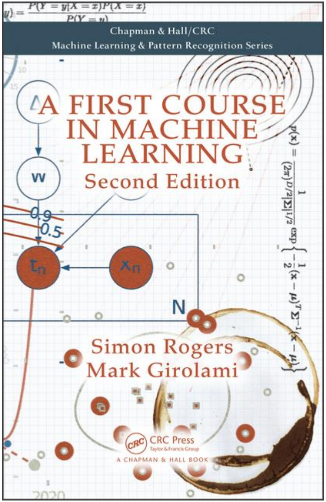
Introduction to Machine Learning

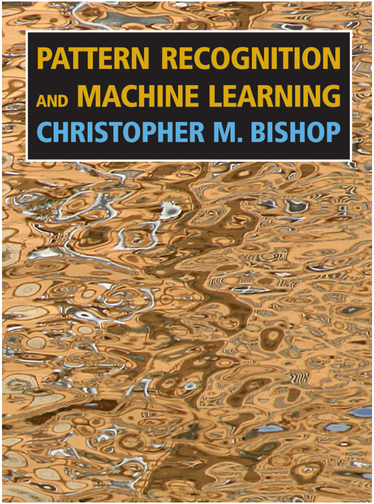
Mauricio A. Álvarez

Machine Learning and Adaptive Intelligence
The University of Sheffield

Textbooks

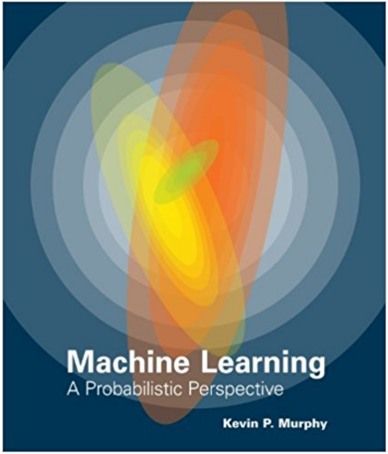


Rogers and Girolami, *A First Course in Machine Learning*, Chapman and Hall/CRC Press, 2nd Edition, 2016.

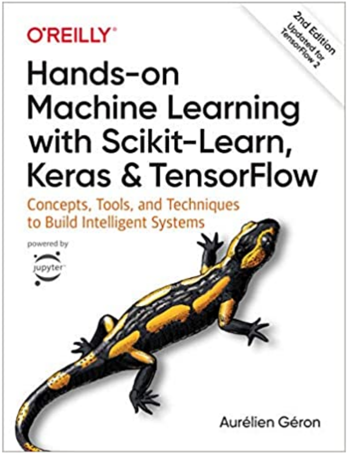


Bishop, *Pattern Recognition and Machine Learning*, Springer-Verlag, 2006.

Textbooks



Murphy, *Machine Learning: A Probabilistic Perspective*, MIT Press, 2012.



Géron, *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow*, O'Reilly, 2nd Edition, 2019.

Contents

Machine learning or Statistical Learning

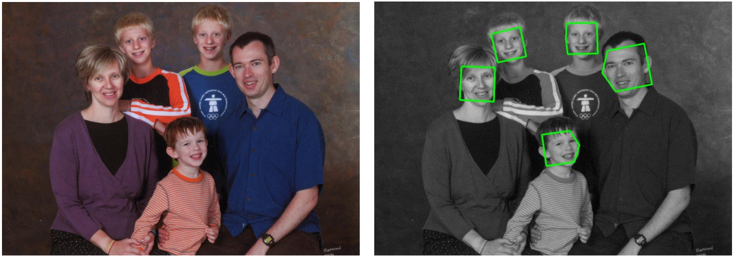
- We would like to design an algorithm that help us to solve different prediction problems.
- The algorithm is designed based on a mathematical model or function, and a dataset.
- Extract knowlegde from data.

Examples of ML problems

Handwritten digit recognition

Examples of ML problems

Face detection and face recognition



From Murphy (2012).

Examples of ML problems

Predicting the age of a person looking at a particular YouTube video.

Examples of ML problems

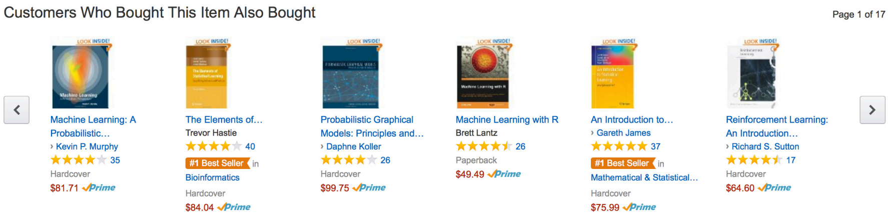
Stock market

Examples of ML problems

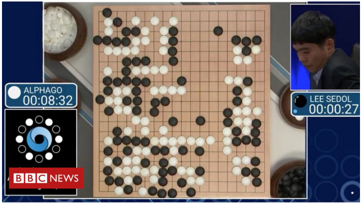
Clustering: segmenting customers in e-commerce

Examples of ML problems

Recommendation systems

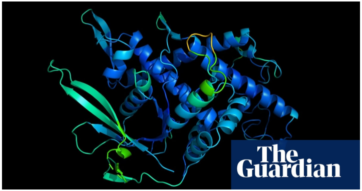


ML has contributed to advances in AI



AlphaGo

Autonomous driving



AlphaFold

Contents

Basic definitions

- Handwritten digit recognition

- Variability

- Each image can be transformed into a vector $\mathbf{x}$ (feature extraction).

- An instance is made of the pair $(\mathbf{x}, y)$, where y is the label of the image.

- Objective: find a function $f(\mathbf{x}, \mathbf{w})$.

Basic definitions

- **Training set**: a set of N images and their labels $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$, to fit the predictive model.

- **Estimation or training phase**: process of getting the values of $\mathbf{w}$ of the function $f(\mathbf{x}, \mathbf{w})$, that best fit the data.

- **Generalisation**: ability to correctly predict the label of new images $\mathbf{x}_*$.

Supervised and unsupervised learning

- **Supervised learning**:
  - Variable y is discrete: *classification*.
  - Variable y is continuous: *regression*.

- **Unsupervised learning**: from the set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$, we only have access to $\mathbf{x}_1, \ldots, \mathbf{x}_N$
  - Find similar groups: *clustering*.
  - Find a probability function for $\mathbf{x}$: *density estimation*.
  - Find a lower dimensionality representation for $\mathbf{x}$: *dimensionality reduction and visualisation*.

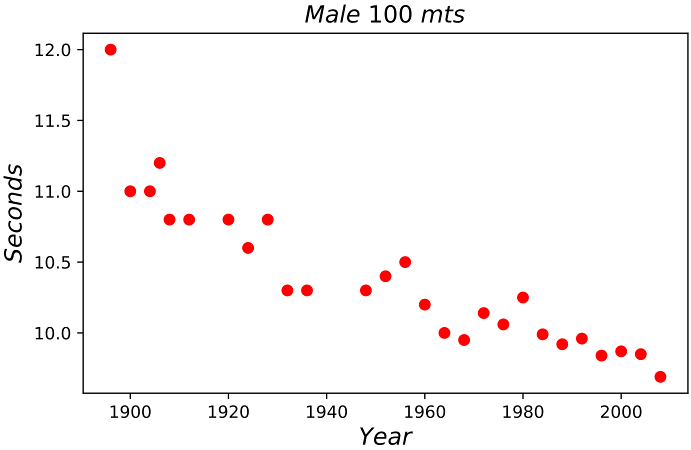
- **Other types of learning**: reinforcement learning, semi-supervised learning, active learning, multi-task learning.

Contents

Olympic 100m Data

Image from Wikimedia Commons http://bit.ly/191adDC.

Dataset



Male 100 mts
12.0
11.5
11.0
10.5
10.0
Seconds
1900
1920
1940
1960
1980
2000
Year

Model

- We will use a linear model $y = f(x, \mathbf{w})$, where y is the time in seconds and x the year of the competition.

- The linear model is given as

$$y = w_1 x + w_0,$$

where w_0 is the intercept and w_1 is the slope.

- We use $\mathbf{w}$ to refer both to w_0 and w_1.

Objective function

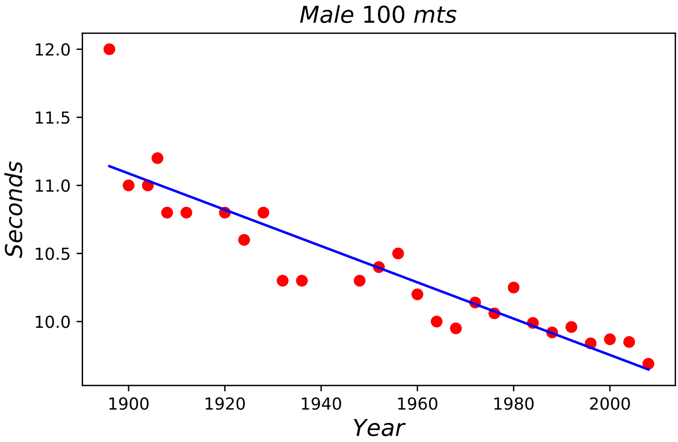
- We use an objetive function to estimate the parameters w_0 and w_1 that best fit the data.

- In this example, we use a a least squares objective function

$$E(w_0, w_1) = \sum_{\forall\, i} (y_i - f(x_i))^2 = \sum_{\forall\, i} [y_i - (w_1 x_i + w_0)]^2.$$

- By minimising the error with respect to **w**, we get the solution as $w_0 = 36.4$ and $w_1 = -1.34 \times 10^{-2}$.

Data and model



Predictions

- We can now use this model for making predictions.
- For example, what does the model predict for 2012?
- If we say $x = 2012$, then

$$\begin{aligned} y = f(x, \mathbf{w}) &= f(x = 2012, \mathbf{w}) \\ &= w_1 x + w_0 = (-1.34 \times 10^{-2}) \times 2012 + 36.4 = 9.59. \end{aligned}$$

- The actual value was 9.63.

Main challenges of machine learning

- Insufficient quantity of training data.
- Nonrepresentative training data.
- Poor-quality data.
- Irrelevant features.
- Overfitting the training data.
- Underfitting the training data.

Contents

Contents

Definition

- A *random variable* (RV) is a *function* that assigns a number to the outcome of a random experiment.

- For example, we toss a coin (random experiment).

- We assign the number 0 to the outcome “tails” and the number “1” to the outcome “heads”.

Discrete and continuous random variables

- A random variable can either be discrete or continuous.

- A **discrete RV** can take a value only from a countable number of distinct values, like $1, 2, 3, \ldots$.

- For example, the number of phone calls received in a call-center from 9:00 to 10:00, the number of COVID patients in the Royal Hallamshire Hospital on May 30, 2020.

- A **continuous RV** can take any value from an infinite possible values within one or more intervals.

- Examples include the time that a cyclist takes to finish the Tour de France; the exchange rate between the british pound and the US dollar on June 30, 2020.

Notation

- We use capital letters to denote random variables, e.g. $X, Y, Z, \ldots$.
- We use lowercase letters to denote the values that the random variable takes, $x, y, z, \ldots$.

Contents

Probability mass function

- A discrete RV X is completely defined by a set of values it can take, $x_1, x_2, \ldots, x_n$, and their corresponding probabilities.

- The probability that $X = x_i$ is denoted as $P(X = x_i)$ for $i = 1, \ldots, n$, and it is known as the *probability mass function* (pmf).

- Properties

  1. $P(X = x_i) \geq 0, \quad i = 1, \ldots, n.$
  2. $\sum_{i=1}^{n} P(X = x_i) = 1.$

Two discrete RVs

- In machine learning, we are usually interested in more than one random variable.

- Consider two RVs X and Y taking values $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_m$, respectively.

- These two random variables can be fully described with **a joint probability mass function** $P(X = x_i, Y = y_j)$ specifying the probability of $X = x_i$ and $Y = y_j$.

- Properties

  1. $P(X = x_i, Y = y_j) \geq 0, \quad i = 1, \ldots, n, j = 1, \ldots, m.$
  2. $\sum_{i=1}^{n} \sum_{j=1}^{m} P(X = x_i, Y = y_j) = 1.$

Rules of probability

- **Marginal**

$$P(X = x_i) = \sum_{j=1}^{m} P(X = x_i, Y = y_j).$$

We obtain the probability of $P(X = x_i)$ regardless of the value of Y. This is also known as the **sum rule of probability**.

- **Conditional**

$$P(X = x_i | Y = y_j) = \frac{P(X = x_i, Y = y_j)}{P(Y = y_j)}, \quad P(Y = y_j) \neq 0.$$

- From the above expression, we can also write

$$P(X = x_i, Y = y_j) = P(X = x_i | Y = y_j) P(Y = y_j).$$

This expression is also known as the **product rule of probability**.

How do we compute $P(X = x_i)$ from data?

- A way to compute the probability $P(X = x_i)$ is to repeat an experiment several times, say N, see how many outcomes we get for which $X = x_i$, say $n_{X=x_i}$ and then approximate the probability as

$$P(X = x_i) \approx \frac{n_{X=x_i}}{N}.$$

- We expect the approximation to become an equality when $N \to \infty$,

$$P(X = x_i) = \lim_{N\to\infty} \frac{n_{X=x_i}}{N}.$$

What about $P(X = x_i, Y = y_j)$ and $P(X = x_i | Y = y_j)$?

- We can follow a similar procedure to compute $P(X = x_i, Y = y_j)$,

$$P(X = x_i, Y = y_j) = \lim_{N \to \infty} \frac{n_{X=x_i, Y=y_j}}{N},$$

  where $n_{X=x_i, Y=y_j}$ is the number of times we observe a simultaneous occurence of $X = x_i$ and $Y = y_j$.

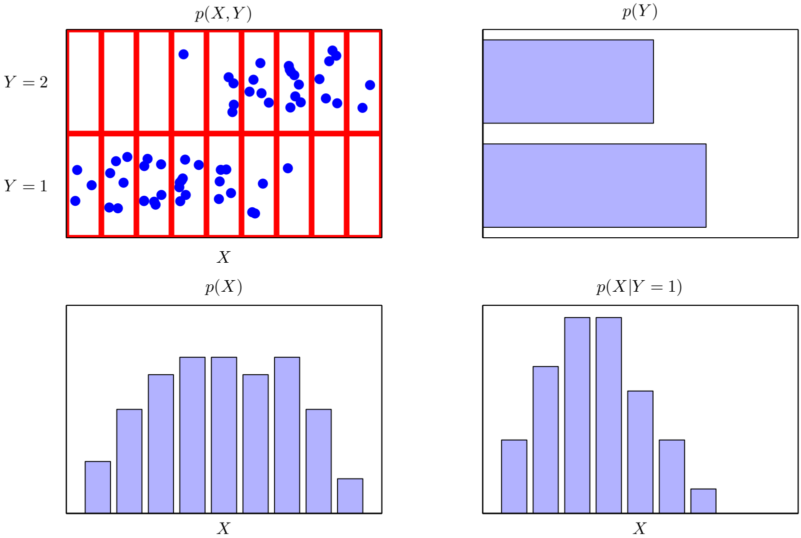
- To compute $P(X = x_i | Y = y_j)$, we can use the definition of the conditional probability

$$P(X = x_i | Y = y_j) = \frac{P(X = x_i, Y = y_j)}{P(Y = y_j)} \approx \frac{\frac{n_{X=x_i, Y=y_j}}{N}}{\frac{n_{Y=y_j}}{N}} = \frac{n_{X=x_i, Y=y_j}}{n_{Y=y_j}}.$$

- In the limit $N \to \infty$,

$$P(X = x_i | Y = y_j) = \lim_{N \to \infty} \frac{n_{X=x_i, Y=y_j}}{n_{Y=y_j}}.$$

Examples of the different pmf



From Bishop (2006).

Statistical independence

Two discrete RVs are *statistically independent* if

$$P(X = x_i, Y = y_j) = P(X = x_i)P(Y = y_j), \quad i = 1, \ldots, n \;\; j = 1, \ldots, m.$$

Bayes theorem

- Bayes theorem allows to go from $P(X = x)$ to $P(X = x|Y = y)$.

- According to Bayes theorem

$$P(X = x|Y = y) = \frac{P(Y = y|X = x)P(X = x)}{P(Y = y)}$$

Example: Bayes theorem

There are two barrels in front of you. Barrel One contains 20 apples and 4 oranges. Barrel Two contains 4 apples and 8 oranges. You choose a barrel randomly and select a fruit. It is an apple. What is the probability that the barrel was Barrel One?

Answer (I)

- There are two random variables involved.

- Let B be the random variable associated to picking one of the barrels. So B can either be “One” or “Two”.

- Let F be the random variables associated to picking a fruit. So F can either be “Apple” (A) or “Orange” (O).

- The probability we want to compute is the conditional probability $P(B = \text{One} | F = A)$.

Answer (II)

- The statement says "You choose a barrel randomly" which means that $P(B = \text{One}) = P(B = \text{Two}) = \frac{1}{2}$.

- Since we want to go from $P(B = \text{One})$ to $P(B = \text{One}|F = A)$, we can use Bayes theorem,

$$P(B = \text{One}|F = A) = \frac{P(F = A|B = \text{One})P(B = \text{One})}{P(F = A)}.$$

- We need to compute $P(F = A|B = \text{One})$ and $P(F = A)$.

Answer (III)

- Using the sum rule of probability and the product rule of probability

$$
\begin{aligned}
P(F = A) = \sum P(F = A, B) = \sum P(F = A|B)P(B) \\
= P(F = A|B = \text{One})P(B = \text{One}) \\
+ P(F = A|B = \text{Two})P(B = \text{Two}).
\end{aligned}
$$

- From the statement,

$$
\begin{aligned}
P(F = A|B = \text{One}) = \frac{20}{24} \\
P(F = A|B = \text{Two}) = \frac{4}{12}
\end{aligned}
$$

- We then have $P(F = A) = \frac{20}{24}\frac{1}{2} + \frac{4}{12}\frac{1}{2}$.

Answer (IV)

We can finally compute $P(B = \text{One}|F = A)$

$$P(B = \text{One}|F = A) = \frac{P(F = A|B = \text{One})P(B = \text{One})}{P(F = A)}$$
$$= \frac{\frac{20}{24}\frac{1}{2}}{\frac{20}{24}\frac{1}{2} + \frac{4}{12}\frac{1}{2}}$$
$$= \frac{\frac{20}{24}}{\frac{20}{24} + \frac{4}{12}} = \frac{5}{7} \approx 0.71$$

Expected value and statistical moments

- The expected value of a function of a discrete RV, $g(X)$ is defined as

$$E\{g(X)\} = \sum_{i=1}^{n} g(x_i) P(X = x_i).$$

- Two expected values or *statistical moments* of the discrete RV X, used frequently are the *mean* μ_X and the *variance* σ_X^2,

$$\mu_X = E\{X\} = \sum_{i=1}^{n} x_i P(X = x_i),$$

$$\begin{aligned}\sigma_X^2 &= \mathrm{var}\{X\} = E\{(X - \mu_X)^2\} = \sum_{i=1}^{n} (x_i - \mu_X)^2 P(X = x_i) \\ &= E\{X^2\} - \mu_X^2\end{aligned}$$

- The squared root of the variance, σ_X, is known as the *standard deviation*.

Example: Expected values

- Consider the following discrete RV X and its pmf. Compute μ_X and σ_X^2.

X	1	2	3	4
$P(X)$	0.3	0.2	0.1	0.4

- For the mean μ_X, we have

$$\mu_X = \sum_{i=1}^{n} x_i P(X = x_i) = (1)(0.3) + (2)(0.2) + (3)(0.1) + (4)(0.4) = 2.6.$$

- For the variance, we first compute $E\{X^2\}$ and then use $\sigma_X^2 = E\{X^2\} - \mu_X^2$.
- To compute $E\{X^2\}$, we can use $E\{g(X)\}$, where $g(X) : X \to X^2$,

$$E\{X^2\} = \sum_{i=1}^{n} x_i^2 P(X = x_i) = (1)^2(0.3) + (2)^2(0.2) + (3)^2(0.1) + (4)^2(0.4) = 8.4.$$

- We finally get $\sigma_X^2 = E\{X^2\} - \mu_X^2 = 8.4 - (2.6)^2 \approx 1.64$.

Notation

- When referring to the probability $P(X = x)$, we usually simply write $P(x)$.

- Likewise, instead of writing $P(X = x, Y = y)$, we simply write $P(x, y)$.

Contents

Probability density function

- A continuous RV X takes values within one or more intervals of the real line.

- We use **probability density functions** (pdf), $p_X(x)$, to describe a continuous RV X.

- Properties of a pdf
  1. $p_X(x) \geq 0$.
  2. $\int_{-\infty}^{\infty} p_X(x)\mathrm{d}x = 1$.
  3. $P(X \leq a) = \int_{-\infty}^{a} p_X(x)\mathrm{d}x$.
  4. $P(a \leq X \leq b) = \int_{a}^{b} p_X(x)\mathrm{d}x$.

Two continuous RVs

- As it was the case for discrete RVs, in ML, we are interested in analysing more than one continuous RV.

- We can use a **joint probability density function**, $p_{X,Y}(x,y)$ to fully characterise two continuous random variables X and Y.

- Properties of a joint pdf
  1. $p_{X,Y}(x,y) \geq 0$.
  2. $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p_{X,Y}(x,y) \mathrm{d}x \mathrm{d}y = 1$.
  3. $P(X \leq a, Y \leq c) = \int_{-\infty}^{a} \int_{-\infty}^{c} p_{X,Y}(x,y) \mathrm{d}x \mathrm{d}y$.
  4. $P(a \leq X \leq b, c \leq Y \leq d) = \int_{a}^{b} \int_{c}^{d} p_{X,Y}(x,y) \mathrm{d}x \mathrm{d}y$.

Rules of probability (continuous RVs)

- **Sum rule of probability.** In the case of continuous RVs, we replace the sums we had before with an integral

$$p_X(x) = \int_{-\infty}^{\infty} p_{X,Y}(x,y)\mathrm{d}y,$$

where $p_X(x)$ is known as the **marginal pdf.**
- **Product rule of probability.** The conditional pdf can be obtained as

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

which can also be written as

$$p_{X,Y}(x,y) = p_{X|Y}(x|y)p_Y(y).$$

The conditional pdf in this last form is known as the product rule of probability for two continuous RVs.

Bayes theorem and statistical independence

- For the case of continuous RVs, Bayes theorem follows as

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

- We say that two continuous RVs X and Y are statistically independent if

$$p_{X,Y}(x,y) = p_X(x)p_Y(y).$$

Expected values and statistical moments

For continuous RVs, expected values are computed as

$$
\begin{aligned}
E\{g(X)\} &= \int_{-\infty}^{\infty} g(x) p_X(x) \mathrm{d}x, \\
\mu_X = E\{X\} &= \int_{-\infty}^{\infty} x p_X(x) \mathrm{d}x, \\
\sigma_X^2 = \mathrm{var}\{X\} &= E\{(X - \mu_X)^2\} = \int_{-\infty}^{\infty} (x - \mu_X)^2 p_X(x) \mathrm{d}x. \\
&= E\{X^2\} - \mu_X^2.
\end{aligned}
$$

Notation

We have been using $p_X(x)$ or $p_{X,Y}(x, y)$ to refer to pdfs. We will normally drop the subindex for the RVs and simply use $p(x)$ or $p(x, y)$ to refer to the pdfs.

Contents

What if we don't have the pmf or pdf?

- Discrete RVs. In practice, we can use data to compute the probabilities $P(X = x_i)$ or $P(X = x_i, Y = y_j)$ by applying the definitions we saw before.

- Notice that those definitions are valid in the limit $N \to \infty$.

- Continuous RVs. In pratice, we assume a particular model for the pdf, eg. a Gaussian pdf, and estimate the parameters of that pdf, e.g. the mean and variance for the Gaussian pdf.

- There are advanced methods to model both pmf and pdfs but we will not study those in this module.

What about moments?

- We can estimate μ_X and σ_X^2 when we have access to observations of the random variable X, $x_1, x_2, \cdots, x_N$, but no access to the pmf or the pdf.
- In statistics, these are called "estimators" for μ_X and σ_X^2, denoted as $\widehat{\mu}_X$ and $\widehat{\sigma^2}_X$.
- An estimator for μ_X is given as

$$\widehat{\mu}_X = \frac{1}{N}\sum_{k=1}^{N} x_k.$$

- An estimator for σ_X^2 is given as

$$\widehat{\sigma^2}_X = \frac{1}{N-1}\sum_{k=1}^{N}(x_k - \widehat{\mu}_X)^2.$$

What if we have more than two RVs?

- In ML, we are usually faced with problems where we have more than two RVs.
- In fact, there are applications of ML in Natural Language Processing, speech processing, computer vision, computational biology, etc. where we can have hundreds of thousands or even millions of RVs.
- The ideas that we saw before can be extended to these cases and we will see some examples in the following lectures.