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.

- 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:

$$Y = \begin{cases} 1 & \text{with probability } \theta \\ 0 & \text{with probability } 1 - \theta \end{cases}$$

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, $f(y_1, ..., y_n | \theta)$ gives the probability of observing a particular sample, given θ .

• 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 $L(\theta)$.

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

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

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

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

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

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

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

• **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 (θ) may have only one global maximum, but multiple *local maxima*.

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- The main *regularity conditions* (now assumed to hold) are as follows:
 - The first three derivatives of log f(y|θ) with respect to θ are continuous and finite for almost all y and for all θ;
 - So For all values of θ , $\left| \frac{\partial^3 \log f(y|\theta)}{\partial \theta_j \partial \theta_k \partial \theta_l} \right|$ is limited by a function that has finite expectation;
 - The domain of *y* does not depend on θ ;
 - **9** θ is an interior point to the compact parameter space Θ .

- 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

$$S(\theta) = \frac{\partial \log L(\theta)}{\partial \theta} = \sum_{i=1}^{n} \frac{\partial \log f(y_i|\theta)}{\partial \theta} = \sum_{i=1}^{n} s_i(\theta),$$

$$H(\theta) = \frac{\partial^2 \log L(\theta)}{\partial \theta \partial \theta'} = \sum_{i=1}^{n} \frac{\partial^2 \log f(y_i|\theta)}{\partial \theta \partial \theta'} = \sum_{i=1}^{n} H_i(\theta).$$

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

- Under the assumed regularity conditions the MLE possesses the following properties:
 - Consistency: plim $\hat{\theta} = \theta$;
 - Symptotic normality: $\sqrt{n} (\hat{\theta} \theta) \xrightarrow{d} \mathcal{N}(0, \mathcal{I}(\theta)^{-1});$
 - Asymptotic efficiency: if $\tilde{\theta}$ is a regular consistent asymptotically normal estimator such that $\sqrt{n} (\tilde{\theta} \theta) \xrightarrow{d} \mathcal{N}(0, \Omega)$, 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 $[\mathcal{I}(\theta)]^{-1}$;
 - **Invariance:** If $c(\theta)$ is a continuous and continuously differentiable one-to-one function, the MLE of $\gamma = c(\theta)$ is $c(\hat{\theta})$.
- **Example:** in the Bernoulli case $\mathcal{I}(\theta)^{-1} = \theta(1-\theta)$, therefore $\sqrt{n} (\hat{\theta} \theta) \xrightarrow{d} \mathcal{N}(0, \theta(1-\theta));$

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Proof of the asymptotic normality

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

$$rac{\partial \log L(\hat{ heta})}{\partial heta} = 0, \ \sum_{i=1}^n rac{\partial \log f(y_i|\hat{ heta})}{\partial heta} = 0$$

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

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

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

Proof of the asymptotic normality

• Write

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

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

- Now we can apply a Central Limit Theorem for random samples to obtain $\sqrt{n}\hat{S}(\theta) \xrightarrow{d} \mathcal{N}(0, B)$ where $B = \operatorname{Var}[s_i(\theta)] = \operatorname{E}[s_i(\theta)s_i(\theta)']$
- Recall that if $x \sim \mathcal{N}(0, C)$ then $Dx \sim \mathcal{N}(0, DCD')$.

• Hence

$$\sqrt{n} \left(\hat{\theta} - \theta \right) \xrightarrow{d} \mathcal{N} \left(0, A^{-1} B A^{-1} \right)$$
$$A = \mathbf{E} \left[-H_i \left(\theta \right) \right] \qquad B = \mathbf{E} \left[s_i(\theta) s_i(\theta)' \right]$$

• For correctly specified models, $B = E[-H_i(\theta)] = A = \mathcal{I}(\theta)$ 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 $\mathcal{I}(\theta)$
 - *Expected Information*: If the form of the expected values of the second derivatives of the log-likelihood function is known, then we can evaluate *I*(θ) at θ̂.
 - **Observed** *Information*: Simply use $-\hat{H}(\hat{\theta})$.
 - Outer Product of the Gradient (OPG): Because of the information matrix identity, we can also use $n^{-1} \sum_{i=1}^{n} s_i(\hat{\theta}) s_i(\hat{\theta})'$.
- The *OPG* is notorious for its poor finite sample performance.



- 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



• $\hat{\theta}$ 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:

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

• 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.

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

The 3 classical test principles

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

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

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 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*:

$$\lambda = rac{\mathcal{L}(ilde{ heta})}{\mathcal{L}(\hat{ heta})}.$$

Test statistic

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

• Under the null hypothesis:

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

The Lagrange Multiplier (LM) or Score Test

- How close is $S(\tilde{\theta})$ 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:

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