Chapter 3
Best Linear Unbiased Estimation

C. R. Henderson

1984 - Guelph

In Chapter 2 we discussed linear unbiased estimation of $\mathbf{k}'\boldsymbol{\beta}$, having determined that it is estimable. Let the estimate be $\mathbf{a}'\mathbf{y}$, and if $\mathbf{k}'\boldsymbol{\beta}$ is estimable, some $\mathbf{a}$ exists such that

$$E(\mathbf{a}'\mathbf{y}) = \mathbf{k}'\boldsymbol{\beta}.$$

Assuming that more than one $\mathbf{a}$ gives an unbiased estimator, which one should be chosen? The most common criterion for choice is minimum sampling variance. Such an estimator is called the best linear unbiased estimator (BLUE).

Thus we find $\mathbf{a}'$ such that $E(\mathbf{a}'\mathbf{y}) = \mathbf{k}'\boldsymbol{\beta}$ and, in the class of such estimators, has minimum sampling variance. Now

$$Var(\mathbf{a}'\mathbf{y}) = \mathbf{a}'(Var(\mathbf{y}))\mathbf{a} = \mathbf{a}'\mathbf{V}\mathbf{a},$$

where $Var(\mathbf{y}) = \mathbf{V}$, assumed known, for the moment.

For unbiasedness we require $\mathbf{a}'\mathbf{X} = \mathbf{k}'$. Consequently we find $\mathbf{a}$ that minimizes $\mathbf{a}'\mathbf{V}\mathbf{a}$ subject to $\mathbf{a}'\mathbf{X} = \mathbf{k}'$. Using a Lagrange multiplier, $\boldsymbol{\theta}$, and applying differential calculus we need to solve for $\mathbf{a}$ in equations

$$\begin{pmatrix} \mathbf{V} & \mathbf{X} \\ \mathbf{X}' & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \boldsymbol{\theta} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{k} \end{pmatrix}.$$

This is a consistent set of equations if and only if $\mathbf{k}'\boldsymbol{\beta}$ is estimable. In that case the unique solution to $\mathbf{a}$ is

$$\mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{k}.$$

A solution to $\boldsymbol{\theta}$ is

$$-(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{k},$$

and this is not unique when $\mathbf{X}$ and consequently $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$ is not full rank. Nevertheless the solution to $\mathbf{a}$ is invariant to the choice of a g-inverse of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$. Thus, BLUE of $\mathbf{k}'\boldsymbol{\beta}$ is

$$\mathbf{k}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}.$$

But let

$$\boldsymbol{\beta}^o = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y},$$

where $\boldsymbol{\beta}^o$ is any solution to

$$(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})\boldsymbol{\beta}^o = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

known as generalized least squares (GLS) equations, Aitken (1935). Superscript 0 is used to denote some solution, not a unique solution. Therefore BLUE of $\mathbf{k}'\boldsymbol{\beta}$ is $\mathbf{k}'\boldsymbol{\beta}^o$.

Let us illustrate with

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 1 & 2 \\ 1 & 3 & 6 \end{pmatrix},$$

and $\mathbf{y}' = (5\ 2\ 4\ 3)$. Suppose $Var(\mathbf{y}) = \mathbf{I}\sigma_e^2$. Then the GLS equations are

$$\sigma_e^{-2} \begin{pmatrix} 4 & 7 & 14 \\ 7 & 15 & 30 \\ 14 & 30 & 60 \end{pmatrix} \quad \boldsymbol{\beta}^o = \begin{pmatrix} 14 \\ 22 \\ 44 \end{pmatrix} \sigma_e^{-2}.$$

A solution is

$$(\boldsymbol{\beta}^o)' = (56 \quad -10 \quad 0)/11.$$

Then BLUE of $(0 \ \ 1 \ \ 2)\boldsymbol{\beta}$, which has been shown to be estimable, is

$$(0 \ \ 1 \ \ 2)(56 \quad -10 \quad 0)'/11 = -10/11.$$

Another solution to $\boldsymbol{\beta}^o$ is

$$(56 \quad 0 \quad -5)'/11.$$

Then BLUE of $(0 \ \ 1 \ \ 2)\boldsymbol{\beta}$ is $-10/11$, the same as the other solution to $\boldsymbol{\beta}^o$.

1 Mixed Model Method For BLUE

One frequent difficulty with GLS equations, particularly in the mixed model, is that $\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$ is large and non-diagonal. Consequently $\mathbf{V}^{-1}$ is difficult or impossible to compute by usual methods. It was proved by Henderson *et al*. (1959) that

$$\mathbf{V}^{-1} = \mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{Z}(\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1})^{-1}\mathbf{Z}'\mathbf{R}^{-1}.$$

Now if $\mathbf{R}^{-1}$ is easier to compute than $\mathbf{V}^{-1}$, as is often true, if $\mathbf{G}^{-1}$ is easy to compute, and $(\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1})^{-1}$ is easy to compute, this way of computing $\mathbf{V}^{-1}$ may have important advantages. Note that this result can be obtained by writing equations, known as Henderson's mixed model equations (1950) as follows,

$$\begin{pmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} \end{pmatrix} \begin{pmatrix} \boldsymbol{\beta}^o \\ \hat{\mathbf{u}} \end{pmatrix} = \begin{pmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \end{pmatrix}.$$

Note that if we solve for $\hat{\mathbf{u}}$ in the second equation and substitute this in the first we get

$$\begin{aligned} & \mathbf{X}'[\mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{Z}(\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1})^{-1}\mathbf{Z}'\mathbf{R}^{-1}]\mathbf{X}\boldsymbol{\beta}^o \\ = & \mathbf{X}'[\mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{Z}(\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1})^{-1}\mathbf{Z}'\mathbf{R}^{-1}]\mathbf{y}, \end{aligned}$$

or from the result for $\mathbf{V}^{-1}$

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\boldsymbol{\beta}^o = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y}.$$

Thus, a solution to $\boldsymbol{\beta}^o$ in the mixed model equations is a GLS solution. An interpretation of $\hat{\mathbf{u}}$ is given in Chapter 5. The mixed model equations are often well suited to an iterative solution. Let us illustrate the mixed model method for BLUE with

$$\mathbf{X} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 1 \\ 1 & 3 \end{pmatrix}, \ \mathbf{Z} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \mathbf{G} = \begin{pmatrix} .1 & 0 \\ 0 & .1 \end{pmatrix},$$

and

$$\mathbf{R} = \mathbf{I}, \ \ \mathbf{y}' = [5\ 4\ 3\ 2].$$

Then the mixed model equations are

$$\begin{pmatrix} 4 & 7 & 3 & 1 \\ 7 & 15 & 4 & 3 \\ 3 & 4 & 13 & 0 \\ 1 & 3 & 0 & 11 \end{pmatrix} \begin{pmatrix} \boldsymbol{\beta}^o \\ \hat{\mathbf{u}} \end{pmatrix} = \begin{pmatrix} 14 \\ 22 \\ 12 \\ 2 \end{pmatrix}.$$

The solution is [286 $-$ 50 2 $-$ 2]'/57. In this case the solution is unique because $\mathbf{X}$ has full column rank.

Now consider a GLS solution.

$$\mathbf{V} = [\mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}] = \begin{pmatrix} 1.1 & .1 & .1 & 0 \\ .1 & 1.1 & .1 & 0 \\ .1 & .1 & 1.1 & 0 \\ 0 & 0 & 0 & 1.1 \end{pmatrix}.$$

$$\mathbf{V}^{-1} = \frac{1}{143} \begin{pmatrix} 132 & -11 & -11 & 0 \\ -11 & 132 & -11 & 0 \\ -11 & -11 & 132 & 0 \\ 0 & 0 & 0 & 130 \end{pmatrix}.$$

Then $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\boldsymbol{\beta}^o = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$ becomes

$$\frac{1}{143} \begin{pmatrix} 460 & 830 \\ 830 & 1852 \end{pmatrix} \boldsymbol{\beta}^o = \frac{1}{143} \begin{pmatrix} 1580 \\ 2540 \end{pmatrix}.$$

The solution is (286 $-$ 50)/57 as in the mixed model equations.

2 Variance of BLUE

Once having an estimate of $\mathbf{k}'\boldsymbol{\beta}$ we should like to know its sampling variance. Consider a set of estimators, $\mathbf{K}'\boldsymbol{\beta}^o$.

$$\begin{aligned} Var(\mathbf{K}'\boldsymbol{\beta}^o) &= Var[\mathbf{K}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}] \\ &= \mathbf{K}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{V}\mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{K} \\ &= \mathbf{K}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{K} \;\; \text{provided } \mathbf{K}'\boldsymbol{\beta} \text{ is estimable.} \end{aligned}$$

The variance is invariant to the choice of a g-inverse provided $\mathbf{K}'\boldsymbol{\beta}$ is estimable. We can also obtain this result from a g-inverse of the coefficient matrix of the mixed model equations. Let a g-inverse of this matrix be

$$\begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{21} & \mathbf{C}_{22} \end{pmatrix}.$$

Then

$$Var(\mathbf{K}'\boldsymbol{\beta}^o) = \mathbf{K}'\mathbf{C}_{11}\mathbf{K}.$$

This result can be proved by noting that

$$\begin{aligned} \mathbf{C}_{11} &= (\mathbf{X}'[\mathbf{R}^{-1}-\mathbf{R}^{-1}\mathbf{Z}(\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}+\mathbf{G}^{-1})^{-1}\mathbf{Z}'\mathbf{R}^{-1}]\mathbf{X})^{-} \\ &= (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}. \end{aligned}$$

Using the mixed model example, let

$$\mathbf{K}' = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

A g-inverse (regular inverse) of the coefficient matrix is

$$\frac{1}{570}\begin{pmatrix} 926 & -415 & -86 & 29 \\ -415 & 230 & 25 & -25 \\ -86 & 25 & 56 & 1 \\ 29 & -25 & 1 & 56 \end{pmatrix}.$$

Then

$$Var(\mathbf{K}'\boldsymbol{\beta}^o) = \frac{1}{570}\left(\begin{array}{rr} 926 & -415 \\ -415 & 230 \end{array} \right].$$

The same result can be obtained from the inverse of the GLS coefficient matrix because

$$\left(143^{-1}\begin{pmatrix} 460 & 830 \\ 830 & 1852 \end{pmatrix} \right)^{-1} = \frac{1}{570}\begin{pmatrix} 926 & -415 \\ -415 & 230 \end{pmatrix}.$$

3 Generalized Inverses and Mixed Model Equations

Earlier in this chapter we found that BLUE of $\mathbf{K}'\boldsymbol{\beta}$, estimable, is $\mathbf{K}'\boldsymbol{\beta}^o$, where $\boldsymbol{\beta}^o$ is any solution to either GLS or mixed model equations. Also the sampling variance requires a g-inverse of the coefficient matrix of either of these sets of equations. We define $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^-$ as a g-inverse of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$. There are various types of generalized inverses, but the one we shall use is defined as follows.

$\mathbf{A}^-$ is a g-inverse of $\mathbf{A}$ provided that

$$\mathbf{A}\ \mathbf{A}^-\mathbf{A} = \mathbf{A}.$$

Then if we have a set of consistent equations,

$$\mathbf{A}\ \mathbf{p} = \mathbf{z},$$

a solution to $\mathbf{p}$ is

$$\mathbf{A}^-\mathbf{z}.$$

We shall be concerned, in this chapter, only with g-inverses of singular, symmetric matrices characteristic of GLS and mixed model equations.

3.1 First type of g-inverse

Let $\mathbf{W}$ be a symmetric matrix with order, s, and rank, $t < s$. Partition $\mathbf{W}$ with possible re-ordering of rows (and the same re-ordering of columns) as

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_{11} & \mathbf{W}_{12} \\ \mathbf{W}'_{12} & \mathbf{W}_{22} \end{pmatrix},$$

where $\mathbf{W}_{11}$ is a non-singular matrix with order t. Then $\mathbf{W}^- = \begin{pmatrix} \mathbf{W}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$.

It is of interest that for this type of $\mathbf{W}^-$ it is true that $\mathbf{W}^-\mathbf{W}\ \mathbf{W}^- = \mathbf{W}^-$ as well as $\mathbf{W}\ \mathbf{W}^-\mathbf{W} = \mathbf{W}$. This is called a reflexive g-inverse. To illustrate, suppose $\mathbf{W}$ is a GLS coefficient matrix,

$$\mathbf{W} = \begin{pmatrix} 4 & 7 & 8 & 15 \\ 7 & 15 & 17 & 32 \\ 8 & 17 & 22 & 39 \\ 15 & 32 & 39 & 71 \end{pmatrix}.$$

This matrix has rank 3 and the upper 3×3 is non-singular with inverse

$$30^{-1} \begin{pmatrix} 41 & -18 & -1 \\ -18 & 24 & -12 \\ -1 & -12 & 11 \end{pmatrix}.$$

Therefore a g-inverse is

$$30^{-1}\begin{pmatrix} 41 & -18 & -1 & 0 \\ -18 & 24 & -12 & 0 \\ -1 & -12 & 11 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Another g-inverse of this type is

$$30^{-1}\begin{pmatrix} 41 & -17 & 0 & -1 \\ -17 & 59 & 0 & -23 \\ 0 & 0 & 0 & 0 \\ -1 & -23 & 0 & 11 \end{pmatrix}.$$

This was obtained by inverting the full rank submatrix composed of rows (and columns) 1, 2, 4 of $\mathbf{W}$. This type of g-inverse is described in Searle (1971b).

In the mixed model equations a comparable g-inverse is obtained as follows. Partition $\mathbf{X}'\mathbf{R}^{-1}\mathbf{X}$ with possible re-ordering of rows (and columns) as

$$\begin{pmatrix} \mathbf{X}_1'\mathbf{R}^{-1}\mathbf{X}_1 & \mathbf{X}_1'\mathbf{R}^{-1}\mathbf{X}_2 \\ \mathbf{X}_2'\mathbf{R}^{-1}\mathbf{X}_1 & \mathbf{X}_2'\mathbf{R}^{-1}\mathbf{X}_2 \end{pmatrix}$$

so that $\mathbf{X}_1'\mathbf{R}^{-1}\mathbf{X}_1$ has order r and is full rank. Compute

$$\begin{pmatrix} \mathbf{X}_1'\mathbf{R}^{-1}\mathbf{X}_1 & \mathbf{X}_1'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X}_1 & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}+\mathbf{G}^{-1} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{C}_{00} & \mathbf{C}_{02} \\ \mathbf{C}_{02}' & \mathbf{C}_{22} \end{pmatrix}.$$

Then a g-inverse of the coefficient matrix is $\begin{pmatrix} \mathbf{C}_{00} & \mathbf{0} & \mathbf{C}_{02} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{C}_{02}' & \mathbf{0} & \mathbf{C}_{22} \end{pmatrix}$. We illustrate with a mixed model coefficient matrix as follows.

$$\begin{pmatrix} 5 & 8 & -8 & 3 & 2 \\ 8 & 16 & -16 & 4 & 4 \\ -8 & -16 & 16 & -4 & -4 \\ 3 & 4 & -4 & 8 & 0 \\ 2 & 4 & -4 & 0 & 7 \end{pmatrix}$$

where $\mathbf{X}$ has 3 columns and $\mathbf{Z}$ has 2. Therefore $\mathbf{X}'\mathbf{R}^{-1}\mathbf{X}$ is the upper 3 x 3 submatrix. It has rank 2 because the 3rd column is the negative of the second. Consequently find a g-inverse by inverting the matrix with the 3rd row and column deleted. This gives

$$560^{-1}\begin{pmatrix} 656 & -300 & 0 & -96 & -16 \\ -300 & 185 & 0 & 20 & -20 \\ 0 & 0 & 0 & 0 & 0 \\ -96 & 20 & 0 & 96 & 16 \\ -16 & -20 & 0 & 16 & 96 \end{pmatrix}.$$

With this type of g-inverse the solution to $\boldsymbol{\beta}^o$ is $(\boldsymbol{\beta}_1^o \ \ \mathbf{0})'$, where $\boldsymbol{\beta}_1^o$ has r elements. Only the first p rows of the mixed model equations contribute to lack of rank of the mixed model matrix. The matrix has order $p+q$ and rank $r+q$, where $r =$ rank of $\mathbf{X}$, $p =$ columns in $\mathbf{X}$, and $q =$ columns in $\mathbf{Z}$.

3.2 Second type of g-inverse

A second type of g-inverse is one which imposes restrictions on the solution to $\boldsymbol{\beta}^o$. Let $\mathbf{M}'\boldsymbol{\beta}$ be a set of $p-r$ linearly independent, non-estimable functions of $\boldsymbol{\beta}$. Then a g-inverse for the GLS matrix is obtained as follows $\begin{pmatrix} \mathbf{X}'\mathbf{V}^{-1}\mathbf{X} & \mathbf{M} \\ \mathbf{M}' & \mathbf{O} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{12}' & \mathbf{C}_{22} \end{pmatrix}$.

$\mathbf{C}_{11}$ is a reflexive g-inverse of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$. This type of solution is described in Kempthorne (1952). Let us illustrate GLS equations as follows.

$$\begin{pmatrix} 11 & 5 & 6 & 3 & 8 \\ 5 & 5 & 0 & 2 & 3 \\ 6 & 0 & 6 & 1 & 5 \\ 3 & 2 & 1 & 3 & 0 \\ 8 & 3 & 5 & 0 & 8 \end{pmatrix} \boldsymbol{\beta}^o = \begin{pmatrix} 12 \\ 7 \\ 5 \\ 8 \\ 4 \end{pmatrix}.$$

This matrix has order 5 but rank only 3. Two independent non-estimable functions are needed. Among others the following qualify

$$\begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix} \boldsymbol{\beta}.$$

Therefore we invert

$$\begin{pmatrix} 11 & 5 & 6 & 3 & 8 & 0 & 0 \\ 5 & 5 & 0 & 2 & 3 & 1 & 0 \\ 6 & 0 & 6 & 1 & 5 & 1 & 0 \\ 3 & 2 & 1 & 3 & 0 & 0 & 1 \\ 8 & 3 & 5 & 0 & 8 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{pmatrix},$$

which is

$$244^{-1} \begin{pmatrix} 28 & -1 & 1 & 13 & -13 & -122 & -122 \\ -1 & 24 & -24 & -7 & 7 & 122 & 0 \\ 1 & -24 & 24 & 7 & -7 & 122 & 0 \\ 13 & -7 & 7 & 30 & -30 & 0 & 122 \\ -13 & 7 & -7 & -30 & 30 & 0 & 122 \\ -122 & 122 & 122 & 0 & 0 & 0 & 0 \\ -122 & 0 & 0 & 122 & 122 & 0 & 0 \end{pmatrix}.$$

The upper 5 x 5 submatrix is a g-inverse. This gives a solution

$$\boldsymbol{\beta}^o \;=\; (386 \;\; 8 \;\; -8 \;\; 262 \;\; -262)'/244.$$

A corresponding g-inverse for the mixed model is as follows

$$\begin{pmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} & \mathbf{M} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}+\mathbf{G}^{-1} & 0 \\ \mathbf{M}' & 0 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} & \mathbf{C}_{13} \\ \mathbf{C}_{12}' & \mathbf{C}_{22} & \mathbf{C}_{23} \\ \mathbf{C}_{13}' & \mathbf{C}_{23} & \mathbf{C}_{33} \end{pmatrix}.$$

Then

$$\begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{12}' & \mathbf{C}_{22} \end{pmatrix}$$

is a g-inverse of the mixed model coefficient matrix. The property of $\boldsymbol{\beta}^o$ coming from this type of g-inverse is

$$\mathbf{M}'\boldsymbol{\beta}^o = \mathbf{0}.$$

3.3 Third type of g-inverse

A third type of g-inverse uses $\mathbf{M}$ of the previous section as follows. $(\mathbf{X}\text{'}\mathbf{V}^{-1}\mathbf{X} + \mathbf{M}\mathbf{M}')^{-1} = \mathbf{C}$. Then $\mathbf{C}$ is a g-inverse of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$. In this case $\mathbf{C}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})\mathbf{C} \neq \mathbf{C}$. This is described in Rao and Mitra (1971).

We illustrate with the same GLS matrix as before and

$$\mathbf{M}' = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

as before.

$$(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X} + \mathbf{M}\mathbf{M}') = \begin{pmatrix} 11 & 5 & 6 & 3 & 8 \\ 5 & 6 & 1 & 2 & 3 \\ 6 & 1 & 7 & 1 & 5 \\ 3 & 2 & 1 & 4 & 1 \\ 8 & 3 & 5 & 1 & 9 \end{pmatrix}$$

with inverse

$$244^{-1} \begin{pmatrix} 150 & -62 & -60 & -48 & -74 \\ -62 & 85 & 37 & -7 & 7 \\ -60 & 37 & 85 & 7 & -7 \\ -48 & -7 & 7 & 91 & 31 \\ -74 & 7 & -7 & 31 & 91 \end{pmatrix},$$

which is a g-inverse of the GLS matrix. The resulting solution to $\boldsymbol{\beta}^o$ is the same as the previous section.

The corresponding method for finding a g-inverse of the mixed model matrix is $\begin{pmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X}+\mathbf{M}\mathbf{M}' & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}+\mathbf{G}^{-1} \end{pmatrix}^{-1} = \mathbf{C}$. Then $\mathbf{C}$ is a g-inverse. The property of the solution to $\boldsymbol{\beta}^o$ is

$$\mathbf{M}'\boldsymbol{\beta}^o = \mathbf{0}.$$

4 Reparameterization

An entirely different method for dealing with the not full rank $\mathbf{X}$ problem is reparameterization. Let $\mathbf{K}'\boldsymbol{\beta}$ be a set of r linearly independent, estimable functions of $\boldsymbol{\beta}$. Let $\hat{\boldsymbol{\alpha}}$ be BLUE of $\mathbf{K}'\boldsymbol{\beta}$. To find $\hat{\boldsymbol{\alpha}}$ solve $(\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\mathbf{K}(\mathbf{K}'\mathbf{K})^{-1}\hat{\boldsymbol{\alpha}} = (\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$. $\hat{\boldsymbol{\alpha}}$ has a unique solution, and the regular inverse of the coefficient matrix is $Var(\hat{\boldsymbol{\alpha}})$. This corresponds to a model

$$E(\mathbf{y}) = \mathbf{X} \;\; \mathbf{K}(\mathbf{K}'\mathbf{K})^{-1}\boldsymbol{\alpha}.$$

This method was suggested to me by Gianola (1980).

From the immediately preceding example we need 3 estimable functions. An independent set is

$$\begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 & 1/2 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix}.$$

The corresponding GLS equations are

$$\begin{pmatrix} 11 & -.50 & -2.50 \\ -.5 & 2.75 & .75 \\ -2.5 & .75 & 2.75 \end{pmatrix} \hat{\boldsymbol{\alpha}} = \begin{pmatrix} 12 \\ 1 \\ 2 \end{pmatrix}.$$

The solution is

$$\hat{\boldsymbol{\alpha}}' = (193 \;\; 8 \;\; 262)/122.$$

This is identical to

$$\begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 & 1/2 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix} \boldsymbol{\beta}^o$$

from the previous solution in which

$$\begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix} \boldsymbol{\beta}^o$$

was forced to equal $\mathbf{0}$.

The corresponding set of equations for mixed models is

$$\begin{pmatrix} (\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{X}'\mathbf{R}^{-1}\mathbf{X}\mathbf{K}(\mathbf{K}'\mathbf{K})^{-1} & (\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X}\mathbf{K}(\mathbf{K}'\mathbf{K})^{-1} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{\alpha}} \\ \hat{\mathbf{u}} \end{pmatrix} = \begin{pmatrix} (\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \end{pmatrix}.$$

5 Precautions in Solving Equations

Precautions must be observed in the solution to equations, especially if there is some doubt about the rank of the matrix. If a supposed g-inverse is calculated, it may be advisable to check that $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A}$. Another check is to regenerate the right hand sides as follows. Let the equations be

$$\mathbf{C}\hat{\boldsymbol{\alpha}} = \mathbf{r}.$$

Having computed $\hat{\boldsymbol{\alpha}}$, compute $\mathbf{C}\hat{\boldsymbol{\alpha}}$ and check that it is equal, except for rounding error, to $\mathbf{r}$.