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 $X_1 \sim \mathbb{P}_{\theta^*}$: $\theta^*$ 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 $\theta^*$.
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 $x \in E$,

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

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

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

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

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

# Properties of Total variation

- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) =$ $\mathrm{TV}(\mathbb{P}_{\theta'}, \mathbb{P}_\theta)$ (symmetric)
- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \geq$ $0$, $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \leq 1$ (positive)
- If $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = 0$ then $\mathbb{P}_\theta = \mathbb{P}_{\theta'}$ (definite)
- $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \leq$ $\mathrm{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta''}) + \mathrm{TV}(\mathbb{P}_{\theta''}, \mathbb{P}_{\theta'})$ (triangle inequality)

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

# Exercises

Compute:

**a)** $\mathsf{TV}(\mathsf{Ber}(0.5), \mathsf{Ber}(0.1)) =$ $\frac{1}{2}\left[ |P_{0.5}(0) - P_{0.1}(0)| + |P_{0.5}(1) - P_{0.1}(1)| \right]$

$E = \{0,1\}$

$= \frac{1}{2}\left[\underbrace{|.5 - .9|}_{0.4} + |.5 - .1|\right] = \frac{0.8}{2} = 0.4$

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

$0.4$

**c)** $\mathsf{TV}(\mathsf{Exp}(1), \mathsf{Unif}[0,1]) =$ $\frac{1}{e}$

**d)** $\mathsf{TV}(X, X + a) =$ $1$ $\quad \Big| \overbrace{\mathbb{P}(X \in \{0,1\})}^{=1} - \overbrace{\mathbb{P}(X+a \in \{0,1\})}^{=0} \Big| = 1$

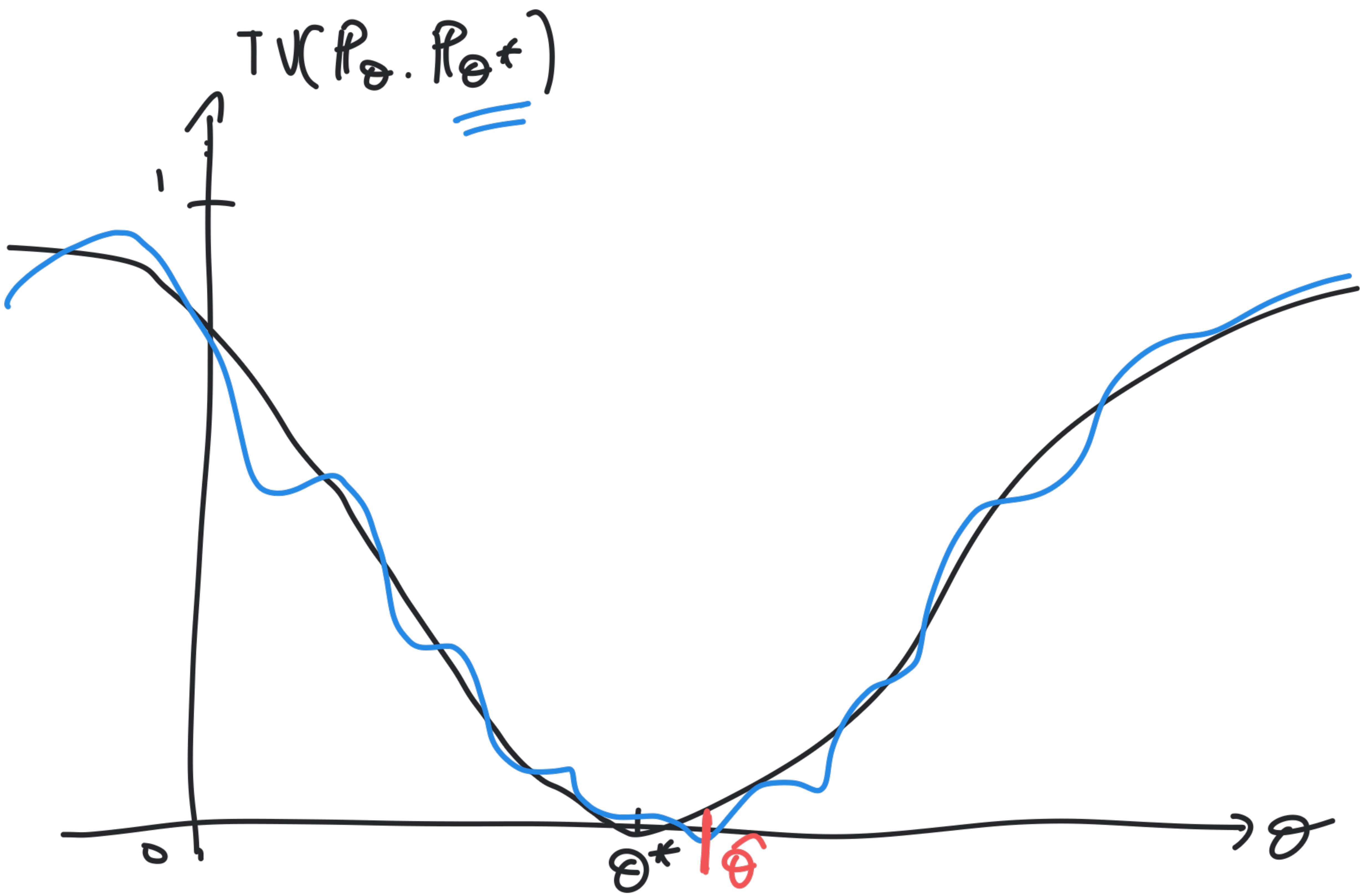
for any $a \in (0,1)$, where $X \sim \mathsf{Ber}(0.5)$

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

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

# An estimation strategy

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




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

# 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!

$\theta^*$ unique minimizer of $\theta \mapsto \mathsf{KL}(\mathbb{P}_{\theta^*}, \mathbb{P}_\theta)$

# Maximum likelihood estimation

# Estimating the KL

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

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

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

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

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

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

(blue curve)

# Maximum likelihood

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

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

This is the **maximum likelihood principle**.

# Likelihood, Discrete case (1)

Let $\left(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\right)$ 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:

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

$$= \prod_{i=1}^{n} \mathbb{P}_\theta [X_i = x_i]$$

# Likelihood for the Bernoulli model

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

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

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

# Likelihood for the Poisson model

**Example 2 (Poisson model):**

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

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

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

$$\mathbb{P}_\lambda(X_i = x_i) = \frac{\lambda^{x_i}}{x_i!} e^{-\lambda}$$

$$\Rightarrow \underbrace{L(x_1 \ldots x_n; \lambda)}_{\prod_{i=1}^{n} \mathbb{P}_\lambda(X_i = x_i)} = \frac{\lambda^{\sum_{i=1}^n x_i}}{\prod_{i=1}^{n} x_i!} e^{-n\lambda}$$

# 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 $f_\theta$.

## Definition

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

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

# Likelihood for the Gaussian model

**Example 1 (Gaussian model):** If $X_1, \ldots, X_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$, 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 $X_1, \ldots, X_n \sim \mathsf{Exp}(\lambda)$, $\lambda > 0$.

**a)** What is $E$? $(0, \infty)$

**b)** What is $\Theta$? $(0, \infty)$

**c)** Find the likelihood of the model.

$$L(x_1, \ldots, x_n; \lambda) = \lambda^n e^{-\lambda \sum_{i=1}^{n} x_i} \mathbb{1}(\min_i x_i > 0)$$

# Exercise

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

**a)** What is $E$?

$[0, \infty)$

**b)** What is $\Theta$?

$[0, \infty)$

**c)** Find the likelihood of the model.

$$L(x_1, \ldots, x_n ; b) = \frac{1}{b^n} \mathbb{1}\left(\max_i X_i \leq b\right)$$

# 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 $\theta$ 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

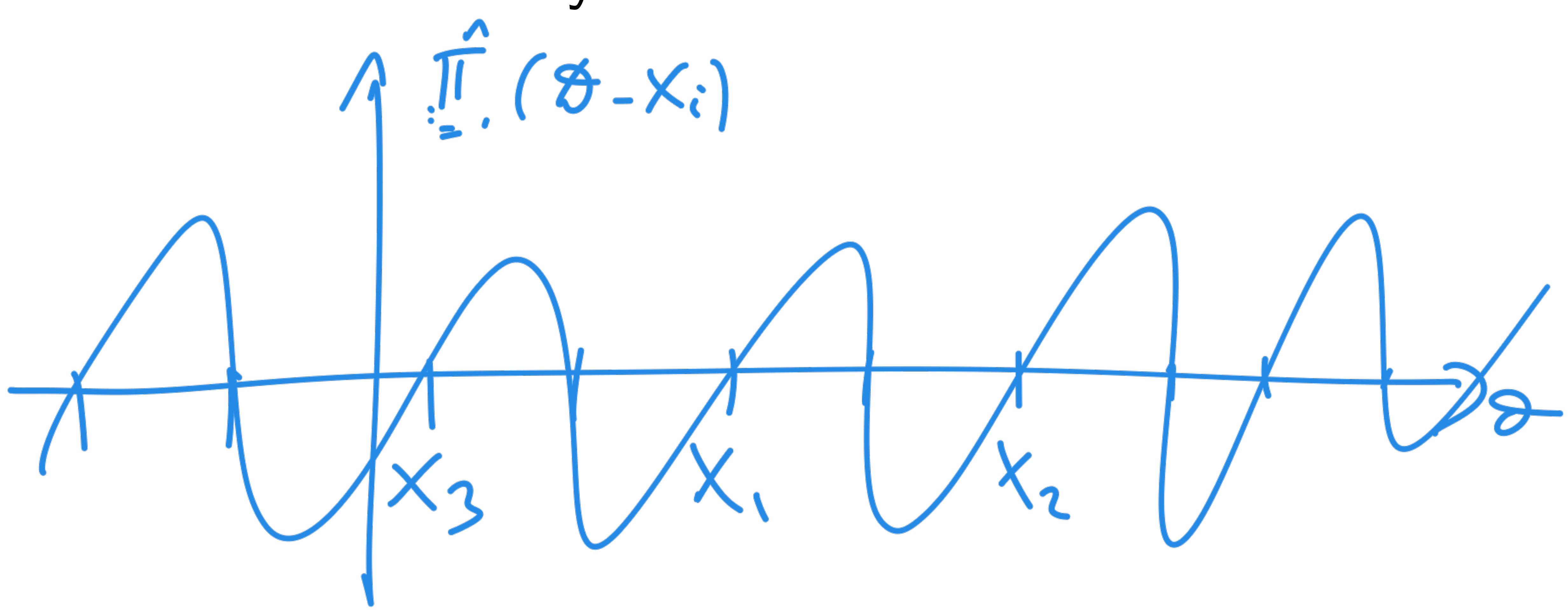
OPTIMIZATION

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:

- $\Theta = \mathbb{R}$, $h(\theta) = -\theta^2$, $h'(\theta) = -2\theta$, $h''(\theta) = -2 < 0$ (s. concave)
- $\Theta = (0, \infty)$, $h(\theta) = \sqrt{\theta}$, $h'(\theta) = \frac{1}{2\sqrt{\theta}}$, $h''(\theta) = -\frac{1}{4\theta^{3/2}} < 0$ (s. concave)
- $\Theta = (0, \infty)$, $h(\theta) = \log\theta$, $h'(\theta) = \frac{1}{\theta}$, $h''(\theta) = -\frac{1}{\theta^2} < 0$ (s. concave)
- $\Theta = [0, \pi]$, $h(\theta) = \sin(\theta)$, $h'(\theta) = \cos(\theta)$, $h''(\theta) = -\sin(\theta) \leq 0$ (concave)
- $\Theta = \mathbb{R}$, $h(\theta) = 2\theta - 3$, $h'(\theta) = 2$, $h''(\theta) = 0 \begin{cases} \leq 0 \\ \geq 0 \end{cases}$ Both

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

$x \neq 0$

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

$$\boxed{h'(\theta) = 0\,,}$$

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: $(\hat{\mu}_n, \hat{\sigma}_n^2) = \left(\bar{X}_n, \hat{S}_n\right)$.

$$\hat{S}_n = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2$$

# Consistency of maximum likelihood estimator

Under mild regularity conditions, we have

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

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

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

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

Technical conditions allow to transfer this convergence to the minimizers.

# Covariance

$$\hat{\theta} = \begin{pmatrix} \overline{X}_n \\ \hat{S}_n \end{pmatrix}$$

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

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

# Properties

- $\text{Cov}(X, \cancel{X}) =$ Var$(X)$
- $\text{Cov}(X, Y) = \text{Cov}(Y, X)$ ✓
- If $X$ and $Y$ are independent, then $\text{Cov}(X, Y) = 0$

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

Rademacher

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

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

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

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

Conditionally on $X$

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

# Covariance matrix

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

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

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

The term on the $i$th row and $j$th column is

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

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

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

$$\mathrm{Cov}(AX + B) = \mathrm{Cov}(AX) = A\,\mathrm{Cov}(X)\,A^\top = A\Sigma A^\top$$

# The multivariate Gaussian distribution

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

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

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 $\Sigma$. We write

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

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

$$f(x) = f(x^{(1)}, \dots, x^{(d)}) = \frac{1}{(2\pi\det(\Sigma))^{d/2}} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right)$$

[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 $\mathbb{E}[X] = \mu$, $\mathsf{Cov}(X) = \Sigma$,

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

$$I_d = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$$

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 $\theta$. Then,

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

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:

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

Assume that $\ell$ 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 $X \sim \mathrm{Ber}(p)$.

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

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

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

# 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 $\theta$;
3. $\theta^*$ is not on the boundary of $\Theta$;
4. $I(\theta)$ is invertible in a neighborhood of $\theta^*$;
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. $\mathbb{P}_{\theta^*}$;
- $\sqrt{n}\left(\hat{\theta}_n^{MLE} - \theta^*\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d\left(0, I(\theta^*)^{-1}\right)$ 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 $\left(E, (\mathbb{P}_\theta)_{\theta \in \Theta}\right)$.

- 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 $\hat{m}_k = \overline{X_n^k} = \frac{1}{n}\sum_{i=1}^{n} X_i^k$, $\quad 1 \leq k \leq d$.
- From LLN,

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

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

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

Assume $M$ is one to one:

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

## Definition

Moments estimator of $\theta$:

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

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 $\Sigma(\theta) = \text{Cov}_\theta(X_1, X_1^2, \ldots, X_1^d)$ 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. e.g. $g_k(x) = \cos(2\pi k x)$
- 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

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

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

# 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 $\mu^*$ 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 $\mu^*$, such that:

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

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

# Examples (1)

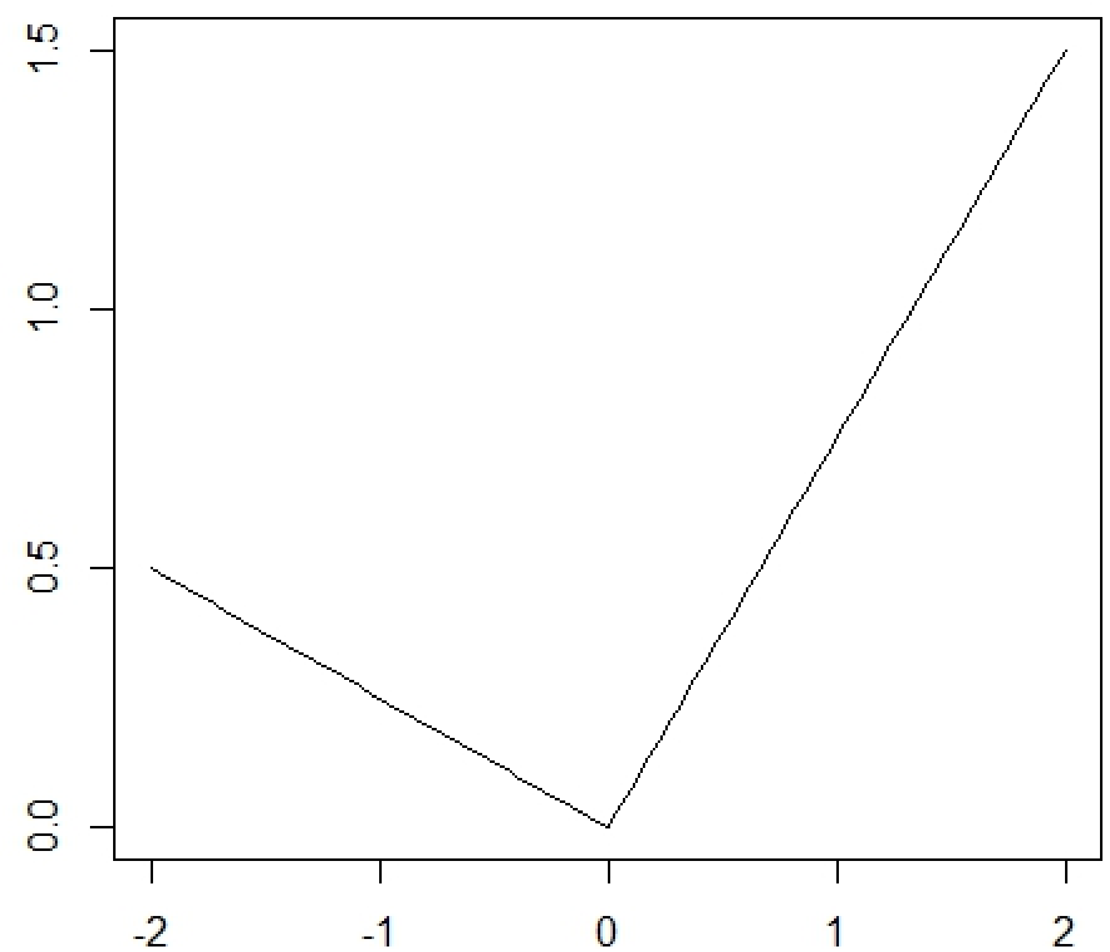
- If $E = \mathcal{M} = \mathbb{R}$ and $\rho(x, \mu) = (x - \mu)^2$, for all $x \in \mathbb{R}, \mu \in \mathbb{R}$:
  $\mu^* =$ $\mathbb{E}[X]$
- If $E = \mathcal{M} = \mathbb{R}^d$ and $\rho(x, \mu) = \|x - \mu\|_2^2$, for all $x \in \mathbb{R}^d, \mu \in \mathbb{R}^d$: $\mu^* =$ $\mathbb{E}[X] \in \mathbb{R}^d$
- If $E = \mathcal{M} = \mathbb{R}$ and $\rho(x, \mu) = |x - \mu|$, for all $x \in \mathbb{R}, \mu \in \mathbb{R}$:
  $\mu^*$ 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 $x \in \mathbb{R}, \mu \in \mathbb{R}$ : $\mu^*$ is a $\alpha$-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., $\theta^*$ is the true value of the parameter).

# Definition

replace $\mathbb{E}$ with $\frac{1}{n}\sum_{i=1}^{n}$

- 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 $\mu = \theta$),

$$J(\theta) = K(\theta) = I(\theta) \qquad \text{(Fisher information)}$$

# Asymptotic normality

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

1. $\mu^*$ 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:

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

# 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 $\Delta$-method
- For MLE, asymptotic covariance matrix is the inverse Fisher information matrix