REML Estimation and Linear Mixed Models
Solution sheet 1

Sue Welham
Rothamsted Research
Harpenden UK AL5 2JQ

1. Derive the effective replications λ_{ij} for the RCBD

For the randomized complete block design with g treatments and r replicates (blocks), we have model

$$y_{ij} = b_i + \mu_j + e_{ij}$$

for $i = 1 \ldots r$, $j = 1 \ldots g$, $n = rg$.

Or in matrix notation

$$\boldsymbol{y} = \boldsymbol{X\tau} + \boldsymbol{Zu} + \boldsymbol{e}$$

for

- $\boldsymbol{y} = (y_{11}\ y_{21} \ldots y_{r1}\ y_{12} \ldots y_{rg})'$
- $\boldsymbol{X} = \boldsymbol{I}_g \otimes \boldsymbol{1}_r$
- $\boldsymbol{Z} = \boldsymbol{1}_g \otimes \boldsymbol{I}_r$
- $\boldsymbol{\tau} = (\mu_1 \ldots \mu_g)'$
- $\boldsymbol{u} = (b_1 \ldots b_r)'$
- $\boldsymbol{e} = (e_{11}\ e_{21} \ldots e_{r1}\ e_{12} \ldots e_{rg})'$

Then

$$\boldsymbol{P}_0 = \frac{1}{n}(\boldsymbol{1}_n\boldsymbol{1}_n' = \frac{1}{n}(\boldsymbol{1}_g\boldsymbol{1}_g' \otimes \boldsymbol{1}_r\boldsymbol{1}_r')$$
$$\boldsymbol{P}_1 = \frac{1}{g}(\boldsymbol{1}_g\boldsymbol{1}_g' \otimes \boldsymbol{I}_r) - \frac{1}{n}(\boldsymbol{1}_g\boldsymbol{1}_g' \otimes \boldsymbol{1}_r\boldsymbol{1}_r')$$
$$\boldsymbol{P}_2 = (\boldsymbol{I}_g \otimes \boldsymbol{I}_r) - \frac{1}{g}(\boldsymbol{1}_r\boldsymbol{1}_r' \otimes \boldsymbol{I}_r)$$

and

$$\boldsymbol{T}_1 = \frac{1}{g}\boldsymbol{1}_g\boldsymbol{1}_g'; \quad \boldsymbol{T}_2 = \boldsymbol{I}_g - \frac{1}{g}\boldsymbol{1}_g\boldsymbol{1}_g'$$

Consider $\boldsymbol{X}'\boldsymbol{P}_i\boldsymbol{X}$ for $i = 0, 1, 2$:

$$\begin{aligned}\boldsymbol{X}'\boldsymbol{P}_0\boldsymbol{X} &= (\boldsymbol{I}_g \otimes \boldsymbol{1}_r')\frac{1}{n}(\boldsymbol{1}_n\boldsymbol{1}_n' = \frac{1}{n}(\boldsymbol{1}_g\boldsymbol{1}_g' \otimes \boldsymbol{1}_r\boldsymbol{1}_r')(\boldsymbol{I}_g \otimes \boldsymbol{1}_r) \\ &= \frac{r^2}{n}\boldsymbol{1}_g\boldsymbol{1}_g' = \boldsymbol{r}\boldsymbol{T}_1\end{aligned}$$

$$
\begin{aligned}
\boldsymbol{X}'\boldsymbol{P}_1\boldsymbol{X} &= (\boldsymbol{I}_g \otimes \mathbf{1}_r')\frac{1}{n}(\mathbf{1}_n\mathbf{1}_n' = \frac{1}{n}(\mathbf{1}_g\mathbf{1}_g' \otimes \mathbf{1}_r\mathbf{1}_r')(\boldsymbol{I}_g \otimes \mathbf{1}_r) \\
&= \frac{r^2}{n}\mathbf{1}_g\mathbf{1}_g' = \boldsymbol{r}\boldsymbol{T}_1
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{X}'\boldsymbol{P}_0\boldsymbol{X} &= (\boldsymbol{I}_g \otimes \mathbf{1}_r')\frac{1}{g}(\mathbf{1}_g\mathbf{1}_g' \otimes \boldsymbol{I}_r) - \frac{1}{n}(\mathbf{1}_g\mathbf{1}_g' \otimes \mathbf{1}_r\mathbf{1}_r')(\boldsymbol{I}_g \otimes \mathbf{1}_r) \\
&= \frac{1}{g}(\mathbf{1}_g\mathbf{1}_g' \otimes \mathbf{1}_r') - \frac{r}{n}(\mathbf{1}_g\mathbf{1}_g' \otimes \mathbf{1}_r') \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{X}'\boldsymbol{P}_2\boldsymbol{X} &= (\boldsymbol{I}_g \otimes \mathbf{1}_r')(\boldsymbol{I}_g \otimes \boldsymbol{I}_r) - \frac{1}{g}(\mathbf{1}_r\mathbf{1}_r' \otimes \boldsymbol{I}_r)(\boldsymbol{I}_g \otimes \mathbf{1}_r) \\
&= r\boldsymbol{I}_g - \frac{r}{g}\mathbf{1}_g\mathbf{1}_g' = \boldsymbol{r}\boldsymbol{T}_2
\end{aligned}
$$

Hence

$$
\begin{array}{lll}
\lambda_{01} = r & \lambda_{11} = 0 & \lambda_{21} = 0 \\
\lambda_{02} = 0 & \lambda_{12} = 0 & \lambda_{22} = r
\end{array}
$$

2. Show that $\frac{\partial \boldsymbol{P}}{\partial\theta} = -\boldsymbol{P}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{P}$ for $\boldsymbol{P} = \boldsymbol{H}^{-1} - \boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-}\boldsymbol{X}\boldsymbol{H}^{-1}$, with $\boldsymbol{H} = \boldsymbol{H}(\theta)$

We need to use the results:

$$
\begin{aligned}
\frac{\partial \boldsymbol{H}^{-1}}{\partial\theta} &= \boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{H}^{-1} \\
\frac{\partial(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}}{\partial\theta} &= (\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{X}\boldsymbol{H}^{-1}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}
\end{aligned}
$$

Then

$$
\begin{aligned}
\frac{\partial \boldsymbol{P}}{\partial\theta} &= \frac{\partial \boldsymbol{H}^{-1}}{\partial\theta} - \frac{\partial \boldsymbol{H}^{-1}}{\partial\theta}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1} \\
&\quad -\boldsymbol{H}^{-1}\boldsymbol{X}\frac{\partial(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}}{\partial\theta}\boldsymbol{X}'\boldsymbol{H}^{-1} - \boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\frac{\partial \boldsymbol{H}^{-1}}{\partial\theta} \\
&= -\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{H}^{-1} + \boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1} \\
&\quad -\boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{X}\boldsymbol{H}^{-1}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1} \\
&\quad +\boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{H}^{-1} \\
&= -\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{P} + \boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{P} \\
&= -\boldsymbol{P}\frac{\partial \boldsymbol{H}}{\partial\theta}\boldsymbol{P}.
\end{aligned}
$$

3. Derive the form of the inverse coefficient matrix from the mixed model equations

For the simple variance components mixed model, the mixed model equations take the form:

$$\begin{bmatrix} \boldsymbol{X}'\boldsymbol{X} & \boldsymbol{X}'\boldsymbol{Z} \\ \boldsymbol{Z}'\boldsymbol{X} & \boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1} \end{bmatrix} \begin{pmatrix} \boldsymbol{\tau} \\ \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} \boldsymbol{X}'\boldsymbol{y} \\ \boldsymbol{Z}'\boldsymbol{y} \end{pmatrix}$$

To get the inverse of the coefficient matrix we use the results: for $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{D}$ conformal with $\boldsymbol{A}$ and $\boldsymbol{D}$ invertible:

$$(\boldsymbol{A}+\boldsymbol{B}'\boldsymbol{D}\boldsymbol{B})^{-1} = \boldsymbol{A}^{-1} - \boldsymbol{A}^{-1}\boldsymbol{B}'(\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}'+\boldsymbol{D}^{-1})^{-1}\boldsymbol{B}\boldsymbol{A}^{-1}$$

and

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B}^T & \boldsymbol{D} \end{bmatrix}^{-1} = \begin{bmatrix} \boldsymbol{P}^{-1} & -\boldsymbol{P}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} \\ -\boldsymbol{D}^{-1}\boldsymbol{B}^T\boldsymbol{P}^{-1} & \boldsymbol{D}^{-1}+\boldsymbol{D}^{-1}\boldsymbol{B}^T\boldsymbol{P}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} \end{bmatrix}$$

This gives the result

$$(\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1} = \boldsymbol{G} - \boldsymbol{G}\boldsymbol{Z}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G}.$$

with

$$\boldsymbol{Z}(\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1} = \boldsymbol{Z}\boldsymbol{G} - \boldsymbol{Z}\boldsymbol{G}\boldsymbol{Z}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} = \boldsymbol{Z}\boldsymbol{G} - (\boldsymbol{H}-\boldsymbol{I})\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} = \boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G}$$

Substituting these results into the mixed model coefficient matrix:

$$\boldsymbol{P} = \boldsymbol{X}'\boldsymbol{X} - \boldsymbol{X}'\boldsymbol{Z}(\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1}\boldsymbol{Z}'\boldsymbol{X} = \boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X}$$

Hence

$$\begin{aligned} \boldsymbol{P}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} &= (\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Z}(\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1} \\ (\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{D}^{-1}+\boldsymbol{D}^{-1}\boldsymbol{B}'\boldsymbol{P}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} &= (\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1} + (\boldsymbol{Z}'\boldsymbol{Z}+\boldsymbol{G}^{-1})^{-1}\boldsymbol{Z}'\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} \\ &= \boldsymbol{G} - \boldsymbol{G}\boldsymbol{Z}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G}\boldsymbol{G}\boldsymbol{Z}\boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} \\ &= \boldsymbol{G} - \boldsymbol{G}\boldsymbol{Z}'\boldsymbol{P}^{-1}\boldsymbol{Z}\boldsymbol{G}. \end{aligned}$$

Hence the inverse coefficient matrix is

$$\begin{bmatrix} (\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1} & -(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{Z}\boldsymbol{G} \\ -\boldsymbol{G}\boldsymbol{Z}'\boldsymbol{H}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}^{-1}\boldsymbol{X})^{-1} & \boldsymbol{G}-\boldsymbol{G}\boldsymbol{Z}'\boldsymbol{P}\boldsymbol{Z}\boldsymbol{G} \end{bmatrix}$$

as required.