

Longitudinal Data Analysis:

Whiteboard Interlude III

Here we are just considering the **simple linear regression model**:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \stackrel{\text{ind.}}{\sim} N(0, \sigma_\varepsilon^2).$$

Note that

$$y_i \sim N(\beta_0 + \beta_1 x_i, \sigma_\varepsilon^2)$$

so the likelihood is

$$\mathcal{L}(\beta_0, \beta_1, \sigma_\varepsilon^2) = \prod_{i=1}^n \left\{ (2\pi\sigma_\varepsilon^2)^{-1/2} e^{-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma_\varepsilon^2}} \right\}.$$

Straightforward algebra then leads to the matrix algebraic expression for the log-likelihood:

$$\ell(\boldsymbol{\beta}, \sigma_\varepsilon^2) = -\frac{1}{2\sigma_\varepsilon^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) - \frac{n}{2} \ln(2\pi\sigma_\varepsilon^2)$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \quad \text{and} \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \cdot & \cdot \\ \cdot & \cdot \\ 1 & x_n \end{bmatrix}.$$

For all $\sigma_\varepsilon^2 > 0$, the maximum likelihood estimator of $\boldsymbol{\beta}$ is

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

(as shown earlier in the course).

The **profile log-likelihood** for σ_ε^2 is

$$\begin{aligned}\ell_P(\sigma_\varepsilon^2) &= -\frac{1}{2\sigma_\varepsilon^2}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) - \frac{n}{2}\ln(2\pi\sigma_\varepsilon^2) \\ &= -\frac{1}{2}(\sigma_\varepsilon^2)^{-1}\text{RSS} - \frac{n}{2}\ln(\sigma_\varepsilon^2) - \frac{n}{2}\ln(2\pi)\end{aligned}$$

where

$$\begin{aligned}\text{RSS} &= (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \mathbf{y}^T(\mathbf{I} - \mathbf{H})\mathbf{y}\end{aligned}$$

and

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T.$$

$$\frac{\partial}{\partial\sigma_\varepsilon^2}\ell_P(\sigma_\varepsilon^2) = \frac{1}{2}(\sigma_\varepsilon^2)^{-2}\text{RSS} - \frac{n}{2}(\sigma_\varepsilon^2)^{-1}$$

which is zero if and only if

$$\sigma_\varepsilon^2 = \frac{\text{RSS}}{n}.$$

This leads to

$$\hat{\sigma}_{\varepsilon,\text{ML}}^2 = \frac{\text{RSS}}{n}.$$

Results for expectations of quadratic forms

lead to

$$E(\text{RSS}) = (n - 2)\sigma_\varepsilon^2.$$

$$E(\hat{\sigma}_{\varepsilon,\text{ML}}^2) = \left(\frac{n - 2}{n}\right)\sigma_\varepsilon^2$$

so the maximum likelihood estimator of σ_ε^2 is slightly **biased**.

It is common to instead use

$$\frac{\text{RSS}}{n - 2}$$

to estimate σ_ε^2 .

This corresponds to maximising the **restricted** log-likelihood.

i.e. the **restricted maximum likelihood (REML)** estimator of σ_ε^2 is:

$$\hat{\sigma}_{\varepsilon, \text{REML}}^2 = \frac{\text{RSS}}{n - 2}.$$

The actual restricted log-likelihood is:

$$\ell_R(\sigma_\varepsilon^2) = \ell_P(\sigma_\varepsilon^2) - \frac{1}{2} \log |(1/\sigma_\varepsilon^2) \mathbf{X}^T \mathbf{X}|.$$

The expression for $\ell_R(\sigma_\varepsilon^2)$ can be derived using

- “contrast” arguments that account for estimation of the regression coefficients vector β . One of the course reference books, McCulloch & Searle (2000), has the details.

- the theory of **modified profile likelihood**. (e.g. look up via **Google** or **Wikipedia**).

