

# Intelligent Systems

Chapter 8: Clustering

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# About this Chapter



#### Content

- Basics
- Hierarchical Clustering
- c-Means
- Further techniques
- Cluster evaluation
- Conclusion
- Further readings

#### Goals

Students should be able to:

- explain the basic idea of clustering.
- classify and compare different clustering methods.
- make a comprehensible selection of an algorithm.
- evaluate clustering results using appropriate metrics.

# Agenda



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- Basics
- Hierarchical Clustering
- c-Means
- Further techniques
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### **Basics**



### Clustering

- Subdivision of a set of given patterns into groups (clusters)
- I.e. a task of unsupervised learning
- In contrast to classification, which is used to predict class affiliation (with the help of examples).
- Typically, the result of the process is to summarise similar patterns:
  - Homogeneity within clusters:
    - → Patterns belonging to the same cluster should be as similar as possible.
  - Heterogeneity between clusters:
    - → Patterns assigned to different clusters should be as different as possible.

# Basics (2)



### Clustering (continued)

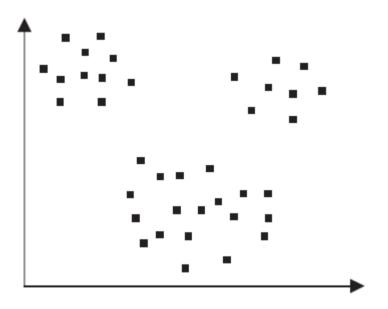
- There are no specifications as to which patterns belong in which clusters.
- The most important tool in clustering is the distance (or similarity) between two patterns
- For time series: clustering using a similarity measure on time series (or using a suitable representation/model)

# Basics (3)

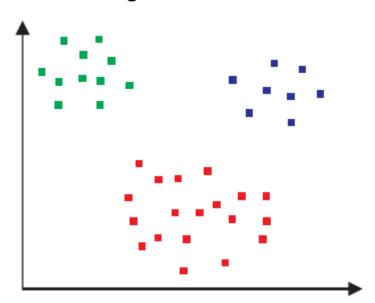


#### Example:

#### Data set:



#### Clustering result:

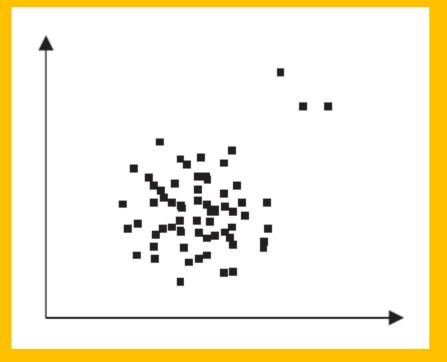


# Basics (4)



#### Question:

 Consider the following example – what are the main problems for clustering illustrated here?



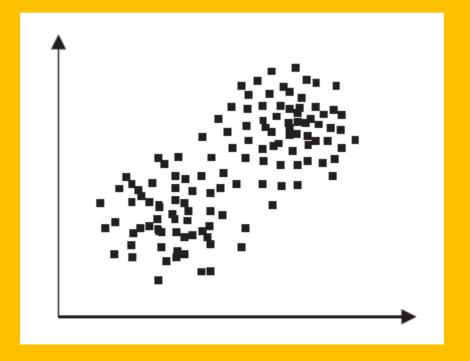
Solution

# Basics (5)



### Question:

How many clusters do you identify in this example?

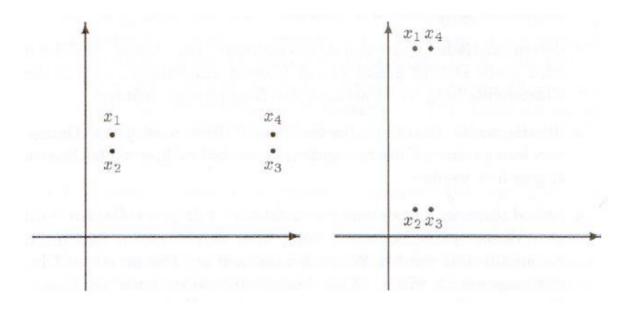


### Basics (6)



#### **Problem**

- Intuitive cluster assignment depends on the scaling of the individual axes / attributes.
- Example: Same pattern, different scaling



### Basics (7)



### Interesting aspects of clustering:

- Treatment of outliers Elimination? Formation of own clusters?
- The clustering result depends on the pre-processing of the data (e.g. scaling).
- Interpretation of the clustering results experts must assign a meaning (label if necessary) to the clusters.
- The number of clusters is sometimes difficult to determine or decide.
- Clustering does not have a "correct" or "optimal" result the quality of the result usually depends on the task at hand.
- With dynamic data records (time-varying data), the assignment of patterns to clusters can change over time.
- ...?

# Basics (8)



#### Terms (after [Höppner, Klawonn, Kruse 1997]):

- Incomplete cluster analysis methods:
  - Representation or projection techniques
  - Multidimensional data are subject to dimension reduction, e.g. by main component analysis
  - Data is displayed graphically, e.g. 2- or 3-dimensionally.
  - Cluster formation takes place manually by viewing the data
- Deterministic cluster analysis methods:
  - Each pattern is assigned to exactly one cluster.
  - Cluster division defines partition of data

#### Terms (continued):

- Overlapping cluster analysis methods:
  - Each sample is assigned to at least one cluster
  - Each sample may be assigned to more than one cluster
- Probabilistic cluster analysis methods:
  - For each sample, a probability distribution over the clusters is determined, indicating the probability with which a sample is assigned to a cluster
  - The sum of the assignment probabilities of a sample must be one
- Possibilistic cluster analysis methods:
  - Pure fuzzy clustering algorithms that work with membership grades instead of probabilities
  - Degree of membership of the sample to the cluster in question
  - Each sample may therefore be assigned to several clusters with certain degrees of membership
  - The secondary condition that the sum of the degrees of membership of a sample to the clusters must be one is often dropped

# Basics (10)



### Terms (continued):

- Hierarchical cluster analysis methods:
  - Procedure bottom-up: Samples are initially assigned to a cluster, clusters are summarised step-by-step.
  - Top-down approach: Initially all samples are combined into one cluster, clusters are broken down step by step.
  - Hierarchical clustering procedures are generally defined in procedural terms, i.e.
     by rules on when clusters are to be split up or grouped together

# Basics (11)



#### Terms (continued):

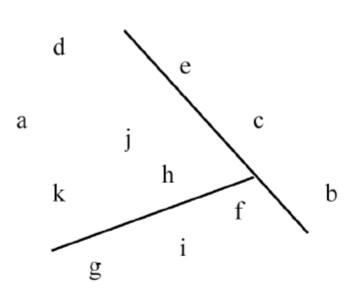
- Cluster analysis method with objective function:
  - Use an objective function to be optimised that assigns a quality or error value to each possible clustering
  - A set of clusters and the assignments of samples to these is sought that receives the best rating.
  - An optimisation problem must be solved (at least approximately)
- Partitioning cluster analysis techniques:
  - A desired number of clusters is predefined
  - Procedures assign all samples to a cluster in each step and try to gradually improve the quality of clustering by rearranging them.

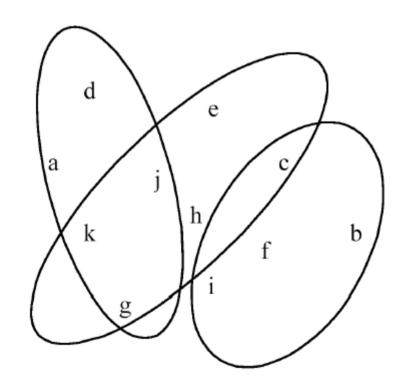
# Basics (12)



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#### Representation of clusters





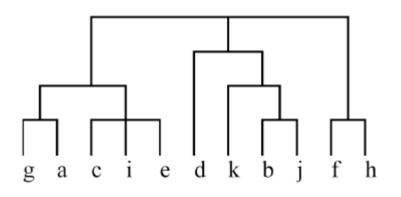
# Basics (13)



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#### Representation of clusters

	1	2	3
a	0.4	0.1	0.5
b		0.8	0.1
c	0.3	0.3	0.4
d	0.1	0.1	0.8
e	0.4	0.2	0.4
f	0.1	0.4	0.5
g	0.7	0.2	0.1
h	0.5	0.4	0.1



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# Agenda



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- c-Means
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Single-Linkage, Complete-Linkage and Average-Linkage are agglomerative, hierarchical cluster analysis methods.

#### Hierarchical cluster analysis methods:

- Bottom-up approach: agglomerative
- Top-down approach: dividing, divisive

# Hierarchical Clustering (2)



#### Agglomerative hierarchical methods:

- These methods assign each sample to its own cluster at the beginning.
- Then, in each step of the process, two clusters are searched for a specific optimality criterion, which are then merged to form a cluster.
- This procedure can be continued until the desired number of clusters is reached.

# Hierarchical Clustering (3)



### Agglomerative hierarchical methods:

- A major advantage and at the same time a disadvantage of these hierarchical cluster methods is that the large solution space is very quickly narrowed down, but the merger decisions made at an early stage can no longer be revised.
- These algorithms therefore sometimes tend to find poor local optima.

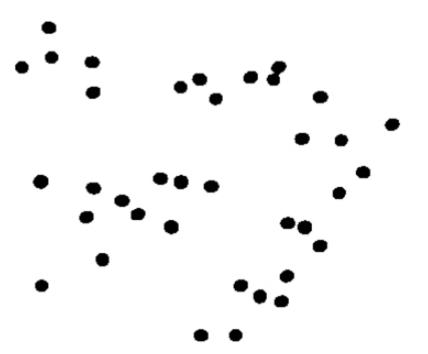
# Hierarchical Clustering (4)



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#### Approach:

1. Assign each point to its own cluster

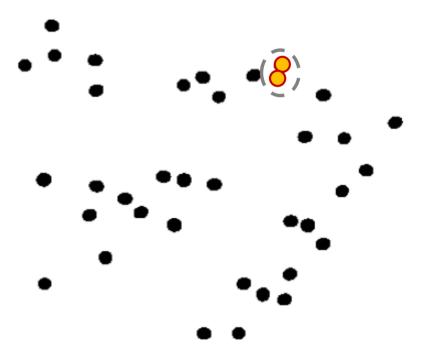


# Hierarchical Clustering (5)



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- 1. Assign each point to its own cluster
- 2.Identify the most similar pair of clusters

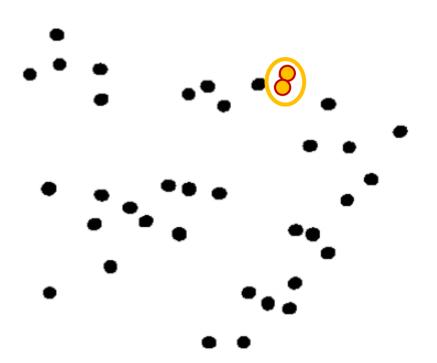


# Hierarchical Clustering (6)



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- 1. Assign each point to its own cluster
- 2.Identify the most similar pair of clusters
- 3.Create new cluster by merging the two identified ones

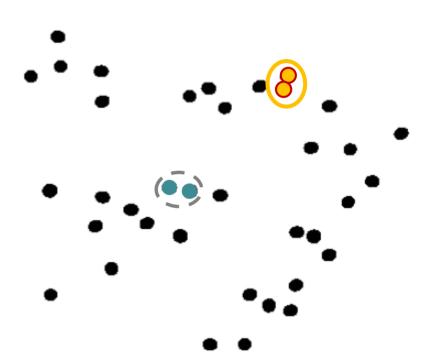


# Hierarchical Clustering (7)



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- 1. Assign each point to its own cluster
- 2.Identify the most similar pair of clusters
- 3.Create new cluster by merging the two identified ones
- 4. Repeat this step

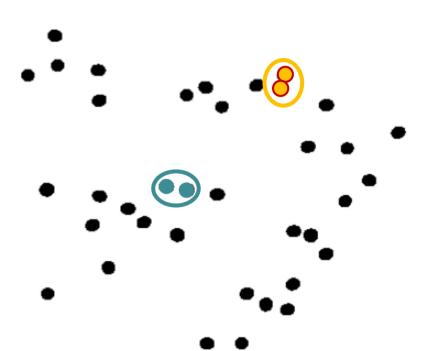


# Hierarchical Clustering (8)



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- 1. Assign each point to its own cluster
- 2.Identify the most similar pair of clusters
- 3.Create new cluster by merging the two identified ones
- 4.Repeat this step ...
- ... until all samples are part of one large cluster ...



# Hierarchical Clustering (9)



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### What does "similarity of clusters" even mean?

- Let  $C_i$  and  $C_j$  with  $i \neq j$  and  $C_i \cap C_j = \emptyset$  be two clusters of samples (data points)  $x_n \in \mathbb{R}^D$  with n = 1, ..., N and  $D \in \mathbb{N}$ .
- The following criteria are defined to assess the similarity of the two clusters:

$$\delta_{\min} \left( \mathcal{C}_i, \mathcal{C}_j \right) := \min_{\mathbf{x}_n \in \mathcal{C}_i, \, \mathbf{x}_l \in \mathcal{C}_j} \left\{ \| \mathbf{x}_k - \mathbf{x}_l \| \right\}$$

$$\delta_{\max} \left( \mathcal{C}_i, \mathcal{C}_j \right) := \max_{\mathbf{x}_k \in \mathcal{C}_i, \, \mathbf{x}_l \in \mathcal{C}_j} \left\{ \left\| \mathbf{x}_k - \mathbf{x}_l \right\| \right\}$$

### Hierarchical Clustering (10)



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C) 
$$\delta_{\text{avg}}\left(\mathcal{C}_{i}, \mathcal{C}_{j}\right) := \frac{1}{|\mathcal{C}_{i}| \cdot |\mathcal{C}_{j}|} \cdot \sum_{\mathbf{x}_{k} \in \mathcal{C}_{i}, \, \mathbf{x}_{l} \in \mathcal{C}_{j}} \|\mathbf{x}_{k} - \mathbf{x}_{l}\|$$

• The criteria  $\delta_{min}$ ,  $\delta_{max}$  or  $\delta_{avg}$  are called nearest neighbour, farthest neighbour or average neighbour.

# Hierarchical Clustering (11)



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#### Single Linkage

• Given is a set of patterns  $x_n \in \mathbb{R}^D$  with n = 1, ..., N and  $D \in \mathbb{N}$  as well as a desired number c of clusters to be detected, where  $N \ge c$  applies.

#### Process:

1. In a first step, a partition of the data consisting of *N* clusters is formed by assigning a pattern to each cluster:

$$C_n \coloneqq \{x_n\}$$

# Hierarchical Clustering (12)



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### Single Linkage – Process:

- 2. These clusters are now being gradually merged:
  - Determine the two clusters that are most similar according to the closest neighbor criterion:

 $(C_k, C_l)$  with the property

$$\left(\forall_{(\mathcal{C}_{k'},\mathcal{C}_{l'})}: \delta_{\min}\left(\mathcal{C}_{k},\mathcal{C}_{l}\right) \leq \delta_{\min}\left(\mathcal{C}_{k'},\mathcal{C}_{l'}\right)\right)$$

- Combine the two clusters  $C_k$  and  $C_l$  to one, so that a new partition of the data results.
- If the number of all clusters of the new partition is greater than the desired number c, then go back to step (a).

# Hierarchical Clustering (13)



#### Single Linkage: Evaluation

- Advantage of the process:
  - Outliers are recognised, because they are inserted only very late or not at all into a cluster.
- Disadvantage of the method:
  - Only two close samples at a time decide on the fusion of two clusters.
  - This can result in concatenations or chain-like structures (chaining effect)
    in which there are samples that are less similar to each other than to
    samples of other clusters.

# Hierarchical Clustering (14)



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#### Complete linkage

- Procedure as for single linkage, but step 2 a) is replaced by:
  - Determine the two clusters that are most similar according to the most distant neighbour criterion:

 $(C_k, C_l)$  with the property

$$(\forall_{(\mathcal{C}_{k'},\mathcal{C}_{l'})}: \delta_{\max}(\mathcal{C}_k,\mathcal{C}_l) \leq \delta_{\max}(\mathcal{C}_{k'},\mathcal{C}_{l'}))$$

# Hierarchical Clustering (15)



Complete Linkage: Evaluation

- Advantage:
  - Unlike single linkage, chaining cannot occur.
  - This ensures more homogeneous clusters.
- Disadvantage:
  - Outliers are integrated earlier and are no longer so easily detected.





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#### Average Linkage

- Procedure as for single/complete linkage, but step 2 a) is replaced by:
  - Determine the two clusters that are most similar according to the average neighbour criterion:

 $(C_k, C_l)$  with the property

$$(\forall_{(\mathcal{C}_{k'},\mathcal{C}_{l'})}: \delta_{\text{avg}}(\mathcal{C}_k,\mathcal{C}_l) \leq \delta_{\text{avg}}(\mathcal{C}_{k'},\mathcal{C}_{l'}))$$

# Hierarchical Clustering (18)



### Average Linkage: Evaluation

- In many cases this procedure leads to good results.
- Average linkage is therefore a good compromise.

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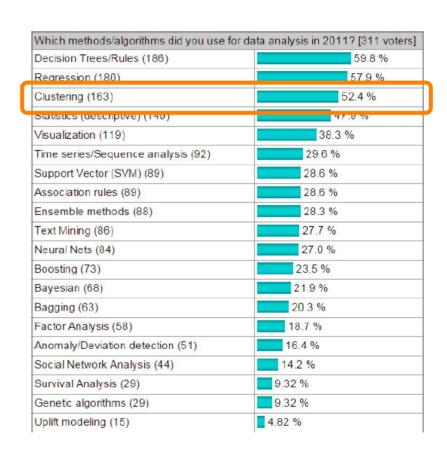
#### **C-Means**



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### c-Means algorithm

- Also: k-Means or simply clustering
- Was introduced by J. B. MacQueen in 1967.
- Is one of the most common data mining algorithms



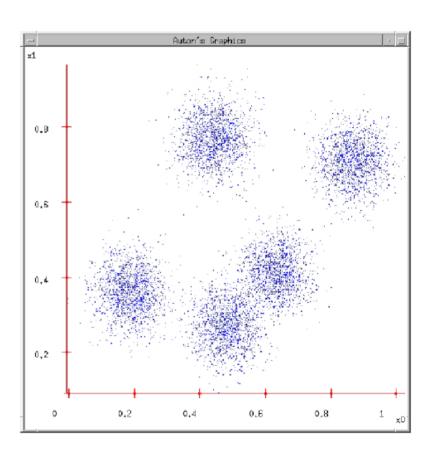
## C-Means (2)



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### c-Means

 Given is data, ask user how many clusters to form (here: c = 5).

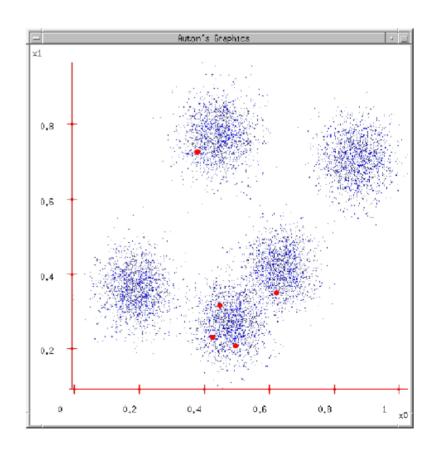


### C-Means (3)



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- Given is data, ask user how many clusters to form (here: c = 5).
- Choose c initial cluster centres.

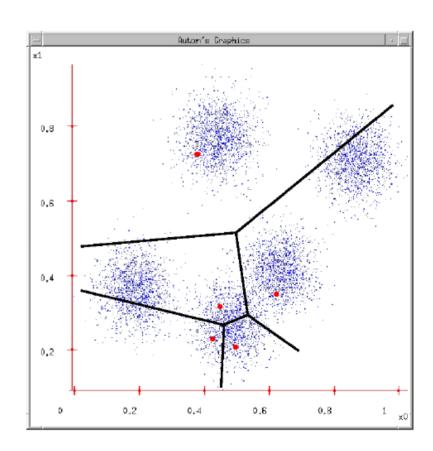


### C-Means (4)



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- Given is data, ask user how many clusters to form (here: c = 5).
- Choose c initial cluster centres.
- Form clusters by determining for each sample which is the nearest cluster centre.

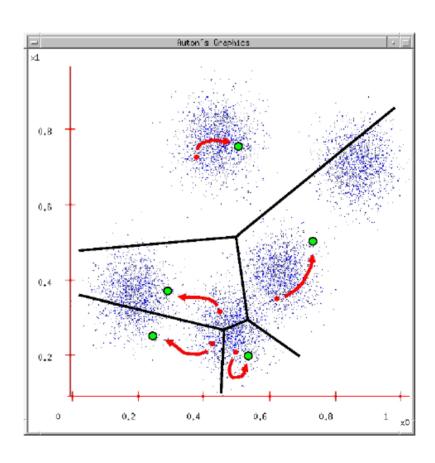


### C-Means (5)



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- Given is data, ask user how many clusters to form (here: c = 5).
- Choose c initial cluster centres.
- Form clusters by determining for each sample which is the nearest cluster centre.
- For each cluster, calculate the mean value of the assigned samples.

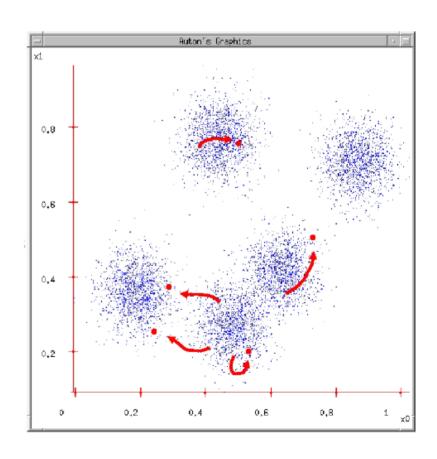


### C-Means (6)



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- Given is data, ask user how many clusters to form (here: c = 5).
- Choose c initial cluster centres.
- Form clusters by determining for each sample which is the nearest cluster centre.
- For each cluster, calculate the mean value of the assigned samples.
- Repeat assignment and centre determination until stopping criterion is reached.



## C-Means (7)



- Advantages:
  - Simple, easy to understand
  - All samples are automatically assigned to clusters
  - Process terminates
- Disadvantages:
  - Convergence in local minimum possible
  - Number of clusters to be determined manually
  - All samples must be assigned to clusters.
  - Sensitive to outliers
  - Sensitive to choice of initial cluster centres

## C-Means (8)



### Questions about c-Means:

- Which objective function is optimised here?
- Does the process terminate?
- Is there an optimal clustering?
- How should the process start?
- How can the number of centres be determined automatically?

## C-Means (9)

#### c-Means

- Given is a set of samples  $x_n \in \mathbb{R}^D$  with n = 1, ..., N and  $D \in \mathbb{N}$  as well as a desired number c of clusters to be detected, where  $N \ge c$  applies.
- The clusters are designated  $C_i$ , their centres  $c_i$  ( $c_i \in \mathbb{R}^D$ , i = 1, 2, ..., c).
- The clusters are initialised with  $C_i := \emptyset$ . A target function value  $\mathcal{E}$  is  $\mathcal{E} := \infty$ .
- Process:
  - In a first step, cluster centres are determined by assigning a randomly selected pattern to each centre:

$$c_i \coloneqq x_n$$

Each sample is selected at most once.

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### c-Means process (ctd.):

2. Each of the *N* samples is now assigned to that cluster, where the distance to the centre head is minimal:

$$C_i := C_i \cup x_n$$
 - exactly in the case if:

$$\forall_{c_j} : \|x_n - c_i\| \le \|x_n - c_j\|$$

Afterwards, all c cluster centres are updated (re-calculated):

$$c_i \coloneqq \frac{1}{|C_i|} \sum_{x_n \in C_i} x_n$$

## C-Means (11)



### c-Means process (Forts.):

4. If the result of the target value function has been decreased:

$$\mathcal{E} = \sum_{i=1,\dots,c} \sum_{x_n \in C_i} ||x_n - c_i||$$

go to Step 2. Again:  $C_i = \emptyset$ .

Otherwise: Stop.

#### Remark:

Other distance measures (e.g. Manhattan, ...) are possible, too!

## C-Means (12)



#### c-Means properties:

- Cluster centres are only moved if the value of the target function decreases as a result.
  - → Process is descending with respect to the target function value.
- Number of possibilities to assign patterns to clusters is finite.
  - → Process terminates.
- Process is "greedy" in the sense that in each run the currently best assignment of samples to centres is selected.
  - → Process can converge in local minimum.

## C-Means (13)



#### Number *c* of clusters:

- Start with low value of c and repetition of the process with increasing c.
- In doing so, studying the improvements of the target function value.
- Decision for c e.g. with knee/elbow approach / rule.

### Choice of starting points:

- Repetition of the procedure with different centre initialisations.
- "Skilful" selection of the initial centres.

## C-Means (14)



#### Heuristic to select the initial centres:

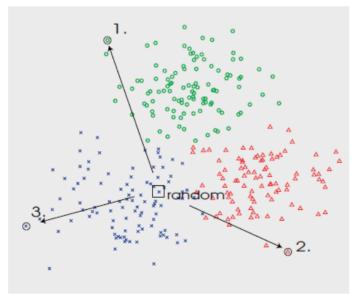
- Select a sample randomly
- As the first initial cluster centre, select a sample that is far away from the first selected sample.
- ...
- Select as i-th initial cluster centre a sample that is far from the previously selected samples
- ...
- ... until all c initial cluster centres are determined.

## C-Means (15)

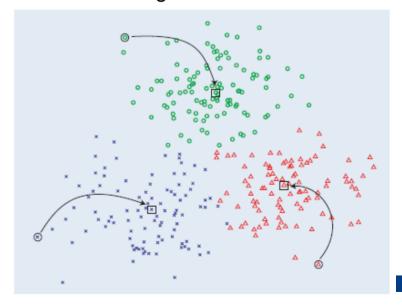


### Heuristic for choosing cluster centres

#### Choosing initial cluster centres



#### Clustering result



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## C-Means (16)



#### Comments:

- Application of c-means to recognise structures in data with one-dimensional data is a promising method for quantisation (buckets)
- Related processes:
  - Vector quantisation
  - Learning Vector Quantisation (LVQ)
  - Competition learning / Online-c-means
  - Self-Organising Maps (SOM)

### C-Means (17)



#### c-Medoids

- Problem: Result of c-means can be significantly affected by outliers.
- Idea: use medians instead of averages
- Example:
  - Average value of 1, 3, 5, 7, 9 is 5
  - Average value of 1, 3, 5, 7, 1009 is 205
  - Median of 1, 3, 5, 7, 1009 is 5
- Other variants (e.g. Fuzzy c-Means) known....

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### Further techniques



### Nearest Neighbour Clustering

- · Cf. hierarchical, agglomerative clustering
- The process starts with a randomly selected sample assigned to a newly created cluster.
- For each sample a different sample is searched in an existing cluster, so that the distance to this sample is minimal.
- If this distance is smaller than a specified threshold value, the corresponding clusters are combined, otherwise a new cluster is formed.

## Further techniques (2)



#### Clustering with Gaussian Mixture Models:

- It is assumed that clusters are generated by Gaussian random processes, i.e. they can also be modelled by a combination of several Gaussian distributions.
- Instead of using degrees of affiliation (like in fuzzy logic) one works with probabilities
- Parameters of the Gauss functions are determined again in an iterative procedure (EM: Expectation Maximisation) (see c-means).

## Further techniques (3)



#### **DBSCAN**

Everything is related to everything else, but near things are more related than distant things. [First geographical law, Waldo Tobler, 1970]

## Further techniques (4)



### **DBSCAN:**

- Density-Based Spatial Clustering of Applications with Noise
- Density-based spatial cluster analysis with noise
- Basic idea similar to Nearest Neighbour Clustering, i.e. neighbouring samples are combined to form a cluster.
- In addition, however, the number of adjacent samples is taken into account and individual samples at the edge are explicitly recognised as noise (or outliers).

We will discuss this technique in detail in the chapter about anomaly / novelty detection...!

### Further techniques (5)



#### **OPTICS**

- Ordering Points To Identify the Clustering Structure
- Based on DBSCAN
- Also density-based algorithm for cluster analysis, further development of DBSCAN
- Fixes weakness of DBSCAN: can detect clusters of different density
- Eliminates to a large extent the  $\varepsilon$  parameter (neighborhood length) of DBSCAN
- Idea: Arranges the points of the data set linearly, so that spatially adjacent points in this order follow each other closely, and determines the so-called "reachability distance".

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### Cluster evaluation



#### Evaluation of clustering methods:

- Usual: Evaluation by experts or with regard to a target function with test data
- Sensible evaluation is often only possible in the application
- Some algorithms already work with target functions (e.g. c-means), others do not (e.g. single linkage).
- Examples of criteria:
  - Dunn's Index,
  - Davies Bouldin Index,
  - SD Index,
  - Minimal Description Length,
  - Category utility,
  - **–** ...

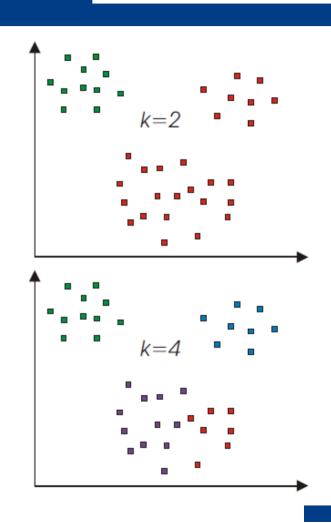
## Cluster evaluation (2)



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#### Evaluation criteria for clusters

- Evaluation of the clustering results: Which partitioning "fits" best with the data?
- Quantitative evaluation of the clustering results
- Search for optimal set of parameters (depending on clustering method):
  - number of clusters (c-means, c-medoids, fuzzy-c-means, ...)
  - Radii (BIRCH, DBSCAN, DENCLUE,...)
  - Maximum number of neighbours (CLARANS, ...)



## Cluster evaluation (3)



Cluster evaluation: subdivision into ...

- External criteria
  - Comparison of the cluster structure found with a predefined structure
  - Assumptions about underlying data are necessary
- Internal criteria
  - Only the clustering itself and the data are taken into account.
- Relative criteria (commonly used)
  - Evaluation of several (successive) cluster structures
  - Use of the same algorithm, but with different parameter sets

## Cluster evaluation (4)



### Relative criteria

- Basic idea: For a clustering algorithm, P is the set of its parameters.
   Among the generated cluster structures, search for the best one with regard to the selected evaluation criterion f.
- There are two cases:
  - 1. P does not contain the number of clusters
    - Start the clustering algorithm for a wide range of parameters.
    - Select the largest range for which the number of k clusters remains constant.
    - Select the mean value from the range found.

### Cluster evaluation (5)



#### Relative criteria (ctd.)

- There are two cases:
  - 2. P does contain the number of clusters
    - Start the clustering algorithm for all c at a user-specified interval  $[c_{MIN}, c_{MAX}]$ .
    - For each c, vary the remaining parameters.
    - Define the function  $\hat{f}(c)$  that contains the optimal value for each c.
    - Determine optimum based on the function  $\hat{f}(c)$  (e.g. by visualising the function  $\hat{f}(c)$ ).
- If the evaluation criterion has no rising or falling trend
  - → Search for maximum or minimum
- In the presence of a trend:
  - Search for a significant change in the curve of  $\hat{f}(c)$  (strong local increase or decrease, so-called knee).
  - No knee can be an indication that there is no cluster structure!

## Cluster evaluation (6)



### Examples:

- Dunn's Index
- Davies Bouldin Index

## Cluster evaluation (7)



#### **Dunn's Index**

- Dunn, 1974
- Search for compact and well separated clusters
- Very popular, widely used
- Basic idea: For compact and well separated clusters, the distance between the clusters should be large (high inter-cluster distance) and the diameter of the respective cluster should be small (small intracluster distance).

## Cluster evaluation (8)



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### Dunn's Index $D_c$ for c Cluster:

$$D_c := \min_{i=1,\dots,c} \left\{ \min_{j=i+1,\dots,c} \left\{ \frac{\delta(\mathcal{C}_i, \mathcal{C}_j)}{\max_{m=1,\dots,c} \operatorname{diam}(\mathcal{C}_m)} \right\} \right\}$$

with the dissimilarity measure

$$\delta(\mathcal{C}_i, \mathcal{C}_j) := \min_{\mathbf{x} \in \mathcal{C}_i, \mathbf{y} \in \mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$$

- d(x, y) is a distance measure which measures the distance (= dissimilarity) of the two samples x and y.
- $diam(C_m)$  is the diameter of the cluster  $C_m$  and can be defined as

$$\operatorname{diam}(\mathcal{C}_m) := \max_{\mathbf{x}, \mathbf{y} \in \mathcal{C}_m} d(\mathbf{x}, \mathbf{y})$$

### Cluster evaluation (9)



#### **Dunn's Index**

- Analysis:
  - Large values for Dunn's Index indicate compact and well separated clusters.
  - The c, for which  $D_c$  is the largest, is assumed to be the best cluster structure.
- Disadvantages
  - High computational effort (quadratic in the number of clusters)
  - high susceptibility to outliers, as outliers can easily influence  $max_{m=1,\dots,c}diam(C_m)$ .
  - Improvements are possible (reduction of runtime and lower sensitivity to outliers).

### Cluster evaluation (10)



#### **DB** Index

- Davies & Bouldin, 1979
- Basic idea as with Dunn's Index: Individual clusters should be as compact as
  possible with the greatest possible distance between the clusters at the same
  time.
- Very popular and widely used criterion.
- Approach: Consider scattering within clusters in relation to the distance between clusters.

## Cluster evaluation (11)



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Davies Bouldin Index  $DB_c$  for c Cluster

$$DB_c := \frac{1}{c} \sum_{i=1}^{c} R_i$$

with

$$R_i \coloneqq \max_{\substack{j=1,\dots,c\\i\neq j}} R_{ij}$$

for

$$i = 1, ..., c$$

#### Remark:

• For  $R_{ij}$  must hold: The smaller the value, the better the separation of clusters.

## Cluster evaluation (12)



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### DB Index (continued)

• Let  $d_{ij}$  be a measure of dissimilarity (distance measure) for two clusters  $C_i$  and  $C_j$ , e.g. measured by the distance of the cluster centres (mean values)  $c_i$  and  $c_j$ :

$$d_{ij} \coloneqq \left\| c_i - c_j \right\|$$

• and  $s_i$  is the scattering (or spread) of the cluster  $C_i$ , e.g. the mean distance of all data points of a cluster to the respective cluster centre.

### Cluster evaluation (13)

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### DB Index (continued)

- R\_ij must be a similarity measure for two clusters that meets the following conditions:
  - 1.  $R_{ii} \ge 0$
  - 2.  $R_{ij} = R_{ji}$
  - 3. If  $s_i = 0$  and  $s_i = 0$  then  $R_{ij} = 0$
  - 4. If  $s_j > s_k$  and  $d_{ij} = d_{ik}$  then  $R_{ij} > R_{ik}$
  - 5. If  $s_j = s_k$  and  $d_{ij} < d_{ik}$  then  $R_{ij} > R_{ik}$
- $R_{ij}$  is therefore especially non-negative and symmetrical.

## Cluster evaluation (14)



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A simple measure that meets the conditions, is

$$R_{ij} \coloneqq \frac{s_i + s_j}{d_{ij}}$$

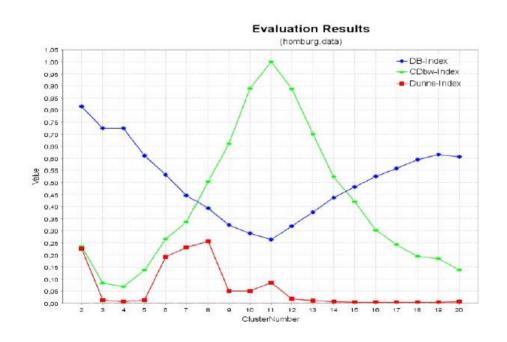
### Analysis:

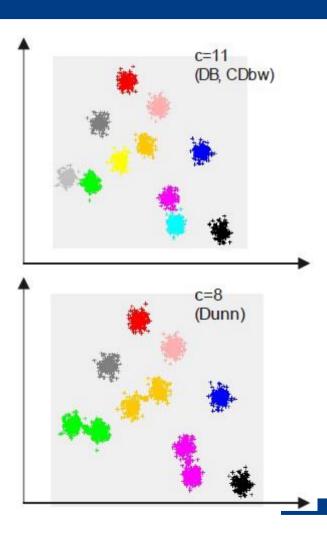
- DB<sub>c</sub> measures the average similarity between a cluster and its most similar cluster.
- The goal is to find clusters that are as dissimilar as possible, i.e. search for the minimum  $DB_c$
- High computational effort
- For further alternatives for scattering within clusters and the spacing of clusters, see: [Davies & Bouldin, 1979]

### Cluster evaluation (15)



Example: 11 clusters in 2 dimensions





# Agenda



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- Basics
- Hierarchical Clustering
- c-Means
- Further techniques
- Cluster evaluation
- Conclusion
- Further readings



### Conclusion



- Basic idea of clustering: Finding natural groups in data
- First basic approach: Hierarchical clustering
- Probably the most popular approach: c-Means (and c-Medoids)
- Other different clustering methods
- Evaluation of clustering results using appropriate metrics:
   In particular Dunn's Index and Davies-Bouldin Index

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# Further readings



- [EKSX96] Ester, Kriegel, Sander, Xu, A density-based algorithm for discovering clusters in large spatial databases with noise, 1996
- [HKK97] Höppner, Frank, Frank Klawonn, and Rudolf Kruse. Fuzzy-Clusteranalyse: Verfahren für die Bilderkennung, Klassifizierung und Datenanalyse. Vieweg+ Teubner Verlag, 1997
- [MQ67] MacQueen, James. "Some methods for classification and analysis of multivariate observations." Proceedings of the fifth Berkeley symposium on mathematical statistics and probability. Vol. 1. No. 14. 1967
- [Dunn74] Dunn, Joseph C. "Well-separated clusters and optimal fuzzy partitions." *Journal of cybernetics* 4.1 (1974): 95-104.
- [DB79] Davies, David L., and Donald W. Bouldin. "A cluster separation measure." *IEEE transactions on pattern analysis and machine intelligence* 2 (1979): 224-227.

End



• Questions....?