Aglomerative Clustering and Clustering Evaluation

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Hierarchical clustering

Each observation starts in its own cluster, and clusters are successively merged together.

The linkage criteria:

- **Mimimum (Single linkage)** minimizes the minimum distance between pairs of clusters.

$$d_{single} = \min\{d(x_i, x_j),\ i \in A, j \in B\}$$

- **Maximum (Complete linkage)** minimizes the maximum distance between pairs of clusters.

$$d_{complete} = \max\{d(x_i, x_j),\ i \in A, j \in B\}$$

- **Average linkage** minimizes the average of the distances between all observations of pairs of clusters.

$$d_{average} = \frac{1}{|A| \cdot |B|} \sum_{i \in A} \sum_{j \in B} d(x_i, x_j)$$

- **Cenroid linkage** minimizes the distance between centers of clusters.

$$d_{centroid} = d\left(\frac{1}{|A|} \sum_{i \in A} x_i, \frac{1}{|B|} \sum_{i \in B} x_i\right)$$

Hierarchical clustering

- **Ward linkage** is a variance minimizing approach. The distance between two clusters A and B is how much the sum of saquares will increase when we merge them. It is similar to the k-means objective function but tackled with an agglomerative hierarchical approach.

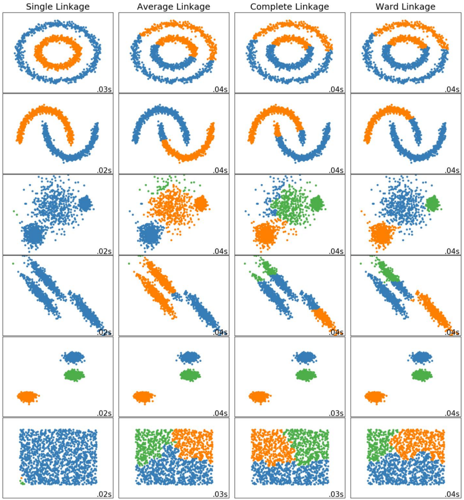
  $$d_{Ward}(A,B) = \sum_{i \in A \cup B} ||x_i - m_{A \cup B}||^2 - \sum_{i \in A} ||x_i - m_A||^2 - \sum_{i \in B} ||x_i - m_B||^2,$$

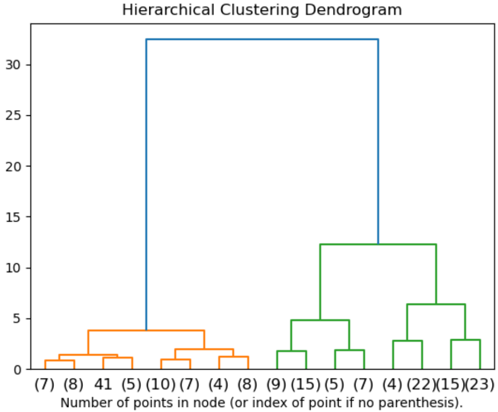
  where m_X is the mean (center) of cluster X. It also corresponds to the squared distance between the centers of the clusters

  $$d_{Ward}(A,B) = \frac{n_A n_B}{n_A + n_B} ||m_A - m_B||^2,$$

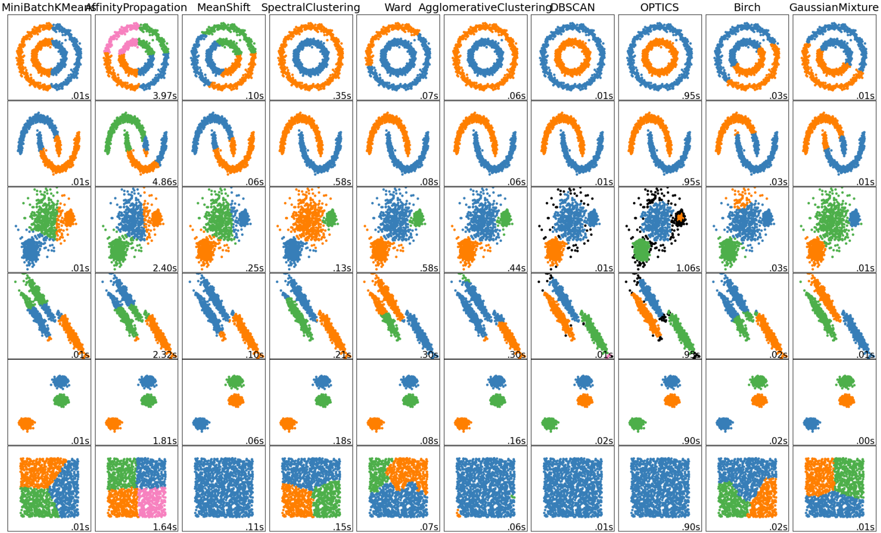
  where n_A and n_B are number of points in clusters A and B, respectively.

Hierarchical clustering





Clustering Methods Comparison



Clustering Evaluation

If you have a testing data available with annotated gold label:

Rosenberg and Hirschberg (2007) define the following objectives for any cluster assignment:

- **Homogeneity** – each cluster contains only members of a single class
- **Completeness** – all members of a given class are assigned to the same cluster
- **V-measure** – their harmonic mean

If you do not have any labelled data:

- **Silhouette coefficient** – "unsupervised" consistency within clusters of data

Homogeneity

Homogeneity – To what extent each cluster contains only members of a single class?

$$h = 1 - \frac{H(C|K)}{H(C)}$$

$H(C|K)$ is the conditional entropy of the cluster assignments given the classes:

$$H(C|K) = -\sum_{c=1}^{|C|}\sum_{k=1}^{|K|}\frac{n_{c,k}}{n}\log\frac{n_{c,k}}{n_k}$$

$H(C)$ is the entropy of the classes:

$$H(C) = -\sum_{c=1}^{|C|}\frac{n_c}{n}\log\frac{n_c}{n}$$

Completeness

Completeness – To what extent all members of a given class are assigned to the same cluster?

$$c = 1 - \frac{H(K|C)}{H(K)}$$

$H(K|C)$ is the conditional entropy of the classes given the cluster assignments:

$$H(K|C) = -\sum_{c=1}^{|C|} \sum_{k=1}^{|K|} \frac{n_{c,k}}{n} \log \frac{n_{c,k}}{n_c}$$

$H(K)$ is the entropy of the clusters:

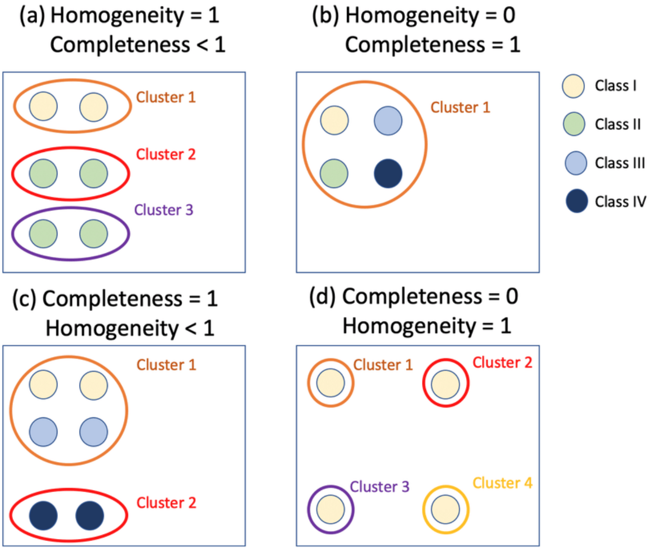
$$H(K) = -\sum_{k=1}^{|K|} \frac{n_k}{n} \log \frac{n_k}{n}$$

V-measure

V-measure – Harmonic mean of homogeneity and comleteness:

$$v = \frac{2 \cdot h \cdot c}{h + c}$$

Homogeneity and Completeness



Silhouette coefficient

How similar an object is to its own cluster (cohesion) compared to other clusters (separation)

Values between -1 and 1

The Silhouette Coefficient s for a single sample is then given as:

$$s_i = \frac{b_i - a_i}{max(a_i, b_i)}, \quad a_i = \frac{1}{C_I - 1} \sum_{j \in C_I, i \neq j} d(i,j), \quad b_i = \min_{J \neq I} \frac{1}{C_J} \sum_{j \in C_J} d(i,j)$$

- a is the mean distance between a sample and all other points in the same cluster
- b is the mean distance between a sample and all other points in the next nearest cluster

The mean over all points of a cluster is a measure of how tightly grouped all the points in the cluster are. Thus the mean over all data of the entire dataset is a measure of how appropriately the data have been clustered.

https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html