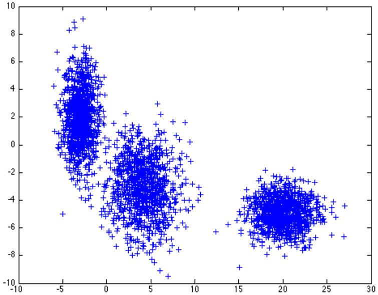
Clustering

Automatic set grouping of objects (clusters)

September 2021

Thomas Corpetti

What is clustering ?



From a dataset : group homogeneous sets of data : clusters

- Group them by their similarity with respect to a model (generative methods)
- Separate them with respect to their dissimilarity (discriminative methods)

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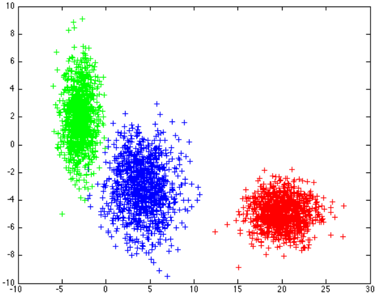

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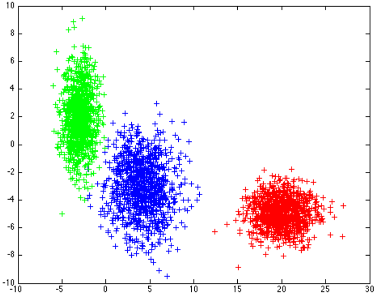

- Inside a cluster :

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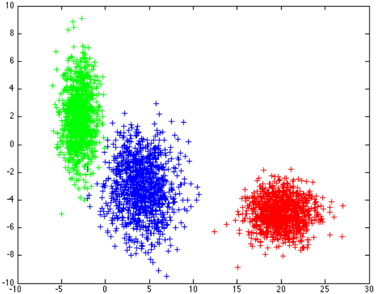

- Inside a cluster : high similarity

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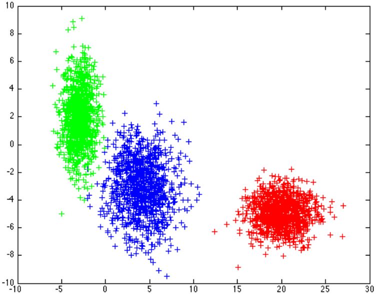

- Inside a cluster : high similarity
- Between clusters :

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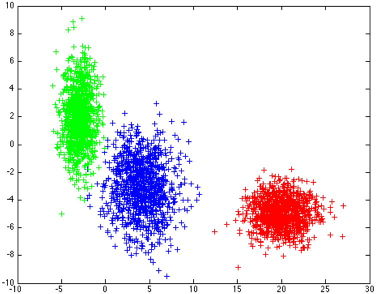

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- Between clusters : low similarity (high dissimilarity)

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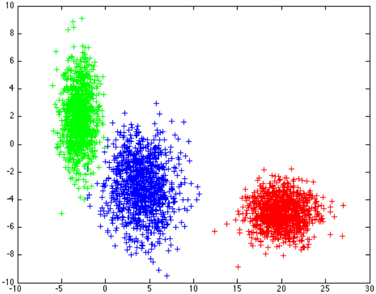

- Inside a cluster : high similarity
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$\Longrightarrow$ Distance/metric of prime importance

Applications

Large range of applications

- Web : similar web-pages
- Social-networks : group of users
- Bio-informatics : identify species
- Marketing : types of clients
- Climatology : types of weather
- Image processing : homogeneous areas
- ...

Main families of clustering

- Centroid : create several clusters and evaluate their quality depending on some centroids (k-means, k-medoids, PAM, ...)
- Hierarchical : group in a hierarchical way data (AGNES, DIANA, ...)
- Density : rely on the adequacy of data with respect to a certain density (DBSCAN)
- Model-based : one model for each cluster
- Spectral : based on a graph-representation of data

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General ideas

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1 Introduction

2 Partitioning
- K-means
- Evaluation / Computations / Characterisation of clusters
- K-medoids

3 Hierarchical Clustering
- Principes
- Agglomerative
- Divisive

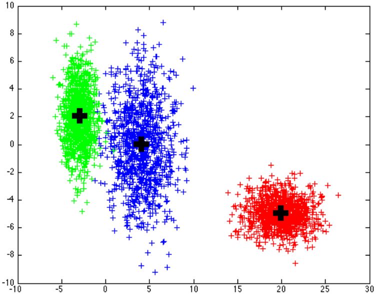
4 Density based clustering
- Principles

5 Model based clustering
- Principles

6 Spectral clustering (graph-based)
- Principles

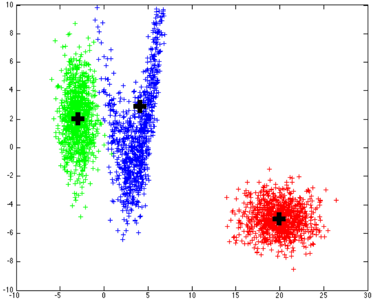
Centroid

- Construct k clusters from n objects
- Many criteria
  - k-means (MacQueen'67) : rely on the center to create clusters



Centroid

- Construct k clusters from n objects
- Many criteria
  - k-means (MacQueen'67) : rely on the center to create clusters
  - k-medoids or PAM (Partition around medoids) : rely on specific data to create clusters



Main idea

- Create k-partitions : each data is associated with the closest center of partition
- Also called quantification algorithm of Lloyd-Max

- We start from a **data matrix** X of dimension $N \times P$ (N points of dimension P)
- Le number of clusters k is a *hyperparameter*, supposed to be known

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K-means

- Formalisation : find the partition $\mathcal{S}^* = \{S1, ..., S_k\}$ such that

$$\mathcal{S}^* = \arg\min_{\mathcal{S}} \sum_{i=1}^{k} \sum_{x_j \in S_i} \|x_j - \mu_i\|^2$$

with μ_i the average of points in S_i

- $\Longrightarrow$ Tricky optimization problem

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Standard algorithm

1. Iteration $p = 0$: find k initial means $\mu_i^p, \forall i = 1...k$ (usually randomly)
2. For each iteration p, until convergence
   1. Each point x_j is assigned to partition S_i^p if its distance with center μ_i^p is minimal :

$$S_i^p = \left\{ x_j : \|x_j - \mu_i^p\| \leqslant \|x_j - \mu_{i^*}^p\|,\ \forall i^* = 1...k \right\}$$

   2. Update the mean of each partition

$$\mu_{i^*}^{p+1} = \frac{1}{\mathrm{card}(S_i^p)} \sum_{x_j \in S_i^p} x_j$$

   3. $p = p + 1$

Note : the convergence can be low $\Longrightarrow$ find some heuristics

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K-means : some notes

Pros

- Cost-function always decreasing along iterations
- Simple and efficient

Coins

- Discontinuous data (what is a "centroid" in this case) ?
- How to fix the number of clusters ?

Variations, alternative approaches

- Monte-Carlo
- Fix k with cross validation

In each case : centers are not guarantee to be part of the dataset

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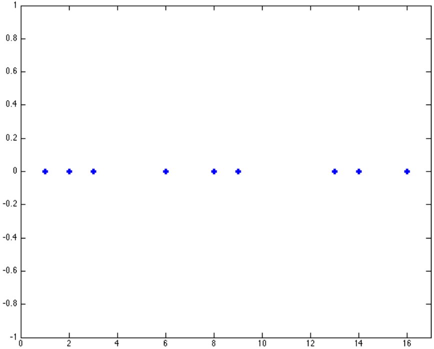
K-means : exercice

Apply a k-mean with 3 clusters for the $1D$ dataset :

$$P = \{1, 2, 3, 6, 8, 9, 13, 14, 16\}$$

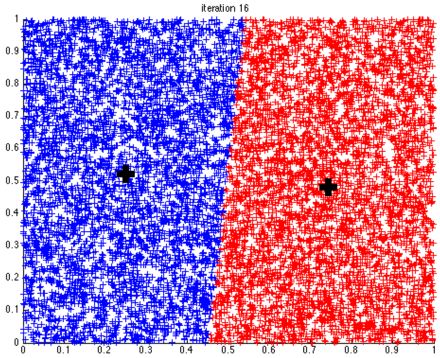
With initial means

$$\mu_1^0 = 1, \mu_2^0 = 2, \mu_3^0 = 3$$



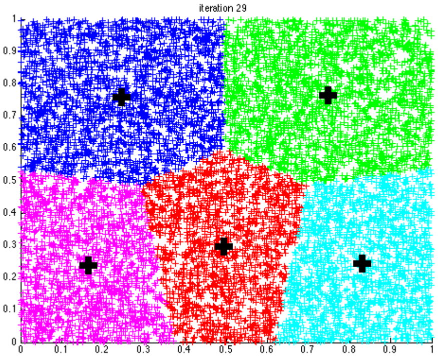
K-means : illustrations

Uniform random set : 2 partitions



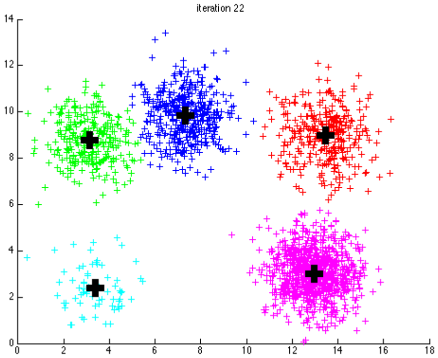
K-means : illustrations

Uniform random set : 5 partitions



K-means : illustrations

Point cloud with 5 clusters



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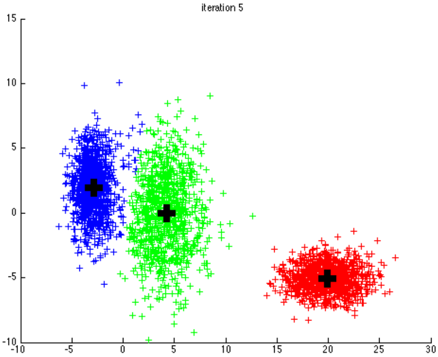

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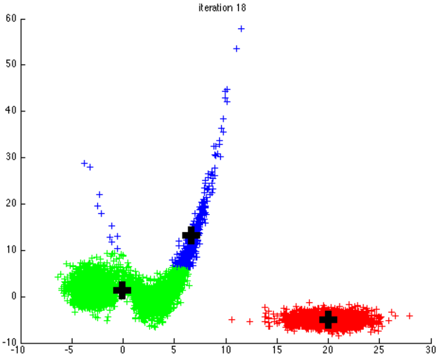

What about images

create a point cloud with R, G, B coef, and may be spatial coordinates

R	G	B	X	Y
212	80	12	180	341
222	34	49	180	342
190	23	423	180	343
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...	...	...	...	...
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To impose spatial consistency

- one can add X, Y coordinates ;
- one can also filter images

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Computation on clusters

How to characterise a cluster ? How to compare partitions ?

- Characterisation :
  - Inertia inside a cluster S_i composed of points $x_1, ..., x_M$ of M :

$$\mathcal{I}_i = \sum_{k=1}^{M} p(x_k) d(x_k, \mu_i)$$

with

- $d(.,.)$: a distance function ;
- μ_i : center of the cluster ;
- $p(x_k)$: probability of point x_k

Note : If all points have similar probability, $p(x_k) = 1/M$

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  - "Intra-class" intertia (of all clusters S) :

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$\Longrightarrow$ sum of all cluster intertia

  - "Inter-class" intertia (between all clusters S) :

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How to compare partitions

- Let's take all pair of points (x_m, x_n) and let's have a look of their partitions with two methods. Four possibilities :

Class with method 1 \ Class with method 2	same	different
same	a	b
different	c	d

- Rand index :

$$R = \frac{a+d}{a+b+c+d} = \frac{a+d}{C_2^N}$$

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Exercise

- We have a set of 5 points $\{x_1, x_2, x_3, x_4, x_5\}$, and 2 clustering methods gave the following partitions :

  - $S_1 = \{1, 1, 2, 2, 2\}$
  - $S_2 = \{1, 2, 2, 1, 2\}$

- What is the Rand index ?

K-medoids

General ideas

- Find most representative centroids (medoids) in the cluster
- Principle : iteratively replace medoids if the global distance is reduced

- More robust with respect to outliers

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      Note : exactly the same than k-means
   2. For each class i, choose randomly some non-medoids (or all) μ_j^p
      - Compute the replace cost of μ_i^p by μ_j^p

      $\Longrightarrow$ If the cost is lower, μ_i^p is replaced by μ_j^p

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K-medoids : some notes

Pros

- Cost-function always decreasing along iterations
- Simple and efficient
- The cluster centroids (medoids) are interpretable

Coins

- How to fix the number of clusters ?

Variations, alternative approaches

- Monte-Carlo
- Fix k with cross validation

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Apply the K-medoids method with 2 clusters on the $1D$ dataset :

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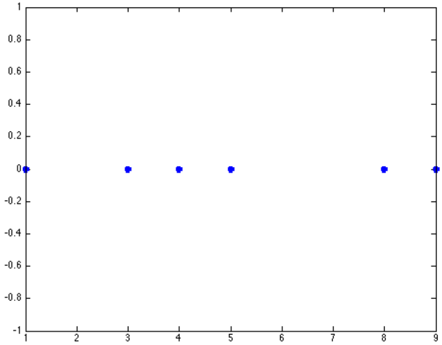
With initial medoids

$$\mu_1^0 = 1, \mu_2^0 = 8$$



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- Principles

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Hierarchical Clustering

Two main types :

1. Clustering agglomerative (bottom-up) : all points are in distincts clusters that are merged based on some criteria
2. Clustering divisive : all points are in a single cluster which is split depending on some criteria

$\Longrightarrow$ Important question : what is the distance between two clusters. Is it :

- The smallest distance between points of each clusters
- The largest distance between points of each clusters
- The distance between the mean of each cluster
- The average between all pairwise distances
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Hierarchical Agglomerative Clustering

Starting point : distance matrix

- From a set of N points of dimension P, the (symmetric) distance matrix is :

$$M = \begin{bmatrix} 0 & D(1,2) & . & D(1,N) \\ D(2,1) & 0 & . & D(2,N) \\ . & . & 0 & . \\ D(N,1) & D(N,2) & . & 0 \end{bmatrix}$$

Algorithm

1. Group all distances lower than a given threshold together
2. Recompute a distance matrix with the new dataset

Stop criteria to define

Main family : AGNES (AGglomerative NESting)

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1. Start from a large cluster that embeds all data
2. Divise it if not consistent

How to divise it ? $\Longrightarrow$ Less used algorithm

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Density based clustering

Basic assumptions

1. A cluster is a “dense” area
2. Data are composed of various clusters separated by less-dense areas

Principles

1. Two points are potentially in the same cluster if the are separated by a distance less than a radius fixed by the user
2. Each cluster has a minimal size

Main problem : in case of too much noise : all points in the same cluster

Pros : no need to compute means

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- Divisive

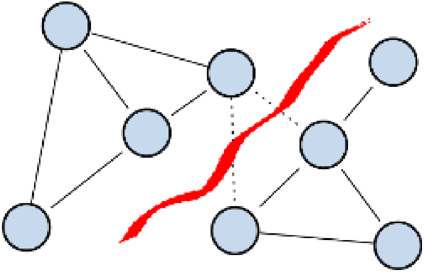
4 Density based clustering
- Principles

5 Model based clustering
- Principles

6 Spectral clustering (graph-based)
- Principles

Spectral clustering

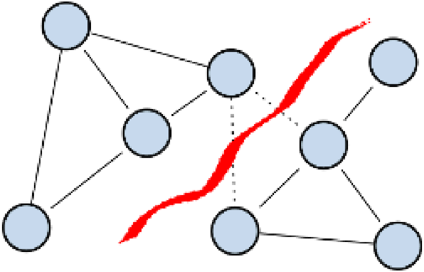
Data are represented on graphes



- The distance between each vertices is computed based on the similarity between points
- Perform “cut” on graphes

Spectral clustering

Data are represented on graphes



- The distance between each vertices is computed based on the similarity between points
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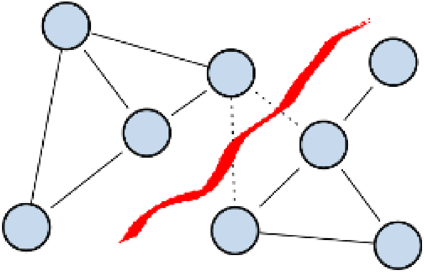
Spectral clustering

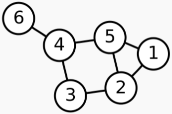
Data are represented on graphes



- The distance between each vertices is computed based on the similarity between points
- Perform "cut" on graphes

Graph theory

source : Wikipedia

Graphe	Représentation par une matrice d'adjacence	Représentation par une matrice laplacienne (non normalisée)
	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

- Based on Adjency and Laplacian matrix, one can characterise the structure of data