Proof of the above equality:

$$\int L(\theta; x) \mathrm{d}x = 1$$

Take a derivative with respect to θ.

$$\int \frac{\partial L(\theta; x)}{\partial \theta} \mathrm{d}x = 0$$

(We assume that (i) the domain of x does not depend on θ and (ii) the derivative $\dfrac{\partial L(\theta; x)}{\partial \theta}$ exists.)

Rewriting the above equation, we obtain:

$$\int \frac{\partial \log L(\theta; x)}{\partial \theta} L(\theta; x) \mathrm{d}x = 0,$$

i.e.,

$$\mathrm{E}\left(\frac{\partial \log L(\theta; X)}{\partial \theta}\right) = 0.$$

Again, differentiating the above with respect to θ, we obtain:

$$\int \frac{\partial^2 \log L(\theta; x)}{\partial\theta\partial\theta'} L(\theta; x)\mathrm{d}x + \int \frac{\partial \log L(\theta; x)}{\partial\theta} \frac{\partial L(\theta; x)}{\partial'\theta}\mathrm{d}x$$
$$= \int \frac{\partial^2 \log L(\theta; x)}{\partial\theta\partial\theta'} L(\theta; x)\mathrm{d}x + \int \frac{\partial \log L(\theta; x)}{\partial\theta} \frac{\partial \log L(\theta; x)}{\partial\theta'} L(\theta; x)\mathrm{d}x$$
$$= \mathrm{E}\Big(\frac{\partial^2 \log L(\theta; X)}{\partial\theta\partial\theta'}\Big) + \mathrm{E}\Big(\frac{\partial \log L(\theta; X)}{\partial\theta} \frac{\partial \log L(\theta; X)}{\partial\theta'}\Big) = 0.$$

Therefore, we can derive the following equality:

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

where the second equality utilizes $\mathrm{E}\left(\frac{\partial \log L(\theta; X)}{\partial\theta}\right) = 0$.

3. **Cramer-Rao Lower Bound (**クラメール・ラオの下限**)**: $(I(\theta))^{-1}$

Suppose that an estimator of θ is given by $s(X)$.

The expectation of $s(X)$ is:

$$\mathrm{E}(s(X)) = \int s(x) L(\theta; x) \mathrm{d}x.$$

Differentiating the above with respect to θ,

$$\begin{aligned}\frac{\partial \mathrm{E}(s(X))}{\partial \theta} &= \int s(x) \frac{\partial L(\theta; x)}{\partial \theta} \mathrm{d}x = \int s(x) \frac{\partial \log L(\theta; x)}{\partial \theta} L(\theta; x) \mathrm{d}x \\ &= \mathrm{Cov}\left(s(X), \frac{\partial \log L(\theta; X)}{\partial \theta} \right)\end{aligned}$$

For simplicity, let $s(X)$ and θ be scalars.

Then,

$$\begin{aligned}\left(\frac{\partial \mathrm{E}(s(X))}{\partial \theta} \right)^2 &= \left(\mathrm{Cov}\left(s(X), \frac{\partial \log L(\theta; X)}{\partial \theta} \right) \right)^2 = \rho^2 \mathrm{V}\left(s(X) \right) \mathrm{V}\left(\frac{\partial \log L(\theta; X)}{\partial \theta} \right) \\ &\leq \mathrm{V}\left(s(X) \right) \mathrm{V}\left(\frac{\partial \log L(\theta; X)}{\partial \theta} \right),\end{aligned}$$

where ρ denotes the correlation coefficient between $s(X)$ and $\dfrac{\partial \log L(\theta; X)}{\partial \theta}$, i.e.,

$$\rho = \frac{\mathrm{Cov}\left(s(X), \dfrac{\partial \log L(\theta; X)}{\partial \theta}\right)}{\sqrt{\mathrm{V}\left(s(X)\right)}\sqrt{\mathrm{V}\left(\dfrac{\partial \log L(\theta; X)}{\partial \theta}\right)}}.$$

Note that $|\rho| \leq 1$.

Therefore, we have the following inequality:

$$\left(\frac{\partial \mathrm{E}(s(X))}{\partial \theta}\right)^2 \leq \mathrm{V}(s(X))\,\mathrm{V}\left(\frac{\partial \log L(\theta; X)}{\partial \theta}\right),$$

i.e.,

$$\mathrm{V}(s(X)) \geq \frac{\left(\dfrac{\partial \mathrm{E}(s(X))}{\partial \theta}\right)^2}{\mathrm{V}\left(\dfrac{\partial \log L(\theta; X)}{\partial \theta}\right)}$$

Especially, when $\mathrm{E}(s(X)) = \theta$,

$$\mathrm{V}(s(X)) \geq \frac{1}{-\mathrm{E}\left(\dfrac{\partial^2 \log L(\theta; X)}{\partial \theta^2}\right)} = (I(\theta))^{-1}.$$

Even in the case where $s(X)$ is a vector, the following inequality holds.

$$\mathrm{V}(s(X)) \geq (I(\theta))^{-1},$$

where $I(\theta)$ is defined as:

$$\begin{aligned} I(\theta) &= -\mathrm{E}\left(\frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'}\right) \\ &= \mathrm{E}\left(\frac{\partial \log L(\theta; X)}{\partial \theta} \frac{\partial \log L(\theta; X)}{\partial \theta'}\right) = \mathrm{V}\left(\frac{\partial \log L(\theta; X)}{\partial \theta}\right). \end{aligned}$$

The variance of any unbiased estimator of θ is larger than or equal to $(I(\theta))^{-1}$.

4. Asymptotic Normality of MLE:

Let $\tilde{\theta}$ be MLE of θ.

As n goes to infinity, we have the following result:

$$\sqrt{n}(\tilde{\theta} - \theta) \longrightarrow N\left(0, \lim_{n\to\infty}\left(\frac{I(\theta)}{n}\right)^{-1}\right),$$

where it is assumed that $\lim_{n\to\infty}\left(\frac{I(\theta)}{n}\right)$ converges.

That is, when n is large, $\tilde{\theta}$ is approximately distributed as follows:

$$\tilde{\theta} \sim N\left(\theta, (I(\theta))^{-1}\right).$$

Suppose that $s(X) = \tilde{\theta}$.

When n is large, $\mathrm{V}(s(X))$ is approximately equal to $(I(\theta))^{-1}$.

5. **Optimization (最適化):**

MLE of θ results in the following maximization problem:

$$\max_{\theta} \quad \log L(\theta; x).$$

We often have the case where the solution of θ is not derived in closed form.

$\Longrightarrow$ Optimization procedure

$$0 = \frac{\partial \log L(\theta; x)}{\partial \theta} = \frac{\partial \log L(\theta^*; x)}{\partial \theta} + \frac{\partial^2 \log L(\theta^*; x)}{\partial \theta \partial \theta'}(\theta - \theta^*).$$

Solving the above equation with respect to θ, we obtain the following:

$$\theta = \theta^* - \left(\frac{\partial^2 \log L(\theta^*; x)}{\partial \theta \partial \theta'}\right)^{-1} \frac{\partial \log L(\theta^*; x)}{\partial \theta}.$$

Replace the variables as follows:

$$\theta \longrightarrow \theta^{(i+1)}$$

$$\theta^* \longrightarrow \theta^{(i)}$$

Then, we have:

$$\theta^{(i+1)} = \theta^{(i)} - \left(\frac{\partial^2 \log L(\theta^{(i)}; x)}{\partial\theta\partial\theta'}\right)^{-1} \frac{\partial \log L(\theta^{(i)}; x)}{\partial\theta}.$$

$\Longrightarrow$ **Newton-Raphson method (ニュートン・ラプソン法)**

Replacing $\dfrac{\partial^2 \log L(\theta^{(i)}; x)}{\partial\theta\partial\theta'}$ by $\mathrm{E}\left(\dfrac{\partial^2 \log L(\theta^{(i)}; x)}{\partial\theta\partial\theta'}\right)$, we obtain the following optimization algorithm:

$$\begin{aligned}
\theta^{(i+1)} &= \theta^{(i)} - \left(\mathrm{E}\left(\frac{\partial^2 \log L(\theta^{(i)}; x)}{\partial\theta\partial\theta'}\right)\right)^{-1} \frac{\partial \log L(\theta^{(i)}; x)}{\partial\theta} \\
&= \theta^{(i)} + \left(I(\theta^{(i)})\right)^{-1} \frac{\partial \log L(\theta^{(i)}; x)}{\partial\theta}
\end{aligned}$$

$\Longrightarrow$ **Method of Scoring (スコア法)**

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

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

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

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

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

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

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

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:

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

In the case where X and $g(Y)$ are $n \times 1$ vectors, $\left| \frac{\mathrm{d}g(y)}{\mathrm{d}y} \right|$ 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:

$$f_y(y) = \left|\frac{\mathrm{d}x}{\mathrm{d}y}\right| f_x(g(y)) = |-\exp(-y)| = \exp(-y)$$

5. Given the observed data $y_1, y_2, \cdots, y_n$, the likelihood function $L(\beta_1,\ \beta_2,\ \sigma^2|y_1,\ y_2,\ \cdots,\ y_n)$, or the log-likelihood function $\log L(\beta_1,\ \beta_2,\ \sigma^2|y_1,\ y_2,\ \cdots,\ y_n)$ is maximized with respect to $(\beta_1, \beta_2, \sigma^2)$.

Solve the following three simultaneous equations:

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

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

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

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:

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

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:

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

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

   Transformation of Variables from u to y:

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

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

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

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

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

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

We obtain MLE of β and σ^2:

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

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

4. Fisher's information matrix is:

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

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

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

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