Machine Learning I

Review on Probability and Statistics

Souhaib Ben Taieb

February 17, 2022

University of Mons

Overview

Probability

Random variables

Discrete random variables

Continuous random variables

Multivariate random variables

Conditional distributions

Conditional expectations

Random vectors

Inference

References

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

Probability

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** are to which we want to attach probability.
- 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 possbile outcomes* of our measurements.

Sample space and events

- We toss one coin 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 $\omega = HT$. 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**
- $\mathcal{F} = 2^{\Omega}$ is the **space of events** (or event space)[1]
- $\mathbb{P}$ is the **probability measure/distribution** that maps an event $A \in \mathcal{F}$ to a real value between zero and one

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

Probability axioms

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

1. *Non-negativity*: $\mathbb{P}(A) \geq 0, \forall A \subseteq \Omega$
2. *Unity of Ω*: $\mathbb{P}(\Omega) = 1$
3. *Additivity*: For all disjoint events $A, B \in \mathcal{F}$ (i.e. $A \cap B = \varnothing$), we have that, $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$.

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

- $\mathbb{P}(\varnothing) = 0$
- $A \subset B \implies \mathbb{P}(A) \leq \mathbb{P}(B)$
- $0 \leq \mathbb{P}(A) \leq 1$
- $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

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

Probability properties

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

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

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

$$
\begin{aligned}
&A \subseteq B \\
&\implies B = A \cup (B \backslash A) \quad (A \cap (B \backslash A) = \varnothing) \\
&\implies \mathbb{P}(B) = \mathbb{P}(A) + \mathbb{P}(B \backslash A) \quad \text{(Axiom 3)} \\
&\implies \mathbb{P}(B) \geq \mathbb{P}(A) \quad \text{(Axiom 1)}
\end{aligned}
$$

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:

$$\mathbb{P}(A) = \mathbb{P}(\{w_1, w_2, \ldots, w_k\}) = \sum_{i=1}^{k} \mathbb{P}(\{w_i\})$$

- 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 less than five. What is $\mathbb{P}(A)$?

Conditional probability

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

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

Note: $\mathbb{P}(A|B) \neq \mathbb{P}(B|A) \quad$ (in general)

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

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

More generally, we have

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

Independence of events

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

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

A set of events $A_j (j \in J)$ are called **mutually independent** if

$$\mathbb{P}\left(\bigcap_{j \in J} A_j\right) = \prod_{j \in J} \mathbb{P}(A_j).$$

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 sometimes 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 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

$$\begin{align}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \tag{1} \\
&= 1 - \mathbb{P}(T \cap T \cap T \cap \cdots \cap T) \tag{2} \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \tag{3} \\
&= 1 - (1/2)^{10} \tag{4}
\end{align}$$

Exercise

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

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

Law of total probability

Let $A_1, A_2, \ldots, A_n$ be a partition of Ω. What is the probability of B?

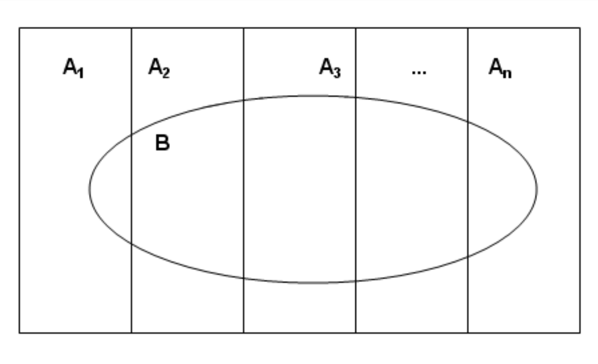


Image source: `https://mathwiki.cs.ut.ee/probability/04_total_probability`

Law of total probability

Let $A_1, A_2, \ldots, A_n$ be a partition of Ω. Then, for any $B \subseteq \Omega$, we have that

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

The **law of total probability** is a combination of **additivity** and **conditional probability**. In fact, we have

$$\begin{aligned}
\mathbb{P}(B) &= \mathbb{P}((B \cap A_1) \cup (B \cap A_2) \cup \cdots \cup (B \cap A_k)) \\
&= \sum_{i=1}^{n} \mathbb{P}(B \cap A_i) \\
&= \sum_{i=1}^{n} \mathbb{P}(B|A_i)\mathbb{P}(A_i)
\end{aligned}$$

Bayes' Rule

(**Bayes' Rule**) Let $A_1, A_2, \ldots, A_n$ be a partition of Ω. Then, we have that

$$\mathbb{P}(A_i|B) = \frac{\mathbb{P}(B|A_i)\mathbb{P}(A_i)}{\sum_{i=1}^{n} \mathbb{P}(B|A_i)\mathbb{P}(A_i)}$$

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

Bayes' Rule is a combination of **conditional probability** and the **law of total probability**:

$$\mathbb{P}(A_i|B) = \frac{\mathbb{P}(A_i \cap B)}{\mathbb{P}(B)} = \frac{\mathbb{P}(B|A_i)\mathbb{P}(A_i)}{\mathbb{P}(B)}$$

Example

Suppose there are three types of emails: $A_1 =$ SPAM, $A_2 =$ Low Priority and $A_3 =$ 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 the event that an email contains the word "free", then $\mathbb{P}(B|A_1) = 0.9, \mathbb{P}(B|A_2) = 0.1, \mathbb{P}(B|A_3) = 0.1$. When we receive an email containing the word "free", what is the probability that it is a spam?

Random variables

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

$$\Omega = \{\underbrace{HHH}_{\substack{\downarrow \\ 3}}, \underbrace{HHT}_{\substack{\downarrow \\ 2}}, \underbrace{HTH}_{\substack{\downarrow \\ 2}}, \underbrace{THH}_{\substack{\downarrow \\ 2}}, \underbrace{TTH}_{\substack{\downarrow \\ 1}}, \underbrace{THT}_{\substack{\downarrow \\ 1}}, \underbrace{HTT}_{\substack{\downarrow \\ 1}}, \underbrace{TTT}_{\substack{\downarrow \\ 0}}\}$$

These summary statistics are called **random variables**. Specifically, a random variable is a function from the sample space Ω to the reals.

Random variables

A random variable can be seen as a **mapping** between a distribution on Ω to a distribution on the reals (or the range of the random variable, $\mathcal{X} \subseteq \mathbb{R}$). Formally, we have that for some subset $S \subseteq \mathcal{X}$,

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

For the previous example, we have

$$\Omega = \{\underbrace{HHH}_{\substack{\downarrow \\ 3}}, \underbrace{HHT}_{\substack{\downarrow \\ 2}}, \underbrace{HTH}_{\substack{\downarrow \\ 2}}, \underbrace{THH}_{\substack{\downarrow \\ 2}}, \underbrace{TTH}_{\substack{\downarrow \\ 1}}, \underbrace{THT}_{\substack{\downarrow \\ 1}}, \underbrace{HTT}_{\substack{\downarrow \\ 1}}, \underbrace{TTT}_{\substack{\downarrow \\ 0}}\}$$

and

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

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

In the following, we will use $\mathbb{P}$ to denote probability.

Discrete random variables

Probability mass function

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

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

What is the PMF of the previous coin flip example?

A function p_X is a PMF if and only if

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

Some important discrete distributions

- Discrete **uniform** distribution on K categories ($X \in \{C_1, C_2, \dots, C_K\}$). The PMF is given by

$$p_X(x) = \frac{1}{k}, \qquad \forall x \in \{C_1, C_2, \dots, C_K\}$$

- The **Bernouilli** distribution with parameter $p \in [0, 1]$ ($X \in \{0, 1\}$). The PMF 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

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

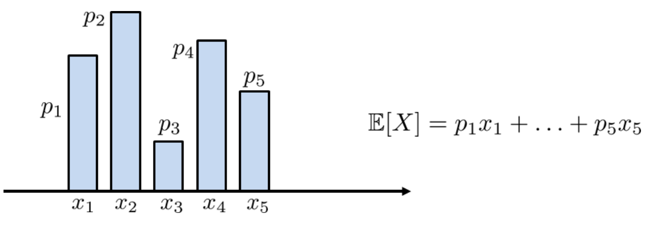


Image source: Introduction to Probability for Data Science, Stanley H. Chan.

Expectation and its properties

For any function g, we have

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

For any function g and h,

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

For any constant c,

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

For any constant c,

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

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

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

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

Useful properties of the variance include:

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

Continuous random variables

Probability density function

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

The **probability density function** (PDF) of a continuous random variable X is a function f_X, when integrated over an interval $[a, b]$, yields the probability of obtaining $a \leq X \leq b$:

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

A PDF has the following properties:

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

Note that $f_X(x)$ is not the probability of having $X = x$. In fact, we can have $f_X(x) > 1$.

Some important continuous distributions

- 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 $X \sim \mathcal{U}[a, b]$.
- **Gaussian** 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, we have

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

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

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

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

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

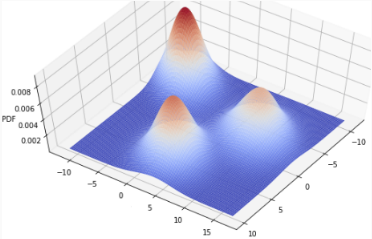
where $\mu_X = \mathbb{E}[X]$. The **standard deviation** of X is $\sqrt{\mathrm{Var}(X)}$.

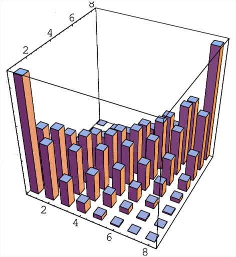
See the useful properties of the variance introduced previously.

Multivariate random variables

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** PDF or PMF.





More than one random variable?

An image from a dataset can be represented by a high-dimensional vector.

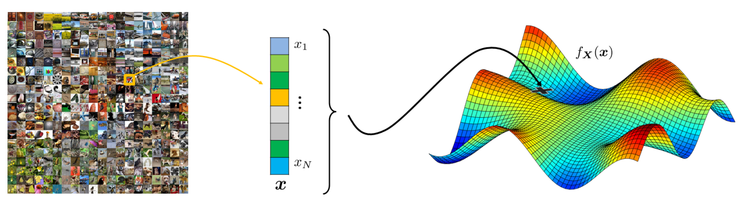


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

Joint distributions

- $f_X(x)$
- $f_{X_1,X_2}(x_1, x_2)$
- $f_{X_1,X_2,X_3}(x_1, x_2, x_3)$
- $\ldots$
- $f_{X_1,\ldots,X_n}(x_1, \ldots, x_n)$
- We often just write $f_X(x)$ when the dimensionality is clear from context.

Joint PMF

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

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

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

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

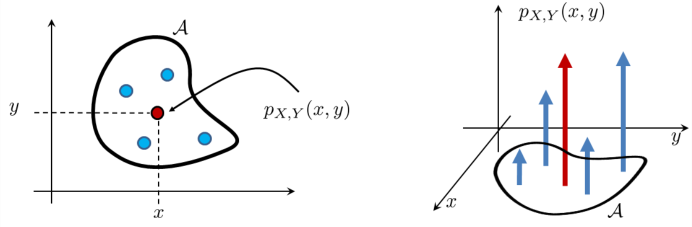


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

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

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

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 $A \subseteq \mathcal{X} \times \mathcal{Y}$.

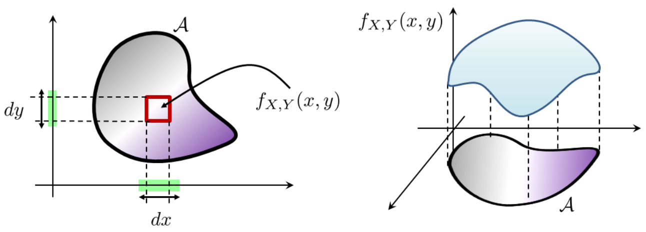


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

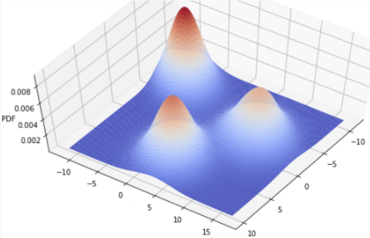
Marginal distribution

The **marginal PMF** is 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 PDF** is defined as

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



Independence

If two random variables X and Y are **independent**, then

$$p_{X,Y}(x, y) = p_X(x)p_Y(y), \qquad \text{and } f_{X,Y}(x, y) = f_X(x)f_Y(y)$$

If a sequence of random variables $X_1, \ldots, X_N$ are independent, then their joint PDF (or joint PMF) can be factorized:

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

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.
2. All $X_1, \ldots, X_N$ have the same distribution.

Joint 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, 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

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

Joint expectations

Let $g(X, Y) = XY$, we have

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

If X and Y are continuous, we have

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

Covariance

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

$$\begin{aligned} \text{Cov}(X, Y) &= \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] && (5) \\ &= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y], && (6) \end{aligned}$$

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

Note that $\text{Cov}(X, X) = \text{Var}(X)$.

Useful properties

For any X and Y, we have

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

and

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

If X and Y are independent, then

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

Correlation

Let X and Y be two random variables. The **correlation coefficient** is

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

where $-1 \leq \rho \leq 1$.

- When $X = Y$ (fully correlated), $\rho = 1$.
- When $X = -Y$ (fully correlated), $\rho = -1$.
- When X and Y are uncorrelated then $\rho = 0$.

Independence vs correlation

Consider the following two statements:

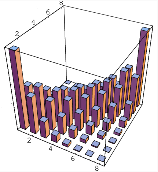
1. X and Y are independent;
2. $\mathrm{Cov}(X, Y) = 0$.

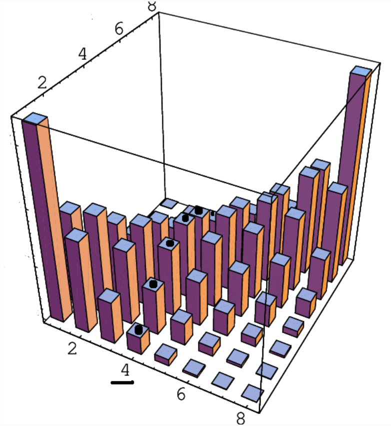
We have

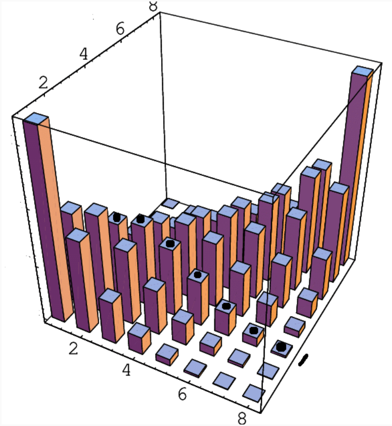
- (1) $\implies$ (2) (independence $\implies$ uncorrelated)
- (2) $\not\Longrightarrow$ (1) (uncorrelated $\not\Longrightarrow$ independence)
- Independence is a stronger condition than correlation

Conditional distributions

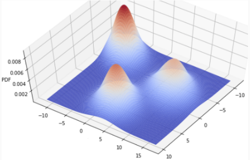
Conditional distributions

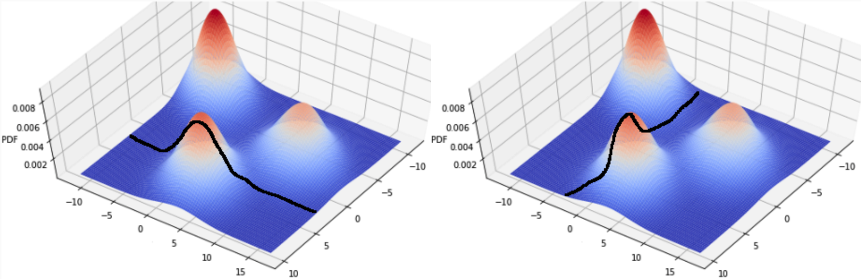






Conditional distributions





Conditional distributions

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

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

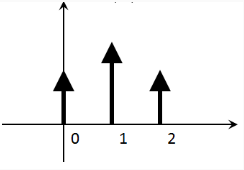
Let X and Y be two continuous random variables. The **conditional PDF** of Y given X is

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

Example

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

$p_Y(y)$:



$p_{Y|X}(y|x = 1)$:

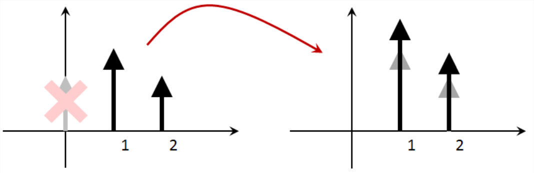


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

Conditional distributions

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

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

and

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

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

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

and

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

Conditional expectations

Conditional expectations

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

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

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

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

The summation/integration is taken w.r.t. y, because $X = x$ is given and fixed.

Law of Total Expectation

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

$$\mathbb{E}[Y] = \sum_{x \in \mathcal{X}} \mathbb{E}[Y|X = x] p_X(x) \text{ or } \mathbb{E}[Y] = \int_{\mathcal{X}} \mathbb{E}[Y|X = x] f_X(x) dx$$

Note the difference between

$$h(x) = \mathbb{E}_{Y|X}[Y|X = x], \quad \text{(A deterministic function in } x\text{)}$$

and

$$h(X) = \mathbb{E}_{Y|X}[Y|X]. \quad \text{(A function of the random variable } X\text{)}$$

The **law of total expectation** can also be written as

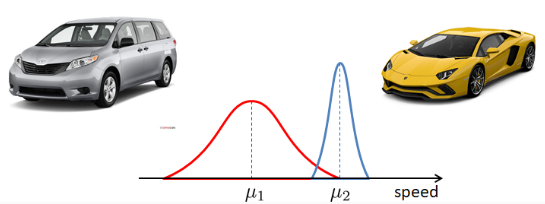
$$\mathbb{E}[Y] = \mathbb{E}_X[\mathbb{E}_{Y|X}[Y|X]].$$

Example

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



Random vectors

Random vectors

Random vector:

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

Joint PDF:

$$f_X(x) = f_{X_1, X_2, \dots, X_n}(x_1, x_2, \dots, x_n)$$

Probability:

$$\mathbb{P}(X \in A) = \int_A f_X(x) dx$$

Mean vector and covariance matrix

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

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

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

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

Diagonal covariance matrix

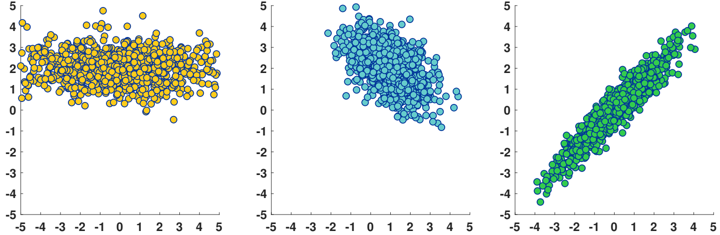
If the coordinates $X_1, X_2, \ldots, X_n$ are *uncorrelated*, the covariance matrix is a **diagonal** matrix:

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

Multivariate Gaussian

A d-dimensional **joint Gaussian** has a PDF:

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



$(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \begin{bmatrix} 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.5 \end{bmatrix}$ $\quad \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$ $\quad \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 & 1.9 \\ 1.9 & 2 \end{bmatrix}$

Inference

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 θ.

Given $X_1, X_2, \ldots, X_n \sim p_X$, 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* $\hat{\theta} = \bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$ is an estimator for the expectation ($\theta = \mathbb{E}[X]$).

Properties of estimators

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

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

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

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

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

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

i.e., its standard deviation.

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

Example - The sample mean

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

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

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

Example - The sample mean

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

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

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

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

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 independent measurements are **essential**? The extreme case of non-independence is when $X_1 = X_2 = \cdots = X_n$, for which we have
$$\mathrm{Var}(\bar{X}_n) = \sigma_X^2.$$

Inference

Let $y_1, y_2, \ldots, y_n \sim p_Y$. 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, but some are useful**".

Maximum likelihood estimation

Let us restrict ourselves to a set of possible distributions $p(y; \boldsymbol{\theta})$, described by a finite number of parameters $\boldsymbol{\theta} \in \boldsymbol{\Theta}$.

An example for $y \in \mathbb{R}$ is

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

where $\boldsymbol{\theta} = (\mu, \sigma)^T$, and, for $y \in \{0, 1\}$,

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

where $\boldsymbol{\theta} = \alpha$.

The goal of maximum likelihood estimation is to select the distribution $p(y; \boldsymbol{\theta})$ that is **most likely** to have generated the sample $y_1, y_2, \ldots, y_n$.

Maximum likelihood estimation

The **likelihood function** is defined as

$$\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}) &\equiv \mathcal{L}(\boldsymbol{\theta}; y_1, y_2, \ldots, y_n) && (7)\\
&= p(y_1, y_2, \ldots, y_n; \boldsymbol{\theta}) && (8)\\
&= \Pi_{i=1}^{n} p(y_i; \boldsymbol{\theta}). && (9)
\end{aligned}$$

The **maximum likelihood estimator**, or MLE – denoted by $\hat{\boldsymbol{\theta}}$ – is the value of $\boldsymbol{\theta}$ that maximizes $\mathcal{L}(\boldsymbol{\theta})$. Note that $\hat{\boldsymbol{\theta}}$ also maximizes the **log-likelihood function** $\log \mathcal{L}(\boldsymbol{\theta})$. We write

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

where $\boldsymbol{\Theta}$ 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

$$y_1, \ldots, y_n \sim p(y; \alpha),$$

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

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

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-ikelihood at $\hat{\alpha}$ is indeed negative, i.e. $(\log\mathcal{L})''(\hat{\alpha}) < 0$.