

Algorithms. Matching

Part II. Preference model.

B9 - Algorithms Matching

M-ALG-102

Introduction

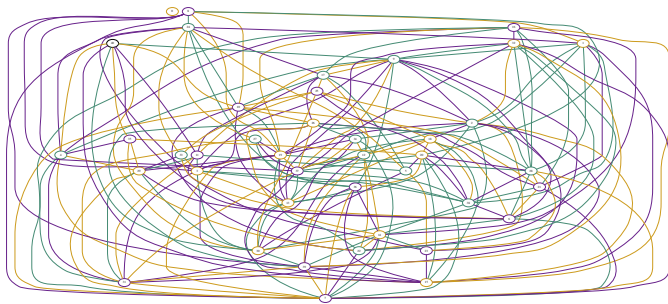


Figure: Graph

Introduction

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

We will need (the installation of these packages should work with pip) :

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

Day 2

Compatibility graphs

- Simple geometrical data

- Complex data

Probability distributions

- Reminders on probabilities

- Analyzing a distribution

- Optimization and Maximum Likelihood

- Gradients

Multivariate analysis and clustering

- Correlation

- Kmeans clustering

Similarities and Spectral Clustering

- Similarities

- Spectral Clustering

Additional considerations and conclusions

Compatibility graphs

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- ▶ If two nodes were related, they were linked by an edge in the graph.

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**.

Compatibility graphs

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

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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.

Example applications

- ▶ Social networks management
- ▶ Recommendations

Building compatibility graphs

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

Building a graph from simple data

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

Euclidian distance and compatibility

Consider the following data :

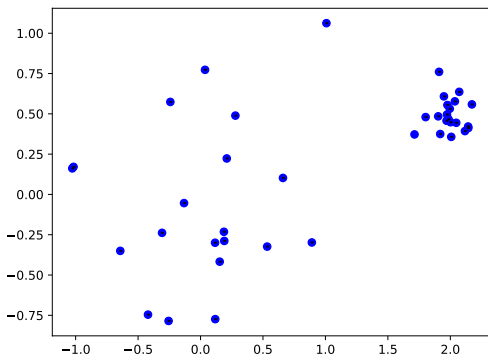


Figure: Data : we would like to define **edge** between some of them

Is this set of edges a good solution ?

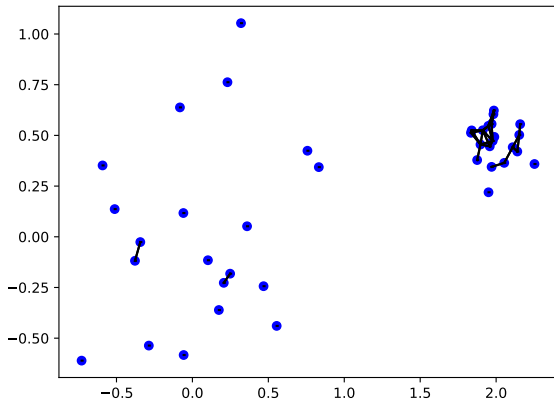


Figure: Some definition of edges

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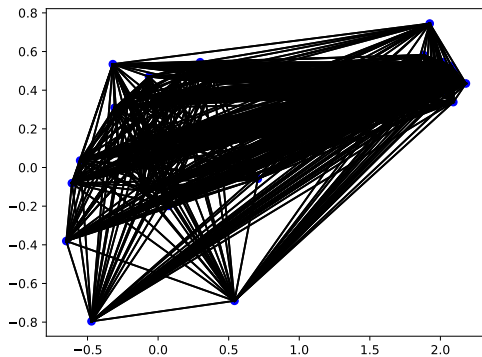
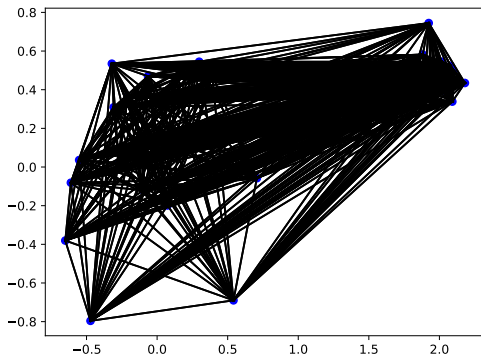


Figure: Some definition of edges

Euclidian distance and compatibility

Here, all we know about the data is their **euclidian distance** :



This one looks ok

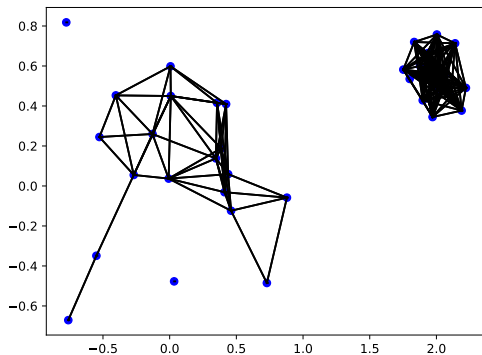
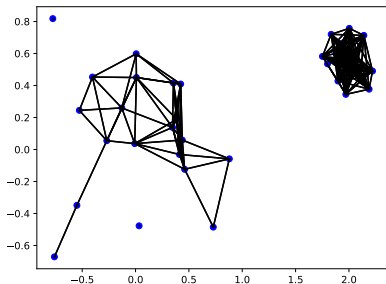


Figure: A proposition of edges

Backboard

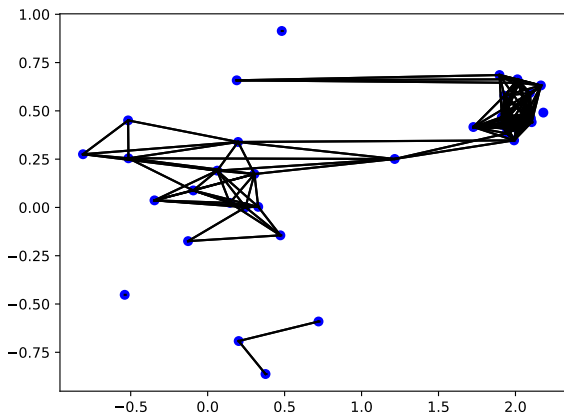
- ▶ Euclidian distance and threshold.

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



Exercice 2 : Changing the distance

- ▶ Assess the impact of changing the distance used. Possible choices :
 - ▶ $L1$ distance (Manhattan)
 - ▶ $|||_{\infty}$ distance (backboard)
 - ▶ custom distance
- ▶ use **build_graph_other_distance.py** and edit the distances used at the end of the file.
- ▶ Try several values for the threshold.



General notion of a distance

- ▶ Let us generalize what we experimentally studied.

Examples of distances

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

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- ▶ L1 : $\|x - y\|_1 = \sum_{k=1}^p |x_k - y_k|$ (Manhattan distance)
- ▶ weighted L1 : $\sum_{k=1}^p w_k |x_k - y_k|$

Hamming distance

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

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)

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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- ▶ **separate the values** : $\forall x, y, d(x, y) = 0 \Leftrightarrow x = y$
- ▶ respect the **triangular inequality**
 $\forall x, y, z, d(x, y) \leq d(x, z) + d(y, z)$

Building compatibility graphs for more complex data

- ▶ We will do the same with more complex data:
 - ▶ possibly more dimensions
 - ▶ possibility categorical variables

Random variables

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

Random variables

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- ▶ For instance :
 - ▶ the result of a dice throw

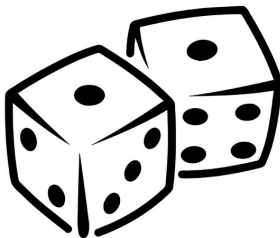


Figure: Dice

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 - ▶ waiting time with RATP



Figure: Some metro station

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 - ▶ waiting time with RATP
 - ▶ weather



Figure: Weather in November

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- ▶ For instance :
 - ▶ the result of a dice throw
 - ▶ waiting time with RATP
 - ▶ weather
 - ▶ number of cars taking the periphrique at the same time

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What are the differences between these random variables ?

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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

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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

- ▶ 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

- ▶ 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

- ▶ Periphrique :

Probability distributions

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

Continuous variables

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

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- ▶ One needs to use **probability densities**. Formally, the probability of being between x and $x + dx$ is $p(x)dx$.

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 probably of being between x and $x + dx$ is $p(x)dx$.
- ▶ Let's see some examples

Uniform discrete

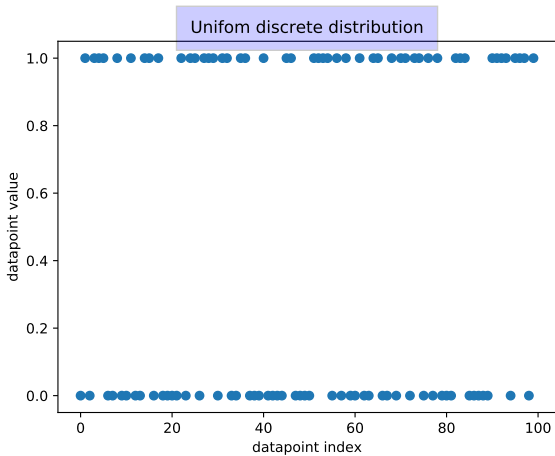


Figure: Uniform discrete distribution

Bernoulli

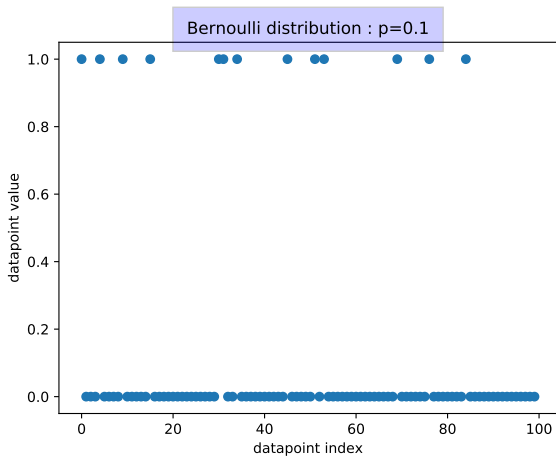


Figure: Bernoulli distribution

Bernoulli p

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

Bernoulli

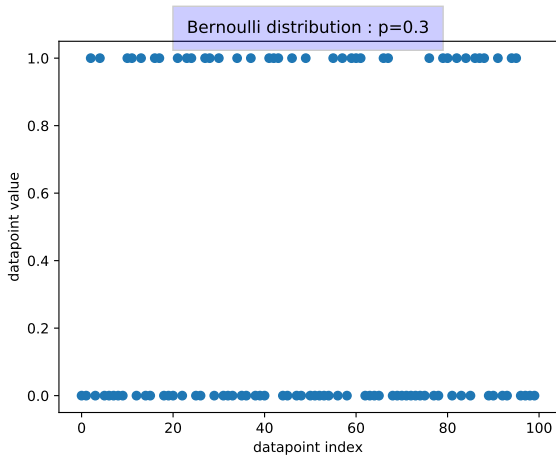


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Bernoulli

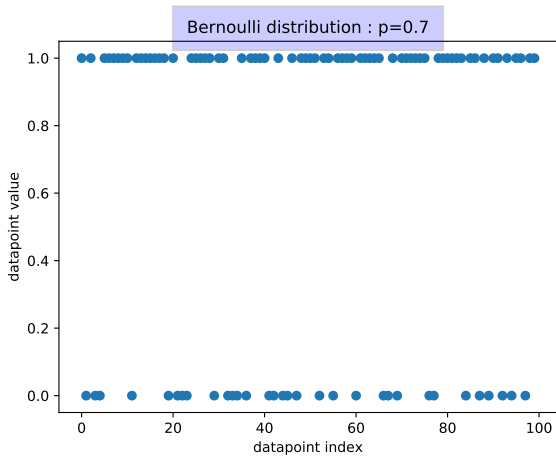


Figure: Bernoulli Distribution

Uniform continuous

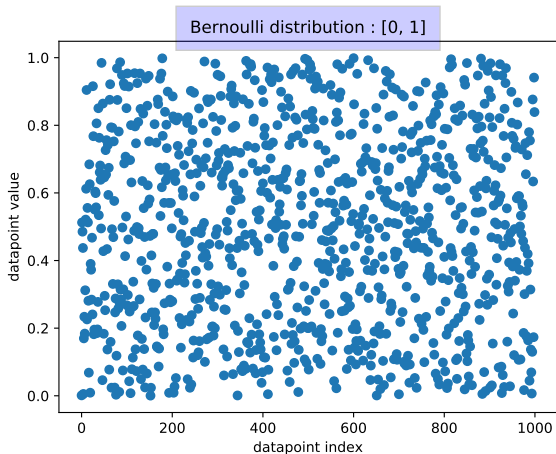


Figure: Uniform continuous distribution

Uniform continuous

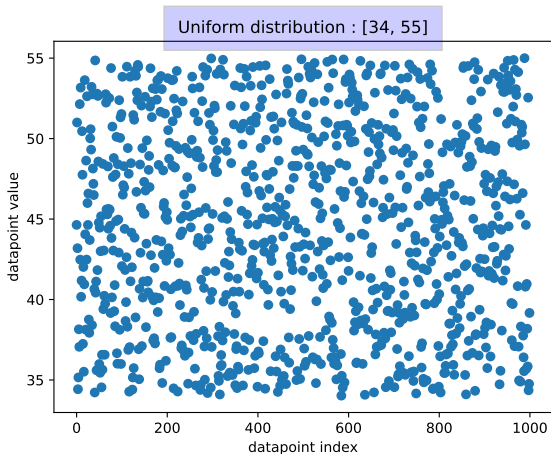


Figure: Uniform continuous distribution

Normal

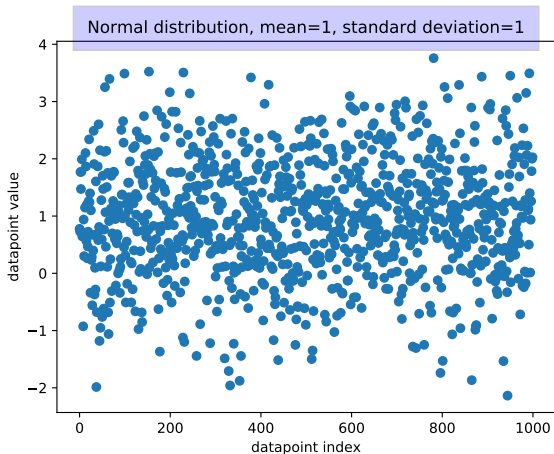


Figure: Normal distribution

Normal

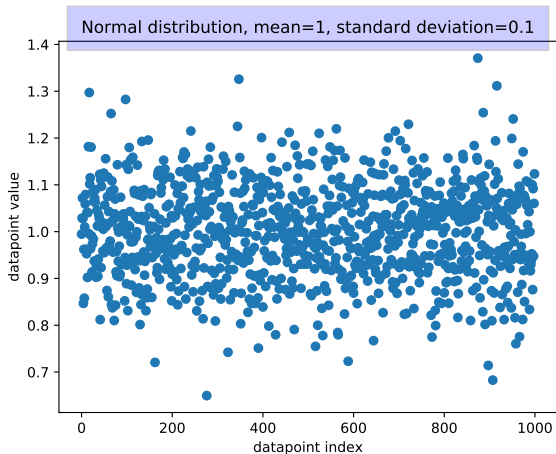


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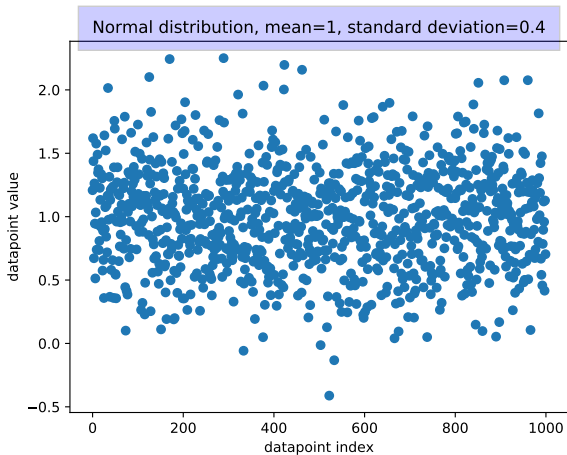


Figure: Normal distribution

White noise

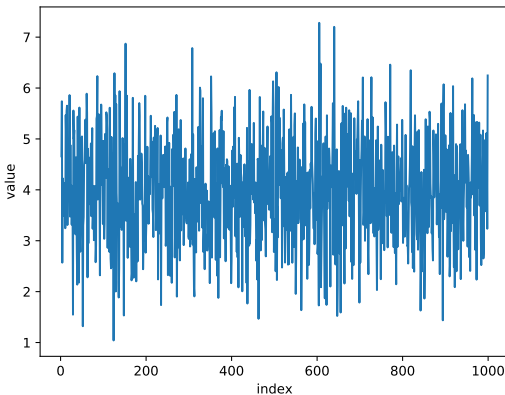


Figure: White noise

Histograms

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

Histograms

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It is informative, but often a **histogram** tells more.

Uniform discrete

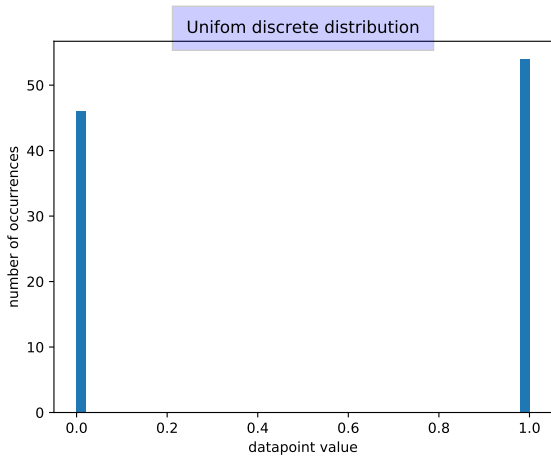


Figure: Histogram 1

Bernoulli

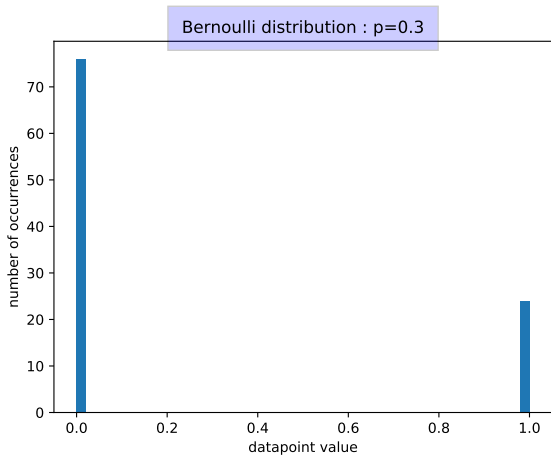


Figure: Histogram 2

Uniform continuous

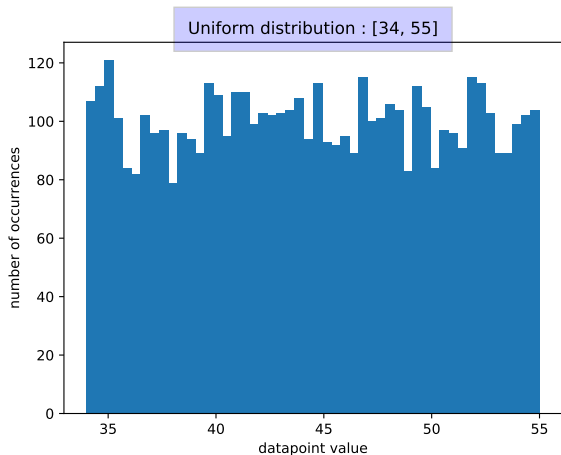


Figure: Histogram 3

Normal

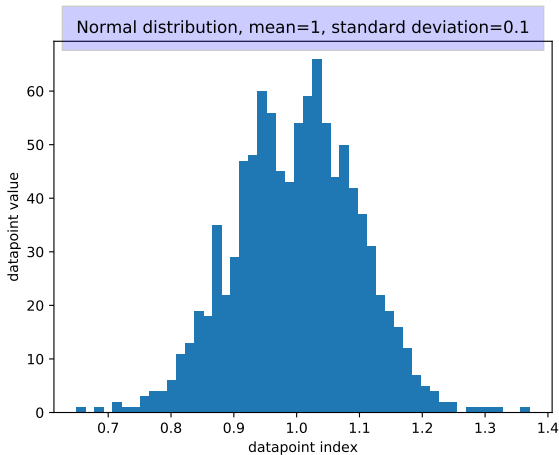


Figure: Histogram 4

Exercice 3 : Analyzing a distribution I put values in the file **mysterious_distro_1.csv**

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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)

Exercise 4 : Analyzing a distribution When you have guessed the kind of distribution it is, you need to find 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**

Distribution 1

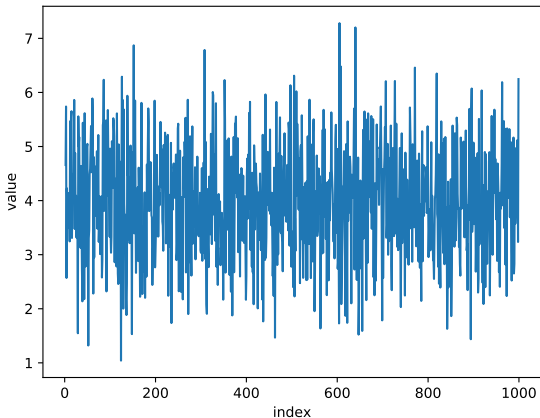


Figure: The data we analyze

histograms

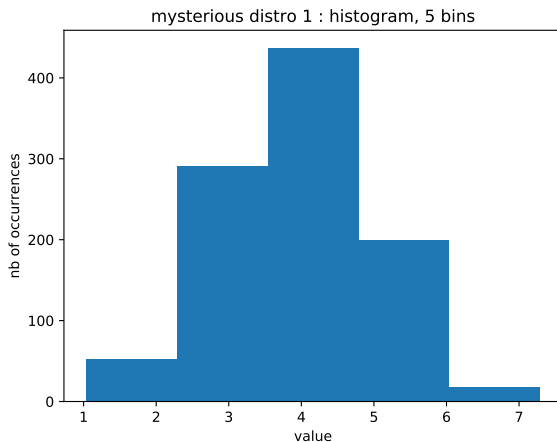


Figure: 5 bins

histograms

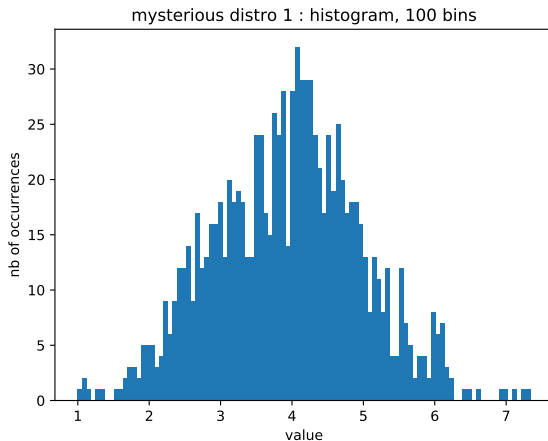


Figure: 100 bins

histograms

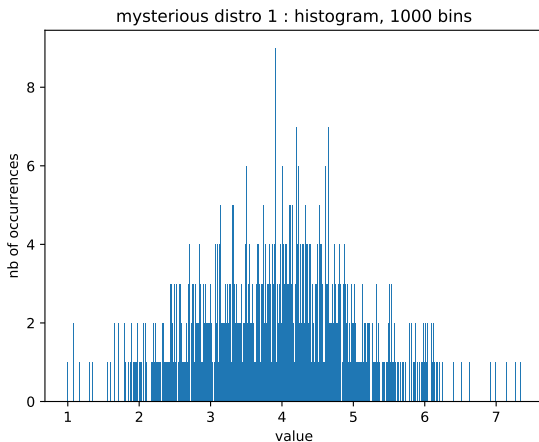


Figure: 1000 bins (too many)

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

Exercice 4 : Second example Let's try to perform the same analysis on the file **mysterious_distro_2.csv** using **read_myst_2.py**.

Second example

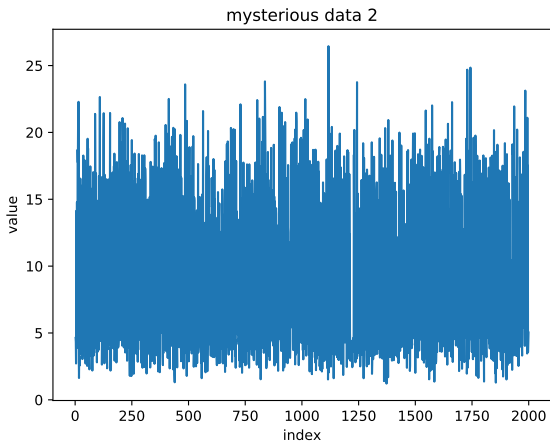


Figure: Second distribution

Multimodal distribution

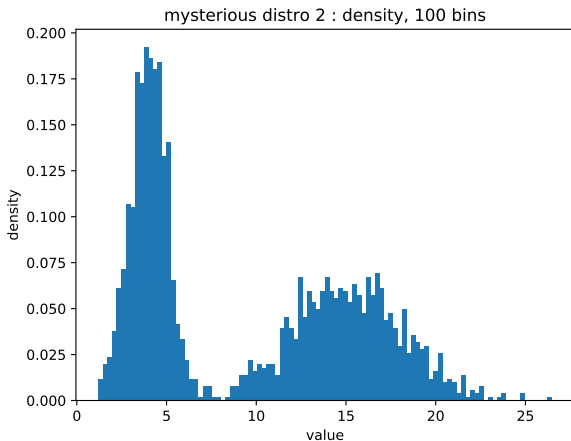


Figure: This distribution has several **modes**

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

Fitting

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

Fitting

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:

- ▶ 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) .

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

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

Maximum Likelihood

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

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

Maximum Likelihood

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

$$L(\theta) = \prod_{i=1}^n p(x_i|\theta) \quad (2)$$

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

Remark on max-likelihood

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

Why ?

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**.

Remark on max-likelihood

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

Example 1

Exercise 5: 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 ?

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$$L = p(1|p)p(0|p) \tag{5}$$

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

Example 2

Exercice 6 : 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) ?

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$$L = p(2.5|\mu, \sigma)p(3.5|\mu, \sigma) \quad (6)$$

Example 2

Exercise 6 : We observe the data (2.5, 3.5). We assume that these data come from a normal law of parameters μ and σ .

$$\begin{aligned} L &= p(2.5|\mu, \sigma)p(3.5|\mu, \sigma) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{2.5-\mu}{\sigma})^2} \times \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{3.5-\mu}{\sigma})^2} \end{aligned} \quad (7)$$

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We want to show that the likelihood is maximum for :

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

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.

Max Likelihood

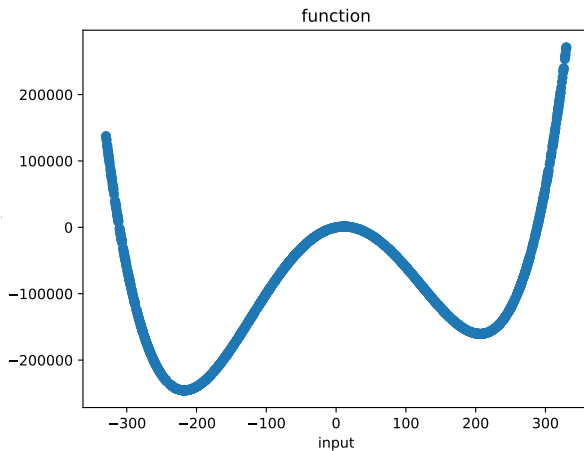
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Max Likelihood

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Most common method : **gradient descent**.

Notion of optimization



Gradient descent

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Gradient descent

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- ▶ If $f'(x) > 0$, the function grows around x .
- ▶ If $f'(x) < 0$, the function decreases around x .
- ▶ If x is a local extremum, $f'(x) = 0$

Gradient descent

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- ▶ 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 ?

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.

$$\nabla_f(x, y) = \left(\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y} \right) \quad (9)$$

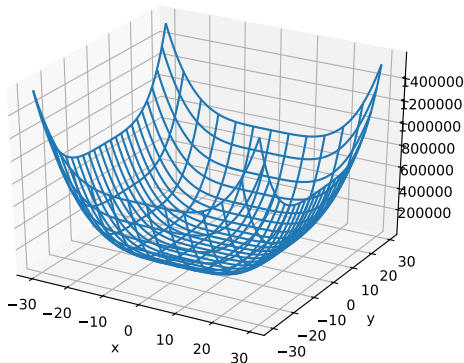
We want x to **minimise** f . We perform, until some criteria is satisfied :

$$x \leftarrow x - \alpha \nabla_f(x) \quad (10)$$

α is a small parameter called the learning rate.

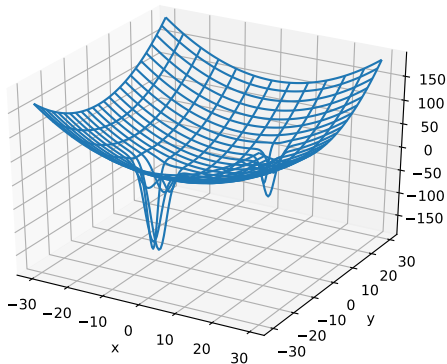
Gradient

Exercise 6: Using the gradient algorithm We will use the algorithm on two functions.



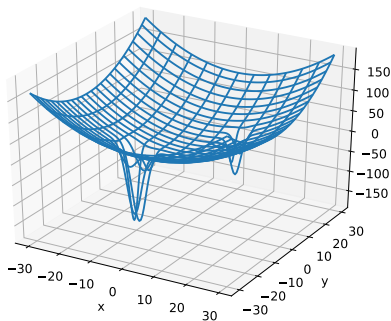
Gradient

Exercise 6: Using the gradient algorithm We will use the algorithm on two functions.



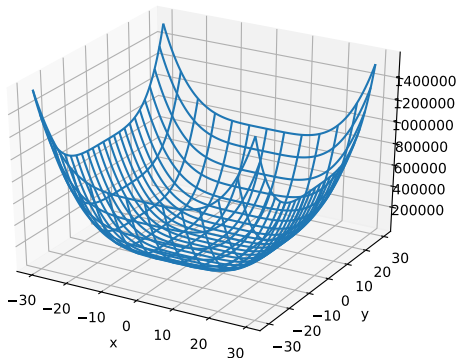
Gradient

Exercise 6: Using the gradient algorithm `cd ./gradient` and use the files `gradient.py` and `gradient_2.py` in order to implement the algorithm to find **minima**.



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.

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2. Examples ?

Multidimensional vectors

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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.

Correlation, expected value

- ▶ Let us introduce these two important quantities (backboard).

$$\text{var}(X) = E((X - E(X))^2) \quad (11)$$

Correlation, expected value

- ▶ Let us introduce these two important quantities (backboard).

$$\text{var}(X) = E((X - E(X))^2) \quad (12)$$

$$\text{cov}(X, Y) = E((X - E(X))(Y - E(Y))) \quad (13)$$

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

Exercise 6 : Which dimensions of the distribution are correlated ?

Correlation matrix

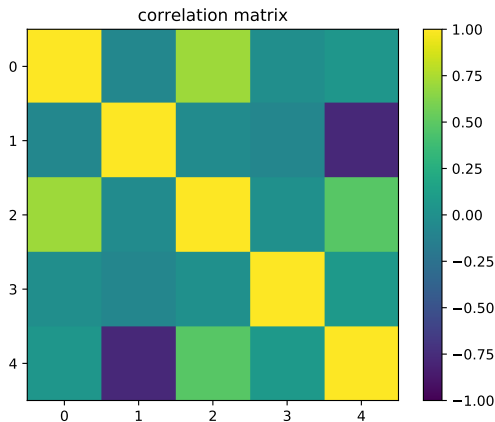


Figure: Correlation matrix for the distribution

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

Pandas

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

K means clustering

- A famous unsupervised clustering method

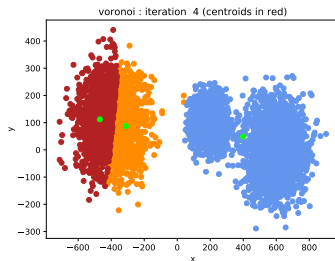


Figure: K means clustering

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 ?

Kmeans clustering

Exercise 7 : Implementing kmeans

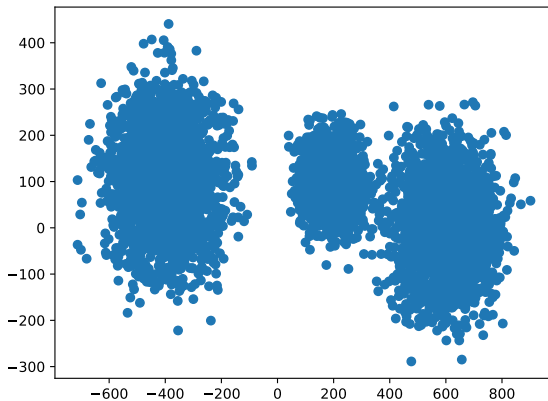


Figure: Data we want to cluster

Kmeans clustering

Exercise 7 : 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:

Kmeans

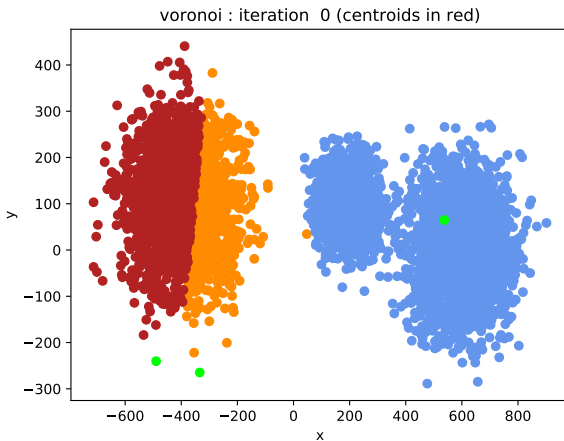


Figure: Voronoi 0th iteration

Kmeans

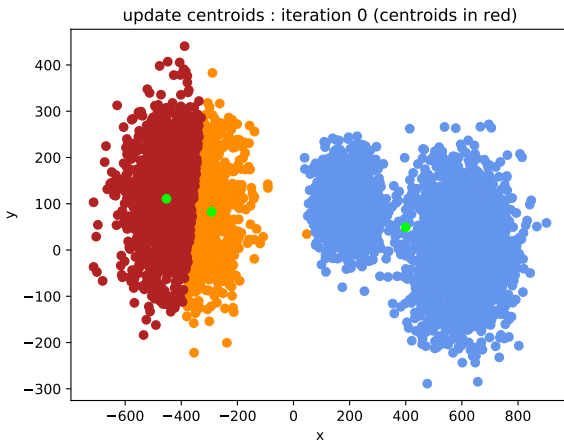


Figure: Centroids 0th iteration

Kmeans

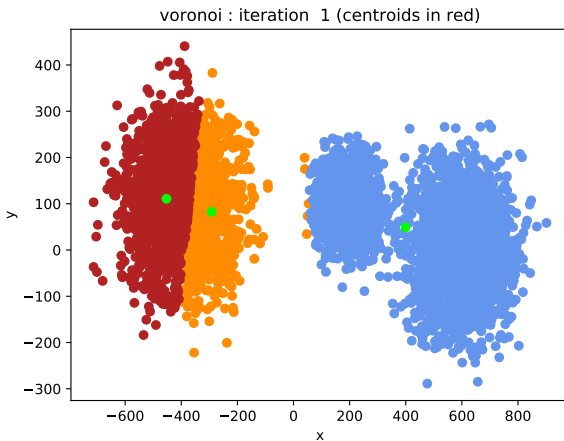


Figure: Voronoi 1st iteration

Kmeans

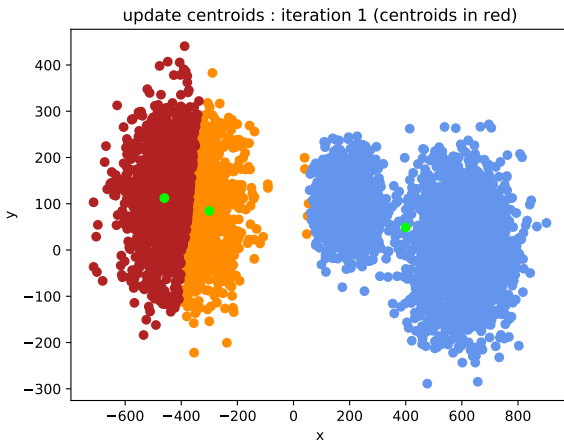


Figure: Centroids 1st iteration

Kmeans and initialization

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

Similarities

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

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- ▶ But sometimes you do not have access to a distance between the points.

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- ▶ 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**.

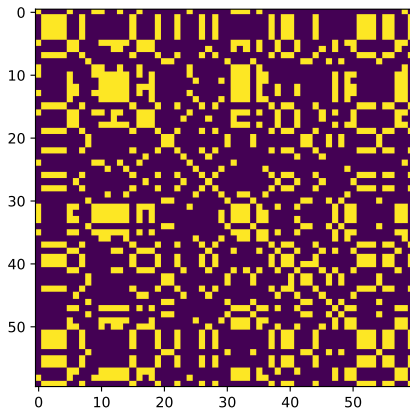
Similarities

- ▶ 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**.

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 $S_{ij} = 0$.

Adjacency matrix



Similarities

Differences between similarities and distances:

- ▶ A similarity S is not always symmetrical.

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- ▶ 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 .

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.

Similarities

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

Similarities

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

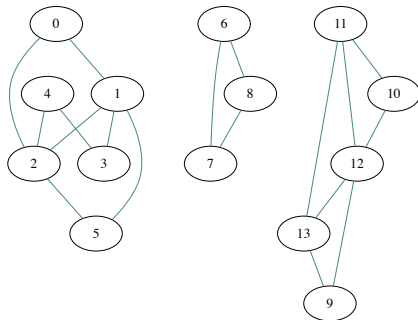
$$S_{ij} = \exp(-d_{ij}) \quad (14)$$

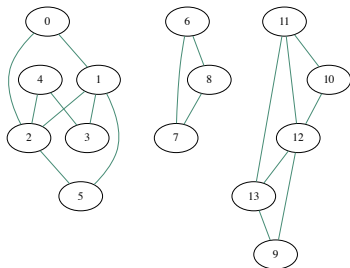
Spectral Clustering

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

Exercise

We will perform Spectral Clustering on this graph :





Please **cd spectral_clustering** and use **vanilla_spectral_clustering** 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.

Spectral clustering

Can you guess some drawbacks of the method ?

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.

Heuristic

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

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:

$$NCut(\mathcal{C}) = \sum_{k=1}^K \frac{Cut(C_k, V \setminus C_k)}{d_{C_k}} \quad (15)$$

Normalization

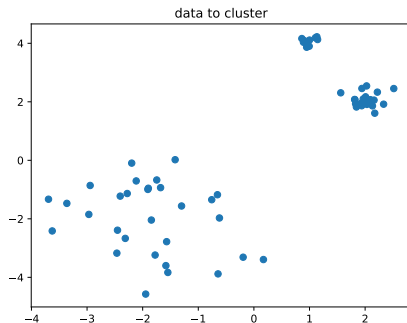
- ▶ The normalization is useful in order to take the **weight** (degree) of a cluster into account.

Normalized cut and clustering

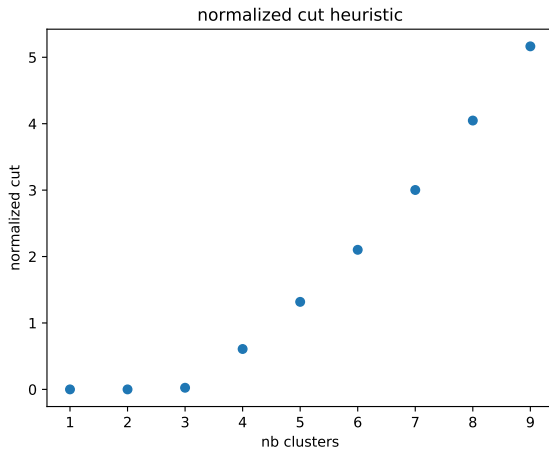
Let's see how the normalized cut can help us choose the right number of clusters (backboard).

Heuristic

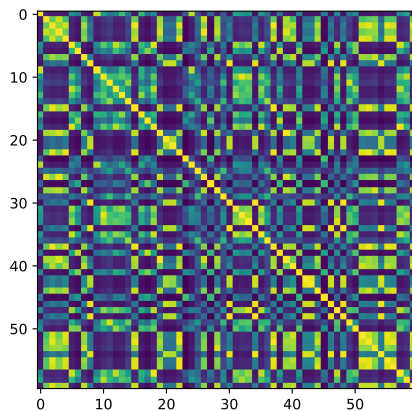
Exercise 8 : Exercise : normalized vut elbow Please use the criterion in the file **normalized_cut.py** in order to guess the relevant number of clusters in order to process the data contained in **data/**



Normalized cuts



Similarity



Example

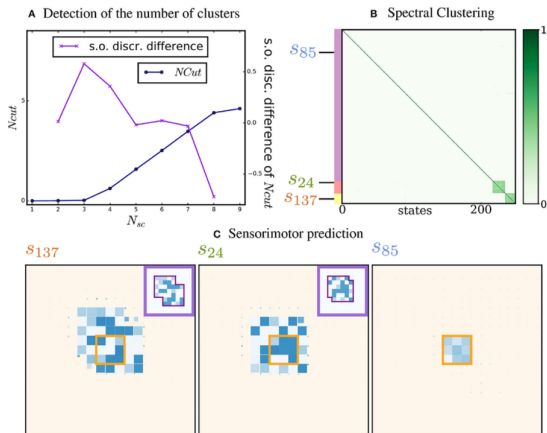


Figure: In a), the elbow method is used to choose the number of clusters.
[Le Hir et al., 2018]

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

Other interesting notions

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

Conclusion

Different kinds of problems exist :

- ▶ P problems where exact polynomial solutions exist (max matching)
- ▶ For other problems :
 - ▶ exhaustive search works but is too slow
 - ▶ to solve the problem a balance between rapidity and quality must be found.
- ▶ Evaluating the quality of a result is not an easy task.

Project

- ▶ Description of the project

Questions ?

References



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