

18.6501x Fundamentals of Statistics

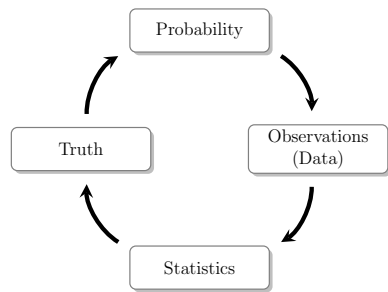
This is a cheat sheet for statistics based on the online course given by Prof. Philippe Rigollet. Compiled by Janus B. Advincula.

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

Law of Large Numbers

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i \xrightarrow[n \rightarrow \infty]{\mathbb{P}, a.s.} \mu.$$

Central Limit Theorem

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

Equivalently,

$$\sqrt{n} (\bar{X}_n - \mu) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma^2).$$

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

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

The Gaussian Distribution

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

- $X \sim \mathcal{N}(\mu, \sigma^2)$
- $\mathbb{E}[X] = \mu$
- $\text{Var}(X) = \sigma^2 > 0$

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 $a, b \in \mathbb{R}$,
$$aX + b \sim \mathcal{N}(a\mu + b, a^2\sigma^2).$$
- Standardization:** If $X \sim \mathcal{N}(\mu, \sigma^2)$, then
$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1)$$

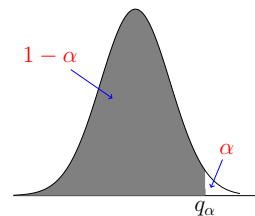
We can compute probabilities from the CDF of $Z \sim \mathcal{N}(0, 1)$:

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

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

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

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



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

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

Convergence in Probability

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

Convergence in Distribution

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

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 $(T_n)_{n \geq 1}$ 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):

$$T_n \xrightarrow[n \rightarrow \infty]{(d)} T \implies \mathbb{P}(a \leq T_n \leq b) \xrightarrow[n \rightarrow \infty]{} \mathbb{P}(a \leq T \leq b)$$

Addition, Multiplication, Division

Assume

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

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

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

Slutsky's Theorem

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

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

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

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

Continuous Mapping Theorem

If f is a continuous function, then

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

Foundation of Inference

Statistical Model

Let the observed outcome of a statistical experiment be a *sample* X_1, \dots, 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*;
- $(\mathbb{P}_\theta)_{\theta \in \Theta}$ 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 $\exists \theta$ such that $\mathbb{P} = \mathbb{P}_\theta$. 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 $\Theta = \Theta_1 \times \Theta_2$, where Θ_1 is finite dimensional and Θ_2 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 θ 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., $\bar{X}_n, \max_i X_i$, etc.

Estimator of θ Any statistic whose expression does not depend on θ

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

$$\hat{\theta}_n \overset{\mathbb{P} \text{ (resp. a.s.)}}{\underset{n \rightarrow \infty}{\rightarrow}} \theta \quad (\text{w.r.t. } \mathbb{P}).$$

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

$$\sqrt{n} \left(\hat{\theta}_n - \theta \right) \overset{(d)}{\underset{n \rightarrow \infty}{\rightarrow}} \mathcal{N} \left(0, \sigma^2 \right)$$

Bias of an Estimator

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

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

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

Jensen’s Inequality

- If the function $f(x)$ is convex,

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

- If the function $g(x)$ is concave,

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

Quadratic 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, \dots, X_n , and assume $\Theta \subseteq \mathbb{R}$. Let $\alpha \in (0, 1)$.

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

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

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

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

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

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

$$\sqrt{n} \frac{\bar{R}_n - p}{\sqrt{p(1-p)}} \overset{(d)}{\underset{n \rightarrow \infty}{\rightarrow}} \mathcal{N}(0, 1)$$

- It yields

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

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

Three solutions:

- Conservative bound
- Solving the (quadratic) equation for p
- Plug-in

The Delta Method

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

$$\sqrt{n} (Z_n - \theta) \overset{(d)}{\underset{n \rightarrow \infty}{\rightarrow}} \mathcal{N} \left(0, \sigma^2 \right)$$

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

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

$$\sqrt{n} (g(Z_n) - g(\theta)) \overset{(d)}{\underset{n \rightarrow \infty}{\rightarrow}} \mathcal{N} \left(0, (g'(\theta))^2 \sigma^2 \right).$$

Introduction to Hypothesis Testing

Statistical Formulation Consider a sample X_1, \dots, X_n of i.i.d. random variables and a statistical model $(E, (\mathbb{P}_\theta)_{\theta \in \Theta})$. Let Θ_0 and Θ_1 be disjoint subsets of Θ .

Consider the two hypotheses:

- $H_0 : \theta \in \Theta_0$
- $H_1 : \theta \in \Theta_1$

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 ψ :

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

- Type 1 error** of a test ψ :

$$\begin{aligned} \alpha_\psi : \Theta_0 &\rightarrow \mathbb{R} \quad (\text{or } [0, 1]) \\ \theta &\mapsto \mathbb{P}_\theta [\psi = 1] \end{aligned}$$

- Type 2 error** of a test ψ :

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

- Power** of a test ψ :

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

Level, test statistic and rejection region

- A test ψ has level α if

$$\alpha_\psi(\theta) \leq \alpha, \quad \forall \theta \in \Theta_0.$$

- A test ψ has asymptotic level α if

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

- 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 ψ_α is the smallest (asymptotic) level α at which ψ_α 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, \dots, X_n . Assume that there exists $\theta^* \in \Theta$ such that $X_1 \sim \mathbb{P}_{\theta^*}$.

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

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

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

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

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

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

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

Properties of Total Variation

- $\text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = \text{TV}(\mathbb{P}_{\theta'}, \mathbb{P}_\theta)$ **symmetric**
- $\text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \geq 0, \text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \leq 1$ **positive**
- If $\text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) = 0$, then $\mathbb{P}_\theta = \mathbb{P}_{\theta'}$ **definite**
- $\text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}) \leq \text{TV}(\mathbb{P}_\theta, \mathbb{P}_{\theta''}) + \text{TV}(\mathbb{P}_{\theta''}, \mathbb{P}_{\theta'})$ **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}_θ and $\mathbb{P}_{\theta'}$ is defined by

KL (P_theta, P_theta') = { sum_{x in E} p_theta(x) log (p_theta(x) / p_theta'(x)) if E is discrete; integral_E f_theta(x) log (f_theta(x) / f_theta'(x)) dx if E is continuous }

KL-divergence is also known as **relative entropy**.

Properties of KL-divergence

- KL (P_theta, P_theta') != KL (P_theta', P_theta) in general
- KL (P_theta, P_theta') >= 0
- If KL (P_theta, P_theta') = 0, then P_theta = P_theta' (definite)
- KL (P_theta, P_theta') <= KL (P_theta, P_theta'') + KL (P_theta'', P_theta') in general

Maximum Likelihood Estimation

Likelihood, Discrete Case Let (E, (P_theta)_theta in Theta) be a statistical model associated with a sample of i.i.d. r.v. X_1, ..., 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 x Theta -> R; (x_1, ..., x_n; theta) -> P_theta [X_1 = x_1, ..., X_n = x_n] = product_{i=1}^n P_theta [X_i = x_i]

Likelihood, Continuous Case Let (E, (P_theta)_theta in Theta) be a statistical model associated with a sample of i.i.d. r.v. X_1, ..., X_n. Assume that all the P_theta have density f_theta.

Definition The likelihood of the model is the map L defined as

L : E^n x Theta -> R; (x_1, ..., x_n; theta) -> product_{i=1}^n f_theta(x_i)

Maximum Likelihood Estimator Let X_1, ..., X_n be an i.i.d. sample associated with a statistical model (E, (P_theta)_theta in Theta) and let L be the corresponding likelihood.

Definition The maximum likelihood estimator of theta is defined as

theta_n^MLE = argmax_{theta in Theta} L (X_1, ..., X_n, theta),

provided it exists.

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

theta_n^MLE = argmax_{theta in Theta} log L (X_1, ..., X_n, theta),

Concave and Convex Functions

A twice-differentiable function h : Theta subset R -> R is said to be **concave** if its second derivative satisfies

h''(theta) <= 0, for all 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) >= 0 (h''(theta) > 0).

Multivariate Concave Functions More generally, for a multivariate function:

h : Theta subset R^d -> R, d >= 2, define the

- **gradient vector:**

nabla h(theta) = (partial h(theta) / partial theta_1, ..., partial h(theta) / partial theta_d)^T in R^d

- **Hessian matrix:**

Hh(theta) = (partial^2 h(theta) / partial theta_1 partial theta_1, ..., partial^2 h(theta) / partial theta_1 partial theta_d, ..., partial^2 h(theta) / partial theta_d partial theta_1, ..., partial^2 h(theta) / partial theta_d partial theta_d) in R^{d x d}

h is concave <=> x^T Hh(theta) x <= 0, for all x in R^d, theta in Theta

h is strictly concave <=> x^T Hh(theta) x < 0, for all x in R^d, theta in Theta

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

theta_n^MLE ->_{n -> inf} P theta*

Covariance In general, when theta subset R^d, d >= 2, its coordinates are not necessarily independent. The covariance between two random variables X and Y is

Cov(X, Y) := E [(X - E[X]) (Y - E[Y])] = E [XY] - E[X] E[Y]

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 = (X^{(1)}, ..., X^{(d)})^T in R^d

is given by

Sigma = Cov (X) = E [(X - E[X]) (X - E[X])^T].

This is a matrix of size d x d.

If X in R^d and A, B are matrices:

Cov (AX + B) = Cov (AX) = A Cov (X) A^T = A Sigma_X A^T

The Multivariate Gaussian Distribution If (X, T)^T is a Gaussian vector then its PDF depends on 5 parameters:

E[X], Var(X), E[Y], Var(Y), and Cov(X, Y).

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

X ~ N_d (mu, Sigma).

It has PDF over R^d given by:

f(x) = 1 / ((2pi)^d det (Sigma))^{1/2} exp (- 1/2 (x - mu)^T Sigma^{-1} (x - mu))

The Multivariate CLT Let X_1, ..., X_n in R^d be independent copies of a random vector X such that E[X] = mu, Cov (X) = Sigma, then

sqrt(n) (X_bar_n - mu) ->_{n -> inf} N_d (0, Sigma)

Multivariate Delta Method Let (T_n)_{n >= 1} sequence of random vectors in R^d such that

sqrt(n) (T_n - theta) ->_{n -> inf}^{(d)} N_d (0, Sigma),

for some theta in R^d and some covariance Sigma in R^{d x d}. Let g : R^d -> R^k (k >= 1) be continuously differentiable at theta. Then,

sqrt(n) (g (T_n) - g (theta)) ->_{n -> inf}^{(d)} N (0, nabla g(theta)^T Sigma nabla g(theta)),

where nabla g(theta) = partial g(theta) / partial theta = (partial g_j / partial theta_i)_{1 <= i <= d, 1 <= j <= k} in R^{d x k}

Fisher Information

Define the log-likelihood for one observation as

l(theta) = log L_1 (X, theta), theta in Theta subset 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) = E [nabla l(theta) nabla l(theta)^T] - E [nabla l(theta)] E [nabla l(theta)]^T = -E [Hl(theta)].

If Theta subset R, we get

I(theta) = Var [l'(theta)] = -E [l''(theta)].

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 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, theta_n^MLE satisfies

- theta_n^MLE ->_{n -> inf} P theta* w.r.t. P_theta*;
- sqrt(n) (theta_n^MLE - theta*) ->_{n -> inf}^{(d)} N_d (0, I^{-1} (theta*)) w.r.t. P_theta*.

The Method of Moments

Moments

Let X_1, ..., X_n be an i.i.d. sample associated with a statistical model (E, (P_theta)_theta in Theta). Assume that E subset R and Theta subset R^d, for some d >= 1.

Population Moments Let m_k(theta) = E_theta [X_1^k], 1 <= k <= d.

Empirical Moments Let m_k = X_bar_n^k = 1/n sum_{i=1}^n X_i^k, 1 <= k <= d.

From LLN,

m_k ->_{n -> inf}^{P/a.s.} m_k(theta)

More compactly, we say that the whole vector converges:

(m_1, ..., m_d) ->_{n -> inf}^{P/a.s.} (m_1(theta), ..., 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}(m_1(\theta), \dots, m_d(\theta))

Moments estimator of \theta:

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

provided it exists.

Generalized Method of Moments

Applying the multivariate CLT and Delta method yields:

Theorem

\sqrt{n}(\hat{\theta}_n^{MM} - \theta) \xrightarrow[n \to \infty]{(d)} \mathcal{N}(0, \Gamma(\theta)),

where \Gamma(\theta) = \left[\frac{\partial M^{-1}}{\partial \theta} M(\theta) \right]^{\top} \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_1, \dots, 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 \ge 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}[\rho(X_1, \mu)]

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

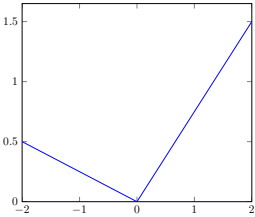
Examples (1)

- 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{P}.

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{P}.

Check Function

C_\alpha = \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).

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^\top}.

- Under some regularity conditions, J(\mu) = \mathbb{E} \left[\frac{\partial^2 \rho(X_1, \mu)}{\partial \mu \partial \mu^\top} \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) \quad (\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 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}(0, J(\mu^*)^{-1} K(\mu^*) J(\mu^*)^{-1})

Hypothesis Testing

Parametric Hypothesis Testing

Hypotheses

H_0 : \Delta_c = \Delta_d \quad \text{vs.} \quad H_1 : \Delta_d > \Delta_c

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

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

Then,

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

where \hat{\sigma}_d^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^2 and \hat{\sigma}_c^2 = \frac{1}{m-1} \sum_{i=1}^m (Y_i - \bar{Y}_m)^2

We get the following test at asymptotic level \alpha:

R_\psi = \left\{ \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\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 + \dots + Z_d^2, where Z_1, \dots, 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] + \dots + \mathbb{E}[Z_d^2] = d
- \text{Var}(V) = \text{Var}(Z_1^2) + \dots + \text{Var}(Z_d^2) = 2d

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

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

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

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

\tilde{S}_n = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^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, \dots, X_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2) where both \mu and \sigma^2 are unknown. We want to test:

H_0 : \mu = 0 \quad \text{vs.} \quad H_1 : \mu \neq 0

Test statistic:

T_n = \sqrt{n} \frac{\bar{X}_n}{\sqrt{\tilde{S}_n}} = \frac{\sqrt{n} \bar{X}_n - \mu}{\sqrt{\frac{\sigma}{\tilde{S}_n}}}

Since \sqrt{n} \frac{\bar{X}_n}{\sigma} \sim \mathcal{N}(0, 1) (under H_0) and \frac{\tilde{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 (1 - \frac{\alpha}{2})-quantile of t_{n-1}.

Student’s T test (one-sample, one-sided)

$H_0 : \mu \leq \mu_0 \quad \text{vs.} \quad H_1 : \mu > \mu_0$

Test statistic:

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

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

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

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

Two-sample T-test

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

Welch-Satterthwaite formula

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

Wald’s Test

A test based on the MLE Consider an i.i.d. sample X_1, \dots, 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. θ^* is the true parameter.

Consider the following hypotheses:

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

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

If H_0 is true, then

$$\sqrt{n} \, I \left(\widehat{\theta}_n^{\text{MLE}} \right)^{\frac{1}{2}} \left(\widehat{\theta}_n^{\text{MLE}} - \theta_0 \right) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}_d(0, \mathbb{I}_d)$$

Wald’s test

$$T_n := n \left(\widehat{\theta}_n^{\text{MLE}} - \theta_0 \right)^\top I \left(\widehat{\theta}_n^{\text{MLE}} \right) \left(\widehat{\theta}_n^{\text{MLE}} - \theta_0 \right) \xrightarrow[n \rightarrow \infty]{(d)} \chi_d^2$$

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

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

where q_α is the $(1 - \alpha)$ -quantile of χ_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 $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \mathbb{P}_{\theta^*}$, and consider the associated statistical model $(E, (\mathbb{P}_\theta)_{\theta \in \mathbb{R}^d})$. Suppose that \mathbb{P}_θ is a discrete probability distribution with pmf given by p_θ .

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

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

Likelihood function

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

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, \dots, X_n with statistical model $(E, (\mathbb{P}_\theta)_{\theta \in \Theta})$, where $\Theta \subseteq \mathbb{R}^d$ ($d \geq 1$). Suppose the null hypothesis has the form

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

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

Let

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

and

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

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:

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

Wilk’s Theorem Assume H_0 is true and the MLE technical conditions are satisfied. Then,

$$T_n \xrightarrow[n \rightarrow \infty]{(d)} \chi_{d-r}^2$$

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

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

where q_α is the $(1 - \alpha)$ -quantile of χ_{d-r}^2 .

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 $E = \{a_1, \dots, a_K\}$ 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 $X \sim \mathbb{P}_\mathbf{p}$,

$$\mathbb{P}_\mathbf{p} [X = a_j] = p_j, \quad j = 1, \dots, K.$$

Let $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \mathbb{P}_\mathbf{p}$, for some unknown $\mathbf{p} \in \Delta_K$, and let $\mathbf{p}^0 \in \Delta_K$ be fixed.

We want to test:

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

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

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

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

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

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 $N_j = \# \{i = 1, \dots, n : X_i = a_j\}$.

- Let $\widehat{\mathbf{p}}$ be the MLE:

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

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

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

Theorem Under H_0 :

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

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

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

It completely characterizes the distribution of X_1 .

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

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

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

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

Glivenko-Cantelli Theorem (Fundamental theorem of statistics)

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

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

$$\sqrt{n} (F_n(t) - F(t)) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, F(t) (1 - F(t)))$$

Donsker’s Theorem If F is continuous, then

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

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

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

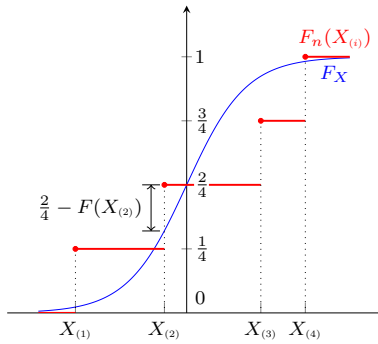
KS test with asymptotic level α :

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

where q_α is the $(1 - \alpha)$ -quantile of Z .

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

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



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

$$\begin{aligned} d^2(F_n, F) &= \int_{\mathbb{R}} [F_n(t) - F(t)]^2 dF(t) \\ &= \mathbb{E}_{X \sim F} [|F_n(X) - F(X)|^2] \end{aligned}$$

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

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

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

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_n is close to that of F or, equivalently, if the plot of F_n^{-1} is close to F^{-1} .
- Check if the points

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

are near the line $y = x$.

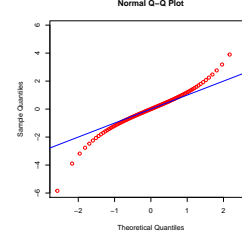
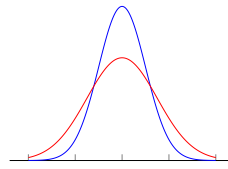
- F_n is not technically invertible but we define

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

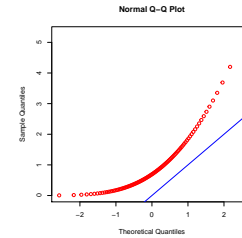
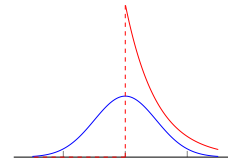
the i^{th} largest observation.

Four patterns

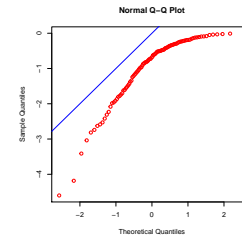
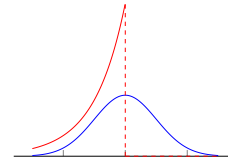
1. heavy tails



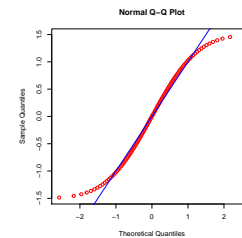
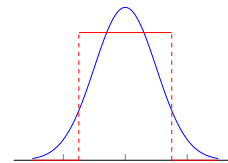
2. right skewed



3. left skewed



4. light tails



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

Bayes' formula

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

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

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

- Hence,

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

- The posterior distribution is

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

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 Θ .
- If Θ is bounded, this is the uniform prior on Θ .
- If Θ is unbounded, this does not define a proper PDF on Θ .
- An **improper prior** on Θ is a measurable, non-negative function $\pi(\cdot)$ defined on Θ 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, \dots, X_n in the frequentist approach (provided it exists).

Examples

- Bernoulli experiment: $\pi_J(\theta) \propto \frac{1}{\sqrt{p(1-p)}}$, $p \in (0, 1)$: 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

Bayesian Statistics

Introduction to Bayesian Statistics

Prior and Posterior

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

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

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

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

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

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

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

Bayesian confidence region and *confidence interval* are two **distinct** notions.

Bayesian estimation

- **Posterior mean**: $\hat{\theta}^{(\pi)} = \int_{\Theta} \theta \pi(\theta | X_1, \dots, X_n) d\theta$
 - **MAP (maximum a posteriori)**: $\hat{\theta}^{\text{MAP}} = \underset{\theta \in \Theta}{\operatorname{argmax}} \pi(\theta | X_1, \dots, X_n)$
- It is the point that maximizes the posterior distribution, provided it is unique.

Linear Regression

Modeling Assumptions $(X_i, Y_i), i = 1, \dots, n$, 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

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

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

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

Restrict to *simple* functions. The simplest is

$$f(x) = a + bx \quad \text{linear (or affine) function}$$

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

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

which gives

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

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

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

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

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

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**:

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

The **response** or **dependent variable** is Y_i with

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

and $\boldsymbol{\beta}_1^*$ is called the **intercept**.

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

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{i=1}^n (Y_i - \mathbf{X}_i^\top \boldsymbol{\beta})^2$$

LSE in Matrix Form

- Let $\mathbf{Y} = (Y_1, \dots, Y_n)^\top \in \mathbb{R}^n$.
- Let \mathbb{X} be the $n \times p$ matrix whose rows are $\mathbf{X}_1^\top, \dots, \mathbf{X}_n^\top$. \mathbb{X} is called the **design matrix**.
- Let $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_n)^\top \in \mathbb{R}^n$, the unobserved noise. Then,

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

- The LSE $\hat{\boldsymbol{\beta}}$ satisfies

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{Y} - \mathbb{X} \boldsymbol{\beta}\|_2^2.$$

Closed Form Solution Assume that $\text{rank}(\mathbb{X}) = p$. Then,

$$\hat{\boldsymbol{\beta}} = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top \mathbf{Y}.$$

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

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

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

Statistical Inference To make inference, we need more assumptions.

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

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

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

Properties of LSE

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

$$\hat{\boldsymbol{\beta}} \sim \mathcal{N}_p(\boldsymbol{\beta}^*, \sigma^2 (\mathbb{X}^\top \mathbb{X})^{-1})$$

- Quadratic Risk of $\hat{\boldsymbol{\beta}}$:

$$\mathbb{E}[\|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*\|_2^2] = \sigma^2 \text{tr}((\mathbb{X}^\top \mathbb{X})^{-1})$$

- Prediction Error:

$$\mathbb{E}[\|\mathbf{Y} - \mathbb{X} \hat{\boldsymbol{\beta}}\|_2^2] = \sigma^2 (n - p)$$

- Unbiased estimator of σ^2 :

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

Significance Tests

- Test whether the j^{th} explanatory variable is significant in the linear regression.
- $H_0 : \beta_j = 0$ v.s. $H_1 : \beta \neq 0$
- If γ_j ($\gamma_j > 0$) is the j^{th} diagonal coefficient of $(\mathbb{X}^\top \mathbb{X})^{-1}$:

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

- Let $T_n^{(j)} = \frac{\hat{\beta}_j}{\sqrt{\hat{\sigma}^2 \gamma_j}}$.

- Test with non-asymptotic level $\alpha \in (0, 1)$:

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

where $q_{\frac{\alpha}{2}}(t_{n-p})$ 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.

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

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

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:**

$$g(\mu(x)) = x^\top \beta$$
where g is called **link function** and $\mu(x) = \mathbb{E}[Y|X = x]$ 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

- η_1, \dots, η_k and $B(\theta)$
- T_1, \dots, T_k , and $h(y) \in \mathbb{R}^q$

such that the density function of \mathbb{P}_θ 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 form **discrete** exponential families of distributions with PMF:

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

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 (α, β): $\frac{\beta^\alpha}{\Gamma(\alpha)} y^{-\alpha-1} e^{-\frac{\beta}{y}}$
- Inverse Gaussian (μ, σ^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 ϕ is known, this is a one-parameter exponential family with θ being the **canonical parameter**.
- If ϕ is unknown, this may /may not be a two-parameter exponential family.
- ϕ is called **dispersion parameter**.

Expected value Note that

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

which leads to

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

Variance

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

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

$$\mathbb{E}[Y|X = x] = f(X^\top \beta)$$

Link function β is the parameter of interest. A **link function** g relates the linear predictor $X^\top \beta$ to the mean parameter μ ,

$$X^\top \beta = g(\mu) = g(\mu(X)).$$

g is required to be monotone increasing and differentiable

$$\mu = g^{-1}(X^\top \beta)$$

Canonical Link The function g that links the mean μ to the canonical parameter θ 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

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

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

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

The canonical link for the Bernoulli distribution is the **logit link**.

Model and Notation

Let $(X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i = 1, \dots, n$ 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 β : Given a link function g , note the following relationship between β and θ :

$$\theta_i = (b')^{-1}(\mu_i) = (b')^{-1} \left(g^{-1}(X_i^\top \beta) \right) \equiv h(X_i^\top \beta)$$

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

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

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

$$\ell_n(\mathbf{Y}, \mathbb{X}, \beta) = \sum_i \frac{Y_i X_i^\top \beta - b(X_i^\top \beta)}{\phi} + \text{constant}$$

Strict concavity The log-likelihood $\ell(\theta)$ is **strictly concave** (if $\text{rank}(\mathbb{X}) = p$) 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!