

which is called GLS (Generalized Least Squares) estimator.

b is rewritten as follows:

$$b = \beta + (X^{\star\prime} X^{\star})^{-1} X^{\star\prime} u^{\star} = \beta + (X' \Omega^{-1} X)^{-1} X' \Omega^{-1} u$$

The mean and variance of b are given by:

$$E(b) = \beta,$$

$$V(b) = \sigma^2 (X^{\star\prime} X^{\star})^{-1} = \sigma^2 (X' \Omega^{-1} X)^{-1}.$$

6. Suppose that the regression model is given by:

$$y = X\beta + u, \quad u \sim N(0, \sigma^2 \Omega).$$

In this case, when we use OLS, what happens?

$$\hat{\beta} = (X'X)^{-1} X'y = \beta + (X'X)^{-1} X'u$$

$$V(\hat{\beta}) = \sigma^2(X'X)^{-1}X'\Omega X(X'X)^{-1}$$

Compare GLS and OLS.

(a) Expectation:

$$E(\hat{\beta}) = \beta, \quad \text{and} \quad E(b) = \beta$$

Thus, both $\hat{\beta}$ and b are unbiased estimator.

(b) Variance:

$$V(\hat{\beta}) = \sigma^2(X'X)^{-1}X'\Omega X(X'X)^{-1}$$

$$V(b) = \sigma^2(X'\Omega^{-1}X)^{-1}$$

Which is more efficient, OLS or GLS?.

$$\begin{aligned}
V(\hat{\beta}) - V(b) &= \sigma^2(X'X)^{-1}X'\Omega X(X'X)^{-1} - \sigma^2(X'\Omega^{-1}X)^{-1} \\
&= \sigma^2\left((X'X)^{-1}X' - (X'\Omega^{-1}X)^{-1}X'\Omega^{-1}\right)\Omega \\
&\quad \times \left((X'X)^{-1}X' - (X'\Omega^{-1}X)^{-1}X'\Omega^{-1}\right)' \\
&= \sigma^2 A\Omega A'
\end{aligned}$$

Note that A is $k \times n$ and Ω is $n \times n$.

Ω is the variance-covariance matrix of u , which is a positive definite matrix.

Therefore, except for $\Omega = I_n$, $A\Omega A'$ is also a positive definite matrix.

(From $\Omega = PP'$ and $A\Omega A' = AP(AP)'$, we have $xAP(xAP)' = \sum_{i=1}^k z_i^2 > 0$ for $x \neq 0$, where x is $1 \times k$, $z = xAP$ is $1 \times k$ and $z = (z_1, z_2, \dots, z_k)$.)

This implies that $V(\hat{\beta}_i) - V(b_i) > 0$ for the i th element of β .

Accordingly, b is more efficient than $\hat{\beta}$.

7. If $u \sim N(0, \sigma^2 \Omega)$, then $b \sim N(\beta, \sigma^2 (X' \Omega^{-1} X)^{-1})$.

Consider testing the hypothesis $H_0 : R\beta = r$.

$$R : G \times k, \quad \text{rank}(R) = G \leq k.$$

$$Rb \sim N(R\beta, \sigma^2 R(X' \Omega^{-1} X)^{-1} R').$$

Therefore, the following quadratic form is distributed as:

$$\frac{(Rb - r)'(R(X' \Omega^{-1} X)^{-1} R')^{-1}(Rb - r)}{\sigma^2} \sim \chi^2(G)$$

8. Because $(y^* - X^* b)'(y^* - X^* b)/\sigma^2 \sim \chi^2(n - k)$, we obtain:

$$\frac{(y - Xb)' \Omega^{-1} (y - Xb)}{\sigma^2} \sim \chi^2(n - k)$$

9. Furthermore, from the fact that b is independent of $y - Xb$, the following F distribution can be derived:

$$\frac{(Rb - r)'(R(X'\Omega^{-1}X)^{-1}R')^{-1}(Rb - r)/G}{(y - Xb)'\Omega^{-1}(y - Xb)/(n - k)} \sim F(G, n - k)$$

10. Let b be the unrestricted GLSE and $\tilde{b}$ be the restricted GLSE.

Their residuals are given by e and $\tilde{u}$, respectively.

$$e = y - Xb, \quad \tilde{u} = y - X\tilde{b}$$

Then, the F test statistic is written as follows:

$$\frac{(\tilde{u}'\Omega^{-1}\tilde{u} - e'\Omega^{-1}e)/G}{e'\Omega^{-1}e/(n - k)} \sim F(G, n - k)$$

8.1 Example: Mixed Estimation (Theil and Goldberger Model)

A generalization of the restricted OLS $\implies$ Stochastic linear restriction:

$$r = R\beta + v, \quad E(v) = 0 \text{ and } V(v) = \sigma^2\Psi$$

$$y = X\beta + u, \quad E(u) = 0 \text{ and } V(u) = \sigma^2 I_n$$

Using a matrix form,

$$\begin{pmatrix} y \\ r \end{pmatrix} = \begin{pmatrix} X \\ R \end{pmatrix} \beta + \begin{pmatrix} u \\ v \end{pmatrix}, \quad E \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ and } V \begin{pmatrix} u \\ v \end{pmatrix} = \sigma^2 \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}$$

For estimation, we do not need normality assumption.

Applying GLS, we obtain:

$$\begin{aligned} b &= \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} X \\ R \end{pmatrix} \right)^{-1} \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} y \\ r \end{pmatrix} \right) \\ &= (X'X + R'\Psi^{-1}R)^{-1} (X'y + R'\Psi^{-1}r). \end{aligned}$$

Mean and Variance of b : b is rewritten as follows:

$$\begin{aligned} b &= \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} X \\ R \end{pmatrix} \right)^{-1} \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} y \\ r \end{pmatrix} \right) \\ &= \beta + \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} X \\ R \end{pmatrix} \right)^{-1} \begin{pmatrix} u \\ v \end{pmatrix} \end{aligned}$$

Therefore, the mean and variance are given by:

$$E(b) = \beta \quad \implies \quad b \text{ is unbiased.}$$

$$\begin{aligned} V(b) &= \sigma^2 \left((X' \quad R') \begin{pmatrix} I_n & 0 \\ 0 & \Psi \end{pmatrix}^{-1} \begin{pmatrix} X \\ R \end{pmatrix} \right)^{-1} \\ &= \sigma^2 (X'X + R'\Psi^{-1}R)^{-1} \end{aligned}$$

9 Maximum Likelihood Estimation (MLE, 最尤法^{さいゆうほう})

→ Review

1. The distribution function of $\{X_i\}_{i=1}^n$ is $f(x; \theta)$, where $x = (x_1, x_2, \dots, x_n)$.

θ is a vector or matrix of unknown parameters, e.g., $\theta = (\mu, \Sigma)$, where $\mu = E(X_i)$ and $\Sigma = V(X_i)$.

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 independently and identically distributed.

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

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

Thus, MLE satisfies the following two conditions:

- (a) $\frac{\partial \log L(\theta; x)}{\partial \theta} = 0. \implies$ Solution of θ : $\tilde{\theta} = \tilde{\theta}(x)$
- (b) $\frac{\partial^2 \log L(\theta; x)}{\partial \theta \partial \theta'}$ is a negative definite matrix.

2. $x = (x_1, x_2, \dots, x_n)$ are used as the observations (i.e., observed data).

$X = (X_1, X_2, \dots, X_n)$ denote the random variables associated with the joint distribution $f(x; \theta) = \prod_{i=1}^n f(x_i; \theta)$.

3. Replacing x by X , we obtain the maximum likelihood **estimator** (MLE, which is the same word as the maximum likelihood **estimate**).

That is, MLE of θ satisfies the following two conditions:

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

4. **Fisher's information matrix** (フィッシャーの情報行列) or simply **information matrix**, denoted by $I(\theta)$, is given by:

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

where we have the following equality:

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

Note that $E(\cdot)$ and $V(\cdot)$ are expected with respect to X .

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.)

(*) Differentiation of Composite Functions (合成関数の微分) or Chain rule (連鎖律):

$$\frac{\partial \log L(\theta; x)}{\partial \theta} = \frac{\partial \log L(\theta; x)}{\partial L(\theta; x)} \frac{\partial L(\theta; x)}{\partial \theta} = \frac{1}{L(\theta; x)} \frac{\partial L(\theta; x)}{\partial \theta}$$

i.e.,

$$\frac{\partial L(\theta; x)}{\partial \theta} = \frac{\partial \log L(\theta; x)}{\partial \theta} L(\theta; x)$$

Rewriting the above equation, we obtain:

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

i.e.,

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

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

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

Therefore, we can derive the following equality:

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

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

5. **Cramer-Rao inequality (クラメール・ラオの不等式)** is given by:

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

where $s(X)$ denotes an unbiased estimator of θ .

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

Proof:

The expectation of $s(X)$ is:

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

Differentiating the above with respect to θ ,

$$\frac{\partial E(s(X))}{\partial \theta} = \int s(x) \frac{\partial L(\theta; x)}{\partial \theta} dx = \int s(x) \frac{\partial \log L(\theta; x)}{\partial \theta} L(\theta; x) dx$$

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

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

Then,

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

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

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

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