Introduction to Machine Learning and Data Science

2. Review of Probability and Statistics

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References

- **Introduction to Probability for Data Science**, Stanley H. Chan. [Link] (Book, slides and videos)
- **Probability Theory Review for Machine Learning (CS229)**, Samuel Ieong. [Link]
- **All of Statistics**, Larry Wasserman. [Link]

Outline

Sample space and events

- When we speak about probability, we often refer to the probability of **an event of uncertain nature** taking place.
- We first need to clarify what the **possible events** to which we want to attach probability are.
- We often conduct an experiment, i.e., take some measurements of a **random (stochastic) process**.
- Our measurements take values in some set Ω, the **sample space** (or the outcome space), which defines *all possible outcomes* of our measurements.

Sample space and events

- We toss one coin. Two outcomes: *heads* (H) or *tails* (T).
  - $\Omega = \{H, T\}$.
- We toss two coins:
  - $\Omega = \{HH, HT, TH, TT\}$.
- We measure the reaction time to some stimulus:
  - $\Omega = (0, \infty)$.

Sample space and events

An **event** A is a subset of Ω ($A \subseteq \Omega$), i.e., it is a subset of possible outcomes of our experiment. We say that an event A **occurs** if the outcome of our experiment belongs to the set A.

- Let $\Omega = \{HH, HT, TH, TT\}$, and consider the following events:
  - $A_1 = \{HH, TH, TT\}$ and $A_2 = \{TH, TT\}$.

  We observe $\omega = HH$. Which events did occur?

- Let $\Omega = (0, \infty)$, and consider the following events:
  - $A_1 = (3, 6)$, $A_2 = (1, 2)$ and $A_3 = (2, 8)$.

  We observe $\omega = 4$. Which events did occur?

Probability space

A **probability space** is defined by the triple $(\Omega, \mathcal{F}, \mathbb{P})$ where

- Ω is the **sample space**,
- $\mathcal{F}$ is the **space of events** (or event space); we abusively[1] assume here that $\mathcal{F} = 2^{\Omega}$,
- $\mathbb{P}$ is the **probability measure/distribution** that maps an event $A \in \mathcal{F}$ to a real value between 0 and 1.

[1] 2^S is the set of all subsets of S, including S and the empty set $\emptyset$. Note that $\mathcal{F} = 2^{\Omega}$ is not mathematically sound in general, but it is sufficient for our practical purposes.

Probability axioms

A **probability distribution** is a mapping from events to real numbers that satisfy certain **axioms**:

1. *Non-negativity*:

$$\forall A \in \mathcal{F}, \mathbb{P}(A) \geq 0.$$

2. *Unity of* Ω:

$$\mathbb{P}(\Omega) = 1.$$

3. σ*-additivity*. For all *disjoint* events $A_1, A_2, \ldots \in \mathcal{F}$ (i.e., for all $i \neq j$, $A_i \cap A_j = \emptyset$), we have that

$$\mathbb{P}\left(\bigcup_{i=1}^{+\infty} A_i\right) = \sum_{i=1}^{+\infty} \mathbb{P}(A_i).$$

Probability properties

Using set theory and the probability axioms, we can show several useful and intuitive properties of probability distributions.

- $\mathbb{P}(\emptyset) = 0$.
- For all $A, B \in \mathcal{F}$, $A \subset B \implies \mathbb{P}(A) \leq \mathbb{P}(B)$.
- For all $A \in \mathcal{F}$, $0 \leq \mathbb{P}(A) \leq 1$.
- For all $A \in \mathcal{F}$, $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$.
- For all $A, B \in \mathcal{F}$, $P(A \cup B) = P(A) + P(B) - P(A \cap B)$.

All of these properties can be understood via a **Venn diagram**.

Probability properties

- $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$.

$$\begin{aligned}
&\mathbb{P}(\Omega) = 1 \quad (\textbf{Axiom } 2) \\
&\iff \mathbb{P}(A \cup A^c) = 1, \quad \forall A \subseteq \Omega \\
&\iff \mathbb{P}(A^c) + \mathbb{P}(A) = 1 \quad (\textbf{Axiom } 3) \\
&\iff \mathbb{P}(A^c) = 1 - \mathbb{P}(A).
\end{aligned}$$

- $A \subseteq B \implies \mathbb{P}(A) \leq \mathbb{P}(B)$.

$$\begin{aligned}
&A \subseteq B \\
&\implies B = A \cup (B \backslash A) \\
&\implies \mathbb{P}(B) = \mathbb{P}(A) + \mathbb{P}(B \backslash A) \quad (\textbf{Axiom } 3, \text{ using that } A \cap (B \backslash A) = \emptyset) \\
&\implies \mathbb{P}(B) \geq \mathbb{P}(A) \quad (\textbf{Axiom } 1).
\end{aligned}$$

Probability of an event (discrete case)

- The probability of any event $A = \{\omega_1, \omega_2, \ldots, \omega_k\}$ ($\omega \in \Omega$) is the sum of the probabilities of its elements:

$$\mathbb{P}(A) = \mathbb{P}(\{\omega_1, \omega_2, \ldots, \omega_k\}) = \sum_{i=1}^{k} \mathbb{P}(\{\omega_i\}).$$

- If Ω consists of n equally likely outcomes (i.e., a uniform distribution), then the probability of any event A is

$$\mathbb{P}(A) = \frac{|A|}{|\Omega|} = \frac{|A|}{n}.$$

- Suppose we toss a **fair** dice twice. The sample space is $\Omega = \{(t_1, t_2) : t_1, t_2 = 1, 2, \ldots, 6\}$. Let A be the event that the sum of two tosses being < 5. What is $\mathbb{P}(A)$?

Conditional probability

If $\mathbb{P}(B) > 0$, the **conditional probability** of A *given* B is

$$\mathbb{P}(A \mid B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}.$$

Note that $\mathbb{P}(A \mid B) \neq \mathbb{P}(B \mid A)$ (in general).

The **chain rule** can be obtained by rewriting the above expression as follows:

$$\mathbb{P}(A \cap B) = \mathbb{P}(B)\mathbb{P}(A \mid B) = \mathbb{P}(A)\mathbb{P}(B \mid A).$$

More generally, we have

$$\mathbb{P}(A_1 \cap A_2 \cap A_3 \dots) = \mathbb{P}(A_1)\mathbb{P}(A_2 \mid A_1)\mathbb{P}(A_3 \mid A_1 \cap A_2) \dots$$

Independence of events

Two events A and B are **independent** if

$$\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B).$$

A finite set of events $(A_j)_{j \in J}$ are **mutually independent** if for all subsets $I \subseteq J$,

$$\mathbb{P}\left(\bigcap_{i \in I} A_i\right) = \prod_{i \in I} \mathbb{P}(A_i).$$

Conditional probability gives another interpretation of independence: A and B are independent if the *unconditional probability* is the **same** as the *conditional probability*.

When combined with other properties of probability, independence can often **simplify the calculation** of the probability of certain events.

Example

Consider a **fair** coin. What is the probability of *at least one head in the first 10 (**independent**) tosses*?

Let A be the event "at least one head in 10 tosses". Then, A^c is the event "No heads in 10 tosses" (all 10 tosses being tails).

We have

$$\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T_1 \cap T_2 \cap \cdots \cap T_{10}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T_i) \qquad \text{(independent tosses)} \\
&= 1 - \left(\frac{1}{2}\right)^{10} \qquad \text{(fair coin)}.
\end{aligned}$$

Exercise

Consider tossing a **fair** dice. Let A be the event that the result is an odd number, and $B = \{1, 2, 3\}$.

- Compute $\mathbb{P}(A \mid B)$.
- Compute $\mathbb{P}(A)$.
- Are A and B independent?

Law of total probability

Let $A_1, A_2, \ldots, A_n \in \mathcal{F}$ be a *partition* of Ω. Then, for any $B \in \mathcal{F}$, we have that

$$\mathbb{P}(B) = \sum_{i=1}^{n} \mathbb{P}(B \cap A_i) = \sum_{i=1}^{n} \mathbb{P}(B \mid A_i)\mathbb{P}(A_i).$$

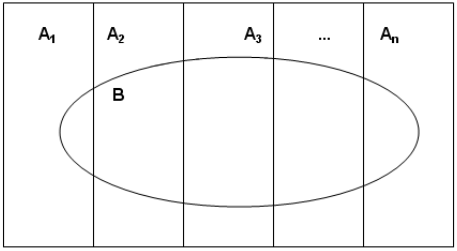


Image source: https://mathwiki.cs.ut.ee/probability/04_total_probability

Law of total probability: proof

The **law of total probability** is a combination of additivity and conditional probability. We have

$$\begin{aligned}\mathbb{P}(B) &= \mathbb{P}((B \cap A_1) \cup (B \cap A_2) \cup \cdots \cup (B \cap A_k)) \\ &= \sum_{i=1}^{n} \mathbb{P}(B \cap A_i) \qquad \text{(since events } (B \cap A_i)_i \text{ are disjoint)} \\ &= \sum_{i=1}^{n} \mathbb{P}(B \mid A_i)\mathbb{P}(A_i).\end{aligned}$$

Bayes' Rule

Let $A, B \in \mathcal{F}$ be two events with positive probability. **Bayes' rule** states that

$$\mathbb{P}(A \mid B) = \frac{\mathbb{P}(B \mid A)\mathbb{P}(A)}{\mathbb{P}(B)}.$$

Roughly, Bayes' rule allows us to calculate $\mathbb{P}(A \mid B)$ from $\mathbb{P}(B \mid A)$. This is useful when $\mathbb{P}(A \mid B)$ is *not obvious to calculate* but $\mathbb{P}(B \mid A)$ is easy to obtain.

Bayes' rule follows from the definition of conditional probability (two uses):

$$\mathbb{P}(A \mid B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)} = \frac{\mathbb{P}(B \mid A)\mathbb{P}(A)}{\mathbb{P}(B)}.$$

Example

Suppose there are exactly three types of emails:

- $A_1 =$ Spam,
- $A_2 =$ Low Priority,
- $A_3 =$ High Priority.

Based on previous experience, we have

$$\mathbb{P}(A_1) = 0.85,\ \mathbb{P}(A_2) = 0.1,\ \mathbb{P}(A_3) = 0.05.$$

Let B be the event that an email contains the word "free", then

$$\mathbb{P}(B \mid A_1) = 0.9,\ \mathbb{P}(B \mid A_2) = 0.1,\ \mathbb{P}(B \mid A_3) = 0.1.$$

When we receive an email containing the word "free", **what is the probability that it is a spam**?

Outline

Random variables

Often we are interested in dealing with *summaries of experiments* rather than the actual *outcome*.

For instance, suppose we toss a coin three times. But we may only be interested in a "summary", such as the number of heads. We have

$$\begin{array}{c} \Omega \\ \downarrow \\ \mathbb{R} \end{array} = \{\underbrace{HHH}_{\downarrow 3}, \underbrace{HHT}_{\downarrow 2}, \underbrace{HTH}_{\downarrow 2}, \underbrace{THH}_{\downarrow 2}, \underbrace{TTH}_{\downarrow 1}, \underbrace{THT}_{\downarrow 1}, \underbrace{HTT}_{\downarrow 1}, \underbrace{TTT}_{\downarrow 0}\}.$$

These summary statistics are called **random variables**. Specifically, a random variable X is a (measurable) *function* from the sample space Ω to the real numbers:

$$X : \Omega \to \mathbb{R}.$$

Random variables

A random variable (r.v.) can be seen as a **mapping** between

- a distribution on Ω,

to

- a distribution on the reals (or the *range* $\mathcal{X} \subseteq \mathbb{R}$ of the r.v.).

Formally, we have that for some subset $S \subseteq \mathcal{X}$,

$$\mathbb{P}_X(X \in S) = \mathbb{P}(\{\omega \in \Omega \mid X(\omega) \in S\}).$$

Random variables

$$\begin{array}{c} \Omega = \{\underbrace{HHH}_{3}, \underbrace{HHT}_{2}, \underbrace{HTH}_{2}, \underbrace{THH}_{2}, \underbrace{TTH}_{1}, \underbrace{THT}_{1}, \underbrace{HTT}_{1}, \underbrace{TTT}_{0}\}. \\ \downarrow \\ \mathbb{R} \end{array}$$

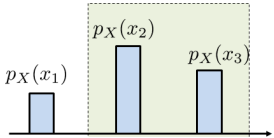
For the previous example, we have

$$\mathbb{P}_X(X = 0) = 1/8, \quad \mathbb{P}_X(X = 1) = 3/8,$$

$$\mathbb{P}_X(X = 2) = 3/8, \quad \mathbb{P}_X(X = 3) = 1/8.$$

Outline

Probability mass function



A random variable is **discrete** if its image $\mathcal{X}$ is a countable set.

The **probability mass function** (PMF) of a discrete random variable X is a function which specifies the *probability* of obtaining a number x. We denote the PMF as

$$p_X(x) = \mathbb{P}(X = x).$$

A function p_X is a PMF if and only if

1. $\forall x \in \mathcal{X}, p_X(x) \geq 0$,
2. $\sum_{x \in \mathcal{X}} p_X(x) = 1$.

What is the PMF of the previous coin flip example?

Some important discrete distributions

- The discrete **uniform** distribution on K categories. The PMF of $X \in \{C_1, C_2, \ldots, C_K\}$ is given by
$$p_X(x) = \frac{1}{k}, \qquad \forall x \in \{C_1, C_2, \ldots, C_K\}.$$
- The **Bernoulli** distribution with parameter $p \in [0, 1]$. The PMF of $X \in \{0, 1\}$ is given by
$$p_X(x) = \begin{cases} p & \text{if } x = 1 \\ 1 - p & \text{if } x = 0 \end{cases} = p^x(1-p)^{1-x}.$$
It can represent a coin toss when the coin has bias p, where 1 denotes *heads* and 0 denotes *tails*.
- Other important distributions: Binomial, Geometric, Poisson, etc.
- The symbol "$\sim$" denotes "distributed as", i.e., $X \sim \text{Ber}(p)$ means that X has a Bernoulli distribution with parameter p.

Expectation

The **expectation** of a random variable X is

$$\mathbb{E}[X] = \sum_{x \in \mathcal{X}} x \; p_X(x).$$

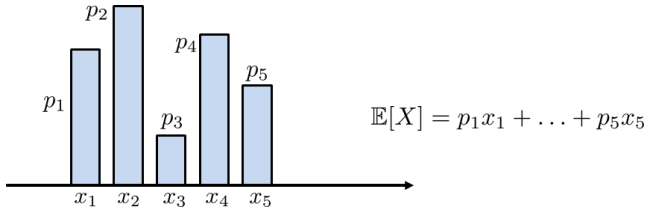


Image source: Introduction to Probability for Data Science, Stanley H. Chan.

Expectation and its properties

For any function $g\colon \mathbb{R} \to \mathbb{R}$, we have

$$\mathbb{E}[g(X)] = \sum_{x \in \mathcal{X}} g(x)\ p_X(x).$$

For any functions $g\colon \mathbb{R} \to \mathbb{R}$ and $h\colon \mathbb{R} \to \mathbb{R}$,

$$\mathbb{E}[g(X) + h(X)] = \mathbb{E}[g(X)] + \mathbb{E}[h(X)].$$

For any constant $c \in \mathbb{R}$,

$$\mathbb{E}[cX] = c\mathbb{E}[X].$$

For any constant $c \in \mathbb{R}$,

$$\mathbb{E}[X + c] = \mathbb{E}[X] + c.$$

Moments and variance

The k-th **moment** of a random variable X is

$$\mathbb{E}[X^k] = \sum_{x \in \mathcal{X}} x^k \; p_X(x).$$

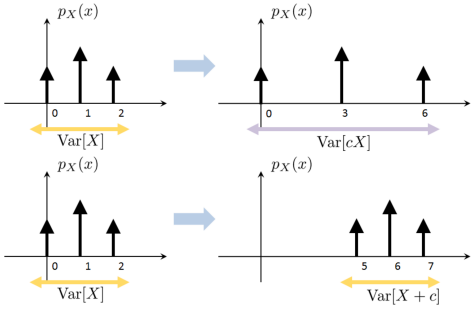
The **variance** of a random variable X is

$$\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2].$$

The **standard deviation** of X, often denoted σ, is $\sqrt{\mathrm{Var}(X)}$.

Useful properties of the variance include:

- $\mathrm{Var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2$,
- $\mathrm{Var}(cX) = c^2\mathrm{Var}(X)$,
- $\mathrm{Var}(X + c) = \mathrm{Var}(X)$.



Outline

Probability density function

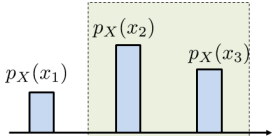


Image source: Introduction to Probability for Data Science, Stanley H. Chan.

A random variable is **continuous** if its image $\mathcal{X}$ is an uncountable set.

The **probability density function** (PDF) of a continuous random variable X is a function $f_X : \mathcal{X} \to [0, +\infty)$, when integrated over an interval $[a, b]$, yields the probability of obtaining $\{x \in \mathcal{X} \mid a \leq x \leq b\}$:

$$\mathbb{P}(a \leq X \leq b) = \int_a^b f_X(x)dx.$$

A PDF must satisfy the following properties:

$$(1) \quad \forall x \in \mathcal{X}, f_X(x) \geq 0, \qquad (2) \quad \int_{\mathcal{X}} f_X(x)dx = 1.$$

Note: $f_X(x)$ is not the probability that $X = x$ (e.g., we can have $f_X(x) > 1$).

Some important continuous distributions

- The continuous **uniform** distribution on interval $[a, b]$. The PDF is given by

$$f_X(x) = \frac{1}{b-a} \quad (x \in [a, b]).$$

  We write $X \sim \mathcal{U}[a, b]$.
- The **Gaussian** or **normal** distribution. With a location (mean) μ and scale (standard deviation) σ, the PDF is given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (x \in \mathbb{R}).$$

  We write $X \sim \mathcal{N}(\mu, \sigma^2)$.

Expectation and its properties

The **expectation** of a continuous random variable X is given by

$$\mathbb{E}[X] = \int_{\mathcal{X}} x f_X(x) dx.$$

For any function $g\colon \mathcal{X} \to \mathbb{R}$, we have

$$\mathbb{E}[g(X)] = \int_{\mathcal{X}} g(x) f_X(x) dx.$$

Let $I_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A \end{cases}$. Then, we have

$$\mathbb{E}[I_A(X)] = \int_{\mathcal{X}} I_A(x) f_X(x) dx = \int_A f_X(x) dx = \mathbb{P}(X \in A).$$

Moments and variance

The k-th **moment** of a continuous random variable X is

$$\mathbb{E}[X^k] = \int_{\mathcal{X}} x^k \; f_X(x) dx.$$

The **variance** of a continuous random variable X is

$$\text{Var}(X) = \mathbb{E}[(X - \mu_X)^2] = \int_{\mathcal{X}} (x - \mu_X)^2 \; f_X(x) dx,$$

where $\mu_X = \mathbb{E}[X]$. The **standard deviation** of X is $\sqrt{\text{Var}(X)}$.

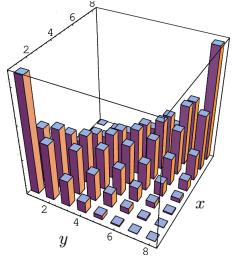
The properties of variance introduced previously still hold in this case.

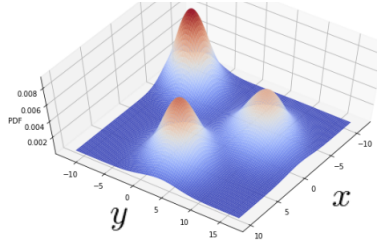
Exercise. If $X \sim \mathcal{U}[a, b]$, what is $\mathbb{E}[X]$ and $\text{Var}(X)$?

Outline

More than one random variable?

- **Multivariate** random variables or **random vectors** are ubiquitous in modern data analysis.
- The uncertainty in the random vector is characterized by a **joint** PMF or PDF.
- We first focus in this section on **bivariate** random variables.





Important concepts

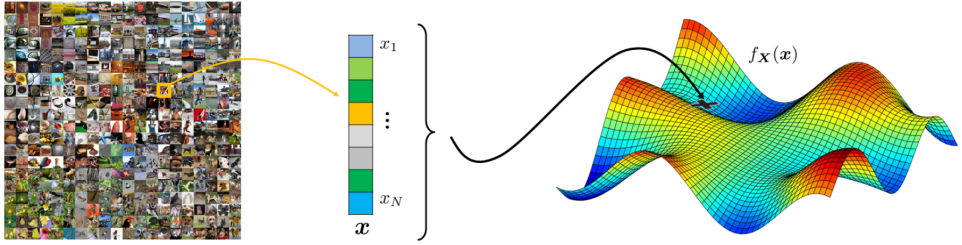
- Joint distribution
- Marginal distribution
- Independence
- Joint expectations
- Covariance and correlation
- Conditional distribution
- Conditional expectations

What are joint distributions?

One random variable is characterized by a PDF f_X (or PMF p_X), whose input x is single-dimensional.

We can characterize N random variables $X_1, \ldots, X_N$ using a PDF $f_{X_1,\ldots,X_N}$ that takes as an input an N-dimensional vector $\mathbf{x} = (x_1, \ldots, x_N)$.

Why do we need more than one dimension?



For instance, the ImageNet dataset consists of images, which can be represented as a 3-dimensional array of pixels of size $224 \times 224 \times 3$. Each pixel is a random variable, and the joint distribution of all pixels characterizes the distribution over all images.

Joint PMF

Let X and Y be two **discrete** random variables. The **joint PMF** of X and Y is defined as

$$p_{X,Y}(x,y) = \mathbb{P}(X = x \text{ and } Y = y).$$

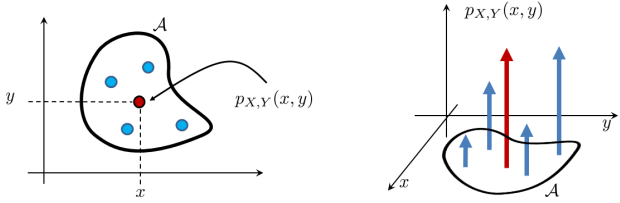


Image source: Introduction to Probability for Data Science, Stanley H. Chan.

For any $A \subseteq \mathcal{X} \times \mathcal{Y}$, we have

$$\mathbb{P}((X,Y) \in A) = \sum_{(x,y)\in A} p_{X,Y}(x,y).$$

Example

Let X be a coin flip, Y be a dice. Find the **joint PMF**.

The *sample space* of X is $\{0, 1\}$. The *sample space* of Y is $\{1, 2, 3, 4, 5, 6\}$. The joint PMF is

			Y			
	1	2	3	4	5	6
X = 0	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$
X = 1	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$

Equivalently, we have

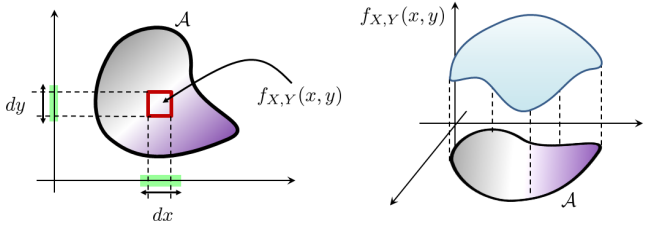
$$p_{X,Y}(x, y) = \frac{1}{12} \text{ for all } x \in \{0, 1\}, y \in \{1, 2, 3, 4, 5, 6\}.$$

Joint PDF

Let X and Y be two **continuous** random variables. The **joint PDF** of X and Y is a function $f_{X,Y}(x,y)$ that can be integrated to yield a probability:

$$\mathbb{P}((X,Y) \in A) = \int_A f_{X,Y}(x,y)dx\ dy,$$

for any (measurable) $A \subseteq \mathcal{X} \times \mathcal{Y}$.



Exercise. Consider a uniform joint PDF $f_{X,Y}(x,y)$ defined on the square $[0,2]^2$ with $f_{X,Y}(x,y) = 1/4$ for all $(x,y) \in [0,2]^2$. Find (i) $\mathbb{P}([a,b] \times [c,d])$ for $0 \leq a \leq b \leq 2$ and $0 \leq c \leq d \leq 2$, and (ii) $\mathbb{P}(X + Y \leq 2)$.

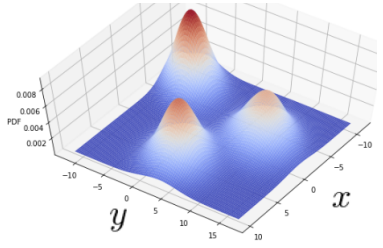
Marginal distribution

The **marginal PMFs** of discrete r.v. are defined as

$$p_X(x) = \sum_{y \in \mathcal{Y}} p_{X,Y}(x, y) \text{ and } p_Y(y) = \sum_{x \in \mathcal{X}} p_{X,Y}(x, y),$$

and the **marginal PDFs** of continuous r.v. are defined as

$$f_X(x) = \int_{\mathcal{Y}} f_{X,Y}(x, y) dy \text{ and } f_Y(y) = \int_{\mathcal{X}} f_{X,Y}(x, y) dx.$$



Marginal PDFs: exercise

Assume the joint PDF of X and Y is given by

$$f_{X,Y}(x,y) = \begin{cases} x + \frac{3}{2}y^2 & \text{if } 0 \leq x \leq 1, 0 \leq y \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

Find the marginal PDFs of X and Y.

Independence

Two random variables X and Y are **independent** if for all x, y, we have

$$p_{X,Y}(x,y) = p_X(x)p_Y(y) \text{ (discrete case) or } f_{X,Y}(x,y) = f_X(x)f_Y(y) \text{ (continuous case).}$$

A sequence of random variables $X_1, \ldots, X_N$ are **independent** if their joint PDF (or joint PMF) can be **factorized**:

$$f_{X_1,\ldots,X_n}(x_1,\ldots,x_n) = \prod_{j=1}^{n} f_{X_j}(x_j).$$

Exercise. Consider two random variables X and Y with joint PDF

$$f_{X,Y}(x,y) = \frac{1}{2\pi\sigma^2} e^{-\frac{x^2+y^2}{2\sigma^2}}.$$

Show that X and Y are independent.

Independent and Identically Distributed (i.i.d.)

A collection of random variables $X_1, \ldots, X_N$ are called **independent and identically distributed (i.i.d.)** if

1. all $X_1, \ldots, X_N$ are **independent**, and
2. all $X_1, \ldots, X_N$ have the **same distribution**.

Example: N distinct coin tosses ($X_1, \ldots, X_N \sim \text{Ber}(p)$).

Example: Let θ be a deterministic number that was sent through a noisy channel. We model the noise as an additive Gaussian random variable with mean 0 and variance σ^2. Supposing we have observed measurements $X_i = \theta + W_i$, for $i = 1, \ldots, N$, where $W_i \sim \mathcal{N}(0, \sigma^2)$. Then, the joint PDF of $X_1, \ldots, X_N$ is

$$\begin{aligned} f_{X_1,\ldots,X_N}(x_1, \ldots, x_N) &= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\theta)^2}{2\sigma^2}} \\ &= \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i-\theta)^2}. \end{aligned}$$

Multivariate expectations

Recall that the expectation of a discrete random variable X is given by

$$\mathbb{E}[X] = \sum_{x \in \mathcal{X}} x \; p_X(x).$$

How about the expectation for two variables?

Let X and Y be two *discrete* random variables. For any function $g \colon \mathbb{R}^2 \to \mathbb{R}$, the **joint expectation** is

$$\mathbb{E}[g(X, Y)] = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} g(x, y) \; p_{X,Y}(x, y).$$

If X and Y are *continuous*, we have

$$\mathbb{E}[g(X, Y)] = \int_{\mathcal{Y}} \int_{\mathcal{X}} g(x, y) \; f_{X,Y}(x, y) \; dx \; dy.$$

Joint expectation

Let $g(X, Y) = XY$. If X and Y are **discrete**, the **joint expectation** is

$$\mathbb{E}[XY] = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} xy \; p_{X,Y}(x, y).$$

If X and Y are **continuous**, we have

$$\mathbb{E}[XY] = \int_{\mathcal{Y}} \int_{\mathcal{X}} xy \; f_{X,Y}(x, y) dx dy.$$

Remark. Why do we consider $\mathbb{E}[XY]$ in particular, and not, e.g., $\mathbb{E}[X + Y]$? It has good properties (it defines an *inner product* in the space of random variables) and is related to the notion of *covariance*.

Covariance

Let X and Y be two random variables. Then the **covariance of X and Y** is

$$\begin{aligned}\mathrm{Cov}(X, Y) &= \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] \\ &= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y],\end{aligned}$$

where $\mu_X = E[X]$ and $\mu_Y = E[Y]$.

Note that $\mathrm{Cov}(X, X) = \mathrm{Var}(X)$. Hence, the covariance is a **generalization** of the variance.

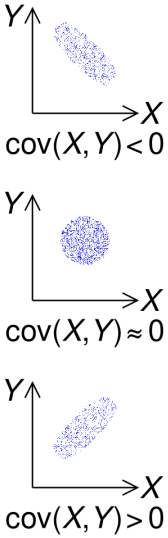


Image source: https://en.wikipedia.org/wiki/Covariance#/media/File:Covariance_trends.svg

Useful properties

For any X and Y, we have

$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y],$$

and

$$\mathrm{Var}[X + Y] = \mathrm{Var}[X] + 2\mathrm{Cov}(X, Y) + \mathrm{Var}[Y].$$

If X and Y are **independent**, then

$$\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y].$$

Correlation coefficient

Let X and Y be two random variables. Assume $\text{Var}[X], \text{Var}[Y] \neq 0$ (*why is this a reasonable assumption?*). The **correlation coefficient** is

$$\rho = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)\text{Var}(Y)}},$$

and always lies between -1 and 1 (which can be shown using Cauchy-Schwarz inequality).

- When $X = Y$ (**perfect positive correlation**), $\rho = 1$.
- When $X = -Y$ (**perfect negative correlation**), $\rho = -1$.
- When X and Y are **uncorrelated** then $\rho = 0$.

Independence vs correlation

Consider the following two statements:

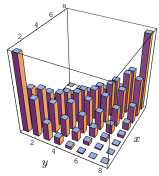
1. X and Y are independent;
2. X and Y are uncorrelated (i.e., $\mathrm{Cov}(X, Y) = 0$; the correlation coefficient is 0).

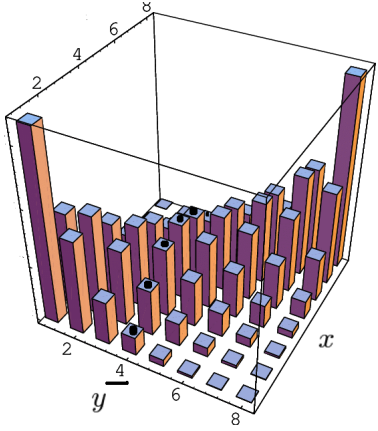
We have

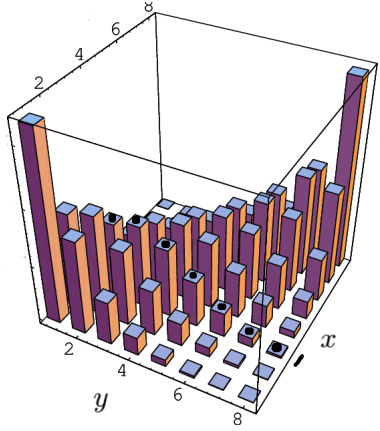
- (1) $\implies$ (2) (independence $\implies$ uncorrelated)
- (2) $\not\implies$ (1) (uncorrelated $\not\implies$ independence)
- Independence is a **stronger** condition than uncorrelation.

Outline

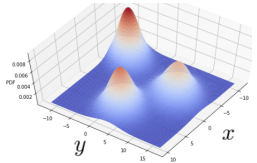
Conditional distributions

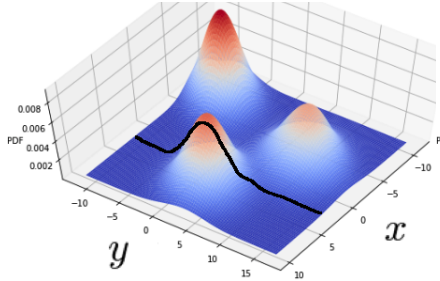


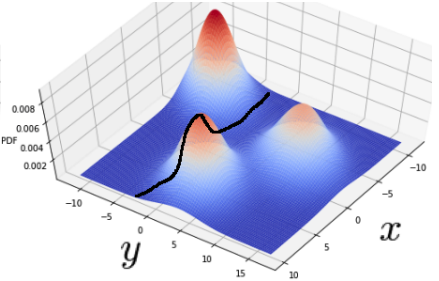




Conditional distributions







Conditional distributions

Let X and Y be two **discrete** random variables. The **conditional PMF** of Y given X is

$$p_{Y|X}(y \mid x) = \frac{p_{X,Y}(x,y)}{p_X(x)}.$$

We can see it as $\mathbb{P}(Y = y \mid X = x)$.

Let X and Y be two **continuous** random variables. The **conditional PDF** of Y given X is

$$f_{Y|X}(y \mid x) = \frac{f_{X,Y}(x,y)}{f_X(x)}.$$

Example

Consider **two coins** which can take values in $\{0, 1\}$. Let X be the *sum* of the two coins and Y be the *value of the first coin*.

- What is $p_X(\cdot)$?
- What is $p_{X|Y}(\cdot \mid y = 1)$?

Conditional distributions

Let X and Y be two **discrete** random variables. For any (measurable) $A \subseteq \mathcal{Y}$, we have

$$\mathbb{P}(Y \in A \mid X = x) = \sum_{y \in A} p_{Y|X}(y \mid x),$$

and

$$\mathbb{P}(Y \in A) = \sum_{x \in \mathcal{X}} \mathbb{P}(Y \in A \mid X = x) p_X(x).$$

Let X and Y be two **continuous** random variables. For any $A \subseteq \mathcal{Y}$, we have

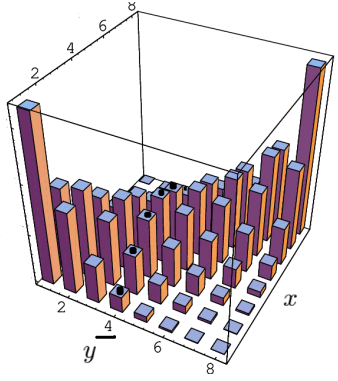
$$\mathbb{P}(Y \in A \mid X = x) = \int_A f_{Y|X}(y \mid x) dy,$$

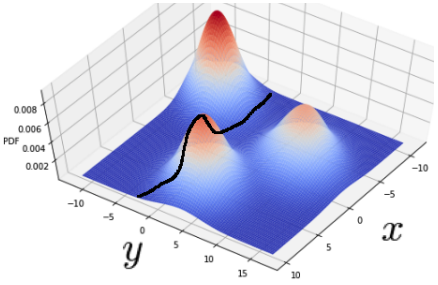
and

$$\mathbb{P}(Y \in A) = \int_{\mathcal{X}} \mathbb{P}(Y \in A \mid X = x) f_X(x) dx.$$

Outline

Conditional expectations





Conditional expectations

For a **discrete** random variable X, the **conditional expectation** of X given Y is

$$\mathbb{E}[X \mid Y = y] = \sum_{x \in \mathcal{X}} x \, p_{X|Y}(x \mid y).$$

For a **continuous** random variable X, the conditional expectation of X given Y is

$$\mathbb{E}[X \mid Y = y] = \int_{\mathcal{X}} x \, f_{X|Y}(x \mid y) dx.$$

The summation/integration is taken w.r.t. x, because $Y = y$ is **fixed**.

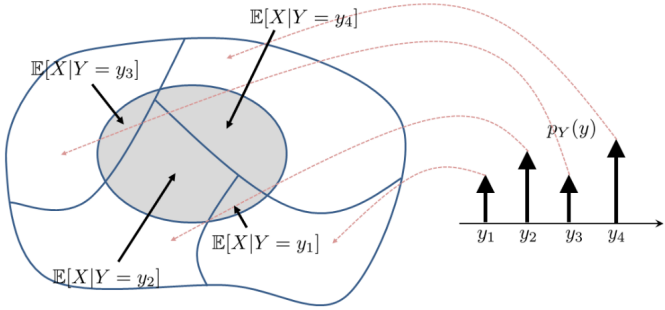
Law of Total Expectation

The **law of total expectation**[2] is a decomposition rule which allows to decompose the computation of $\mathbb{E}[X]$ into **conditional expectations** that are smaller/easier to compute.

$$\mathbb{E}[X] = \sum_{y \in \mathcal{Y}} \mathbb{E}[X \mid Y = y] \; p_Y(y),$$

or

$$\mathbb{E}[X] = \int_{\mathcal{Y}} \mathbb{E}[X \mid Y = y] \; f_Y(y) dy.$$



[2] Also known as the **law of iterated expectations** and the **tower rule**.

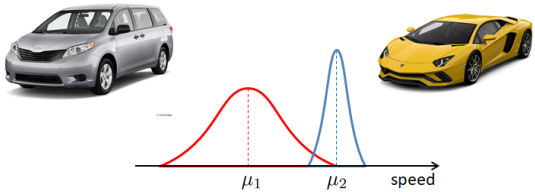
Example

Suppose there are two classes of cars. Let $C \in \{1, 2\}$ be the **class** and $S \in \mathbb{R}$ be the **speed**.

We know that

- $\mathbb{P}(C = 1) = p$,
- When $C = 1$, $S \sim \mathcal{N}(\mu_1, \sigma_1^2)$,
- When $C = 2$, $S \sim \mathcal{N}(\mu_2, \sigma_2^2)$.

You see a car on the freeway, what is its **average speed**?



Outline

Random vectors

Random vector:

$$\boldsymbol{X} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{pmatrix} \text{ and } \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

We assume that, by default, vectors are column vectors; we use $\boldsymbol{x}^T$ to denote the transpose of $\boldsymbol{x}$, which is a row vector

Joint PDF:

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n).$$

Probability:

$$\mathbb{P}(\boldsymbol{X} \in A) = \int_A f_{\boldsymbol{X}}(\boldsymbol{x}) dx.$$

Mean vector and covariance matrix

Let $\boldsymbol{X} = (X_1, X_2, \ldots, X_n)^T$ be a random vector. The **expectation** is

$$\boldsymbol{\mu} = \mathbb{E}[\boldsymbol{X}] = \begin{pmatrix} \mathbb{E}[X_1] \\ \mathbb{E}[X_2] \\ \vdots \\ \mathbb{E}[X_n] \end{pmatrix}.$$

The **covariance** matrix is

$$\boldsymbol{\Sigma} = \begin{pmatrix} \mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) & \ldots & \mathrm{Cov}(X_1, X_n) \\ \mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) & \ldots & \mathrm{Cov}(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}(X_n, X_1) & \mathrm{Cov}(X_n, X_2) & \ldots & \mathrm{Var}(X_n) \end{pmatrix},$$

which can be written in a more compact way as

$$\boldsymbol{\Sigma} = \mathbb{E}[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T].$$

Covariance matrix: properties

The covariance matrix is **symmetric**: $\mathbf{\Sigma} = \mathbf{\Sigma}^T$. This is due to the symmetry of the covariance operator: $\mathrm{Cov}(X, Y) = \mathrm{Cov}(Y, X)$.

If the coordinates $X_1, X_2, \ldots, X_n$ are *uncorrelated* (or pairwise independent, which is stronger), the covariance matrix is a **diagonal** matrix:

$$\mathbf{\Sigma} = \begin{pmatrix} \mathrm{Var}(X_1) & 0 & \ldots & 0 \\ 0 & \mathrm{Var}(X_2) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \mathrm{Var}(X_n) \end{pmatrix}.$$

Multivariate Gaussian distribution

A multivariate Gaussian distribution is characterized by a mean vector $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$.[3] The PDF of a d-dimensional **multivariate Gaussian** is given by

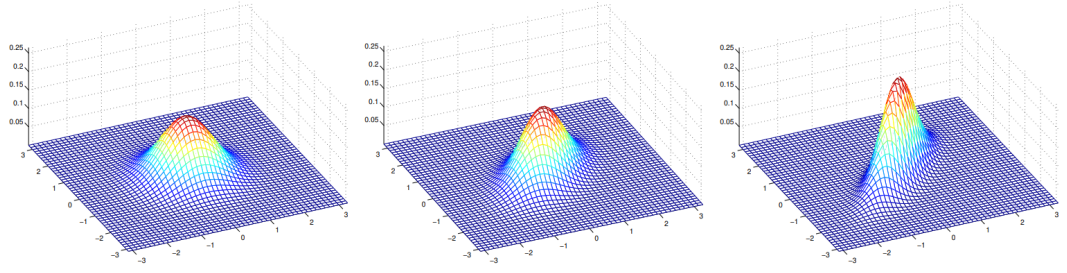
$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left\{ -\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right\},$$

where $\boldsymbol{d}$ is the dimension of the random vector $\boldsymbol{X}$, and $|\boldsymbol{\Sigma}|$ is the determinant of the covariance matrix $\boldsymbol{\Sigma}$.

Exercise. Check that it gives the correct PDF when the components X_i are independent!

[3] The covariance matrix must be symmetric and *positive semi-definite*.

Multivariate Gaussian: examples

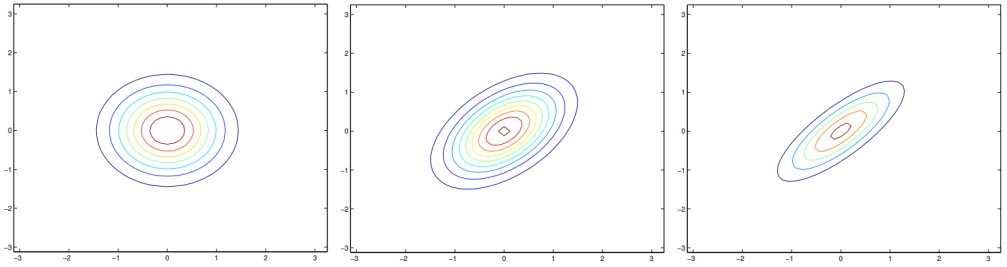


The figures above show the PDFs of Gaussians with mean 0 and with covariance matrix respectively

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}.$$

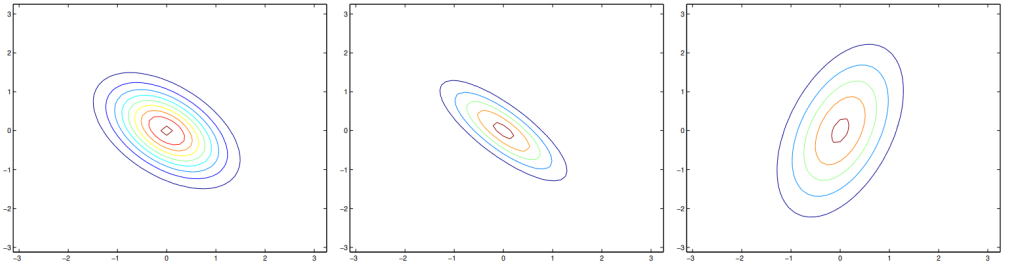
Multivariate Gaussian: examples

Other point of view: the *contours* of the above Gaussians are



Multivariate Gaussian: examples

Here are the contours of the PDF of other multivariate Gaussians of mean 0:

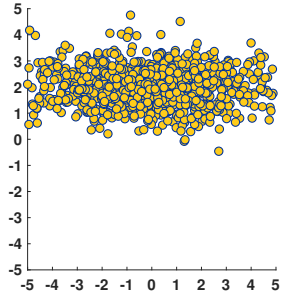


Try to guess (roughly) their covariance matrix!
Answer:

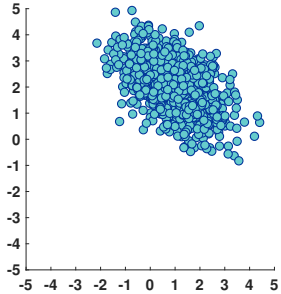
$$\Sigma = \begin{pmatrix} 1 & -0.5 \\ -0.5 & 1 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 1 & -0.8 \\ -0.8 & 1 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 3 & 0.8 \\ 0.8 & 1 \end{pmatrix}.$$

Multivariate Gaussian: examples

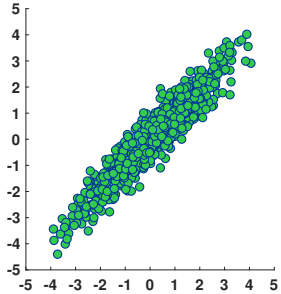
Third type of plot, obtained by sampling many points from Gaussians:



$$(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \begin{bmatrix} 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.5 \end{bmatrix}$$



$$\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$$



$$\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 & 1.9 \\ 1.9 & 2 \end{bmatrix}$$

Outline

Estimators

A central concept of machine learning (or statistics) is to **learn (or estimate)** certain properties about some underlying (stochastic) process on the basis of *samples* (data).

Point estimation refers to calculating a single "best guess" of the value of an unknown quantity of interest, which could be a **parameter** or a **density function**. We typically use $\hat{\theta}$ to denote a point estimator for a fixed parameter θ.

Given $X_1, X_2, \ldots, X_n \overset{\text{i.i.d.}}{\sim} p_X$, a (point) **estimator** is a function of the observed sample, i.e.

$$\hat{\theta} = T(X_1, X_2, \ldots, X_n),$$

so that $\hat{\theta}$ is a *random variable*.

For example, the *sample mean* $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$ is an estimator for the expectation ($\theta = \mathbb{E}[X]$).

Bias of an estimator

The **bias of an estimator** is given by

$$b(\hat{\theta}) = \mathbb{E}[\hat{\theta}] - \theta = \mathbb{E}[\hat{\theta} - \theta].$$

An estimator is **unbiased** if $b(\hat{\theta}) = 0$.

Other properties of estimators

The **variance of an estimator** is given by

$$v(\hat{\theta}) = \mathbb{E}[(\hat{\theta} - \mathbb{E}[\hat{\theta}])^2].$$

The **standard error of an estimator** is given by

$$\mathsf{se}(\hat{\theta}) = \sqrt{v(\hat{\theta})},$$

i.e., its standard deviation.

The **sampling distribution** of an estimator is the probability distribution of the estimator.

Example – The sample mean

Let $X_1, X_2, \ldots, X_n \overset{\text{i.i.d.}}{\sim} p_X$, with $\mathbb{E}[X] = \mu_X$ and $\text{Var}(X) = \sigma_X^2$. The *sample mean* estimator is defined as

$$\overline{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

What are the bias and variance of $\overline{X}_n$?

- Since $\mathbb{E}[\overline{X}_n] = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[X_i] = \frac{1}{n} \sum_{i=1}^{n} \mu_X = \mu_X$, $\bar{X}_n$ is unbiased, i.e., the bias is equal to zero.
- Also, using the fact that $\text{Var}(\frac{1}{n} \sum_{i=1}^{n} X_i) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{Cov}(X_i, X_j)$, we can show (how?) that

  $$\text{Var}(\overline{X}_n) = \frac{\sigma_X^2}{n}.$$

  The variance decreases as the sample size n increases!

More on the sample mean

- The variance of the *average* is **much smaller** that the variance of the *individual* random variables.
  - This is one of the core principles of statistics and help us learn various quantities reliably by making **repeated independent measurements**.
- Why are *independent* measurements **essential**?
  - The extreme case of non-independence is when $X_1 = X_2 = \cdots = X_n$, for which we have (how?)

$$\mathrm{Var}(\overline{X}_n) = \sigma_X^2.$$

Inference

Let $y_1, y_2, \ldots, y_n \overset{\text{i.i.d.}}{\sim} p_Y$. How can we estimate p_Y?

- We often **assume** that the sample was generated from some (parametric) model.
- When we specify a model, we hope that it can provide a useful **approximation** to the data generation mechanism.
- The George Box quote is worth remembering in this context: "**all models are wrong; the practical question is how wrong do they have to be to not be useful**".

Maximum likelihood estimation

Let $y_1, y_2, \ldots, y_n \overset{\text{i.i.d.}}{\sim} p_Y$. How can we estimate p_Y?

- Let us restrict ourselves to a set of **possible distributions** $p(y; \theta)$, described by a finite number of parameters $\theta \in \mathbb{R}^d$.
- The goal of **maximum likelihood estimation** is to select the distribution $p(y; \theta)$ that is **most likely** to have generated the sample $y_1, y_2, \ldots, y_n$.

Maximum likelihood estimation

An example of a set of possible distributions for a **continuous variable** ($y \in \mathbb{R}$) is

$$\left\{ p(y; \mu; \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{ -\frac{(y-\mu)^2}{2\sigma^2} \right\} \mid \mu \in \mathbb{R}, \sigma > 0 \right\},$$

where $\boldsymbol{\theta} = (\mu, \sigma)^T$ and $d = 2$. What is this distribution?

An example of a set of possible distributions for a **discrete variable** ($y \in \{0, 1\}$) is

$$\left\{ p(y; \alpha) = \alpha^y (1-\alpha)^{1-y} : 0 \leq \alpha \leq 1 \right\},$$

where $\boldsymbol{\theta} = \alpha$ and $d = 1$. What is this distribution?

Maximum likelihood estimation

The **likelihood function** is defined as

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &\equiv \mathcal{L}(\boldsymbol{\theta}; y_1, y_2, \ldots, y_n) \\ &= p(y_1, y_2, \ldots, y_n; \boldsymbol{\theta}) \\ &= \prod_{i=1}^{n} p(y_i; \boldsymbol{\theta}).\end{aligned}$$

The **maximum likelihood estimator**, or MLE — denoted by $\hat{\boldsymbol{\theta}}$ — is the value of $\boldsymbol{\theta}$ that maximizes $\mathcal{L}(\boldsymbol{\theta})$.

Log-likelihood

Working with a big product may not be convenient for practical computations. But note that $\hat{\theta}$ also maximizes the **log-likelihood function** $\log(\mathcal{L}(\theta))$! This is due to the fact that the logarithm is a **non-decreasing** function. This can be used to make a product into a sum, which is, e.g., easier to differentiate.

We write

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmax}}\ \mathcal{L}(\theta) = \underset{\theta \in \Theta}{\operatorname{argmax}}\ \log(\mathcal{L}(\theta)),$$

where Θ is the parameter space.

Example

We observe $y_1, \ldots, y_n$ where $y_i \in \{0, 1\}$ with unknown PMF p_Y. If we assume

$$y_1, \ldots, y_n \overset{\text{i.i.d.}}{\sim} p(y; \alpha),$$

where

$$p(y; \alpha) = \alpha^y (1 - \alpha)^{1-y}$$

with $0 \leq \alpha \leq 1$.

What is the maximum likelihood estimate $\hat{\alpha}$?

Example

The **likelihood function** is given by

$$\begin{aligned}\mathcal{L}(\alpha; y_1, \ldots, y_n) &= p(y_1, \ldots, y_n; \alpha) \\ &= \prod_{i=1}^{n} p(y_i; \alpha) \\ &= \prod_{i=1}^{n} \alpha^{y_i}(1-\alpha)^{1-y_i} \\ &= \alpha^{\sum_{i=1}^{n} y_i}(1-\alpha)^{\sum_{i=1}^{n}(1-y_i)},\end{aligned}$$

and the **log-likelihood function** is given by

$$\begin{aligned}\log\, \mathcal{L}(\alpha; y_1, \ldots, y_n) &= \sum_{i=1}^{n} y_i \log(\alpha) + (1-y_i)\log(1-\alpha) \\ &= n\bar{y}\log(\alpha) + n(1-\bar{y})\log(1-\alpha),\end{aligned}$$

where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.

Example

The first derivative of the log-likelihood is given by

$$(\log\mathcal{L})'(\alpha) = n\bar{y}\frac{1}{\alpha} - n(1-\bar{y})\frac{1}{1-\alpha}.$$

A necessary condition for a maximum is given by

$$(\log\mathcal{L})'(\alpha) = 0 \iff \hat{\alpha} = \bar{y}.$$

We can verify that it is indeed a maximum by checking that the second derivative of the log-likelihood at $\hat{\alpha}$ is indeed negative, i.e., $(\log\mathcal{L})''(\hat{\alpha}) < 0$.

Overview

Probability

Random variables

Discrete random variables

Continuous random variables

Multivariate random variables

Conditional distributions

Conditional expectations

Random vectors (more than two variables)

Inference