Statistical Learning with High-dimensional Data

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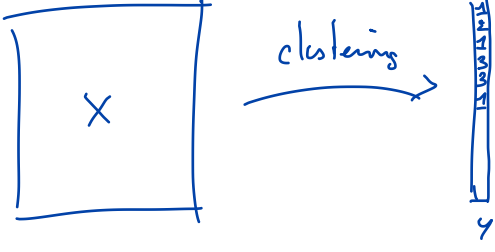
Clustering :

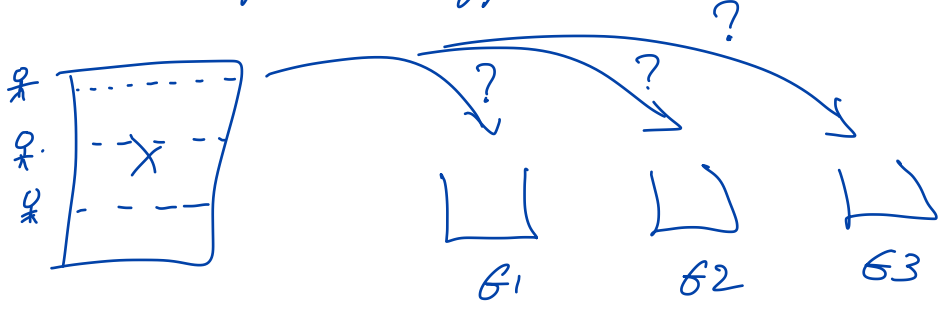
The goal of clustering is to be able to predict from X a categorical variable Y

X —learning→ Y = the group memberships of the observations



⚠ From the conceptual point of view, clustering is far more difficult than supervised classif.

Clustering is based on a simple idea of assigning individuals to groups (such that people who behave similarly are in the same group) but which have a combinatorial aspect which makes the problem difficult!



Clustering methods ?

- k means
- hierarchical clustering
- EM algorithm for GMM
- ...

The k-means algorithm:

The algo: for a fixed value k

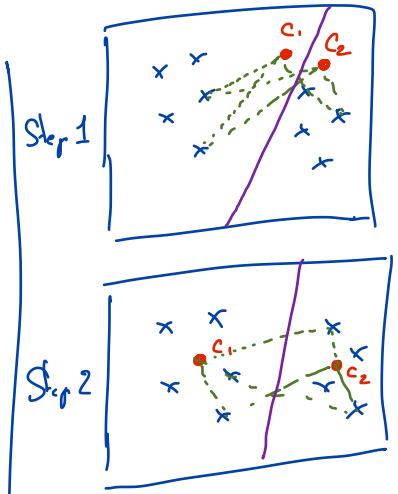
initialization: . pick k centers

loop: (i) compute the distances between all individuals and the k centers

(ii) assign each individual to the closest center and recompute the centers of each group.

stop: when the groups are stable (no more changes!)

$k = 2$



↳ stop: because the group assignements are already stable!

K-means is very simple and works very well most of the time, but requires to select k externally.

One approach to select k is to rely on the elbow method computed on the evolution of a clustering quality criterion:

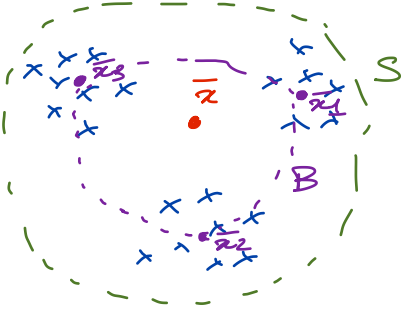
$$J(k) = \frac{B(k)}{S}$$

between variance

which has to be maximized

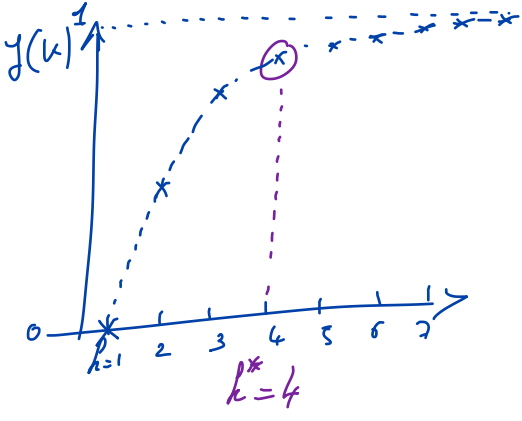
$J(k) \to 1$

variance of the data



$$S = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^t(x_i - \bar{x}), \quad B = \frac{1}{n}\sum_{k=1}^{K} n_k (\bar{x}_k - \bar{x})^t(\bar{x}_k - \bar{x})$$

To select the most appropriate k, we compute $J(k)$ for all possible values of k for the k-means and we look for the elbow of the curve.



Here $k^* = 4$ realises a compromise between an efficient clustering in terms of $J(k)$ with a small number of clusters.

Summary on k-means:

⊕ simple and efficient algorithm (→ reference technique)

⊕ the centers can be easily interpreted as the average individual of each group.

⊕ in combination to the elbow method, you can select k.

⊖ it is sensitive to the initialization and to outliers.

⊖ k-means tends to produce clusters of the same size.

Hierarchical clustering:

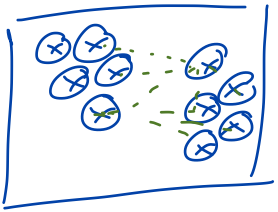
The algo:

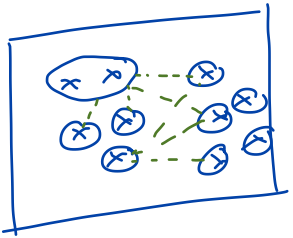
initialization: each individual is assigned to its own group.

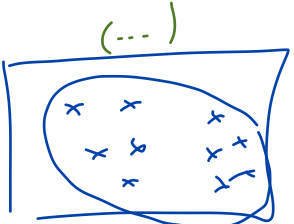
loop: (i) compute the distances between all groups

(ii) gather the two groups that are the closest ones

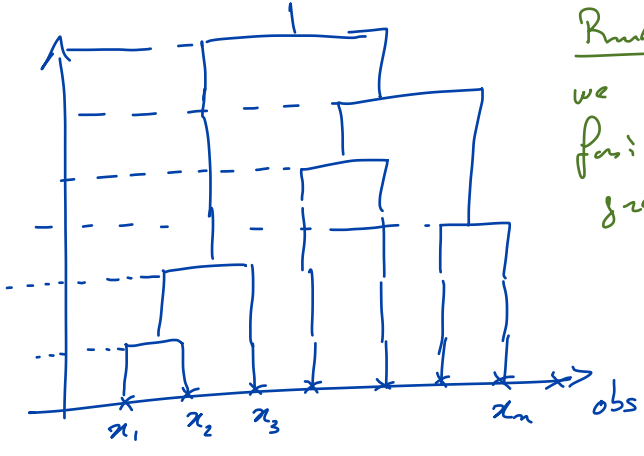
stop: when it remains only one group.







HC is generating a hierarchy of clustering with $k \in [1, n]$ groups. Interestingly, the hierarchy can be easily visualized thanks to a dendrogram:



Rmk: at each level, we have a unique fusion between two groups.

HC is in fact a family of algorithms, because we have several possibilities for the distance between groups.

- the **complete linkage**:

$$d(A,B) = \max \{ d(a,b) \,/\, a \in A, b \in B \}$$

- the **single linkage**:

$$d(A,B) = \min \{ d(a,b) \,/\, a \in A, b \in B \}$$

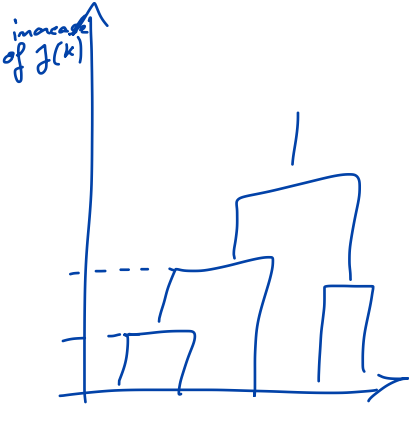
- the **centroid dist**:

$$d(A,B) = d(\bar{a}, \bar{b})$$

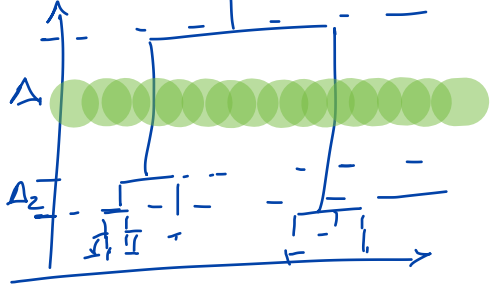
- the **Ward dist**:

$$d(A,B) = \frac{d(\bar{a}, \bar{b})}{\frac{1}{n_A} + \frac{1}{n_B}}$$

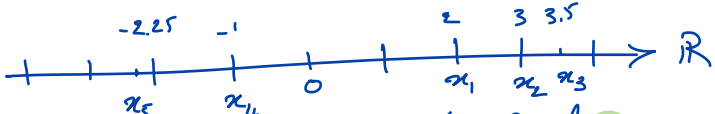
in HC, the elbow technique can also be applied to select k. Interestingly, it has been incorporated in most dendrograms produced by softwares like R



we pick the clustering with the largest gap



Exercise :

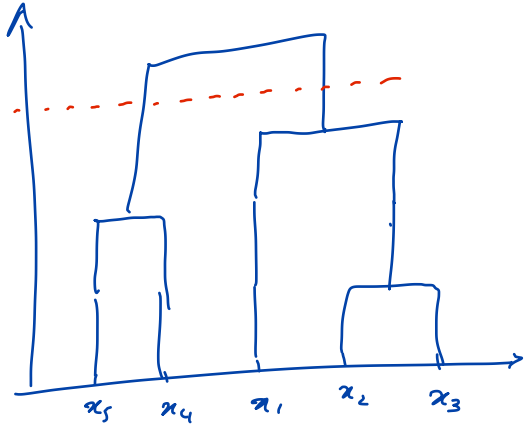


↳ apply HC on these data with the complete linkage

	x_2	x_3	x_4	x_5
x_1	1	1.5	3	4.25
x_2		0.5	4	5.25
x_3			4.5	5.75
x_4				1.25

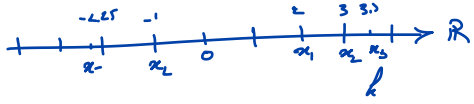
	x_{23}	x_4	x_5
x_1	1.5	3	4.25
x_{23}		4.5	5.75
x_4			1.25

	x_{23}	x_{45}
x_1	1.5	4.25
x_{23}		5.75



$$d(x_1, x_{23}) = \max\{d(x_1, x_2), d(x_1, x_3)\}$$
$$= \max\{1, 1.5\} = 1.5$$

Let's now apply k-means on the same data ($k = 2$) with x_1 and x_2 as initial centers.

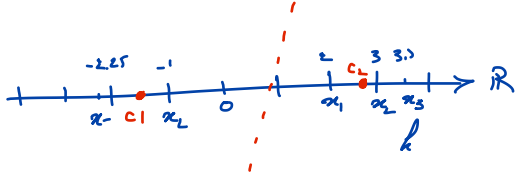


	x_1	x_2	x_3	x_4	x_5
$c_1 = x_1$	0	1	1.5	3	4.25
$c_2 = x_2$	1	0	0.5	4	5.25

↳ $c_1 = \text{mean}(x_1, x_4, x_5) = -0.41$

$c_2 = \text{mean}(x_2, x_3) = 3.25$

	x_1	x_2	x_3	x_4	x_5
c_1	2.41	3.41	3.91	0.39	1.64
c_2	1.25	0.25	0.25	4.25	5.5



↳ $c_1 = \text{mean}(x_4, x_5)$

$c_2 = \text{mean}(x_1, x_2, x_3)$

Summary on hierachical clustering:

⊕ the dendrogram is a very appreciated tool for visualizing the clustering hierarchy

⊕ a flexible tool thanks to the different group distances

⊕ the ability to choose K thanks to the elbow method directly within the dendrogram.

⊖ high algorithmic complexity ($\mathcal{O}(n^2 \log n)$)
↳ not possible to use it for $n > 10\,000$

DANGER some people use kmean as a pretreatment before applying hclust on the centers.