

9.1 MLE: The Case of Single Regression Model

The regression model:

$$y_i = \beta_1 + \beta_2 x_i + u_i,$$

1. $u_i \sim N(0, \sigma^2)$ is assumed.
2. The density function of u_i is:

$$f(u_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2} u_i^2\right).$$

Because u_1, u_2, \dots, u_n are mutually independently distributed, the joint density function of u_1, u_2, \dots, u_n is written as:

$$\begin{aligned} f(u_1, u_2, \dots, u_n) &= f(u_1)f(u_2) \cdots f(u_n) \\ &= \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n u_i^2\right) \end{aligned}$$

3. Using the transformation of variable ($u_i = y_i - \beta_1 - \beta_2 x_i$), the joint density function of y_1, y_2, \dots, y_n is given by:

$$\begin{aligned} f(y_1, y_2, \dots, y_n) &= \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_1 - \beta_2 x_i)^2\right) \\ &\equiv L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n). \end{aligned}$$

$L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)$ is called the likelihood function.

$\log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)$ is called the log-likelihood function.

$$\begin{aligned} \log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n) \\ = -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_1 - \beta_2 x_i)^2 \end{aligned}$$

4. Transformation of Variable (変数変換) — Review:

Suppose that the density function of a random variable X is $f_x(x)$.

Defining $X = g(Y)$, the density function of Y , $f_y(y)$, is given by:

$$f_y(y) = f_x(g(y)) \left| \frac{dg(y)}{dy} \right|.$$

In the case where X and $g(Y)$ are $n \times 1$ vectors, $\left| \frac{dg(y)}{dy} \right|$ should be replaced by $\left| \frac{\partial g(y)}{\partial y'} \right|$, which is an absolute value of a determinant of the matrix $\frac{\partial g(y)}{\partial y'}$.

Example: When $X \sim U(0, 1)$, derive the density function of $Y = -\log(X)$.

$$f_x(x) = 1$$

$X = \exp(-Y)$ is obtained.

Therefore, the density function of Y , $f_y(y)$, is given by:

$$f_y(y) = \left| \frac{dx}{dy} \right| f_x(g(y)) = |-\exp(-y)| = \exp(-y)$$

5. **[Going back to 3]:** Given the observed data y_1, y_2, \dots, y_n , the likelihood function $L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)$, or the log-likelihood function $\log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)$ is maximized with respect to $(\beta_1, \beta_2, \sigma^2)$.

Solve the following three simultaneous equations:

$$\frac{\partial \log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)}{\partial \beta_1} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \beta_1 - \beta_2 x_i) = 0,$$

$$\frac{\partial \log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)}{\partial \beta_2} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \beta_1 - \beta_2 x_i) x_i = 0,$$

$$\frac{\partial \log L(\beta_1, \beta_2, \sigma^2 | y_1, y_2, \dots, y_n)}{\partial \sigma^2} = -\frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (y_i - \beta_1 - \beta_2 x_i)^2 = 0.$$

The solutions of $(\beta_1, \beta_2, \sigma^2)$ are called the maximum likelihood estimates, denoted by $(\tilde{\beta}_1, \tilde{\beta}_2, \tilde{\sigma}^2)$.

The maximum likelihood estimates are:

$$\tilde{\beta}_2 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad \tilde{\beta}_1 = \bar{y} - \tilde{\beta}_2 \bar{x}, \quad \tilde{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \tilde{\beta}_1 - \tilde{\beta}_2 x_i)^2.$$

The MLE of σ^2 is divided by n , not $n - 2$.

9.2 MLE: The Case of Multiple Regression Model I

1. Multivariate Normal Distribution: $X : n \times 1$ and $X \sim N(\mu, \Sigma)$

The density function of X is:

$$f(x) = (2\pi)^{n/2} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(x - \mu)' \Sigma^{-1} (x - \mu)\right).$$

2. Regression model: $y = X\beta + u, \quad u \sim N(0, \sigma^2 I_n)$

Transformation of Variables from u to y :

$$f_u(u) = (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2}u'u\right)$$

$$\begin{aligned} f_y(y) &= f_u(y - X\beta) \left| \frac{\partial u}{\partial y'} \right| \\ &= (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2}(y - X\beta)'(y - X\beta)\right) \\ &= L(\theta; y, X), \end{aligned}$$

where $\theta = (\beta, \sigma^2)$, because of $\frac{\partial u}{\partial y'} = I_n$.

Therefore, the log-likelihood function is:

$$\log L(\theta; y, X) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(y - X\beta)'(y - X\beta),$$

Note that $|\Sigma|^{-1/2} = |\sigma^2 I_n|^{-1/2} = \sigma^{-n/2}$.

$$3. \max_{\theta} \log L(\theta; y, X)$$

$$\text{(FOC)} \quad \frac{\partial \log L(\theta; y, X)}{\partial \theta} = 0$$

$$\text{(SOC)} \quad \frac{\partial^2 \log L(\theta; y, X)}{\partial \theta \partial \theta'} \text{ is a negative definite matrix.}$$

We obtain MLE of β and σ^2 :

$$\tilde{\beta} = (X'X)^{-1}X'y, \quad \tilde{\sigma}^2 = \frac{(y - X\tilde{\beta})'(y - X\tilde{\beta})}{n},$$

where $\tilde{\sigma}^2$ is divided by n , not $n - k$.

4. Fisher's information matrix is:

$$I(\theta) = -E\left(\frac{\partial^2 \log L(\theta; y, X)}{\partial \theta \partial \theta'}\right)$$

The inverse of the information matrix, $I(\theta)^{-1}$, provides a lower bound of the variance - covariance matrix for unbiased estimators of θ .

$$I(\theta)^{-1} = \begin{pmatrix} \sigma^2(X'X)^{-1} & 0 \\ 0 & \frac{2\sigma^4}{n} \end{pmatrix}$$

For large n , we approximately obtain: $\begin{pmatrix} \tilde{\beta} \\ \tilde{\sigma}^2 \end{pmatrix} \sim N\left(\begin{pmatrix} \beta \\ \sigma^2 \end{pmatrix}, \begin{pmatrix} \sigma^2(X'X)^{-1} & 0 \\ 0 & \frac{2\sigma^4}{n} \end{pmatrix}\right)$.

9.3 MLE: The Case of Multiple Regression Model II

1. Regression model: $y = X\beta + u$, $u \sim N(0, \sigma^2\Omega)$

Transformation of Variables from u to y :

$$f_u(u) = (2\pi\sigma^2)^{-n/2} |\Omega|^{-1/2} \exp\left(-\frac{1}{2\sigma^2} u' \Omega^{-1} u\right)$$

$$f_y(y) = f_u(y - X\beta) \left| \frac{\partial u}{\partial y'} \right|$$

$$\begin{aligned}
&= (2\pi\sigma^2)^{-n/2} |\Omega|^{-1/2} \exp\left(-\frac{1}{2\sigma^2} (y - X\beta)' \Omega^{-1} (y - X\beta)\right) \\
&= L(\theta; y, X),
\end{aligned}$$

where $\theta = (\beta, \sigma^2)$, because of $\frac{\partial u}{\partial y'} = I_n$.

The log-likelihood function is:

$$\log L(\theta; y, X) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2} \log |\Omega| - \frac{1}{2\sigma^2} (y - X\beta)' \Omega^{-1} (y - X\beta),$$

where $\theta = (\beta, \sigma^2)$.

$$2. \quad \max_{\theta} \log L(\theta; y, X)$$

$$\text{(FOC)} \quad \frac{\partial \log L(\theta; y, X)}{\partial \theta} = 0$$

$$\text{(SOC)} \quad \frac{\partial^2 \log L(\theta; y, X)}{\partial \theta \partial \theta'}$$
 is a negative definite matrix.

Then, we obtain MLE of β and σ^2 :

$$\tilde{\beta} = (X'\Omega^{-1}X)^{-1}X'\Omega^{-1}y, \quad \tilde{\sigma}^2 = \frac{(y - X\tilde{\beta})'\Omega^{-1}(y - X\tilde{\beta})}{n}$$

3. Fisher's information matrix is defined as:

$$I(\theta) = -E\left(\frac{\partial^2 \log L(\theta; y, X)}{\partial \theta \partial \theta'}\right)$$

The inverse of the information matrix, $I(\theta)^{-1}$, provides a lower bound of the variance - covariance matrix for unbiased estimators of θ , which is given by:

$$I(\theta)^{-1} = \begin{pmatrix} \sigma^2(X'\Omega^{-1}X)^{-1} & 0 \\ 0 & \frac{2\sigma^4}{n} \end{pmatrix}$$