4.6 Appendix: Derivation of BLUP

Consider the mixed linear model

$$y = Xb + Zu + e$$

with $E(y) = Xb$, $E(u) = 0$ and $E(e) = 0$, $var(u) = U$ and $var(e) = R$, hence $var(y) = V = ZUZ^T + R$

4.6.1 Predictions

Breeding values u are to be predicted by a statistic which is a function of the data y. At this point, we are restricting ourselves on linear functions of the data. The predictions are called $\hat{u}$

Suppose, we want to predict breeding values u with a linear function of the data y corrected for some vector k. As a formula this can be written as

$$\hat{u} = M \cdot (y - k)$$

where M is an unknown matrix and k an unknown vector of corrections. The unknowns M and k are determined using the properties of BLUP.

4.6.2 Unbiasedness

The BLUP $\hat{u}$ has the property of unbiasedness. This means

$$E[\hat{u}] = E[u]$$

According to the previously made definition of breeding value, we set $E[u] = 0$. Inserting the above definition of $\hat{u}$ and taking expectations, leads to

$$E[\hat{u}] = E[M \cdot (y - k)] = M \cdot (E[y] - E[k])$$

Due to the unbiasedness property, we want $E[\hat{u}] = 0$. This leads to $E[y] = E[k]$. Because, k is expected to be a constant vector of corrections, we can set

$$k = E[y]$$

In the definition of the linear mixed effects model, we saw that $E[y] = X\beta$. The BLUP $\hat{u}$ of our breeding values has now the form

$$\hat{u} = M \cdot (y - E[y])$$

4.6.3 Minimal Prediction Error Variance (Best)

The third condition that is satisfied by the BLUP $\hat{u}$ is that of minimal prediction error variance. More formally that means

$$var(u - \hat{u}) \rightarrow \text{Minimum}$$

For reasons of simplicity, we are looking at the case of just one breeding value u_i and one observation y_i for animal i. This reduces M to a scalar factor which is to be determined such that the prediction error variance (PEV) is minimal.

$$\begin{aligned}
PEV = var(u_i - \hat{u}_i) &= var(u_i) + var(\hat{u}_i) - 2 * cov(u_i, \hat{u}_i) \\
&= var(u_i) + var(M(y_i - E[y_i])) - 2 * cov(u_i, (M(y_i - E[y_i]))) \\
&= var(u_i) + M^2 * var(y_i - E[y_i]) - 2 * M * cov(u_i, (y_i - E[y_i])) \\
&= var(u_i) + M^2 * var(y_i) - 2 * M * cov(u_i, y_i)
\end{aligned}$$

The factor M is found by taking the first derivative of PEV with respect to M.

$$\frac{\partial PEV}{\partial M} = 2 * M * var(y_i) - 2 * cov(u_i, y_i)$$

The value $\widehat{M}$ for which PEV is minimal is found by setting $\partial PEV / \partial M$ to 0.

$$\begin{aligned}
0 &= 2 * \widehat{M} * var(y_i) - 2 * cov(u_i, y_i) \\
\widehat{M} &= cov(u_i, y_i) * (var(y_i))^{-1}
\end{aligned}$$

This result can be generalized by going back to the original vector valued variables and the mixed model

$$y = X\beta + Zu + e.$$

Hence

- y is a vector of length n with phenotypic observations
- u is a vector of length q with breeding values

Expected values and variance-covariance matrices for the two vectors y and u are given by

- $E[y] = X\beta$
- $E[u] = 0$
- var(y) = V
- var(u) = U
- cov(u, y^T) = UZ^T

The matrix $\widehat{M}$ can be written as

$$\widehat{M} = UZ^T V^{-1}$$

Inserting the value for matrix M to the BLUP $\hat{u}$ and using $E[y] = X\beta$ yields

$$\hat{u} = UZ^T V^{-1}(y - X\beta)$$

The vector β of fixed effects and regression coefficients is not known. But because $X\hat{\beta}$ with $\hat{\beta}$ being the general least squares solution for β, the above used unbiasedness property does also hold for $X\hat{\beta}$. Therefore we can write the BLUP $\hat{u}$ as

$$\hat{u} = UZ^T V^{-1}(y - X\hat{\beta})$$

with $\hat{\beta} = (X^T V{-}1X)^{-}X^T V^{-1}y$