



Algorithms. Matching

Part II. Preference model.

B9 - Algorithms Matching

M-ALG-102

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└ Introduction

Introduction

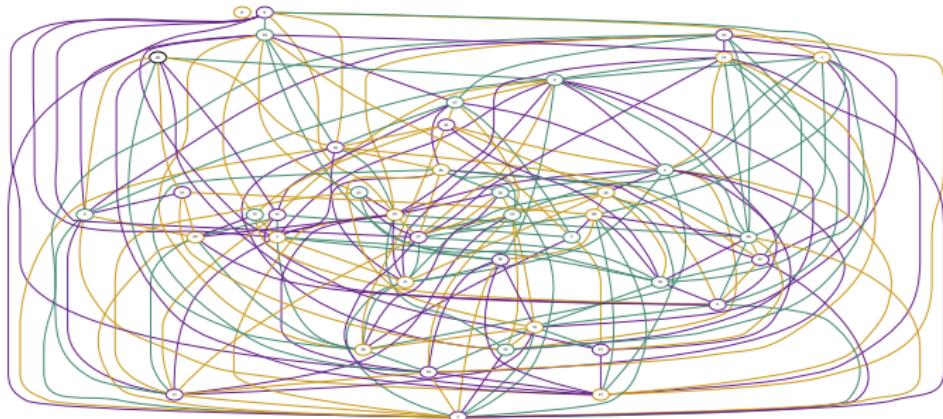


Figure – Graph

...

└ Introduction

Introduction

<https://github.com/nlehir/ALGO2>

We will use :

- ▶ networkx
- ▶ matplotlib
- ▶ pandas
- ▶ sklearn
- ▶ optionnally : ipdb



Compatibility graphs

Simple geometrical data

Non geometrical data

Probability distributions

Reminders on probabilities

Analyzing a distribution

Optimization and Maximum Likelihood

Gradients

Multivariate analysis and clustering

Correlation

Dimension reduction

Correlation and causality

Scatter matrix

Clustering

Kmeans clustering

Similarities

Spectral Clustering

Additional considerations and conclusions

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Compatibility graphs

- ▶ Yesterday we processed graphs describing **relationship between data**
- ▶ If two nodes were related, they were linked by an edge in the graph.

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Compatibility graphs

- ▶ Yesterday we processed graphs describing **relationship between data**
- ▶ If two nodes were related, they were linked by an edge in the graph.
- ▶ Today we are interested in building such graphs directly from the data, we call them **compatibility graphs**.

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└ Compatibility graphs

Compatibility graphs

We are interested in building **compatibility graphs**.

Given two nodes in a graph, should there be an edge between them ?

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Compatibility graphs

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Given two nodes in a graph, should there be an edge between them ?

Note : it is not the same problem as the matching problem. In the matching problem, the edges are already defined.

...

└ Compatibility graphs

Compatibility graphs

We are interested in building **compatibility graphs**.

Given two nodes in a graph, should there be an edge between them ?

Note : it is not the same problem as the matching problem. In the matching problem, the edges are already defined.

However, once the edges are built, we can apply a matching to it.

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└ Compatibility graphs

Example applications

- ▶ Social networks management
- ▶ Recommendations

...

└ Compatibility graphs

Building compatibility graphs

- ▶ We will build graphs first from simple data
- ▶ Then from more complex data.

...

└ Compatibility graphs

 └ Simple geometrical data

Building a graph from simple data

- ▶ We will first build a graph from simple data in the 2D space.

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- Compatibility graphs

- Simple geometrical data

Euclidian distance and compatibility

Consider the following data :

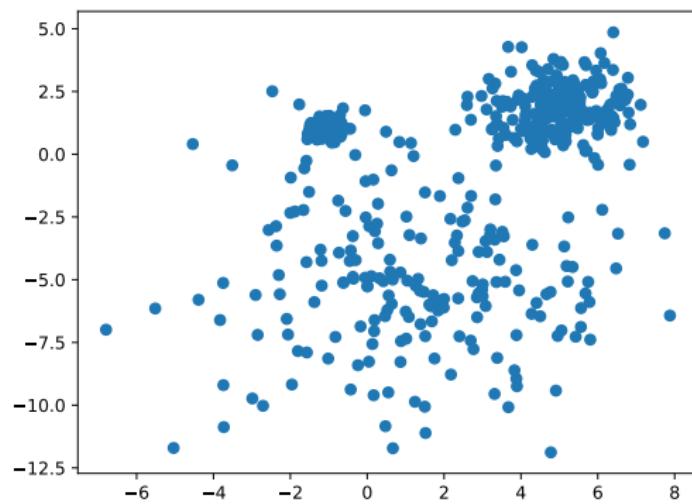


Figure – Data : we would like to define **edge** between some of them

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└ Compatibility graphs

└ Simple geometrical data

Is this set of edges a good solution ?

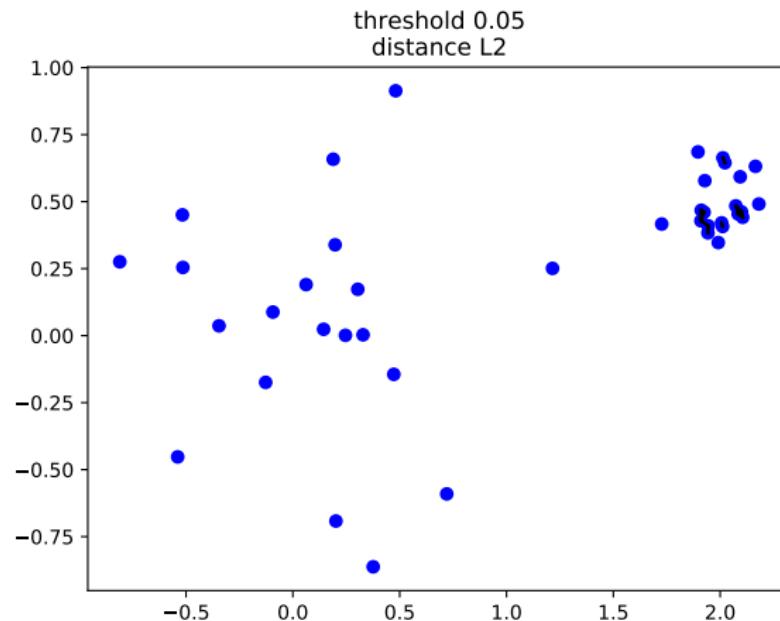


Figure – Some definition of edges

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└ Compatibility graphs

└ Simple geometrical data

Is this set of edges a good solution ?

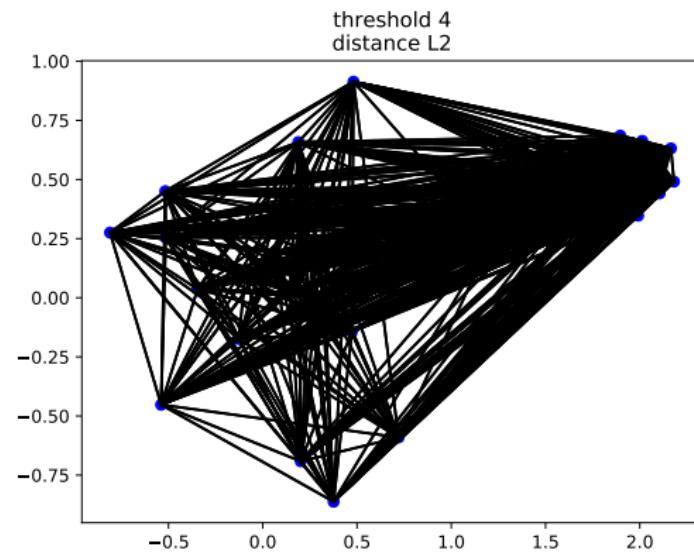


Figure – Some definition of edges

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└ Compatibility graphs

└ Simple geometrical data

This one looks ok

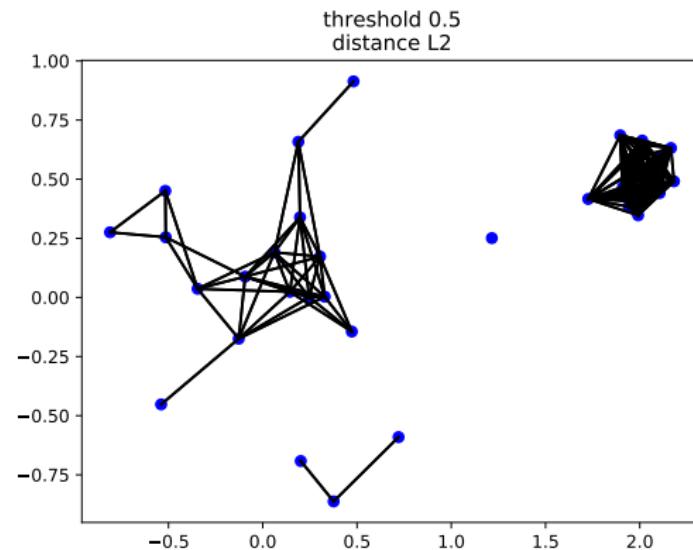


Figure – A proposition of edges

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└ Compatibility graphs

 └ Simple geometrical data

Backboard

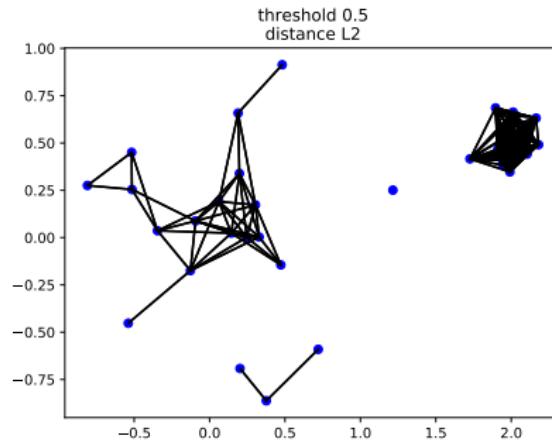
- ▶ Euclidian distance and threshold.

...

└ Compatibility graphs

└ Simple geometrical data

Exercice 1: Setting a threshold cd **compatibility_simple** and set the threshold used in **build_graph_1.py** to draw relevant edges between the nodes. Feel free to use another dataset !



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- └ Compatibility graphs

- └ Simple geometrical data

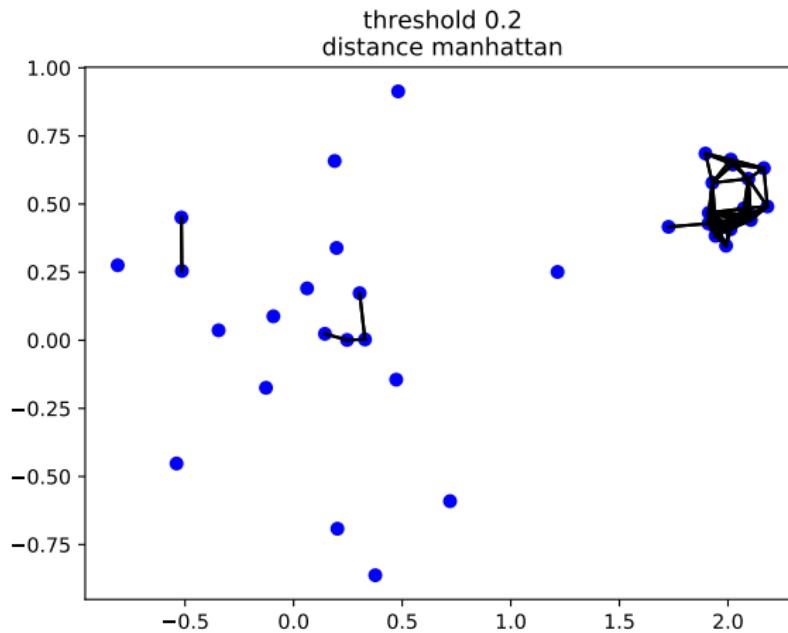
Exercice 2 : Changing the distance

- ▶ Assess the impact of changing the distance used. Possible choices :
 - ▶ L_1 distance (Manhattan)
 - ▶ $\| \cdot \|_\infty$ distance (backboard)
 - ▶ custom distance
- ▶ use **build_graph_2.py** and edit the distances used at the end of the file.
- ▶ Try several values for the threshold.

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└ Compatibility graphs

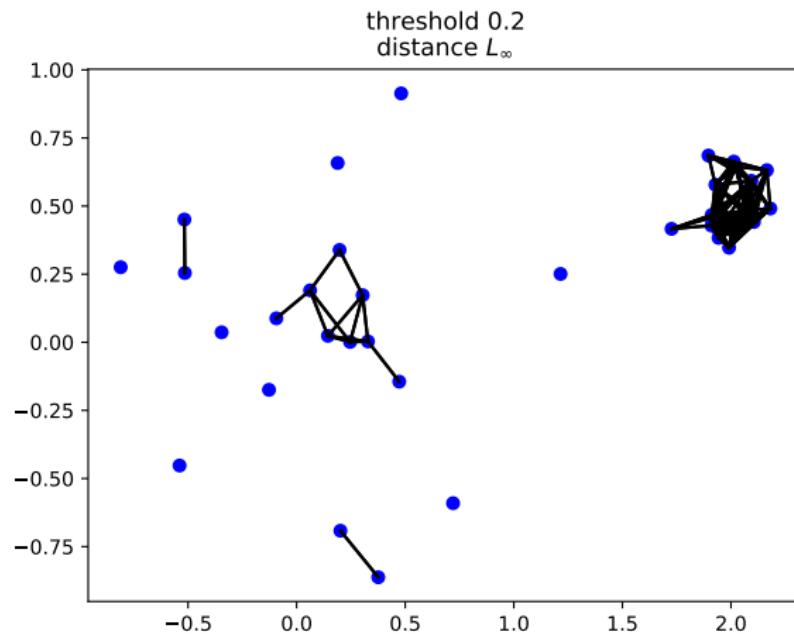
└ Simple geometrical data



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└ Compatibility graphs

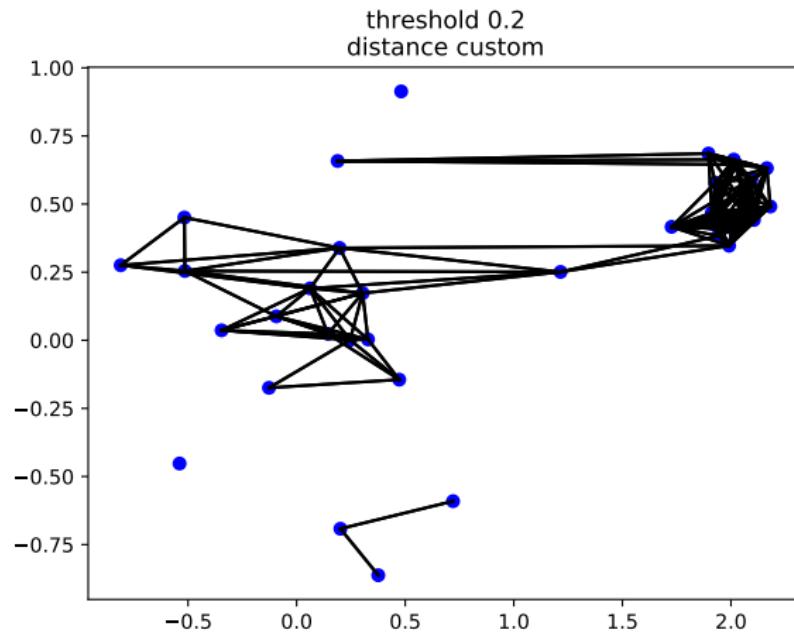
└ Simple geometrical data



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└ Compatibility graphs

└ Simple geometrical data



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└ Compatibility graphs

└ Simple geometrical data

General notion of a distance

- ▶ Let us generalize what we experimentally studied.

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└ Compatibility graphs

└ Simple geometrical data

Examples of distances

$x = (x_1, \dots, x_p)$ and $y = (y_1, \dots, y_p)$ are p -dimensional **vectors**.

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- └ Compatibility graphs

- └ Simple geometrical data

Examples of distances

$x = (x_1, \dots, x_p)$ and $y = (y_1, \dots, y_p)$ are p -dimensional vectors.

- ▶ $L_2 : ||x - y||_2 = \sqrt{\sum_{k=1}^p (x_k - y_k)^2}$ (Euclidian distance,
2-norm distance)

...

└ Compatibility graphs

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Examples of distances

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- ▶ $L_1 : ||x - y||_1 = \sum_{k=1}^p |x_k - y_k|$ (Manhattan distance, 1-norm distance)

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└ Compatibility graphs

└ Simple geometrical data

Examples of distances

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- ▶ weighted $L_1 : \sum_{k=1}^p w_k |x_k - y_k|$

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└ Compatibility graphs

└ Simple geometrical data

Examples of distances

$x = (x_1, \dots, x_p)$ and $y = (y_1, \dots, y_p)$ are p -dimensional vectors.

- ▶ L2 : $\|x - y\|_2 = \sqrt{\sum_{k=1}^p (x_k - y_k)^2}$ (Euclidian distance, 2-norm distance)
- ▶ L1 : $\|x - y\|_1 = \sum_{k=1}^p |x_k - y_k|$ (Manhattan distance, 1-norm distance)
- ▶ weighted L_1 : $\sum_{k=1}^p w_k |x_k - y_k|$
- ▶ L_∞ : $\max(x_1, \dots, x_n)$ (infinity norm distance)

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└ Compatibility graphs

└ Simple geometrical data

Hamming distance

- ▶ $\#\{x_i \neq y_i\}$ (Hamming distance)

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└ Compatibility graphs

└ Simple geometrical data

Hamming distance and edit distance

- ▶ $\#\{x_i \neq y_i\}$ (Hamming distance)
- ▶ linked to **edit distance** : used to quantify how dissimilar two strings are by counting the number of operations needed to transform one into the other (several variants exist)

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└ Compatibility graphs

└ Simple geometrical data

General definition of a distance

A **distance** on a set E is an application $d : E \times E \rightarrow \mathbb{R}_+$ that must :

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- └ Compatibility graphs

- └ Simple geometrical data

General definition of a distance

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- ▶ be **symmetrical** : $\forall (x, y) \in E^2, d(x, y) = d(y, x)$

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- └ Compatibility graphs

- └ Simple geometrical data

General definition of a distance

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- ▶ **separate the values** : $\forall (x, y) \in E^2, d(x, y) = 0 \Leftrightarrow x = y$

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└ Compatibility graphs

└ Simple geometrical data

General definition of a distance

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- ▶ **separate the values** : $\forall (x, y) \in E^2, d(x, y) = 0 \Leftrightarrow x = y$
- ▶ respect the **triangular inequality**

$$\forall (x, y, z) \in E^3, d(x, y) \leq d(x, z) + d(z, y)$$

Building compatibility graphs for non geometrical data

- ▶ Some data are not geometric
- ▶ Some features are not numbers, but could for instance be strings, or categories (categorical data)
- ▶ We will use **pandas** process the data from a **csv** file and build a compatibility graph.
- ▶ You can use
compatibility_graphs_other_data/build_graph.py or
the notebook.

...

└ Compatibility graphs

 └ Non geometrical data

Non geometrical data

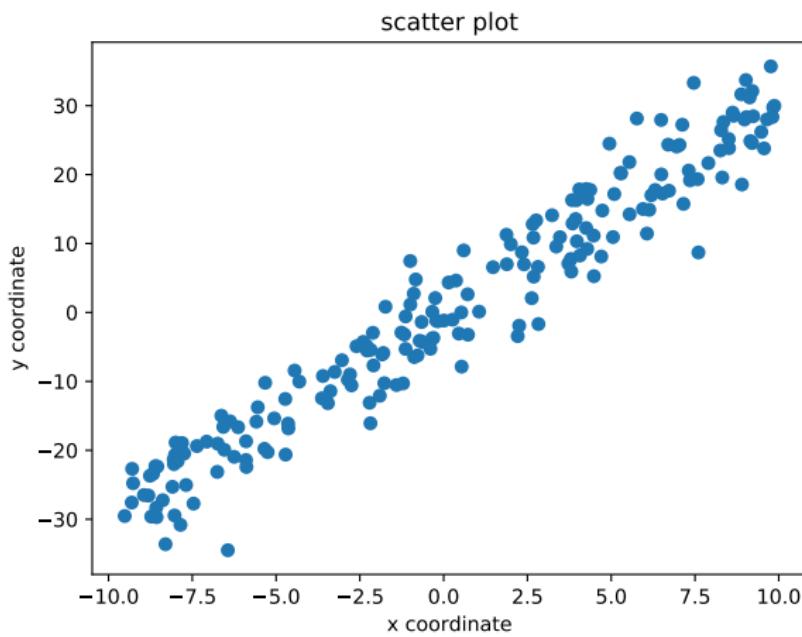
Exercice 3 : Experiment with the data, the threshold in order to build different graphs

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- Probability distributions

- Reminders on probabilities

Random variables

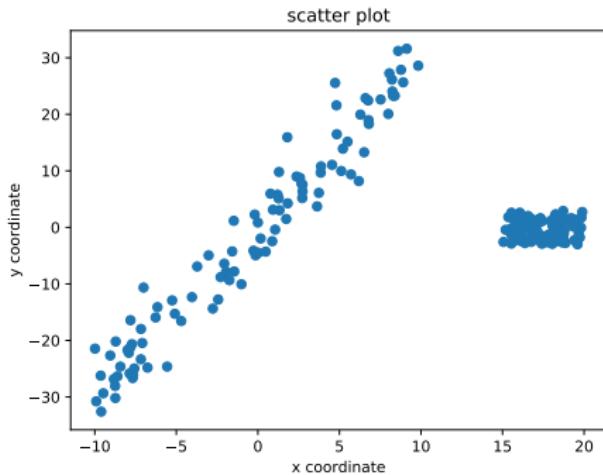


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- Probability distributions

- Reminders on probabilities

Random variables



We want to analyse how the data are **distributed**. For instance the x coordinate, the y coordinate.

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└ Probability distributions

 └ Reminders on probabilities

Random variables

- ▶ A **random variable** is a quantity that can take several values

...

- Probability distributions

- Reminders on probabilities

Random variables

- ▶ A **random variable** is a quantity that can take several values
- ▶ For instance :
 - ▶ the result of a dice throw



Figure – Dice

...

└ Probability distributions

 └ Reminders on probabilities

Random variables

- ▶ A **random variable** is a quantity that can take several values
- ▶ For instance :
 - ▶ the result of a dice throw
 - ▶ waiting time with RATP



Figure – Some metro station

...

- Probability distributions

- Reminders on probabilities

Random variables

- ▶ A **random variable** is a quantity that can take several values
- ▶ For instance :
 - ▶ the result of a dice throw
 - ▶ waiting time with RATP
 - ▶ weather



Figure – Weather in November

...

└ Probability distributions

 └ Reminders on probabilities

Random variables

- ▶ A **random variable** is a quantity that can take several values
- ▶ For instance :
 - ▶ the result of a dice throw
 - ▶ waiting time with RATP
 - ▶ weather
 - ▶ number of cars taking the périphérique at the same time

...

└ Probability distributions

 └ Reminders on probabilities

Random variables

What are the differences between these random variables ?

...

└ Probability distributions

 └ Reminders on probabilities

Random variables

What are the differences between these random variables ?

- ▶ Some are **continuous**, others **discrete**
- ▶ **continuous** :

...

└ Probability distributions

 └ Reminders on probabilities

Random variables

What are the differences between these random variables ?

- ▶ Some are **continuous**, others **discrete**
- ▶ **continuous** : weather, RATP

...

- Probability distributions

- Reminders on probabilities

Random variables

What are the differences between these random variables ?

- ▶ Some are **continuous**, others **discrete**
- ▶ **continuous** : weather, RATP
- ▶ **discrete** : dice (6 possibilities), number of cars (> 10000)

...

└ Probability distributions

 └ Reminders on probabilities

Probability distributions

- ▶ A random variable is linked to a **probability distribution**.

...

└ Probability distributions

 └ Reminders on probabilities

Probability distributions

- ▶ A random variable is linked to a **probability distribution**.
- ▶ It quantifies the probability of observing one outcome.

...

- Probability distributions

- Reminders on probabilities

Probability distributions

- ▶ A random variable is linked to a **probability distribution**, which is a function P
- ▶ It quantifies the probability of observing one outcome.
- ▶ For a discrete variable : each possible outcome is associated with a number between 0 and 1

...

- Probability distributions

- Reminders on probabilities

Probability distributions

- ▶ For a dice game, the possible outcomes are in the set $\{1, 2, 3, 4, 5, 6\}$
- ▶ For a dice game : $P(1) = ?$ $P(2) = ?$ $P(3) = ?$ $P(4) = ?$
 $P(5) = ?$ $P(6) = ?$

...

└ Probability distributions

└ Reminders on probabilities

Probability distributions

- ▶ For a dice game, the possible outcomes are in the set $\{1, 2, 3, 4, 5, 6\}$
- ▶ For a dice game : $P(1) = \frac{1}{6}$, $P(2) = \frac{1}{6}$, $P(3) = \frac{1}{6}$, $P(4) = \frac{1}{6}$,
 $P(5) = \frac{1}{6}$, $P(6) = \frac{1}{6}$
- ▶ This is called a **uniform distribution**

...

└ Probability distributions

 └ Reminders on probabilities

Probability distributions

- ▶ Peripherique :

...

└ Probability distributions

 └ Reminders on probabilities

Probability distributions

- ▶ Peripherique : probably a time-dependent very complicated distribution

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└ Probability distributions

 └ Reminders on probabilities

Continuous variables

- ▶ How would you model a continuous variable ? Can you assign a number to a waiting time or a weather ?

...

- Probability distributions

- Reminders on probabilities

Continuous variables

- ▶ How would you model a continuous variable? Can you assign a number to a waiting time or a weather?
- ▶ One needs to use **probability densities**. Formally, the probability of being between x and $x + dx$ is $p(x)dx$.

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- Probability distributions

- Reminders on probabilities

Continuous variables

- ▶ How would you model a continuous variable? Can you assign a number to a waiting time or a weather?
- ▶ One needs to use **probability densities**. Formally, the probability of being between x and $x + dx$ is $p(x)dx$.
- ▶ Let's see some examples

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- Probability distributions

- Reminders on probabilities

Uniform discrete

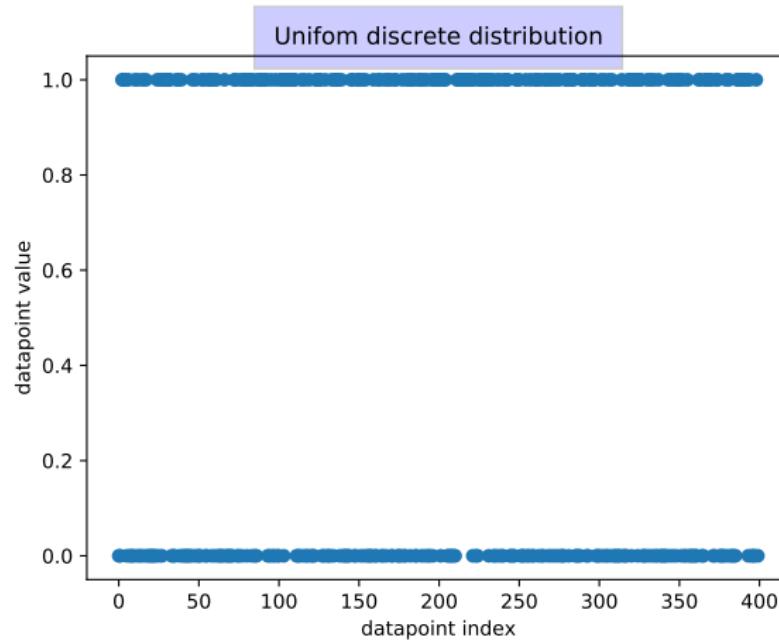


Figure – Uniform discrete distribution with 2 values

Uniform discrete

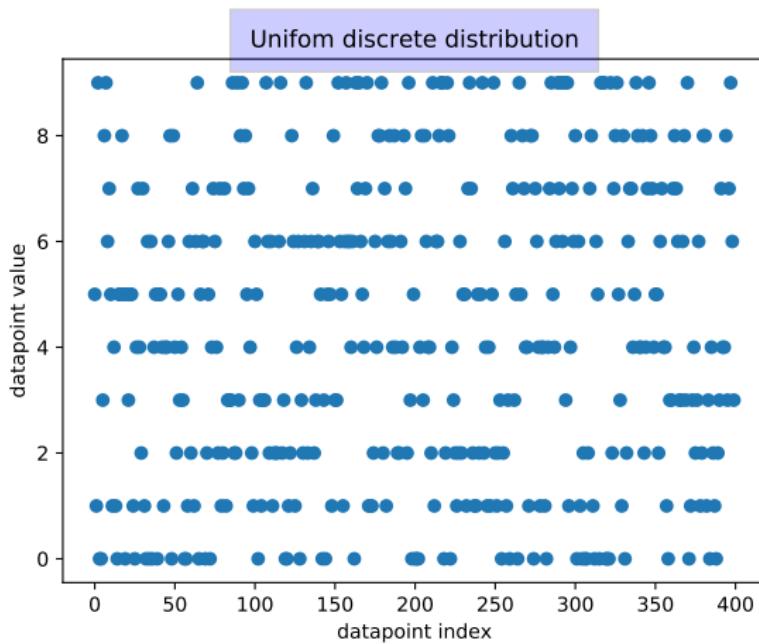


Figure – Uniform discrete distribution with 10 values

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- Probability distributions

- Reminders on probabilities

Bernoulli

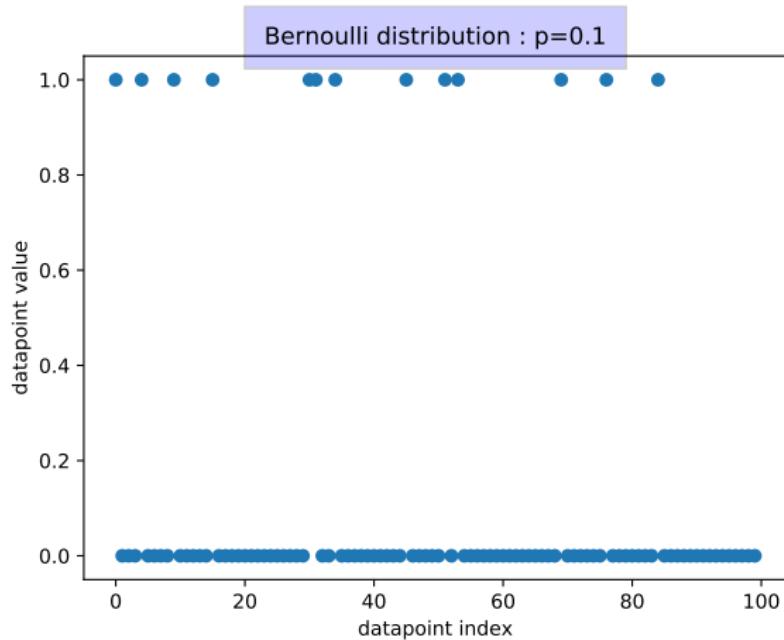


Figure – Bernoulli distribution

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- └ Probability distributions

- └ Reminders on probabilities

Bernoulli p

- ▶ With probability p , $X = 1$
- ▶ With probability $1 - p$, $X = 0$

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- Probability distributions

- Reminders on probabilities

Bernoulli

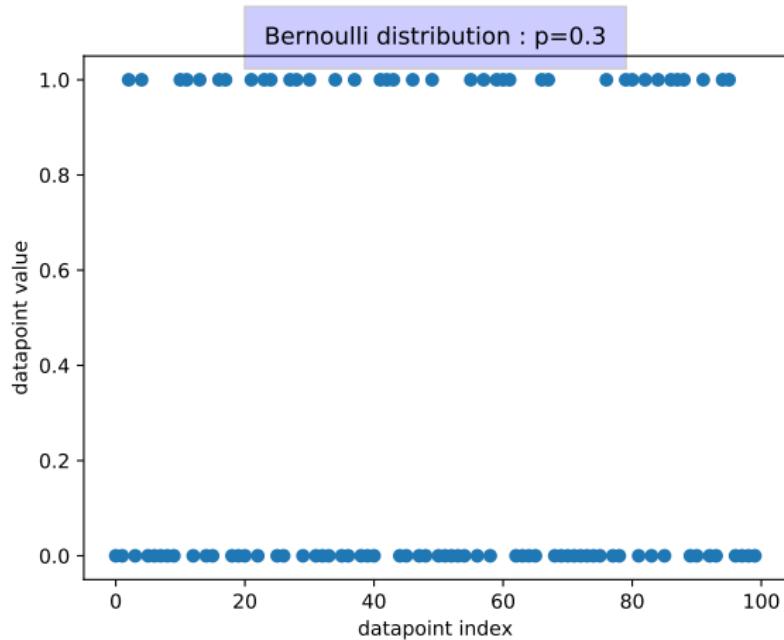


Figure – Bernoulli Distribution

Bernoulli

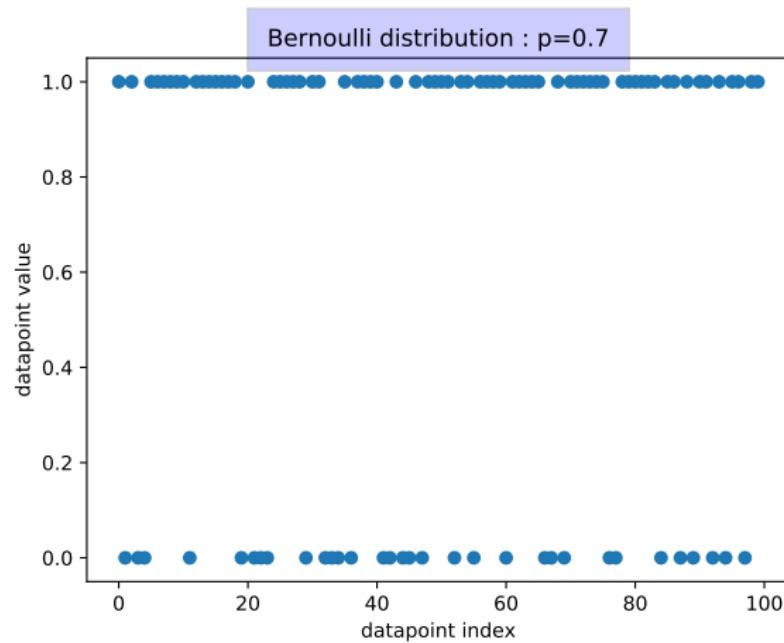


Figure – Bernoulli Distribution

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- Probability distributions

- Reminders on probabilities

Uniform continuous

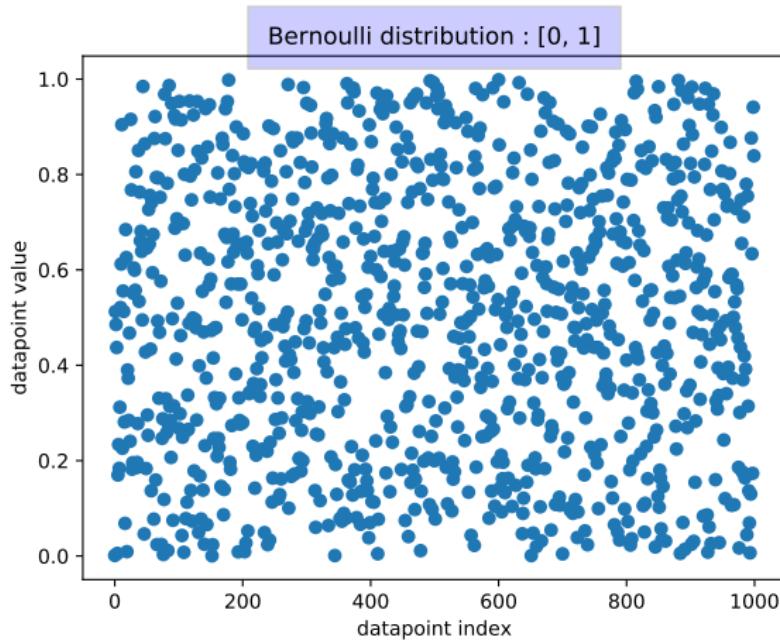


Figure – Uniform continuous distribution

...

- Probability distributions

- Reminders on probabilities

Uniform continuous

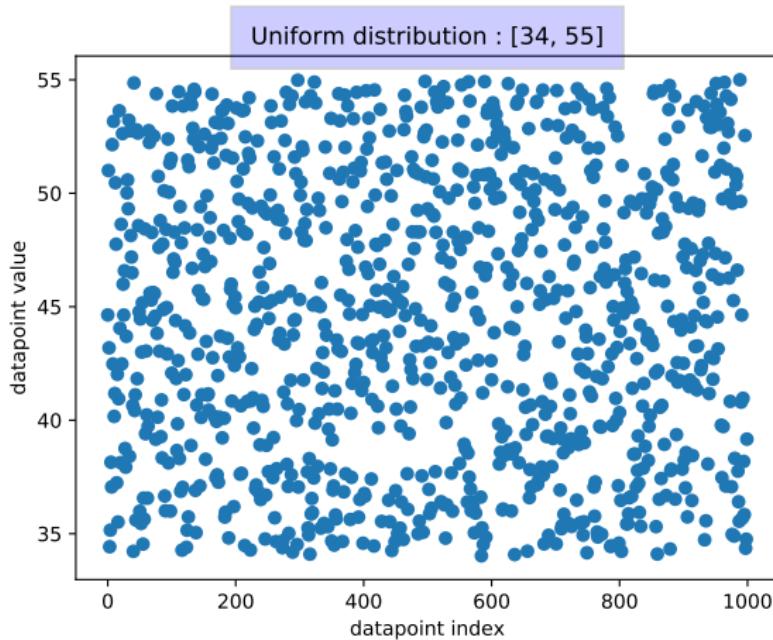


Figure – Uniform continuous distribution

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- Probability distributions

- Reminders on probabilities

Uniform continuous

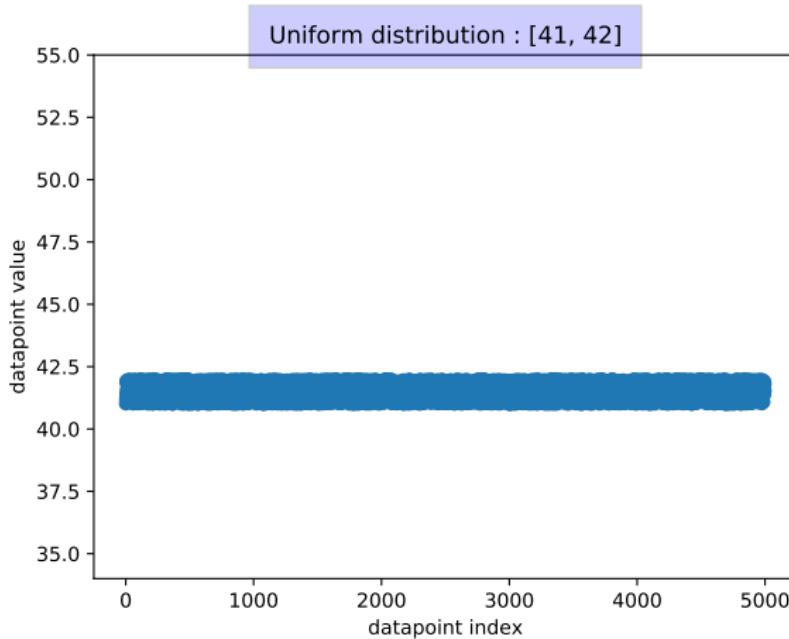


Figure – Uniform continuous distribution

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- Probability distributions

- Reminders on probabilities

Normal

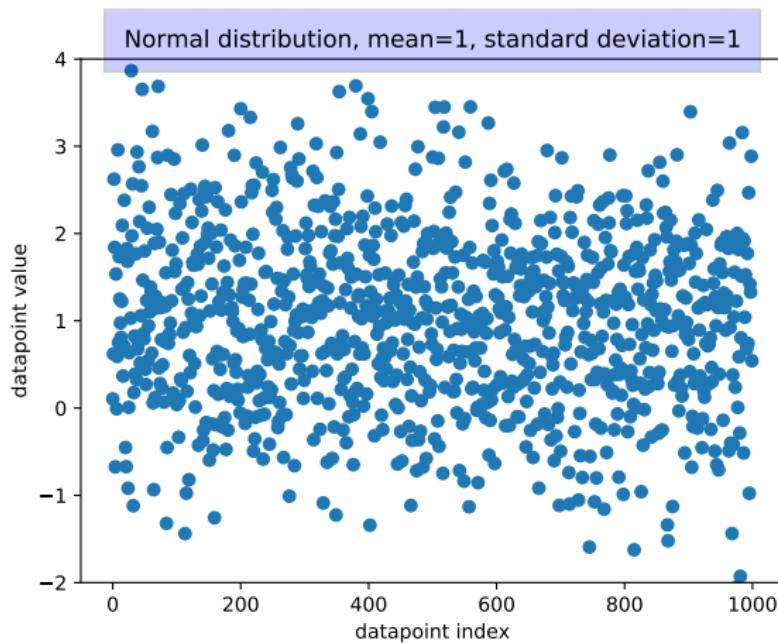


Figure – Normal distribution

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- Probability distributions

- Reminders on probabilities

Normal

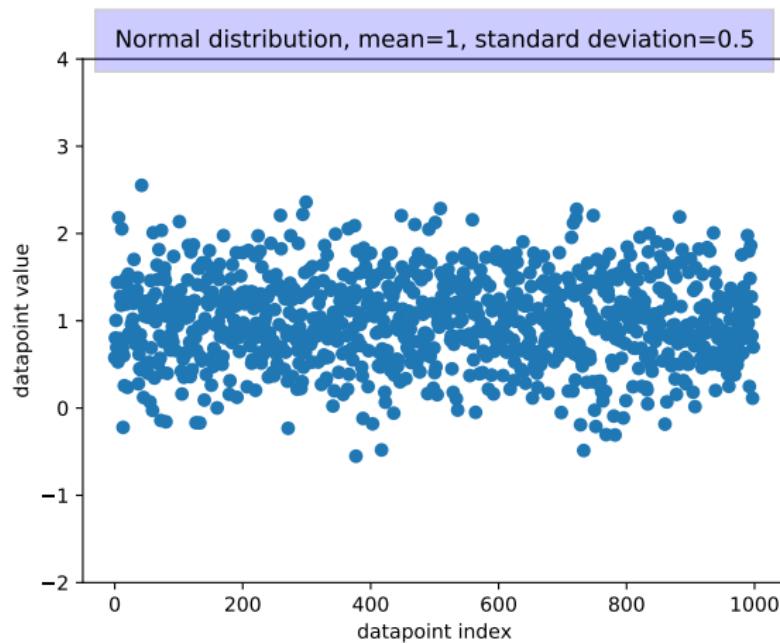


Figure – Normal distribution

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- Probability distributions

- Reminders on probabilities

Normal

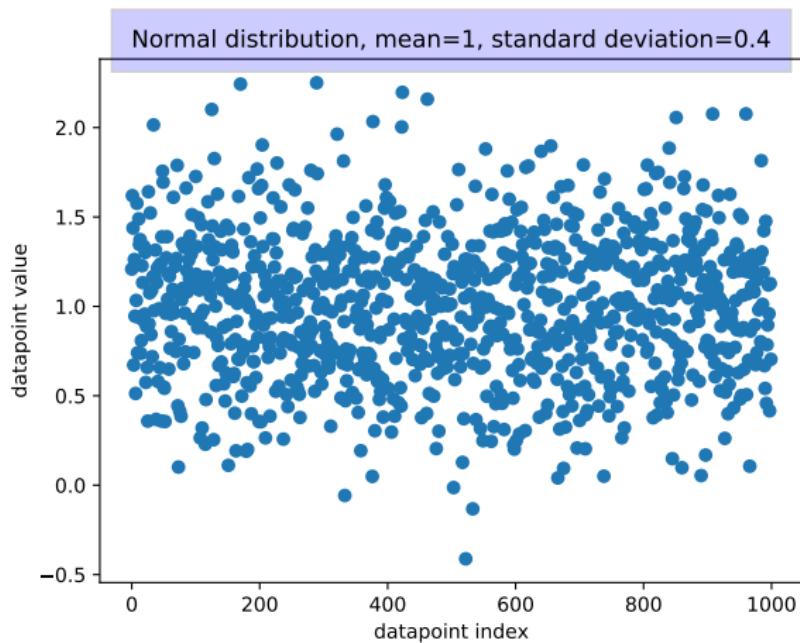


Figure – Normal distribution

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- Probability distributions

- Reminders on probabilities

White noise

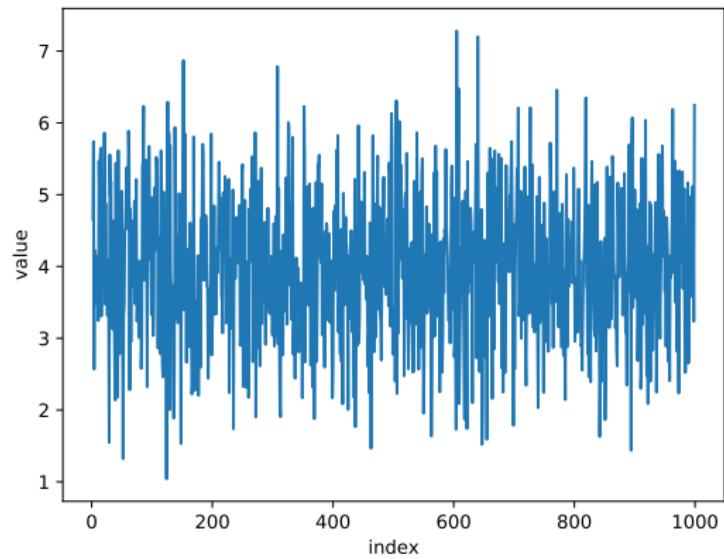


Figure – White noise

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└ Probability distributions

 └ Reminders on probabilities

Histograms

Is looking at the raw dataset really **informative** ?

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└ Probability distributions

 └ Reminders on probabilities

Histograms

Is looking at the raw dataset really **informative** ?
It is informative, but often a **histogram** tells more.

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- Probability distributions

- Reminders on probabilities

Uniform discrete

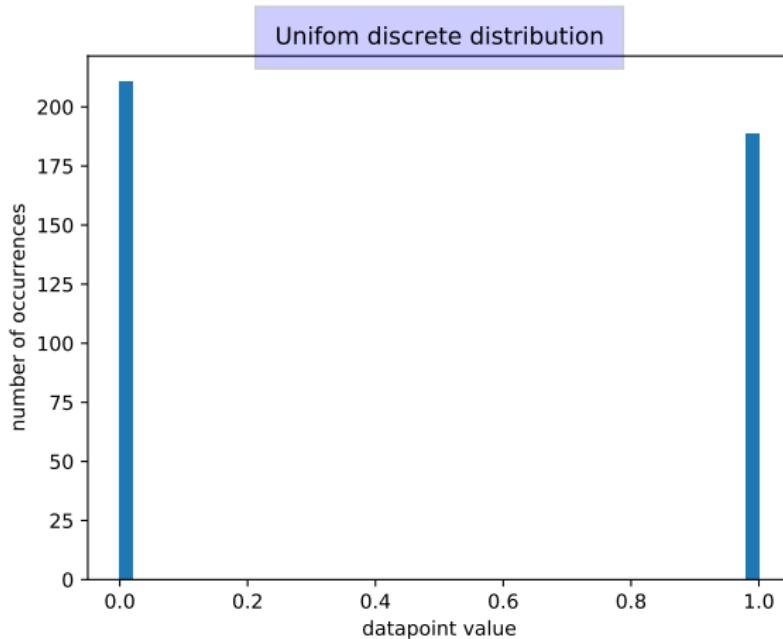


Figure – Histogram 1

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- Probability distributions

- Reminders on probabilities

Uniform discrete

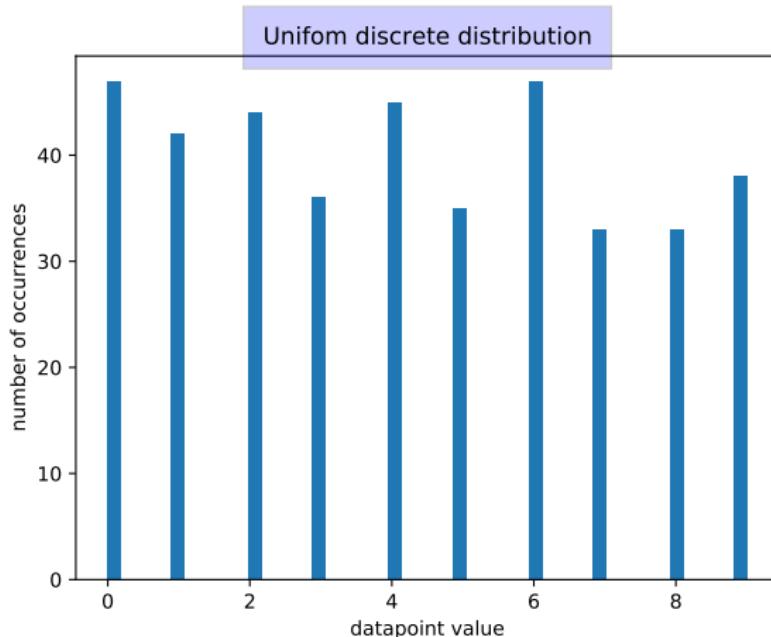


Figure – Historgram 1

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- Probability distributions

- Reminders on probabilities

Bernoulli

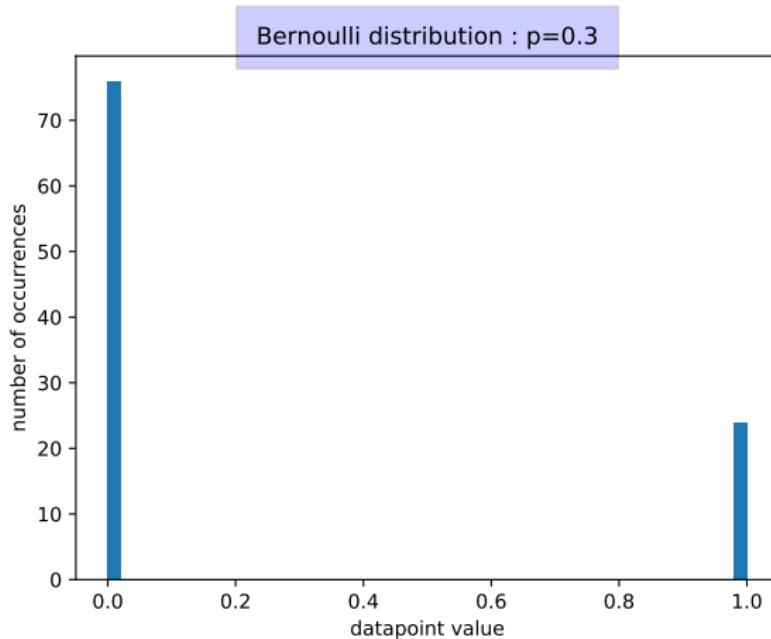


Figure – Histogram 2

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- Probability distributions

- Reminders on probabilities

Uniform continuous

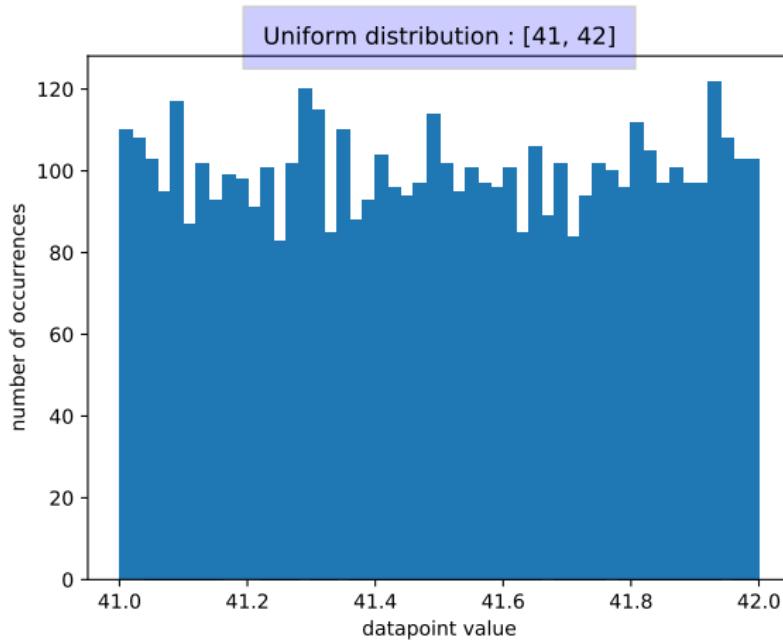


Figure – Histogram 3

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- Probability distributions

- Reminders on probabilities

Normal

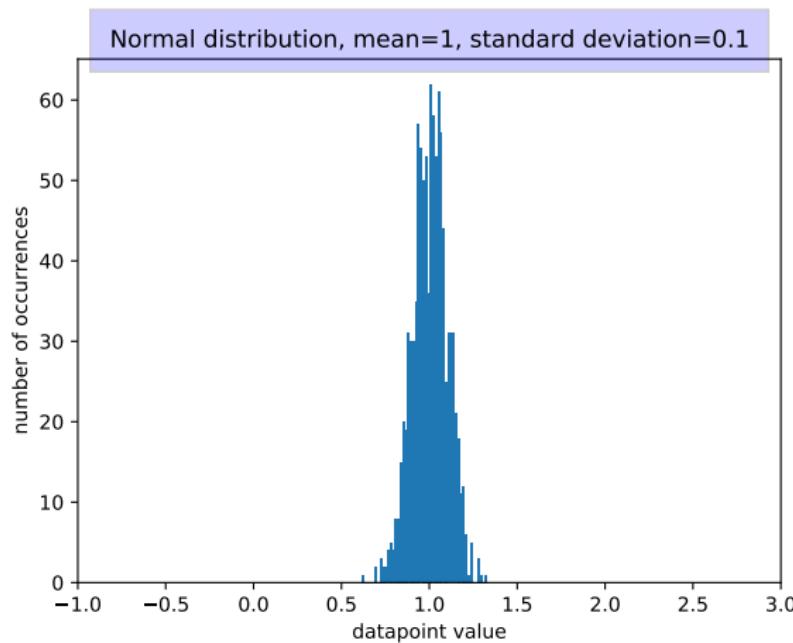


Figure – Historgram 4

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- Probability distributions

- Reminders on probabilities

Normal

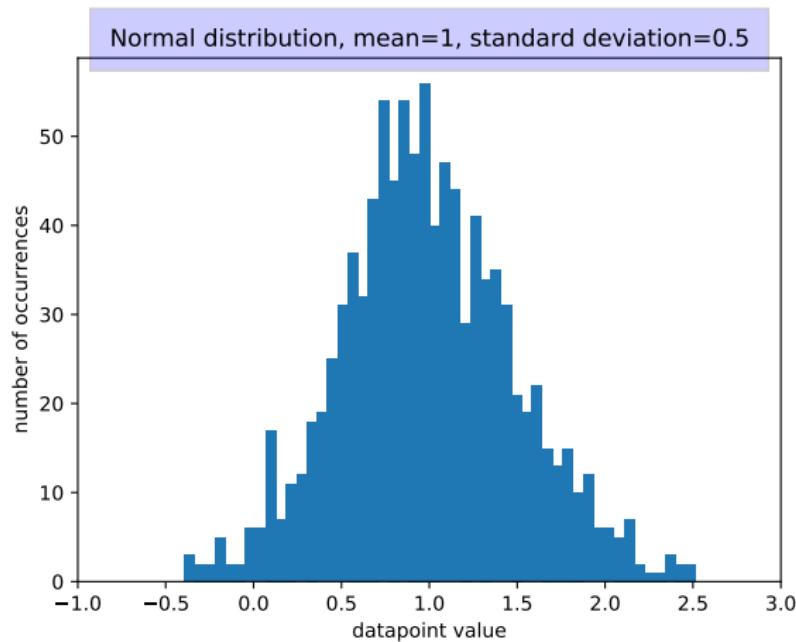


Figure – Histogram 4

...

└ Probability distributions

 └ Analyzing a distribution

Exercice 4 : Analyzing a distribution I put values in the file
mysterious_distro_1.csv

...

- └ Probability distributions
 - └ Analyzing a distribution

Exercice 4 : Analyzing a distribution I put values in the file
mysterious_distro_1.csv

Can you analyze these values in terms of a **distribution** ?

Use **read_myst_1.py** to analyze the distribution (suggestion :
change the number of bins used)

...

Exercice 5 : Analyzing a distribution When you have guessed the kind of distribution it is, you need to finds its **parameters**.

- ▶ its mean
- ▶ its standard deviation

This is called **fitting** a distribution to a dataset : it's a classical machine learning problem.

To do so, uncomment the last section of the script

read_myst_1.py

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- └ Probability distributions
 - └ Analyzing a distribution

Distribution 1

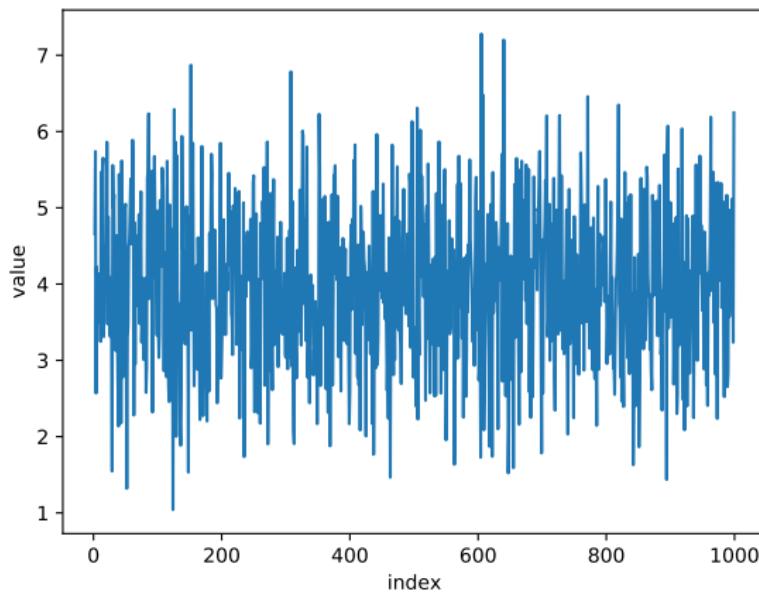


Figure – The data we analyze

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- └ Probability distributions
 - └ Analyzing a distribution

histograms

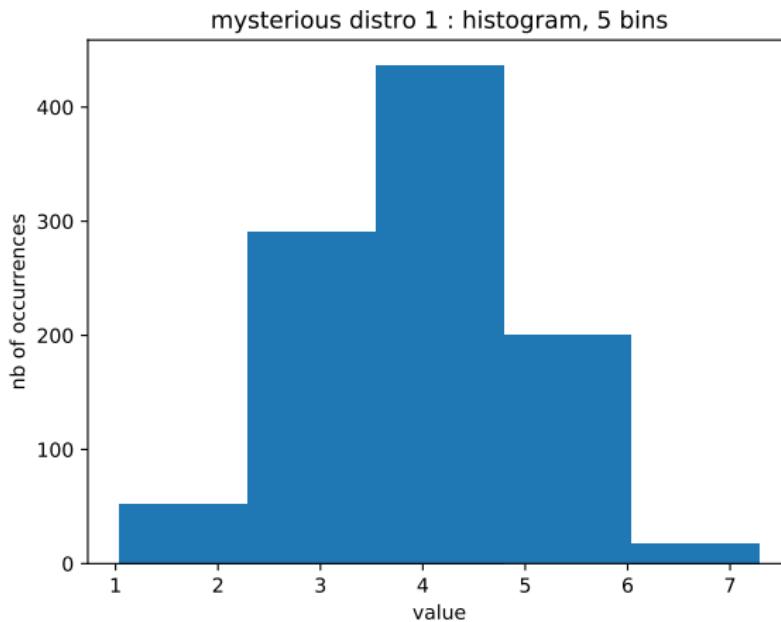


Figure – 5 bins

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- └ Probability distributions
 - └ Analyzing a distribution

histograms

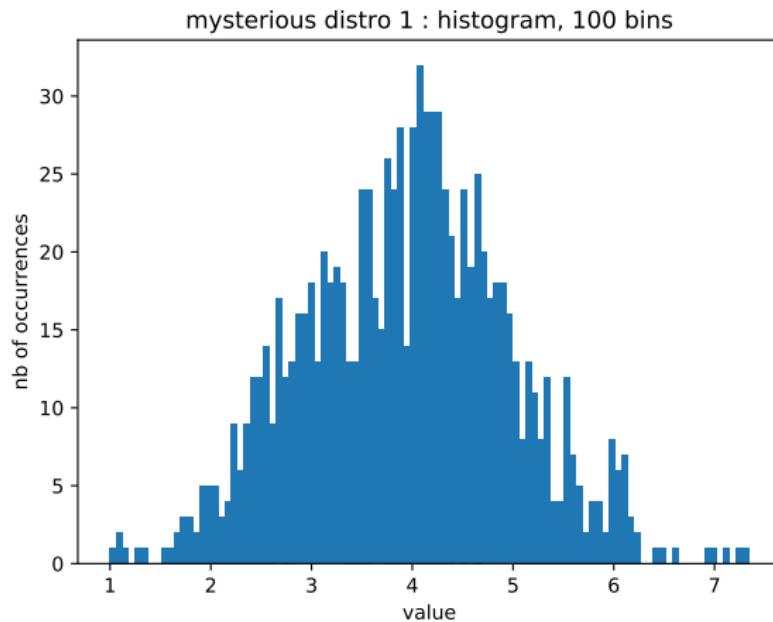


Figure – 100 bins

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- └ Probability distributions
 - └ Analyzing a distribution

histograms

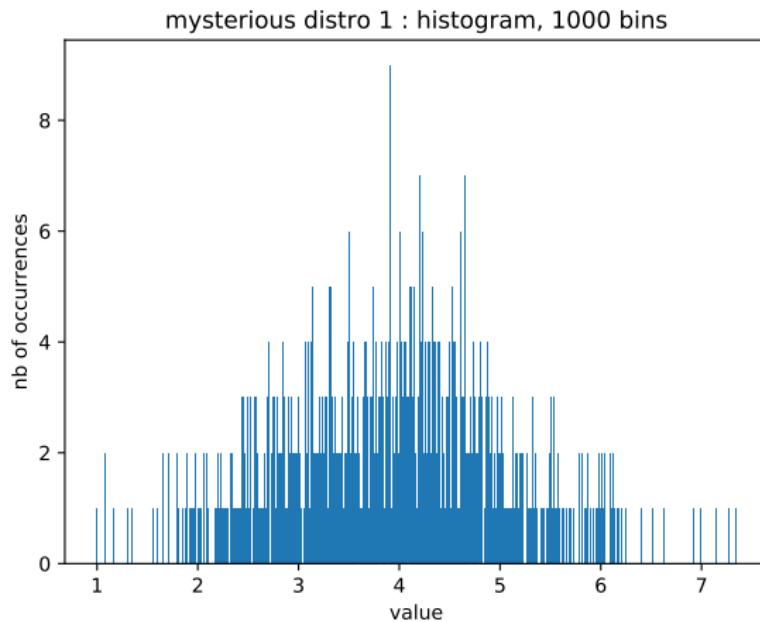


Figure – 1000 bins (too many)

Normal distribution

```
import csv
import numpy as np

file_name = 'mysterious_distro_1.csv'

mean = 4
std_dev = 1
nb_point = 1000

with open('csv_files/' + file_name, 'w') as csvfile:
    filewriter = csv.writer(csvfile, delimiter=',')
    for point in range(1, nb_point):
        random_variable = np.random.normal(loc=mean, scale=std_dev)
        filewriter.writerow([str(point), str(random_variable)])
```

Figure – **create_normal.py** : Creation of the distribution

...

- └ Probability distributions
- └ Analyzing a distribution

Exercice 5 : Second example Let's try to perform the same analysis on the file **mysterious_distro_2.csv** using **read_myst_2.py**.

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- └ Probability distributions
 - └ Analyzing a distribution

Second example

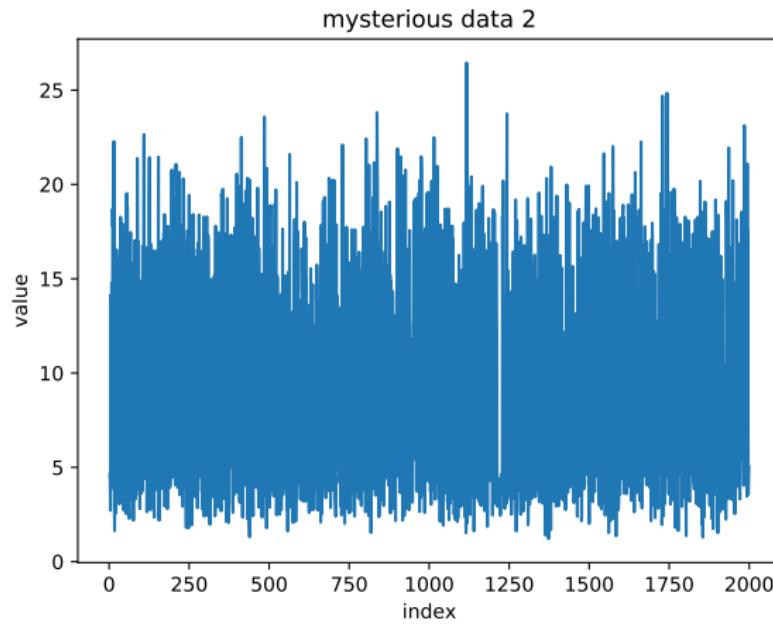


Figure – Second distribution

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- └ Probability distributions
 - └ Analyzing a distribution

Multimodal distribution

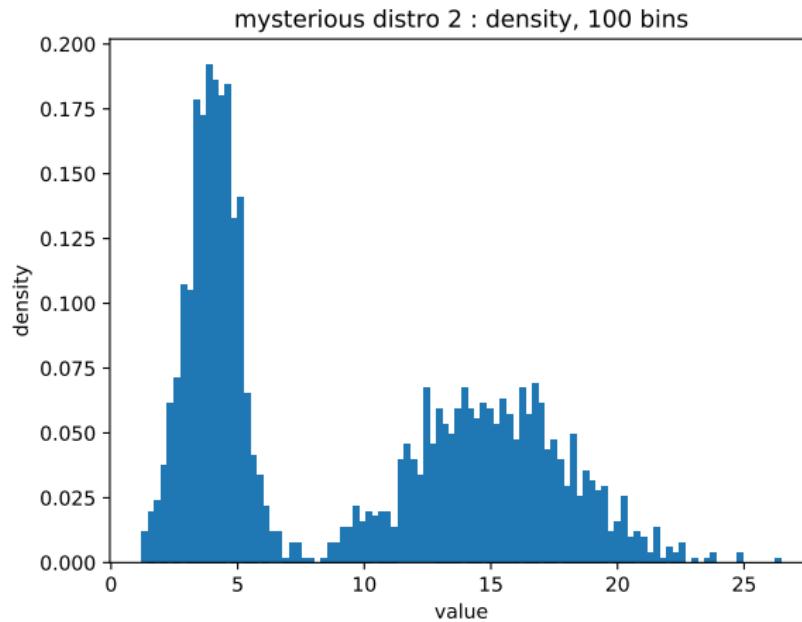


Figure – This distribution has several **modes**

Multimodal distribution

```
mean_1 = 4
std_dev_1 = 1
nb_point_1 = 1000

mean_2 = 15
std_dev_2 = 3
nb_point_2 = 1000

nb_point = nb_point_1 + nb_point_2

with open('csv_files/' + file_name, 'w') as csvfile:
    filewriter = csv.writer(csvfile, delimiter=',')
    for point in range(1, nb_point):
        if random.randint(1, 2) == 1:
            random_variable = np.random.normal(loc=mean_1, scale=std_dev_1)
            filewriter.writerow([str(point), str(random_variable)])
        else:
            random_variable = np.random.normal(loc=mean_2, scale=std_dev_2)
            filewriter.writerow([str(point), str(random_variable)])
```

Figure – **create_bimodal.py** : Generation of multimodal distribution

...

└ Probability distributions

 └ Optimization and Maximum Likelihood

Fitting

In most cases, it won't be that straightforward to fit a distribution :

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Fitting

In most cases, it won't be that straightforward to fit a distribution :

- ▶ what distribution do we want to use ?
- ▶ even if we know the right shape of the distribution, how to choose the parameters ?

Maximum Likelihood

The **Maximum Likelihood** method is one example method used in Machine Learning.

Say you observe a dataset (x_1, \dots, x_n) .

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Maximum Likelihood

The **Maximum Likelihood** method is one example method used in Machine Learning.

Say you observe a dataset (x_1, \dots, x_n) .

You first need to choose a **model** (which is the distribution) of your dataset, p .

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Maximum Likelihood

The **Maximum Likelihood** method is one example method used in Machine Learning.

Say you observe a dataset (x_1, \dots, x_n) .

You first need to choose a **model** (which is the distribution) of your dataset, p .

Then, you must optimize the **parameters of this model**, noted θ .

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Maximum Likelihood

The **likelihood** (vraisemblance) of your model is

$$L(\theta) = p(x_1, \dots, x_n | \theta) \tag{1}$$

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Maximum Likelihood

The **likelihood** (vraisemblance) of your model is

$$L(\theta) = p(x_1, \dots, x_n | \theta) \quad (2)$$

If (x_1, \dots, x_n) are conditionally independant, then it writes :

$$L(\theta) = \prod_{i=1}^n p(x_i | \theta) \quad (3)$$

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Maximum Likelihood

The **likelihood** (vraisemblance) of your model is

$$L(\theta) = \prod_{i=1}^n p(x_i|\theta) \tag{4}$$

This is the function that you want to **maximise**.

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Remark on max-likelihood

Most of the time it's written this way : "minimise $-\log L(\theta)$ "

Because the log **transforms the product into a sum**, which is easier to **derivate**.

$$-\log L(\theta) = - \sum_{i=1}^n \log(p(x_i|\theta)) \quad (5)$$

Example 1

Exercice 6: We observe the data $(1, 0)$. We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p . What is the likelihood of these observations as a function of p ?

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Example 1

Exercice 6: We observe the data $(1, 0)$. We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p . What is the likelihood of these observations as a function of p ?

$$L = p(1|p)p(0|p) \quad (6)$$

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Example 1

Exercice 6: We observe the data $(1, 0)$. We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p . What is the likelihood of these observations as a function of p ?

$$L = p(1|p)p(0|p) \quad (7)$$

For which value of p is this likelihood **maximum**?

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Example 2

Exercice 7 : We observe the data $(2.5, 3.5)$. We assume that these data come from a normal law of parameters μ and σ .
What is the likelihood of (μ, σ) ?

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Example 2

Exercice 7 : We observe the data $(2.5, 3.5)$. We assume that these data come from a normal law of parameters μ and σ .

$$L = p(2.5|\mu, \sigma)p(3.5|\mu, \sigma) \quad (8)$$

...

└ Probability distributions

└ Optimization and Maximum Likelihood

Example 2

Exercice 7 : We observe the data $(2.5, 3.5)$. We assume that these data come from a normal law of parameters μ and σ .

$$\begin{aligned} L &= p(2.5|\mu, \sigma)p(3.5|\mu, \sigma) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{2.5-\mu}{\sigma}\right)^2} \times \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{3.5-\mu}{\sigma}\right)^2} \end{aligned} \tag{9}$$

...

Probability distributions

Optimization and Maximum Likelihood

Example 2

Exercice 7 : We observe the data $(2.5, 3.5)$. We assume that these data come from a normal law of parameters μ and σ .

$$\begin{aligned} L &= p(2.5|\mu, \sigma)p(3.5|\mu, \sigma) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{2.5-\mu}{\sigma}\right)^2} \times \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{3.5-\mu}{\sigma}\right)^2} \end{aligned} \quad (10)$$

We wan show that the likelihood is maximum for :

- ▶ $\hat{\mu} = \frac{2.5+3.5}{2}$
- ▶ $\hat{\sigma}^2 = \frac{(2.5-\hat{\mu})^2 + (3.5-\hat{\mu})^2}{2}$

...

└ Probability distributions

└ Gradients

Max Likelihood

In the case of very large datasets, and large numbers of parameters (tens, hundredths, more), most of the time an **analytic solution** is not available.

...

- Probability distributions

- Gradients

Max Likelihood

In the case of very large datasets, and large numbers of parameters (tens, hundredths, more), most of the time an **analytic solution** is not available. So how can we **maximize** the likelihood ?

...

└ Probability distributions

└ Gradients

Max Likelihood

In the case of very large datasets, and large numbers of parameters (tens, hundredths, more), most of the time an **analytic solution** is not available. So how can we **maximize** the likelihood ?

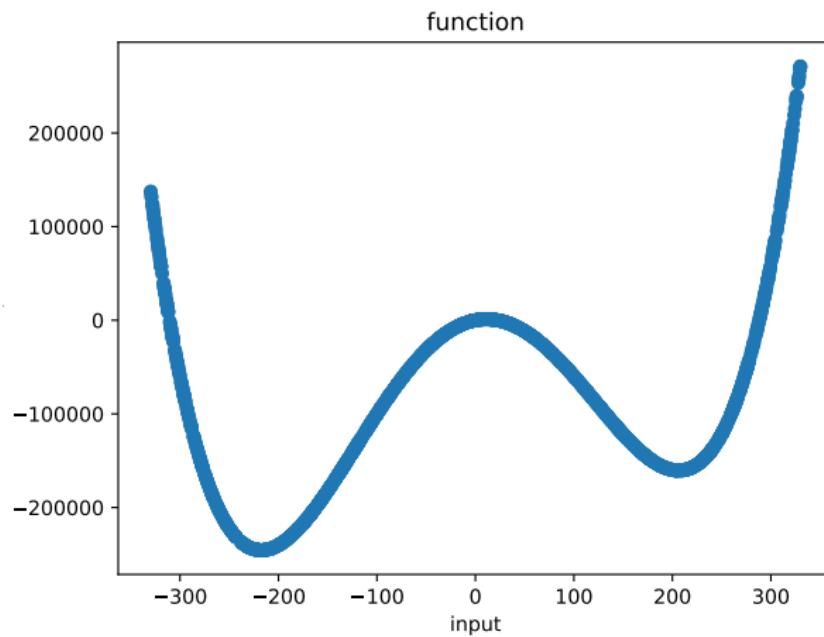
Most common method : **gradient descent**.

...

Probability distributions

Gradients

Notion of optimization



...

└ Probability distributions

└ Gradients

Gradient descent

- ▶ In the case a function $f : \mathbb{R} \rightarrow \mathbb{R}$, we can study its variations by computing its derivative f' , **if it exists**

...

└ Probability distributions

└ Gradients

Gradient descent

- ▶ In the case a function $f : \mathbb{R} \rightarrow \mathbb{R}$, we can study its variations by computing its derivative f' , **if it exists**
- ▶ If $f'(x) > 0$, the function grows around x .
- ▶ If $f'(x) < 0$, the function decreases around x .
- ▶ If x is a local extremum, $f'(x) = 0$

...

└ Probability distributions

└ Gradients

Gradient descent

- ▶ In the case a function $f : \mathbb{R} \rightarrow \mathbb{R}$, we can study its variations by computing its derivative f' , **if it exists**
- ▶ If $f'(x) > 0$, the function grows around x .
- ▶ If $f'(x) < 0$, the function decreases around x .
- ▶ If x is a local extremum, $f'(x) = 0$
- ▶ Is the reciprocal true ?

...

└ Probability distributions

└ Gradients

Gradient

- ▶ The **gradient** is similar to a derivative but in the case of a function with several inputs, such as (μ, θ) .
- ▶ Then we store the **partial derivative** with respect to each input in a **vector** called the gradient.

Gradient descent

Consider a function f that has 2 parameters as inputs.

$$\nabla_f(x, y) = \left(\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y} \right) \quad (11)$$

We want x to **minimise** f . We perform, until some criteria is satisfied :

$$x \leftarrow x - \alpha \nabla_f(x) \quad (12)$$

α is a small parameter called the learning rate.

...

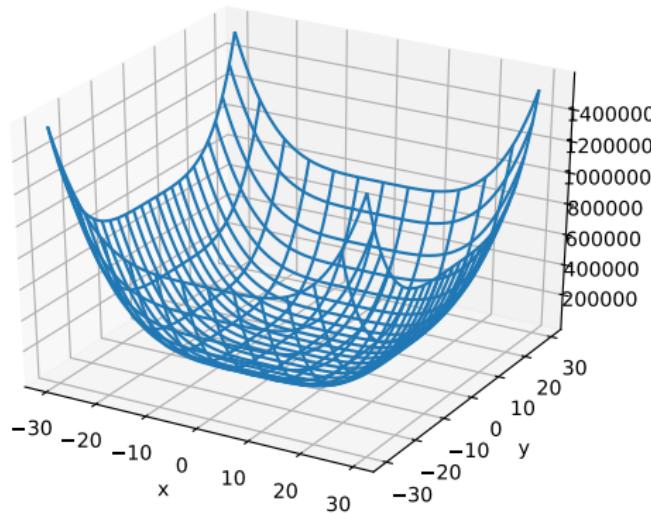
Probability distributions

Gradients

Gradient

Exercice 7 : Implementing the gradient algorithm

We will use the algorithm on two functions.

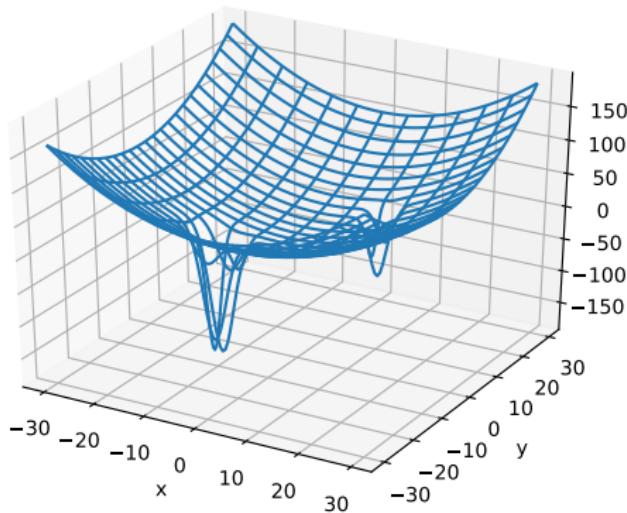


...

Gradient

Exercice 7 : Implementing the gradient algorithm

We will use the algorithm on two functions.

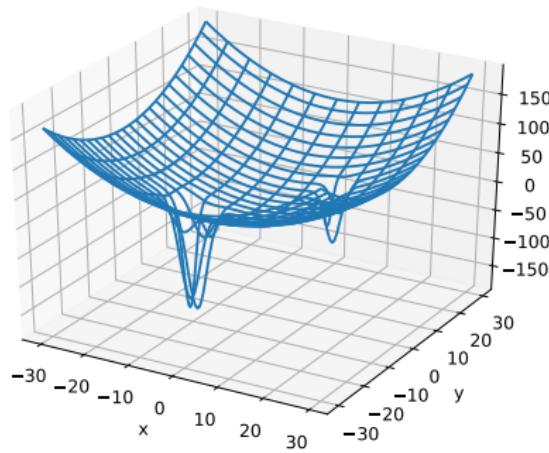


...

Gradient

Exercice 7 : Implementing the gradient algorithm

cd ./gradient and use the files **gradient.py** and **gradient_2.py** in order to implement the algorithm to find **minima**.



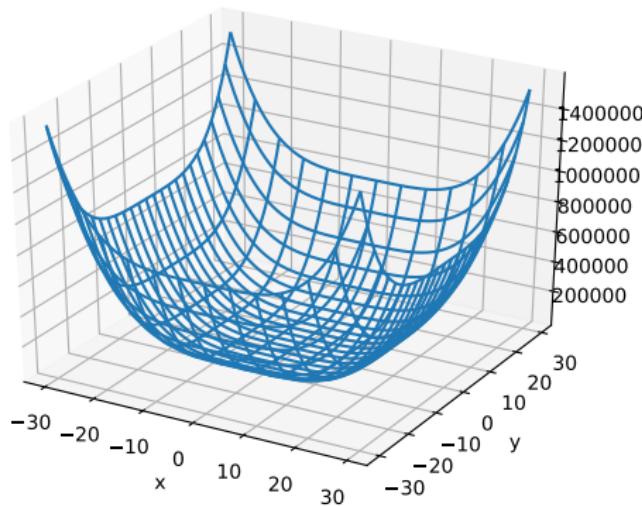
...

Probability distributions

Gradients

The gradient descent

Experiment with it, try to change all the parameters and to break it again. Is it stable?



Multidimensional vectors

We can consider data that live in higher dimensional spaces than 2.

Multidimensional vectors

We can consider data that live in higher dimensional spaces than 2.
Examples ?

Multidimensional vectors

We can consider data that live in higher dimensional spaces than 2.
Examples ?

- ▶ images
- ▶ sensor that receives **multimodal information**

Correlation

Sometimes the components of a multidimensional vector (x_1, \dots, x_n) are not independent.

...

Correlation

Sometimes the components of a multidimensional vector (x_1, \dots, x_n) are not independent.

To study this, we can use the **covariance** of the two components, or the **correlation** which is actually clearer.

...

└ Multivariate analysis and clustering

└ Correlation

Expected value (espérance)

- ▶ For a discrete random variable X that takes the values x_i with probability p_i :

$$E(X) = \sum_{i=1}^n p_i x_i \quad (13)$$

- ▶ For a continuous random variable X with density $p(x)$:

$$E(X) = \int x p(x) dx \quad (14)$$

Expected value (espérance)

Exercice 7 : Computing an expected value

- ▶ For a discrete random variable X that takes the values x_i with probability p_i :

$$E(X) = \sum_{i=1}^n p_i x_i \quad (15)$$

- ▶ For a continuous random variable X with density $p(x)$:

$$E(X) = \int x p(x) dx \quad (16)$$

Compute the expected value of the dice game.

Variance

$$\text{var}(X) = E((X - E(X))^2) \quad (17)$$

...

Variance and Covariance

$$\text{var}(X) = E\left(\left(X - E(X)\right)^2\right) \quad (18)$$

$$\text{cov}(X, Y) = E\left(\left(X - E(X)\right)\left(Y - E(Y)\right)\right) \quad (19)$$

Example

Look at the data contained in **mysterious_distro_3.csv**
They contain a random variable with 5 dimensions. Some of these dimensions are correlated.
Think for instance to physics : temperature and pressure, etc. If you have measurements of temperature and pressure, the two would probably be **correlated**.

Correlation

Exercice 8 : Which dimensions of the distribution are correlated ?

...

- Multivariate analysis and clustering

- Correlation

Correlation matrix

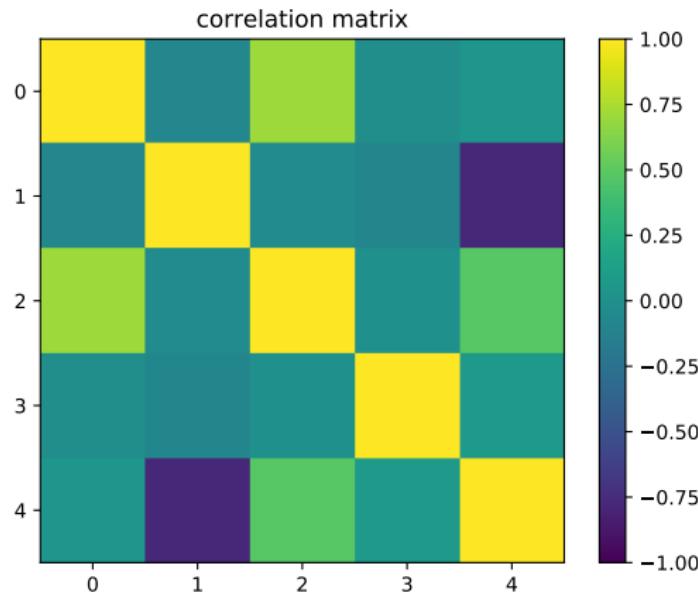


Figure – Correlation matrix for the distribution

Generation of the data

```
mean_1 = 4
std_dev_1 = 1

mean_2 = 15
std_dev_2 = 3

mean_3 = -5
std_dev_3 = 2

mean_noise = 0
noise_std_dev = 1

nb_point = 1000

with open('csv_files/' + file_name, 'w') as csvfile:
    filewriter = csv.writer(csvfile, delimiter=',')
    for point in range(1, nb_point):
        noise = np.random.normal(loc=mean_noise, scale=noise_std_dev)
        random_variable_1 = np.random.normal(loc=mean_1, scale=std_dev_1)
        random_variable_2 = np.random.normal(loc=mean_2, scale=std_dev_2)
        random_variable_3 = random_variable_1 + noise
        random_variable_4 = np.random.normal(loc=mean_3, scale=std_dev_3)
        random_variable_5 = -0.4 * random_variable_2 + noise
        filewriter.writerow([str(point),
                            str(random_variable_1),
                            str(random_variable_2),
                            str(random_variable_3),
                            str(random_variable_4),
                            str(random_variable_5)])
```

Figure – Multidimensional random variable

...

└ Multivariate analysis and clustering

 └ Dimension reduction

Removing dimensions

- ▶ Sometimes given a question and a dataset, not all dimensions of the data are **relevant**
- ▶ It is possible that only one or two of them are sufficient to answer the given question

...

- Multivariate analysis and clustering

- Dimension reduction

Removing dimensions

- ▶ Sometimes given a question and a dataset, not all dimensions of the data are **relevant**
- ▶ It is possible that only one or two of them are sufficient to answer the given question
- ▶ We will illustrate this with the titanic dataset and the pandas library

Titanic Dataset

- The dataset contains the list of passengers and several informations on each of them :

PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
1	0	3	Braund, Mr. Owen Harris	male	22	1	0	A/5 21171	7.25	S	
2	1	1	Curtis, Mrs. John Bradley (Florence Briggs Thayer)	female	38	1	0	PC 17399	71.2033	C86	C
3	1	3	Heikkinen, Miss. Laina	female	26	0	0	STON/O2. 3101282	7.925	S	
4	1	1	Holtedahl, Mrs. Jacques Heude (July May Heude)	female	35	1	0	113833	33.1	C133	S
5	0	3	Allen, Mr. William Henry	male	35	0	0	373493	8.95	S	
6	0	3	Horan, Ms. James	male	0	0	0	330877	8.4983	Q	
7	0	1	McCarthy, Ms. Timothy J	male	54	0	0	17460	51.8625	C46	S
8	0	3	Palsson, Master Gustaf Leonard	male	2	3	1	349699	21.075	S	
9	1	3	Johnson, Mrs. Oscar W (Elsieast Vilhelmina Berg)	female	27	0	2	347742	11.1333	S	
10	1	2	Nasser, Mrs. Nicholas (Adele Ahola)	female	14	1	0	237736	30.0708	C	
11	1	3	Sandstrom, Miss. Marguerite Rut	female	4	1	1	MM 35648	16.7	G8	S
12	1	3	Burnett, Miss. Elizabeth	female	58	0	0	113983	26.95	C103	S
13	0	3	Saundercock, Mr. William Henry	male	20	0	0	A/5 215	8.95	S	
14	0	3	Andersen, Mr. Anderson John	male	39	1	5	347082	31.275	S	
15	0	3	Vestrum, Miss. Hilda Aneade Adolfa	female	14	0	0	350486	7.8542	S	
16	1	2	Hewlett, Mrs. (Mary D KIngcome)	female	55	0	0	248785	16	S	
17	0	3	Rice, Master Eugene	male	2	4	1	302623	26.125	Q	
18	1	2	Williams, Mr. Charles Eugene	male	0	0	0	244373	13	S	
19	0	3	Vander Valken, Mrs. Julia (Elinia Maria Vandervoordt)	female	31	1	0	349783	18	S	
20	1	3	Masseveldt, Mrs. Patricia	female	0	0	0	2649	7.225	C	
21	0	2	Payne, Mr. Joseph J	male	35	0	0	239885	26	S	
22	1	2	Beauchamp, Mr. Lawrence	male	34	0	0	249698	13	D56	S
23	1	3	McGowan, Miss. Anna "Annie"	female	15	0	0	330923	0.8202	Q	
24	1	1	Shaper, Mr. William Thompson	male	26	0	0	113788	35.5	A6	S
25	0	3	Peterson, Miss. Tatanya Daniels	female	8	3	1	346699	21.075	S	
26	1	3	Asplund, Mrs. Carl Oscar (Selma Augusta Emilia Johansson)	female	36	1	5	341037	31.3675	S	
27	0	3	Erick, Mr. Farred Charles	male	0	0	0	2631	7.225	C	
28	0	1	Perkins, Mr. Charles Alexander	male	19	5	2	19988	281	C25 C25 C27	S
29	1	3	O'Dwyer, Miss. Ellen "Nellie"	female	0	0	0	330999	7.8792	Q	
30	0	3	Todoroff, Mr. Leonti	male	0	0	0	349218	7.8958	S	
31	0	1	Urschutz, Dr. Max E	male	40	0	0	PC 17601	27.7508	C	
32	1	3	Spicer, Mrs. William Augustus (Maria Eugenia)	female	1	0	0	PC 17569	146.5208	B76	C
33	1	3	Glynn, Miss. Mary Augusta	female	0	0	0	235677	7.75	Q	
34	0	2	Wheeler, Miss. Edward H	male	66	0	0	CA 24579	16.5	S	
35	0	1	Hoyos, Mr. Bolivar Jose	male	28	1	0	PC 17604	82.1708	C	
36	0	1	Hansen, Mr. Alexander Oskar	male	42	1	0	113799	52	S	
37	1	3	Horne, Mr. Harry	male	0	0	2077	7.2292	C		
38	0	3	Caro, Mr. Ernest Charles	male	21	0	0	A/5 2123	8.95	S	
39	0	3	Vander Valken, Miss. Augusta Maria	female	18	2	0	345784	18	S	
40	1	3	Nicole-Yerrell, Miss. Junilia	female	14	1	0	2651	11.2417	C	

...

Titanic Dataset

- ▶ The dataset contains the list of passengers and several informations on each of them :

PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket
1	0	3	Braund, Mr. Owen Harris	male	22	1	0	A/5 21171
2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Thayer)	female	38	1	0	PC 17599
3	1	3	Heikkinen, Miss. Laina	female	26	0	0	STON/O2. 31
4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35	1	0	113803
5	0	3	Allen, Mr. William Henry	male	35	0	0	373450
6	0	3	Moran, Mr. James	male	0	0	0	330877
7	n	1	McCarthy, Mr. Timothy J	male	34	n	n	17463

Figure – Titanic dataset : can be found here

<https://www.kaggle.com/c/titanic/data>

Pandas

- ▶ The pandas library is used to study large datasets with python
- ▶ We will use the **Dataframe** structure to process the titanic dataset
- ▶ `cd multivariate_analysis/titanic/` and use the file `pandas_infos.py` to load the dataset to a dataframe and print general information on the dataframe.

Pandas

```
---  
all info on passenger 25  
PassengerId                      26  
Survived                           1  
Pclass                            3  
Name      Asplund, Mrs. Carl Oscar (Selma Augusta Emilia...  
Sex                                female  
Age                               38  
SibSp                             1  
Parch                             5  
Ticket                          347077  
Fare                            31.3875  
Cabin                           NaN  
Embarked                         S  
Name: 25, dtype: object  
---  
age of passenger 25  
38.0
```

Figure – Some passenger that survived

Exercice 9 : Prediction

We would like to know if there is a criterion that can help to predict if a passenger survived or not.

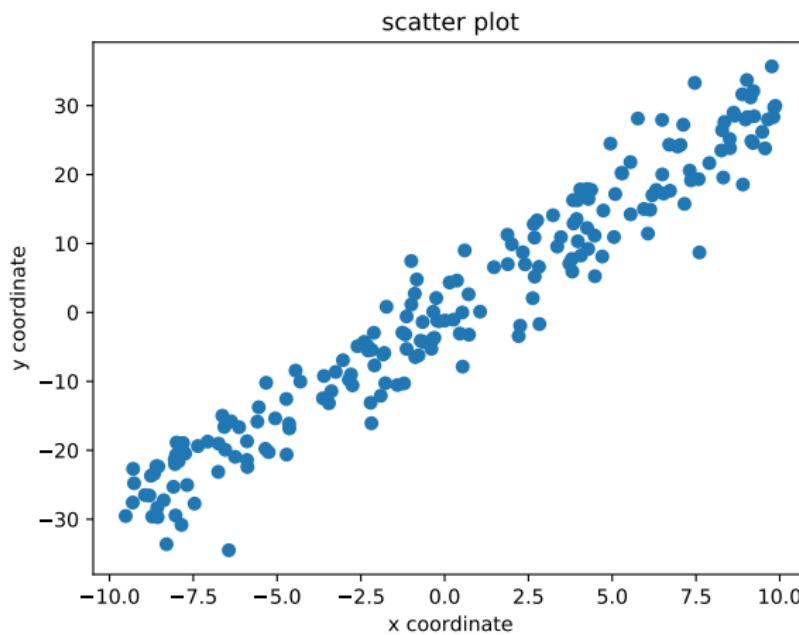
Ideally, we would like to remove dimensions that are useless for this problem.

...

- Multivariate analysis and clustering

- Dimension reduction

Scatter plot (nuage de points)

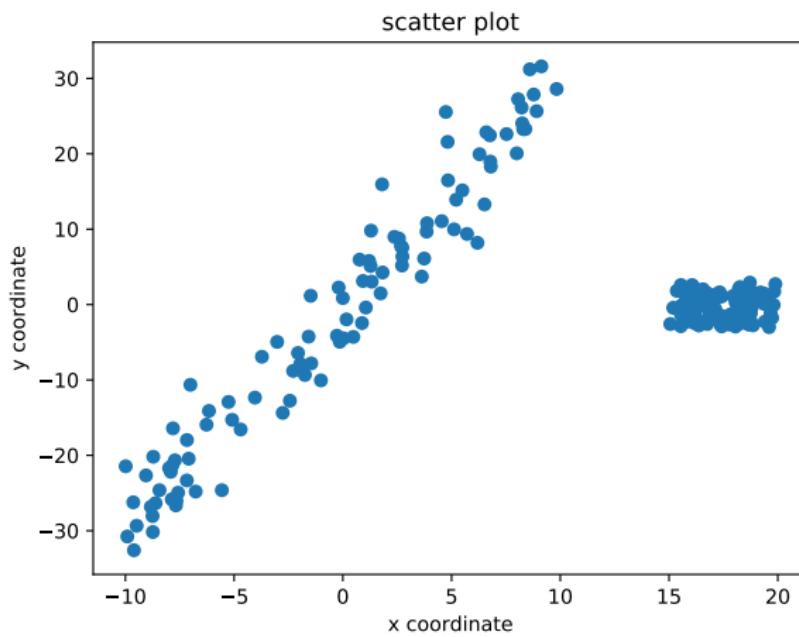


...

- Multivariate analysis and clustering

- Dimension reduction

Scatter plot (nuage de points)



...

└ Multivariate analysis and clustering

 └ Dimension reduction

Exercice 9 : Prediction

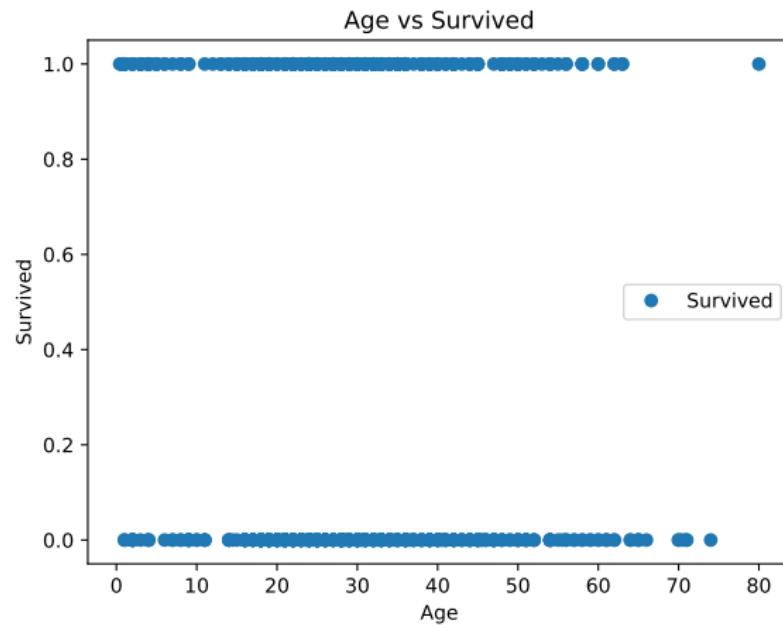
`cd multivariate_analysis/titanic/.`

Use the file `scatter_titanic.py` to see if one column is sufficient to predict survival. We use the `seaborn` lib.

...

- Multivariate analysis and clustering

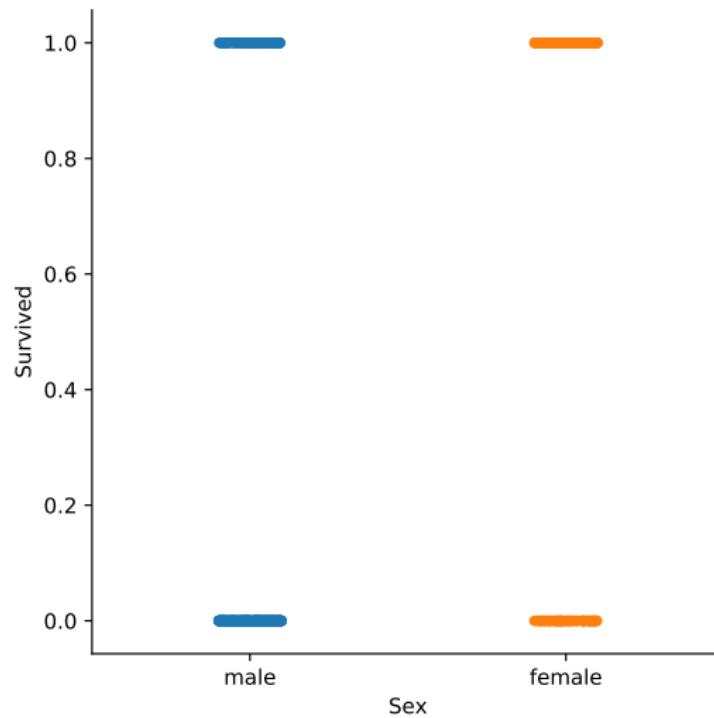
- Dimension reduction



...

- Multivariate analysis and clustering

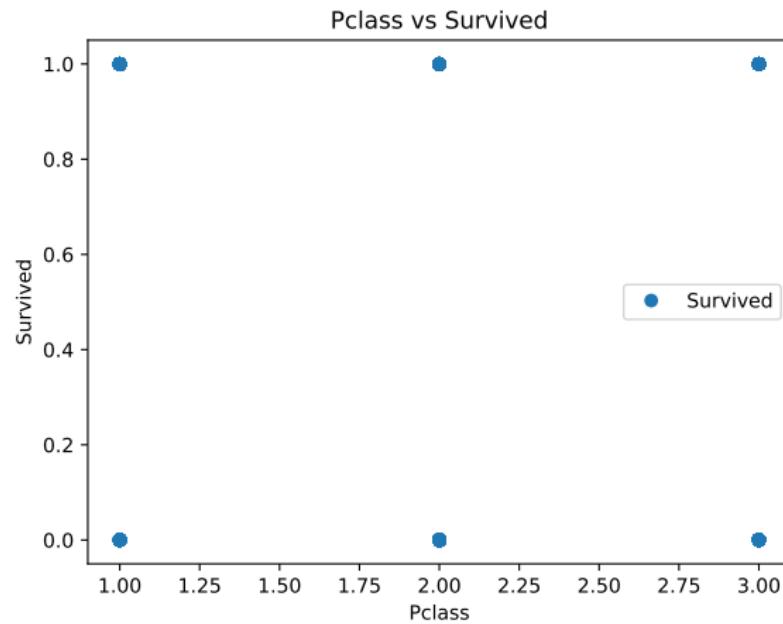
- Dimension reduction



...

- Multivariate analysis and clustering

- Dimension reduction



Exercice 9 : Prediction

How could we plot 3 variables on the same graph ?

...

└ Multivariate analysis and clustering

 └ Dimension reduction

Exercice 9 : Prediction

How could we plot 3 variables on the same graph ?

Use the file **scatter_titanic_color.py** in order to color the datapoint in a $2D$ space as a function of survival.

...

- Multivariate analysis and clustering

- Dimension reduction

Exercice 9 : Prediction

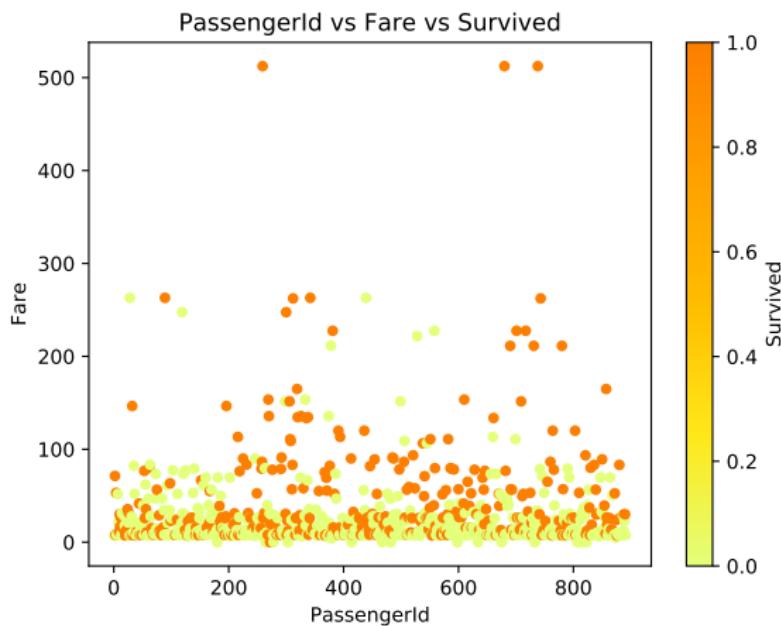


Figure – Not much information

Exercice 9 :

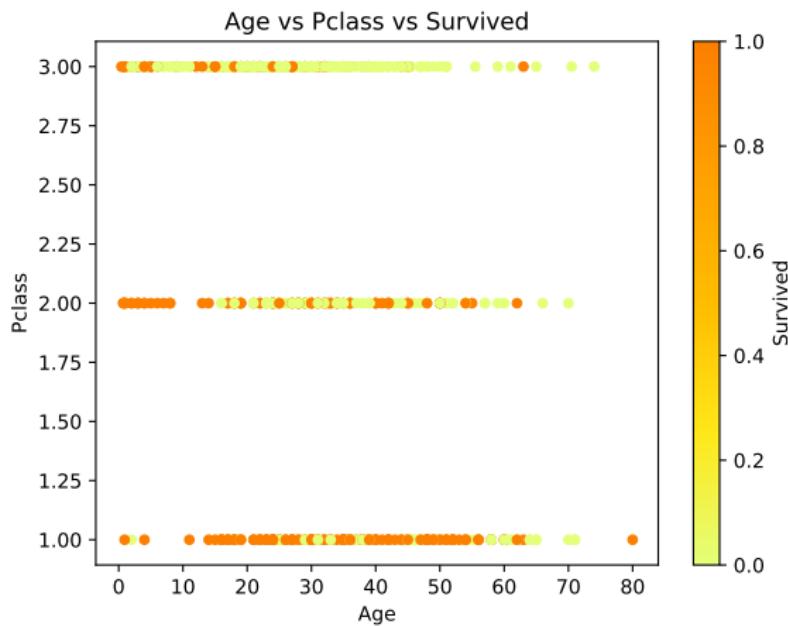


Figure – There seems to be a link between class and survival

Remark : we did not have to use pandas to solve this problem.

Warning

- ▶ Some times removing dimensions can lead to a **misinterpretation**

...

- └ Multivariate analysis and clustering
 - └ Correlation and causality

Exercice 10 :

`cd multivariate_analysis/causality/.`

- ▶ Load the dataset `grades.csv` and study it using `process_grades.py`
- ▶ What columns are correlated ?

Exercice 10 :

- ▶ **cd causality**
- ▶ Load the dataset **grades.csv** and study it using **process_grades.py**
- ▶ What columns are correlated ?
- ▶ Plot the grade as a function of the height.

...

- Multivariate analysis and clustering

- Correlation and causality

Exercice 10 :

- ▶ Load the dataset `grades.csv` and study it using `process_grades.py`
- ▶ What columns are correlated ?
- ▶ Plot the grade as a function of the height.
- ▶ Plot the grade as a function of the age.

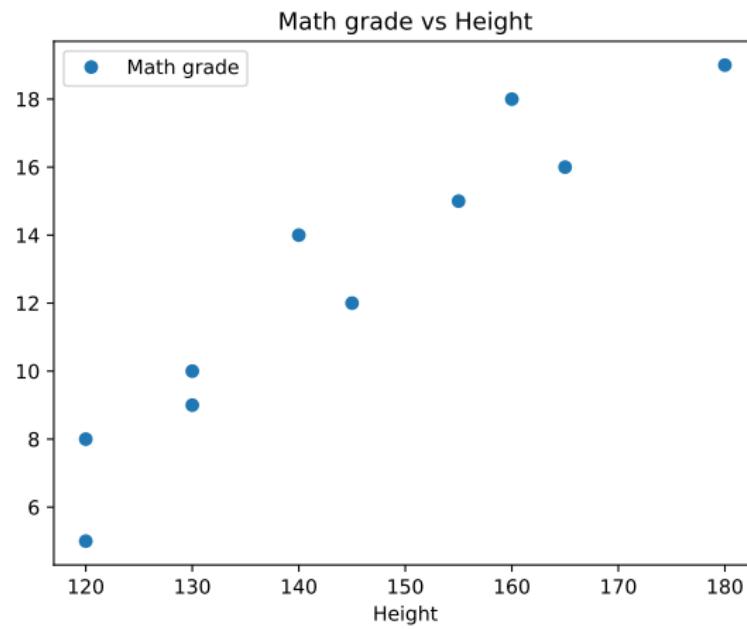
Exercice 10 :

- ▶ Load the dataset **grades.csv** and study it using **process_grades.py**
- ▶ What columns are correlated ?
- ▶ Plot the grade as a function of the height.
- ▶ Plot the grade as a function of the age.
- ▶ Which one of these plots does not make sense ?

...

- └ Multivariate analysis and clustering
 - └ Correlation and causality

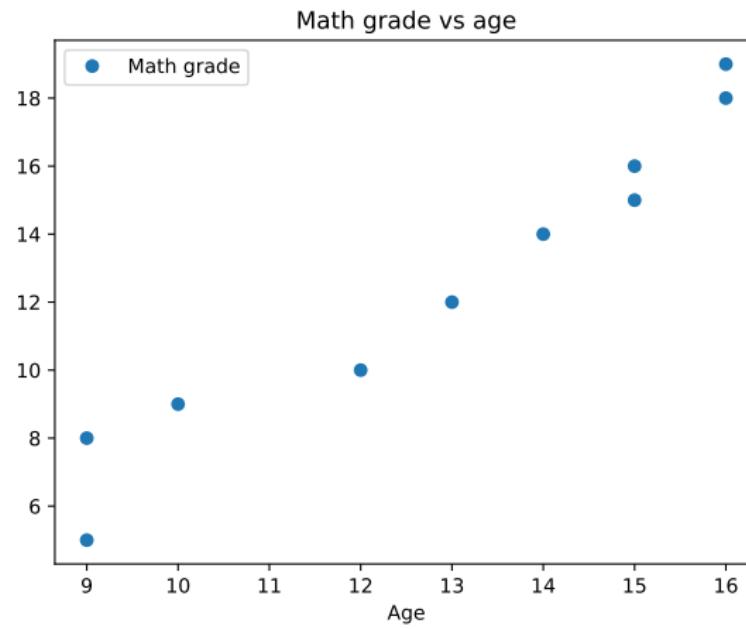
Correlation and causality



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- └ Multivariate analysis and clustering
 - └ Correlation and causality

Correlation and causality

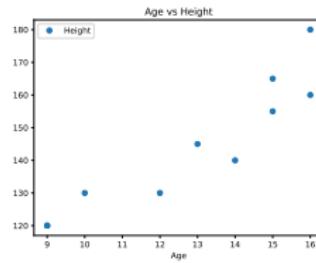


Conclusion

- ▶ The height of a student is actually not linked to his/her grade
- ▶ If we plot the grade as a function of the height There is a **hidden variable** which is the age of the student
- ▶ Correlation is different than causality.

Scatter matrix

- ▶ Let us generalize the idea of a scatter plot.



- ▶ Given a dataset, we can build all the possible scatter plots and store them in a matrix, called the **scatter matrix**.

Scatter matrix

- ▶ Let us generalize the idea of a scatter plot.

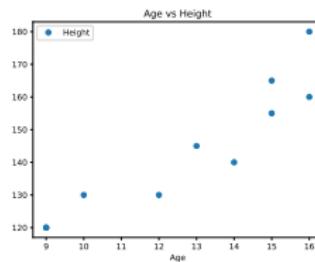
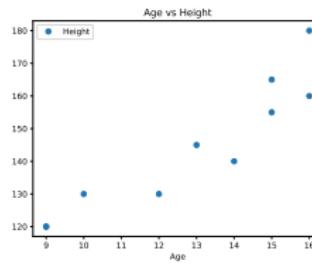


Figure – Exemple scatter plot

- ▶ Given a dataset, we can build all the possible scatter plots and store them in a matrix, called the **scatter matrix**.
- ▶ What will happen on the diagonal of the matrix ?

Scatter matrix

- ▶ Let us generalize the idea of a scatter plot.



- ▶ Given a dataset, we can build all the possible scatter plots and store them in a matrix, called the **scatter matrix**.
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Scatter matrix

- ▶ Let us generalize the idea of a scatter plot.
- ▶ Given a dataset, we can build all the possible scatter plots and store them in a matrix, called the **scatter matrix**.
- ▶ What will happen on the diagonal of the matrix ?

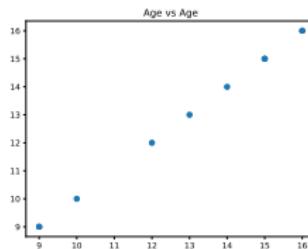


Figure – Variable plotted against itsself : All the points are on the $y = x$ line

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└ Multivariate analysis and clustering

└ Scatter matrix

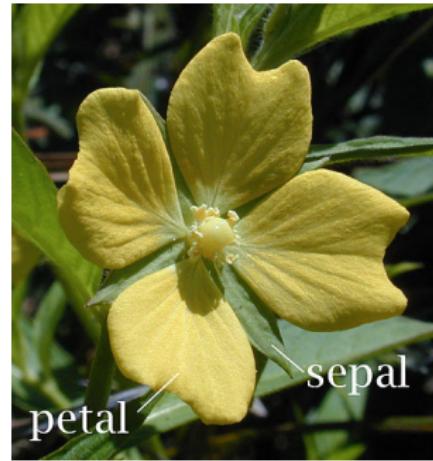
Scatter matrix

- ▶ Let us generalize the idea of a scatter plot.
- ▶ Given a dataset, we can build all the possible scatter plots and store them in a matrix, called the **scatter matrix**.
- ▶ On the diagonal, one can plot histograms or the density probability
- ▶ The scatter plot can be a good way to start analyzing a dataset when we don't know which variables could be correlated

...

Iris dataset

- ▶ 150 samples of iris flower
- ▶ 3 species
- ▶ 4 attributes : petal width and length, sepal width and length



...

Exercice 11: Iris dataset : scatter matrix
cd multivariate_analysis/titanic/.

- ▶ use `iris_scatter_matrix.py` to plot the scatter matrix of the iris dataset with seaborn.
- ▶ Is there a variable that can discriminate between the species ?

...

Multivariate analysis and clustering

Scatter matrix

Exercice 11: Iris dataset : scatter matrix

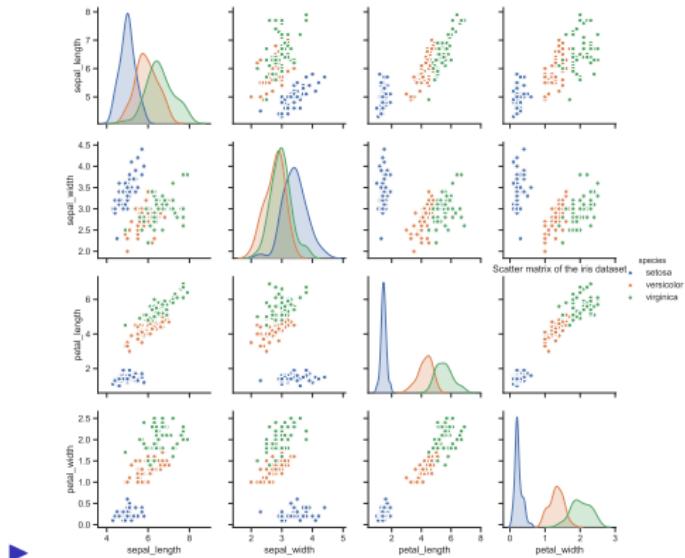


Figure – Plotted in `iris_scatter_matrix.py`

Exercice 11: Iris dataset : scatter matrix

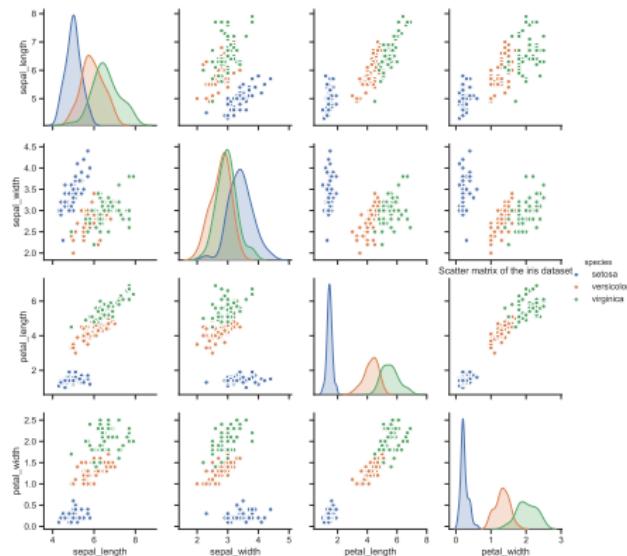


Figure – It seems that **petal width** is a parameter that separates the three species. On the contrary, **sepal width** is not able to do so.

Titanic dataset : scatter matrix

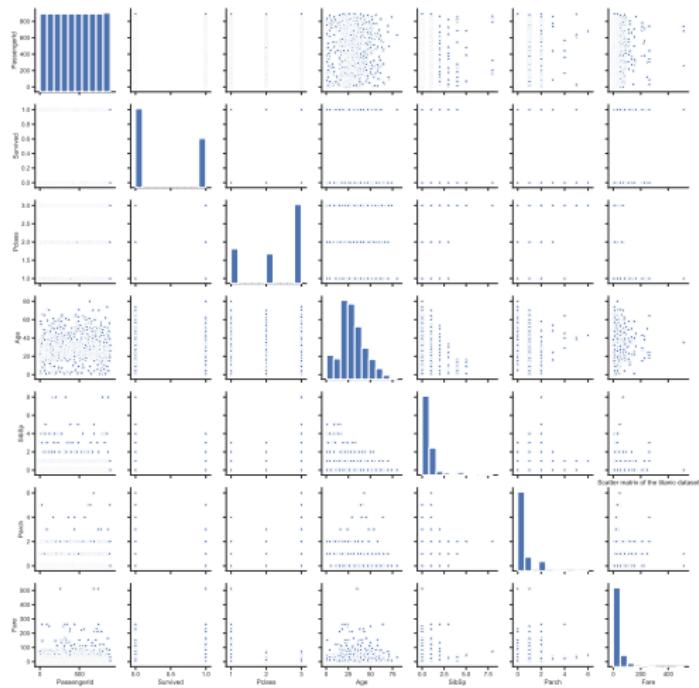


Figure – Titanic dataset scatter matrix

K means clustering

- ▶ A famous unsupervised clustering method

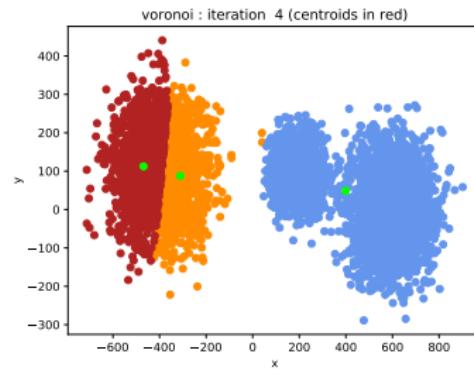


Figure – K means clustering

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└ Clustering

└ Kmeans clustering

Kmeans

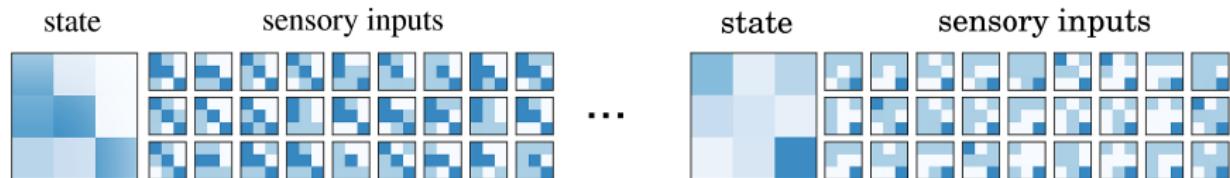


Figure – Other example of kmeans clustering, this time in 9 dimensions
[Le Hir et al., 2018]

Kmeans : Expectation Maximisation algorithm

- ▶ Classical Machine Learning algorithm (EM)
- ▶ Blackboard
- ▶ What could be the drawbacks of this algorithm ?

...

└ Clustering

└ Kmeans clustering

Kmeans clustering

Exercice 12: **Implementing kmeans**

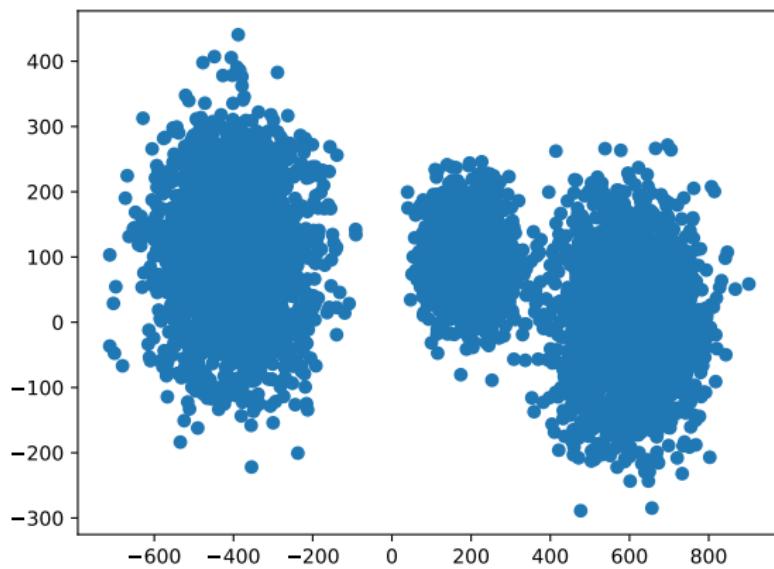


Figure 12: Data points to cluster

Kmeans clustering

Exercice 12 : Implementing kmeans cd ./kmeans

- ▶ Modify the `k_means.py` file so that it performs the kmeans algorithm.
- ▶ There are **two mistake series :**
 - ▶ line 64
 - ▶ around line 84

you will need to fix them.

You should obtain something like this :

...

└ Clustering

└ Kmeans clustering

Kmeans

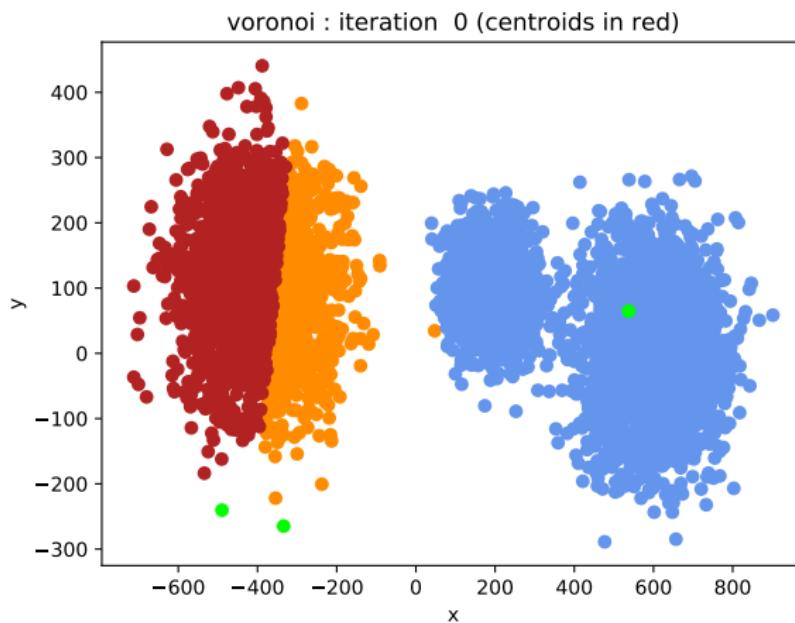


Figure – Voronoi 0th iteration

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└ Clustering

└ Kmeans clustering

Kmeans

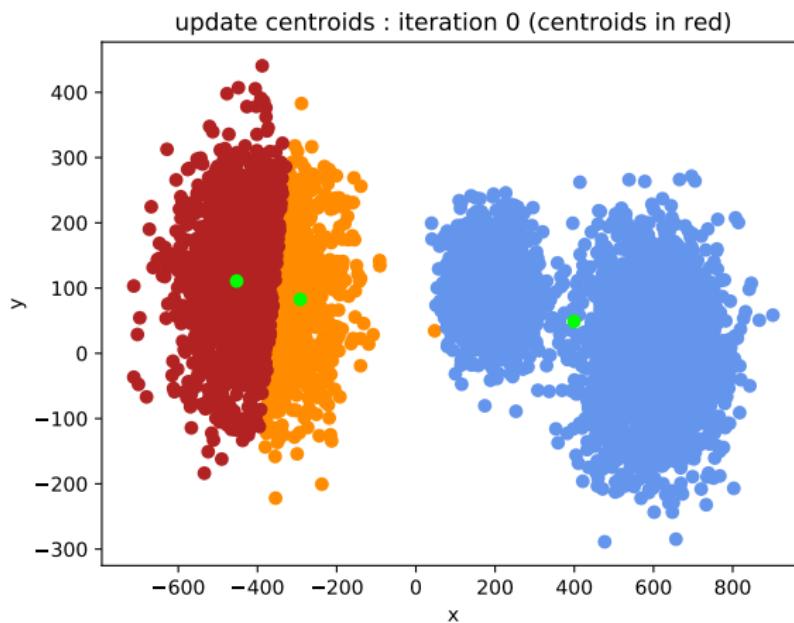


Figure – Centroids 0th iteration

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└ Clustering

└ Kmeans clustering

Kmeans

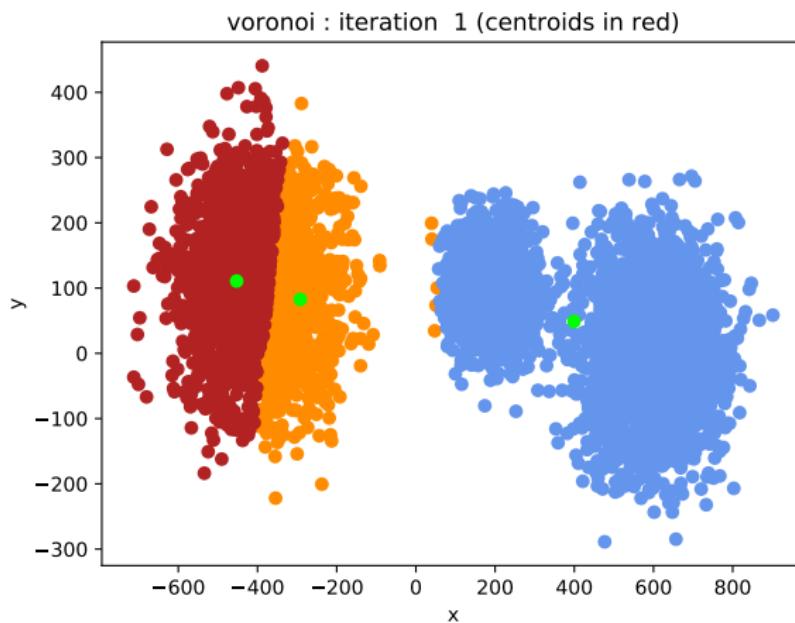


Figure – Voronoi 1st iteration

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└ Clustering

└ Kmeans clustering

Kmeans

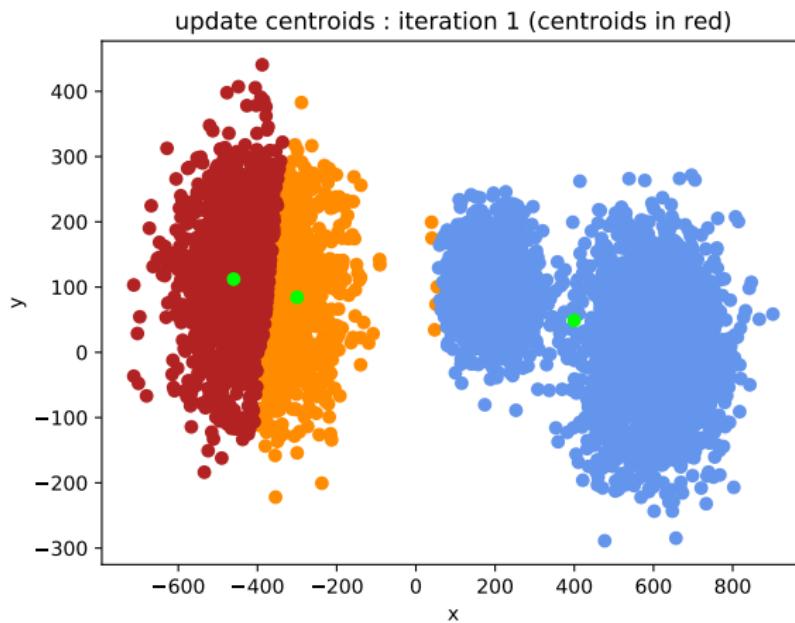


Figure – Centroids 1st iteration

...

└ Clustering

 └ Kmeans clustering

Kmeans and initialization

Note that when launching the algorithm several times, the result may differ.

...

└ Clustering

 └ Kmeans clustering

Sklearn

Exercice 13 : Perform the kmeans algorithm using **sklearn**.

...

└ Clustering

 └ Similarities

Similarities

- ▶ The kmeans were based on a notion of **distance between points**

...

└ Clustering

└ Similarities

Similarities

- ▶ The kmeans were based on a notion of **distance between points**
- ▶ But sometimes you do not have access to a distance between the points (like this morning, when we introduced **dissimilarities**)

...

└ Clustering

└ Similarities

Similarities

- ▶ The kmeans were based on a notion of **distance between points**
- ▶ But sometimes you do not have access to a distance between the points.
- ▶ You might need to work with something that is more general, for instance a **similarity**.

...

└ Clustering

└ Similarities

Similarities

- ▶ When working with distances, two points that "look the same" should be separated by a **small distance** .
- ▶ When working with a similarity, two points that "look the same" should have a **high similarity**.

...

└ Clustering

└ Similarities

Example of similarity : adjacency

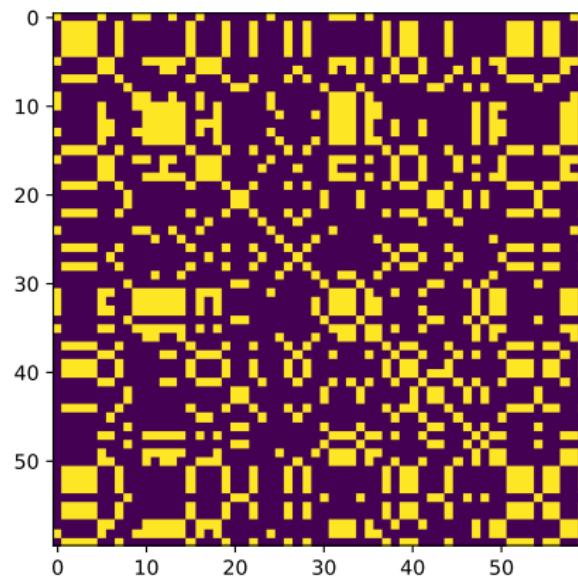
- ▶ An example of similarity is the relationship of **adjacency**.
- ▶ If i and j are related by an edge, $S_{ij} = 1$.
- ▶ Otherwise $S_{ij} = 0$.

...

└ Clustering

└ Similarities

Adjacency matrix



...

└ Clustering

└ Similarities

Similarities

Differences between similarities and distances :

- ▶ A similarity S is not always symmetrical.

...

└ Clustering

└ Similarities

Similarities

Differences between similarities and distances :

- ▶ A similarity S is not always symmetrical.
- ▶ Indeed, in a **directed graph**, having a directed edge between i and j does not mean that we have an edge between j and i .

...

└ Clustering

└ Similarities

Similarities

Differences between similarities and distances :

- ▶ A similarity S is not always symmetrical.
- ▶ Indeed, in a **directed graph**, having a directed edge between i and j does not mean that we have an edge between j and i .
- ▶ $S_{ij} = 0$ does not mean that $i = j$, it is rather the contrary.

...

└ Clustering

└ Similarities

Similarities

- ▶ A similarity is a more general notion than a distance. Given a distance between two points, we can deduce a similarity.

...

└ Clustering

└ Similarities

Similarities

- ▶ A similarity is a more general notion than a distance. Given a similarity between two points, we can deduce a similarity.
- ▶ For instance this way, if d_{ij} is the distance between i and j :

$$S_{ij} = \exp(-d_{ij}) \quad (20)$$

...

└ Clustering

└ Spectral Clustering

Spectral Clustering

- ▶ A clustering method that works with similarities
- ▶ It performs a low dimensional embedding of the similarity matrix, followed by a Kmeans

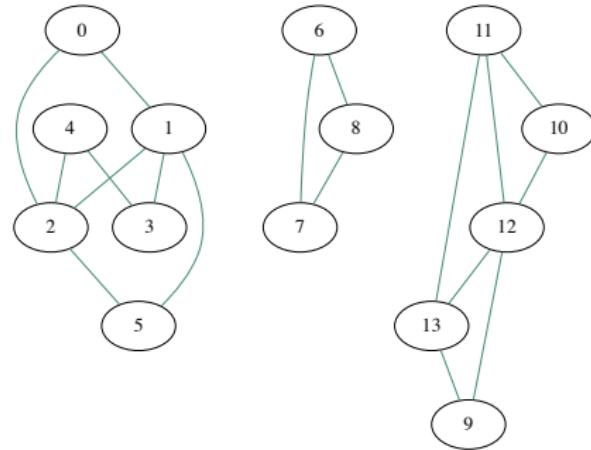
...

└ Clustering

└ Spectral Clustering

Exercise

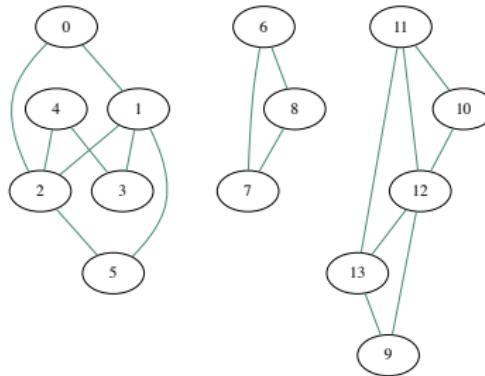
We will perform Spectral Clustering on this graph :



...

└ Clustering

└ Spectral Clustering



Please `cd spectral_clustering/` and use `vanilla_spectral_clustering.py` in order to apply spectral clustering. You first need to input the right **affinity matrix** or **similarity matrix** and then use the **sklearn** library. You also need to **tune the number of clusters**. doc : check the **sklearn** page for Spectral Clustering.

...

└ Clustering

 └ Spectral Clustering

Spectral clustering

Can you guess some drawbacks of the method ?

...

└ Clustering

└ Spectral Clustering

Spectral clustering

Can you guess some drawbacks of the method ?

- ▶ Need to provide the number of clusters.
- ▶ Not adapted to a large number of clusters.
- ▶ kmeans step : so depends on a random initialization.

...

└ Clustering

 └ Spectral Clustering

Heuristic

- ▶ We would like a criterion in order to justify the number of clusters used.

...

└ Clustering

└ Spectral Clustering

Normalized cut : a measurement of the quality of a clustering

- ▶ The **cut of a cluster** is the number of outside connections (connections with other clusters).
- ▶ The **degree** of a node is its number of adjacent edges
- ▶ The **degree of a cluster** is the sum of the degrees of its nodes.
- ▶ The **normalized cut** of a clustering is :

$$NCut(\mathcal{C}) = \sum_{k=1}^K \frac{Cut(C_k, V \setminus C_k)}{d_{C_k}} \quad (21)$$

...

└ Clustering

 └ Spectral Clustering

Normalization

- ▶ The normalization is useful in order to take the **weight** (degree) of a cluster into account.

...

└ Clustering

 └ Spectral Clustering

Normalized cut and clustering

Let's see how the normalized cut can help us choose the right number of clusters (backboard).

...

└ Clustering

└ Spectral Clustering

Heuristic

Exercice 14: Normalized but elbow :

Please use the criterion in the file **normalized_cut.py** in order to guess the relevant number of clusters in order to process the data contained in **data/**. These data are generated by **generate_data.py**.

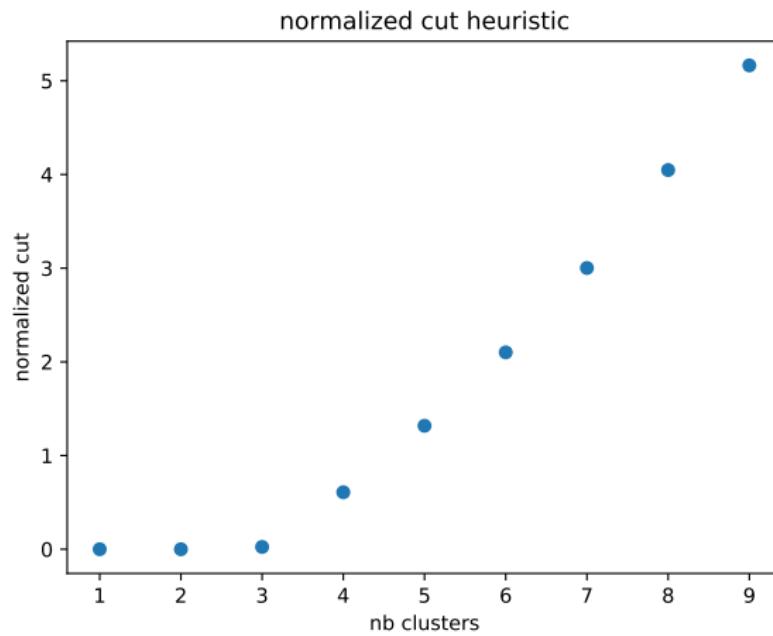


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└ Clustering

└ Spectral Clustering

Normalized cuts



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└ Clustering

└ Spectral Clustering

Normalized cuts

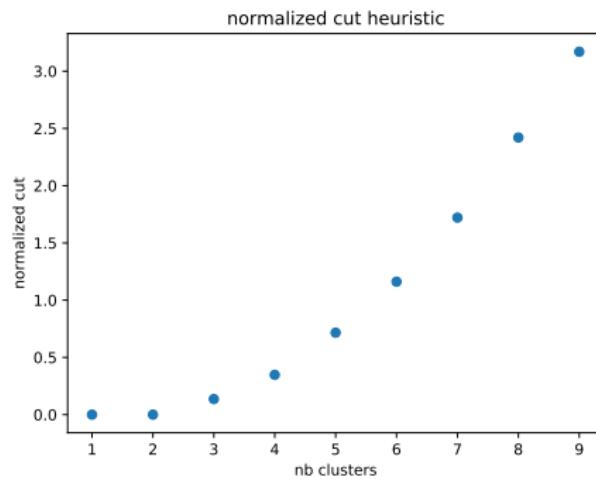


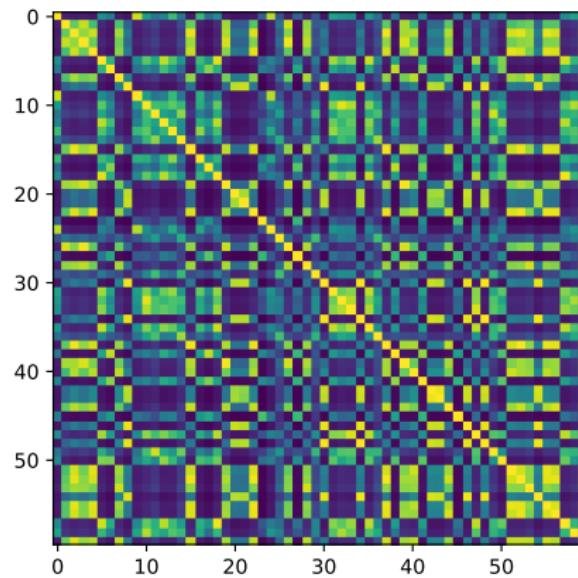
Figure – If the standard deviations in the dataset are larger, it is harder to identify a relevant number of clusters.

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└ Clustering

└ Spectral Clustering

Similarity



Example

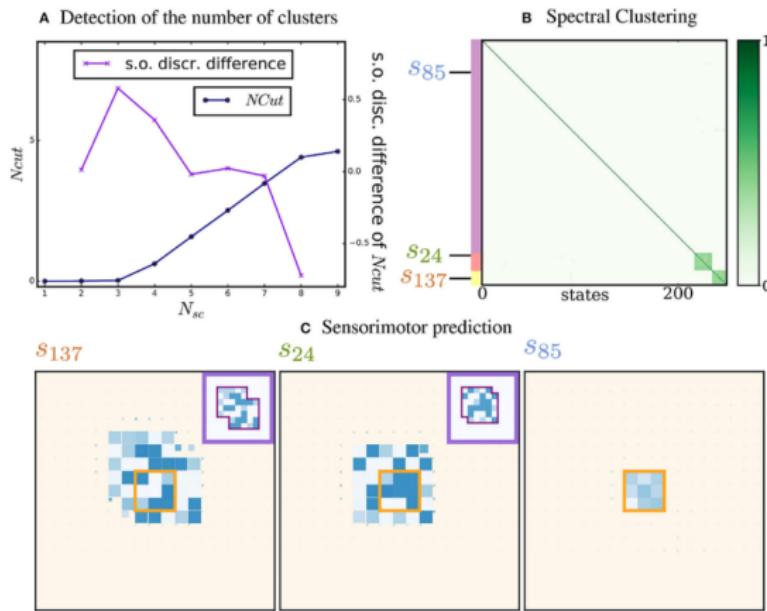


Figure – In a), the elbow method is used to choose the number of clusters. [Le Hir et al., 2018]

...

Other methods to evaluate the quality of a clustering

- ▶ Stability of the result when launching the algorithm many times
- ▶ Separation of the clusters (the mean distance between pairs of centroids is large)
- ▶ Ratio inter / intra
- ▶ Silhouette coefficient

...

└ Additional considerations and conclusions

Other interesting notions

- ▶ Agglomerative clustering (CHA : classification Hierarchique Ascendante)
- ▶ Xmeans : improvement of k means
- ▶ If you know more about probabilities :
 - ▶ Latent variables and variational learning
 - ▶ Auto Encoders
 - ▶ Boltzmann Machines

Project

- ## ► Description of the project

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└ Additional considerations and conclusions

Questions ?

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└ Additional considerations and conclusions

References

-  Le Hir, N., Sigaud, O., and Laflaqui  re, A. (2018).
Identification of Invariant Sensorimotor Structures as a
Prerequisite for the Discovery of Objects.
Frontiers in Robotics and AI, 5(June) :1–14.