Appendix A

Properties of the eblups

Here we derive the correct measure of variability of the eblups as discussed in Chapter 4 using the variance operator. Using $\text{Var}(b) = B$ and the expression in (4.12) we first note that $\text{Cov}(Ae, b) = 0$, $\text{Cov}(A\beta, b) = 0$, and $\text{Cov}(Ab, b) = A\text{Var}(b)$ for any matrix $A$. Then we can show that

$$\text{Cov}(\hat{b}, b) = \text{Cov}(BZ'V^{-1}(y - X\hat{\beta}), b)$$

$$= \text{Cov}(BZ'V^{-1}(X\beta + Zb + \epsilon - X\hat{\beta}), b)$$

$$= \text{Cov}(BZ'V^{-1}Zb, b) - \text{Cov}(BZ'V^{-1}X\hat{\beta}, b)$$

$$= BZ'V^{-1}Z\text{Var}(b) - \text{Cov}(BZ'V^{-1}X(X'V^{-1}X)^{-1}X'V^{-1}y, b)$$

$$= BZ'V^{-1}ZB - \text{Cov}(BZ'V^{-1}X(X'V^{-1}X)^{-1}X'V^{-1}(X\beta + Zb + \epsilon), b)$$

$$= BZ'V^{-1}ZB - BZ'V^{-1}X(X'V^{-1}X)^{-1}X'V^{-1}Z\text{Var}(b)$$

$$= BZ'V^{-1}ZB - BZ'V^{-1}X(X'V^{-1}X)^{-1}X'V^{-1}ZB = \text{Var}(\hat{b}).$$

(A.1)
Then we have

\[
\begin{align*}
\text{Var}(\hat{b} - b) &= \text{Var}(\hat{b}) + \text{Var}(b) - 2\text{Cov}(\hat{b}, b) \\
&= \text{Var}(\hat{b}) + \text{Var}(b) - 2\text{Var}(\hat{b}) \\
&= \text{Var}(b) - \text{Var}(\hat{b}) \\
&= \mathbf{B} - \text{Var}(\hat{b}),
\end{align*}
\]

which is equivalent to the expression in (4.13).
Appendix B

Sum of the eblups

Theorem B.1. The sum of the random deviations from the linear mixed model, $\hat{b}_i$, is equal to the zero vector when $X_i = Z_i$, for $i = 1, 2, \ldots, m$.

Proof. We first set $X_i = Z_i$ and noted that we can interchange between the model formulation in terms of the individual profiles (unstacked form) and the model formulation using stacked matrices (stacked form). For example, we have $\sum_{i=1}^m X_i'V_iX_i = X'V^{-1}X$ and $\sum_{i=1}^m X_i'V_iy_i = X'V^{-1}y$ where $X$ is a $(\sum_{i=1}^m n_i)$ by $p$ stacked matrix of the $X_i's$, $V = ZBZ' + R = diag(V_i)$ with $B = diag(D)$, $R = diag(R_i)$, and $Z$ is a block diagonal matrix containing all the $Z_i$ matrices. Then using (4.7) and (4.8) with the estimated values in place of the known values and doing some manipulation gives
\[
\sum_{i=1}^{m} \hat{b}_i = \sum_{i=1}^{m} \left[ DZ_i'V_i^{-1} \left( y_i - X_i\hat{\beta}_{MIX} \right) \right] \\
= \sum_{i=1}^{m} DX_i'V_i^{-1}y_i - \sum_{i=1}^{m} DX_iV_i^{-1}X_i (X'VX)^{-1} X'V^{-1}y \\
= DX'V^{-1}y - D (X'V^{-1}X) (X'VX)^{-1} X'V^{-1}y \\
= DX'V^{-1}y - DX'V^{-1}y \\
= 0. \quad (B.1)
\]

Notice that this proof does not require that \(X_i\) be the same for each profile. Nor does it require that the profiles have the same number of measurements (i.e. \(n_i\) does not have to be the same for all the profiles). As a result it is obvious that the average of the random deviations is zero

\[
\bar{\beta} = \frac{\sum_{i=1}^{m} \hat{b}_i}{m} = 0, \quad (B.2)
\]

and that

\[
\hat{\beta}_{MIX} = \frac{\sum_{i=1}^{m} \hat{\beta}_{i,MIX}}{m} = \frac{\sum_{i=1}^{m} (\hat{\beta}_{MIX} + \hat{b}_i)}{m} = \frac{\sum_{i=1}^{m} \hat{\beta}_{MIX}}{m} = \frac{m\hat{\beta}_{MIX}}{m} = \hat{\beta}_{MIX}. \quad (B.3)
\]

In Theorem B.2, we extend the results of Theorem B.1 to the case where the \(Z_i\) matrix is not equivalent to the \(X_i\) matrix but that the columns of \(Z_i\) are contained in \(X_i\), thus \(X_i\) may also have some additional columns not contained in \(Z_i\).

**Theorem B.2.** The sum of the random deviations from the mixed model, \(\hat{b}_i\), is equal to the zero vector when the \(Z_i\) matrix is contained within the \(X_i\) matrix.

**Proof.** We set the partitioned matrix \(X_i = [X_{1,i} X_{2,i}] = [Z_i X_{2,i}]\) where \(Z_i = X_{1,i}\) and then using (4.7) and (4.8) with the estimated values in place of the known values and doing some
manipulation gives

\[
\sum_{i=1}^{m} \hat{b}_i = \sum_{i=1}^{m} \left[ DZ_i'V_i^{-1} \left( y_i - X_i\hat{\beta}_{MIX} \right) \right]
\]

\[
= D \left[ \sum_{i=1}^{m} Z_i'V_i^{-1}y_i - \sum_{i=1}^{m} Z_i'V_i^{-1} [X_{1,i}|X_{2,i}] \hat{\beta}_{MIX} \right]
\]

\[
= D \left[ \sum_{i=1}^{m} X_{1,i}'V_i^{-1}y_i - \sum_{i=1}^{m} X_{1,i}'V_i^{-1}[X_{1,i}|X_{2,i}] \hat{\beta}_{MIX} \right]
\]

\[
= D \left[ X_1'V^{-1}y - [X_1'V^{-1}X_1|X_1'V^{-1}X_2] (X'VX)^{-1} X'V^{-1}y \right], \quad \text{(B.4)}
\]

where \(X_1\) and \(X_2\) are stacked matrices of \(X_{1,i}\) and \(X_{2,i}\) respectively.

We now turn attention to the partitioned matrix in the right hand side of the expression and show that

\[
(X'VX)^{-1} = A^{-1}
\]

\[
= \begin{bmatrix}
    A_{11} & A_{12} \\
    A_{21} & A_{22}
\end{bmatrix}^{-1}
\]

\[
= \begin{bmatrix}
    X_1'V^{-1}X_1 & X_1'V^{-1}X_2 \\
    X_2'V^{-1}X_1 & X_2'V^{-1}X_2
\end{bmatrix}^{-1}. \quad \text{(B.5)}
\]

Then using a common result (2.50 of Rencher, 2000) to take the inverse of the partitioned matrix we have

\[
A^{-1} = \begin{bmatrix}
    A_{11}^{-1} + A_{11}^{-1}A_{12}B^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}B^{-1} \\
    -B^{-1}A_{21}A_{11}^{-1} & B^{-1}
\end{bmatrix}
\]

\[
= \begin{bmatrix}
    (X_1'V^{-1}X_1)^{-1} + (X_1'V^{-1}X_1)^{-1}X_1'V^{-1}X_2B^{-1}X_2'V^{-1}X_1 (X_1'V^{-1}X_1)^{-1} - (X_1'V^{-1}X_1)^{-1}X_1'V^{-1}X_2B^{-1} \\
    -B^{-1}X_2'V^{-1}X_1 (X_1'V^{-1}X_1)^{-1}
\end{bmatrix}
\]

\[
- B^{-1}X_2'V^{-1}X_1 (X_1'V^{-1}X_1)^{-1}
\]

\[
B^{-1}, \quad \text{147}
\]
where $B = A_{22} - A_{21}A_{11}^{-1}A_{12} = (X'_2V^{-1}X_2) - X'_2V^{-1}X_1(X'_1V^{-1}X_1)^{-1}X'_1V^{-1}X_2$ has an inverse. This inverse of the partitioned matrix also requires the existence of inverses of $A_{11}$ and $A_{22}$. These inverses exist because $A$ has an inverse and by Theorem 2.6F of Rencher (2000) which says the square submatrices of a partitioned matrix have inverses if the whole matrix itself has an inverse. Thus the right hand side of (B.4) can be written as

$$[X'_1V^{-1}X_1|X'_1V^{-1}X_2](X'VX)^{-1}X'V^{-1}y =$$

$$\begin{bmatrix}
1 + X'_1V^{-1}X_2B^{-1}X'_2V^{-1}X_1(X'_1V^{-1}X_1)^{-1} & -X'_1V^{-1}X_2B^{-1} \\
-(X'_1V^{-1}X_2)B^{-1}X'_2V^{-1}X_1(X'_1V^{-1}X_1)^{-1} & (X'_1V^{-1}X_2)B^{-1}
\end{bmatrix}\begin{bmatrix}
X'_1V^{-1}y \\
X'_2V^{-1}y
\end{bmatrix}.$$  \hspace{1cm} (B.6)

Now multiplying this last result into the earlier expression for the blups in (B.4) gives us

$$\sum_{i=1}^{m} \hat{b}_i = D\left[X'_iV^{-1}y - [X'_iV^{-1}X_1|X'_iV^{-1}X_2](X'VX)^{-1}X'V^{-1}y\right]$$

$$= DX'_1V^{-1}y - DX'_1V^{-1}y + DX'_1V^{-1}X_2B^{-1}X'_2V^{-1}X_1(X'_1V^{-1}X_1)^{-1}X'_1V^{-1}y$$

$$-DX'_1V^{-1}X_2B^{-1}X'_2V^{-1}y - DX'_1V^{-1}X_2B^{-1}X'_2V^{-1}X_1(X'_1V^{-1}X_1)^{-1}X'_1V^{-1}y$$

$$+DX'_1V^{-1}X_2B^{-1}X'_2V^{-1}y$$

$$= DX'_1V^{-1}y - DX'_1V^{-1}y$$

$$= 0.$$  

Thus the eblups sum to zero for balanced and unbalanced data and/or whether or not $X_i$ is the same for each profile as long as $Z_i$ is equal to or contained within $X_i$. Note that Theorems B.1 and B.2 will hold whether or not $V_i$ (and consequently $D$) are replaced with estimates or are assumed to be known.
Appendix C

Dependence of $T^2$ on eblups

Theorem C.1. If $\sum_{i=1}^{m} \mathbf{b}_i = \mathbf{0}$, then the $T^2_{1,i,\text{MIX}}$ and $T^2_{2,i,\text{MIX}}$ statistics in (5.2) and (5.5) depend only on the $\hat{\mathbf{b}}_i$, the random components.

Proof. Starting with (5.2) and using the results from Appendix B we have

$$T^2_{1,i,\text{MIX}} = \left( \hat{\beta}_{i,\text{MIX}} - \bar{\beta}_{\text{MIX}} \right)' S^{-1}_{1,\text{MIX}} \left( \hat{\beta}_{i,\text{MIX}} - \bar{\beta}_{\text{MIX}} \right) \text{ for } i = 1, 2, \ldots, m$$

$$= \left[ \left( \hat{\beta}_{\text{MIX}} + \hat{\mathbf{b}}_i \right) - \left( \hat{\beta}_{\text{MIX}} \right) \right]' \left[ \frac{\sum_{i=1}^{m} \left( \left( \hat{\beta}_{\text{MIX}} + \hat{\mathbf{b}}_i \right) - \bar{\beta}_{\text{MIX}} \right) \left( \left( \hat{\beta}_{\text{MIX}} + \hat{\mathbf{b}}_i \right) - \bar{\beta}_{\text{MIX}} \right)'}{m - 1} \right]^{-1} \left( \hat{\beta}_{\text{MIX}} + \hat{\mathbf{b}}_i \right) - \left( \hat{\beta}_{\text{MIX}} \right) \text{ (because } \hat{\beta}_{\text{MIX}} = \bar{\beta}_{\text{MIX}} \right)$$

$$= \hat{\mathbf{b}}_i \left( \frac{\sum_{i=1}^{m} \hat{\mathbf{b}}_i \hat{\mathbf{b}}'_i}{m - 1} \right)^{-1} \hat{\mathbf{b}}_i \text{ for } i = 1, 2, \ldots, m. \quad \text{(C.1)}$$
Starting with (5.5) we have
\[
T_{2,i,MIX}^2 = (\hat{\beta}_{i,MIX} - \bar{\beta}_{MIX})' S_{2,MIX}^{-1} (\hat{\beta}_{i,MIX} - \bar{\beta}_{MIX}) \text{ for } i = 1, 2, \ldots, m
\]
\[
= \left( (\hat{\beta}_{MIX} + \hat{b}_i) - (\bar{\beta}_{MIX}) \right)' \sum_{i=1}^m \left( (\hat{\beta}_{MIX} + \hat{b}_i) - (\bar{\beta}_{MIX} + \hat{b}_{i+1}) \right) \left( (\hat{\beta}_{MIX} + \hat{b}_i) - (\bar{\beta}_{MIX} + \hat{b}_i) \right)' \times \frac{2(m-1)}{m-1} - \hat{b}_i \text{ for } i = 1, 2, \ldots, m.
\]

Theorem C.2. The \(T_{2,i,MIX}^2\) and \(T_{2,2,i,MIX}^2\) statistics in (5.2) and (5.5) depend only on the eblups, \(\hat{b}_i\), and their average, \(\bar{b}\), no matter the value of \(X_i\) and \(Z_i\).

Proof. In the most general situation, we have 3 components that make up the \(T_{2,i,MIX}^2\) and \(T_{2,2,i,MIX}^2\) statistics. The first component consisting of both random and fixed effects, comprises the columns of \(Z_i\) and \(X_i\) that are equal to each other, the second component consisting of only fixed effects, comprises the columns in \(X_i\) that are not in \(Z_i\), and the third component consisting of only random effects, comprises the columns in \(Z_i\) that are not in \(X_i\). Theorem C.1 shows that if there are only the first two components present that the eblups sum to zero and that provides the simplification noted above.

We note that once \(\hat{\beta}_{MIX}\) and \(\hat{b}_i\) are obtained in the most general situation that we can partition \(\hat{\beta}_{i,MIX}\) into the 3 components. Thus we have \(\hat{\beta}_{i,MIX} = \hat{\beta}_{MIX} + \hat{b}_i = \begin{bmatrix} \hat{\beta}_{MIX,1} + \hat{b}_{i,1} \\ \hat{b}_{i,2} \\ \hat{\beta}_{MIX,2} \end{bmatrix}\), where \(\hat{\beta}_{MIX,1}\) and \(\hat{b}_{i,1}\) are ax1 vectors corresponding to the columns in \(X_i\) and \(Z_i\) that are equivalent, \(\hat{b}_{i,2}\) is the cx1 vector corresponding to the columns in \(Z_i\) that are not in \(X_i\), and \(\hat{\beta}_{MIX,2}\) is a bx1 vector corresponding to the columns in \(X_i\) that are not in \(Z_i\). Thus \(X_i\) is a
\( n_i \) by \((a + b)\) matrix and \( Z_i \) is a \( n_i \) by \((a + c)\) matrix. We also have

\[
\overline{\beta}_{i,MIX} = \frac{\sum_{i=1}^{m} \hat{\beta}_{i,MIX}}{m} = \begin{bmatrix} \hat{\beta}_{MIX,1} + \sum_{i=1}^{m} \hat{b}_{i,1} \\ \sum_{i=1}^{m} \hat{b}_{i,2} \\ \hat{\beta}_{MIX,2} \end{bmatrix} = \begin{bmatrix} \hat{\beta}_{MIX,1} + \bar{b}_{i,1} \\ \bar{b}_{i,2} \\ \hat{\beta}_{MIX,2} \end{bmatrix} \text{ for } i = 1, 2, \ldots, m, \tag{C.3}
\]

and

\[
\hat{\beta}_{i,MIX} - \overline{\beta}_{i,MIX} = \begin{bmatrix} \hat{b}_{i,1} + \bar{b}_{i,1} \\ \hat{b}_{i,2} - \bar{b}_{i,2} \end{bmatrix} = \begin{bmatrix} \hat{b}_{i} - \bar{b} \\ 0 \end{bmatrix} \text{ for } i = 1, 2, \ldots, m. \tag{C.4}
\]

The resulting \( T^2_{1,i,MIX} \) statistics is then given by

\[
T^2_{1,i,MIX} = (\hat{\beta}_{i,MIX} - \overline{\beta}_{i,MIX})' S^{-1}_{1,MIX} (\hat{\beta}_{i,MIX} - \overline{\beta}_{i,MIX}) \text{ for } i = 1, 2, \ldots, m
\]

\[
= \left[ (\hat{b}_{i} - \bar{b})' \right] \frac{\sum_{i=1}^{m} (\hat{b}_{i} - \bar{b})' (\hat{b}_{i} - \bar{b})}{m - 1} \left[ \begin{array}{c} \hat{b}_{i} - \bar{b} \\ 0 \end{array} \right]^{-1} \left[ \begin{array}{c} \hat{b}_{i} - \bar{b} \\ 0 \end{array} \right]. \tag{C.5}
\]

The previous expression contains a matrix without an inverse because of the column of zeros. However, because the matrix is block diagonal, it is a simple matter to calculate the generalized inverse by simply taking the inverse of the non-zero portion of the matrix. We can then rewrite the above expression as

\[
T^2_{1,i,MIX} = \left[ (\hat{b}_{i} - \bar{b})' \right] \left( \frac{\sum_{i=1}^{m} (\hat{b}_{i} - \bar{b})' (\hat{b}_{i} - \bar{b})}{m - 1} \right)^{-1} \left[ \begin{array}{c} \hat{b}_{i} - \bar{b} \\ 0 \end{array} \right] \left[ \begin{array}{c} \hat{b}_{i} - \bar{b} \\ 0 \end{array} \right]. \tag{C.6}
\]
By similar arguments we can show that

$$\hat{\beta}_{i+1, MIX} - \hat{\beta}_{i, MIX} = \begin{bmatrix} \hat{b}_{i+1} - \hat{b}_i \\ 0 \end{bmatrix}, \quad (C.7)$$

and

$$T^2_{2,i, MIX} = (\hat{b}_i - \bar{b})' \left[ \sum_{i=1}^{m-1} (\hat{b}_{i+1} - \hat{b}_i)' (\hat{b}_{i+1} - \hat{b}_i) / 2(m-1) \right]^{-1} (\hat{b}_i - \bar{b}) \text{ for } i = 1, 2, \ldots, m, \quad (C.8)$$

which is similar to the same result obtained for $T^2_{2,i, MIX}$ in Theorem C.1.

The results of Theorem C.1 and C.2 imply that for a given set of data, we only need to consider the random components when calculating the $T^2_{1,i, MIX}$ and $T^2_{2,i, MIX}$ statistics. This simplifies the calculations needed to determine the properties of multivariate control charts.
Appendix D

Regression Equivariance in the Linear Mixed Model

Following the convention of Rousseeuw and Leroy (1987), an estimator, $T$ is regression equivariant, if for the response vector, $y_i$, the regressors, $x_i$, and an arbitrary vector, $v$,

$$T(x_i; y_i + x_i'v) = T(x_i; y_i) + v \forall i.$$  \hspace{0.5cm} (D.1)

Regression equivariance is important because it allows us to arbitrarily pick parameter values to generate $y_i$ for simulation studies without loss of generality. For example in a simple linear regression model, the least squares estimators are regression equivariant, which would allow us to pick an arbitrary slope and intercept for simulation studies, and still obtain the same conclusions from the study.

We show here the regression equivariance of the estimator of fixed effects and of the predictor of random effects for the linear mixed model. We use the stacked form of the model from (4.6), the estimator of the fixed effects in (4.9), and the predictor of random
effects in (4.10).

Suppose the response vector $y$ was changed by some arbitrary amount that is a function of the regressors, $X$. The resulting response vector is given by $\tilde{y} = y + Xv$ where $v$ is some arbitrary $px1$ vector.

Then the resulting estimator of the fixed effects is given by

$$\tilde{\beta} = (X'V^{-1}X)V^{-1}(y + Xv)$$

$$= X'V^{-1}XV^{-1}y + X'V^{-1}XV^{-1}Xv$$

$$= \beta + v.$$  \hspace{1cm} (D.2)

As a result of the definition in (D.1) the estimator of the fixed effects is regression equivariant.

Now consider the predictor of the random effects given in (4.10). If the response vector is changed by some arbitrary amount so that we have $\tilde{y}$ then we can show that the resulting predictor of random effects is given by

$$\tilde{b} = BZ'V^{-1}(\tilde{y} - X\tilde{\beta})$$

$$= BZ'V^{-1}(y + Xv - X(\beta + v))$$

$$= BZ'V^{-1}(y - X\beta)$$

$$= \hat{b}.$$  \hspace{1cm} (D.3)

Thus the predicted random effects are unchanged when the response vector has been changed by some arbitrary amount.