K-Means clustering

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Outline

1. Cluster analysis
2. K-Means algorithm
3. K-Means for categorical data
4. Fuzzy C-Means
5. Clustering of variables
6. Conclusion
7. References

Cluster analysis

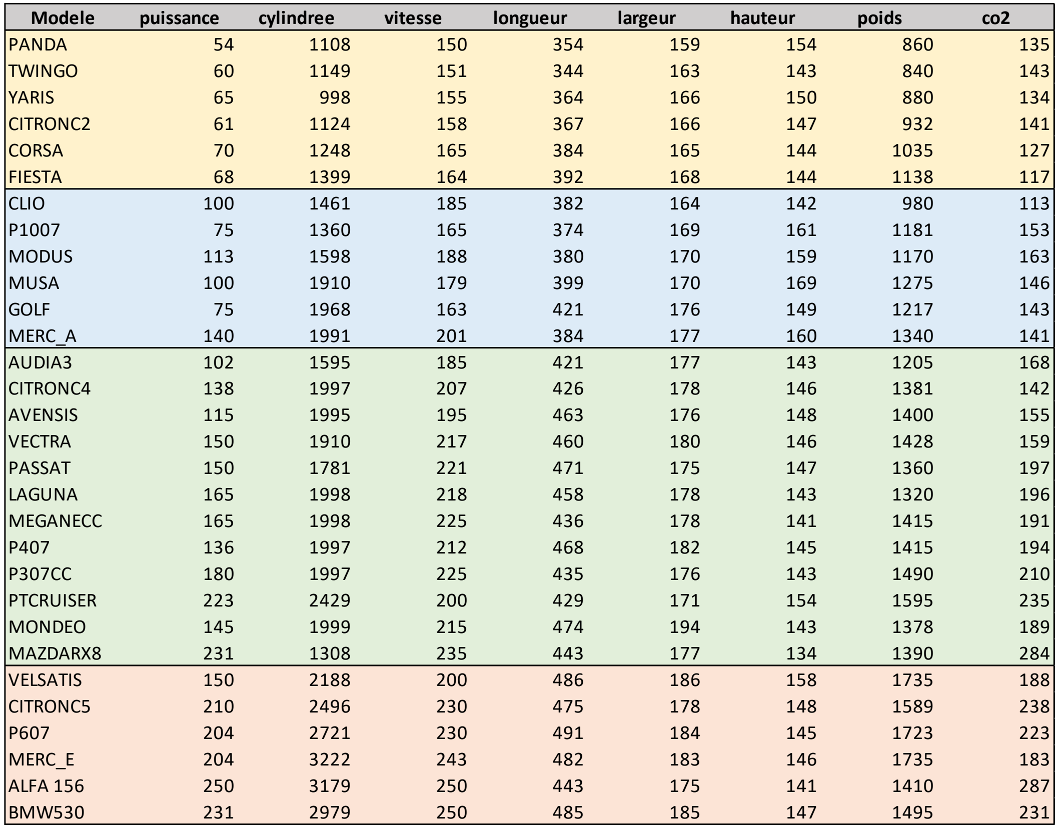
Clustering, unsupervised learning

Cluster analysis

Also called: clustering, unsupervised learning, typological analysis

Input variables, used for the creation of the clusters

Often (but not always) numeric variables



Modele	puissance	cylindree	vitesse	longueur	largeur	hauteur	poids	co2
PANDA	54	1108	150	354	159	154	860	135
TWINGO	60	1149	151	344	163	143	840	143
YARIS	65	998	155	364	166	150	880	134
CITRONC2	61	1124	158	367	166	147	932	141
CORSA	70	1248	165	384	165	144	1035	127
FIESTA	68	1399	164	392	168	144	1138	117
CLIO	100	1461	185	382	164	142	980	113
P1007	75	1360	165	374	169	161	1181	153
MODUS	113	1598	188	380	170	159	1170	163
MUSA	100	1910	179	399	170	169	1275	146
GOLF	75	1968	163	421	176	149	1217	143
MERC_A	140	1991	201	384	177	160	1340	141
AUDIA3	102	1595	185	421	177	143	1205	168
CITRONC4	138	1997	207	426	178	146	1381	142
AVENSIS	115	1995	195	463	176	148	1400	155
VECTRA	150	1910	217	460	180	146	1428	159
PASSAT	150	1781	221	471	175	147	1360	197
LAGUNA	165	1998	218	458	178	143	1320	196
MEGANECC	165	1998	225	436	178	141	1415	191
P407	136	1997	212	468	182	145	1415	194
P307CC	180	1997	225	435	176	143	1490	210
PTCRUISER	223	2429	200	429	171	154	1595	235
MONDEO	145	1999	215	474	194	143	1378	189
MAZDARX8	231	1308	235	443	177	134	1390	284
VELSATIS	150	2188	200	486	186	158	1735	188
CITRONC5	210	2496	230	475	178	148	1589	238
P607	204	2721	230	491	184	145	1723	223
MERC_E	204	3222	243	482	183	146	1735	183
ALFA 156	250	3179	250	443	175	141	1410	287
BMW530	231	2979	250	485	185	147	1495	231

Goal: Identifying the set of objects with similar characteristics

We want that:

(1) The objects in the same group are more similar to each other

(2) Thant to those in other groups

For what purpose?

→ Identify underlying structures in the data

→ Summarize behaviors or characteristics

→ Assign new individuals to groups

→ Identify totally atypical objects

The aim is to detect the set of "similar" objects, called groups or clusters.

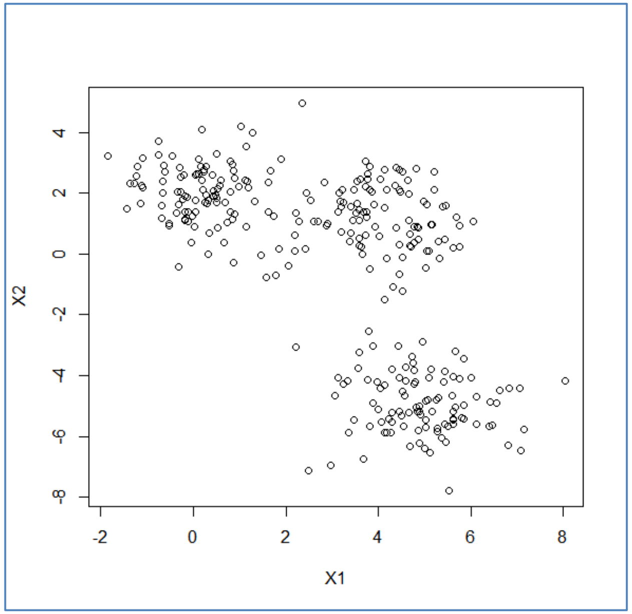
"Similar" should be understood as "which have close characteristics".

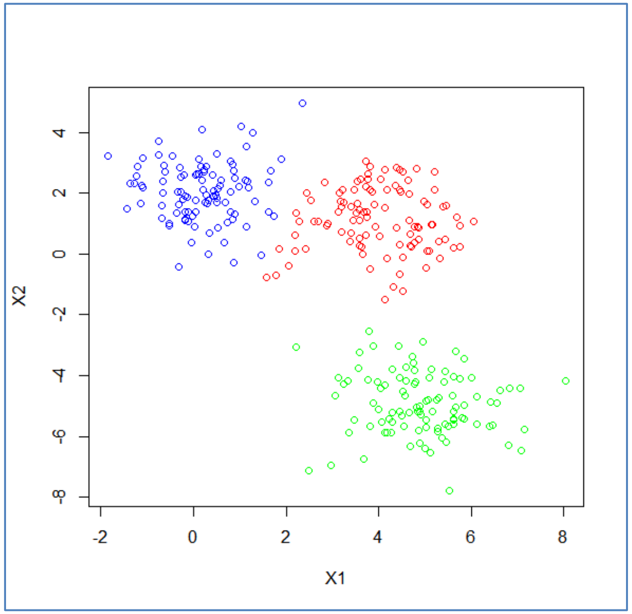
Cluster analysis

Example into a two dimensional representation space

We "perceive" the groups of instances (data points) into the representation space.

The clustering algorithm has to identify the “natural” groups (clusters) which are significantly different (distant) from each other.





2 key issues ⇨

1. Determining the number of clusters
2. Delimiting these groups by machine learning algorithm

Characterizing the partition

Within-cluster sum of squares (variance)

Huygens theorem

$$\text{TOTAL.SS} = \text{BETWEEN-CLUSTER.SS} + \text{WITHIN-CLUSTER.SS}$$

$$\text{T} = B + W$$

$$\sum_{i=1}^{n} d^2(i,G) = \underbrace{\sum_{k=1}^{K} n_k d^2(G_k,G)} + \underbrace{\sum_{k=1}^{K}\sum_{i=1}^{n_k} d^2(i,G_k)}$$

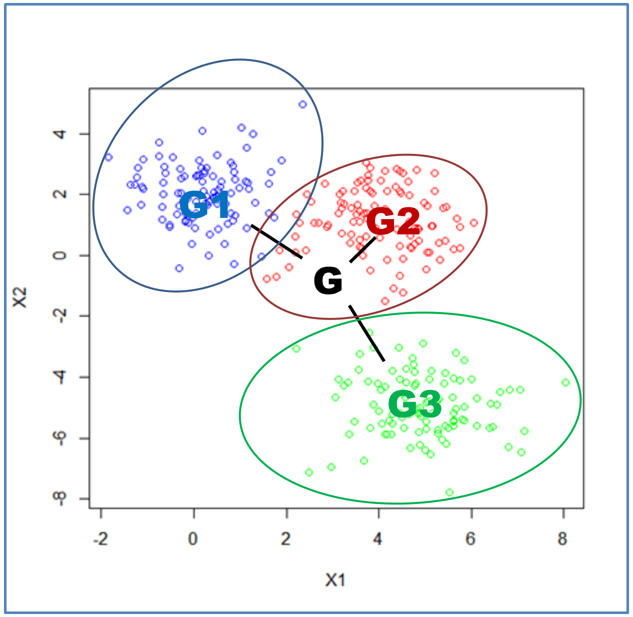
Dispersion of the clusters' centroids around the overall centroid.

Clusters separability indicator.

Dispersion inside the clusters.

Clusters compacity indicator.

Give crucial role to the centroids



Note: *Since the instances are attached to a group according to their proximity to their centroid, the shape of the clusters tends to be spherical.*

d() is a distance measurement characterizing the proximity between individuals. E.g. Euclidean distance or Euclidean distance weighted by the inverse of variance (pay attention to outliers)

The aim of the cluster analysis would be to minimize the within-cluster sum of squares (W), to a fixed number of clusters.

Partitioning-based clustering

Generic iterative relocation clustering algorithm

Main steps

- Set the number of clusters K
- Set a first partition of the data
- **Relocation.** Move objects (instances) from one group to another to obtain a better partition
- The aim (implicitly or explicitly) is to optimize some objective function evaluating the partitioning
- Provides an unique partitioning of the objects (unique solution)

But can be depending on other parameters such as the maximum diameter of the clusters. Remains an open problem often.

Often in a random fashion. But can also start from another partition method or rely on considerations of distances between individuals (e.g., the K most distant individuals from each other).

By processing all individuals, or by attempting to have random exchanges (more or less) between groups.

The within-cluster sum of squares (W) can be a relevant objective function

We have a unique solution for a given value of K. And not a hierarchy of partitions as for HAC (hierarchical agglomerative clustering) for example.

K-Means clustering algorithm

Each group is represented by its centroid

K-Means algorithm

Lloyd (1957), Forgy (1965), MacQueen (1967)

Iterative refinement technique

```
Input: X (n instances, p variables), K #groups

Initialize K centroids for the groups ($G_k$)

REPEAT

    Assignment. Assign each observation to the
    group with the closest centroid

    Update. Recalculate centroids from
    individuals attached to the groups

UNTIL Convergence

Output: A partition of the instances in K
groups characterized by their centroids Gk
```

Can be K randomly chosen individuals.
Or, K centroids calculated from a random partition of individuals in K groups.

MacQueen variation: Update the centroid for each processed individual. It accelerates the convergence, but the result depends on the order of the individuals.

Crucial property : the within-cluster sum of squares decreases at each step (when we update the centroids G_k)

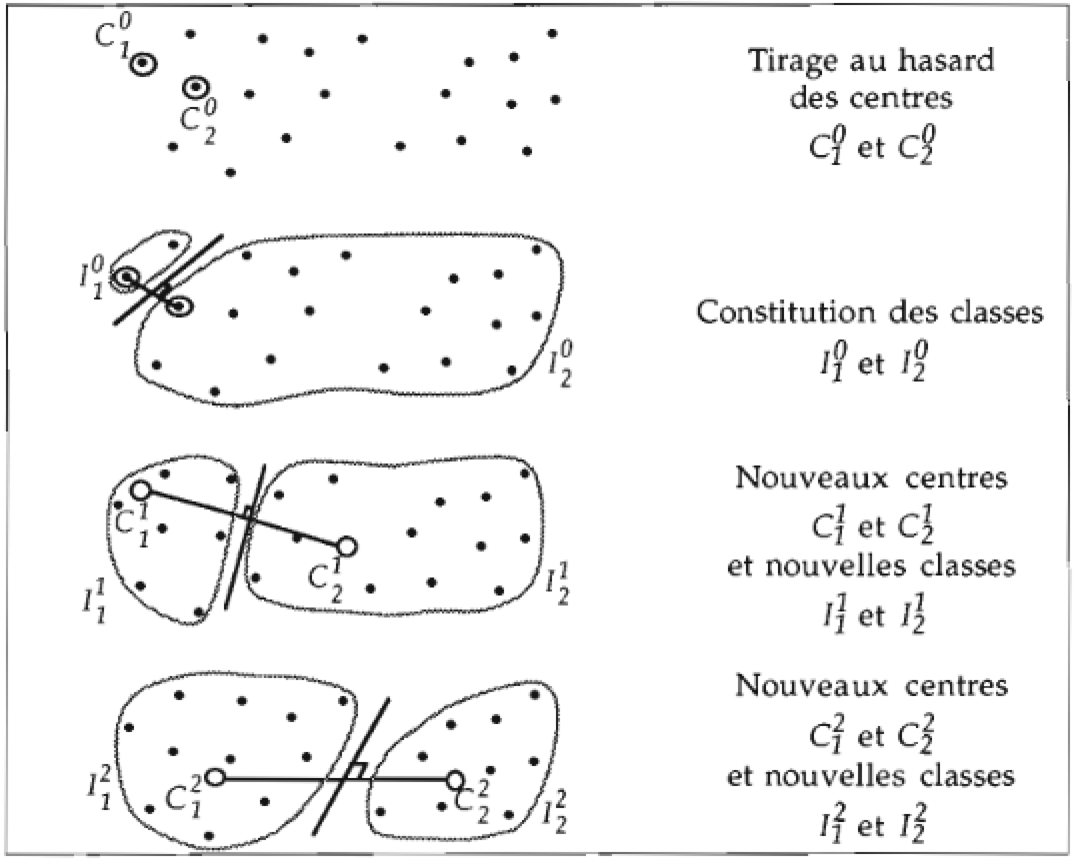
Fixed number of iterations
Or no assignment no longer change
Or when W does not decrease
Or when G_k are no longer modified

The approach minimizes implicitly the within-cluster sum of squares W

(A rewrite in the form of explicit optimization is possible. See Gan and al., p. 163)

K-Means algorithm

Example



Lebart et al., 1995 ; page 149.

K-Means approach

Pros and cons

Pros

Scalability: Ability to process very large dataset. Only the centroids coordinates must be stored in memory. Linear complexity according to the number of instances (no need to calculate the pairwise distance between the individuals).

Cons

But the computing time may be high because we can process many times each individual.

There is no guarantee that the algorithm reaches to the global optimum of W.

The solution depends on the initial values of the centroids.

Try several starting configurations and choose the one that results in a solution with the lowest W.

The solution may depend on the order of the individuals into the dataset (MacQueen variant)

Rearranging randomly the individuals before processing them in order to not be dependent on a predefined order of the observations into the database.

K-Means approach

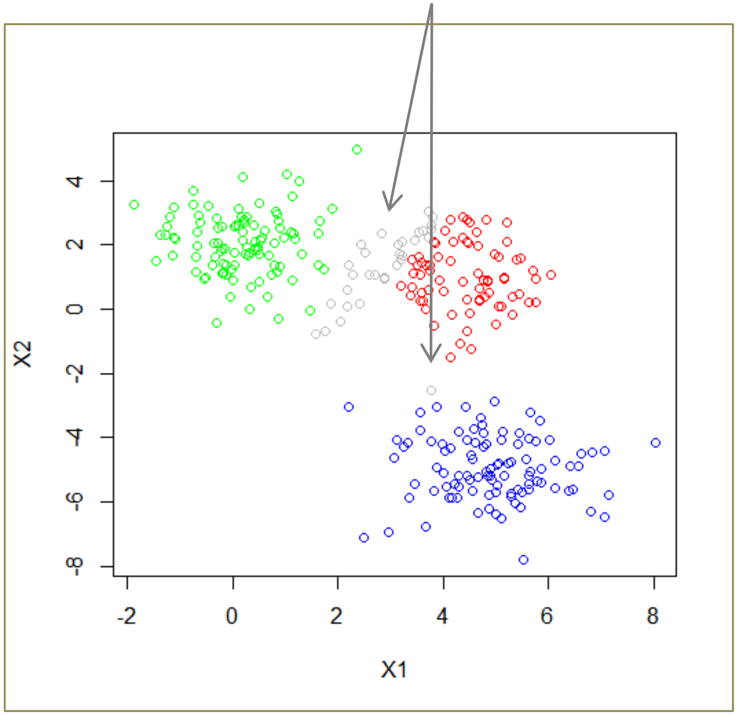
“Strong pattern” concept

Two (or more) executions of the algorithm on the same data can result in (slightly) different solutions. The idea is to combine them to observe the stable groupings, symptomatic of a real structuring of the data i.e. stable grouping = strong pattern.

		2ème exécution		
		C1	**C2**	**C3**
1ère exécution	**C1**	30	0	72
	C2	0	99	1
	C3	98	0	0

We observe the consistency between clusters. C3 for the 1st attempt corresponds to C1 for the 2nd one, etc.

The indecision areas (in grey) correspond to boundary zones between classes. "Weak pattern".

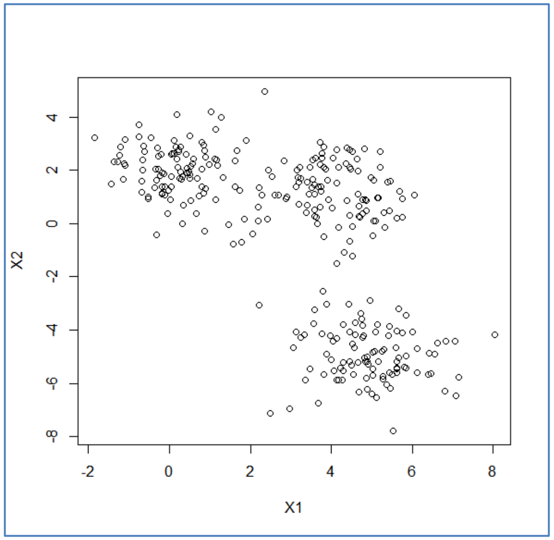


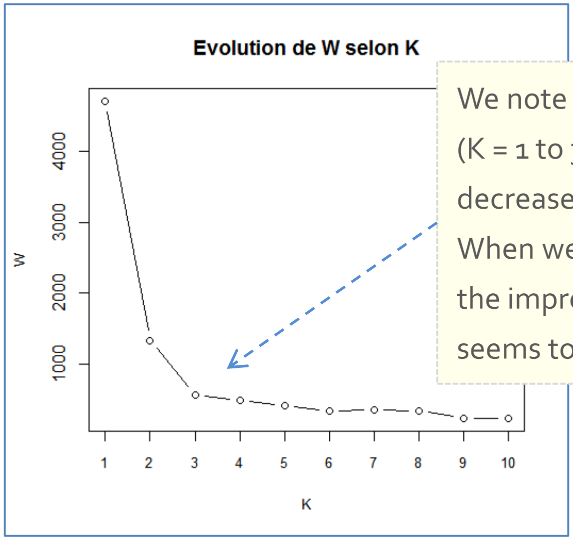
We can multiply executions and combinations, but the calculations become quickly intractable.

K-Means algorithm

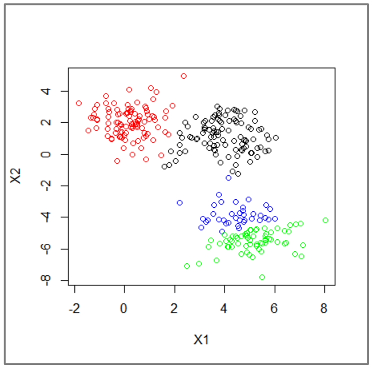
Determining the number of clusters – The elbow method

Principle: A simple strategy to identify the number of classes is to start K = 1 and increase K gradually. We analyze the evolution of within-cluster sum of squares (W). We have an "elbow" when the adding of an additional cluster does not decrease significantly W.





We note that for the first values of K (K = 1 to 3), the adding of a cluster decreases strongly the W criterion. When we move from K = 3 to K = 4, the improvement is low. K = 3 seems to be the right solution.

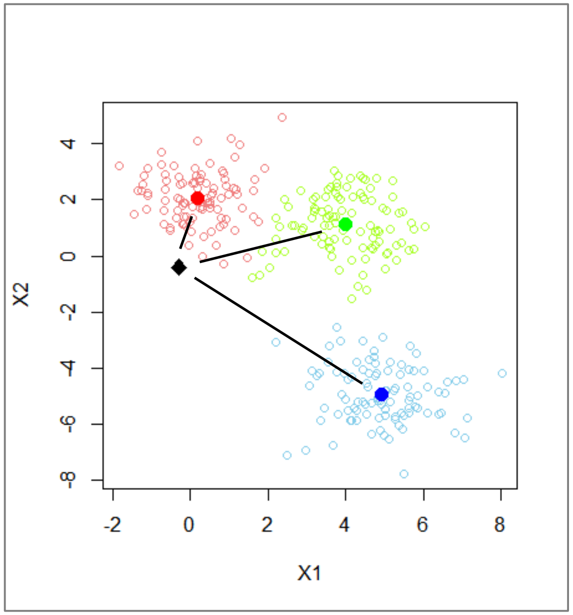


If we set K = 4 clusters, we observe that the additional subdivision is artificial.

K-Means approach

Deployment – Assigning a new instance to a cluster

Goal: Predicting the cluster membership of a new instance. The procedure must be consistent with the modeling approach.



In the sense of distance to conditional centroids, the new individual « ♦ » is assigned to the "red" cluster.

Solution 1: Assign the individual to the cluster of which the centroid is the closest. The approach is consistent with the k-means principle.

Solution 2 : Try to reproduce the assignment process using a supervised learning algorithm, among other things discriminant analysis. QDA (quadratic) or LDA (linear) if the clusters are of similar shapes.

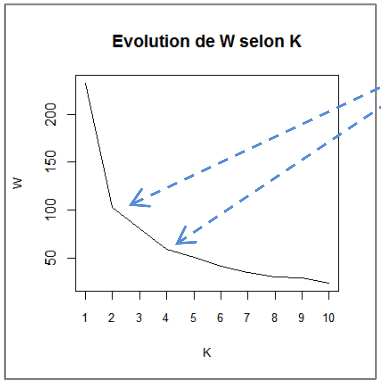
E.g. For our example dataset, QDA can assign perfectly the instances to the right cluster.

		Affectation QDA		
		C1	C2	C3
Classes K-Means	C1	102	0	0
	C2	0	100	0
	C3	0	0	98

Resubstitution confusion matrix

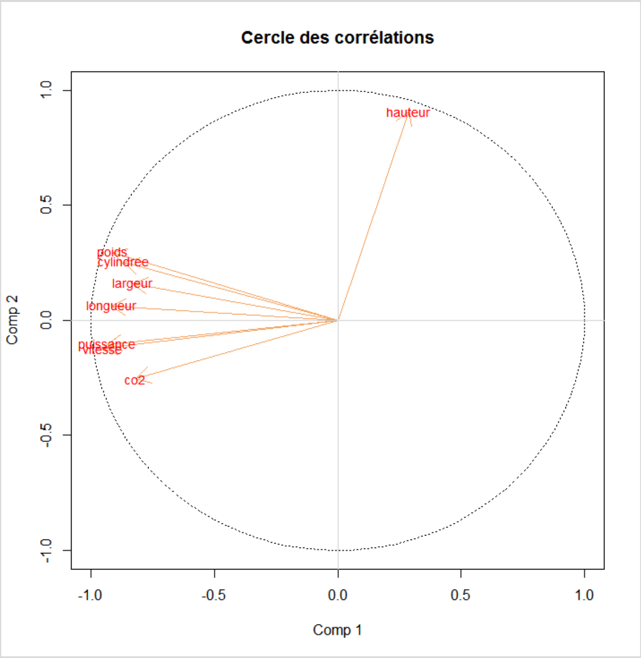
K-Means algorithm

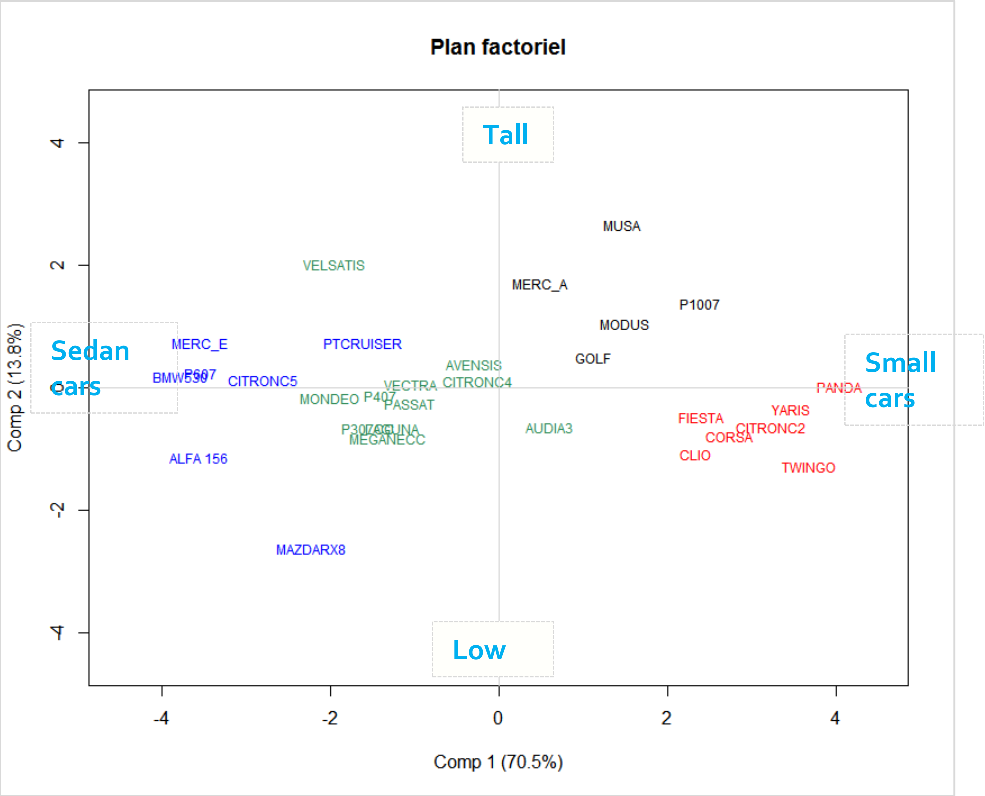
“Cars” dataset



K = 2 or K = 4 are possible partitions. We choose K = 4 because this solution will be confirmed by complementary analysis (PCA - principal component analysis).

The solution seems to consistent. But we see that there are singular cars (Vel Satis, Mazda RX8), and some associations ask questions (Golf among the multipurpose vehicle, PTCruiser among the sedans).





The correlation circle enables to understand the nature of the factors and, thus, the location of the cars (graph on the right…)

K-Means for categorical data

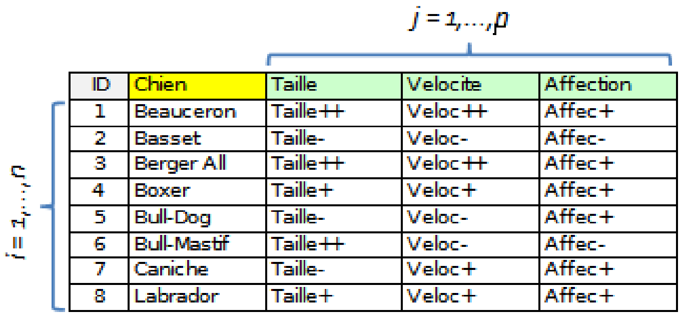
Strategy for the handling of categorical variables

CHI-squared distance (1)

Using dummy variables

A table of categorical variables can be transformed in a table of dummy variables, then in a table of frequencies (row profile).

Dog dataset (Tenenhaus, 2006 ; page 254)



ID	Chien	Taille	Velocite	Affection
1	Beauceron	Taille++	Veloc++	Affec+
2	Basset	Taille-	Veloc-	Affec-
3	Berger All	Taille++	Veloc++	Affec+
4	Boxer	Taille+	Veloc+	Affec+
5	Bull-Dog	Taille-	Veloc-	Affec+
6	Bull-Mastif	Taille++	Veloc-	Affec-
7	Caniche	Taille-	Veloc+	Affec+
8	Labrador	Taille+	Veloc+	Affec+

$$M = \sum_{j=1}^{p} m_j = 8$$

$m_1 = 3$ $m_2 = 3$ $m_3 = 2$

$p = 3$

$n = 8$

Chien	Taille-	Taille+	Taille++	Veloc-	Veloc+	Veloc++	Affec-	Affec+	Somme
Beauceron	0	0	1	0	0	1	0	1	3
Basset	1	0	0	1	0	0	1	0	3
Berger All	0	0	1	0	0	1	0	1	3
Boxer	0	1	0	0	1	0	0	1	3
Bull-Dog	1	0	0	1	0	0	0	1	3
Bull-Mastif	0	0	1	1	0	0	1	0	3
Caniche	1	0	0	0	1	0	0	1	3
Labrador	0	1	0	0	1	0	0	1	3
Somme	3	2	3	3	3	2	2	6	24

x_{ik}

$n_1 = 3$

$$\sum_{k=1}^{M} n_k = n \times p = 8 * 3 = 24$$

The distance between 2 individuals can be measured.

The centroid has a meaning, it is the "medium" profile.

The distance to the centroid (O) can also be measured.

$$\frac{x_{ik}}{p}$$

Chien	Taille-	Taille+	Taille++	Veloc-	Veloc+	Veloc++	Affec-	Affec+
Beauceron	0.000	0.000	0.333	0.000	0.000	0.333	0.000	0.333
Basset	0.333	0.000	0.000	0.333	0.000	0.000	0.333	0.000
Berger All	0.000	0.000	0.333	0.000	0.000	0.333	0.000	0.333
Boxer	0.000	0.333	0.000	0.000	0.333	0.000	0.000	0.333
Bull-Dog	0.333	0.000	0.000	0.333	0.000	0.000	0.000	0.333
Bull-Mastif	0.000	0.000	0.333	0.333	0.000	0.000	0.333	0.000
Caniche	0.333	0.000	0.000	0.000	0.333	0.000	0.000	0.333
Labrador	0.000	0.333	0.000	0.000	0.333	0.000	0.000	0.333
Profil moyen	0.125	0.083	0.125	0.125	0.125	0.083	0.083	0.250

Barycentre (O)

$$\frac{n_k}{n \times p}$$

Chi-squared distance (2)

Formulas

$$\frac{x_{ik}}{p}$$

Chien	Taille-	Taille+	Taille++	Veloc-	Veloc+	Veloc++	Affec-	Affec+
Beauceron	0.000	0.000	0.333	0.000	0.000	0.333	0.000	0.333
Basset	0.333	0.000	0.000	0.333	0.000	0.000	0.333	0.000
Berger All	0.000	0.000	0.333	0.000	0.000	0.333	0.000	0.333
Boxer	0.000	0.333	0.000	0.000	0.333	0.000	0.000	0.333
Bull-Dog	0.333	0.000	0.000	0.333	0.000	0.000	0.000	0.333
Bull-Mastif	0.000	0.000	0.333	0.333	0.000	0.000	0.333	0.000
Caniche	0.333	0.000	0.000	0.000	0.333	0.000	0.000	0.333
Labrador	0.000	0.333	0.000	0.000	0.333	0.000	0.000	0.333

Barycentre (O)

$$\frac{n_k}{n \times p}$$

Profil moyen	0.125	0.083	0.125	0.125	0.125	0.083	0.083	0.250

The differences between rare categories are intensified

$$d^2(beauceron, basset) = \sum_{k=1}^{M} \frac{1}{\frac{n_k}{n \times p}} \left(\frac{x_{1k}}{p} - \frac{x_{2k}}{p} \right)^2 = \frac{1}{0.125}(0.000 - 0.333)^2 + \cdots + \frac{1}{0.250}(0.333 - 0.000)^2 = 5.778$$

$$d^2(basset, O) = \frac{1}{0.125}(0.333 - 0.125)^2 + \frac{1}{0.083}(0.333 - 0.083)^2 + \cdots + \frac{1}{0.250}(0.000 - 0.250)^2 = 2.111$$

"Basset" is closer to "medium dog" than "beauceron".

K-Means algorithm

With the chi-squared distance

The algorithm remains the same but…

```
Input: X (n instances, p variables), K #groups

Initialize K centroids for the groups ($G_k$)

REPEAT

    Assignment. Assign each observation to the
    group with the closest centroid

    Update. Recalculate centroids from
    individuals attached to the groups

UNTIL Convergence

Output: A partition of the instances in K
groups characterized by their centroids $G_k$
```

Using the chi-squared distance

The centroid of the cluster is the "medium profile"

K-Modes algorithm

Another approach for dealing with categorical data

Principle: (1) Defining a distance measure adapted to categorical variables. (2) A cluster is represented by a synthetic profile defined by the modal values for each variable.

```
Input: X (n obs., p variables), K #classes

Initialize K representative individuals of the
clusters $M_k$ (by choosing K individuals randomly)

REPEAT

    Allocation. Assign each observation to the
    group with the closest centroid

    Update. Recalculate the modes $M_k$ for each
    cluster

UNTIL Convergence

Output: A partition of the individuals in K groups
characterized by their modes $M_k$
```

$$d(i,i') = \sum_{j=1}^{p} \delta\left(v_{ij}, v_{i'j}\right), \text{ où } \delta(i,i') = \begin{cases} 0 \; si \; v_{ij} = v_{i'j} \\ 1 \; si \; v_{ij} \neq v_{i'j} \end{cases}$$

Formula for the distance measurement between pairs of individuals (v_{ij} *is the value for the individual i and the variable* V_j)

The description of the representative individual M_k is based on the modal values for each variable (for the individuals belonging to the cluster).

Example

Chien	Taille	Velocite	Affection	Agressivite
Basset	Taille-	Veloc-	Affec-	Agress+
Bull-Dog	Taille-	Veloc-	Affec+	Agress-
Caniche	Taille-	Veloc+	Affec+	Agress-
Chihuahua	Taille-	Veloc-	Affec+	Agress-
Cocker	Taille+	Veloc-	Affec+	Agress+

Représentant	**Taille-**	**Veloc-**	**Affec+**	**Agress-**

Note: We have to be careful. The results can be very unstable. The mode – and thus the description of the representative individual – can be modified with one or two individuals in more or less into the clusters.

Minimization of a criterion similar to W

$$Q = \sum_{k=1}^{K} \sum_{i=1}^{n_k} d(i, M_k)$$

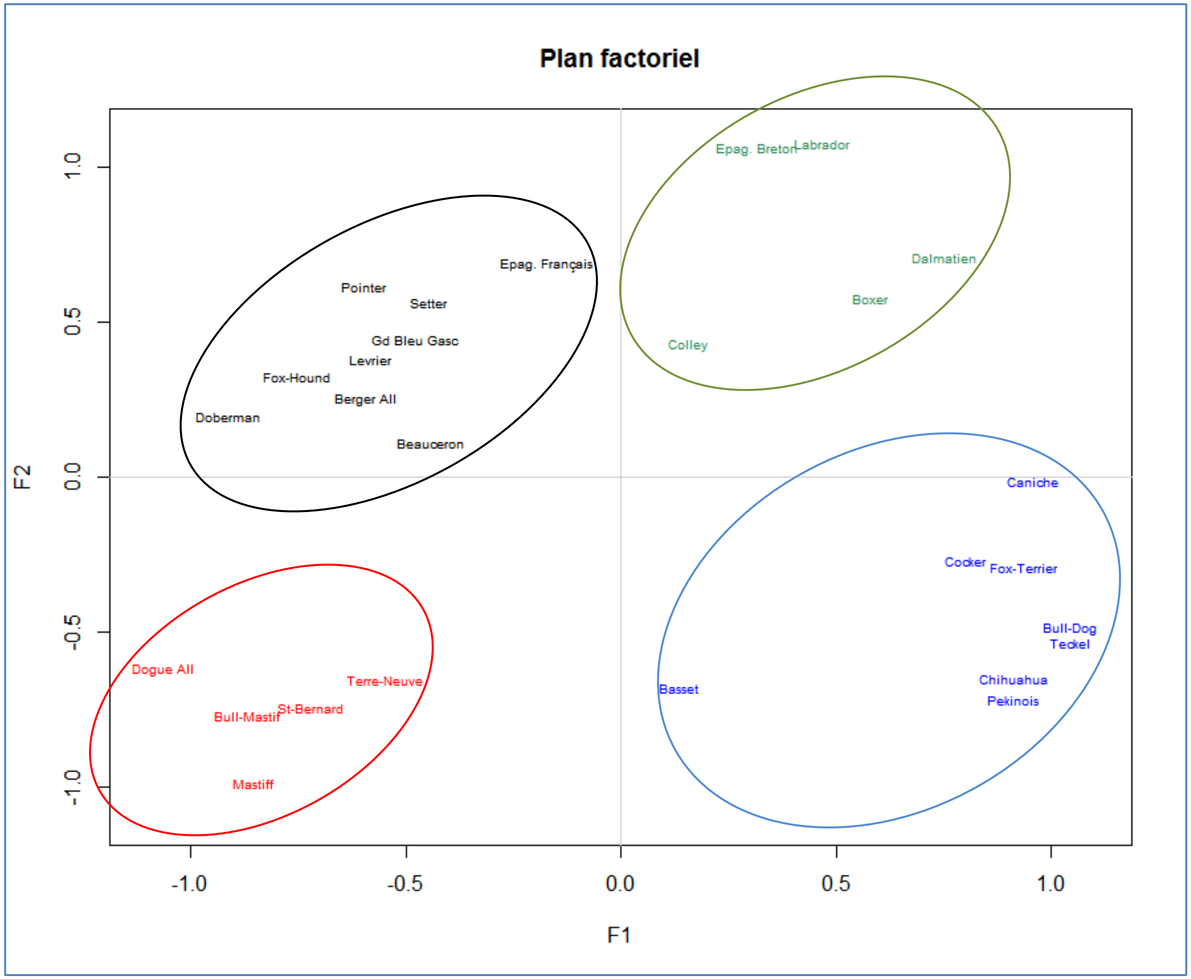
Tandem Analysis

Factor analysis + clustering

Principle: Using a dimensions-reduction technique (multiple correspondence analysis for categorical variables) to create a new representation space with numeric variables. Performing the k-means from these variables. The approach can be extended to a mix of numeric and categorical variables with the factor analysis for mixed data.

"Dog" dataset (Tenenhaus, 2006 ; page 254)

The 4 clusters in the representation space defined by the two-first factors of multiple correspondence analysis.



Note: Using only a small number of factors enables to remove the "noise" of the data. But the number of factors to retain becomes an additional parameter of the algorithm.

Fuzzy C-Means

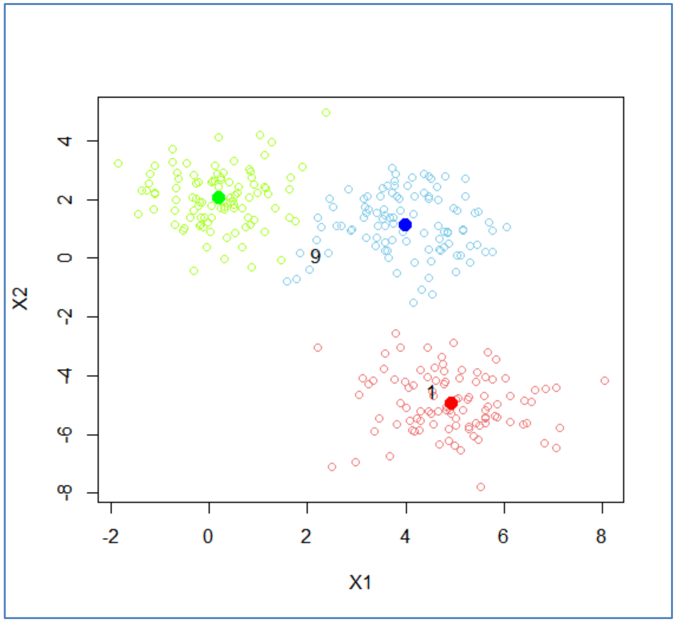
Instead of each data point belongs to an unique cluster (crisp or hard clustering), it can potentially belongs to multiple clusters to varying degrees (fuzzy or soft clustering)

Fuzzy C-Means

Cluster membership indicator

Issue: K-means approach necessarily assigns a data point at an unique cluster. All would have the same credibility. This is questionable for some individuals for which the distances to two or more centroids are very similar.

Solution: Introduce a cluster membership indicator.



For data points "1" and "9", we note that depending on the distance from the centroids, the degree of membership to the clusters may differ.

E.g.

N° point	Bleu	Rouge	Vert
1	0.011	0.983	0.006
9	0.472	0.105	0.423

How to proceed to get this kind of indicator?

It must act during the prediction of the cluster membership, but also during the modeling to “smooth” the construction of the clusters (weighting of the calculation of centroids)

Knowing that it is always possible to carry out a "crisp" assignment by taking the max of the level of membership.

Fuzzy C-Means

Algorithme (Dunn, 1973 ; Bezdek, 1981)

Principle: Introducing a table of cluster membership Ω of dimension (n x K) [n number of observations, K number of clusters].

➔ The values of Ω are defined between `[0 ; 1]`, the sum for each row (individual) is equal to 1.

```
Input: X (n obs., p variables), K #classes

Initialize randomly the values of the Ω matrix

REPEAT

      Representation. Calculate the centroids G_k
      by taking into account the cluster
      membership

      Update. Recalculate the cluster
      membership for each individual

UNTIL Convergence

Output: A table with, for each individual, a
vector measuring the clusters membership
```

$$G_{kj} = \frac{\sum_{i=1}^{n} \omega_{ik}^{m} x_j}{\sum_{i=1}^{n} \omega_{ik}^{m}}$$

The value of j (j = 1,…, p ; number of variables) of the centroid coordinates G_k

$$\omega_{ik} = \frac{1}{\sum_{l=1}^{K} \left(\frac{\|x_i - G_k\|}{\|x_i - G_l\|} \right)^{\frac{2}{m-1}}}$$

*To obtain ω_{ik} the degree of membership of the cluster **k** for the individual n°**i**, we compare its distance to G_k with its distance to the other centroids (G_l, l = 1…K)*

When the cluster membership matrix Ω is no longer substantially modified.

Minimization of a criterion similar to W

$$Q = \sum_{i=1}^{n} \sum_{k=1}^{K} \omega_{ik}^{m} \times \|x_i - G_k\|^2$$

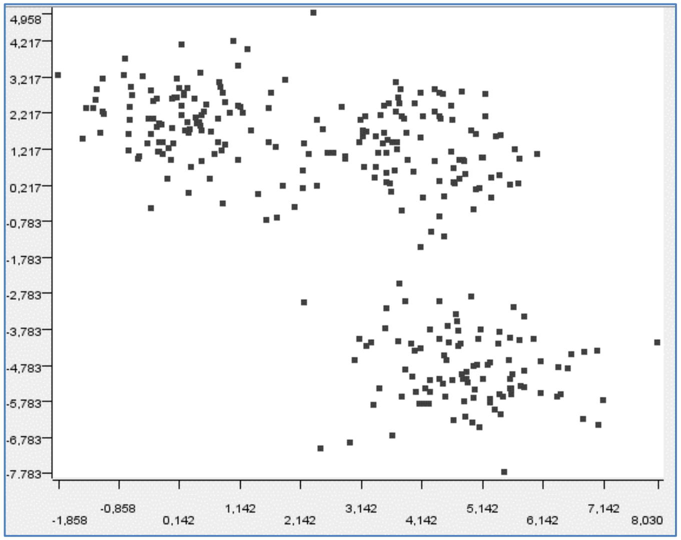
The « *fuzzifier* » parameter (**m** , m ≥ 1) determines the level of cluster fuzziness. The higher is m, the smoother is the clusters membership. Conversely, m= 1, we have the "crisp" K-Means (ω_{ik} = 0 or 1). In the absence of experimentation or domain knowledge, m is commonly set to 2

!

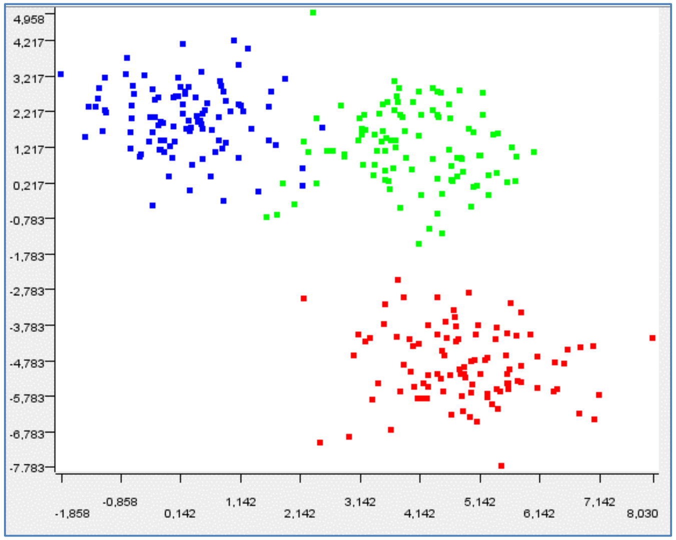
Fuzzy C-Means

Example into two dimensional representation space

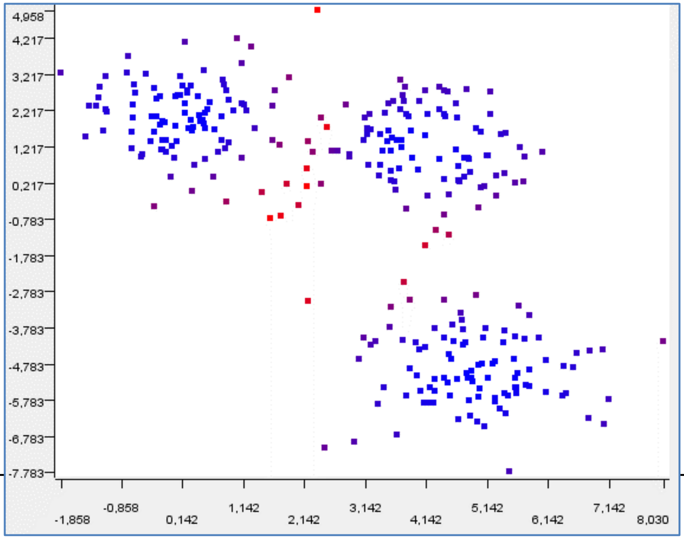
Example of data points



Fuzzy c-means knows how to build a "crisp" partition by associating each individual to the cluster maximizing the degree of membership.

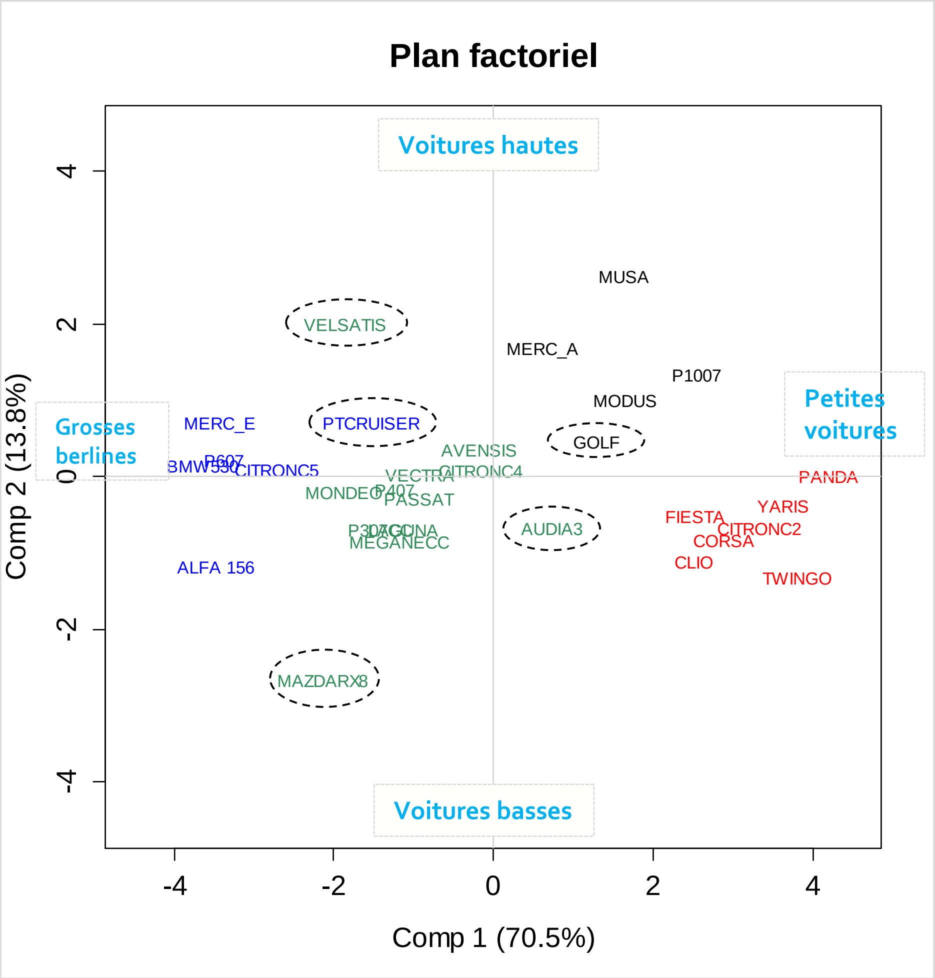


But it knows to put in perspective the results. Here, we distinct the high level of membership (≈ 1, blue points) and the low level of membership (≈ 1/3, red points).



Fuzzy C-Means

Cars dataset



Results of Fuzzy C-Means in the first two-dimensional representation space of principal component analysis (PCA). We observe that "Mazda RX8" belong to another cluster here, compared with the crisp K-Means.

We note that the membership of some cars to their cluster is not really clear (VELSATIS, MAZDA RX8, PT CRUISER, GOLF, AUDI A3). We understand why when we perform a PCA (Figure opposite).

Modele	cluster_0	cluster_1	cluster_2	cluster_3	Winner	MAX
P607	0.870	0.023	0.013	0.094	cluster_0	**0.870**
MERC_E	0.718	0.061	0.035	0.186	cluster_0	**0.718**
CITRONC5	0.878	0.020	0.011	0.091	cluster_0	**0.878**
PTCRUISER	0.409	0.187	0.081	0.323	cluster_0	**0.409**
BMW530	0.845	0.032	0.019	0.105	cluster_0	**0.845**
ALFA 156	0.613	0.094	0.065	0.228	cluster_0	**0.613**
GOLF	0.080	0.422	0.271	0.227	cluster_1	**0.422**
P1007	0.033	0.701	0.202	0.065	cluster_1	**0.701**
MUSA	0.052	0.755	0.106	0.087	cluster_1	**0.755**
MODUS	0.013	0.909	0.049	0.029	cluster_1	**0.909**
MERC_A	0.063	0.725	0.082	0.130	cluster_1	**0.725**
PANDA	0.033	0.172	0.736	0.059	cluster_2	**0.736**
TWINGO	0.020	0.074	0.866	0.039	cluster_2	**0.866**
CITRONC2	0.003	0.017	0.973	0.007	cluster_2	**0.973**
YARIS	0.012	0.067	0.897	0.025	cluster_2	**0.897**
FIESTA	0.028	0.129	0.775	0.068	cluster_2	**0.775**
CORSA	0.008	0.035	0.939	0.018	cluster_2	**0.939**
CLIO	0.038	0.136	0.740	0.086	cluster_2	**0.740**
AUDIA3	0.097	0.245	0.230	0.428	cluster_3	**0.428**
AVENSIS	0.113	0.177	0.083	0.628	cluster_3	**0.628**
P407	0.074	0.032	0.017	0.877	cluster_3	**0.877**
CITRONC4	0.106	0.165	0.081	0.649	cluster_3	**0.649**
MONDEO	0.288	0.113	0.072	0.526	cluster_3	**0.526**
VECTRA	0.068	0.045	0.023	0.865	cluster_3	**0.865**
PASSAT	0.099	0.060	0.032	0.808	cluster_3	**0.808**
VELSATIS	0.351	0.191	0.077	0.381	cluster_3	**0.381**
LAGUNA	0.058	0.023	0.014	0.905	cluster_3	**0.905**
MEGANECC	0.106	0.041	0.026	0.826	cluster_3	**0.826**
P307CC	0.209	0.060	0.035	0.695	cluster_3	**0.695**
MAZDARX8	0.355	0.135	0.116	0.395	cluster_3	**0.395**

Clustering of variables

Detecting subsets (clusters) of correlated variables

K-Means clustering around latent components

Vigneau & Qannari, 2003.

Objective: Highlight the underlying structures that organize the data. Detect redundancies and allow to reduce the dimensionality.

```
Input: X (n obs., p variables), K #classes

Initialize the clusters $C_k$ with K variables chosen randomly

REPEATE

    Allocation. Assign each variable to the nearest
    cluster i.e. that minimizes its distance to the
    representative variable characterizing the cluster

    Update. Recalculate the synthetic variable which is
    used as representative variable ($U_k$ = latent component)

Until Convergence

Output: A partition of the variables in K groups
characterized by the latent variables $U_k$
```

The square of the correlation coefficient r² may be used as similarity measure. Thus, the distance can be measured with (1 – r²).

We use the 1st component U_k of the PCA as representative variable of the cluster n°k of p_k variables. Indeed U_k is such that it maximizes

$$\lambda_k = \sum_{j=1}^{p_k} r^2\left(X_j, U_k\right)$$

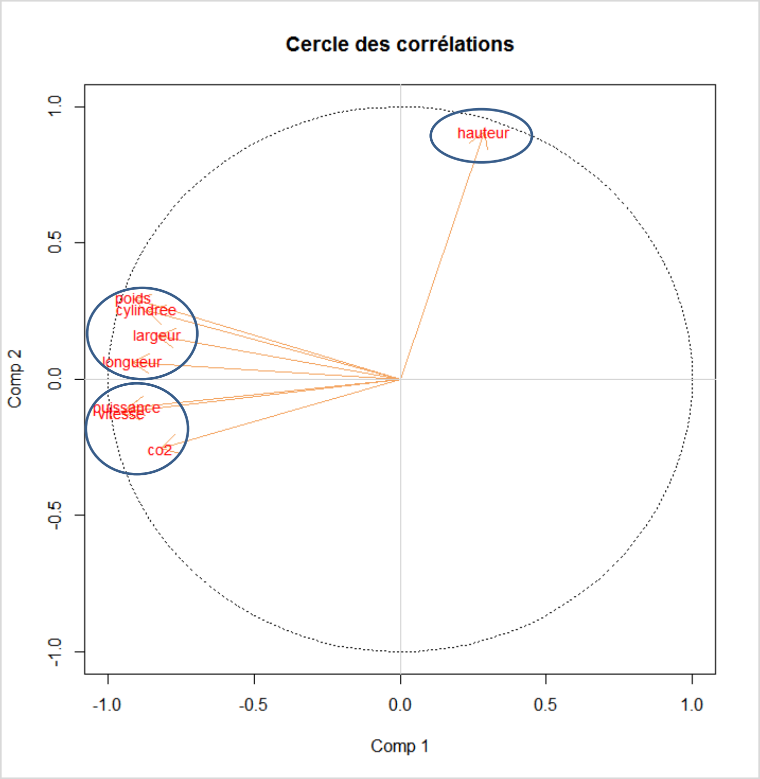
λ_k is computed by the diagonalization of the correlation matrix.

The 1st main component (**latent component**, latent variable) of the PCA is the best summary that one can have of a group of variables (like the centroid in the space of the individuals). !

Clustering variables

Processing “Cars dataset” with Tanagra – 3 clusters

Variable factor map (Two first dimensions)

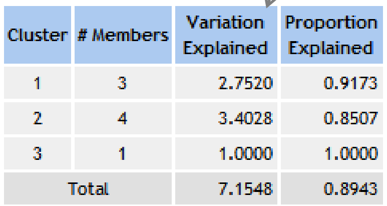


Cluster 1 and Cluster 2 are close with regard to the correlations.

Eigen value related to the 1st component of the cluster

Quality of the representation of the cluster by its 1st component (λ_k/p_k). It states the compacity of the cluster.

Cluster summary

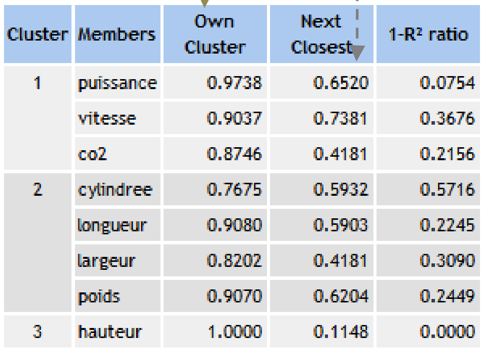


Cluster	# Members	Variation Explained	Proportion Explained
1	3	2.7520	0.9173
2	4	3.4028	0.8507
3	1	1.0000	1.0000
Total		7.1548	0.8943

Squared correlation of the variable with the latent component of its group.

The highest squared correlation of the variable with the other latent components.

Cluster members and R-square values

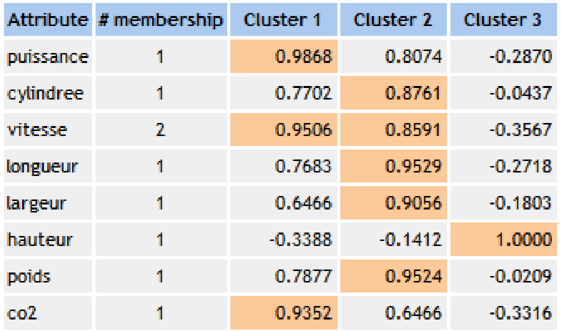


Cluster	Members	Own Cluster	Next Closest	1-R² ratio
1	puissance	0.9738	0.6520	0.0754
	vitesse	0.9037	0.7381	0.3676
	co2	0.8746	0.4181	0.2156
2	cylindree	0.7675	0.5932	0.5716
	longueur	0.9080	0.5903	0.2245
	largeur	0.8202	0.4181	0.3090
	poids	0.9070	0.6204	0.2449
3	hauteur	1.0000	0.1148	0.0000

$$1 - R^2 ratio = \frac{1 - R^2\ own}{1 - R^2\ next}$$

Level of membership to its group. Good membership if (1-R²) ≈ 0 ; (1-R²) > 1 is bad.

Cluster correlations -- Structure



Attribute	# membership	Cluster 1	Cluster 2	Cluster 3
puissance	1	0.9868	0.8074	-0.2870
cylindree	1	0.7702	0.8761	-0.0437
vitesse	2	0.9506	0.8591	-0.3567
longueur	1	0.7683	0.9529	-0.2718
largeur	1	0.6466	0.9056	-0.1803
hauteur	1	-0.3388	-0.1412	1.0000
poids	1	0.7877	0.9524	-0.0209
co2	1	0.9352	0.6466	-0.3316

Correlation of each variable with the latent components of the groups (we observe the sign of the relation here).

Conclusion

- Partitioning clustering methods are often simple and efficient. K-Means is one the most popular approach.

- They can process large datasets but they may be slow because many accesses to the data are needed.
- K-Means approach produce clusters with particular shapes. They are spherical and have approximately the same size.
- The approach may be generalized to databases with categorical and mixed (categorical and numeric) variables.
- The approach may be generalized to clustering of variables.

- The choice of K remains an open issue.
- Summarizing the cluster with only the centroid is not always relevant (see EM algorithm, K-Medoids, etc.).

References

Some books, including state-of-the-art French books

Chandon J.L., Pinson S., « Analyse typologique – Théorie et applications », Masson, 1981.

Diday E., Lemaire J., Pouget J., Testu F., « Eléments d'analyse de données », Dunod, 1982.

Gan G., Ma C., Wu J., « Data Clustering – Theory, Algorithms and Applications », SIAM, 2007.

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Tutorials and other references

"Hierarchical agglomerative clustering", June 2017.

"Clustering variables", September 2014.

"Cluster analysis for mixed data", February 2014.

"Two-step clustering for handling large databases", June 2009.

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