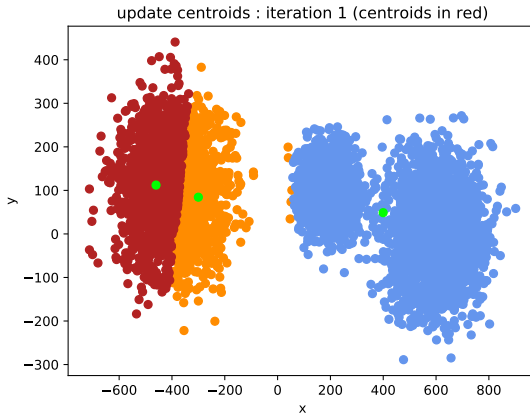


# Machine learning II, unsupervised learning and agents: clustering



Motivation

K-means clustering

Hierarchical clustering

Spectral clustering

## Motivation

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## Clustering (technical definition)

**Clustering** consists in **partitioning** the data.  $\forall i, x_i \in \mathcal{X}^n$ .

$$D_n = \{(x_i)_{i \in [1, \dots, n]}\} \quad (1)$$

A **partition** is a set of  $K$  subsets  $A_k \subset D_n$ , such that



$$\cup_{k \in [1, \dots, K]} A_k = D_n \quad (2)$$



$$\forall k \neq k', A_k \cap A_{k'} = \emptyset \quad (3)$$

# Partitions

- ▶ **Example 1** :  $A$  is the set of even integers,  $B$  the set of odd integers. Is  $(A, B)$  a partition of  $\mathbb{N}$ ?
- ▶ **Example 2** :  $C$  is the set of multiples of 2,  $D$  the set of multiples of 3. Is  $(C, D)$  a partition of  $\mathbb{N}$ ?

## Example : partition of data

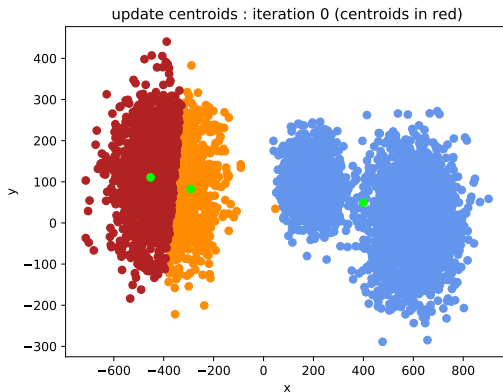


Figure – In this image, each cluster is represented by a color.

## Applications of clustering

Example applications :

- ▶ spam filtering [Sharma and Rastogi, 2014, ]
- ▶ fake news identification  
[Hosseinimotlagh and Papalexakis, 2018, ]
- ▶ marketing and sales
- ▶ document analysis [Zhao and Karypis, 2002, ]
- ▶ traffic classification [Woo et al., 2007, ]

Some of these applications can be considered to be semi-supervised learning.

## Applications of clustering

[https://en.wikipedia.org/wiki/Cluster\\_analysis](https://en.wikipedia.org/wiki/Cluster_analysis)  
[https://datafloq.com/read/  
7-innovative-uses-of-clustering-algorithms/](https://datafloq.com/read/7-innovative-uses-of-clustering-algorithms/)



Many clustering algorithms exist !

`https:  
//scikit-learn.org/stable/modules/clustering.html`

## K means clustering

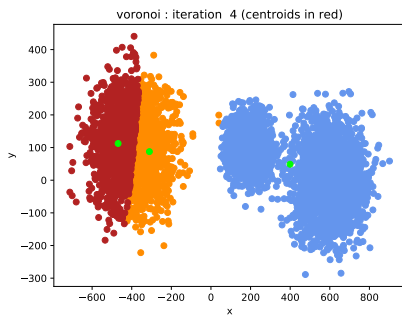


Figure – K means clustering

## K-means

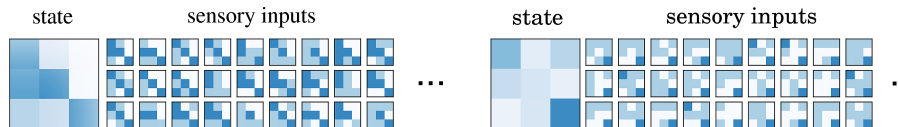


Figure – Other example of k-means clustering, this time in 9 dimensions  
[Le Hir et al., 2018]

## K-means : Expectation Maximisation algorithm

- ▶ Classical Machine Learning algorithm (EM)
- ▶ Discussion on the drawbacks of the algorithm.

Numpy demo.

# K-means clustering

## Exercise 1 : Implementing kmeans

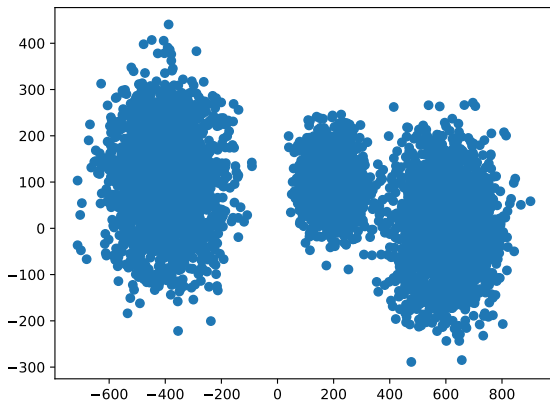


Figure – Data we want to cluster

## K-means clustering

### Exercise 1 : Implementing k-means

`cd ./k_means.`

Edit the `k_means.py` file so that it performs the k-means algorithm, on the example dataset, with 3 clusters.

## K-means

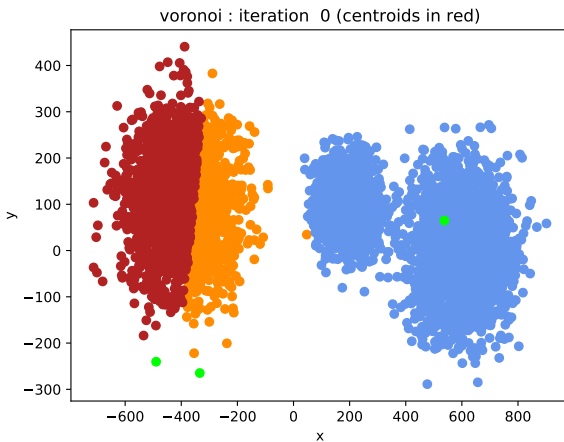


Figure – Voronoi 0th iteration



## K-means

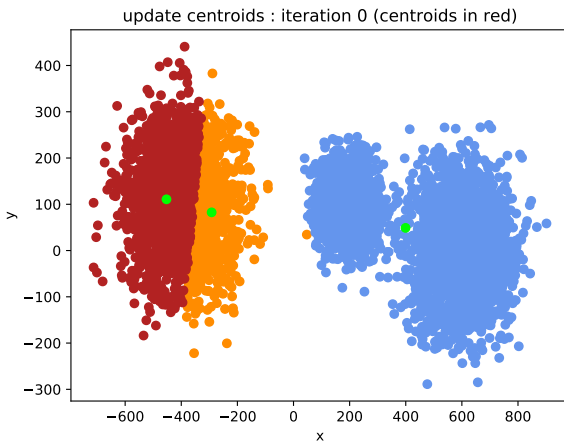


Figure – Centroids 0th iteration

## K-means

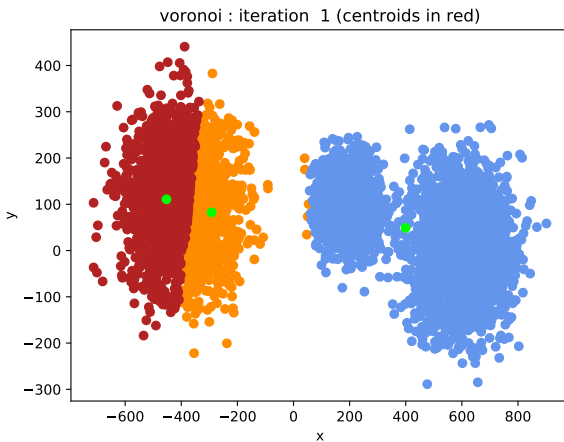


Figure – Voronoi 1st iteration

## K-means

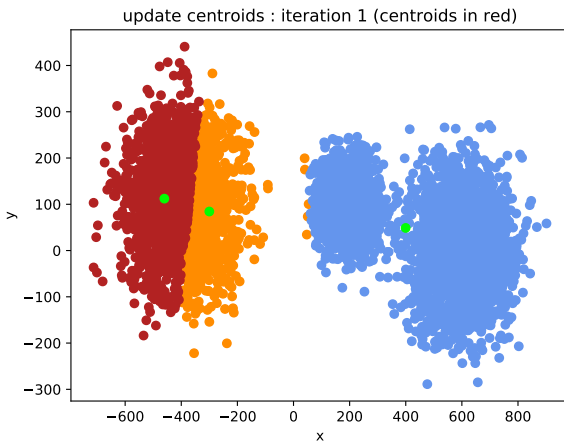


Figure – Centroids 1st iteration

## K-means and initialization

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

## K-means optimization problem

Let us present the optimization problem associated with the k-means algorithm.

## K-means and cost

- ▶ When performing the k-means algorithm, we optimize the **inertia**.
- ▶ if we have  $n$  points,  $x_i$ , each assigned to a centroid  $c_i$ .

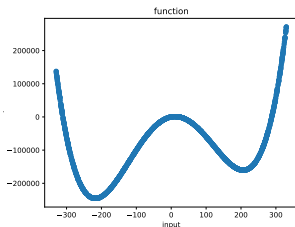
$$I = \sum_{i=1}^n d(x_i, c_i)^2 \quad (4)$$

$$I = \sum_{i=1}^n \|x_i - c_i\|_2^2 \quad (5)$$

$\|$  stands for "norm".

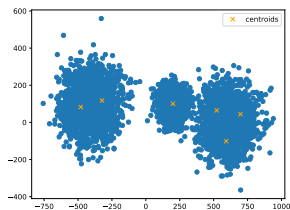
## K-means : Expectation Maximisation algorithm

- What would you do if the algorithm falls in a local optimum ?



**Exercise 2:** Perform the algorithm on the same dataset with scikit-learn (use the file : `k_means_sklearn.py`)

- ▶ Observe the randomness of the result
- ▶ Explore the available parameters :  
<https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html> and find a solution in order to observe a **stable** result.





## Knee/elbow criterion

- ▶ We would like a **heuristic method** in order to be able to assess a relevant number of clusters.

## Knee/elbow criterion

- ▶ **Exercise 3:** use the file `k_means_inertia.py` in order to find a relevant number of clusters for the `data_2.npy`, with scikit-learn and kneed.

<https://github.com/arvkevi/kneed>

Observe the behavior of this method when you run it on a different input dataset (you can generate a new one).

[https://scikit-learn.org/stable/auto\\_examples/cluster/  
plot\\_kmeans\\_assumptions.html](https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_assumptions.html)

Motivation

K-means clustering

**Hierarchical clustering**

Spectral clustering

# Hierarchies

It is possible to perform a clustering in a hierarchical way. This means building a **sequence of clusterings**.

[https://scikit-learn.org/stable/auto\\_examples/cluster/plot\\_agglomerative\\_dendrogram.html](https://scikit-learn.org/stable/auto_examples/cluster/plot_agglomerative_dendrogram.html)

# Hierarchies

`https://docs.scipy.org/doc/scipy/reference/cluster.hierarchy.html`

## Example application of hierarchical clustering

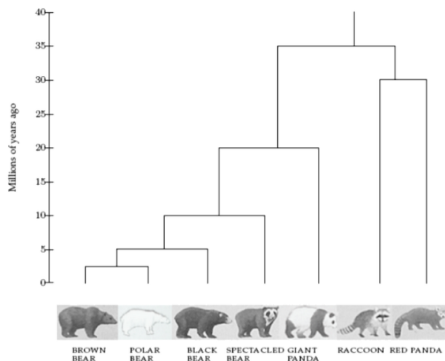


Figure – <https://towardsdatascience.com/hierarchical-clustering-and-its-applications-41c1ad4441a6>

## Treemaps

A **Treemap** is a another representation of hierarchical data in the two-dimensional space (not a clustering though).

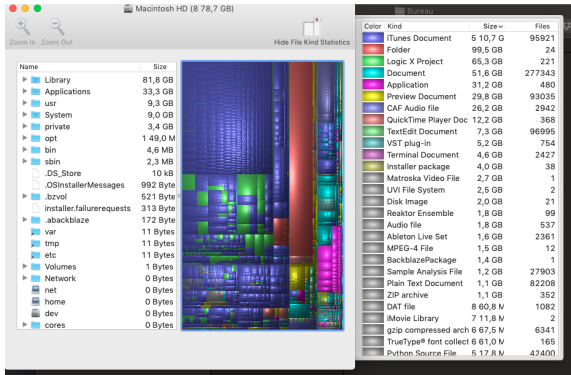


Figure – Disk Inventory X <http://www.derlien.com/>



## Treemaps

A **Treemap** is a another representation of hierarchical data in the two-dimensional space (not a clustering though).

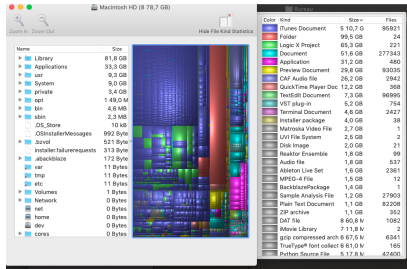


Figure – Disk Inventory X <http://www.derlien.com/>

The size of a rectangle corresponds to its size.

## Building a tree map

`treemap/build_treemap.py` can draw treemap of a folder.

## Building a tree map

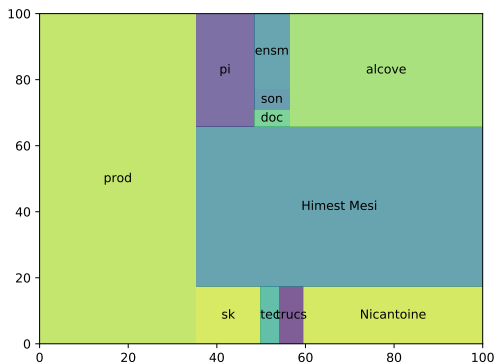


Figure – Treemap of desktop computer (desktop folder)

## Building a tree map

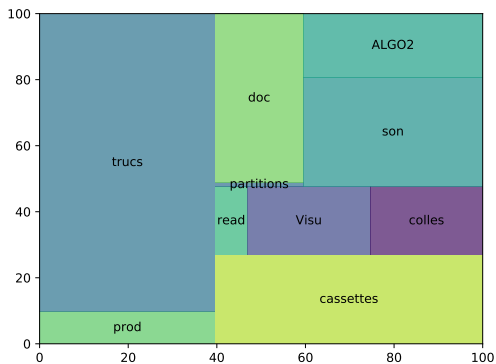


Figure – Treemap of laptop (desktop folder)

# Treemaps

We can again use plotly.

<https://plot.ly/python/treemaps/>

# Hierarchical clustering

We will apply hierarchical clustering to a small example dataset containing addresses.

## Hierarchical clustering

### Exercice 4 : Plotting data

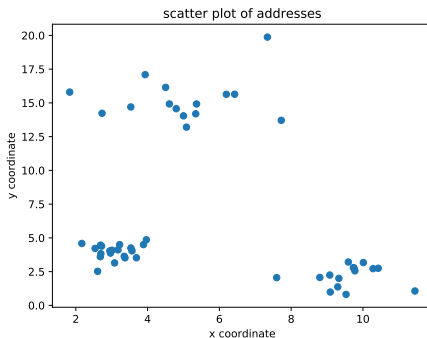
`cd hierarchical_clustering/` and use `hierarchical_clustering.py` in order to show the scatter plot of the data (nuage de points) loaded from `addresses.csv`.

## Scatter plots

Seaborn lib : <https://seaborn.pydata.org/>



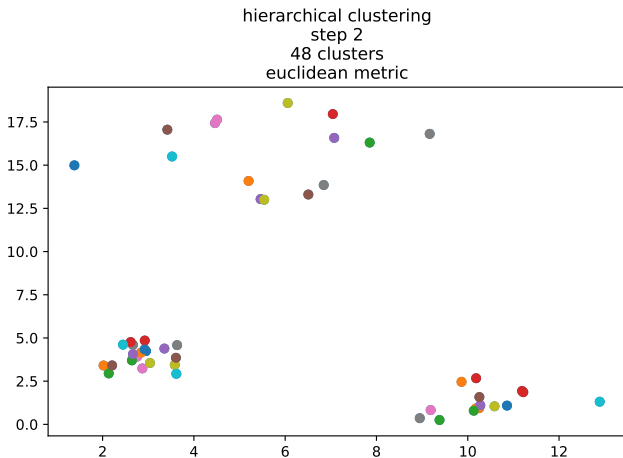
# Hierarchical clustering

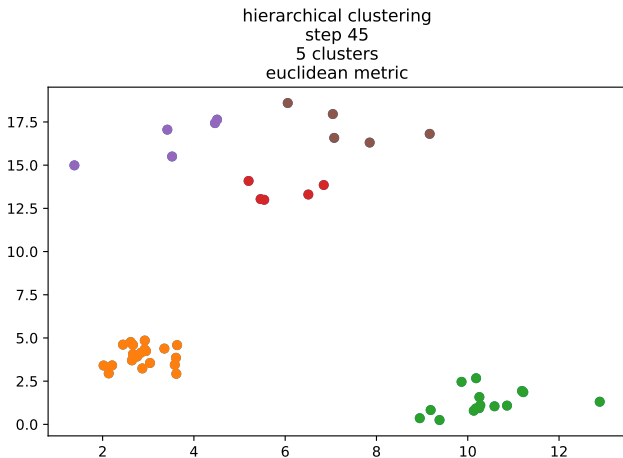


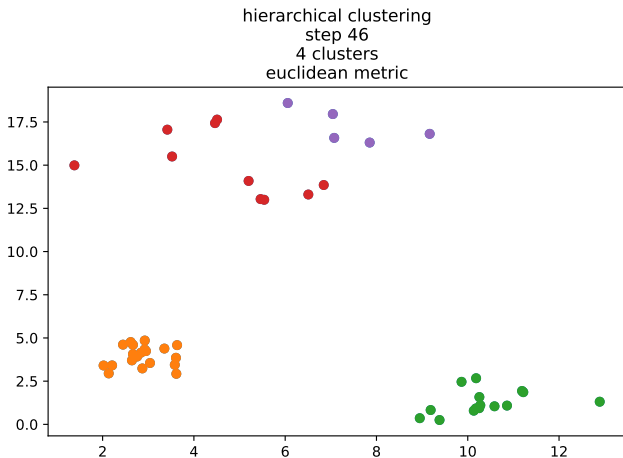
Hierarchical clustering consists in progressively grouping points together in **classes**.

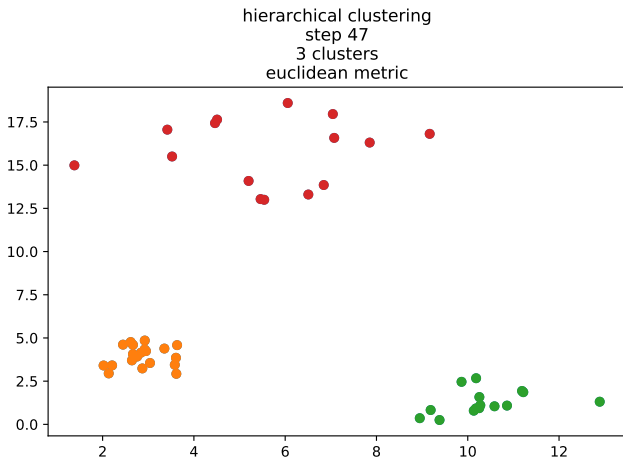
## Hierarchical clustering

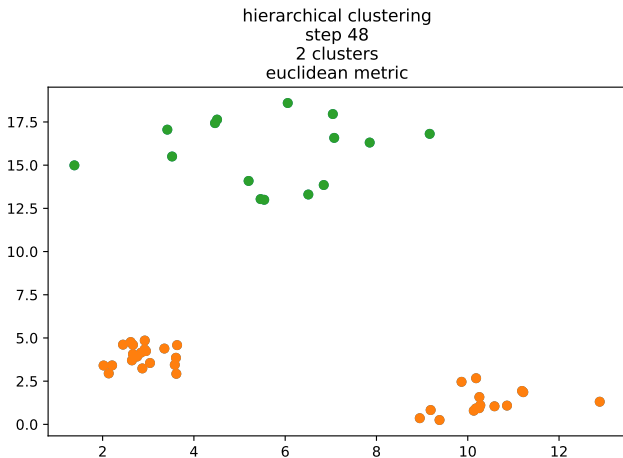
**Exercise 5:** Edit `find_closest_classes()` in order to find the closest classes. Then they can be merged in the while loop.















## Hierarchical clustering

An important aspect of hierarchical clustering is that different criteria can be used in order to merge the classes. The distance between class 1 and class 2 can for instance be :

- ▶ the minimum distance between one point of class 1 and one point of class 2 : **single-linkage clustering**.
- ▶ the average distance between points a class 1 and points a class 2 : **unweighted average linkage clustering**

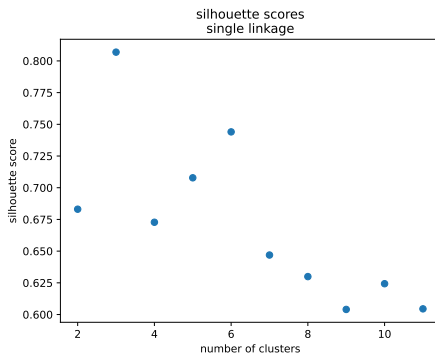
The two methods can lead to a different hierarchy of clusters.

## Average-linkage clustering

**Exercice 6 :** Modify the computation of the distance between classes using the average-linkage criterion.

## Silhouette score

The Silhouette score is another heuristic used in order to choose a relevant number of clusters. File : **hierarchical\_clustering\_silhouette.py**.



Motivation

K-means clustering

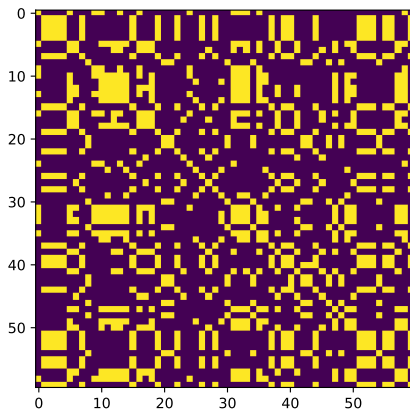
Hierarchical clustering

Spectral clustering

## 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 : **adjacency relationship** in a graph : 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.
- ▶ 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 similarity between two points, we can deduce a distance.
- ▶ For instance this way, if  $d_{ij}$  is the distance between  $i$  and  $j$  :

$$S_{ij} = \exp(-d_{ij}) \quad (6)$$

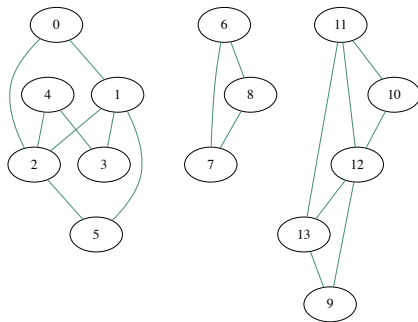


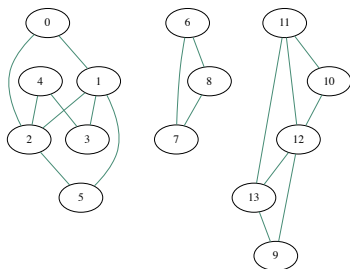
## Spectral Clustering

- ▶ 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 :





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 **scikit-learn** library. **doc** : check the scikit page for Spectral Clustering.

## Spectral clustering

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 :

$$NCut(\mathcal{C}) = \sum_{k=1}^K \frac{Cut(C_k, V \setminus C_k)}{d_{C_k}} \quad (7)$$

## Normalization

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

## Normalized cut and clustering

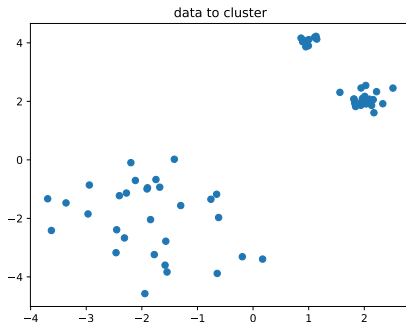
Let's see how the normalized cut can help us choose the right number of clusters (backboard).



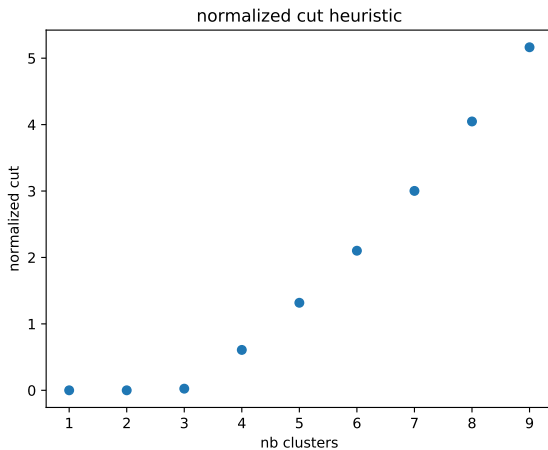
## Heuristic

### Exercise 7 : Normalized but elbow :

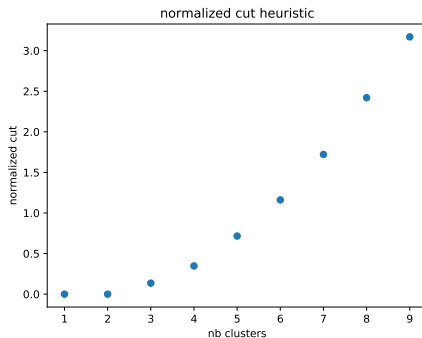
Please use the criterion in the file `normalized_cut.py` in order to guess the relevant number of clusters in order to process the data contained in `data/`. These data are generated by `generate_data.py`.



## Normalized cuts

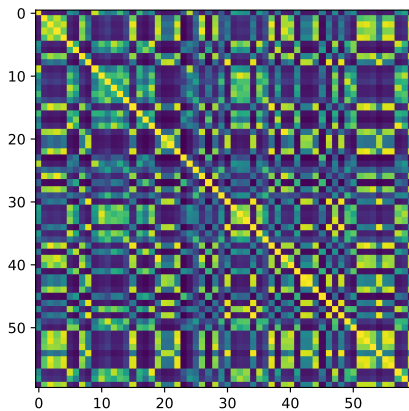


## Normalized cuts

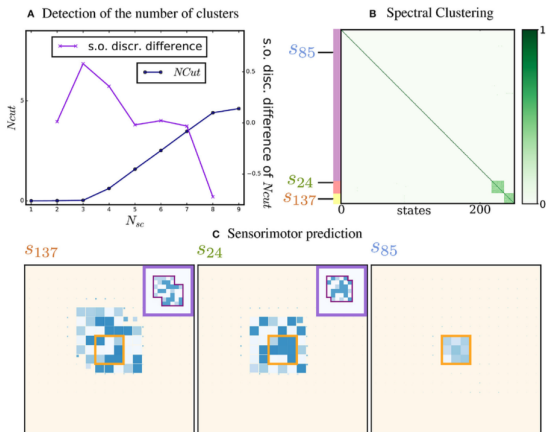


**Figure** – If the standard deviations in the dataset are larger, it is harder to identify a relevant number of clusters.

# 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

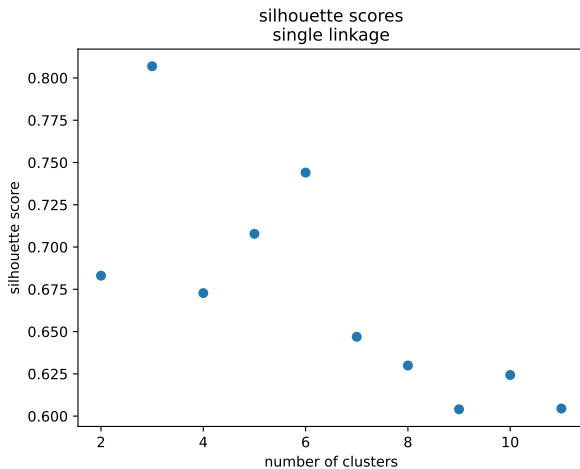
`https://scikit-learn.org/stable/modules/clustering.html`

### Exercise 8 :

Study the silhouette score as a function of the number of clusters for the hierarchical clustering problem.

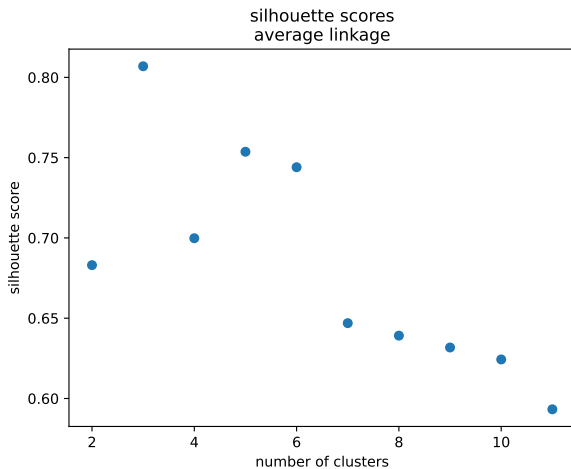
`https://scikit-learn.org/stable/modules/generated/sklearn.metrics.silhouette\_score.html`

## Silhouette coefficient with single linkage







## Silhouette coefficient with average linkage



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