Lecture 10: Hierarchical Agglomerative Clustering

Introduction to Machine Learning

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Definition: hierarchical clustering

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- **Bottom-up approach (agglomerative*)**: Each observation starts in its own cluster, and **pairs of clusters are merged as one moves up the hierarchy**. We need to decide when to **merge** clusters.
- **Top-down approach (divisive*)**: All observations start in one cluster, and **splits are performed recursively as one moves down the hierarchy**. We need to decide when to **split** clusters.

Cluster linkage

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- A measure of dissimilarity between *sets* of observations.

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Among the most popular,

1. Ward
2. Complete
3. Average
4. Single

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$$
\begin{aligned}
W(A,B) &= \sum_{x \in A \cup B} ||x - \mu_{A \cup B}||^2 - \sum_{x \in A} ||x - \mu_A||^2 - \sum_{x \in B} ||x - \mu_B||^2 \\
&= \frac{|A| \times |B|}{|A \cup B|} ||\mu_A - \mu_B||^2
\end{aligned}
$$

Cluster linkage: Complete

Complete linkage

The **complete linkage criterion** minimizes the maximum distance between observations of pairs of clusters.

Cluster linkage: Complete

Complete linkage

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Given a dissimilarity d and two sets A and B,

$$C(A, B) = max_{A \in A, b \in B} d(a, b)$$

Cluster linkage: Single

Single linkage

The **single linkage criterion** minimizes the distance between the closest observations of pairs of clusters.

Cluster linkage: Single

Single linkage

The **single linkage criterion** minimizes the distance between the closest observations of pairs of clusters.

Given a dissimilarity d and two sets A and B,

$$S(A, B) = min_{a \in A, b \in B} d(a, b)$$

Cluster linkage: Average

Average linkage

The **average linkage criterion** minimizes the average of the distances between all observations of pairs of clusters.

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Average linkage

The **average linkage criterion** minimizes the average of the distances between all observations of pairs of clusters.

Given a dissimilarity d and two sets A and B,

$$A(A, B) = \frac{1}{|A| \times |B|} \sum_{a \in A} \sum_{b \in B} d(a, b)$$

Cluster linkage

Question

Compute the linkage criterion of *ward*, *complete*, *average*, *single* between the following sets of $\mathbb{R}^2$ vectors using *Manhattan distance*:

- $A = \{[1, 2], [2, 3], [4, 5]\}$
- $B = \{[3, 1], [4, 5], [1, 5]\}$

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Clusters are assigned by cutting the algorithm at a selected value for the Linkage criterion.

Example

Question

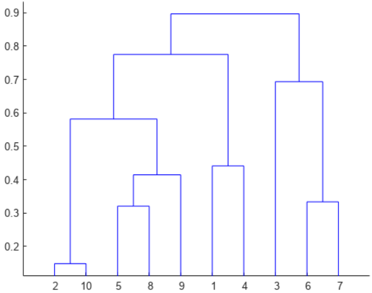
Using single linkage criterion and manhattan distance, perform Hierarchical Agglomerative Clustering on the following dataset. Test different cut-off values for final clusters.

Sepal length	Sepal width	Petal length
5	2	1
4	3	1
6	5	4
7	1	5

Dendrograms

Dendrograms

A **dendrogram*** is a diagram representing a tree. In the case of hierarchical clustering, it consists in representing graphically the clusters and their linkage criterion.



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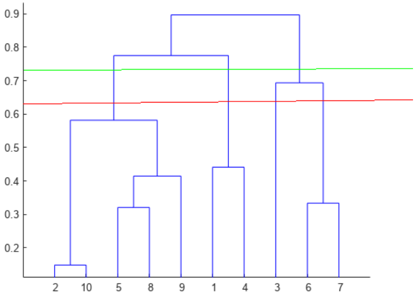

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- The dendogram can show splits that "make sense"
- Plot clustering quality scores *vs* the number of clusters

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- No need to perform the computations again when changing the number of clusters

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Limits

- Number of clusters has to be inferred

Questions

Questions ?