Maximum Likelihood Estimation

- Likelihood function and the ML principle;
- Properties of ML estimators;
- Proof of the asymptotic normality
- Estimators of the information matrix
- Regressors
- Robust covariance matrix estimation;
- Hypothesis testing.

Likelihood function and the ML principle

- Let $f(y; \theta)$ denote the *probability density function/probability function* of the random variable y, given θ. Our objective to to estimate the true parameter vector θ.

- **Example:** A Bernoulli Random variable:

$$Y = \left\{ \begin{array}{ll} 1 & \text{with probability } \theta \\ 0 & \text{with probability } 1 - \theta \end{array} \right.$$

where $\theta \in (0,1)$. Hence

$$f(y; \theta) = \mathcal{P}(Y = y | \theta) = \theta^y (1 - \theta)^{1-y}, \ y = 0, 1$$

- The *joint density* of n iid observations of y is

$$f(y_1, \ldots, y_n | \theta) = \prod_{i=1}^{n} f(y_i; \theta).$$

- If y is a discrete random variable, $f(y_1, \ldots, y_n | \theta)$ gives the probability of observing a particular sample, given θ.

Likelihood function and the ML principle

- Let us now take $f(y_i; \theta)$ as a function of θ given y and write

$$L(\theta|y_1, \ldots, y_n) = \prod_{i=1}^{n} f(y_i; \theta).$$

- This is the *likelihood function*, which gives the likelihood that the population parameter is θ, given the observed sample.

- Note: $L(\theta|y_1, \ldots, y_n)$ is often abbreviated to $L(\theta)$.

Likelihood function and the ML principle

- The *Maximum Likelihood (ML) principle* suggests that estimators of the unknown
  parameters are obtained by maximizing $L(\theta)$ with respect to θ.

$$\hat{\theta} = \arg\max_{\theta \in \Theta} L(\theta).$$

It is often convenient to work with the natural logarithm of the likelihood function $\log L(\theta)$. For example, in the iid case:

$$\log L(\theta|y_1, \ldots, y_n) = \sum_{i=1}^{n} \log f(y_i; \theta);$$

$$\hat{\theta} = \arg\max_{\theta \in \Theta} L(\theta) = \arg\max_{\theta \in \Theta} \log L(\theta)$$

Likelihood function and the ML principle

- Usually $\hat{\theta}$ can be obtained by solving the *likelihood equation*

$$\left. \frac{\partial \log L\left(\theta\right)}{\partial \theta} \right|_{\hat{\theta}} = 0$$

- **Example:** In the Bernoulli case $\mathcal{P}(Y = y|\theta) = \theta^y(1-\theta)^{1-y}$ we have

$$\log L\left(\theta\right) = \sum_{i=1}^{n} y_i \log(\theta) + \sum_{i=1}^{n} (1 - y_i) \log(1 - \theta).$$

the solution is given by $\hat{\theta} = \bar{y} = \sum_{i=1}^{n} y_i / n$.

- Occasionally the ML estimator is *not unique*.
- Also, $\log L\left(\theta\right)$ may have only one global maximum, but multiple *local maxima*.

Likelihood function and the ML principle

- The main *regularity conditions* (now assumed to hold) are as follows:

  1. The first three derivatives of $\log f(y|\theta)$ with respect to θ are continuous and finite for almost all y and for all θ;
  2. For all values of θ, $\left| \partial^3 \log f(y|\theta) / \partial \theta_j \partial \theta_k \partial \theta_l \right|$ is limited by a function that has finite expectation;
  3. The domain of y does not depend on θ;
  4. θ is an interior point to the compact parameter space Θ.

Likelihood function and the ML principle

- In order to proceed, it is interesting to look at some important results (Bartlett identities).

- Define the *score* vector $S(\theta)$ and the *Hessian* matrix $H(\theta)$ as

$$
\begin{aligned}
S(\theta) &= \frac{\partial \log L(\theta)}{\partial \theta} = \sum_{i=1}^{n} \frac{\partial \log f(y_i|\theta)}{\partial \theta} = \sum_{i=1}^{n} s_i(\theta), \\
H(\theta) &= \frac{\partial^2 \log L(\theta)}{\partial \theta \partial \theta'} = \sum_{i=1}^{n} \frac{\partial^2 \log f(y_i|\theta)}{\partial \theta \partial \theta'} = \sum_{i=1}^{n} H_i(\theta).
\end{aligned}
$$

- *First Bartlett identity*: $\mathrm{E}[s_i(\theta)] = 0$.
- Hence $\mathrm{E}[S(\theta)] = 0$
- *Second Bartlett identity:* $\mathrm{Var}[s_i(\theta)] = -\mathrm{E}[H_i(\theta)]$
- $\mathrm{Var}[s_i(\theta)] = \mathrm{E}\left[s_i(\theta) s_i(\theta)'\right]$ defines Fisher's *information matrix*, denoted $\mathcal{I}(\theta)$.
- Hence, the result $\mathrm{Var}[s_i(\theta)] = \mathrm{E}\left[s_i(\theta) s_i(\theta)'\right] = -\mathrm{E}[H_i(\theta)]$ is also called the *information matrix identity*.

Properties of MLE

- Under the assumed regularity conditions the MLE possesses the following properties:

    1. *Consistency*: plim $\hat{\theta} = \theta$;
    2. *Asymptotic normality*: $\sqrt{n}\left(\hat{\theta} - \theta\right) \xrightarrow{d} \mathcal{N}(0, \mathcal{I}(\theta)^{-1})$;
    3. *Asymptotic efficiency*: if $\tilde{\theta}$ is a regular consistent asymptotically normal estimator such that $\sqrt{n}\left(\tilde{\theta} - \theta\right) \xrightarrow{d} \mathcal{N}(0, \Omega)$, then $\Omega - [\mathcal{I}(\theta)]^{-1}$ is positive semi-definite, i.e., under these RC, the MLE asymptotically achieves the *Cramer-Rao* lower bound which is given by $[\mathcal{I}(\theta)]^{-1}$;
    4. *Invariance:* If $c\left(\theta\right)$ is a continuous and continuously differentiable one-to-one function, the MLE of $\gamma = c(\theta)$ is $c\left(\hat{\theta}\right)$.

- **Example:** in the Bernoulli case $\mathcal{I}(\theta)^{-1} = \theta(1-\theta)$, therefore $\sqrt{n}\left(\hat{\theta} - \theta\right) \xrightarrow{d} \mathcal{N}(0, \theta(1-\theta))$;

Proof of the asymptotic normality

- It is enlightening to sketch the proof of the asymptotic normality.
- Under the assumed regularity conditions, we have

$$
\frac{\partial \log L(\hat{\theta})}{\partial \theta} = 0,
$$

$$
\sum_{i=1}^{n} \frac{\partial \log f(y_i|\hat{\theta})}{\partial \theta} = 0
$$

- Expanding this result in a *1st order Taylor series* around θ we have

$$
\sum_{i=1}^{n} \frac{\partial \log f(y_i|\hat{\theta})}{\partial \theta} = \sum_{i=1}^{n} \frac{\partial \log f(y_i|\theta)}{\partial \theta} + \sum_{i=1}^{n} \frac{\partial^2 \log f(y_i|\bar{\theta})}{\partial \theta \partial \theta'} \left(\hat{\theta} - \theta \right) = 0
$$

$$
\sqrt{n} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \frac{\partial \log f(y_i|\theta)}{\partial \theta}}_{\hat{S}(\theta)} + \underbrace{\frac{1}{n} \sum_{i=1}^{n} \frac{\partial^2 \log f(y_i|\bar{\theta})}{\partial \theta \partial \theta'}}_{\hat{H}(\bar{\theta})} \sqrt{n} \left(\hat{\theta} - \theta \right) = 0
$$

where $\bar{\theta} = w\hat{\theta} + (1-w)\theta$ for $0 \leq w \leq 1$.

Proof of the asymptotic normality

- Write

$$\sqrt{n}\left(\hat{\theta} - \theta\right) = \left[-\hat{H}\left(\bar{\theta}\right)\right]^{-1} \sqrt{n}\hat{S}\left(\theta\right)$$

  Notice that, because $\text{plim}\left(\hat{\theta} - \theta\right) = 0$, and we have $\text{plim}\left(\bar{\theta} - \theta_0\right) = 0$ and (under some conditions) $\text{plim} - \hat{H}\left(\bar{\theta}\right) = \text{E}\left[-H_i\left(\theta_0\right)\right] = A$

- Now we can apply a Central Limit Theorem for random samples to obtain $\sqrt{n}\hat{S}\left(\theta\right) \xrightarrow{d} \mathcal{N}\left(0, B\right)$ where $B = \text{Var}\left[s_i\left(\theta\right)\right] = \text{E}\left[s_i(\theta_0)s_i(\theta_0)'\right]$

- Recall that if $x \sim \mathcal{N}\left(0, C\right)$ then $Dx \sim \mathcal{N}\left(0, DCD'\right)$.

- Hence

$$\sqrt{n}\left(\hat{\theta} - \theta\right) \xrightarrow{d} \mathcal{N}\left(0, A^{-1}BA^{-1}\right)$$

$$A = \text{E}\left[-H_i\left(\theta\right)\right] \qquad B = \text{E}\left[s_i(\theta)s_i(\theta)'\right]$$

- For correctly specified models, $B = \text{E}\left[-H_i\left(\theta\right)\right] = A = \mathcal{I}(\theta)$ and

$$\sqrt{n}\left(\hat{\theta} - \theta\right) \xrightarrow{d} \mathcal{N}\left(0, \mathcal{I}(\theta)^{-1}\right);$$

Estimators of the information matrix

- There are three commonly used estimators of $\mathcal{I}(\theta)$
    1. *Expected Information*: If the form of the expected values of the second derivatives of the log-likelihood function is known, then we can evaluate $\mathcal{I}(\theta)$ at $\hat{\theta}$.

    2. *Observed Information*: Simply use $-\hat{H}\left(\hat{\theta}\right)$.
    3. *Outer Product of the Gradient (OPG)*: Because of the information matrix identity, we can also use $n^{-1}\sum_{i=1}^{n} s_i\left(\hat{\theta}\right) s_i\left(\hat{\theta}\right)'$.

- The *OPG* is notorious for its poor finite sample performance.

Regressors

- The previous results are easy to extend to accommodate the presence of covariates.
- Suppose the joint distribution of y and x depends on α, giving $f(y, x|\alpha) = f(y|x, \alpha)g(x|\alpha)$.
- Next, suppose that α can be divided into θ and δ, so that (exogeneity of x) $f(y, x|\alpha) = f(y_i|x_i, \theta)g(x_i|\delta)$.
- For an iid sample $\{(y_i, x_i)\}_{i=1}^{n}$ then

$$\log L(\theta, \delta|y_i, x_i) = \sum_{i=1}^{n} \log f(y_i, x_i|\alpha) = \sum_{i=1}^{n} \log f(y_i|x_i, \theta) + \sum_{i=1}^{n} \log g(x_i|\delta).$$

and the term $\sum_{i=1}^{n} \log g(x_i|\delta)$. can be ignored

Regressors

- $\hat{\theta}$ can then be obtained by maximizing just $\sum_{i=1}^{n} \log f(y_i|x_i, \theta)$ with respect to θ. Therefore, frequently we will work directly with the conditional log-likelihood

$$\log L(\theta|y_i, x_i) = \sum_{i=1}^{n} \log f(y_i|x_i, \theta),$$

and this (under appropriate regularity conditions) will behave to a large extent like a standard log-likelihood.

- However, now $E[-H_i(\theta)] = E\left[-\frac{\partial^2 \log f(y_i|x_i,\theta)}{\partial\theta\partial\theta'}\right] = \mathcal{I}(\theta) = E\left[\frac{\partial \log f(y|x_i,\theta)}{\partial\theta} \frac{\partial \log f(y|x_i,\theta)}{\partial\theta'}\right]$, and so on.

Robust covariance matrix estimation

- If the likelihood function is misspecified, the MLE is generally inconsistent for the parameters of interest.
- However, under very general conditions, plim $\hat{\theta} = \theta^*$, where the *pseudo-true value* θ^* minimizes the Kullback-Leibler divergence, that is

$$\theta^* = \arg\min_c \int_{-\infty}^{+\infty} \left[\log \left(\frac{f_0(y)}{f(y|c)} \right) \right] f_0(y) dy = \arg\min_c E \left[\log \left(\frac{f_0(y)}{f(y|c)} \right) \right].$$

  where $f_0(y)$ is the true distribution of the data.
- The *Kullback–Leibler divergence* (also called relative entropy) is a measure of how one probability distribution is different from a second, reference probability distribution
- That is, the MLE leads to the *best approximation*, in the Kullback-Leibler sense, to $f_0(y)$, the true density.
- However, because the IM identity does not hold, the asymptotic covariance matrix is given by:

$$A^{-1}BA^{-1}, \quad A = \mathrm{E}\left[-H_i\left(\theta^*\right)\right] \qquad B = \mathrm{E}\left[g_i(\theta^*)g_i(\theta^*)'\right].$$

Hypothesis testing

- Consider a general set of restrictions to be tested

$$H_0 : h(\theta) = 0$$

  where:

- θ: vector of parameters in model
- $h(\theta)$: $d \times 1$ vector of restrictions
- $L(\theta)$: likelihood function for model
- $S(\theta) = \sum_{i=1}^{n} s_i(\theta)$ the efficient score
- $\hat{\theta}$ and $\tilde{\theta}$: <u>unrestricted</u> and <u>restricted</u> MLE, respectively (that is $\hat{\theta} = \hat{\theta}_{ml}$ and $\tilde{\theta} = \tilde{\theta}_{ml}$).
- $\hat{\theta}$ is the value of θ that maximizes $\log L(\theta)$
- $\tilde{\theta}$ is the value of θ that maximizes $\log L(\theta)$ and satisfy $h(\theta) = 0$.
- $L(\hat{\theta})$ and $L(\tilde{\theta})$: value of $L(\theta)$ evaluated at $\hat{\theta}$ and $\tilde{\theta}$, respectively.

The 3 classical test principles

Likelihood Ratio Tests:

- Compare $L(\hat{\theta})$ and $L(\tilde{\theta})$ (if $h(\theta) = 0$ then $L(\hat{\theta})$ should be close to $L(\tilde{\theta})$)
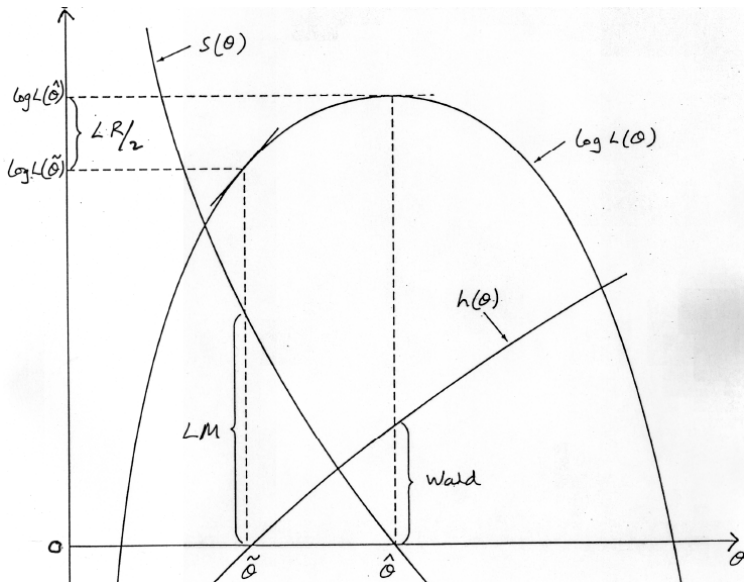
Wald Tests:

- Compare $h(\hat{\theta})$ with 0 (since $h(\tilde{\theta}) = 0$).

Lagrange Multiplier or Score Tests:

- Compare $S(\tilde{\theta})$ with 0 (since $S(\hat{\theta}) = 0$).

Intuition:

The Wald Test

- How close is $h(\hat{\theta})$ to zero (since $h(\tilde{\theta}) = 0$)?
- Test statistic:

$$\mathcal{W} = n \times h(\hat{\theta})' \left[G(\hat{\theta})' \left[\widehat{\mathcal{I}(\theta)} \right]^{-1} G(\hat{\theta}) \right]^{-1} h(\hat{\theta}).$$

where

$$G(\theta) = \frac{\partial h(\theta)}{\partial \theta}.$$

and $\widehat{\mathcal{I}(\theta)}$ is an estimator of $\mathcal{I}(\theta)$.

- Under the null hypothesis:

$$\mathcal{W} \xrightarrow{D} \chi^2(d).$$

Shortcoming: Wald test not invariant to how restrictions are formulated. E.g.: $\beta/(1-\alpha) = 1$ (<u>nonlinear</u> restriction) and $\beta + \alpha - 1 = 0$ (<u>linear</u> restriction) are equivalent restrictions, but may lead to different values of $\mathcal{W}$.
Note: If $h(\theta) = R\theta - q$, and $G(\theta) = R$.

The Likelihood Ratio Test

- How "close" are $\mathcal{L}(\hat{\theta})$ and $\mathcal{L}(\tilde{\theta})$?
- Test is based on the *likelihood ratio*:

$$\lambda = \frac{\mathcal{L}(\tilde{\theta})}{\mathcal{L}(\hat{\theta})}.$$

- Test statistic

$$\begin{aligned}
\mathcal{LR} &= -2\log(\lambda) \\
&= 2\{\log \mathcal{L}(\hat{\theta}) - \log \mathcal{L}(\tilde{\theta})\}
\end{aligned}$$

- Under the null hypothesis:

$$\mathcal{LR} \xrightarrow{D} \chi^2(d)$$

The Lagrange Multiplier (LM) or Score Test

- How close is $S(\widetilde{\theta})$ to zero (since $S(\hat{\theta}) = 0$)?
- Test statistic

$$\mathcal{LM} = S(\widetilde{\theta})' \left[\widehat{\mathcal{I}(\theta)} \right]^{-1} S(\widetilde{\theta})/n$$

- Under the null hypothesis:

$$\mathcal{LM} \xrightarrow{D} \chi^2(d).$$