

2 Maximum Likelihood Estimation (MLE, 最尤法) — More Formally Review

1. We have random variables X_1, X_2, \dots, X_n , which are assumed to be mutually independently and identically distributed.
2. The distribution function of $\{X_i\}_{i=1}^n$ is $f(x; \theta)$, where $x = (x_1, x_2, \dots, x_n)$ and $\theta = (\mu, \Sigma)$.

Note that X is a vector of random variables and x is a vector of their realizations (i.e., observed data).

Likelihood function $L(\cdot)$ is defined as $L(\theta; x) = f(x; \theta)$.

Note that $f(x; \theta) = \prod_{i=1}^n f(x_i; \theta)$ when X_1, X_2, \dots, X_n are mutually independent.

dently and identically distributed.

The maximum likelihood estimator (MLE) of θ is θ such that:

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

MLE satisfies the following two conditions:

- (a) $\frac{\partial \log L(\theta; X)}{\partial \theta} = 0.$
- (b) $\frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'}$ is a negative definite matrix.

3. **Fisher's information matrix** (フィッシャーの情報行列) is defined as:

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

where we have the following equality:

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

Proof of the above equality:

$$\int L(\theta; x)dx = 1$$

Take a derivative with respect to θ .

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

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

Rewriting the above equation, we obtain:

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

i.e.,

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

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

$$\begin{aligned}
 & \int \frac{\partial^2 \log L(\theta; x)}{\partial \theta \partial \theta'} L(\theta; x) dx + \int \frac{\partial \log L(\theta; x)}{\partial \theta} \frac{\partial L(\theta; x)}{\partial \theta'} dx \\
 &= \int \frac{\partial^2 \log L(\theta; x)}{\partial \theta \partial \theta'} L(\theta; x) dx + \int \frac{\partial \log L(\theta; x)}{\partial \theta} \frac{\partial \log L(\theta; x)}{\partial \theta'} L(\theta; x) dx \\
 &= \mathbb{E}\left(\frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'}\right) + \mathbb{E}\left(\frac{\partial \log L(\theta; X)}{\partial \theta} \frac{\partial \log L(\theta; X)}{\partial \theta'}\right) = 0.
 \end{aligned}$$

Therefore, we can derive the following equality:

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

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

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

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

Then, we have the following:

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

Proof:

The expectation of $s(X)$ is:

$$E(s(X)) = \int s(x)L(\theta; x)dx.$$

Differentiating the above with respect to θ ,

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

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

Then,

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

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

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

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

Therefore, we have the following inequality:

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

i.e.,

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

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

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

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

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

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

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

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

5. Asymptotic Normality of MLE:

Let $\tilde{\theta}$ be MLE of θ .

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

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

where it is assumed that $\lim_{n \rightarrow \infty} \left(\frac{I(\theta)}{n}\right)$ 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, $V(s(X))$ is approximately equal to $(I(\theta))^{-1}$.

Practically, we utilize the following approximated distribution:

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

Then, we can obtain the significance test and the confidence interval for θ

6. **Central Limit Theorem:** Let X_1, X_2, \dots, X_n be mutually independently distributed random variables with mean $E(X_i) = \mu$ and variance $V(X_i) = \sigma^2 < \infty$ for $i = 1, 2, \dots, n$.

Define $\bar{X} = (1/n) \sum_{i=1}^n X_i$.

Then, the central limit theorem is given by:

$$\frac{\bar{X} - E(\bar{X})}{\sqrt{V(\bar{X})}} = \frac{\bar{X} - \mu}{\sigma / \sqrt{n}} \rightarrow N(0, 1).$$

Note that $E(\bar{X}) = \mu$ and $V(\bar{X}) = \sigma^2/n$.

That is,

$$\sqrt{n}(\bar{X} - \mu) = \frac{1}{\sqrt{n}} \sum_{i=1}^n (X_i - \mu) \longrightarrow N(0, \sigma^2).$$

Note that $E(\bar{X}) = \mu$ and $nV(\bar{X}) = \sigma^2$.

In the case where X_i is a vector of random variable with mean μ and variance $\Sigma < \infty$, the central limit theorem is given by:

$$\sqrt{n}(\bar{X} - \mu) = \frac{1}{\sqrt{n}} \sum_{i=1}^n (X_i - \mu) \longrightarrow N(0, \Sigma).$$

Note that $E(\bar{X}) = \mu$ and $nV(\bar{X}) = \Sigma$.

7. **Central Limit Theorem II:** Let X_1, X_2, \dots, X_n be mutually independently distributed random variables with mean $E(X_i) = \mu$ and variance $V(X_i) = \sigma_i^2$ for $i = 1, 2, \dots, n$.

Assume:

$$\sigma^2 = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \sigma_i^2 < \infty.$$

Define $\bar{X} = (1/n) \sum_{i=1}^n X_i$.

Then, the central limit theorem is given by:

$$\frac{\bar{X} - E(\bar{X})}{\sqrt{V(\bar{X})}} = \frac{\bar{X} - \mu}{\sigma / \sqrt{n}} \longrightarrow N(0, 1),$$

i.e.,

$$\sqrt{n}(\bar{X} - \mu) = \frac{1}{\sqrt{n}} \sum_{i=1}^n (X_i - \mu) \longrightarrow N(0, \sigma^2).$$

Note that $E(\bar{X}) = \mu$ and $nV(\bar{X}) \longrightarrow \sigma^2$.

In the case where X_i is a vector of random variable with mean μ and variance Σ_i , the central limit theorem is given by:

$$\sqrt{n}(\bar{X} - \mu) = \frac{1}{\sqrt{n}} \sum_{i=1}^n (X_i - \mu) \longrightarrow N(0, \Sigma),$$

where $\Sigma = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \Sigma_i < \infty$.

Note that $E(\bar{X}) = \mu$ and $nV(\bar{X}) \longrightarrow \Sigma$.

[Review of Asymptotic Theories]

- **Convergence in Probability** (確率収束) $X_n \longrightarrow a$, i.e., X converges in probability to a , where a is a fixed number.

- **Convergence in Distribution** (分布収束) $X_n \rightarrow X$, i.e., X converges in distribution to X . The distribution of X_n converges to the distribution of X as n goes to infinity.

Some Formulas

X_n and Y_n : Convergence in Probability

Z_n : Convergence in Distribution

- If $X_n \rightarrow a$, then $f(X_n) \rightarrow f(a)$.
- If $X_n \rightarrow a$ and $Y_n \rightarrow b$, then $f(X_n Y_n) \rightarrow f(ab)$.
- If $X_n \rightarrow a$ and $Z_n \rightarrow Z$, then $X_n Z_n \rightarrow aZ$, i.e., aZ is distributed with mean $E(aZ) = aE(Z)$ and variance $V(aZ) = a^2V(Z)$.

[End of Review]

8. **Weak Law of Large Numbers** (大数の弱法則) — **Review:**

n random variables X_1, X_2, \dots, X_n are assumed to be mutually independently and identically distributed, where $E(X_i) = \mu$ and $V(X_i) = \sigma^2 < \infty$.

Then, $\bar{X} \rightarrow \mu$ as $n \rightarrow \infty$, which is called the **weak law of large numbers**.

→ Convergence in probability

→ Proved by Chebyshev's inequality

9. **Some Formulas of Expectation and Variance in Multivariate Cases**

— **Review:**

A vector of random variable X : $E(X) = \mu$ and $V(X) \equiv E((X - \mu)(X - \mu)') = \Sigma$

Then, $E(AX) = A\mu$ and $V(AX) = A\Sigma A'$.

Proof:

$$E(AX) = AE(X) = A\mu$$

$$\begin{aligned} V(AX) &= E((AX - A\mu)(AX - A\mu)') = E(A(X - \mu)(A(X - \mu))') \\ &= E(A(X - \mu)(X - \mu)'A') = AE((X - \mu)(X - \mu)')A' = AV(X)A' = A\Sigma A' \end{aligned}$$

10. Asymptotic Normality of MLE — Proof:

The density (or probability) function of X_i is given by $f(x_i; \theta)$.

The likelihood function is: $L(\theta; x) \equiv f(x; \theta) = \prod_{i=1}^n f(x_i; \theta)$,

where $x = (x_1, x_2, \dots, x_n)$.

MLE of θ results in the following maximization problem:

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

A solution of the above problem is given by MLE of θ , denoted by $\tilde{\theta}$.

That is, $\tilde{\theta}$ is given by the θ which satisfies the following equation:

$$\frac{\partial \log L(\theta; x)}{\partial \theta} = \sum_{i=1}^n \frac{\partial \log f(x_i; \theta)}{\partial \theta} = 0.$$

Replacing x_i by the underlying random variable X_i , $\frac{\partial \log f(X_i; \theta)}{\partial \theta}$ is taken as the i th random variable, i.e., X_i in the **Central Limit Theorem II**.

Consider applying **Central Limit Theorem II** as follows:

$$\frac{\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} - E\left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}\right)}{\sqrt{V\left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}\right)}} = \frac{\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta} - E\left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta}\right)}{\sqrt{V\left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta}\right)}}.$$

Note that

$$\sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} = \frac{\partial \log L(\theta; X)}{\partial \theta}$$

In this case, we need the following expectation and variance:

$$\mathbb{E}\left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}\right) = \mathbb{E}\left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta}\right) = 0,$$

and

$$\mathbb{V}\left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}\right) = \mathbb{V}\left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta}\right) = \frac{1}{n^2} I(\theta).$$

Note that $\mathbb{E}\left(\frac{\partial \log L(\theta; X)}{\partial \theta}\right) = 0$ and $\mathbb{V}\left(\frac{\partial \log L(\theta; X)}{\partial \theta}\right) = I(\theta)$.

Thus, the asymptotic distribution of

$$\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta} = \frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}$$

is given by:

$$\begin{aligned} & \sqrt{n} \left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} - \mathbb{E} \left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} \right) \right) \\ &= \sqrt{n} \left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta} - \mathbb{E} \left(\frac{1}{n} \frac{\partial \log L(\theta; X)}{\partial \theta} \right) \right) \\ &= \frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta} \longrightarrow N(0, \Sigma) \end{aligned}$$

where

$$\begin{aligned} n \mathbb{V} \left(\frac{1}{n} \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} \right) &= \frac{1}{n} \mathbb{V} \left(\sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta} \right) = \frac{1}{n} \mathbb{V} \left(\frac{\partial \log L(\theta; X)}{\partial \theta} \right) \\ &= \frac{1}{n} I(\theta) \longrightarrow \Sigma. \end{aligned}$$

That is,

$$\frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta} \longrightarrow N(0, \Sigma),$$

where $X = (X_1, X_2, \dots, X_n)$.

Now, replacing θ by $\tilde{\theta}$, consider the asymptotic distribution of

$$\frac{1}{\sqrt{n}} \frac{\partial \log L(\tilde{\theta}; X)}{\partial \theta},$$

which is expanded around $\tilde{\theta} = \theta$ as follows:

$$0 = \frac{1}{\sqrt{n}} \frac{\partial \log L(\tilde{\theta}; X)}{\partial \theta} \approx \frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta} + \frac{1}{\sqrt{n}} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} (\tilde{\theta} - \theta).$$

Therefore,

$$-\frac{1}{\sqrt{n}} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} (\tilde{\theta} - \theta) \approx \frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta} \longrightarrow N(0, \Sigma).$$

The left-hand side is rewritten as:

$$-\frac{1}{\sqrt{n}} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} (\tilde{\theta} - \theta) = \sqrt{n} \left(-\frac{1}{n} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} \right) (\tilde{\theta} - \theta).$$

Then,

$$\begin{aligned} \sqrt{n}(\tilde{\theta} - \theta) &\approx \left(-\frac{1}{n} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} \right)^{-1} \left(\frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta} \right) \\ &\longrightarrow N(0, \Sigma^{-1} \Sigma \Sigma^{-1}) = N(0, \Sigma^{-1}). \end{aligned}$$

Using the law of large number, note that

$$\begin{aligned} -\frac{1}{n} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} &\longrightarrow \lim_{n \rightarrow \infty} \frac{1}{n} \left(-\mathbb{E} \left(\frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'} \right) \right) \\ &= \lim_{n \rightarrow \infty} \frac{1}{n} \left(\mathbb{V} \left(\frac{\partial \log L(\theta; X)}{\partial \theta} \right) \right) = \lim_{n \rightarrow \infty} \frac{1}{n} I(\theta) = \Sigma, \end{aligned}$$

and $\left(\frac{1}{n} \frac{\partial^2 \log L(\theta; X)}{\partial \theta \partial \theta'}\right)^{-1} \left(\frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta}\right)$ has the same asymptotic distribution as $\Sigma^{-1} \left(\frac{1}{\sqrt{n}} \frac{\partial \log L(\theta; X)}{\partial \theta}\right)$.

11. Optimization (最適化):

MLE of θ results in the following maximization problem:

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

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

⇒ 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:

$$\theta \longrightarrow \theta^{(i+1)}, \quad \theta^* \longrightarrow \theta^{(i)}.$$

Then, we have:

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

⇒ Newton-Raphson method (ニュートン・ラフソン法)

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

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

⇒ Method of Scoring (スコア法)