

Clustering

Statistical Natural Language Processing 1

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Winter Semester 2025/2026

Unsupervised learning

- In unsupervised learning, we do not have labels in our training data
- Our aim is to find useful patterns/structure in the data
 - for exploratory study of the data
 - for augmenting / complementing supervised methods
- Close relationships with ‘data mining’, ‘data science / analytics’, ‘knowledge discovery’
- Most unsupervised methods can be cast as graphical models with hidden variables
- Evaluation is difficult: no ‘true’ labels/values

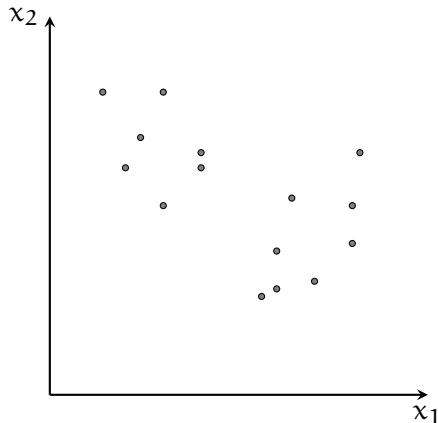
Today's lecture (and later)

- Today: *clustering*, finding related groups of instances
 - k-means
 - hierarchical clustering
 - evaluation
- Later: *clustering*, finding related groups of instances
 - *Density estimation*: finding a probability distribution that explains the data
 - *Dimensionality reduction*: find an accurate/useful lower dimensional representation of the data
 - Unsupervised learning in ANNs (RBMs, autoencoders)

Clustering: why do we do it?

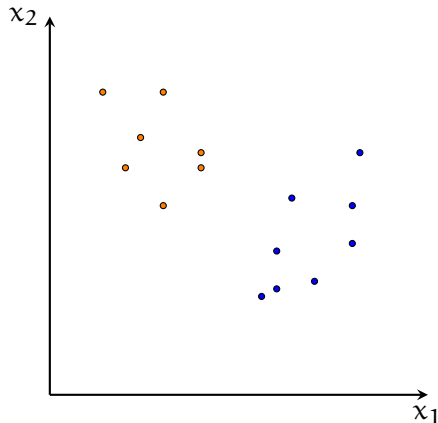
- The aim is to find groups of instances/items that are similar to each other
- Applications include
 - Clustering languages, dialects for determining their relations
 - Clustering (literary) texts, for e.g., authorship attribution
 - Clustering words for e.g., better parsing
 - Clustering documents, e.g., news into topics
 - ...

Clustering in two dimensional space



- Unlike classification, we do not have labels

Clustering in two dimensional space



- Unlike classification, we do not have labels
- We want to find 'natural' groups in the data
- Intuitively, similar or closer data points are grouped together

Similarity and distance

- The notion of distance (similarity) is important in clustering. A distance measure D ,
 - is symmetric: $D(a, b) = D(b, a)$
 - non-negative: $D(a, b) \geq 0$
for all a, b , and it $D(a, b) = 0$ iff $a = b$
 - obeys triangle inequality: $D(a, b) + D(b, c) \geq D(a, c)$
- The choice of distance is application specific
- We will often face with defining distance measures between linguistic units (letters, words, sentences, documents, ...)

Distance measures in Euclidean space

- Euclidean distance:

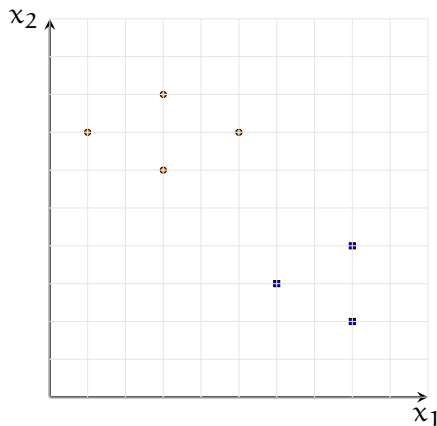
$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{j=1}^k (a_j - b_j)^2}$$

- Manhattan distance:

$$\|\mathbf{a} - \mathbf{b}\|_1 = \sum_{j=1}^k |a_j - b_j|$$

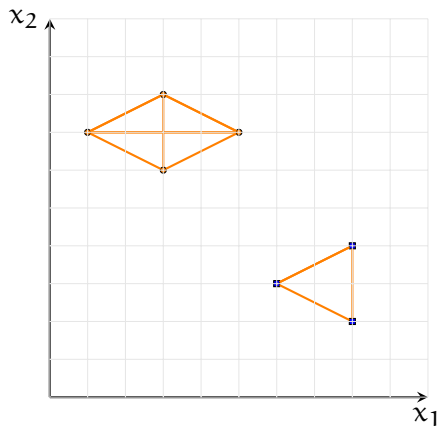
How to do clustering

Most clustering algorithms try to minimize the scatter **within** each cluster. Which is equivalent to maximizing the scatter **between** clusters.



How to do clustering

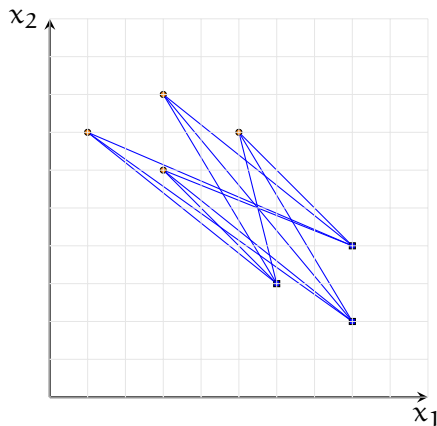
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$$\sum_{k=1}^K \sum_{a \in C_k} \sum_{b \in C_k} d(a, b)$$

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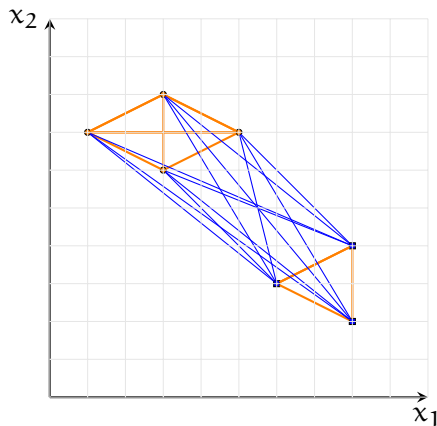


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K-means algorithm

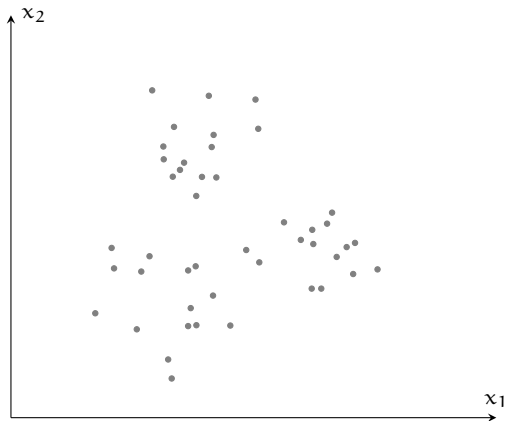
K-means is a popular method for clustering.

1. Randomly choose *centroids*, $m_1, \dots, m_K$, representing K clusters
2. Repeat until convergence
 - Assign each data point to the cluster of the nearest centroid
 - Re-calculate the centroid locations based on the assignments

Effectively, we are finding a *local minimum* of the sum of squared Euclidean distance within each cluster

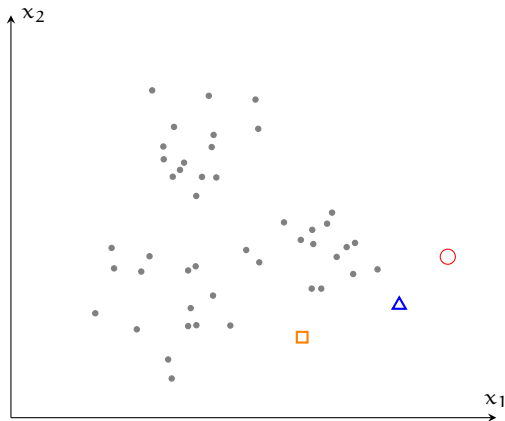
$$\frac{1}{2} \sum_{k=1}^K \sum_{a \in C_k} \sum_{b \in C_k} \|a - b\|^2$$

K-means clustering: visualization



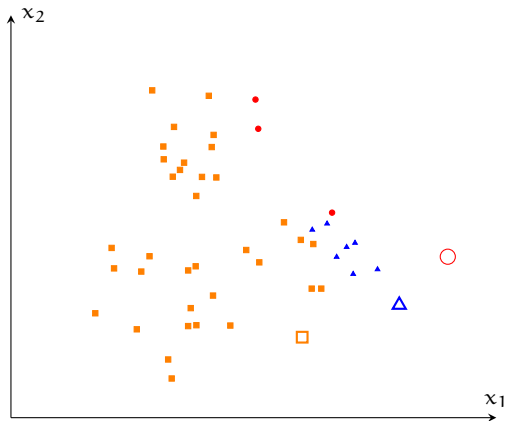
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



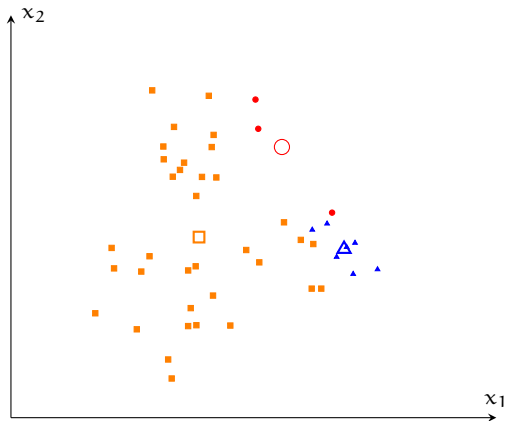
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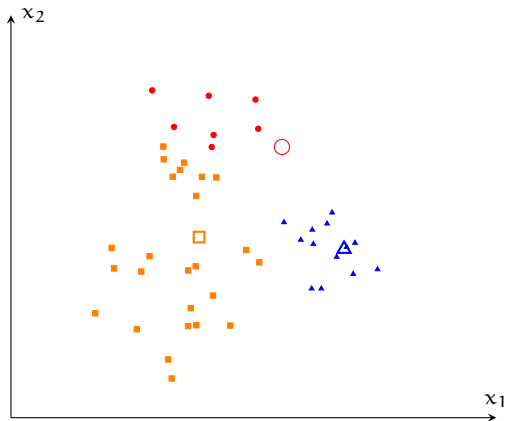
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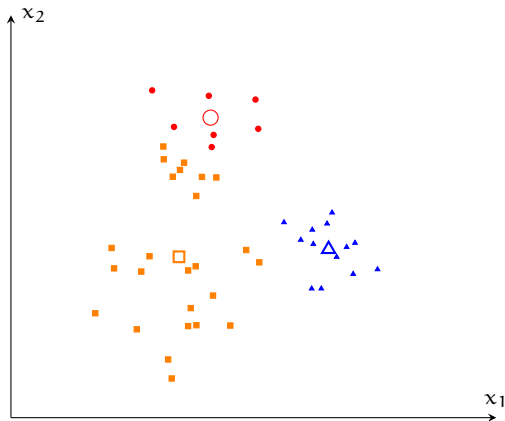
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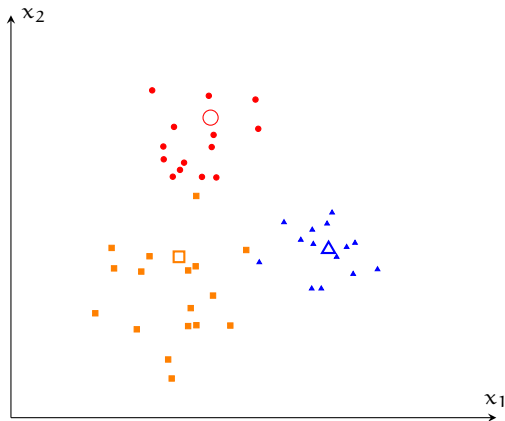
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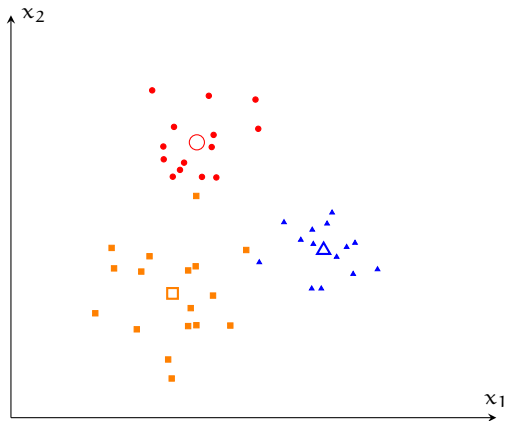
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K-means clustering: visualization



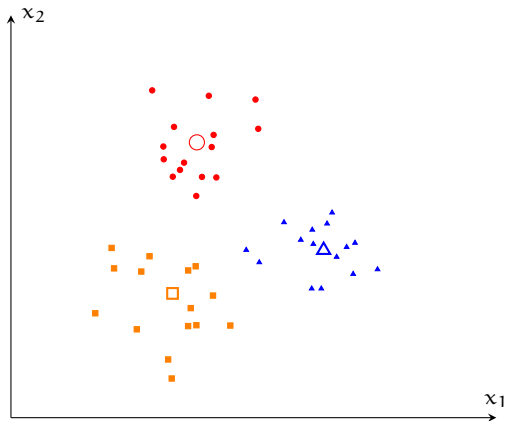
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K-means clustering: visualization



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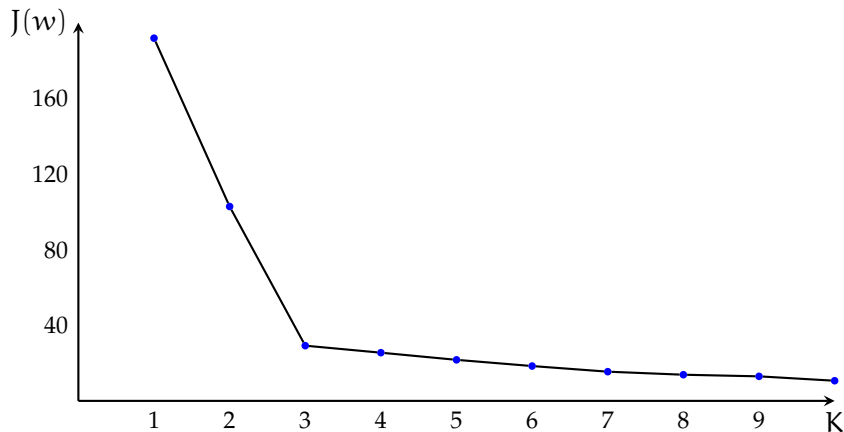
K-means: some issues

- K-means requires the data to be in an Euclidean space
- K-means is sensitive to outliers
- The results are sensitive to initialization
 - There are some smarter ways to select initial points
 - One can do multiple initializations, and pick the best (with lowest within-group squares)
- It works well with approximately equal-size round-shaped clusters
- We need to specify number of clusters in advance

How many clusters?

- The number of clusters is defined for some problems, e.g., classifying news into a fixed set of topics/interests
- For others, there is no clear way to select the best number of clusters
- The error (within cluster scatter) decreases with increasing number of clusters, using a test set or cross validation is not useful either
- A common approach is clustering for multiple K values, and picking where there is an 'elbow' in the graph of the error function

How many clusters?



This plot is sometimes called a *scree plot*.

K-medoids

- K-medoids algorithm is an alternation of K-means
- Instead of calculating centroids, we try to find most typical data point (medoids) at each iteration
- K-medoids can work with distances, does not need feature vectors to be in an Euclidean space
- It is less sensitive to outliers
- It is computationally more expensive than K-means

Hierarchical clustering

- Instead of a flat division to clusters as in K-means, hierarchical clustering builds a hierarchy based on similarity of the data points
- There are two main 'modes of operation':

Bottom-up or *agglomerative* clustering

- starts with individual data points,
- merges the clusters until all data is in a single cluster

Top-down or *divisive* clustering

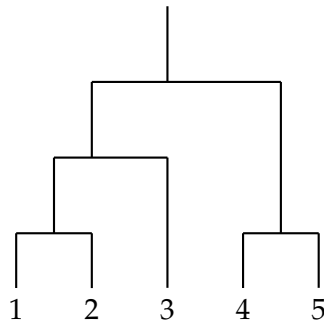
- starts with a single cluster,
- and splits until all leaves are single data points

Hierarchical clustering

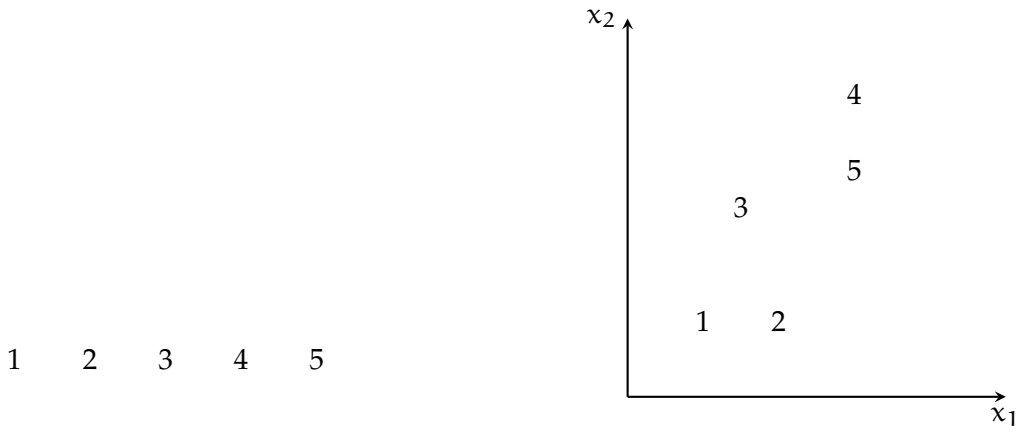
- Hierarchical clustering operates on distances (or similarities)
- The result is a binary tree called *dendrogram*
- Dendrograms are easy to interpret (especially if data is hierarchical)
- The algorithm does not commit to the number of clusters K from the start, the dendrogram can be 'cut' at any height for determining the clusters

Agglomerative clustering

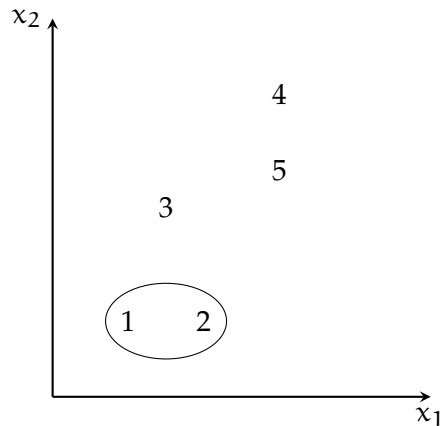
1. Compute the similarity/distance matrix
2. Assign each data point to its own cluster
3. Repeat until no clusters left to merge
 - Pick two clusters that are most similar to each other
 - Merge them into a single cluster



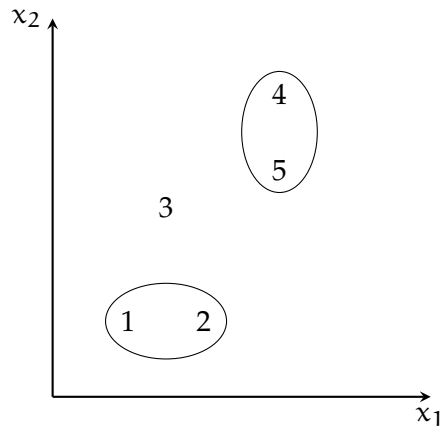
Agglomerative clustering demonstration



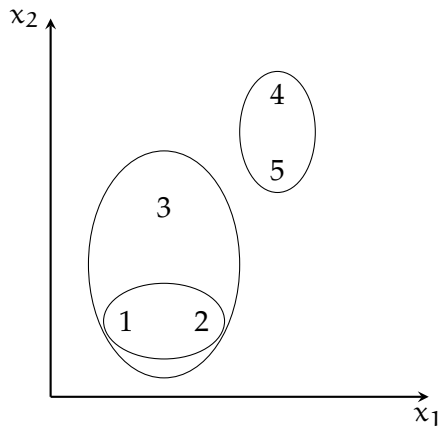
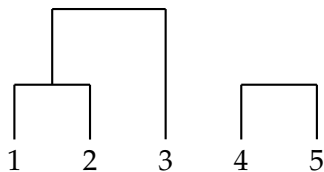
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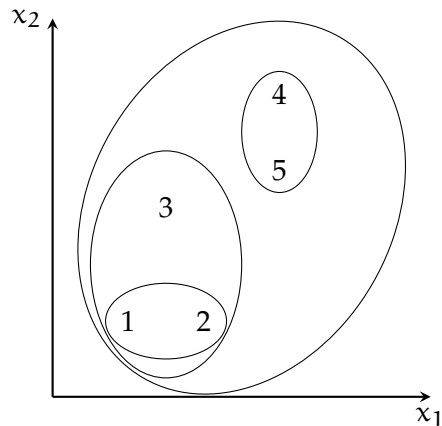
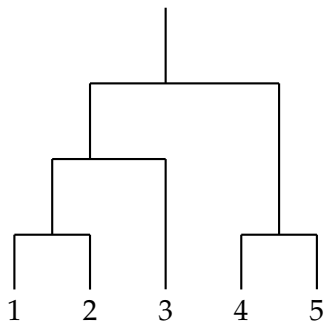
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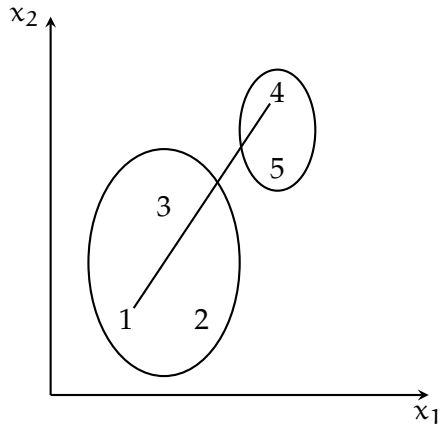


Agglomerative clustering demonstration



How to calculate between cluster distances

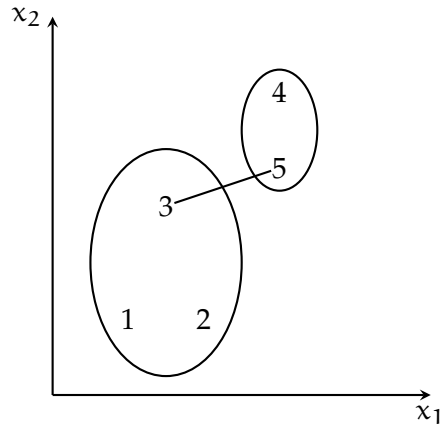
Complete maximal inter-cluster distance



How to calculate between cluster distances

Complete maximal inter-cluster distance

Single minimal inter-cluster distance

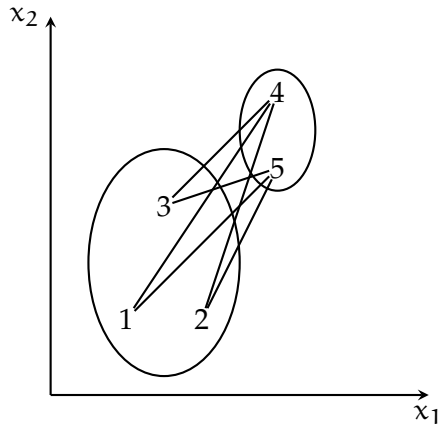


How to calculate between cluster distances

Complete maximal inter-cluster distance

Single minimal inter-cluster distance

Average mean inter-cluster distance



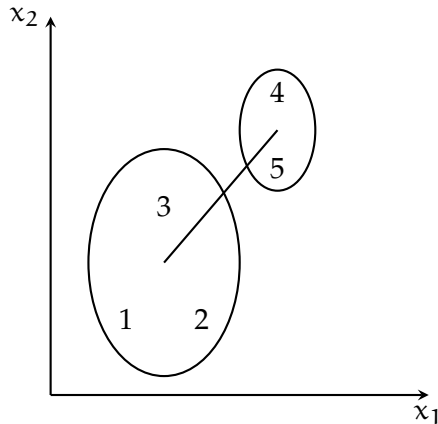
How to calculate between cluster distances

Complete maximal inter-cluster distance

Single minimal inter-cluster distance

Average mean inter-cluster distance

Centroid distance between the
centroids



Note: we only need distances, (feature) vectors are not necessary

Clustering evaluation

Evaluating clustering results is often non-trivial

- Internal evaluation is based a metric that aims to indicate ‘good clustering’: e.g., *Dunn index*, *gap statistic*, *silhouette*
- External metrics can be useful if we have labeled *test* data: e.g., *V-measure*, *B³ed F-score*
- The results can be tested on the target application: e.g., word-clusters evaluated based on their effect on parsing accuracy
- Human judgments, manual evaluation – ‘looks good to me’

Clustering evaluation

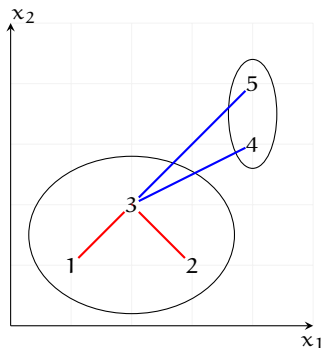
internal metric example: silhouette

$$s_i = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

where

$a(i)$ average distance between object i and objects in the same cluster

$b(i)$ average distance between object i and objects in the *closest* cluster

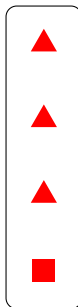


Clustering evaluation

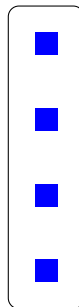
external metrics: general intuition

- We want clusters that contain members of a single gold-standard class (homogeneity)
- We want all members of a class to be in a single cluster (completeness)

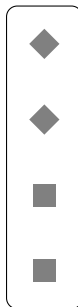
Cluster 1



Cluster 2



Cluster 3



Note the similarity with precision and recall.

Clustering: some closing notes

- Clustering evaluation is not straightforward
- Some clustering methods are unstable, slight changes in the data or parameter choices may change the results drastically
- Approaches against instability include some validation methods, or producing 'probabilistic' dendrograms by running clustering with different options
- Reading suggestion: James et al. (2023, section 12.4)