Machine Learning

Module 8.1 - Unsupervised Learning: clustering

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Clusters

A **cluster** is a group of instances that share some common characteristics measured by the features. They are **similar**.

Unlike classification (supervised learning) where groups are already defined, clustering aims at finding groups that **do not exist a priori**.

Hierarchical clustering and partitioning

Two different approaches:

- Hierarchical clustering: methods based on a **dissimilarity matrix** (hierarchical clustering).
- Partitioning: methods based on the value of the features (K-Means, PAM).

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Concept

Hierarchical clustering algorithms

- Take a **dissimilarity matrix** as input: the features are used to compute dissimilarities between instances. The feature values are not by the algorithm strickly speaking.
- Can be of two types: **agglomerative** (e.g., AGNES) or **divisive** (not treated).

In agglomerative algorithm, once two instances are clustered, they cannot be separated.

AGNES

Accronym for **AGglomerative NESting**: a sequential algorithm:

1. To start each instance is a cluster in itself.
2. Merge the two closest clusters.
3. Repeat 2 until only one cluster remains.

To merge two clusters (2), we need a **linkage method**. To link two clusters, we need **dissimilarities**.

Dissimilarity

A **dissimilarity** between two instances with features x and x' is a function $d(\cdot, \cdot)$ such that

- Non-negativity: $d(x, x') \geq 0$,
- Nullity: $d(x, x') = 0$ iff $x = x'$,
- Symmetry: $d(x, x') = d(x', x)$,

If further it satisfies the triangle inequality,

$$d(x, x') + d(x', x'') \geq d(x, x''),$$

then it is called a **distance**

For numerical features

A general distance: **Minkowski**, $q \geq 1$

$$d(x, x') = \left(\sum_{j=1}^{p} |x_j - x'_j|^q \right)^{1/q}$$

Special cases:

- **Euclidean** for $q = 2$ (the most used),

$$d(x, x') = \sqrt{\sum_{j=1}^{p} (x_j - x'_j)^2}$$

- **Manhattan** for $q = 1$,

$$d(x, x') = \sum_{j=1}^{p} |x_j - x'_j|$$

- **Maximum distance** $q = \infty$,

$$d(x, x') = \max_{j=1,\ldots p} |x_j - x'_j|$$

Numerical features

Example on the `iris` data. The Euclidean distance between instances 1 and 2 is 0.54

```
> iris[1:2,-5]
  Sepal.Length Sepal.Width Petal.Length Petal.Width
1          5.1         3.5          1.4         0.2
2          4.9         3.0          1.4         0.2
> dist(iris[1:2, -5], p=2)
  0.5385165
```

In detail,

$$\sqrt{(5.1-4.9)^2+(3.5-3.0)^2+(1.4-1.4)^2+(0.2-0.2)^2}=0.54$$

Categorical and mixed features types

When categorical features are present in the data set, the **Gower index** can be used. It combines dissimilarities to build a global one:

$$d_{ij} = \frac{\sum_{k=1}^{p} w_k d_{ij,k}}{\sum_{k=1}^{p} w_k}$$

is the dissimilarity between instances i and j over the p features.

The weight w_k are always 1, except if $x_i k$ or $x_j k$ is missing, in which case it is 0. The dissimilarity $d_{ij,k}$ depends on the type of the feature x_k:

- Numerical:

  $$d_{ij,k} = |x_{ik} - x_{jk}|/r_k,$$

  where r_k is the range of variable k,
- Categorical: $d_{ij,k} = 1$ if $x_{ik} \neq x_{jk}$, $d_{ij,k} = 0$ if $x_{ik} = x_{jk}$.

Mixed features types

Example:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Color	Species
1	5.1	3.5	1.4	0.2	mauve	setosa
2	4.9	3.0	1.4	0.2	violet	setosa
3	4.7	3.2	1.3	0.2	violet	virginica

The ranges are respectively $3.6, 2.4, 5.9, 2.4$ (from the full data set).

$$
\begin{aligned}
d_{12} &= \frac{1}{6}\left(\frac{|5.1-4.9|}{3.6}+\frac{|3.5-3.0|}{2.4}+\frac{|1.4-1.4|}{5.9}+\frac{|0.2-0.2|}{2.4}+1+0\right)=0.2106.\\
d_{13} &= 0.3755\\
d_{23} &= 0.1926
\end{aligned}
$$

Linkage

Once the matrix of dissimilarities between all the instances is computed, we use **linkage** to merge the two clusters:

- **Single linkage**: For all pairs of clusters A and B, compute the smallest dissimilarity between each pair of cluster members,

$$d(A, B) = \min\{d(x, x') : x \in A,\ x' \in B\}$$

  Link A and B with the smallest $d(A, B)$.

- **Complete linkage**: For all pairs of clusters A and B, compute the largest dissimilarity between each pair of cluster members,

$$d(A, B) = \max\{d(x, x') : x \in A,\ x' \in B\}$$

  Link A and B with the smallest $d(A, B)$.

- **Ward**'s method: merges the two clusters A and B such that, after the merging, the total within variance is minimum[1].

[1] Other criteria are possible. Several algorithms exists (e.g., Ward 1963, Murtagh and Legendre 2014).

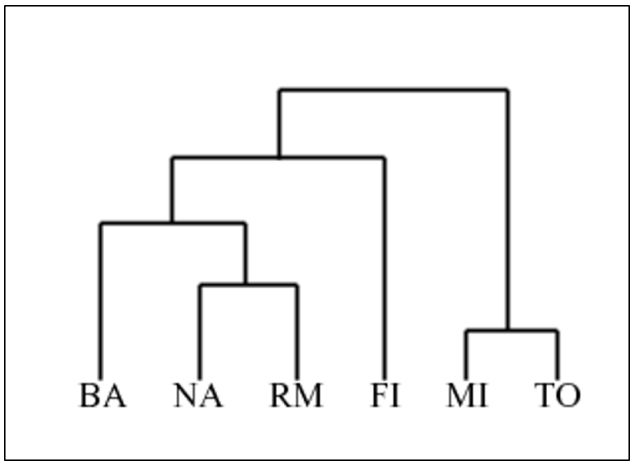
Dendrogram

The **dendrogram** is a graphical representation of the hierarchical clustering. It shows which clusters are grouped at each step k, together with the dissimilarity on the y-axis ate which they have been clustered.

Example

Italian cities: Bari, Firenze, Napoli, Roma, Torino.

	BA	FI	MI	NA	RM	TO
BA	0	662	877	255	412	996
FI	662	0	295	468	268	400
MI	877	295	0	754	564	138
NA	255	468	754	0	219	869
RM	412	268	564	219	0	669
TO	996	400	138	869	669	0



Source: `https://home.deib.polimi.it/matteucc/Clustering/tutorial_html/hierarchical.html`

Divisive hierarchical clustering

AGNES is **agglomerating** because it starts from individual points and run up to a unique cluster, merging clusters one after the other.

It is called "hierarchical" because when an instance is attached to a group, it cannot be separated from it anymore.

There also exist **divisive** hierarchical clustering, **DIANA**, for DIvise ANAlysis. It starts from one unique cluster with all the instances, and splits clusters one after the other, going down to one instance per cluster.

Divise clustering is considered complex because at each step there exist a lot of possibilities to split a cluster.

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Partitioning methods

Unlike the hierarchical clustering, **partitioning methods** apply for a given number of clusters.

From an initial assignment of instances to k clusters, the method allocates the instances to clusters such that a given criterion is optimized.

Two popular methods are

- The **K-means**.
- The **Partitioning Around the Medoid** (PAM).

K-means

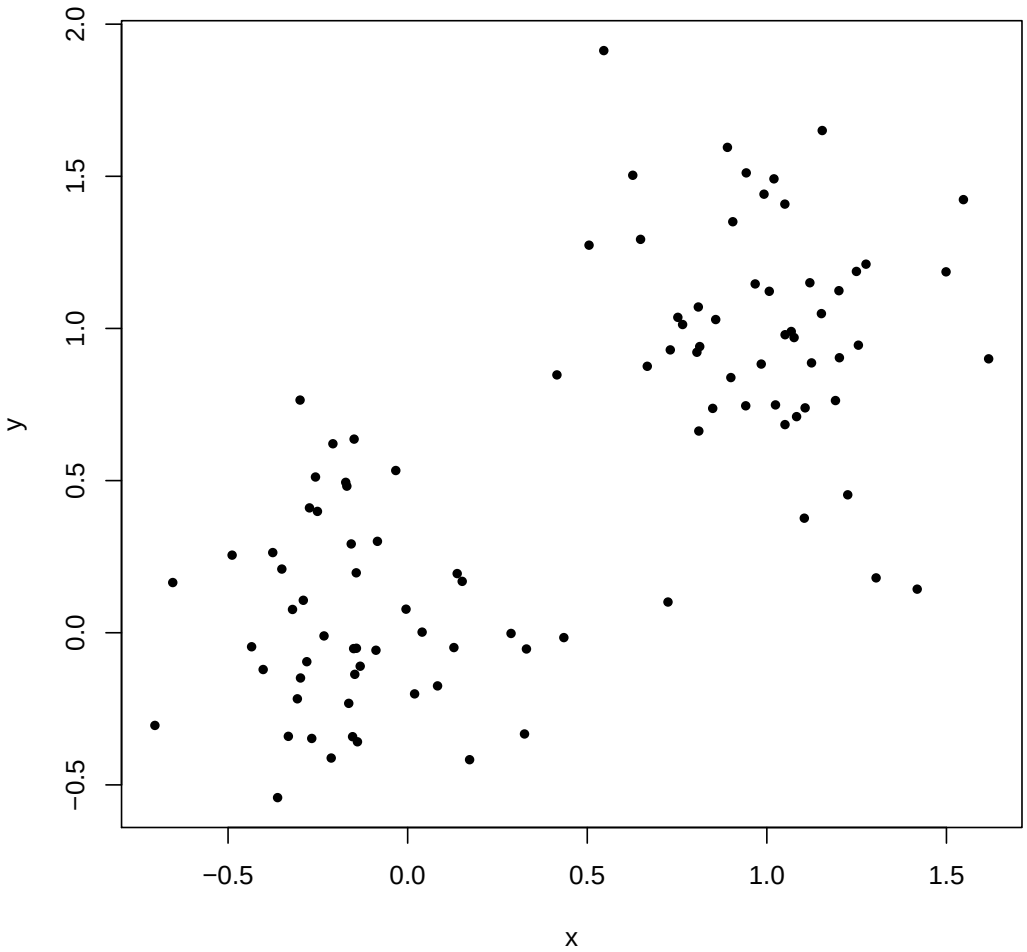
For k clusters:

1. The initial clustering is random: assign each instance to one cluster at random.
2. Compute the centers of the clusters.
3. Each instance is then re-assigned to the cluster with the closest center.
4. Step 2. and 3. are repeated until a convergence criterion is satisfied.

The K-means is suitable for **numerical features only**. The Euclidean distance is often used.

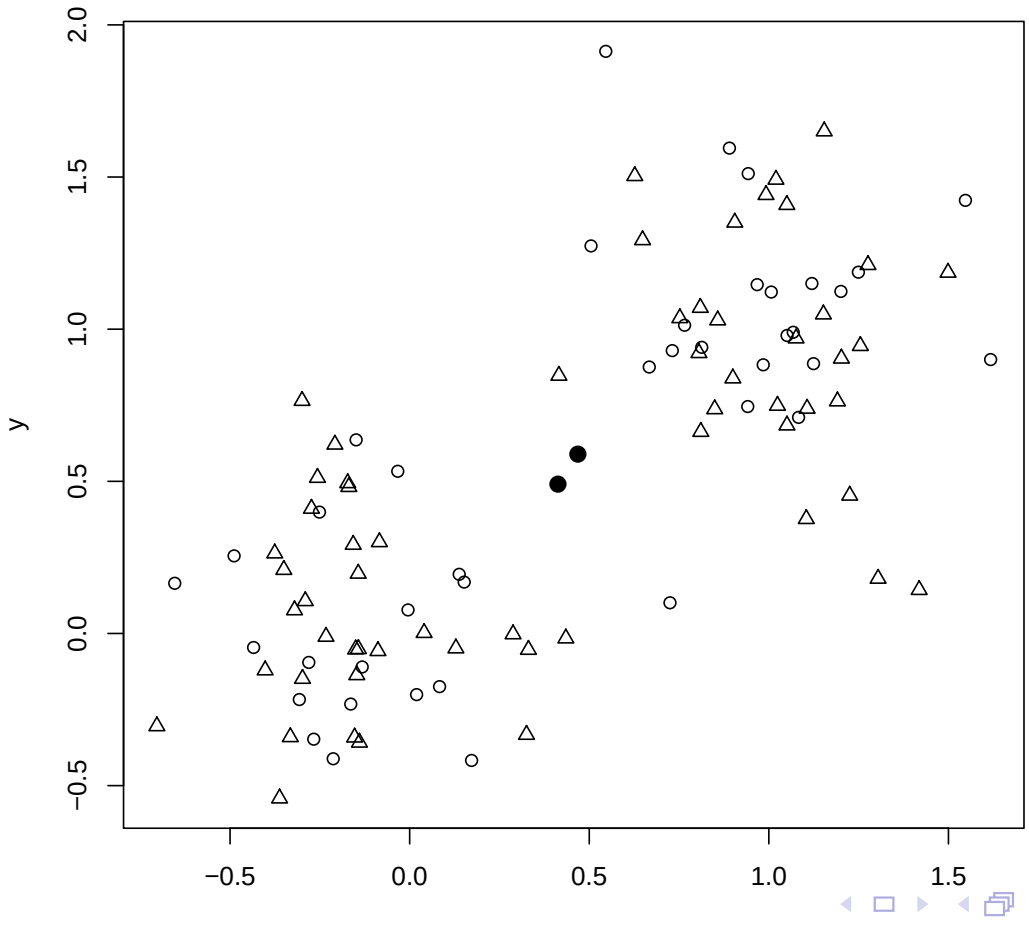
K-means

Illustration on simulated data, with $k = 2$. Below, the data ($p = 2$)



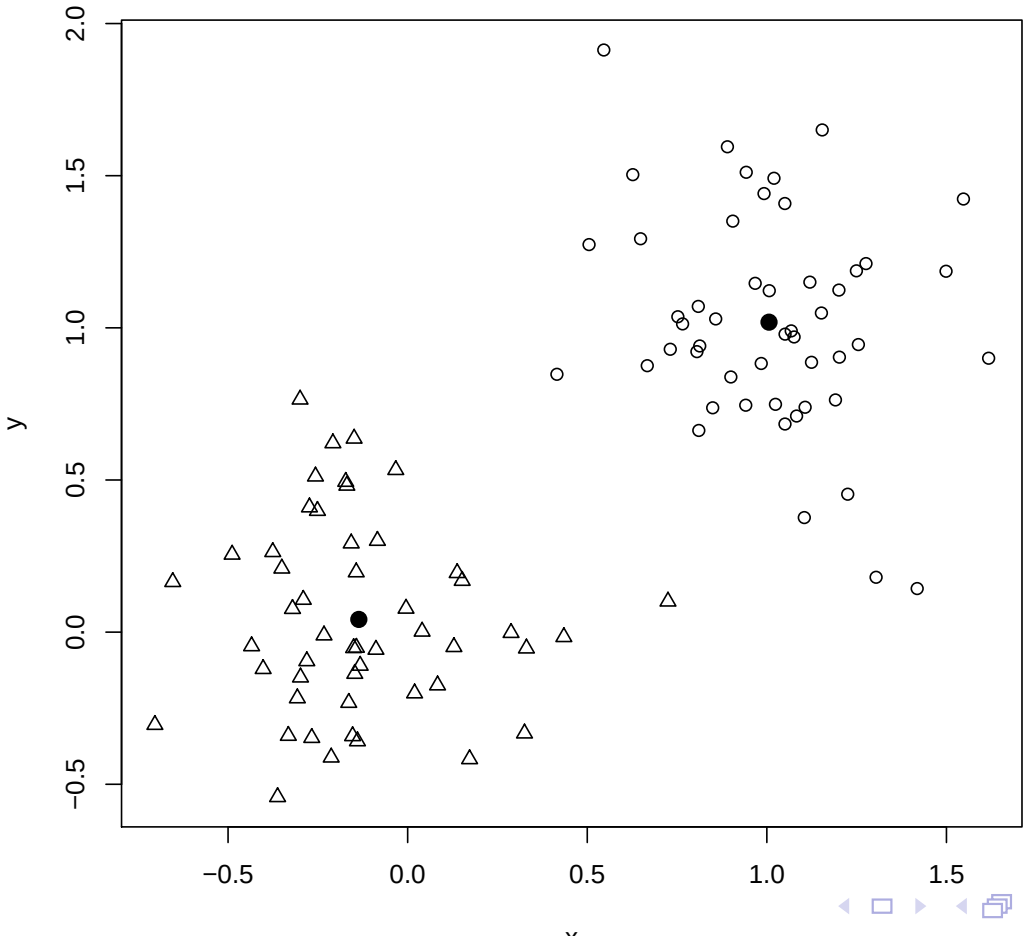
K-means

First step, each instance is randomly assigned (circles and triangles). The centers are computed (dots).



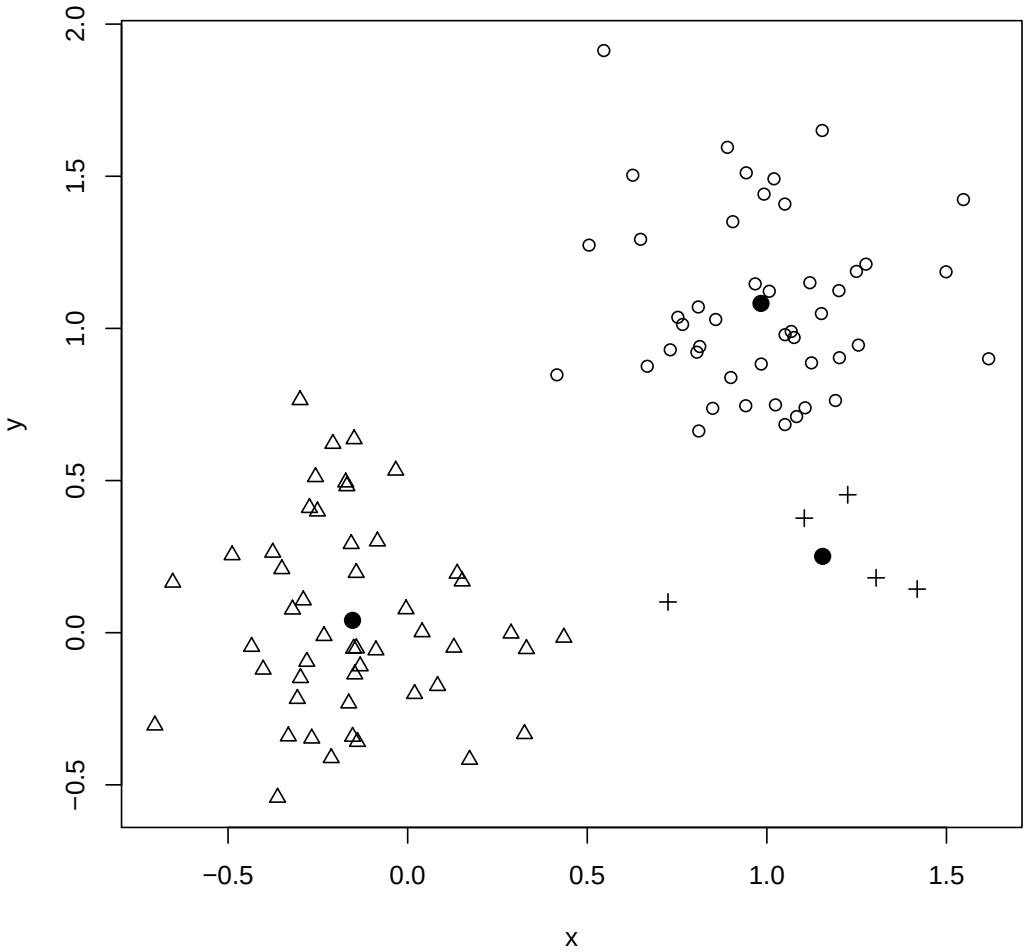
K-means

Next step, instances are re-assigned to the closest center. Then, new centers are computed. The clustering is already finished.



K-means

Illustration for $k = 3$ clusters.



Partitioning Around the Medoid

PAM extends the K-mean to **features of mixed types** (numerical and categorical) by extending the definition of the center of the cluster to **a medoid**.

The medoid of cluster is the most representative instance belonging to it.

The medoid of a cluster A is the instance with smallest sum of dissimilarities with the other instances in the cluster A:

$$m_A = \arg\min_{x \in A} \sum_{y \in A; y \neq x} d_{xy}$$

Unlike for the K-means, where the center is computed by averaging the features values (and thus may not be an instance of the data base), the medoid is an instance of its cluster.

Therefore, PAM can be used for numerical and categorical features.

Example

With the Italian cities, consider the cluster {BA, NA, RM}. Then the medoïd is NA. Indeed, the sum of dissimilarities are

- BA: $d_{BA,NA} + d_{BA,RM} = 255 + 412 = 667$
- NA: $d_{NA,BA} + d_{NA,RM} = 255 + 219 = 474$
- RM: $d_{RM,BA} + d_{RM,NA} = 212 + 219 = 631$

Thus NA is the most representative city of this cluster.

Note that the medoïd of cluster {MI, TO} is either MI or TO (at random).

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Choice or selection?

The number of clusters is often an **arbitrary choice** guided by the domain and the business application. This approach should be preferred if possible.

It is also possible to select of the number of clusters with an index. There are a lot of such index[2].

In this course, we see

- The **total within-cluster sum of squares** (TWSS),
- The **silhouette**.

In practice, the index is computed for a clustering with 1, 2, 3, etc., clusters and the best choice is made.

[2] There are 30 index available in the function `NbClust` in `R`.

Total within-cluster sum of squares

The sum of squares within cluster C, whose center (mean or medoid) is x_C, is the

$$W_C = \sum_{i \in C} \|x_i - x_C\|^2 = \sum_{i \in C} \sum_{j=1}^{p} (x_{ij} - x_{Cj})^2.$$

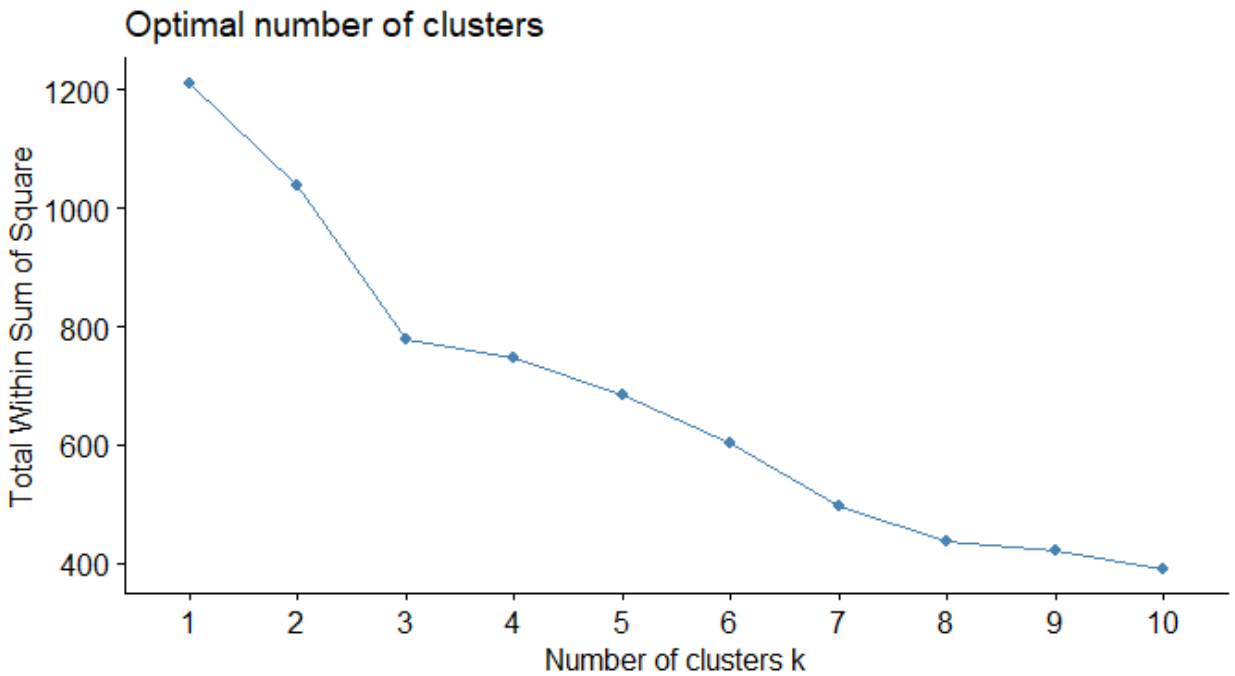
The TWSS is the sum of all W_k over the K clusters $C_1, \ldots, C_K$,

$$\sum_{k=1}^{K} W_{C_k}$$

The Each time a cluster is created ($K \to K+1$), TWSS diminishes. The number of clusters is selected at **an elbow** on the graph.

Example

Clustering on data with TWSS (dendrogram with complete linkage):



$k = 3$ is a good choice here.

Silhouette

The **silhouette** measures how "well" an instance is within its cluster.

Consider an instance x assigned to cluster C. Let $d(x, A)$ be **the dissimilarity from** x **to any cluster** A: the average dissimilarity between x and all the instances in cluster A:

$$d(x, A) = \frac{1}{|A|} \sum_{y \in A} d_{xy}.$$

In particular, $d(x, C)$ **is the dissimilarity from** x **to its cluster**.

A small $d(x, C)$ indicates a good clustering of x within its cluster C.

Silhouette

Now, consider $d(x, \bar{C})$, the smallest average dissimilarities from x to all the clusters to which it is not assigned (all but C):

$$d(x, \bar{C}) = \min_{A \neq C} d(x, A)$$

This measures how x is separated from the other clusters.

A large $d(x, \bar{C})$ indicates a good separation of x from all the other clusters (i.e., the ones in which x is not).

Silhouette

The silhouette of x combines

- $d(x, C)$, how well x is integrated to its cluster C, and
- $d(x, \bar{C})$, how well x is separated from the other clusters.

The silhouette of x is

$$s_x = \frac{d(x, \bar{C}) - d(x, C)}{\max\left\{d(x, \bar{C}), d(x, C)\right\}}$$

The denominator ensures that $-1 \leq s_x \leq 1$.

The larger s_x, the better the clustering of x in C.

Average silhouette

The **average silhouette** of all instances is taken as a measure of the **goodness of the clustering**:

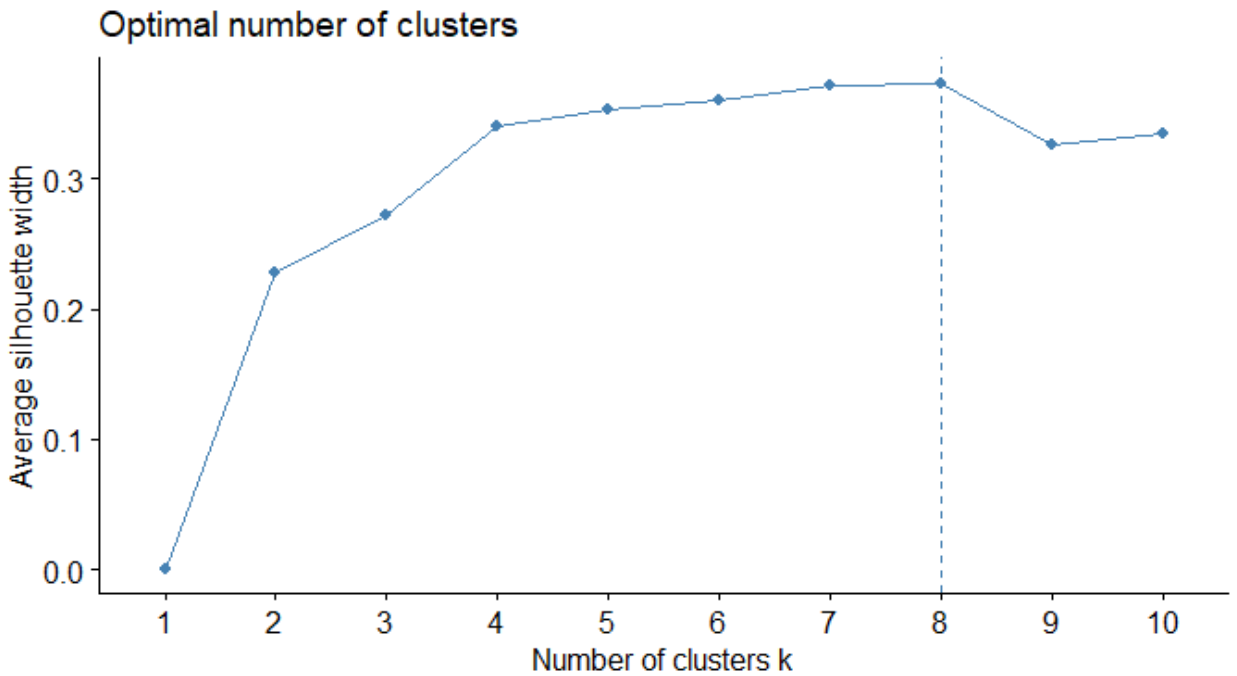
$$s = \frac{1}{n} \sum_{i=1}^{n} s_{x_i}.$$

The larger the average silhouette s, the better the clustering overall. The number of clusters k should maximize the average silhouette.

The average silhouette should not be interpreted for itself.

Example

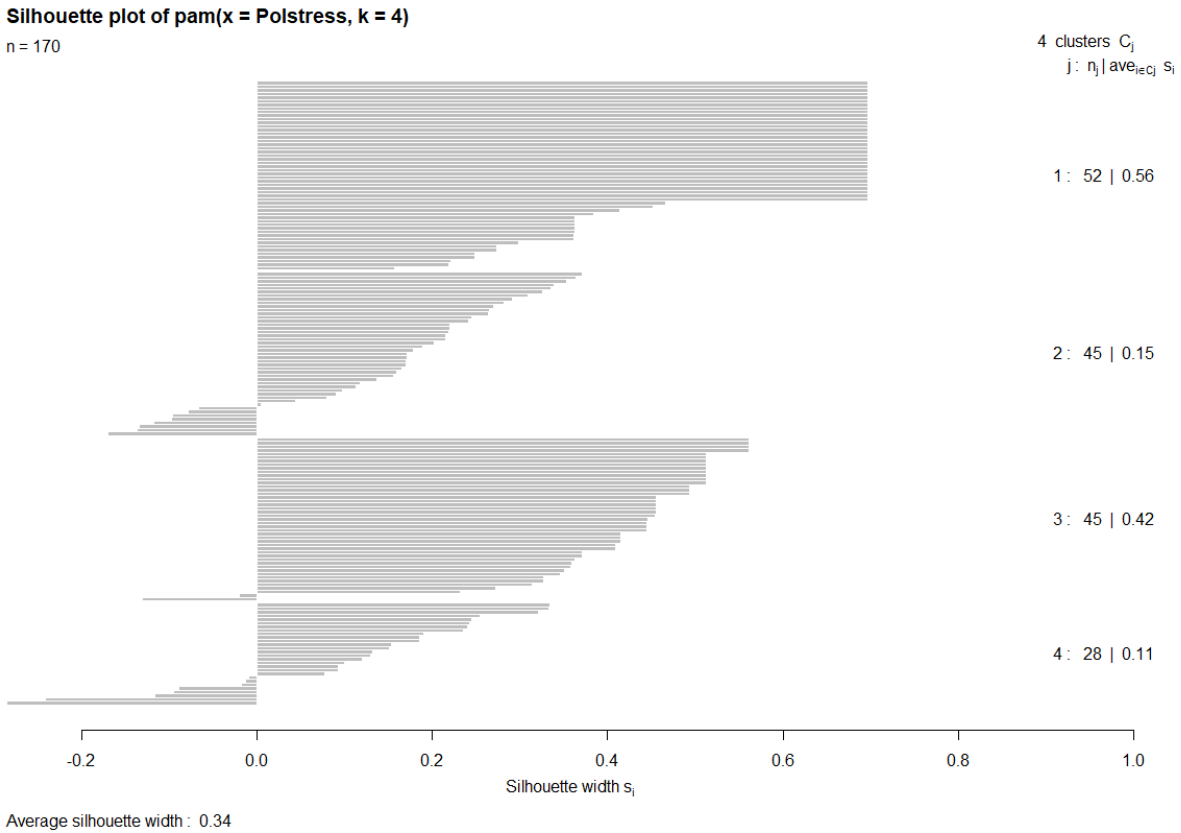
Clustering on data with average silhouette:



$k = 8$ is a good choice here.

Silhouette plot

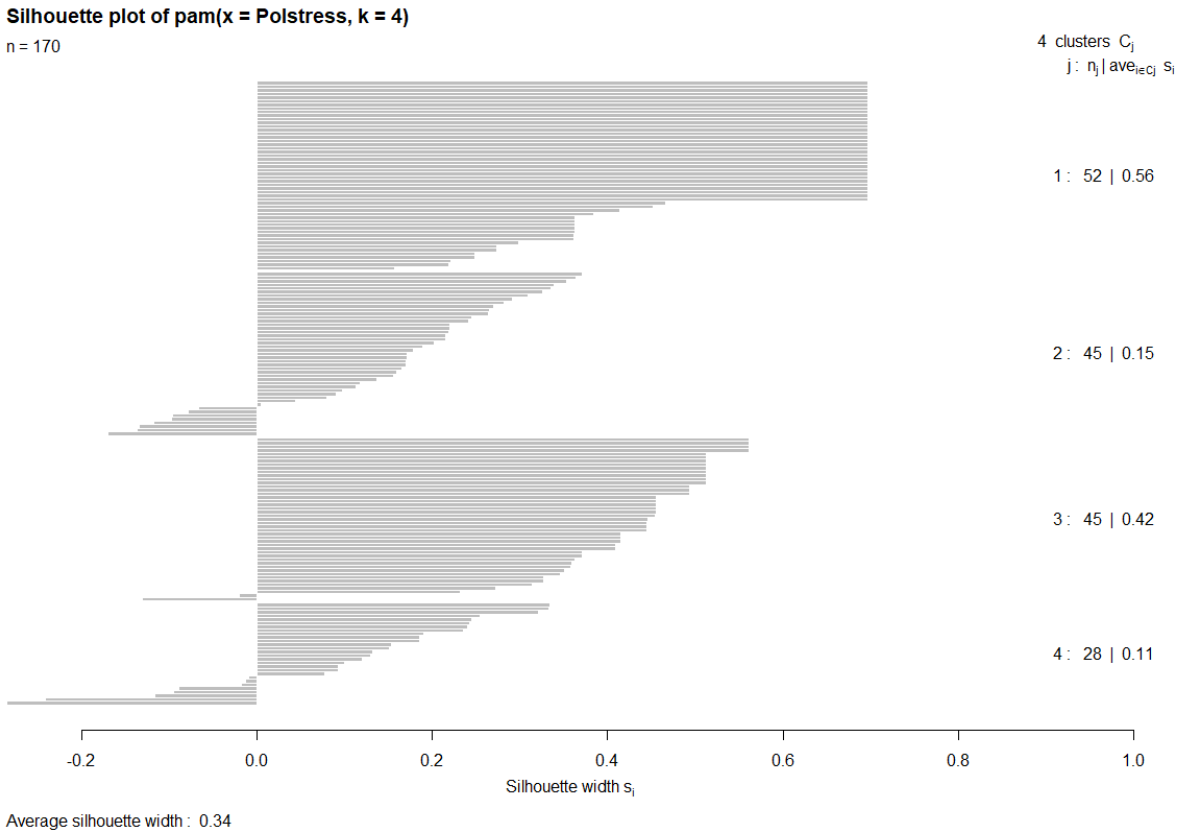
A detailed analysis of the clustering can be obtained using the **silhouette plot** shows: the silhouettes of all the instances.



Clusters 1 and 3 are well formed, Clusters 2 and 3 are less homogeneous.

Silhouette plot

Policemen - PAM $k = 4$



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Interpretation

What are the features behind: what feature/combination of features makes that an individual belong to a cluster.

A usual method consists of representing each feature against the clusters.

Example

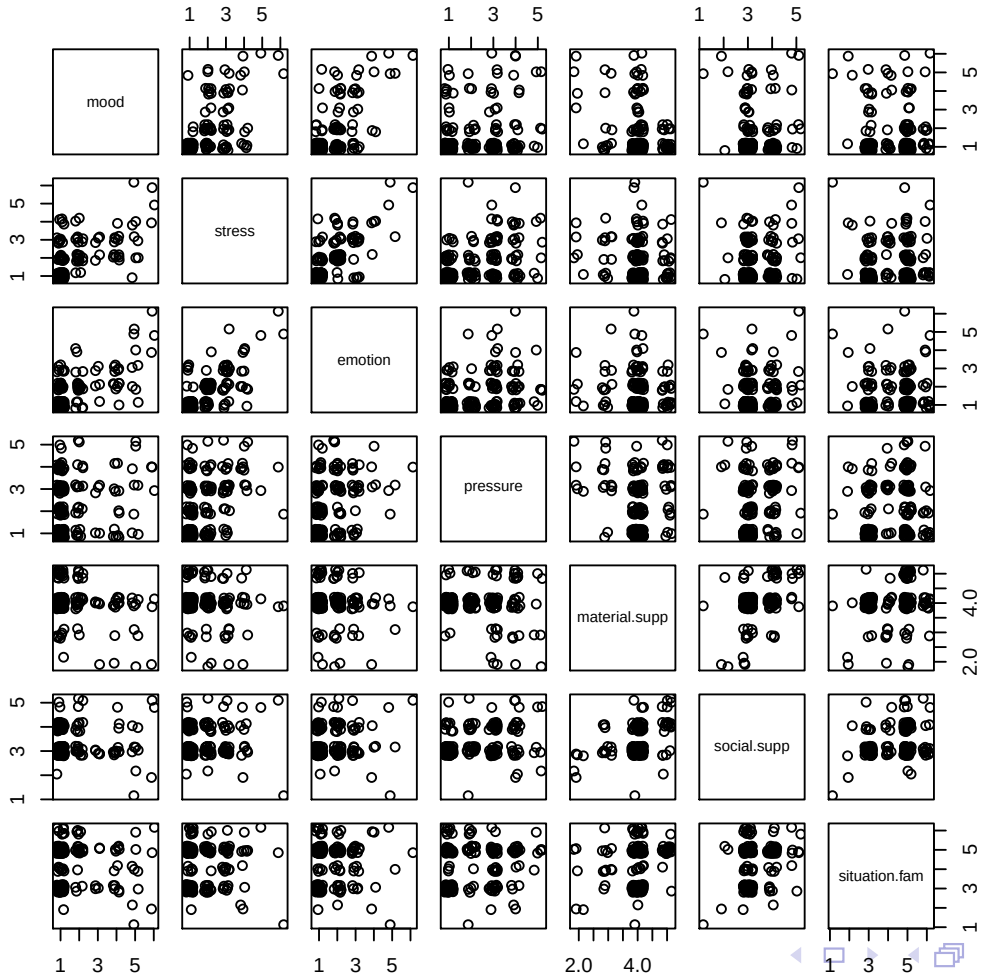
Example: 170 Swiss policemen recorded their emotional state in time using a questionnaire with ordinal scales (1 to 6). The features are

- mood,
- stress,
- emotion,
- pressure,
- social support,
- situation familiarity,
- material support.

There is nothing to predict: the interest is to discover patterns in the data.

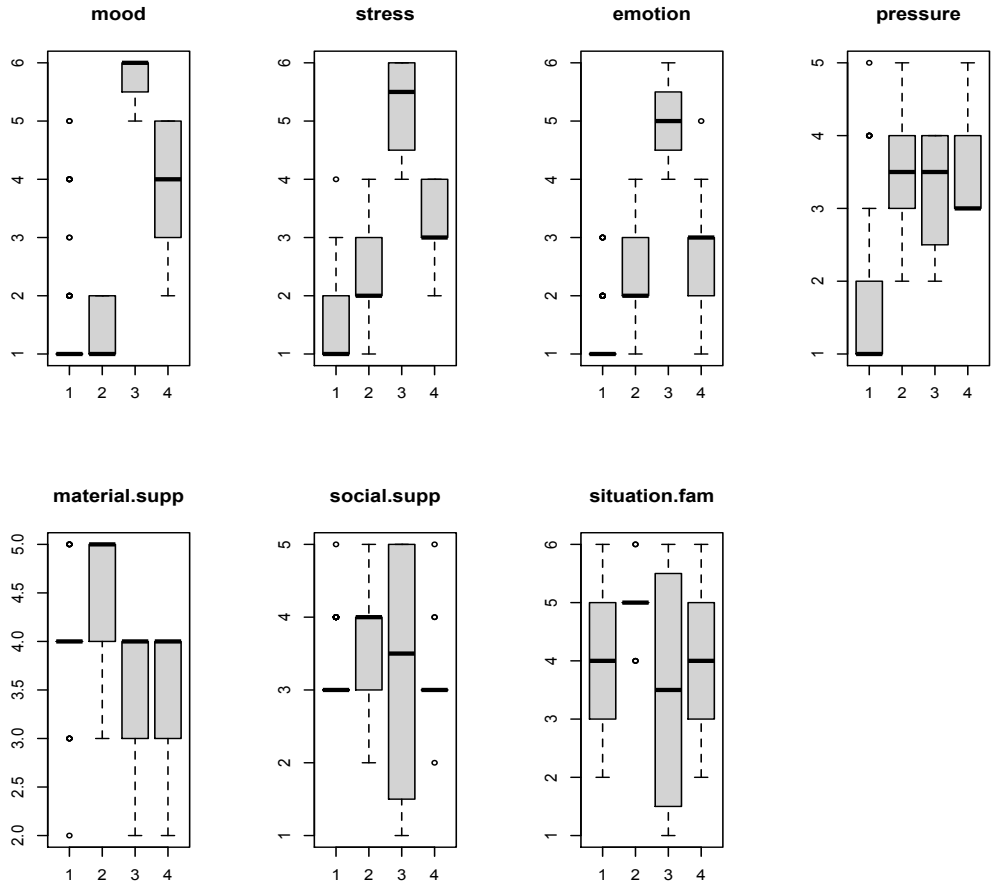
Example

Below the scatter plots of the features (jittering points for more readability).



Example

4 clusters of policemen were formed using AGNES. They can be analyzed by the feature values within each cluster.



Example

Some possible conclusions are

- Policemen in Cluster 3 have large mood, stress, and emotion values.
- Pressure characterizes cluster 1 (low) versus clusters 2 to 4 (medium).
- Mood and stress are associated because clusters 1 to 4 have the same levels of these two features.