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:

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

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・ラプソン法)

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

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

⇒ Method of Scoring (スコア法)

2 Qualitative Dependent Variable (質的従属変数)

- 1. Discrete Choice Model (離散選択モデル)
- 2. Limited Dependent Variable Model (制限従属変数モデル)
- 3. Count Data Model (計数データモデル)

Usually, the regression model is given by:

$$y_i = X_i \beta + u_i, \qquad u_i \sim N(0, \sigma^2), \qquad i = 1, 2, \dots, n,$$

where y_i is a continuous type of random variable within the interval from $-\infty$ to ∞ .

When y_i is discrete or truncated, what happens?

2.1 Discrete Choice Model (離散選択モデル)

2.1.1 Binary Choice Model (二値選択モデル)

Example 1: Consider the regression model:

$$y_i^* = X_i \beta + u_i, \qquad u_i \sim (0, \sigma^2), \qquad i = 1, 2, \dots, n,$$

where y_i^* is unobserved, but y_i is observed as 0 or 1, i.e.,

$$y_i = \begin{cases} 1, & \text{if } y_i^* > 0, \\ 0, & \text{if } y_i^* \le 0. \end{cases}$$

Consider the probability that y_i takes 1, i.e.,

$$P(y_i = 1) = P(y_i^* > 0) = P(u_i > -X_i\beta) = P(u_i^* > -X_i\beta^*) = 1 - P(u_i^* \le -X_i\beta^*)$$
$$= 1 - F(-X_i\beta^*) = F(X_i\beta^*), \quad \text{(if the dist. of } u_i^* \text{ is symmetric.)},$$

where $u_i^* = \frac{u_i}{\sigma}$, and $\beta^* = \frac{\beta}{\sigma}$ are defined.

(*) β^* can be estimated, but β and σ^2 cannot be estimated separately (i.e., β and σ^2 are not identified).

The distribution function of u_i^* is given by $F(x) = \int_0^x f(z)dz$.

If
$$u_i^*$$
 is standard normal, i.e., $u_i^* \sim N(0, 1)$, we call **probit model**. $F(x) = \int_{-\infty}^x (2\pi)^{-1/2} \exp(-\frac{1}{2}z^2) dz$, $f(x) = (2\pi)^{-1/2} \exp(-\frac{1}{2}x^2)$.

If u_i^* is logistic, we call **logit model**.

$$F(x) = \frac{1}{1 + \exp(-x)}, \qquad f(x) = \frac{\exp(-x)}{(1 + \exp(-x))^2}.$$

We can consider the other distribution function for u_i^* .

Likelihood Function: y_i is the following Bernoulli distribution:

$$f(y_i) = (P(y_i = 1))^{y_i} (P(y_i = 0))^{1 - y_i} = (F(X_i \beta^*))^{y_i} (1 - F(X_i \beta^*))^{1 - y_i}, \qquad y_i = 0, 1.$$

[Review — Bernoulli Distribution (ベルヌイ分布)]

Suppose that X is a Bernoulli random variable. the distribution of X, denoted by f(x), is:

$$f(x) = p^{x}(1-p)^{1-x},$$
 $x = 0, 1.$

The mean and variance are:

$$\mu = E(X) = \sum_{x=0}^{1} xf(x) = 0 \times (1-p) + 1 \times p = p,$$

$$\sigma^2 = V(X) = E((X - \mu)^2) = \sum_{x=0}^{1} (x - \mu)^2 f(x) = (0 - p)^2 (1 - p) + (1 - p)^2 p = p(1 - p).$$

[End of Review]

The likelihood function is given by:

$$L(\beta^*) = f(y_1, y_2, \dots, y_n) = \prod_{i=1}^n f(y_i) = \prod_{i=1}^n (F(X_i \beta^*))^{y_i} (1 - F(X_i \beta^*))^{1-y_i},$$

The log-likelihood function is:

$$\log L(\beta^*) = \sum_{i=1}^{n} (y_i \log F(X_i \beta^*) + (1 - y_i) \log(1 - F(X_i \beta^*))),$$

Solving the maximization problem of $\log L(\beta^*)$ with respect to β^* , the first order condition is:

$$\frac{\partial \log L(\beta^*)}{\partial \beta^*} = \sum_{i=1}^n \left(\frac{y_i X_i' f(X_i \beta^*)}{F(X_i \beta^*)} - \frac{(1 - y_i) X_i' f(X_i \beta^*)}{1 - F(X_i \beta^*)} \right)
= \sum_{i=1}^n \frac{X_i' f(X_i \beta^*) (y_i - F(X_i \beta^*))}{F(X_i \beta^*) (1 - F(X_i \beta^*))} = \sum_{i=1}^n \frac{X_i' f_i (y_i - F_i)}{F_i (1 - F_i)} = 0,$$

where $f_i \equiv f(X_i\beta^*)$ and $F_i \equiv F(X_i\beta^*)$. Remember that $f(x) \equiv \frac{dF(x)}{dx}$.

The second order condition is:

$$\frac{\partial^{2} \log L(\beta^{*})}{\partial \beta^{*} \partial \beta^{*'}} = \sum_{i=1}^{n} \frac{X_{i}' \frac{\partial f_{i}}{\partial \beta^{*}} (y_{i} - F_{i})}{F_{i}(1 - F_{i})} + \sum_{i=1}^{n} \frac{X_{i}' f_{i} \frac{\partial (f_{i} - F_{i})}{\partial \beta^{*}}}{F_{i}(1 - F_{i})} + \sum_{i=1}^{n} X_{i}' f_{i} (y_{i} - F_{i}) \frac{\partial (F_{i}(1 - F_{i}))^{-1}}{\partial \beta^{*}}$$

$$= \sum_{i=1}^{n} \frac{X_{i}' X_{i} f_{i}' (y_{i} - F_{i})}{F_{i}(1 - F_{i})} - \sum_{i=1}^{n} \frac{X_{i}' X_{i} f_{i}^{2}}{F_{i}(1 - F_{i})} + \sum_{i=1}^{n} X_{i}' f_{i} (y_{i} - F_{i}) \frac{X_{i} f_{i}(1 - 2F_{i})}{(F_{i}(1 - F_{i}))^{2}}$$

is a negative definite matrix.

For maximization, the method of scoring is given by:

$$\begin{split} \beta^{*(j+1)} &= \beta^{*(j)} + \left(-\mathrm{E} \Big(\frac{\partial^2 \log L(\beta^{*(j)})}{\partial \beta^* \partial \beta^{*'}} \Big) \right)^{-1} \frac{\partial \log L(\beta^{*(j)})}{\partial \beta^*} \\ &= \beta^{*(j)} + \left(\sum_{i=1}^n \frac{X_i' X_i (f_i^{(j)})^2}{F_i^{(j)} (1 - F_i^{(j)})} \right)^{-1} \sum_{i=1}^n \frac{X_i' f_i^{(j)} (y_i - F_i^{(j)})}{F_i^{(j)} (1 - F_i^{(j)})}, \end{split}$$

where $F_i^{(j)} = F(X_i \beta^{*(j)})$ and $f_i^{(j)} = f(X_i \beta^{*(j)})$. Note that $I(\beta^*) = -\mathbb{E}\left(\frac{\partial^2 \log L(\beta^*)}{\partial \beta^* \partial \beta^{*'}}\right) = \sum_{i=1}^n \frac{X_i' X_i f_i^2}{F_i (1 - F_i)}.$

because of $E(y_i) = F_i$.

It is known that

$$\sqrt{n}(\hat{\beta}^* - \beta^*) \longrightarrow N\left(0, \lim_{n \to \infty} \left(-\frac{1}{n} \mathbb{E}\left(\frac{\partial^2 \log L(\beta^*)}{\partial \beta^* \partial \beta^{*'}}\right)\right)^{-1}\right),$$

where $\hat{\beta}^* \equiv \lim_{i \to \infty} \beta^{*(j)}$ denotes MLE of β^* .

Practically, we use the following normal distribution:

$$\hat{\beta}^* \sim N(\beta^*, I(\hat{\beta}^*)^{-1}),$$

where
$$I(\hat{\beta}^*) = -\mathbb{E}\left(\frac{\partial^2 \log L(\hat{\beta}^*)}{\partial \beta^* \partial \beta^{*'}}\right) = \sum_{i=1}^n \frac{X_i' X_i \hat{f}_i^2}{\hat{F}_i (1 - \hat{F}_i)}, \ \hat{f}_i = f(X_i \hat{\beta}^*) \text{ and } \hat{F}_i = F(X_i \hat{\beta}^*).$$

Thus, the significance test for β^* and the confidence interval for β^* can be constructed.

Another Interpretation: This maximization problem is equivalent to the nonlinear least squares estimation problem from the following regression model:

$$y_i = F(X_i \beta^*) + u_i,$$

where $u_i = y_i - F_i$ takes $u_i = 1 - F_i$ with probability $P(y_i = 1) = F(X_i\beta^*) = F_i$ and $u_i = -F_i$ with probability $P(y_i = 0) = 1 - F(X_i\beta^*) = 1 - F_i$.

Therefore, the mean and variance of u_i are:

$$E(u_i) = (1 - F_i)F_i + (-F_i)(1 - F_i) = 0,$$

$$\sigma_i^2 = V(u_i) = E(u_i^2) - (E(u_i))^2 = (1 - F_i)^2 F_i + (-F_i)^2 (1 - F_i) = F_i (1 - F_i).$$

The weighted least squares method solves the following minimization problem:

$$\min_{\beta^*} \sum_{i=1}^n \frac{(y_i - F(X_i \beta^*))^2}{\sigma_i^2}.$$

The first order condition is:

$$\sum_{i=1}^{n} \frac{X_{i}' f(X_{i} \beta^{*})(y_{i} - F(X_{i} \beta^{*}))}{\sigma_{i}^{2}} = \sum_{i=1}^{n} \frac{X_{i}' f_{i}(y_{i} - F_{i})}{F_{i}(1 - F_{i})} = 0,$$

which is equivalent to the first order condition of MLE.

Thus, the binary choice model is interpreted as the nonlinear least squares.

Prediction:
$$E(y_i) = 0 \times (1 - F_i) + 1 \times F_i = F_i \equiv F(X_i \beta^*).$$

Example 2: Consider the two utility functions: $U_{1i} = X_i \beta_1 + \epsilon_{1i}$ and $U_{2i} = X_i \beta_2 + \epsilon_{2i}$.

A linear utility function is problematic, but we consider the linear function for simplicity of discussion.

We purchase a good when $U_{1i} > U_{2i}$ and do not purchase it when $U_{1i} < U_{2i}$.

We can observe $y_i = 1$ when we purchase the good, i.e., when $U_{1i} > U_{2i}$, and $y_i = 0$ otherwise.

$$P(y_i = 1) = P(U_{1i} > U_{2i}) = P(X_i(\beta_1 - \beta_2) > -\epsilon_{1i} + \epsilon_{2i})$$

$$= P(-X_i\beta^* < \epsilon_i^*) = P(-X_i\beta^{**} < \epsilon_i^{**}) = 1 - F(-X_i\beta^{**}) = F(X_i\beta^{**})$$

where
$$\beta^* = \beta_1 - \beta_2$$
, $\epsilon_i^* = \epsilon_{1i} - \epsilon_{2i}$, $\beta^{**} = \frac{\beta^*}{\sigma^*}$ and $\epsilon_i^{**} = \frac{\epsilon_i^*}{\sigma^*}$.

We can estimate β^{**} , but we cannot estimate ϵ_i^* and σ^* , separately.

Mean and variance of ϵ_i^{**} are normalized to be zero and one, respectively.

If the distribution of ϵ_i^{**} is symmetric, the last equality holds.

We can estimate β^{**} by MLE as in Example 1.

Example 3: Consider the questionnaire:

$$y_i = \begin{cases} 1, & \text{if the } i \text{th person answers YES,} \\ 0, & \text{if the } i \text{th person answers NO.} \end{cases}$$

Consider estimating the following linear regression model:

$$y_i = X_i \beta + u_i.$$

When $E(u_i) = 0$, the expectation of y_i is given by:

$$E(y_i) = X_i \beta.$$

Because of the linear function, $X_i\beta$ takes the value from $-\infty$ to ∞ .

However, $E(y_i)$ indicates the ratio of the people who answer YES out of all the people, because of $E(y_i) = 1 \times P(y_i = 1) + 0 \times P(y_i = 0) = P(y_i = 1)$.

That is, $E(v_i)$ has to be between zero and one.

Therefore, it is not appropriate that $E(y_i)$ is approximated as $X_i\beta$.

The model is written as:

$$y_i = P(y_i = 1) + u_i,$$

where u_i is a discrete type of random variable, i.e., u_i takes $1 - P(y_i = 1)$ with probability $P(y_i = 1)$ and $-P(y_i = 1)$ with probability $1 - P(y_i = 1) = P(y_i = 0)$.

Consider that $P(y_i = 1)$ is connected with the distribution function $F(X_i\beta)$ as follows:

$$P(y_i = 1) = F(X_i\beta),$$

where $F(\cdot)$ denotes a distribution function such as normal dist., logistic dist., and so on. \longrightarrow probit model or logit model.

The probability function of y_i is:

$$f(y_i) = F(X_i\beta)^{y_i} (1 - F(X_i\beta))^{1-y_i} \equiv F_i^{y_i} (1 - F_i)^{1-y_i}, \quad y_i = 0, 1.$$

The joint distribution of y_1, y_2, \dots, y_n is:

$$f(y_1, y_2, \dots, y_n) = \prod_{i=1}^n f(y_i) = \prod_{i=1}^n F_i^{y_i} (1 - F_i)^{1 - y_i} \equiv L(\beta),$$

which corresponds to the likelihood function. --> MLE

Example 4: Ordered probit or logit model:

Consider the regression model:

$$y_i^* = X_i \beta + u_i, \qquad u_i \sim (0, 1), \qquad i = 1, 2, \dots, n,$$

where y_i^* is unobserved, but y_i is observed as $1, 2, \dots, m$, i.e.,

$$y_{i} = \begin{cases} 1, & \text{if } -\infty < y_{i}^{*} \le a_{1}, \\ 2, & \text{if } a_{1} < y_{i}^{*} \le a_{2}, \\ \vdots, & \\ m, & \text{if } a_{m-1} < y_{i}^{*} < \infty, \end{cases}$$

where a_1, a_2, \dots, a_{m-1} are assumed to be known.

Consider the probability that y_i takes 1, 2, \cdots , m, i.e.,

$$P(y_{i} = 1) = P(y_{i}^{*} \leq a_{1}) = P(u_{i} \leq a_{1} - X_{i}\beta)$$

$$= F(a_{1} - X_{i}\beta),$$

$$P(y_{i} = 2) = P(a_{1} < y_{i}^{*} \leq a_{2}) = P(a_{1} - X_{i}\beta < u_{i} \leq a_{2} - X_{i}\beta)$$

$$= F(a_{2} - X_{i}\beta) - F(a_{1} - X_{i}\beta),$$

$$P(y_{i} = 3) = P(a_{2} < y_{i}^{*} \leq a_{3}) = P(a_{2} - X_{i}\beta < u_{i} \leq a_{3} - X_{i}\beta)$$

$$= F(a_{3} - X_{i}\beta) - F(a_{2} - X_{i}\beta),$$

$$\vdots$$

$$P(y_{i} = m) = P(a_{m-1} < y_{i}^{*}) = P(a_{m-1} - X_{i}\beta < u_{i})$$

$$= 1 - F(a_{m-1} - X_{i}\beta).$$

Define the following indicator functions:

$$I_{i1} = \begin{cases} 1, & \text{if } y_i = 1, \\ 0, & \text{otherwise.} \end{cases} \qquad I_{i2} = \begin{cases} 1, & \text{if } y_i = 2, \\ 0, & \text{otherwise.} \end{cases} \qquad \cdots \qquad I_{im} = \begin{cases} 1, & \text{if } y_i = m, \\ 0, & \text{otherwise.} \end{cases}$$

More compactly,

$$P(y_i = j) = F(a_j - X_i\beta) - F(a_{j-1} - X_i\beta),$$

for $j = 1, 2, \dots, m$, where $a_0 = -\infty$ and $a_m = \infty$.

$$I_{ij} = \begin{cases} 1, & \text{if } y_i = j, \\ 0, & \text{otherwise,} \end{cases}$$

for $j = 1, 2, \dots, m$.

Then, the likelihood function is:

$$L(\beta) = \prod_{i=1}^{n} \left(F(a_1 - X_i \beta) \right)^{I_{i1}} \left(F(a_2 - X_i \beta) - F(a_1 - X_i \beta) \right)^{I_{i2}} \cdots \left(1 - F(a_{m-1} - X_i \beta) \right)^{I_{im}}$$

$$= \prod_{i=1}^{n} \prod_{j=1}^{m} \left(F(a_j - X_i \beta) - F(a_{j-1} - X_i \beta) \right)^{I_{ij}},$$

where $a_0 = -\infty$ and $a_m = \infty$. Remember that $F(-\infty) = 0$ and $F(\infty) = 1$.

The log-likelihood function is:

$$\log L(\beta) = \sum_{i=1}^{n} \sum_{j=1}^{m} I_{ij} \log (F(a_j - X_i \beta) - F(a_{j-1} - X_i \beta)).$$

The first derivative of $\log L(\beta)$ with respect to β is:

$$\frac{\partial \log L(\beta)}{\partial \beta} = \sum_{i=1}^{n} \sum_{j=1}^{m} \frac{-I_{ij}X_{i}' \Big(f(a_{j} - X_{i}\beta) - f(a_{j-1} - X_{i}\beta) \Big)}{F(a_{j} - X_{i}\beta) - F(a_{j-1} - X_{i}\beta)} = 0.$$

Usually, normal distribution or logistic distribution is chosen for $F(\cdot)$.

Example 5: Multinomial logit model:

The *i*th individual has m + 1 choices, i.e., $j = 0, 1, \dots, m$.

$$P(y_i = j) = \frac{\exp(X_i \beta_j)}{\sum_{j=0}^m \exp(X_i \beta_j)} \equiv P_{ij},$$

for $\beta_0 = 0$. The case of m = 1 corresponds to the bivariate logit model (binary choice).

Note that

$$\log \frac{P_{ij}}{P_{i0}} = X_i \beta_j$$

The log-likelihood function is:

$$\log L(\beta_1, \dots, \beta_m) = \sum_{i=1}^n \sum_{j=0}^m d_{ij} \ln P_{ij},$$

where $d_{ij} = 1$ when the *i*th individual chooses *j*th choice, and $d_{ij} = 0$ otherwise.