Machine Learning I

Review of Probability and Statistics

Souhaib Ben Taieb

University of Mons

Overview

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]

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** 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?

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?

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*:

$$\mathbb{P}(A) \geq 0, \quad \forall A \subseteq \Omega$$

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,

$$\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$$

.

Probability axioms

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

1. *Non-negativity*:

$$\mathbb{P}(A) \geq 0, \quad \forall A \subseteq \Omega$$

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,

$$\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$$

.

Probability axioms

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

1. *Non-negativity*:

$$\mathbb{P}(A) \geq 0, \quad \forall A \subseteq \Omega$$

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,

$$\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$$

.

Probability properties

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

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability properties

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

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

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

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

Probability of an event (discrete case)

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

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

- 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 $\Omega = \{(t_1, t_2) : t_1, t_2 = 1, 2, \dots, 6\}$. Let A be the event that the sum of two tosses being less than five. What is $\mathbb{P}(A)$?

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 $\mathbb{P}(A)$?

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

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

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 (**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

$$\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)} \\
&= 1 - (1/2)^{10} \qquad \text{(fair coin)}
\end{aligned}$$

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

$$
\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)} \\
&= 1 - (1/2)^{10} \qquad \text{(fair coin)}
\end{aligned}
$$

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

$$\begin{aligned}\mathbb{P}(A) &= 1 - \mathbb{P}(A^c)\\ &= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}})\\ &= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)}\\ &= 1 - (1/2)^{10} \qquad \text{(fair coin)}\end{aligned}$$

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

$$
\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)} \\
&= 1 - (1/2)^{10} \qquad \text{(fair coin)}
\end{aligned}
$$

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

$$\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)} \\
&= 1 - (1/2)^{10} \qquad \text{(fair coin)}
\end{aligned}$$

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

$$\begin{aligned}
\mathbb{P}(A) &= 1 - \mathbb{P}(A^c) \\
&= 1 - \mathbb{P}(\underbrace{T \cap T \cap T \cap \cdots \cap T}_{10 \text{ times}}) \\
&= 1 - \prod_{i=1}^{10} \mathbb{P}(T) \qquad \text{(independent tosses)} \\
&= 1 - (1/2)^{10} \qquad \text{(fair coin)}
\end{aligned}$$

Exercise

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

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

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

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

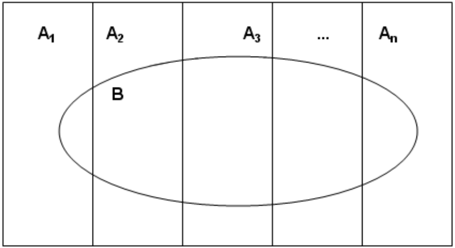


Image source: `https://mathwiki.cs.ut.ee/probability/04_total_probability`

Law of total probability

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

Let $A_1, A_2, \ldots, A_n$ be a partition of Ω. **Bayes' Rule** states 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:

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

Bayes' Rule

Let $A_1, A_2, \ldots, A_n$ be a partition of Ω. **Bayes' Rule** states 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:

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

Example

Suppose there are 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 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**?

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

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

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

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

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* of the r. v., $\mathcal{X} \subseteq \mathbb{R}$)

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

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

Random variables

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

For the previous example, we have

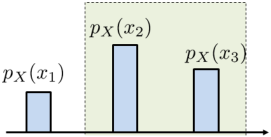
$$\mathbb{P}_X(X = 0) = 1/8, \quad \mathbb{P}_X(X = 1) = 3/8,$$

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

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

Outline

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

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

A function p_X is a PMF if and only if

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

What is the PMF of the previous coin flip example?

Some important discrete distributions

- 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 **Bernouilli** 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.

Some important discrete distributions

- 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 **Bernouilli** 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. $X \sim \mathrm{Ber}(p)$ means that X has a Bernoulli distribution with parameter p.

Some important discrete distributions

- 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 **Bernouilli** 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.

Some important discrete distributions

- 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 **Bernouilli** 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

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

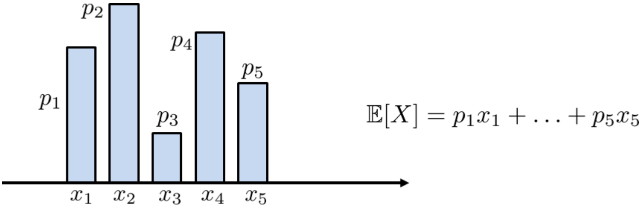


Image source: Introduction to Probability for Data Science, Stanley H. Chan.

Expectation and its properties

For any function g, 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

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

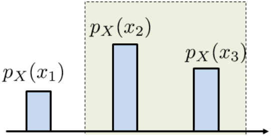
where $\mu_X = \mathbb{E}[X]$. The **standard deviation** of X is $\sqrt{\mathrm{Var}(X)}$.

Useful properties of the variance include:

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

Outline

Probability density function



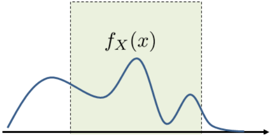


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

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 $\{x : a \leq x \leq b\}$:

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

For a PDF, we have:

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

Note: $f_X(x)$ is not the probability of $X = x$ since 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** 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 $X \sim \mathcal{N}(\mu, \sigma^2)$.

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** 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, 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

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

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

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

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

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

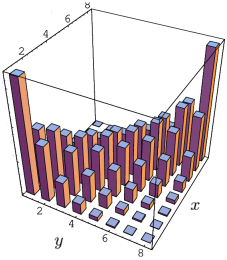
where $\mu_X = \mathbb{E}[X]$. The **standard deviation** of X is $\sqrt{\text{Var}(X)}$.

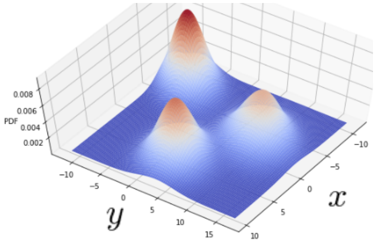
See the useful properties of the variance introduced previously.

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.





Important concepts

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

Joint distributions

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

In the following, we will mainly focus on **bivariate random variables**.

Joint PMF

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

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

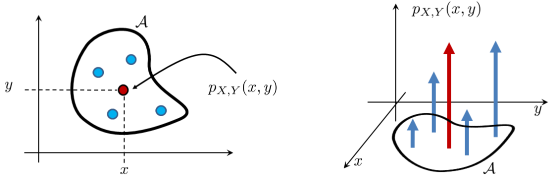


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

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

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

Joint PMF

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

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

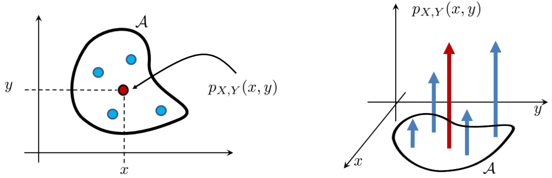


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

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

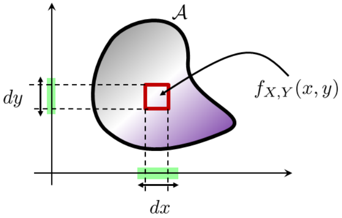
$$p_{X,Y}(x, y) = \frac{1}{12}, \quad x = 0, 1, \quad y = 1, 2, 3, 4, 5, 6.$$

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



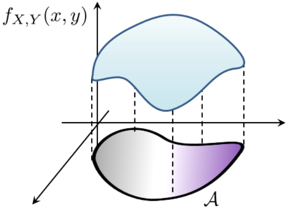


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

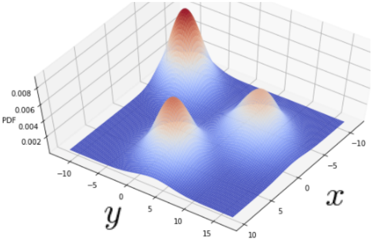
Marginal distribution

The **marginal PMFs** 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** are defined as

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



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 $g(X, Y) = XY$. If X and Y are **discrete**, 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

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

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

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

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

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

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:

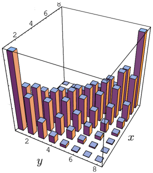
1. X and Y are independent;
2. $\text{Cov}(X, Y) = 0$.

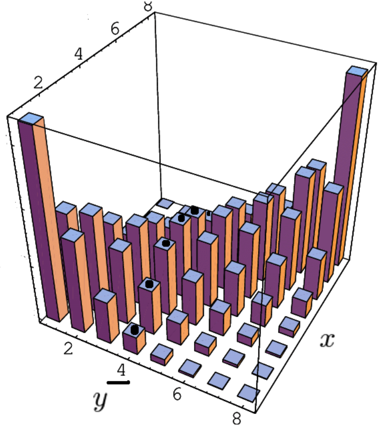
We have

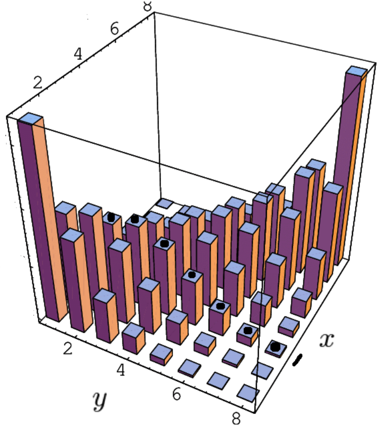
- (1) $\implies$ (2) (independence $\implies$ uncorrelated)
- (2) $\not\Longrightarrow$ (1) (uncorrelated $\not\Longrightarrow$ independence)
- Independence is a **stronger** condition than correlation

Outline

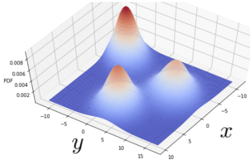
Conditional distributions

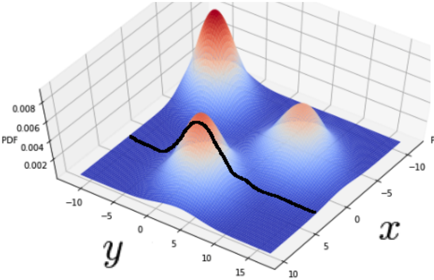


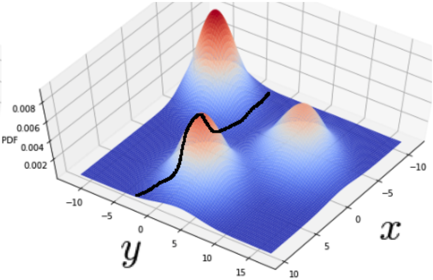




Conditional distributions







Conditional distributions

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

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

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

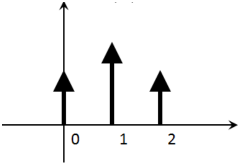
$$f_{Y|X}(y|x) = \frac{f_{Y,X}(x,y)}{f_X(x)}.$$

Example

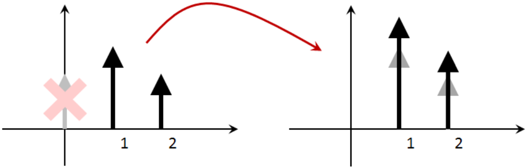
Consier **two coins** which can take values in $\{0,1\}$. Let Y be the *sum* of the two coins, and X, the *value of the first coin*.

- What is $p_Y(y)$?
- What is $p_{Y|X}(y|x=1)$?
- What is $p_{Y,X}(y,x)$??

Example



$p_Y(y)$:



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

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 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

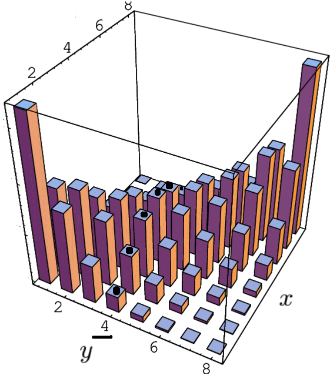
$$\mathbb{P}(Y \in A|X = x) = \int_A f_{Y|X}(y|x) dy,$$

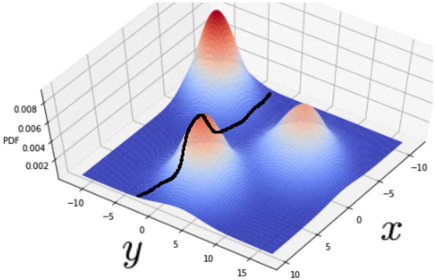
and

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

Outline

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**.

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

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

or

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

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

Law of Total Expectation

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

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

Note the difference between

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

and

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

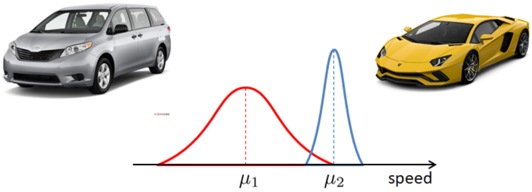
Example

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**?



Outline

Random vectors

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

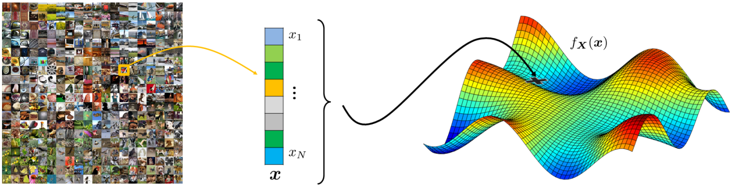


Image source:: Introduction to Probability for Data Science, Stanley H. Chan.

Random vectors

Random vector:

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

Joint PDF:

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

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

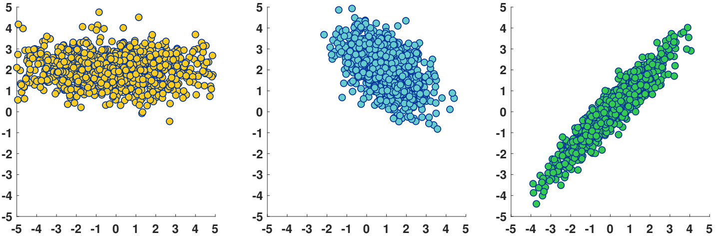
$$\boldsymbol{\Sigma} = \mathbb{E}[(X - \boldsymbol{\mu})(X - \boldsymbol{\mu})^T].$$

Diagonal covariance matrix

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

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

Bivariate Gaussian



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

Multivariate Gaussian

The PDF of a d-dimensional **joint Gaussian** is given by

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

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 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* $\hat{\theta} = \bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$ 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 $X_1, X_2, \ldots, X_n \overset{\text{i.i.d.}}{\sim} p_X$, with $\mathbb{E}[X] = \mu_x$ and $\text{Var}(X) = \sigma_X^2$. The *sample mean* estimator is defined as

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

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 $\text{Var}(\sum_{i=1}^n X_i) = \sum_{i=1}^n \sum_{j=1}^n \text{Cov}(X_i, X_j)$, we can show that $\text{Var}(\bar{X}_n) = \frac{\sigma_X^2}{n}$.

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 $\mathrm{Var}(X) = \sigma_X^2$. 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 $y_1, y_2, \ldots, y_n \overset{\text{i.i.d.}}{\sim} p_Y$. 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, 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

$$\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}) &\equiv \mathcal{L}(\boldsymbol{\theta}; y_1, y_2, \ldots, y_n) && (1) \\
&= p(y_1, y_2, \ldots, y_n; \boldsymbol{\theta}) && (2) \\
&= \Pi_{i=1}^{n} p(y_i; \boldsymbol{\theta}). && (3)
\end{aligned}$$

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

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

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

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

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

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

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. $(\log \mathcal{L})''(\hat{\alpha}) < 0$.