7 Design Matrices of Less Than Full Rank

If $\mathbf{X}_{n\times p}$ has rank $r < p$, there is not a unique solution $\hat{\boldsymbol{\beta}}$ to the normal equations. We have three ways to find *a* solution $\hat{\boldsymbol{\beta}}$ and *the* orthogonal projection $\hat{\mathbf{Y}}$:

1. Reducing the model to one of full rank.
2. Finding a generalized inverse $(\mathbf{X}'\mathbf{X})^{-}$.
3. Imposing identifiability constraints.

7.1 Reducing the Model to One of Full Rank

Let $\mathbf{X}_1$ consist of r linearly independent columns from $\mathbf{X}$ and let $\mathbf{X}_2$ consist of the remaining columns. Then $\mathbf{X_2} = \mathbf{X_1 F}$ because the columns of $\mathbf{X}_2$ are linearly dependent on the columns of $\mathbf{X}_1$.

$$\mathbf{X} = (\mathbf{X_1}, \mathbf{X_2}) = (\mathbf{X_1}, \mathbf{X_1 F}) = \mathbf{X_1}(\mathbf{I_{r\times r}}, \mathbf{F}).$$

This is a special case of the factorization $\mathbf{X} = \mathbf{KL}$, where $\text{rank}(\mathbf{K}_{n\times r}) = r$ and $\text{rank}(\mathbf{L}_{r\times p}) = r$. Now,

$$E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta} = \mathbf{KL}\boldsymbol{\beta} = \mathbf{K}\boldsymbol{\alpha}.$$

Since $\mathbf{K}$ has full rank, the least squares estimate of $\boldsymbol{\alpha}$ is $\hat{\boldsymbol{\alpha}} = (\mathbf{K}'\mathbf{K})^{-\mathbf{1}}\mathbf{K}'\mathbf{Y}$ and the orthogonal projection is $\hat{\mathbf{Y}} = \mathbf{K}\hat{\boldsymbol{\alpha}} = \mathbf{K}(\mathbf{K}'\mathbf{K})^{-\mathbf{1}}\mathbf{K}'\mathbf{Y}$. Therefore, $\mathbf{P} = \mathbf{K}(\mathbf{K}'\mathbf{K})^{-\mathbf{1}}\mathbf{K}'$, i.e. $\mathbf{P} = \mathbf{X_1}(\mathbf{X_1'}\mathbf{X_1})^{-\mathbf{1}}\mathbf{X_1'}$.

7.1 Example: (One-way ANOVA with 2 groups).

$$\begin{pmatrix} Y_{11} \\ \vdots \\ Y_{1n_1} \\ Y_{21} \\ \vdots \\ Y_{2n_2} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{pmatrix} + \begin{pmatrix} \varepsilon_{11} \\ \vdots \\ \varepsilon_{1n_1} \\ \varepsilon_{21} \\ \vdots \\ \varepsilon_{2n_2} \end{pmatrix}$$

Let $\mathbf{X}_1$ consist of the first 2 columns of $\mathbf{X}$. Then

$$\mathbf{X} = \mathbf{X}_1 \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix},$$

and $\mathbf{X}\boldsymbol{\beta} = \mathbf{X}_1\boldsymbol{\alpha}$, where

$$\boldsymbol{\alpha} = \begin{pmatrix} \mu + \alpha_2 \\ \alpha_1 - \alpha_2 \end{pmatrix}.$$

Then

$$\hat{\boldsymbol{\alpha}} = \begin{pmatrix} n & n_1 \\ n_1 & n_1 \end{pmatrix}^{-1} \begin{pmatrix} \sum_j Y_{1j} + \sum_j Y_{2j} \\ \sum_j Y_{1j} \end{pmatrix} = \begin{pmatrix} n_2^{-1} & -n_2^{-1} \\ -n_2^{-1} & n_1^{-1} + n_2^{-1} \end{pmatrix} \begin{pmatrix} \sum_j Y_{1j} + \sum_j Y_{2j} \\ \sum_j Y_{1j} \end{pmatrix}$$

$$= \begin{pmatrix} \bar{Y}_2 \\ \bar{Y}_1 - \bar{Y}_2 \end{pmatrix},$$

and hence $\hat{\mathbf{Y}} = \mathbf{X}_1 \hat{\boldsymbol{\alpha}} = (\bar{Y}_1., \ldots, \bar{Y}_1., \bar{Y}_2., \ldots, \bar{Y}_2.)'$.

7.2 Finding a Generalized Inverse $(\mathbf{X}'\mathbf{X})^-$

Let $\mathbf{X} = (\mathbf{X_1}, \mathbf{X_2})$, where $\mathbf{X}_1$ consists of r linearly independent columns from $\mathbf{X}$. Then a generalized inverse of $\mathbf{X}'\mathbf{X}$ is

$$(\mathbf{X}'\mathbf{X})^- = \begin{pmatrix} (\mathbf{X}_1'\mathbf{X}_1)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

A solution to the normal equations is $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^-\mathbf{X}'\mathbf{Y}$ and $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}'\mathbf{Y} = \mathbf{P}\mathbf{Y}$, where $\mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}'$. Note that this also gives $\mathbf{P} = \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'$. This result is a special case of the following theorem:

7.2 Theorem: Let the matrix $\mathbf{W}_{p\times p}$ have rank r and be partitioned as

$$\mathbf{W} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix},$$

where $\mathbf{A}$ has rank r. Then a generalized inverse of $\mathbf{W}$ is

$$\mathbf{W}^- = \begin{pmatrix} \mathbf{A}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

7.3 Example: (One-way ANOVA with 2 groups, continued). We have

$$\mathbf{X}'\mathbf{X} = \begin{pmatrix} n & n_1 & n_2 \\ n_1 & n_1 & 0 \\ n_2 & 0 & n_2 \end{pmatrix}.$$

If $\mathbf{X}_1$ consists of the first 2 columns of $\mathbf{X}$, then

$$(\mathbf{X}_1'\mathbf{X}_1)^{-1} = \begin{pmatrix} n & n_1 \\ n_1 & n_1 \end{pmatrix}^{-1} = \begin{pmatrix} n_2^{-1} & -n_2^{-1} \\ -n_2^{-1} & n_1^{-1} + n_2^{-1} \end{pmatrix}.$$

and generalized inverse of $\mathbf{X}'\mathbf{X}$ is

$$(\mathbf{X}'\mathbf{X})^- = \begin{pmatrix} n_2^{-1} & -n_2^{-1} & 0 \\ -n_2^{-1} & n_1^{-1} + n_2^{-1} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Now a solution to the normal equations is

$$\hat{\boldsymbol{\beta}} = \begin{pmatrix} n_2^{-1} & -n_2^{-1} & 0 \\ -n_2^{-1} & n_1^{-1} + n_2^{-1} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \sum_j Y_{1j} + \sum_j Y_{2j} \\ \sum_j Y_{1j} \\ \sum_j Y_{2j} \end{pmatrix} = \begin{pmatrix} \bar{Y}_2 \\ \bar{Y}_1 - \bar{Y}_2 \\ 0 \end{pmatrix},$$

and $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = (\bar{Y}_{1\cdot}, \ldots, \bar{Y}_{1\cdot}, \bar{Y}_{2\cdot}, \ldots, \bar{Y}_{2\cdot})'$, as before.

7.3 Imposing Identifiability Constraints

Impose $s = p - r$ constraints on $\boldsymbol{\beta}$ to make $\boldsymbol{\beta}$ uniquely determined (identifiable), i.e. such that for any $\boldsymbol{\theta} \in \mathcal{R}(\mathbf{X})$, there is a unique $\boldsymbol{\beta}$ satisfying

$$\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\theta} \quad \text{and} \quad \mathbf{H}\boldsymbol{\beta} = \mathbf{0}.$$

This can be written

$$\begin{pmatrix} \boldsymbol{\theta} \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{X} \\ \mathbf{H} \end{pmatrix} \boldsymbol{\beta} \equiv \mathbf{G}\boldsymbol{\beta}.$$

Now when is there a unique solution?

7.4 Theorem: A unique solution exists if and only if $\mathbf{G}$ has rank p and the rows of $\mathbf{H}$ are linearly independent of the rows of $\mathbf{X}$.

7.5 Theorem: A unique solution exists if and only if $\mathbf{G}$ has rank p and $\mathbf{H}$ has rank $p - r$.

To estimate $\boldsymbol{\beta}$, we solve $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$ and $\mathbf{H}\hat{\boldsymbol{\beta}} = \mathbf{0}$, i.e. we solve the augmented normal equations $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y}$ and $\mathbf{H}'\mathbf{H}\hat{\boldsymbol{\beta}} = \mathbf{0}$, i.e. $(\mathbf{X}'\mathbf{X} + \mathbf{H}'\mathbf{H})\hat{\boldsymbol{\beta}} = (\mathbf{G}'\mathbf{G})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y}$. Therefore,

$$\hat{\boldsymbol{\beta}} = (\mathbf{G}'\mathbf{G})^{-1}\mathbf{X}'\mathbf{Y}, \text{ and } \hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{P}\mathbf{Y}, \text{ where } \mathbf{P} = \mathbf{X}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{X}'.$$

7.6 Example: (One-way ANOVA with 2 groups, cont.). Set $\alpha_1 + \alpha_2 = 0$, i.e.

$$\mathbf{H}\boldsymbol{\beta} \equiv (0, 1, 1) \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = 0.$$

Suppose $n_1 = n_2 = m$. Then it can be shown that

$$\hat{\boldsymbol{\beta}} = \begin{pmatrix} \bar{Y}_{\cdot\cdot} \\ \frac{1}{2}(\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}) \\ \frac{1}{2}(\bar{Y}_{2\cdot} - \bar{Y}_{1\cdot}) \end{pmatrix}$$

satisfies the normal equations, and clearly satisfies the constraint $\alpha_1 + \alpha_2 = 0$. Therefore, we have as before $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = (\bar{Y}_{1\cdot}, \ldots, \bar{Y}_{1\cdot}, \bar{Y}_{2\cdot}, \ldots, \bar{Y}_{2\cdot})'$.