Key results for solving the General Linear Model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$

(1) **OLS (Ordinary Least Squares)**.

• Residuals are assumed to be uncorrelated and have the same variance, $\mathbf{e} \sim (\mathbf{0}, \sigma_e^2 \mathbf{I})$

• Solve for the vector $\boldsymbol{\beta}$ of unknown fixed effects by minimizing the unweighted sum of squared residuals, $\sum e_i^2$

• OLS estimate of fixed effects:

$$\text{OLS}(\boldsymbol{\beta}) = \widehat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

• Variance-covariance matrix for estimates of fixed effects:

$$\text{Var}(\widehat{\boldsymbol{\beta}}) = (\mathbf{X}^T\mathbf{X})^{-1}\sigma_e^2$$

• Vector of predicted y values

$$\widehat{\mathbf{y}} = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

• Vector of estimated residuals

$$\widehat{\mathbf{e}} = \mathbf{y} - \widehat{\mathbf{y}}$$

• Error Sum of Squares, SS_E, for model

$$\text{SS}_E = \sum_{i=1}^{N} e_i^2 = \widehat{\mathbf{e}}^T\ \widehat{\mathbf{e}} = (\mathbf{y} - \widehat{\mathbf{y}})^T\ (\mathbf{y} - \widehat{\mathbf{y}})$$

• SS_E as a quadratic product

$$\text{SS}_E = \mathbf{y}^T\mathbf{A}\mathbf{y}, \quad \text{where} \quad \mathbf{A} = \mathbf{I} - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$$

• Estimate of the residual variance when there are N observations and p estimated parameters

$$\widehat{\sigma_e^2} = \frac{\text{SS}_E}{N-p}$$

• If $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2\mathbf{I})$, then

$$\frac{\text{SS}_E}{\sigma_e^2} \sim \chi^2_{N-p}$$

• **Confidence intervals:** If $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2\mathbf{I})$, then

$$\widehat{\boldsymbol{\beta}} \sim \text{MVN}(\boldsymbol{\beta}, (\mathbf{X}^T\mathbf{X})^{-1}\sigma_e^2)$$

Hence, a 95% CI for β_i is given by

$$\widehat{\beta}_i \pm 1.96\sqrt{\sigma^2(\widehat{\beta}_i)}, \quad \text{where} \quad \sigma^2(\widehat{\beta}_i) = [(\mathbf{X}^T\mathbf{X})^{-1}\sigma_e^2]_{ii}$$

• **Hypothesis testing:** Assume $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2\mathbf{I})$. Consider a full model with p estimated parameters and a reduced model where q of the parameters are free, but $p-q$ of the β_i in the full model are set to zero (i.e., the reduced model is **nested** within the full model). Under this null, the error sum of squares for the full and reduced models are distributed as

$$\text{SS}_{Ef} \sim \sigma_e^2\chi^2_{N-p}, \quad \text{and} \quad \text{SS}_{Er} \sim \sigma_e^2\chi^2_{N-q}, \quad \text{hence} \quad \text{SS}_{Er} - \text{SS}_{Ef} \sim \sigma_e^2\chi^2_{p-q}$$

Thus

$$\frac{(\text{SS}_{Er} - \text{SS}_{Ef})/(p-q)}{\text{SS}_{Ef}/(N-p)} = \frac{N-p}{p-q}\left(\frac{\text{SS}_{Er}}{\text{SS}_{Ef}} - 1\right) \sim F_{p-q,N-p}$$

(2) **GLS (Generalized Least Squares).**

• Residuals are NOT assumed to be uncorrelated and have the same variance, $\mathbf{e} \sim (\mathbf{0}, \sigma_e^2 \mathbf{R})$

• Solve for the vector $\boldsymbol{\beta}$ of unknown fixed effects by minimizing the appropriately weighted sum of squared residuals, $\sum_i \sum_j w_{ij} e_i e_j$

• GLS estimate of fixed effects:

$$\text{GLS}(\boldsymbol{\beta}) = \widehat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{R}^{-1} \mathbf{y}$$

• Variance-covariance matrix for estimates of fixed effects:

$$\text{Var}(\widehat{\boldsymbol{\beta}}) = (\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \sigma_e^2$$

• Vector of predicted y values

$$\widehat{\mathbf{y}} = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{R}^{-1} \mathbf{y}$$

• Vector of estimated residuals

$$\widehat{\mathbf{e}} = \mathbf{y} - \widehat{\mathbf{y}}$$

• Error Sum of Squares, SS_E

$$\text{SS}_E = \widehat{\mathbf{e}}^T \mathbf{R}^{-1} \widehat{\mathbf{e}}$$

• SS_E as a quadratic product

$$\text{SS}_E = \mathbf{y}^T \mathbf{B} \mathbf{y}, \quad \text{where} \quad \mathbf{B} = \mathbf{R}^{-1}(\mathbf{I} - \mathbf{X}(\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{R}^{-1})$$

• Estimate of the residual variance when there are N observations and p estimated parameters

$$\widehat{\sigma_e^2} = \frac{\text{SS}_E}{N - p}$$

• If $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2 \mathbf{R})$, then

$$\frac{\text{SS}_E}{\sigma_e^2} \sim \chi^2_{N-p}$$

• **Confidence intervals:** If $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2 \mathbf{R})$, then

$$\widehat{\boldsymbol{\beta}} \sim \text{MVN}(\boldsymbol{\beta}, (\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \sigma_e^2)$$

Hence, a 95% CI for β_i is given by

$$\widehat{\beta}_i \pm 1.96\sqrt{\sigma^2(\widehat{\beta}_i)}, \quad \text{where} \quad \sigma^2(\widehat{\beta}_i) = [(\mathbf{X}^T \mathbf{R}^{-1} \mathbf{X})^{-1} \sigma_e^2]_{ii}$$

• **Hypothesis testing:** Assume $\mathbf{e} \sim \text{MVN}(\mathbf{0}, \sigma_e^2 \mathbf{R})$. Consider a full model with p estimated parameters and a reduced model where q of the parameters are free, but $p - q$ of the β_i in the full model are set to zero (i.e., the reduced model is **nested** within the full model). Under this null, the error sum of squares for the full and reduced models are distributed as

$$\text{SS}_{Ef} \sim \sigma_e^2 \chi^2_{N-p}, \quad \text{and} \quad \text{SS}_{Er} \sim \sigma_e^2 \chi^2_{N-q}, \quad \text{hence} \quad \text{SS}_{Er} - \text{SS}_{Ef} \sim \sigma_e^2 \chi^2_{p-q}$$

Thus

$$\frac{(\text{SS}_{Er} - \text{SS}_{Ef})/(p-q)}{\text{SS}_{Ef}/(N-p)} = \frac{N-p}{p-q}\left(\frac{\text{SS}_{Er}}{\text{SS}_{Ef}} - 1\right) \sim F_{p-q, N-p}$$