18.650 – Fundamentals of Statistics

3. Methods for estimation

Goals

In the kiss example, the estimator was **intuitively** the right thing to do: $\hat{p} = \bar{X}_n$.

In view of LLN, since $p = \mathbb{E}[X]$, we have $\bar{X}_n$ so $\hat{p} \approx p$ for n large enough.

If the parameter is $\theta \neq \mathbb{E}[X]$? How do we perform?

1. Maximum likelihood estimation: a generic approach with very good properties
2. Method of moments: a (fairly) generic and easy approach
3. M-estimators: a flexible approach, close to machine learning

Total variation distance

Let $\big(E, (\mathbb{P}_\theta)_{\theta\in\Theta}\big)$ be a statistical model associated with a sample of i.i.d. r.v. $X_1, \ldots, X_n$. Assume that there exists $\theta^* \in \Theta$ such that $X_1 \sim \mathbb{P}_{\theta^*}$: θ^* is the **true** parameter.

Statistician's goal: given $X_1, \ldots, X_n$, find an estimator $\hat\theta = \hat\theta(X_1, \ldots, X_n)$ such that $\mathbb{P}_{\hat\theta}$ is close to $\mathbb{P}_{\theta^*}$ for the true parameter θ^*.

This means: $\big|\mathbb{P}_{\hat\theta}(A) - \mathbb{P}_{\theta^*}(A)\big|$ is **small** for all $A \subset E$.

Definition

The *total variation distance* between two probability measures $\mathbb{P}_\theta$ and $\mathbb{P}_{\theta'}$ is defined by

$$\mathsf{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \max_{A\subset E}\big|\mathbb{P}_\theta(A) - \mathbb{P}_{\theta'}(A)\big|.$$

Total variation distance between discrete measures

Assume that E is discrete (i.e., finite or countable). This includes Bernoulli, Binomial, Poisson, ...

Therefore X has a PMF (probability mass function):
$\mathbb{P}_\theta(X = x) = p_\theta(x)$ for all $x \in E$,

$$p_\theta(x) \geq 0 \,, \quad \sum_{x \in E} p_\theta(x) = 1 \,.$$

The total variation distance between $\mathbb{P}_\theta$ and $\mathbb{P}_{\theta'}$ is a simple function of the PMF's p_θ and $p_{\theta'}$:

$$\mathsf{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \frac{1}{2} \sum_{x \in E} \left| p_\theta(x) - p_{\theta'}(x) \right| .$$

Total variation distance between continuous measures

Assume that E is continuous. This includes Gaussian, Exponential, ...

Assume that X has a density $\mathbb{P}_\theta(X \in A) = \int_A f_\theta(x)dx$ for all $A \subset E$.

$$f_\theta(x) \geq 0, \quad \int_E f_\theta(x)dx = 1\,.$$

The total variation distance between $\mathbb{P}_\theta$ and $\mathbb{P}_{\theta'}$ is a simple function of the densities f_θ and $f_{\theta'}$:

$$\mathsf{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \frac{1}{2}\int_E \big|f_\theta(x) - f_{\theta'}(x)\big|dx\,.$$

Properties of Total variation

- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \mathrm{TV}(\mathbb{P}_{\theta'}, \mathbb{P}_\theta)$ (symmetric)
- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \geq 0$ (positive)
- If $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = 0$ then $\mathbb{P}_\theta = \mathbb{P}_{\theta'}$ (definite)
- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \leq \mathrm{TV}(P_\theta, P_{\theta''}) + \mathrm{TV}(P_{\theta'}, P_{\theta''})$ (triangle inequality)

These imply that the total variation is a *distance* between probability distributions.

Exercises

Compute:

a) $\text{TV}(\text{Ber}(0.5), \text{Ber}(0.1)) =$

b) $\text{TV}(\text{Ber}(0.5), \text{Ber}(0.9)) =$

c) $\text{TV}(\text{Exp}(1), \text{Unif}[0,1]) =$

d) $\text{TV}(X, X+a) =$ 1 $\quad$ $TV(P,Q)=1$ if P, Q have disjoint support

for any $a \in (0,1)$, where $X \sim \text{Ber}(0.5)$

$\bar{X} \in \{0, \frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n}\}$ discrete

e) $\text{TV}(2\sqrt{n}(\bar{X}_n - 1/2), Z) =$ 1

where $X_i \overset{i.i.d}{\sim} \text{Ber}(0.5)$ and $Z \sim \mathcal{N}(0,1)$

An estimation strategy

Build an estimator $\widehat{\mathsf{TV}}(\mathbb{P}_\theta, \mathbb{P}_{\theta^*})$ for all $\theta \in \Theta$. Then find $\hat{\theta}$ that *minimizes* the function $\theta \mapsto \widehat{\mathsf{TV}}(\mathbb{P}_\theta, \mathbb{P}_{\theta^*})$.

problem: Unclear how to build $\widehat{\mathsf{TV}}(\mathbb{P}_\theta, \mathbb{P}_{\theta^*})$!

Kullback-Leibler (KL) divergence

There are **many** distances between probability measures to replace total variation. Let us choose one that is more convenient.

Definition

The *Kullback-Leibler*[1] *(KL) divergence* between two probability measures $\mathbb{P}_\theta$ and $\mathbb{P}_{\theta'}$ is defined by

$$\mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \begin{cases} \displaystyle\sum_{x \in E} p_\theta(x) \log\left(\frac{p_\theta(x)}{p_{\theta'}(x)}\right) & \text{if } E \text{ is discrete} \\ \displaystyle\int_E f_\theta(x) \log\left(\frac{f_\theta(x)}{f_{\theta'}(x)}\right) dx & \text{if } E \text{ is continuous} \end{cases}$$

[1] KL-divergence is also know as "relative entropy"

Properties of KL-divergence

- $\mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \neq \mathsf{KL}(\mathbb{P}_{\theta'}, \mathbb{P}_\theta)$ in general
- $\mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \geq 0$
- If $\mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = 0$ then $\mathbb{P}_\theta = \mathbb{P}_{\theta'}$ (definite)
- $\mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \not\leq \mathsf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta''}) + \mathsf{KL}(\mathbb{P}_{\theta''}, \mathbb{P}_{\theta'})$ in general

Not a distance.

This is is called a *divergence*.

Asymmetry is the key to our ability to estimate it!

Maximum likelihood estimation

Estimating the KL

$$\mathsf{KL}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta) = \mathbb{E}_{\theta^*}\left[\log\left(\frac{p_{\theta^*}(X)}{p_\theta(X)}\right)\right]$$

$$= \mathbb{E}_{\theta^*}\left[\log p_{\theta^*}(X)\right] - \mathbb{E}_{\theta^*}\left[\log p_\theta(X)\right]$$

So the function $\theta \mapsto \mathsf{KL}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta)$ is of the form:

$$\text{"constant"} - \mathbb{E}_{\theta^*}\left[\log p_\theta(X)\right]$$

Can be estimated: $\mathbb{E}_{\theta^*}[h(X)] \rightsquigarrow \frac{1}{n}\sum_{i=1}^{n} h(X_i)$ (by LLN)

$$\widehat{\mathsf{KL}}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta) = \text{"constant"} - \frac{1}{n}\sum_{i=1}^{n} \log p_\theta(X_i)$$

Maximum likelihood

$$\widehat{\mathsf{KL}}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta) = \text{“constant”} - \frac{1}{n}\sum_{i=1}^{n} \log p_\theta(X_i)$$

$$\begin{aligned}
\min_{\theta\in\Theta} \widehat{\mathsf{KL}}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta) \quad &\Leftrightarrow \quad \min_{\theta\in\Theta} -\frac{1}{n}\sum_{i=1}^{n} \log p_\theta(X_i) \\
&\Leftrightarrow \quad \max_{\theta\in\Theta} \frac{1}{n}\sum_{i=1}^{n} \log p_\theta(X_i) \\
&\Leftrightarrow \quad \max_{\theta\in\Theta} \sum_{i=1}^{n} \log p_\theta(X_i) \\
&\Leftrightarrow \quad \max_{\theta\in\Theta} \prod_{i=1}^{n} p_\theta(X_i)
\end{aligned}$$

This is the **maximum likelihood principle**.

Likelihood, Discrete case (1)

Let $\big(E, (\mathbb{P}_\theta)_{\theta\in\Theta}\big)$ be a statistical model associated with a sample of i.i.d. r.v. $X_1, \ldots, X_n$. Assume that E is discrete (i.e., finite or countable).

Definition

The *likelihood* of the model is the map L_n (or just L) defined as:

$$
\begin{array}{rccl}
L_n : & E^n \times \Theta & \to & \mathbb{R} \\
& (x_1, \ldots, x_n, \theta) & \mapsto & \mathbb{P}_\theta[X_1 = x_1, \ldots, X_n = x_n].
\end{array}
$$

$= \prod_{i=1}^{n} P(x_i|\theta)$

Likelihood for the Bernoulli model

Example 1 (Bernoulli trials): If $X_1, \dots, X_n \overset{iid}{\sim} \mathsf{Ber}(p)$ for some $p \in (0,1)$:

- $E = \{0,1\}$;
- $\Theta = (0,1)$;
- $\forall (x_1, \dots, x_n) \in \{0,1\}^n, \quad \forall p \in (0,1),$

$$
\begin{aligned}
L(x_1, \dots, x_n, p) &= \prod_{i=1}^{n} \mathbb{P}_p[X_i = x_i] \\
&= \prod_{i=1}^{n} p^{x_i}(1-p)^{1-x_i} \\
&= p^{\sum_{i=1}^n x_i}(1-p)^{n-\sum_{i=1}^n x_i}.
\end{aligned}
$$

Likelihood for the Poisson model

Example 2 (Poisson model):
If $X_1, \ldots, X_n \overset{iid}{\sim}$ Poiss(λ) for some $\lambda > 0$:

- $E = \mathbb{N}$;
- $\Theta = (0, \infty)$;
- $\forall (x_1, \ldots, x_n) \in \mathbb{N}^n, \quad \forall \lambda > 0,$

$$L(x_1, \ldots, x_n, p) = e^{-n\lambda} \frac{\lambda^{\sum_{i=1}^n x_i}}{x_1! \ldots x_n!}.$$

Likelihood, Continuous case

Let $\big(E, (\mathbb{P}_\theta)_{\theta\in\Theta}\big)$ be a statistical model associated with a sample of i.i.d. r.v. $X_1, \ldots, X_n$. Assume that all the $\mathbb{P}_\theta$ have density f_θ.

Definition

The *likelihood* of the model is the map L defined as:

$$\begin{array}{cccc} L & : & E^n \times \Theta & \to & \mathbb{R} \\ & & (x_1, \ldots, x_n, \theta) & \mapsto & \prod_{i=1}^n f_\theta(x_i). \end{array}$$

Likelihood for the Gaussian model

Example 1 (Gaussian model): If $X_1, \ldots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$, for some $\mu \in \mathbb{R}, \sigma^2 > 0$:

- $E = \mathbb{R}$;
- $\Theta = \mathbb{R} \times (0, \infty)$
- $\forall (x_1, \ldots, x_n) \in \mathbb{R}^n, \quad \forall (\mu, \sigma^2) \in \mathbb{R} \times (0, \infty)$,

$$L(x_1, \ldots, x_n, \mu, \sigma^2) = \frac{1}{(\sigma\sqrt{2\pi})^n} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^n (x_i - \mu)^2\right).$$

Exercises

Let $\left(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\right)$ be a statistical model associated with $X_1, \ldots, X_n \sim \mathsf{Exp}(\lambda)$.

a) What is E? $[0, +\infty)$

b) What is Θ? $(0, +\infty)$

c) Find the likelihood of the model.

$$L = \prod_{i=1}^{n} \lambda e^{-\lambda x_i}$$

Exercise

Let $\left(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\right)$ be a statistical model associated with $X_1, \ldots, X_n \sim$Unif$[0, b]$ for some $b > 0$.

a) What is E? $[0, +\infty)$

b) What is Θ? $[0, +\infty)$

c) Find the likelihood of the model.

$L = \left(\frac{1}{b}\right)^n$

Maximum likelihood estimator

Let $X_1, \ldots, X_n$ be an i.i.d. sample associated with a statistical model $\big(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\big)$ and let L be the corresponding likelihood.

Definition

The *maximum likelihood estimator* of θ is defined as:

$$\hat{\theta}_n^{MLE} = \underset{\theta \in \Theta}{\operatorname{argmax}} \; L(X_1, \ldots, X_n, \theta),$$

provided it exists.

Remark (log-likelihood estimator): In practice, we use the fact that

$$\hat{\theta}_n^{MLE} = \underset{\theta \in \Theta}{\operatorname{argmax}} \; \log L(X_1, \ldots, X_n, \theta).$$

Interlude: maximizing/minimizing functions

Note that

$$\min_{\theta \in \Theta} -h(\theta) \quad \Leftrightarrow \quad \max_{\theta \in \Theta} h(\theta)$$

In this class, we focus on **maximization**.

Maximization of arbitrary functions can be difficult:

Example: $\theta \mapsto \prod_{i=1}^{n} (\theta - X_i)$

Concave and convex functions

Definition

A function twice differentiable function $h : \Theta \subset \mathbb{R} \to \mathbb{R}$ is said to be *concave* if its second derivative satisfies

$$h''(\theta) \leq 0\,, \qquad \forall\ \theta \in \Theta$$

It is said to be *strictly concave* if the inequality is strict: $h''(\theta) < 0$

Moreover, h is said to be (strictly) *convex* if $-h$ is (strictly) concave, i.e. $h''(\theta) \geq 0$ ($h''(\theta) > 0$).

Examples:

- $\Theta = \mathbb{R}$, $h(\theta) = -\theta^2$,
- $\Theta = (0, \infty)$, $h(\theta) = \sqrt{\theta}$,
- $\Theta = (0, \infty)$, $h(\theta) = \log \theta$,
- $\Theta = [0, \pi]$, $h(\theta) = \sin(\theta)$
- $\Theta = \mathbb{R}$, $h(\theta) = 2\theta - 3$

Multivariate concave functions

More generally for a *multivariate* function: $h : \Theta \subset \mathbb{R}^d \to \mathbb{R}$, $d \geq 2$, define the

- *gradient* vector: $\nabla h(\theta) = \begin{pmatrix} \frac{\partial h}{\partial \theta_1}(\theta) \\ \vdots \\ \frac{\partial h}{\partial \theta_d}(\theta) \end{pmatrix} \in \mathbb{R}^d$
- *Hessian* matrix:

$$\mathbf{H}h(\theta) = \begin{pmatrix} \frac{\partial^2 h}{\partial \theta_1 \partial \theta_1}(\theta) & \cdots & \frac{\partial^2 h}{\partial \theta_1 \partial \theta_d}(\theta) \\ & & \\ \frac{\partial^2 h}{\partial \theta_d \partial \theta_d}(\theta) & \cdots & \frac{\partial^2 h}{\partial \theta_d \partial \theta_d}(\theta) \end{pmatrix} \in \mathbb{R}^{d \times d}$$

h is concave $\quad \Leftrightarrow \quad x^\top \mathbf{H}h(\theta)x \leq 0 \quad \forall x \in \mathbb{R}^d,\ \theta \in \Theta.$

h is strictly concave $\quad \Leftrightarrow \quad x^\top \mathbf{H}h(\theta)x < 0 \quad \forall x \in \mathbb{R}^d,\ \theta \in \Theta.$

$x \neq \vec{0}$

Examples:

- $\Theta = \mathbb{R}^2$, $h(\theta) = -\theta_1^2 - 2\theta_2^2$ or $h(\theta) = -(\theta_1 - \theta_2)^2$
- $\Theta = (0, \infty)$, $h(\theta) = \log(\theta_1 + \theta_2)$,

Optimality conditions

Strictly concave functions are easy to maximize: if they have a maximum, then it is **unique**. It is the unique solution to

$$h'(\theta) = 0\,,$$

or, in the multivariate case

$$\nabla h(\theta) = 0 \in \mathbb{R}^d\,.$$

There are many algorithms to find it numerically: this is the theory of "convex optimization". In this class, often a **closed form formula** for the maximum.

Exercises

a) Which one of the following functions are concave on $\Theta = \mathbb{R}^2$?

1. $h(\theta) = -(\theta_1 - \theta_2)^2 - \theta_1\theta_2$
2. $h(\theta) = -(\theta_1 - \theta_2)^2 + \theta_1\theta_2$
3. $h(\theta) = (\theta_1 - \theta_2)^2 - \theta_1\theta_2$
4. Both 1. and 2.
5. All of the above
6. None of the above

b)Let $h : \Theta \subset \mathbb{R}^d \to \mathbb{R}$ be a function whose hessian matrix $\mathbf{H}h(\theta)$ has a positive diagonal entry for some $\theta \in \Theta$. Can h be concave? Why or why not?

Examples of maximum likelihood estimators

- Bernoulli trials: $\hat{p}_n^{MLE} = \bar{X}_n$.
- Poisson model: $\hat{\lambda}_n^{MLE} = \bar{X}_n$.
- Gaussian model: $\left(\hat{\mu}_n, \hat{\sigma}_n^2\right) = \left(\bar{X}_n, \hat{S}_n\right)$.

Consistency of maximum likelihood estimator

Under mild regularity conditions, we have

$$\hat{\theta}_n^{MLE} \xrightarrow[n \to \infty]{\mathbb{P}} \theta^*$$

This is because for all $\theta \in \Theta$

$$\frac{1}{n} L(X_1, \ldots, X_n, \theta) \xrightarrow[n \to \infty]{\mathbb{P}} \text{“constant”} - \mathsf{KL}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta)$$

Moreover, the minimizer of the right-hand side is θ^* if the parameter is identifiable.

Technical conditions allow to transfer this convergence to the minimizers.

Covariance

How about asymptotic normality?

In general, when $\theta \subset \mathbb{R}^d, d \geq 2$, its coordinates are not necessarily independent.

The **covariance** between two random variables X and Y is

$$\begin{aligned}\mathsf{Cov}(X, Y) &= \mathbb{E}\Big[\big(X - \mathbb{E}(X)\big) \cdot \big(Y - \mathbb{E}(Y)\big)\Big] \\ &= \mathbb{E}\big[X \cdot Y\big] - \mathbb{E}[X]\mathbb{E}[Y] \\ &= \mathbb{E}\Big[X \cdot \big(Y - \mathbb{E}(Y)\big)\Big]\end{aligned}$$

Properties

- Cov(X, Y) = Var(X)
- Cov(X, Y) = Cov(Y, X)
- If X and Y are independent, then Cov$(X, Y) = 0$

In general, the **converse is not true** except if $(X, Y)^\top$ is a **Gaussian vector**[2], i.e., $\alpha X + \beta Y$ is Gaussian for all $(\alpha, \beta) \in \mathbb{R}^{\setminus}\{(0, 0)\}$.

Take $X \sim \mathcal{N}(0, 1)$, $B \sim$ Ber$(1/2)$, $R = 2B - 1 \sim$ Rad$(1/2)$. Then

$$Y = R \cdot X \sim \mathcal{N}(0, 1)$$

But taking $\alpha = \beta = 1$, we get

$$X + Y = \begin{cases} 0 & \text{with prob. } 1/2 \\ 2X & \text{with prob. } 1/2 \end{cases}$$

Actually Cov$(X, Y) = 0$ but they are not independent: $|X| = |Y|$

Covariance matrix

The covariance matrix of a random vector $X = (X^{(1)}, \ldots, X^{(d)})^\top \in \mathbb{R}^d$ is given by

$$\Sigma = \mathbf{Cov}(X) = \mathbb{E}\left[\big(X - \mathbb{E}(X)\big)\big(X - \mathbb{E}(X)\big)^\top\right]$$

This is a matrix of size $d \times d$.

The term on the ith row and jth column is

$$\Sigma_{ij} = \mathbb{E}\left[\big(X^{(i)} - \mathbb{E}(X^{(i)})\big)\big(X^{(j)} - \mathbb{E}(X^{(j)})\big)\right] = \mathsf{Cov}(X^{(i)}, X^{(j)})$$

In particular, on the diagonal, we have $\Sigma_{ii} = \mathsf{Cov}(X^{(i)}, X^{(i)}) = \mathsf{Var}(X^{(i)}$

Recall that for $X \in \mathbb{R}$, $\mathsf{Var}(aX + b) = a^2\mathsf{Var}(X)$. Actually, if $X \in \mathbb{R}^d$ and A, B are matrices:

$$\mathsf{Cov}(AX + B) = A\Sigma A^\top$$

The multivariate Gaussian distribution

If $(X, Y)^\top$ is a Gaussian vector then its pdf depends on 5 parameters:

$$\mathbb{E}[X],\ \mathbb{E}[Y],\ \mathsf{Var}(X),\ \mathsf{Var}(Y) \quad \text{and} \quad \mathsf{Cov}(X, Y)$$

More generally, a Gaussian vector[3] $X \in \mathbb{R}^d$, is completely determined by its expected value and $\mathbb{E}[X] = \mu \in \mathbb{R}^d$ covariance matrix Σ. We write

$$X \sim \mathcal{N}_d(\mu, \Sigma).$$

It has pdf over $\mathbb{R}^d$ given by:

$$\frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right)$$

[3] As before, this means that $\alpha^\top X$ is Gaussian for any $\alpha \in \mathbb{R}^d, \alpha \neq 0$.

The multivariate CLT

The CLT may be generalized to averages or random vectors (also vectors of averages).
Let $X_1, \ldots, X_n \in \mathbb{R}^d$ be independent copies of a random vector X such that $\mathbb{E}[X] = \mu$, $\mathsf{Cov}(X) = \Sigma$,

$$\sqrt{n}(\bar{X}_n - \mu) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d(0, \Sigma)$$

Equivalently

$$\sqrt{n}\Sigma^{-1/2}(\bar{X}_n - \mu) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d(0, I_d)$$

Multivariate Delta method

Let $(T_n)_{n\geq 1}$ sequence of random vectors in $\mathbb{R}^d$ such that

$$\sqrt{n}(T_n - \theta) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d(0, \Sigma),$$

for some $\theta \in \mathbb{R}^d$ and some covariance $\Sigma \in \mathbb{R}^{d\times d}$.

Let $g : \mathbb{R}^d \to \mathbb{R}^k$ $(k \geq 1)$ be continuously differentiable at θ.
Then,

$$\sqrt{n}\left(g(T_n) - g(\theta)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_k\big(0, \nabla g(\theta)^\top \Sigma \nabla g(\theta)\big),$$

where $\nabla g(\theta) = \dfrac{\partial g}{\partial \theta}(\theta) = \left(\dfrac{\partial g_j}{\partial \theta_i}\right)_{\substack{1\leq i\leq d\\ 1\leq j\leq k}} \in \mathbb{R}^{d\times k}$.

Fisher Information

Definition: Fisher information

Define the log-likelihood for one observation as:

$$\ell(\theta) = \log L_1(X, \theta), \quad \theta \in \Theta \subset \mathbb{R}^d$$

Assume that ℓ is a.s. twice differentiable. Under some regularity conditions, the *Fisher information* of the statistical model is defined as:

$$I(\theta) = \mathbb{E}\left[\nabla \ell(\theta) \nabla \ell(\theta)^\top\right] - \mathbb{E}\left[\nabla \ell(\theta)\right] \mathbb{E}\left[\nabla \ell(\theta)\right]^\top = -\mathbb{E}\left[\mathbf{H} \ell(\theta)\right].$$

If $\Theta \subset \mathbb{R}$, we get:

$$I(\theta) = \mathsf{var}\left[\ell'(\theta)\right] = -\mathbb{E}\left[\ell''(\theta)\right]$$

Fisher information of the Bernoulli experiment

Let $X \sim \mathsf{Ber}(p)$.

$$\ell(p) = \log(p^X(1-p)^(1-X)) = X\log p + (1-X)\log(1-p)$$

$$\ell'(p) = \frac{X}{p} - \frac{1-X}{1-p} \qquad \mathsf{var}[\ell'(p)] = \frac{1}{p(1-p)}$$

$$= \frac{X-p}{p(1-p)}$$

$$\ell''(p) = -\frac{X}{p^2} - \frac{1-X}{(1-p)^2} \qquad -\mathbb{E}[\ell''(p)] = \frac{1}{p(1-p)}$$

Asymptotic normality of the MLE

Theorem

Let $\theta^* \in \Theta$ (the *true* parameter). Assume the following:

1. The parameter is identifiable.
2. For all $\theta \in \Theta$, the support of $\mathbb{P}_\theta$ does not depend on θ;
3. θ^* is not on the boundary of Θ;
4. $I(\theta)$ is invertible in a neighborhood of θ^*;
5. A few more technical conditions.

Then, $\hat{\theta}_n^{MLE}$ satisfies:

- $\hat{\theta}_n^{MLE} \xrightarrow[n\to\infty]{\mathbb{P}} \theta^*$ w.r.t. $\mathbb{P}_{\theta^*}$;
- $\sqrt{n}\left(\hat{\theta}_n^{MLE} - \theta^*\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\left(0, I(\theta^*)^{-1}\right)$ w.r.t. $\mathbb{P}_{\theta^*}$.

The method of moments

Moments

Let $X_1, \ldots, X_n$ be an i.i.d. sample associated with a statistical model $\big(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\big)$.

- Assume that $E \subseteq \mathbb{R}$ and $\Theta \subseteq \mathbb{R}^d$, for some $d \geq 1$.
- *Population moments*: Let $m_k(\theta) = \mathbb{E}_\theta[X_1^k], \ 1 \leq k \leq d$.
- *Empirical moments*: Let $\hat{m}_k = \overline{X_n^k} = \dfrac{1}{n}\sum_{i=1}^n X_i^k, \quad 1 \leq k \leq d$.
- From LLN, for all k

$$\hat{m}_k \xrightarrow[n\to\infty]{\mathbb{P}/a.s} m_k(\theta)$$

More compactly, we say that the whole vector converges:

$$(\hat{m}_1, \ldots, \hat{m}_d) \xrightarrow[n\to\infty]{\mathbb{P}/a.s} (m_1(\theta), \ldots, m_d(\theta))$$

Moments estimator

Let

$$\begin{array}{rcccl} M & : & \Theta & \to & \mathbb{R}^d \\ & & \theta & \mapsto & M(\theta) = (m_1(\theta), \ldots, m_d(\theta)) \,. \end{array}$$

Assume M is one to one:

$$\theta = M^{-1}(m_1(\theta), \ldots, m_d(\theta)).$$

Definition

Moments estimator of θ:

$$\hat{\theta}_n^{MM} = M^{-1}(\hat{m}_1, \ldots, \hat{m}_d \qquad),$$

provided it exists.

Statistical analysis

- Recall $M(\theta) = (m_1(\theta), \ldots, m_d(\theta))$;
- Let $\hat{M} = (\hat{m}_1, \ldots, \hat{m}_d)$.
- Let $\Sigma(\theta) = \mathsf{Cov}_\theta(X_1, X_1^2, \ldots, X_1^d)$ be the covariance matrix of the random vector $(X_1, X_1^2, \ldots, X_1^d)$, which we assume to exist.
- Assume M^{-1} is continuously differentiable at $M(\theta)$.

Method of moments (5)

Remark: The method of moments can be extended to more general moments, even when $E \not\subset \mathbb{R}$.

- Let $g_1, \ldots, g_d : E \to \mathbb{R}$ be given functions, chosen by the practitioner.
- Previously, $g_k(x) = x^k, \quad x \in E = \mathbb{R}$, for all $k = 1, \ldots, d$.
- Define $m_k(\theta) = \mathbb{E}_\theta[g_k(X)]$, for all $k = 1, \ldots, d$.
- Let $\Sigma(\theta) = \mathsf{Cov}_\theta(g_1(X_1), g_2(X_1), \ldots, g_d(X_1))$ be the covariance matrix of the random vector $(g_1(X_1), g_2(X_1), \ldots, g_d(X_1))$, which we assume to exist.
- Assume M is one to one and M^{-1} is continuously differentiable at $M(\theta)$.

Generalized method of moments

Applying the multivariate CLT and Delta method yields:

Theorem

$$\sqrt{n}\left(\hat{\theta}_n^{MM} - \theta\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\left(0, \Gamma(\theta)\right) \qquad (\text{w.r.t. } \mathbb{P}_\theta),$$

where $\Gamma(\theta) = \left[\frac{\partial M^{-1}}{\partial \theta}\big(M(\theta)\big)\right]^\top \Sigma(\theta) \left[\frac{\partial M^{-1}}{\partial \theta}\big(M(\theta)\big)\right].$

MLE vs. Moment estimator

- Comparison of the quadratic risks: In general, the MLE is more accurate.

- MLE still gives good results if model is misspecified

- Computational issues: Sometimes, the MLE is intractable but MM is easier (polynomial equations)

M-estimation

M-estimators

Idea:

- Let $X_1, \ldots, X_n$ be i.i.d with some unknown distribution $\mathbb{P}$ in some sample space E ($E \subseteq \mathbb{R}^d$ for some $d \geq 1$).
- No statistical model needs to be assumed (similar to ML).
- Goal: estimate some parameter μ^* associated with $\mathbb{P}$, e.g. its mean, variance, median, other quantiles, the true parameter in some statistical model...
- Find a function $\rho : E \times \mathcal{M} \to \mathbb{R}$, where $\mathcal{M}$ is the set of all possible values for the unknown μ^*, such that:

  $$\mathcal{Q}(\mu) := \mathbb{E}\left[\rho(X_1, \mu)\right]$$

  achieves its minimum at $\mu = \mu^*$.

Examples (1)

- If $E = \mathcal{M} = \mathbb{R}$ and $\rho(x, \mu) = (x - \mu)^2$, for all $x \in \mathbb{R}, \mu \in \mathbb{R}$: $\mu^* = \mathbb{E}[X]$

- If $E = \mathcal{M} = \mathbb{R}^d$ and $\rho(x, \mu) = \|x - \mu\|_2^2$, for all $x \in \mathbb{R}^d, \mu \in \mathbb{R}^d$: $\mu^* = \mathbb{E}[X]$

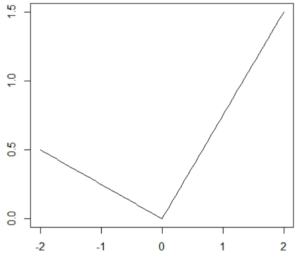
- If $E = \mathcal{M} = \mathbb{R}$ and $\rho(x, \mu) = |x - \mu|$, for all $x \in \mathbb{R}, \mu \in \mathbb{R}$: μ^* is a median of $\mathbb{P}$.

Examples (2)

If $E = \mathcal{M} = \mathbb{R}$, $\alpha \in (0,1)$ is fixed and $\rho(x,\mu) = C_\alpha(x-\mu)$, for all $x \in \mathbb{R}, \mu \in \mathbb{R}$: μ^* is a α-quantile of $\mathbb{P}$.

Check function

$$C_\alpha(x) = \begin{cases} -(1-\alpha)x \text{ if } x < 0 \\ \alpha x \text{ if } x \geq 0. \end{cases}$$



MLE is an M-estimator

Assume that $(E, \{\mathbb{P}_\theta\}_{\theta \in \Theta})$ is a statistical model associated with the data.

Theorem

Let $\mathcal{M} = \Theta$ and $\rho(x, \theta) = -\log L_1(x, \theta)$, provided the likelihood is positive everywhere. Then,

$$\mu^* = \theta^*,$$

where $\mathbb{P} = \mathbb{P}_{\theta^*}$ (i.e., θ^* is the true value of the parameter).

Definition

- Define $\hat{\mu}_n$ as a minimizer of:

$$\mathcal{Q}_n(\mu) := \frac{1}{n}\sum_{i=1}^{n}\rho(X_i,\mu).$$

- Examples: Empirical mean, empirical median, empirical quantiles, MLE, etc.

Statistical analysis

- Let $J(\mu) = \frac{\partial^2 Q}{\partial\mu\partial\mu^\top}(\mu) \quad \left(= \mathbb{E}\left[\frac{\partial^2 \rho}{\partial\mu\partial\mu^\top}(X_1, \mu)\right]\right.$ under some regularity conditions).

- Let $K(\mu) = \text{Cov}\left[\frac{\partial \rho}{\partial\mu}(X_1, \mu)\right]$.

- **Remark:** In the log-likelihood case (write $\mu = \theta$),

  $J(\theta) = K(\theta) = I(\theta)$ Fisher Information

  in general, $J \neq K$

Asymptotic normality

Let $\mu^* \in \mathcal{M}$ (the *true* parameter). Assume the following:

1. μ^* is the only minimizer of the function $\mathcal{Q}$;
2. $J(\mu)$ is invertible for all $\mu \in \mathcal{M}$;
3. A few more technical conditions.

Then, $\hat{\mu}_n$ satisfies:

- $\hat{\mu}_n \xrightarrow[n\to\infty]{\mathbb{P}} \mu^*$;
- $\sqrt{n}\left(\hat{\mu}_n - \mu^*\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\left(0, J(\mu^*)^{-1}K(\mu^*)J(\mu^*)^{-1}\right)$.

M-estimators in robust statistics

Example: Location parameter

If $X_1, \ldots, X_n$ are i.i.d. with density $f(\cdot - m)$, where:

- f is an unknown, positive, even function (e.g., the Cauchy density);
- m is a real number of interest, a *location parameter*;

How to estimate m ?

- M-estimators: empirical mean, empirical median, ...
- Compare their risks or asymptotic variances;
- The empirical median is more *robust*.

Recap

- Three principled methods for estimation: maximum likelihood, Method of moments, M-estimators
- Maximum likelihood is an example of M-estimation
- Method of moments inverts the function that maps parameters to moments
- All methods yield to asymptotic normality under regularity conditions
- Asymptotic covariance matrix can be computed using multivariate Δ-method
- For MLE, asymptotic covariance matrix is the inverse Fisher information matrix