}'\mathbf{G}\mathbf{Z}'\mathbf{P}\mathbf{Y} = \left(\mathbf{a}'\mathbf{B} + \mathbf{s}'\mathbf{G}\mathbf{Z}'\mathbf{P}\right)\mathbf{Y} \qquad (6)$$

To quantify the precision of this as a predictor of l we must consider the random variable

$$\widehat{l} - l$$

The variance of this is the unpleasant (but not impossible) quantity

$$\mathrm{Var}\left(\widehat{l} - l\right) = \mathbf{a}'\mathbf{X}\left(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\right)^{-}\mathbf{X}'\mathbf{a} + \mathbf{s}'\mathbf{G}\mathbf{Z}'\mathbf{P}\mathbf{Z}\mathbf{G}\mathbf{s} - 2\mathbf{a}'\mathbf{B}\mathbf{Z}\mathbf{G}\mathbf{s} \qquad (7)$$

(This variance is from page 256 of McCulloch and Searle.)

Now $\widehat{l}$ of (6) is not available unless one knows covariance matrices. But with estimates of variance components and corresponding matrices, what is available as an approximation to $\widehat{l}$ is

$$\widehat{\widehat{l}} = \left(\mathbf{a}'\widehat{\mathbf{B}} + \mathbf{s}'\widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{P}}\right)\mathbf{Y}$$

A way of making a crude approximation to a measure of precision of the approximate BLUP (as a predictor of l) is to plug estimates into the relationship (7) to produce

$$\widehat{\mathrm{Var}\left(\widehat{l} - l\right)} = \mathbf{a}'\mathbf{X}\left(\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{X}\right)^{-}\mathbf{X}'\mathbf{a} + \mathbf{s}'\widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{P}}\mathbf{Z}\widehat{\mathbf{G}}\mathbf{s} - 2\mathbf{a}'\widehat{\mathbf{B}}\mathbf{Z}\widehat{\mathbf{G}}\mathbf{s}$$