# 18.6501x Fundamentals of Statistics

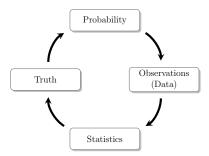
This is a cheat sheet for statistics based on the online course given by Prof. Philippe Rigollet. Compiled by Janus B. Advincula.

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## **Introduction to Statistics**

#### What is Statistics?

**Statistical view** Data comes from a *random process*. The goal is to learn how this process works in order to make predictions or to understand what plays a role in it.



## Statistics vs. Probability

**Probability** Previous studies showed that the drug was 80% effective. Then we can anticipate that for a study on 100 patients, in average 80 will be cured and at least 65 will be cured with 99.99% chances.

**Statistics** Observe that  $\frac{78}{100}$  patients were cured. We (will be able to) conclude that we are 95% confident that for other studies, the drug will be effective on between 69.88% and 86.11% of patients.

## **Probability Redux**

Let  $X_1, \ldots, X_n$  be i.i.d. random variables with  $\mathbb{E}[X] = \mu$  and  $Var(X) = \sigma^2$ .

### Law of Large Numbers

$$\overline{X}_n = \frac{1}{n} \sum_{i=1}^n X_i \xrightarrow{\mathbb{P}, a.s.} \mu.$$

#### Central Limit Theorem

$$\sqrt{n} \frac{\overline{X}_n - \mu}{\sigma} \xrightarrow[n \to \infty]{(d)} \mathcal{N}(0, 1).$$

Equivalently,

$$\sqrt{n}\left(\overline{X}_n - \mu\right) \xrightarrow{(d)} \mathcal{N}\left(0, \sigma^2\right)$$

**Hoeffding's Inequality** Let n be a positive integer and  $X,X_1,\ldots X_n$  be i.i.d. random variables such that  $\mathbb{E}\left[X\right]=\mu$  and  $X\in\left[a,b\right]$  almost surely. Then,

$$\mathbb{P}\left(\left|\overline{X}_n - \mu\right| \ge \epsilon\right) \le 2e^{-\frac{2n\epsilon^2}{(b-a)^2}} \quad \forall \epsilon > 0$$

## The Gaussian Distribution

Because of the CLT, the Gaussian (a.k.a. normal) distribution is ubiquitous in statistics.

- X ~ N (μ, σ²)
- E[X] = μ
- $Var(X) = \sigma^2 > 0$

## Gaussian density (PDF)

$$f_{\mu,\sigma^2}(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

#### **Useful Properties of Gaussian**

It is invariant under affine transformation.

• If  $X \sim \mathcal{N}(\mu, \sigma^2)$ , then for any  $a, b \in \mathbb{R}$ ,

$$aX + b \sim \mathcal{N}\left(a\mu + b, a^2\sigma^2\right).$$

• Standardization: If  $X \sim \mathcal{N}(\mu, \sigma^2)$ , then

$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}\left(0, 1\right)$$

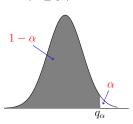
We can compute probabilities from the CDF of  $Z \sim \mathcal{N}(0, 1)$ :

$$\mathbb{P}\left(u \leq X \leq v\right) = \mathbb{P}\left(\frac{u-\mu}{\sigma} \leq Z \leq \frac{v-\mu}{\sigma}\right)$$

• Symmetry: If  $X \sim \mathcal{N}\left(0, \sigma^2\right)$ , then  $-X \sim \mathcal{N}\left(0, \sigma^2\right)$ . If x > 0,  $\mathbb{P}\left(|X| > x\right) = \mathbb{P}\left(X > x\right) + \mathbb{P}\left(-X > x\right) = 2\,\mathbb{P}\left(X > x\right)$ 

**Quantiles** Let  $\alpha \in (0,1)$ . The quantile of order  $1-\alpha$  of a random variable X is the number  $q_\alpha$  such that

$$\mathbb{P}\left(X \leq q_{\alpha}\right) = 1 - \alpha.$$



Let F denote the CDF of X.

- $F(q_{\alpha}) = 1 \alpha$
- If *F* is invertible, then  $q_{\alpha} = F^{-1} (1 \alpha)$
- $\mathbb{P}(X > q_{\alpha}) = \alpha$
- If  $X \sim \mathcal{N}(0,1)$ ,  $\mathbb{P}(|X| > q_{\alpha/2}) = \alpha$

# Three Types of Convergence

Almost Surely (a.s.) Convergence

$$T_n \xrightarrow[n \to \infty]{a.s.} T \iff \mathbb{P}\left[\left\{\omega : T_n(\omega) \xrightarrow[n \to \infty]{} T(\omega)\right\}\right] = 1$$

Convergence in Probability

$$T_n \xrightarrow[n \to \infty]{\mathbb{P}} T \iff \mathbb{P}(|T_n - T| \ge \epsilon) \xrightarrow[n \to \infty]{} 0 \quad \forall \epsilon > 0$$

Convergence in Distribution

$$T_n \xrightarrow[n \to \infty]{(d)} T \iff \mathbb{E}[f(T_n)] \xrightarrow[n \to \infty]{} \mathbb{E}[f(T)]$$

for all continuous and bounded function f.

## **Properties**

- If  $(T_n)_{n\geq 1}$  converges a.s., then it also converges in probability, and the two limits are equal.
- If  $(T_n)_{n>1}$  converges in probability, then it also converges in distribution.
- Convergence in distribution implies convergence in probability if the limit has a density (e.g. Gaussian):

$$T_n \xrightarrow[n \to \infty]{(d)} T \quad \Rightarrow \quad \mathbb{P}(a \le T_n \le b) \xrightarrow[n \to \infty]{} \mathbb{P}(a \le T \le b)$$

## Addition, Multiplication, Division

Assume

$$T_n \xrightarrow[n \to \infty]{a.s./\mathbb{P}} T$$
 and  $U_n \xrightarrow[n \to \infty]{a.s./\mathbb{P}} U$ .

- $T_n + U_n \xrightarrow[n \to \infty]{a.s./\mathbb{P}} T + U$
- $T_n U_n \xrightarrow[n \to \infty]{a.s./\mathbb{P}} TU$
- If, in addition,  $U \neq 0$  a.s., then

$$\frac{T_n}{U_n} \xrightarrow[n \to \infty]{a.s./\mathbb{P}} \frac{T}{U}$$

## Slutsky's Theorem

Let  $(X_n)$ ,  $(Y_n)$  be two sequences of random variables such that

(i) 
$$T_n \xrightarrow[n \to \infty]{(d)} T$$
 and (ii)  $U_n \xrightarrow[n \to \infty]{\mathbb{P}} u$ 

where T is a random variable and u is a given real number. Then,

- $T_n + U_n \xrightarrow[n \to \infty]{(d)} T + u$
- $T_n U_n \xrightarrow[n \to \infty]{(d)} Tu$
- $\bullet \quad \text{If, in addition, } u \neq 0 \text{, then } \frac{T_n}{U_n} \xrightarrow[n \to \infty]{} \frac{T}{u}.$

## **Continuous Mapping Theorem**

If f is a continuous function, then

$$T_n \xrightarrow[n \to \infty]{a.s./\mathbb{P}/(d)} T \Rightarrow f(T_n) \xrightarrow[n \to \infty]{a.s./\mathbb{P}/(d)} f(T).$$

# **Foundation of Inference**

### **Statistical Model**

Let the observed outcome of a statistical experiment be a  $sample\ X_1,\ldots,X_n$  of n i.i.d. random variables in some measurable space E (usually  $E\subseteq\mathbb{R}$ ) and denote by  $\mathbb{P}$  their common distribution. A  $statistical\ model$  associated to that statistical experiment is a pair

$$(E, (\mathbb{P}_{\theta})_{\theta \in \Theta})$$

where

- *E* is called *sample space*;
- (P<sub>θ</sub>)<sub>θ∈Θ</sub> is a family of probability measures on E;
- Θ is any set, called *parameter set*.

## Parametric, Nonparametric and Semiparametric Models

- Usually, we will assume that the statistical model is well-specified, i.e., defined such that ∃θ such that ℙ = ℙ<sub>θ</sub>. This particular θ is called the true parameter and is unknown.
- We often assume that  $\Theta \subseteq \mathbb{R}^d$  for some  $d \geq 1$ . The model is called parametric.
- Sometimes we could have Θ be infinite dimensional, in which case the model is called nonparametric.
- If Θ = Θ<sub>1</sub> × Θ<sub>2</sub>, where Θ<sub>1</sub> is finite dimensional and Θ<sub>2</sub> is infinite dimensional, then we have a semiparametric model. In these models, we only care to estimate the finite dimensional parameter and the infinite dimensional one is called nuisance parameter.

## Identifiability

The parameter  $\theta$  is called *identifiable* if and only if the map  $\theta \in \Theta \mapsto \mathbb{P}_{\theta}$  is injective, i.e.,

$$\theta \neq \theta' \implies \mathbb{P}_{\theta} \neq \mathbb{P}_{\theta'}$$

or equivalently,

$$\mathbb{P}_{\theta} = \mathbb{P}_{\theta'} \implies \theta = \theta'.$$

## **Parameter Estimation**

**Statistic** Any *measurable* function of the sample, e.g.,  $\bar{X}_n$ ,  $\max X_i$ , etc.

**Estimator of**  $\theta$  Any statistic whose expression does not depend on  $\theta$ 

• An estimator  $\hat{\theta}_n$  of  $\theta$  is weakly (resp. strongly) **consistent** if

$$\hat{\theta}_n \xrightarrow[n \to \infty]{\mathbb{P} \text{ (resp. } a.s.)} \theta \quad \text{(w.r.t. } \mathbb{P}\text{)}.$$

• An estimator  $\hat{\theta}_n$  of  $\theta$  is **asymptotically normal** if

$$\sqrt{n}\left(\hat{\theta}_n - \theta\right) \xrightarrow[n \to \infty]{(d)} \mathcal{N}\left(0, \sigma^2\right)$$

#### Bias of an Estimator

• **Bias** of an estimator of  $\hat{\theta}_n$  of  $\theta$ :

bias 
$$(\hat{\theta}_n) = \mathbb{E}[\hat{\theta}_n] - \theta$$

• If bias  $(\hat{\theta}_n) = 0$ , we say that  $\hat{\theta}_n$  is **unbiased**.

### Jensen's Inequality

• If the function f(x) is convex,

$$\mathbb{E}\left[f\left(X\right)\right] > f\left(\mathbb{E}\left[X\right]\right).$$

• If the function g(x) is concave,

$$\mathbb{E}\left[g\left(X\right)\right] \le g\left(\mathbb{E}\left[X\right]\right).$$

#### **Ouadratic Risk**

- We want estimators to have low bias and low variance at the same time.
- The risk (or quadratic risk) of an estimator  $\hat{\theta}_n \in \mathbb{R}$  is

$$R\left(\hat{\theta}_{n}\right) = \mathbb{E}\left[\left|\hat{\theta}_{n} - \theta\right|^{2}\right] = \text{variance} + \text{bias}^{2}$$

• Low quadratic risk means that both bias and variance are small.

### **Confidence Intervals**

Let  $(E, (\mathbb{P}_{\theta})_{\theta \in \Theta})$  be a statistical model based on observations  $X_1, \ldots, X_n$ , and assume  $\Theta \subseteq \mathbb{R}$ . Let  $\alpha \in (0, 1)$ .

• Confidence interval (C.I.) of level  $1 - \alpha$  for  $\theta$ : Any random (depending on  $X_1, \ldots, X_n$ ) interval  $\mathcal{I}$  whose boundaries do not depend on  $\theta$  and such that

$$\mathbb{P}_{\theta} \left[ \mathcal{I} \ni \theta \right] \ge 1 - \alpha, \quad \forall \theta \in \Theta.$$

• C.I. of asymptotic level  $1 - \alpha$  for  $\theta$ : Any random interval  $\mathcal{I}$  whose boundaries do not depend on  $\theta$  and such that

$$\lim_{n \to \infty} \mathbb{P}_{\theta} \left[ \mathcal{I} \ni \theta \right] \ge 1 - \alpha, \quad \forall \theta \in \Theta.$$

**Example** We observe  $R_1, \ldots, R_n \stackrel{\text{iid}}{\sim} \text{Ber}(p)$  for some unknown  $p \in (0, 1)$ .

- Statistical model:  $(\{0,1\}, (Ber(p))_{p \in \{0,1\}})$
- From CLT:

$$\sqrt{n} \frac{\overline{R}_n - p}{\sqrt{p(1-p)}} \xrightarrow[n \to \infty]{(d)} \mathcal{N}(0,1)$$

• It yields

$$\mathcal{I} = \left[ \overline{R}_n - \frac{q \frac{\alpha}{2} \sqrt{p(1-p)}}{\sqrt{n}}, \overline{R}_n + \frac{q \frac{\alpha}{2} \sqrt{p(1-p)}}{\sqrt{n}} \right]$$

• But this is **not** a confidence interval because it depends on *p*!

#### Three solutions:

- 1. Conservative bound
- 2. Solving the (quadratic) equation for p
- 3. Plug-in

## The Delta Method

Let  $(Z_n)_{n\geq 1}$  be a sequence of random variables that satisfies

$$\sqrt{n} (Z_n - \theta) \xrightarrow[n \to \infty]{(d)} \mathcal{N} (0, \sigma^2)$$

for some  $\theta \in \mathbb{R}$  and  $\sigma^2 > 0$  (the sequence  $(Z_n)_{n \geq 1}$  is said to be **asymptotically normal around**  $\theta$ ). Let  $g : \mathbb{R} \to \mathbb{R}$  be continuously differentiable at the point  $\theta$ . Then,

- $(g(Z_n))_{n>1}$  is also asymptotically normal around  $g(\theta)$ .
- · More precisely,

$$\sqrt{n}\left(g\left(Z_{n}\right)-g\left(\theta\right)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\left(0,\left(g'(\theta)\right)^{2}\sigma^{2}\right).$$

## **Introduction to Hypothesis Testing**

**Statistical Formulation** Consider a sample  $X_1,\ldots,X_n$  of i.i.d. random variables and a statistical model  $(E,(\mathbb{P}_{\theta})_{\theta\in\Theta})$ . Let  $\Theta_0$  and  $\Theta_1$  be disjoint subsets of  $\Theta$ .

Consider the two hypotheses:

- H<sub>0</sub> : θ ∈ Θ<sub>0</sub>
- H<sub>1</sub> : θ ∈ Θ<sub>1</sub>

 $H_0$  is the **null hypothesis** and  $H_1$  is the **alternative hypothesis**.

**Asymmetry in the hypotheses**  $H_0$  and  $H_1$  do not play a symmetric role: the data is only used to try to disprove  $H_0$ . Lack of evidence does not mean that  $H_0$  is true.

A test is a statistic  $\psi \in \{0, 1\}$  such that:

- If  $\psi = 0$ ,  $H_0$  is not rejected.
- If  $\psi = 1$ ,  $H_0$  is rejected.

#### Errors

• **Rejection region** of a test  $\psi$ :

$$R_{\psi} = \{ x \in E^n : \psi(x) = 1 \}.$$

• **Type 1 error** of a test  $\psi$ 

$$\alpha_{\psi}: \Theta_0 \rightarrow \mathbb{R} \text{ (or } [0,1])$$

$$\theta \mapsto \mathbb{P}_{\theta} [\psi = 1]$$

• Type 2 error of a test  $\psi$ :

$$\beta_{\psi}: \Theta_1 \rightarrow \mathbb{R}$$
 $\theta \mapsto \mathbb{P}_{\theta} [\psi = 0]$ 

Power of a test ψ:

$$\pi_{\psi} = \inf_{\theta \in \Theta_1} \left( 1 - \beta_{\psi}(\theta) \right)$$

Level, test statistic and rejection region

• A test  $\psi$  has level  $\alpha$  if

$$\alpha_{\psi}(\theta) \le \alpha, \quad \forall \theta \in \Theta_0.$$

• A test  $\psi$  has asymptotic level  $\alpha$  if

$$\lim_{n \to \infty} \alpha_{\psi}(\theta) \le \alpha, \quad \forall \theta \in \Theta_0.$$

· In general, a test has the form

$$\psi = \mathbb{1}\{T_n > c\}$$

for some statistic  $T_n$  and threshold  $c \in \mathbb{R}$ .  $T_n$  is called the **test statistic**. The rejection region is  $R_{\psi} = \{T_n > c\}$ .

**p-value** The (asymptotic) *p*-value of a test  $\psi_{\alpha}$  is the smallest (asymptotic) level  $\alpha$  at which  $\psi_{\alpha}$  rejects  $H_0$ .

# **Methods of Estimation**

#### **Total Variation Distance**

Let  $(E, (\mathbb{P}_{\theta})_{\theta \in \Theta})$  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  $X_1 \sim \mathbb{P}_{\theta^*}$ .

**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  $\theta^*$ .

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

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

**Total Variation Distance between Discrete Measures** Assume that E is discrete (i.e., finite or countable). The total variation distance between  $\mathbb{P}_{\theta}$  and  $\mathbb{P}_{\theta'}$  is

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

**Total Variation Distance between Continuous Measures** Assume that E is continuous. The total variation distance between  $\mathbb{P}_{\theta}$  and  $\mathbb{P}_{\alpha \ell}$  is

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

Properties of Total Variation

•  $TV(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) = TV(\mathbb{P}_{\theta'}, \mathbb{P}_{\theta})$  symmetric

• TV  $(\mathbb{P}_{\theta}, \mathbb{P}_{\alpha'}) > 0$ , TV  $(\mathbb{P}_{\theta}, \mathbb{P}_{\alpha'}) < 1$ 

positive

• If TV  $(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) = 0$ , then  $\mathbb{P}_{\theta} = \mathbb{P}_{\theta'}$  definite

•  $TV(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) \leq TV(\mathbb{P}_{\theta}, \mathbb{P}_{\theta''}) + TV(\mathbb{P}_{\theta''}, \mathbb{P}_{\theta'})$  triangle inequality

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

## Kullback-Leibler (KL) Divergence

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

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

KL-divergence is also known as relative entropy.

### Properties of KL-divergence

- $KL(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) \neq KL(\mathbb{P}_{\theta'}, \mathbb{P}_{\theta})$  in general
- $KL(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) \geq 0$
- If  $KL(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) = 0$ , then  $\mathbb{P}_{\theta} = \mathbb{P}_{\theta'}$  (definite)
- $KL(\mathbb{P}_{\theta}, \mathbb{P}_{\theta'}) \nleq KL(\mathbb{P}_{\theta}, \mathbb{P}_{\theta''}) + KL(\mathbb{P}_{\theta''}, \mathbb{P}_{\theta'})$  in general

## **Maximum Likelihood Estimation**

**Likelihood, Discrete Case** Let  $(E,(\mathbb{P}_{\theta})_{\theta\in\Theta})$  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

$$L_n : E^n \times \Theta \to \mathbb{R}$$

$$(x_1, \dots, x_n; \theta) \mapsto \mathbb{P}_{\theta} [X_1 = x_1, \dots, X_n = x_n]$$

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

**Likelihood, Continuous Case** Let  $(E,(\mathbb{P}_{\theta})_{\theta\in\Theta})$  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

$$L: E^n \times \Theta \to \mathbb{R}$$
 
$$(x_1, \dots, x_n; \theta) \mapsto \prod_{i=1}^n f_{\theta}(x_i)$$

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

**Definition** The maximum likelihood estimator of  $\theta$  is defined as

$$\hat{\theta}_{n}^{\text{MLE}} = \underset{\theta \in \Theta}{\operatorname{argmax}} L\left(X_{1}, \dots, X_{n}, \theta\right),$$

provided it exists.

Log-likelihood Estimator In practice, we use the fact that

$$\hat{\theta}_{n}^{\text{MLE}} = \underset{\theta \in \Theta}{\operatorname{argmax}} \log L\left(X_{1}, \dots, X_{n}, \theta\right),$$

#### Concave and Convex Functions

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

$$h''(\theta) \le 0, \quad \forall \theta \in \Theta.$$

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.  $h''(\theta) \geq 0$  ( $h''(\theta) > 0$ ).

**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:

$$\nabla h(\theta) = \begin{pmatrix} \frac{\partial h(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial h(\theta)}{\partial \theta_d} \end{pmatrix} \in \mathbb{R}^d$$

· Hessian matrix:

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

h is concave  $\iff x^{\mathsf{T}} \mathbb{H} h(\theta) x < 0, \forall x \in \mathbb{R}^d, \theta \in \Theta$ 

h is strictly concave  $\iff x^{\mathsf{T}} \mathbb{H} h(\theta) x < 0, \forall x \in \mathbb{R}^d, \theta \in \Theta$ 

Consistency of Maximum Likelihood Estimator Under mild regularity conditions, we have

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

**Covariance** 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

$$\begin{aligned} \operatorname{Cov}(X,Y) &:= \mathbb{E}\left[ \left( X - \mathbb{E}\left[ X \right] \right) \left( Y - \mathbb{E}\left[ Y \right] \right) \right] \\ &= \mathbb{E}\left[ XY \right] - \mathbb{E}\left[ X \right] \mathbb{E}\left[ Y \right] \end{aligned}$$

#### Properties

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

Covariance Matrix The covariance matrix of a random vector

$$X = \left(X^{(1)}, \dots, X^{(d)}\right)^{\mathsf{T}} \in \mathbb{R}^d$$

is given by

$$\Sigma = \operatorname{Cov}(X) = \mathbb{E}\left[ (X - \mathbb{E}[X]) (X - \mathbb{E}[X])^{\mathsf{T}} \right].$$

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

If  $X \in \mathbb{R}^d$  and A, B are matrices:

$$Cov(AX + B) = Cov(AX) = ACov(X)A^{\mathsf{T}} = A\Sigma_X A^{\mathsf{T}}$$

**The Multivariate Gaussian Distribution** If  $(X, T)^{\mathsf{T}}$  is a Gaussian vector then its PDF depends on 5 parameters:

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

A Gaussian vector  $X \in \mathbb{R}^d$  is completely determined by its expected value and covariance matrix  $\Sigma$ :

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

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

$$f(x) = \frac{1}{((2\pi)^d \det(\Sigma))^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^{\mathsf{T}} \Sigma^{-1} (x-\mu)\right)$$

**The Multivariate CLT** Let  $X_1, \ldots, X_n \in \mathbb{R}^d$  be independent copies of a random vector X such that  $\mathbb{E}[X] = \mu$ , Cov  $(X) = \Sigma$ , then

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

**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  $g: \mathbb{R}^d \to \mathbb{R}^k$   $(k \ge 1)$  be continuously differentiable at  $\theta$ . Then,

$$\sqrt{n}\left(g\left(T_{n}\right)-g\left(\theta\right)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\left(0,\nabla g(\theta)^{\mathsf{T}}\Sigma\,\nabla g(\theta)\right),$$

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

#### Fisher Information

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  $\ell$  is a.s. twice differentiable. Under some regularity conditions, the Fisher information of the statistical model is defined as

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

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

$$I(\theta) = \operatorname{Var} \left[\ell'(\theta)\right] = -\mathbb{E} \left[\ell''(\theta)\right].$$

## 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,  $\hat{\theta}_n^{\text{MLE}}$  satisfies

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

### The Method of Moments

## Moments

Let  $X_1, \ldots, X_n$  be an i.i.d. sample associated with a statistical model  $(E, (\mathbb{P}_{\theta})_{\theta \in \Theta})$ . Assume that  $E \subseteq \mathbb{R}$  and  $\Theta \subseteq \mathbb{R}^d$ , for some  $d \geq 1$ .

**Population Moments** Let  $m_k(\theta) = \mathbb{E}_{\theta} \left[ X_1^k \right]$ ,  $1 \leq k \leq d$ .

**Empirical Moments** Let  $\hat{m}_k = \overline{X_n^k} = \frac{1}{n} \sum_{i=1}^n X_i^k$ ,  $1 \le k \le d$ .

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:

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

## **Moments Estimator**

Let

$$M: \Theta \to \mathbb{R}^d$$
  
 $\theta \mapsto M(\theta) = (m_1(\theta), \dots, m_d(\theta))$ 

Assume M is one-to-one:

$$\theta = M^{-1}\left(m_1(\theta), \dots, m_d(\theta)\right)$$

Moments estimator of  $\theta$ :

$$\widehat{\theta}_n^{\text{MM}} = M^{-1} \left( \widehat{m}_1, \dots, \widehat{m}_d \right)$$

provided it exists.

#### Generalized Method of Moments

Applying the multivariate CLT and Delta method yields:

Theorem

$$\sqrt{n} \left( \widehat{\theta}_n^{\text{MM}} - \theta \right) \xrightarrow[n \to \infty]{(d)} \mathcal{N} \left( 0, \Gamma(\theta) \right),$$

$$\mathcal{N}^{-1} \quad \text{if} \quad \Gamma_{\partial M^{-1}} \quad \text{if} \quad \mathcal{N} \left( 0, \Gamma(\theta) \right),$$

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

#### MLE vs. Moment Estimator

- Comparison of the quadratic risks: In general, the MLE is more accurate.
- MLE still gives good results if the model is misspecified.
- Computational issues: Sometimes, the MLE is intractable but MM is easier (polynomial equations).

### M-Estimation

- Let X<sub>1</sub>,..., X<sub>n</sub> be i.i.d. with some unknown distribution ℙ in some sample space E (E ⊂ ℝ<sup>d</sup> for some d > 1).
- · No statistical model needs to be assumed (similar to ML).
- The goal is to estimate some parameter  $\mu^*$  associated with  $\mathbb{P}$ , e.g. its mean, variance, median, other quantiles, the true parameter in some statistical model, etc.
- We want to 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

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

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

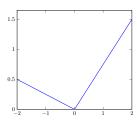
## Examples (1)

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

**Example (2)** If  $E=\mathcal{M}=\mathbb{R}$ ,  $\alpha\in(0,1)$  is fixed and  $\rho(x,\mu)=C_{\alpha}(x-\mu)$ , for all  $x,\mu\in\mathbb{R}$ :  $\mu^*$  is a  $\alpha$ -quantile of  $\mathbb{R}$ .

#### **Check Function**

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



**MLE is an M-estimator** Assume that  $\left(E, (\mathbb{P}_{\theta})_{\theta \in \Theta}\right)$  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).

#### Statistical Analysis

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

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

- Let  $J(\mu) = \frac{\partial^2 Q(\mu)}{\partial \mu \partial \mu^{\mathsf{T}}}$ .
- Under some regularity conditions,  $J(\mu) = \mathbb{E}\left[\frac{\partial^2 \rho(X_1,\mu)}{\partial \mu \partial \mu^\intercal}\right]$
- Let  $K(\mu) = \text{Cov}\left(\frac{\partial \rho(X_1, \mu)}{\partial \mu}\right)$
- · Remark: In the log-likelihood case,

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

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

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

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

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

# **Hypothesis Testing**

# **Parametric Hypothesis Testing**

## Hypotheses

$$H_0: \Delta_c = \Delta_d$$
 vs.  $H_1: \Delta_d > \Delta_c$ 

Since the data is Gaussian by assumption, we don't need the CLT

$$\overline{X}_n \sim \mathcal{N}\left(\Delta_d, \frac{\sigma_d^2}{n}\right)$$
 and  $\overline{Y}_m \sim \mathcal{N}\left(\Delta_c, \frac{\sigma_c^2}{m}\right)$ 

Then,

$$\frac{\overline{X}_n - \overline{Y}_m - (\Delta_d - \Delta_c)}{\sqrt{\frac{\sigma_d^2}{n} + \frac{\sigma_c^2}{m}}} \sim \mathcal{N}(0, 1)$$

**Asymptotic test** Assume that m=cn and  $n\to\infty$ 

Using Slutsky's theorem, we also have

$$\frac{\overline{X}_n - \overline{Y}_m - (\Delta_d - \Delta_c)}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} \quad \xrightarrow[n \to \infty]{(d)} \quad \mathcal{N}(0, 1)$$

where 
$$\widehat{\sigma}_d^2 = \frac{1}{n-1} \sum_{i=1}^n \left( X_i - \overline{X}_n \right)^2$$
 and  $\widehat{\sigma}_c^2 = \frac{1}{m-1} \sum_{i=1}^m \left( Y_i - \overline{Y}_m \right)^2$ 

We get the following test at asymptotic level  $\alpha$ :

$$R_{\psi} = \left\{ \frac{\overline{X}_n - \overline{Y}_m}{\sqrt{\frac{\widehat{\sigma}_d^2}{n} + \frac{\widehat{\sigma}_c^2}{m}}} > q_{\alpha} \right\}$$

## The $\chi^2$ Distribution

**Definition** For a positive integer d, the  $\chi^2$  distribution with d degrees of freedom is the law of the random variable  $Z_1^2 + \cdots + Z_d^2$ , where  $Z_1, \ldots, Z_d \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$ . **Properties** If  $V \sim \chi_k^2$ , then

- $\mathbb{E}[V] = \mathbb{E}[Z_1^2] + \cdots + \mathbb{E}[Z_d^2] = d$
- $\operatorname{Var}(V) = \operatorname{Var}(Z_1^2) + \cdots + \operatorname{Var}(Z_d^2) = 2d$

Sample Variance 
$$S_n = \frac{1}{n} \sum_{i=1}^n \left( X_i - \overline{X}_n \right)^2 = \frac{1}{n} \sum_{i=1}^n X_i^2 - \left( \overline{X}_n \right)^2$$

**Cochran's Theorem** If  $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$ , then

- $\overline{X}_n \perp \!\!\!\perp S_n$ , for all n.
- $\frac{nS_n}{\sigma^2} \sim \chi_{n-1}^2$

We often prefer the unbiased estimator of  $\sigma^2$ :

$$\widetilde{S}_n = \frac{1}{n-1} \sum_{i=1}^n \left( X_i - \overline{X}_n \right)^2 = \frac{n}{n-1} S_n$$

#### Student's T Distribution

**Definition** For a positive integer d, the Student's T distribution with d degrees of freedom (denoted by  $t_d$ ) is the law of the random variable  $\frac{Z}{\sqrt{V/d}}$ , where

$$Z \sim \mathcal{N}(0,1), V \sim \chi_d^2$$
 and  $Z \perp \!\!\! \perp V$ .

Student's T test (one-sample, two-sided)

Let  $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \mathcal{N}\left(\mu, \sigma^2\right)$  where both  $\mu$  and  $\sigma^2$  are unknown. We want to test:  $H_0: \mu = 0$  vs.  $H_1: \mu \neq 0$ 

Test statistic:

$$T_n = \sqrt{n} \frac{\overline{X}_n}{\sqrt{\widetilde{S}_n}} = \frac{\sqrt{n} \frac{\overline{X}_n - \mu}{\sigma}}{\sqrt{\frac{\widetilde{S}_n}{\sigma^2}}}$$

Since  $\sqrt{n}\frac{\overline{X}_n}{\sigma} \sim \mathcal{N}(0,1)$  (under  $H_0$ ) and  $\frac{\widetilde{S}_n}{\sigma^2} \sim \frac{\chi_{n-1}^2}{n-1}$  are independent by Cochran's theorem, we have

$$T_n \sim t_{n-1}$$
.

Student's test with (non-asymptotic) level  $\alpha \in (0, 1)$ :

$$\psi_{\alpha} = \mathbb{1}\left\{ |T_n| > q_{\frac{\alpha}{2}} \right\},\,$$

where  $q_{\frac{\alpha}{2}}$  is the  $\left(1-\frac{\alpha}{2}\right)$ -quantile of  $t_{n-1}$ .

#### Student's T test (one-sample, one-sided)

$$H_0: \mu < \mu_0$$
 vs.  $H_1: \mu > \mu_0$ 

Test statistic:

$$T_n = \sqrt{n} \frac{\overline{X}_n - \mu_0}{\sqrt{\widetilde{S}_n}} \sim t_{n-1} \quad \text{(under } H_0\text{)}$$

Student's test with (non-asymptotic) level  $\alpha \in (0, 1)$ :

$$\psi_{\alpha} = \mathbb{1} \{T_n > q_{\alpha}\}$$

where  $q_{\alpha}$  is the  $(1 - \alpha)$ -quantile of  $t_{n-1}$ .

Two-sample T-test

$$\frac{\overline{X}_n - \overline{Y}_m - (\Delta_d - \Delta_c)}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} \sim t_N$$

Welch-Satterthwaite formula

$$N = \frac{\left(\frac{\widehat{\sigma}_d^2}{n} + \frac{\widehat{\sigma}_c^2}{m}\right)^2}{\frac{\widehat{\sigma}_d^4}{n^2(n-1)} + \frac{\widehat{\sigma}_c^4}{m^2(m-1)}} \ge \min(n, m)$$

#### Wald's Test

A test based on the MLE Consider an i.i.d. sample  $X_1,\ldots,X_n$  with statistical model  $(E,(\mathbb{P}_{\theta})_{\theta\in\Theta})$ , where  $\Theta\subseteq\mathbb{R}^d$   $(d\geq 1)$  and let  $\theta_0\in\Theta$  be fixed and given.  $\theta^*$  is the true parameter.

Consider the following hypotheses:

$$H_0: \theta^* = \theta_0$$
 vs.  $H_1: \theta^* \neq \theta_0$ 

Let  $\widehat{\theta}_n^{\text{MLE}}$  be the MLE. Assume the MLE technical conditions are satisfied.

If  $H_0$  is true, then

$$\sqrt{n}\,I\left(\widehat{\boldsymbol{\theta}}^{\,\mathrm{MLE}}\right)^{\frac{1}{2}}\left(\widehat{\boldsymbol{\theta}}_{n}^{\,\mathrm{MLE}}-\boldsymbol{\theta}_{0}\right) \quad \xrightarrow[n\to\infty]{(d)} \quad \mathcal{N}_{d}\left(\boldsymbol{0},\mathbb{I}_{d}\right)$$

Wald's test

$$T_n := n \left( \widehat{\boldsymbol{\theta}}_n^{\, \mathrm{MLE}} - \boldsymbol{\theta}_0 \right)^{\mathsf{T}} I \left( \widehat{\boldsymbol{\theta}}_n^{\, \mathrm{MLE}} \right) \left( \widehat{\boldsymbol{\theta}}_n^{\, \mathrm{MLE}} - \boldsymbol{\theta}_0 \right) \quad \xrightarrow[n \to \infty]{} \quad \boldsymbol{\chi}_d^2$$

Wald's test with asymptotic level  $\alpha \in (0, 1)$ :

$$\psi=\mathbb{1}\left\{ T_{n}>q_{\alpha}\right\} ,$$

where  $q_{\alpha}$  is the  $(1 - \alpha)$ -quantile of  $\chi_d^2$ .

**Wald's Test in 1 dimension** In one dimension, Wald's test coincides with the two-sided test based on the asymptotic normality of the MLE.

### Likelihood Ratio Test

Basic Form of the Likelihood Ratio Test Let  $X_1,\ldots,X_n\stackrel{\mathrm{iid}}{\sim}\mathbb{P}_{\theta^*}$ , and consider the associated statistical model  $\left(E,\left(\mathbb{P}_{\theta}\right)_{\theta\in\mathbb{R}^d}\right)$ . Suppose that  $\mathbb{P}_{\theta}$  is a discrete probability distribution with pmf given by  $p_{\theta}$ .

In its most basic form, the likelihood ratio test can be used to decide between two hypotheses of the following form:

$$H_0: \theta^* = \theta_0 \text{ vs. } H_1: \theta^* = \theta_1$$

Likelihood function

$$L_n: \mathbb{R}^n \times \mathbb{R}^d \to \mathbb{R}$$
  
 $(x_1, \dots, x_n; \theta) \mapsto \prod_{i=1}^n p_{\theta}(x_i)$ 

The likelihood ratio test in this set-up is of the form

$$\psi_C = \mathbb{1}\left(\frac{L_n(x_1, \dots, x_n; \theta_1)}{L_n(x_1, \dots, x_n; \theta_0)} > C\right)$$

where C is a threshold to be specified.

A test based on the log-likelihood Consider an i.i.d. sample  $X_1,\ldots,X_n$  with statistical model  $\left(E,(\mathbb{P}_{\theta})_{\theta\in\Theta}\right)$ , where  $\Theta\subseteq\mathbb{R}^d$   $(d\geq1)$ . Suppose the null hypothesis has the form

$$H_0: (\theta_{r+1}, \dots, \theta_d) = (\theta_{r+1}^{(0)}, \dots, \theta_d^{(0)}),$$

for some fixed and given numbers  $\theta_{r+1}^{(0)}, \dots, \theta_d^{(0)}$ .

Let

$$\widehat{\theta}_n = \operatorname*{argmax}_{\theta \in \Theta} \ell_n(\theta) \qquad (MLE)$$

and

$$\widehat{\theta}_n^c = \underset{\theta \in \Theta_0}{\operatorname{argmax}} \ell_n(\theta)$$
 (constrained MLE)

where 
$$\Theta_0 = \left\{ \theta \in \Theta : (\theta_{r+1}, \dots, \theta_d) = \left(\theta_{r+1}^{(0)}, \dots, \theta_d^{(0)}\right) \right\}$$

Test statistic:

$$T_n = 2\left(\ell_n\left(\hat{\theta}_n\right) - \ell_n\left(\hat{\theta}_n^c\right)\right).$$

 $\mbox{Wilk's Theorem}$  Assume  $H_0$  is true and the MLE technical conditions are satisfied. Then,

$$T_n \xrightarrow[n \to \infty]{(d)} \chi^2_{d-r}$$

Likelihood ratio test with asymptotic level  $\alpha \in (0, 1)$ :

$$\psi = \mathbb{1}\left\{T_n > q_\alpha\right\},\,$$

where  $q_{\alpha}$  is the  $(1-\alpha)$ -quantile of  $\chi^2_{d-r}$ .

#### **Goodness of Fit Tests**

Let X be a r.v. We want to know if the hypothesized distribution is a good fit for the data.

Key characteristic of Goodness of Fit tests: no parametric modeling.

**Discrete distribution** Let  $E=\{a_1,\ldots,a_K\}$  be a finite space and  $(\mathbb{P}_{\mathbf{p}})_{\mathbf{p}\in\Delta_K}$  be the family of all probability distributions on E.

• 
$$\Delta_K = \left\{ \mathbf{p} = (p_1, \dots, p_K) \in (0, 1)^K : \sum_{j=1}^K p_j = 1 \right\}$$

• For  $\mathbf{p} \in \Delta_K$  and  $X \sim \mathbb{P}_{\mathbf{p}}$ ,

$$\mathbb{P}_{\mathbf{p}}\left[X=a_{j}\right]=p_{j}, \quad j=1,\ldots,K.$$

Let  $X_1,\ldots,X_n\stackrel{\mathrm{iid}}{\sim}\mathbb{P}_{\mathbf{p}}$ , for some unknown  $\mathbf{p}\in\Delta_K$ , and let  $\mathbf{p}^0\in\Delta_K$  be fixed. We want to test:

$$H_0: \mathbf{p} = \mathbf{p}^0$$
 vs.  $H_1: \mathbf{p} \neq \mathbf{p}^0$ 

with asymptotic level  $\alpha \in (0, 1)$ .

The Probability Simplex in K Dimensions The probability simplex in  $\mathbb{R}^K$ , denoted by  $\Delta_K$ , is the set of all vectors  $\mathbf{p} = [p_1, \dots, p_K]^{\mathsf{T}}$  such that

$$\mathbf{p} \cdot \mathbf{1} = \mathbf{p}^\mathsf{T} \mathbf{1} = 1, \quad p_i \geq 0 \quad \text{for all } K$$

where **1** denotes the vector  $\mathbf{1} = (1, \dots, 1)^{\mathsf{T}}$ 

#### Categorical Likelihood

· Likelihood of the model:

$$L_n(X_1, \dots, X_n; \mathbf{p}) = p_1^{N_1} p_2^{N_2} \dots p_K^{N_K}$$
 where  $N_i = \# \{i = 1, \dots, n : X_i = a_i\}$ .

Let \( \hat{\boldsymbol{p}} \) be the MLE:

$$\widehat{\mathbf{p}}_j = \frac{N_j}{n}, \quad j = 1, \dots, K.$$

 $\widehat{\mathbf{p}}$  maximizes  $\log L_n(X_1,\ldots,X_n,\mathbf{p})$  under the constraint.

 $\chi^{\bf 2}$  test  $\,$  If  $H_0$  is true, then  $\sqrt{n}\left(\widehat{\bf p}-{\bf p}^0\right)$  is asymptotically normal, and the following holds:

**Theorem** Under  $H_0$ :

$$T_n = n \sum_{j=1}^n \frac{\left(\widehat{\mathbf{p}}_j - \mathbf{p}_j^0\right)^2}{\mathbf{p}_j^0} \quad \xrightarrow[n \to \infty]{(d)} \quad \chi_{K-1}^2$$

CDF and empirical CDF Let  $X_1, \ldots, X_n$  be i.i.d. real random variables. The CDF of  $X_1$  is defined as

$$F(t) = \mathbb{P}[X_1 \le 1], \quad \forall t \in \mathbb{R}.$$

It completely characterizes the distribution of  $X_1$ .

The **empirical CDF** of the sample  $X_1, \ldots, X_n$  is defined as

$$F_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1} \{X_i \le 1\}$$
  
=  $\frac{\#\{i = 1, \dots, n : X_i \le t\}}{n}$ ,  $\forall t \in \mathbb{R}$ .

**Consistency** By the LLN, for all  $t \in \mathbb{R}$ ,

$$F_n(t) \xrightarrow[n \to \infty]{a.s.} F(t).$$

Glivenko-Cantelli Theorem (Fundamental theorem of statistics)

$$\sup_{t \in \mathbb{R}} |F_n(t) - F(t)| \xrightarrow[n \to \infty]{a.s.} 0$$

**Asymptotic normality** By the CLT, for all  $t \in \mathbb{R}$ ,

$$\sqrt{n}\left(F_n(t) - F(t)\right) \xrightarrow{(d)} \mathcal{N}\left(0, F(t)\left(1 - F(t)\right)\right)$$

**Donsker's Theorem** If *F* is continuous, then

$$\sqrt{n} \sup_{t \in \mathbb{R}} |F_n(t) - F(t)| \xrightarrow{a.s.} \sup_{0 < t < 1} |\mathbf{B}(t)|,$$

where  $\mathbf{B}(t)$  is a Brownian bridge on [0, 1].

## Kolmogorov-Smirnov Test

Let  $T_n = \sup_{t \in \mathbb{R}} \sqrt{n} |F_n(t) - F(t)|$ . By Donsker's theorem, if  $H_0$  is true, then

 $T_n \xrightarrow[n \to \infty]{(d)} Z$ , where Z has a known distribution (supremum of the absolute value of a Brownian bridge).

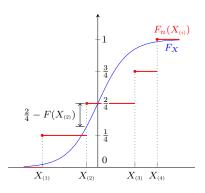
KS test with asymptotic level  $\alpha$ :

$$\delta_{\alpha}^{\text{KS}} = \mathbb{1}\left\{T_n > q_{\alpha}\right\}$$

where  $q_{\alpha}$  is the  $(1 - \alpha)$ -quantile of Z.

Let  $X_{(1)} \leq X_{(2)} \leq \cdots \leq X_{(n)}$  be the reordered sample. The expression for  $T_n$ 

$$T_{n} = \sqrt{n} \max_{i=1,\dots,n} \left\{ \max \left( \left| \frac{i-1}{n} - F^{0}\left(X_{(i)}\right) \right|, \left| \frac{i}{n} - F^{0}\left(X_{(i)}\right) \right| \right) \right\}.$$



**Pivotal Distribution**  $T_n$  is called a **pivotal statistic**: If  $H_0$  is true, the distribution of  $T_n$  does not depend on the distribution of the  $X_i$ 's.

## Other Goodness of Fit Tests

Kolmogorov-Smirnov

$$d(F_n, F) = \sup_{t \in \mathbb{R}} |F_n(t) - F(t)|$$

Cramér-Von Mises

$$d^{2}(F_{n}, F) = \int_{\mathbb{R}} \left[ F_{n}(t) - F(t) \right]^{2} dF(t)$$
$$= \underset{X \sim F}{\mathbb{E}} \left[ \left| F_{n}(X) - F(X) \right|^{2} \right]$$

Anderson-Darling

$$d^{2}(F_{n}, F) \int_{\mathbb{R}} \frac{[F_{n}(t) - F(t)]^{2}}{F(t)(1 - F(t))} dF(t)$$

## Kolmogorov-Lilliefors Test

We want to test if X has a Gaussian distribution with unknown parameters. In this case, Donsker's theorem is *no longer valid*. Instead, we compute the quantiles for the test statistic

$$\sup_{t \in \mathbb{R}} \left| F_n(t) - \Phi_{\hat{\mu}, \hat{\sigma}^2}(t) \right|$$

where  $\hat{\mu}=\overline{X}_n$ ,  $\hat{\sigma}^2=S_n^2$  and  $\Phi_{\hat{\mu},\hat{\sigma}^2}(t)$  is the CDF of  $\mathcal{N}\left(\hat{\mu},\hat{\sigma}^2\right)$ .

They do not depend on unknown parameters.

## Quantile-Quantile (QQ) plots

- Provide a visual way to perform goodness of fit tests.
- Not a formal test but quick and easy check to see if a distribution is plausible.
- Main idea: We want to check visually if the plot of F<sub>n</sub> is close to that of F or, equivalently, if the plot of F<sub>n</sub><sup>-1</sup> is close to F<sup>-1</sup>.
- · Check if the points

$$\left(F^{-1}(\frac{1}{n}), F_n^{-1}(\frac{1}{n})\right), \dots, \left(F^{-1}(\frac{n-1}{n}), F_n^{-1}(\frac{n-1}{n})\right)$$

are near the line y = x.

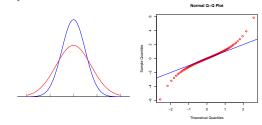
•  $F_n$  is not technically invertible but we define

$$F_n^{-1}(\frac{i}{n}) = X_i,$$

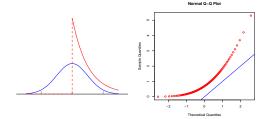
the  $i^{th}$  largest observation.

#### Four patterns

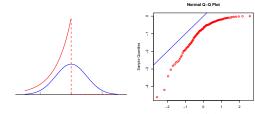
heavy tails



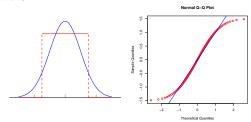
right skewed



3. left skewed



4. light tails



# **Bayesian Statistics**

# **Introduction to Bayesian Statistics**

### Prior and Posterior

• Consider a probability distribution on a parameter space  $\Theta$  with some PDF  $\pi(\cdot)$ : the **prior distribution**.

- Let  $X_1, \ldots, X_n$  be a sample of n random variables.
- Denote by  $L_n(\cdot|\theta)$  the joint PDF of  $X_1,\ldots,X_n$  conditionally on  $\theta$ , where  $\theta\sim\pi$ .
- Remark:  $L_n(X_1, \ldots, X_n | \theta)$  is the likelihood used in the frequentist approach.
- The conditional distribution of  $\theta$  given  $X_1,\ldots,X_n$  is called the **posterior distribution**. Denote by  $\pi(\cdot|X_1,\ldots,X_n)$  its PDF.

#### Bayes' formula

$$\pi(\theta|X_1,\ldots,X_n) \propto \pi(\theta)L_n(X_1,\ldots,X_n|\theta), \quad \forall \theta \in \Theta$$

## Bernoulli experiment with a Beta prior

•  $p \sim \text{Beta}(a, a)$ :

$$\pi(p) \propto p^{a-1} (1-p)^{a-1}, \quad p \in (0,1)$$

• Given  $p, X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{Ber}(p)$ , so

$$L_n(X_1,...,X_n|p) = p^{\sum_{i=1}^n X_i} (1-p)^{n-\sum_{i=1}^n X_i}.$$

Hence.

$$\pi(p|X_1,\ldots,X_n) \propto p^{a-1+\sum_{i=1}^n X_i} (1-p)^{a-1+n-\sum_{i=1}^n X_i}$$

• The posterior distribution is

Beta 
$$\left(a + \sum_{i=1}^{n} X_i, a + n - \sum_{i=1}^{n} X_i\right)$$
 conjugate prior

#### Non-informative Priors

- We can still use a Bayesian approach if we have no prior information about the parameter.
- Good candidate:  $\pi(\theta) \propto 1$ , i.e., constant PDF on  $\Theta$ .
- If  $\Theta$  is bounded, this is the uniform prior on  $\Theta$ .
- If  $\Theta$  is unbounded, this define a proper PDF on  $\Theta$ .
- An improper prior on  $\Theta$  is a measurable, non-negative function  $\pi(\cdot)$  defined on  $\Theta$  that is not integrable:

$$\int \pi(\theta)d\theta = \infty.$$

 In general, one can still define a posterior distribution using an improper prior, using Bayes' formula.

## Jeffreys Prior and Bayesian Confidence Interval

Jeffreys prior is an attempt to incorporate frequentist ideas of likelihood in the Bayesian framework, as well as an example of a **non-informative prior**:

$$\pi_J(\theta) \propto \sqrt{\det I(\theta)}$$

where  $I(\theta)$  is the Fisher information matrix of the statistical model associated with  $X_1, \ldots, X_n$  in the frequentist approach (provided it exists).

#### Examples

- Bernoulli experiment:  $\pi_J(\theta) \propto \frac{1}{\sqrt{p(1-p)}}, \quad p \in (0,1)$ : the prior is  $\text{Beta}(\frac{1}{2},\frac{1}{2})$
- Gaussian experiment:  $\pi_J(\theta) \propto 1, \theta \in \mathbb{R}$ , is an improper prior

Jeffreys prior satisfies a **reparametrization invariance principle**: If  $\eta$  is a reparametrization of  $\theta$  (i.e.,  $\eta=\phi(\theta)$  for some one-to-one map  $\phi$ ), then the PDF  $\tilde{\pi}(\cdot)$  of  $\eta$  satisfies:

$$\tilde{\pi}(\eta) \propto \sqrt{\det \tilde{I}(\eta)},$$

where  $\tilde{I}(\eta)$  is the Fisher information of the statistical model parametrized by  $\eta$  instead of  $\theta$ .

**Bayesian confidence regions** For  $\alpha \in (0,1)$ , a Bayesian confidence region with level  $\alpha$  is a random subset  $\mathcal R$  of the parameter space  $\Theta$ , which depends on the sample  $X_1,\ldots,X_n$ , such that

$$\mathbb{P}\left[\theta \in \mathcal{R}|X_1, \dots, X_n\right] = 1 - \alpha.$$

Note that  $\mathcal{R}$  depends on the prior  $\pi(\cdot)$ .

Bayesian confidence region and confidence interval are two distinct notions.

## Bayesian estimation

- Posterior mean:  $\widehat{\theta}^{(\pi)} = \int_{\Theta} \theta \pi (\theta | X_1, \dots, X_n) d\theta$
- MAP (maximum a posteriori):  $\widehat{\theta}^{\,\mathrm{MAP}} = \mathop{\mathrm{argmax}}_{\theta \in \Theta} \pi(\theta|X_1,\dots,X_n)$

It is the point that maximizes the posterior distribution, provided it is unique.

# **Linear Regression**

**Modeling Assumptions**  $(X_i, Y_i)$ ,  $i = 1, \ldots, n$ , are i.i.d. from some *unknown joint distribution*  $\mathbb{P}$ .  $\mathbb{P}$  can be described entirely by (assuming all exist):

- either a joint PDF h(x, y)
- the marginal density of X,  $h(x) = \int h(x, y) dy$  and the conditional density

$$h(y|x) = \frac{h(x,y)}{h(x)}$$

h(y|x) answers all our questions. It contains all the information about Y given X.

Partial Modeling We can also describe the distribution only partially, e.g. using

- the expectation of  $Y : \mathbb{E}[Y]$
- the conditional expectation of Y given X = x:  $\mathbb{E}[X = x]$ . The function

$$x \mapsto f(x) := \mathbb{E}[Y|X = x] = \int yh(y|x)dy$$

is called **regression function**.

- · other possibilities:
  - the conditional median: m(x) such that

$$\int_{-\infty}^{m(x)} h(y|x)dy = \frac{1}{2}$$

- conditional quantiles
- conditional variance (not information about location)

Linear Regression We focus on modeling the regression function

$$f(x) = \mathbb{E}\left[Y|X=x\right].$$

Restrict to simple functions. The simplest is

$$f(x) = a + bx$$
 linear (or affine) function

**Probabilistic Analysis** Let X and Y be two r.v. (not necessarily independent) with two moments and such that Var(X) > 0. The theoretical linear regression of Y on X is the line  $x \mapsto a^* + b^*x$ , where

$$(a^*, b^*) = \underset{(a,b) \in \mathbb{R}^2}{\operatorname{argmin}} \mathbb{E}\left[ (Y - a - bX)^2 \right]$$

which gives

$$a^* = \frac{\operatorname{Cov}(X, Y)}{\operatorname{Var}(X)}$$

$$b^* = \mathbb{E}[Y] - b^* \mathbb{E}[X] = \mathbb{E}[Y] - \frac{\operatorname{Cov}(X, Y)}{\operatorname{Var}(X)} \mathbb{E}[X]$$

**Noise** The points are not exactly on the line  $x \mapsto a^* + b^* x$  if Var(Y|X=x) > 0. The random variable  $\varepsilon = Y - (a^* + b^* X)$  is called **noise** and satisfies

$$Y = a^* + b^*X + \varepsilon,$$

with  $\mathbb{E}[\varepsilon] = 0$  and  $Cov(X, \varepsilon) = 0$ 

**Statistical Problem** In practice,  $a^*$ ,  $b^*$  need to be estimated from data.

**Least Squares** The **least squares estimator** (LSE) of (a,b) is the minimizer of the sum of squared errors:

$$\sum_{i=1}^{n} (Y_i - a - bX_i)^2.$$

Then,

$$\hat{b} = \frac{\overline{XY} - \overline{X}\,\overline{Y}}{\overline{X^2} - \overline{X}^2}$$

$$\hat{a} = \overline{Y} - \hat{b}\overline{X}$$

## **Multivariate Regression**

We have a vector of explanatory variables or **covariates**:

$$\mathbf{X}_i = egin{pmatrix} X_i^{(1)} \ dots \ X_i^{(p)} \end{pmatrix} \in \mathbb{R}^p.$$

The response or dependent variable is  $Y_i$  with

$$Y_i = \mathbf{X}_i^{\mathsf{T}} \boldsymbol{\beta}^* + \varepsilon_i, \quad i = 1, \dots, n$$

and  $\beta_1^*$  is called the **intercept**.

**Least Squares Estimator** The least squares estimator of  $\beta^*$  is the minimizer of the sum of squared errors

$$\widehat{oldsymbol{eta}} = \operatorname*{argmin}_{eta \in \mathbb{R}^p} \sum_{i=1}^n \left( Y_i - \mathbf{X}_i^\intercal oldsymbol{eta} 
ight)^2$$

LSE in Matrix Form

- Let  $\mathbf{Y} = (Y_1, \dots, Y_n)^{\mathsf{T}} \in \mathbb{R}^n$ .
- Let X be the n × p matrix whose rows are X<sub>1</sub><sup>T</sup>,..., X<sub>n</sub><sup>T</sup>. X is called the design matrix.
- Let  $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_n)^{\mathsf{T}} \in \mathbb{R}^n$ , the unobserved noise. Then,

$$\mathbf{Y} = \mathbb{X}\boldsymbol{\beta}^* + \boldsymbol{\varepsilon}, \quad \boldsymbol{\beta}^* \text{ unknown.}$$

• The LSE  $\widehat{\beta}$  satisfies

$$\widehat{oldsymbol{eta}} = \operatorname*{argmin}_{eta \in \mathbb{R}^p} \lVert \mathbf{Y} - \mathbb{X} oldsymbol{eta} 
Vert_2^2$$

**Closed Form Solution** Assume that rank(X) = p. Then,

$$\widehat{\boldsymbol{\beta}} = (\mathbb{X}^{\mathsf{T}}\mathbb{X})^{-1}\,\mathbb{X}^{\mathsf{T}}\mathbf{Y}.$$

**Geometric Interpretation of the LSE**  $\mathbb{X}\widehat{\boldsymbol{\beta}}$  is the orthogonal projection of  $\mathbf{Y}$  onto the subspace spanned by the columns of  $\mathbb{X}$ :

$$\mathbb{X}\widehat{\boldsymbol{\beta}} = P\mathbf{Y},$$

where  $P = \mathbb{X} (\mathbb{X}^{\mathsf{T}} \mathbb{X})^{-1} \mathbb{X}^{\mathsf{T}}$ .

Statistical Inference To make inference, we need more assumptions.

- The design matrix X is deterministic and rank(X) = p.
- The model is **homoscedastic**:  $\varepsilon_1, \ldots, \varepsilon_n$  are i.i.d.
- The noise vector  $\varepsilon$  is Gaussian:

$$\boldsymbol{\varepsilon} \sim \mathcal{N}_n \left( 0, \sigma^2 \mathbb{I}_n \right)$$

for some known or unknown  $\sigma^2 > 0$ .

## Properties of LSE

- LSE = MSE
- Distribution of  $\widehat{\boldsymbol{\beta}}$ :

$$\widehat{\boldsymbol{\beta}} \sim \mathcal{N}_p\left(\boldsymbol{\beta}^*, \sigma^2\left(\mathbb{X}^\intercal \mathbb{X}\right)^{-1}\right)$$

Quadratic Risk of β:

$$\mathbb{E}\left[\left\|\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right\|_{2}^{2}\right] = \sigma^{2} \mathrm{tr}\left(\left(\mathbb{X}^{\mathsf{T}} \mathbb{X}\right)^{-1}\right)$$

• Prediction Error:

$$\mathbb{E}\left[\left\|\mathbf{Y} - \mathbb{X}\widehat{\boldsymbol{\beta}}\right\|_{2}^{2}\right] = \sigma^{2}\left(n - p\right)$$

• Unbiased estimator of  $\sigma^2$ :

$$\widehat{\sigma}^2 = \frac{\|\mathbf{Y} - \mathbb{X}\widehat{\boldsymbol{\beta}}\|_2^2}{n-p} = \frac{1}{n-p} \sum_{i=1}^n \widehat{\varepsilon}_i^2$$

#### Significance Tests

- Test whether the  $j^{th}$  explanatory variable is significant in the linear regression.
- $H_0: \beta_i = 0 \text{ v.s. } H_1: \beta \neq 0$
- If  $\gamma_i$  ( $\gamma_i > 0$ ) is the  $j^{\text{th}}$  diagonal coefficient of  $(X^{\mathsf{T}}X)^{-1}$ :

$$\frac{\widehat{\beta}_j - \beta_j}{\sqrt{\widehat{\sigma}^2 \gamma_j}} \sim t_{n-p}$$

- Let  $T_n^{(j)} = \frac{\widehat{\beta}_j}{\sqrt{\widehat{\sigma}^2 \gamma_j}}$ .
- Test with non-asymptotic level  $\alpha \in (0, 1)$ :

$$R_{j,\alpha} = \left\{ \left| T_n^{(j)} \right| > q_{\frac{\alpha}{2}} \left( t_{n-p} \right) \right\}$$

where  $q_{\underline{\alpha}}(t_{n-p})$  is the  $(1-\frac{\alpha}{2})$ -quantile of  $t_{n-p}$ .

**Bonferroni's test** Test whether a **group** of explanatory variables is significant in the linear regression.

- $H_0: \beta_i = 0 \ \forall i \in S \text{ v.s. } H_1: \exists i \in S, \beta_i \neq 0 \text{ where } S \subseteq \{1, \dots, p\}.$
- · Bonferroni's test:

$$R_{S,\alpha} = \bigcup_{j \in S} R_{j,\frac{\alpha}{k}}, \text{ where } k = |S|$$

## **Generalized Linear Model**

**Generalization** A generalized linear model (GLM) generalizes normal linear regression models in the following directions:

- 1. Random component:  $Y|X = x \sim$  some distribution
- 2. Regression function:

$$q(\mu(x)) = x^{\mathsf{T}}\beta$$

where g is called link function and  $\mu(x)=\mathbb{E}\left[Y|X=x\right]$  is the regression function.

## **Exponential Family**

A family of distribution  $\{\mathbb{P}_{\theta}: \theta \in \Theta\}$ ,  $\Theta \subset \mathbb{R}^k$  is said to be a k-parameter exponential family on  $\mathbb{R}^q$ , if there exist real-valued functions

- $\eta_1, \ldots, \eta_k$  and  $B(\theta)$
- $T_1, \ldots, T_k$ , and  $h(y) \in \mathbb{R}^q$

such that the density function of  $\mathbb{P}_{\theta}$  can be written as

$$f_{\theta}(y) = \exp\left[\sum_{i=1}^{k} \eta_i(\theta) T_i(y) - B(\theta)\right] h(y)$$

**Examples of discrete distributions** The following distributions for **discrete** exponential families of distributions with PMF:

- Bernoulli (p):  $p^y(1-p)^{1-y}$ ,  $y \in \{0,1\}$
- Poisson ( $\lambda$ ):  $\frac{\lambda^y}{y!}e^{-\lambda}$ ,  $y=0,1,\ldots$

**Examples of continuous distributions** The following distributions form **continuous** exponential families of distributions with PDF:

- Gamma (a, b):  $\frac{1}{\Gamma(a)b^a}y^{a-1}e^{-\frac{y}{b}}$
- Inverse Gamma  $(\alpha, \beta)$ :  $\frac{\beta^{\alpha}}{\Gamma(\alpha)} y^{-\alpha-1} e^{-\frac{\beta}{y}}$
- Inverse Gaussian  $(\mu, \sigma^2)$ :  $\sqrt{\frac{\sigma^2}{2\pi y^3}} \exp\left(-\frac{\sigma^2 (y-\mu)^2}{2\mu^2 y}\right)$

#### **One-parameter Canonical Exponential Family**

$$f_{\theta}(y) = \exp\left(\frac{y\theta - b(\theta)}{\phi} + c(y, \phi)\right)$$

for some known functions  $b(\theta)$  and  $c(y, \phi)$ .

- If  $\phi$  is known, this is a one-parameter exponential family with  $\theta$  being the canonical parameter.
- If  $\phi$  is unknown, this may/may not be a two-parameter exponential family.
- $\phi$  is called **dispersion parameter**.

Expected value Note that

$$\ell(\theta) = \frac{Y\theta - b(\theta)}{\phi} + c(Y; \phi),$$

which leads to

$$\mathbb{E}\left[Y\right] = b'(\theta).$$

Variance

$$Var(Y) = b''(\theta) \cdot \phi$$

In GLM, we have  $Y|X=x\sim$  distribution in exponential family. Then,

$$\mathbb{E}\left[Y|X=x\right] = f\left(X^{\mathsf{T}}\beta\right)$$

**Link function**  $\beta$  is the parameter of interest. A **link function** g relates the linear predictor  $X^{\mathsf{T}}\beta$  to the mean parameter  $\mu$ ,

$$X^{\mathsf{T}}\beta = g(\mu) = g(\mu(X)).$$

g is required to be monotone increasing and differentiable

$$\mu = g^{-1} \left( X^{\mathsf{T}} \beta \right)$$

**Canonical Link** The function g that links the mean  $\mu$  to the canonical parameter  $\theta$  is called **canonical link**:

$$g(\mu) = \theta$$
.

Since  $\mu = b'(\theta)$ , the canonical link is given by

$$g(\mu) = (b')^{-1}(\mu)$$

If  $\phi > 0$ , the canonical link function is strictly increasing.

Example Bernoulli distribution

$$p^{y}(1-p)^{1-y} = \exp\left(y\log\left(\frac{p}{1-p}\right) + \log(1-p)\right)$$
$$= \exp\left(y\theta - \log(1+e^{\theta})\right)$$

Hence, 
$$\theta = \log\left(\frac{p}{1-p}\right)$$
 and  $b(\theta) = \log\left(1+e^{\theta}\right)$  .

$$b'(\theta) = \frac{e^{\theta}}{1 + e^{\theta}} = \mu \quad \iff \quad \theta = \log\left(\frac{\mu}{1 - \mu}\right)$$

The canonical link for the Bernoulli distribution is the logit link

#### Model and Notation

Let  $(X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$ , i = 1, ..., n be independent random pairs such that the conditional distribution of  $Y_i$  given  $X_i = x_i$  has density in the canonical exponential family:

$$f_{\theta_i}(y_i) = \exp\left[\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i, \phi)\right]$$

**Back to**  $\beta$ : Given a link function g, note the following relationship between  $\beta$  and  $\theta$ :

$$\theta_i = (b')^{-1}(\mu_i) = (b')^{-1} \left( g^{-1}(X_i^{\mathsf{T}}\beta) \right) \equiv h\left( X_i^{\mathsf{T}}\beta \right)$$

where h is defined as

$$h = (b')^{-1} \circ g^{-1} = (g \circ b')^{-1}.$$

If g is the canonical link function, h is the **identity**  $g = (b')^{-1}$ .

Log-likelihood The log-likelihood is given by

$$\begin{split} \ell_n\left(\mathbf{Y}, \mathbb{X}, \beta\right) &= \sum_i \frac{Y_i \theta_i - b(\theta_i)}{\phi} + \text{constant} \\ &= \sum_i \frac{Y_i h\left(X_i^\intercal \beta\right) - b\left(h\left(X_i^\intercal \beta\right)\right)}{\phi} + \text{constant} \end{split}$$

When we use the canonical link function, we obtain the expression

$$\ell_{n}\left(\mathbf{Y}, \mathbb{X}, \beta\right) = \sum_{i} \frac{Y_{i} X_{i}^{\mathsf{T}} \beta - b\left(X_{i}^{\mathsf{T}} \beta\right)}{\phi} + \text{constant}$$

Strict concavity The log-likelihood  $\ell(\theta)$  is strictly concave (if  $\mathrm{rank}(\mathbb{X})=p$ ) using the canonical function when  $\phi>0$ . As a consequence, the maximum likelihood estimator is unique.

On the other hand, if another parametrization is used, the likelihood function may not be strictly concaving leading to *several local maxima*.

## **Recommended Resources**

- Probability and Statistics (DeGroot and Schervish)
- Mathematical Statistics and Data Analysis (Rice)
- Fundamentals of Statistics [Lecture Slides] (http://www.edx.org)

Please share this cheatsheet with friends!