Lecture 6: Clustering

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MSA220/MVE441 Statistical Learning for Big Data

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Classification without classes

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Goals

- Find groups in data
- Summarize high-dimensional data
- Data exploration

Clustering

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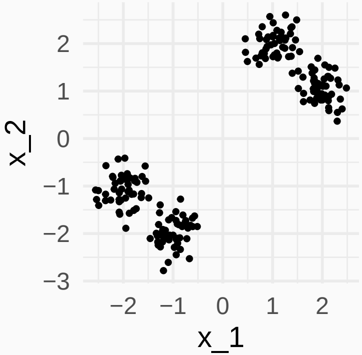

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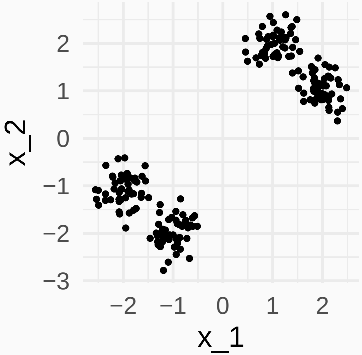

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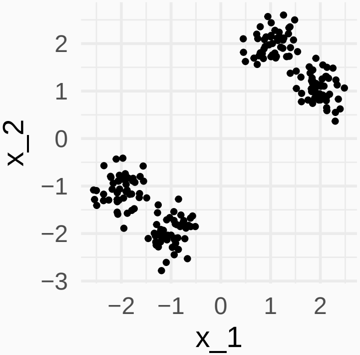

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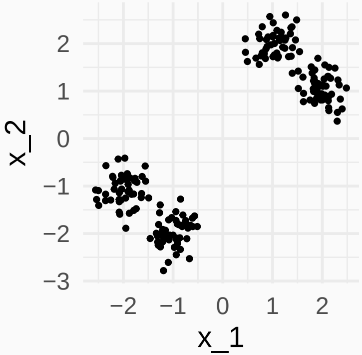

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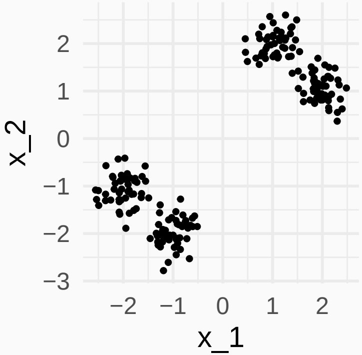

We need to able to measure **dissimilarity** between features to determine which samples/objects are close together or far apart.

Note: In clustering *classes* are often called **labels** and *features* are **attributes**

Dissimilarity measures

A **dissimilarity measure** for features x_1, x_2 is a function such that

$$d(x_1, x_2) \geq 0 \quad \text{and} \quad d(x_1, x_2) = d(x_2, x_1)$$

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Typical examples

- For quantitative features: ℓ_1 or ℓ_2 norm, correlation between whole feature vectors, ...
- For categorical variables with K levels: Loss matrix $\mathbf{L} \in \mathbb{R}^{K \times K}$ such that $\mathbf{L}_{rs} = \mathbf{L}_{sr}$, $\mathbf{L}_{rr} = 0$ and $\mathbf{L}_{rs} \geq 0$. Then $d(r, s) = \mathbf{L}_{rs}$

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Idea: Partition the observations into K groups/clusters so that **pairwise dissimilarities within groups** are **smaller than between groups.**

Note: A partition of the observations is called a **clustering** $C(\mathbf{x}) = i$

Combinatorial Clustering (I)

Total amount of dissimilarity for an arbitrary clustering C

$$T = \underbrace{\sum_{l=1}^{n} \sum_{m<l} D(\mathbf{x}_l, \mathbf{x}_m)}_{\text{Total point scatter}}$$

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Note that T does not depend on the clustering. Therefore

$$W(C) = T - B(C)$$

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As in the case of decision trees/CART looking at all possible partitions and finding the global minimum of $W(C)$ is too computational expensive.

Use **greedy algorithms** to find local minima.

An approximation to Combinatorical Clustering (I)

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$$= \sum_{i=1}^{K} n_i \sum_{\substack{l=1 \\ C(\mathbf{x}_l)=i}}^{n} \|\mathbf{x}_l - \mathbf{m}_i\|^2$$

where

$$n_i = \sum_{l=1}^{n} \mathbb{1}(C(\mathbf{x}_l) = i) \quad \text{and} \quad \mathbf{m}_i = \frac{1}{n_i} \sum_{C(\mathbf{x}_l)=i} \mathbf{x}_l$$

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The goal now is to solve

$$\arg\min_{C} \sum_{i=1}^{K} n_i \sum_{\substack{l=1 \\ C(\mathbf{x}_l)=i}}^{n} \|\mathbf{x}_l - \mathbf{m}_i(C)\|^2$$

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Observation: For a fixed clustering rule C it holds that

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Approximative solution: Consider the larger problem

$$\arg\min_{\substack{C \\ m_i \text{ for } 1 \leq i \leq K}} \sum_{i=1}^{K} n_i \sum_{\substack{l=1 \\ C(\mathbf{x}_l)=i}}^{n} \|\mathbf{x}_l - \mathbf{m}_i\|^2$$

This approximation can be solved iteratively for the clustering C and the cluster centres. This is called the **k-means** algorithm.

Computational procedure:

1. **Initialize:** Randomly choose K observations as cluster centres $\mathbf{m}_i$ and set $J_{\max}$ to a positive integer.
2. For steps $j = 1, \dots, J_{\max}$
   2.1 **Cluster allocation:** $C(\mathbf{x}_l) = \underset{1 \le i \le K}{\arg\min} \|\mathbf{x}_l - \mathbf{m}_i\|^2$
   2.2 **Cluster centre update:** $\mathbf{m}_i = \frac{1}{n_i} \sum_{C(\mathbf{x}_l)=i} \mathbf{x}_l$
   2.3 Stop if clustering C did not change

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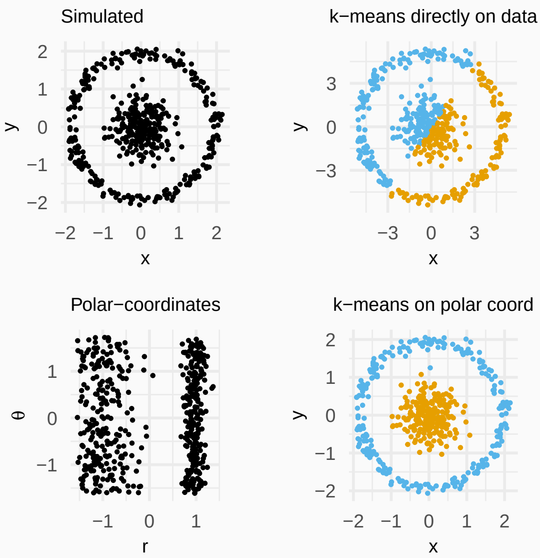
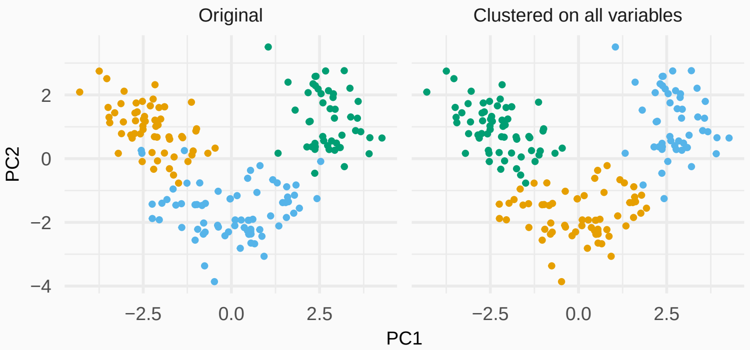
- **Dependence on initial selection:** Run repeatedly to see if k-means provides stable results
- Since k-means uses the ℓ_2 norm it has all the typical problems (**sensitive to outliers and noise**)
- **Clusters tend to be circular:** k-means looks in a circular fashion around each cluster centre and assigns an observation to the closest centre
- **Problems with unequal cluster size:** If some clusters have less samples than others, then k-means tends to add those to the bigger clusters
- **Always finds K clusters** (not unique to k-means)

k-means and circular clusters



Using k-means on the wine dataset

UCI Wine dataset: $K = 3$ classes. Let's see if k-means recovers the classes given only the features/attributes.



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Solve

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Notation: For observed feature vectors $\mathbf{x}_l$ and $\mathbf{x}_m$ set $\mathbf{D}_{l,m} = D(\mathbf{x}_l, \mathbf{x}_m)$. This results in $\mathbf{D} \in \mathbb{R}^{n \times n}$.

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Note: All PAM requires is a matrix of distances $\mathbf{D}$ and no additional distance computations are necessary. Very diverse types of features can be used.

Cluster validation and selection of cluster count

Internal indices

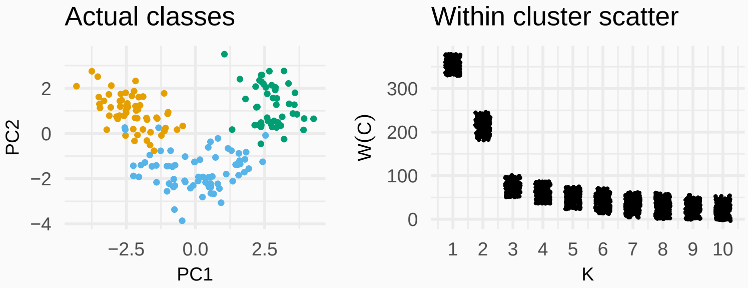
- Focus on between and within cluster scatter
- Aim is to achieve high between cluster scatter and low within cluster scatter

External indices

- Focus on comparison of final clustering with reference classes
- Used to e.g. determine which types of clusters can be found in data, or to evaluate different clustering algorithms on a reference dataset

Examples of internal indices

Elbow heuristic for k-means



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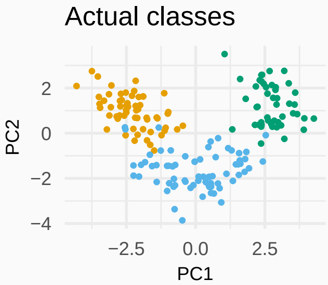

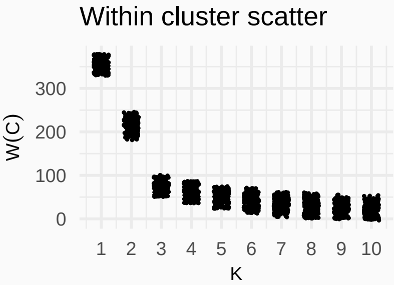

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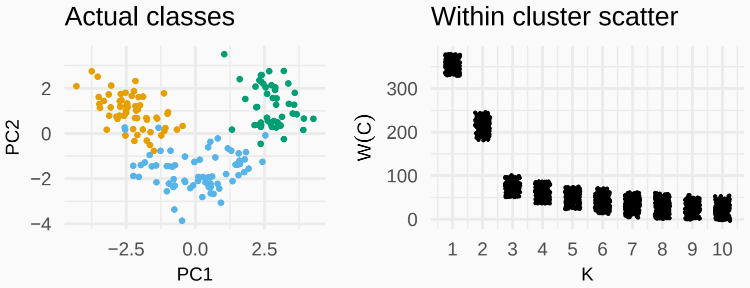

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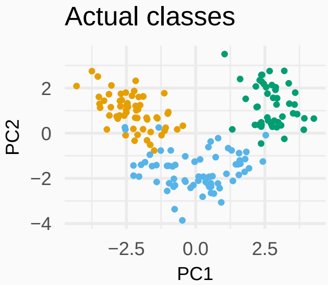

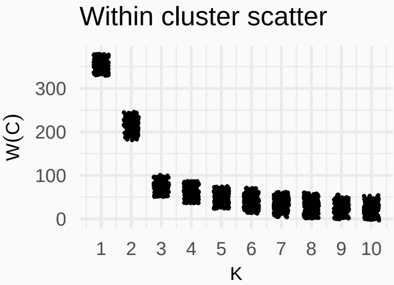

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- K is chosen such that **following decreases are substantially smaller**.

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and overall **average silhouette width:** $S = \dfrac{1}{n} \sum_{l=1}^{n} s_l$.

Notes on silhouette width

- **Interpretation**
  - Close to 1 when observation is well located inside the cluster and separated from the nearest cluster
  - Close to 0 when observation is between two clusters
  - Negative if observation on average closer to another cluster.
    Warning sign: Hints at which observations should be investigated.
  - Average silhouette width should be maximal for a good clustering

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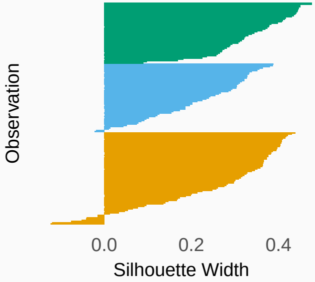
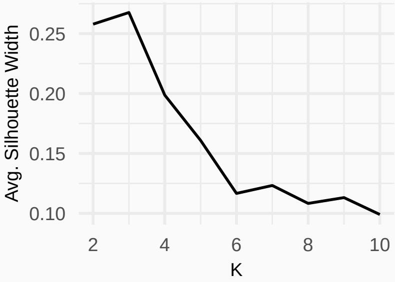
  - Average silhouette width should be maximal for a good clustering
- **Limitations**
  - Needs at least two clusters
  - Based on the same ideas as PAM/k-medoids and therefore considers clusters to be spherical

Silhouette Width: Example

Clustering of the **UCI wine data** using k-medoids with the ℓ_2 metric. Sorted per cluster and arranged in decreasing order of silhouette width.





Silhouette Width: Example

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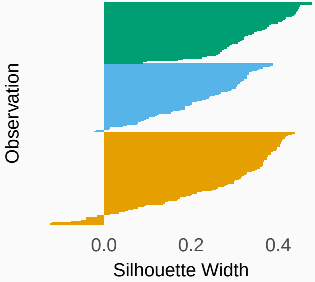

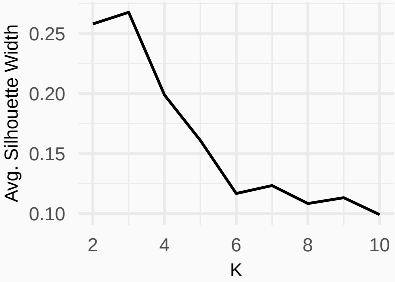

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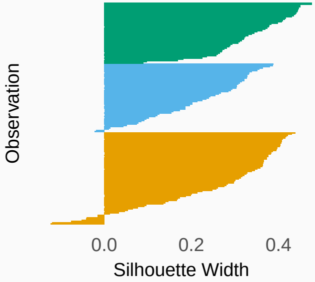
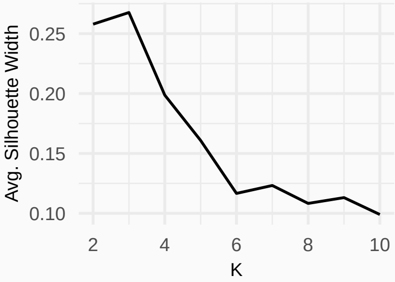
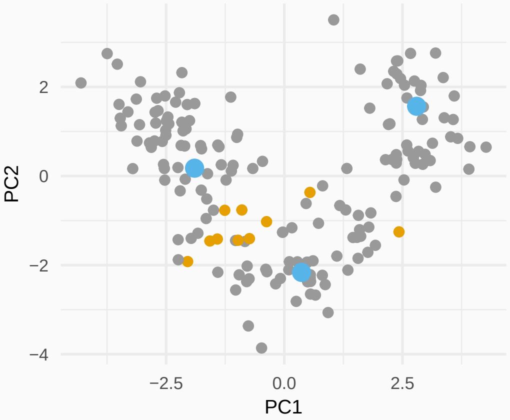


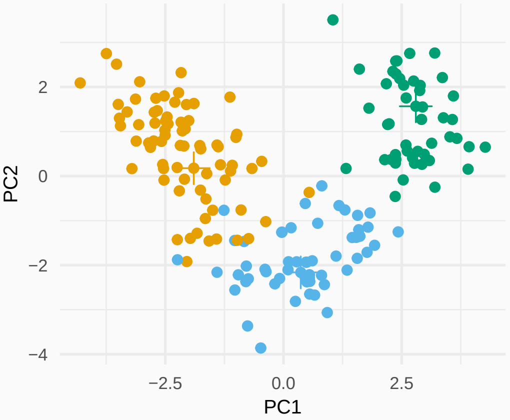


- Silhouette width gives a clear signal that more than three clusters lead to decreasing performance
- However, two and three clusters are indicated of similar quality.

Observations with negative Silhouette width

Observations in orange have negative silhouette width. Cluster medoids are shown in blue.





An example of an external index

Mutual information and entropy

Let C be a clustering for K clusters and c a classification rule for M classes.
Denote $S_i = \{\mathbf{x}_l : C(\mathbf{x}_l) = i\}$, $S^j = \{\mathbf{x}_l : c(\mathbf{x}_l) = j\}$, and $S_i^j = S_i \cap S^j$.

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Mutual Information: Amount of information that can be obtained about one rule by knowing the other rule

$$I(C, c) = \sum_{i=1}^{K} \sum_{j=1}^{M} \mathbb{P}(S_i^j) \log \frac{\mathbb{P}(S_i^j)}{\mathbb{P}(S_i)\,\mathbb{P}(S^j)} \approx \sum_{i=1}^{K} \sum_{j=1}^{M} \frac{|S_i^j|}{n} \log \frac{n|S_i^j|}{|S_i||S^j|}$$

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Entropy: Information present in each rule

$$H(C) = -\sum_{i=1}^{K} \mathbb{P}(S_i) \log \mathbb{P}(S_i) \approx -\sum_{i=1}^{K} \frac{|S_i|}{n} \log \frac{|S_i|}{n}$$

and analogously for c.

Normalised mutual information

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Note that $I(C, c) \leq (H(C) + H(c))/2$ which leads to the definition of **normalised mutual information**

$$\mathrm{NMI}(C, c) = \frac{I(C, c)}{(H(C) + H(c))/2} \in [0, 1].$$

Take-home message

- Clustering is a more challenging problem than classification and needs to answer two questions:
  - What is a cluster?
  - How many clusters are there?
- The clustering algorithm defines what shapes are considered as clusters.
- Clustering results can be validated by external indices and cluster count can be selected through internal indices.