Hierarchical Clustering

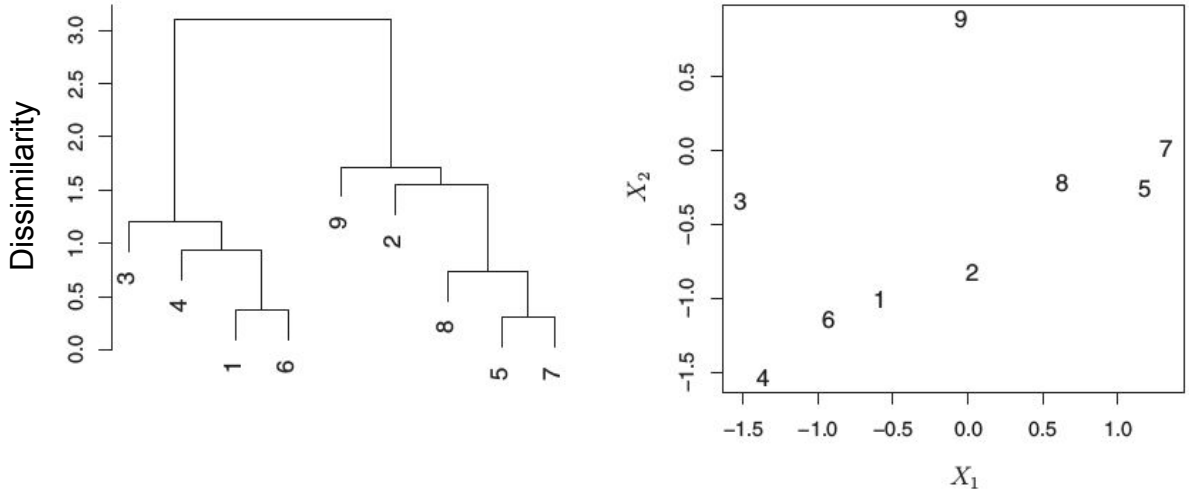
Frank Burkholder

Objectives

- Explain how agglomerative clustering works
- Differentiate hierarchical, agglomerative clustering from Kmeans
- Explain what is shown in a dendrogram
- Be able to perform hierarchical clustering in sklearn

Hierarchical clustering

- Another clustering method (creating groups through *hierarchies*)
- Don’t have to commit to a value of k beforehand
- Results don’t depend on initialization
- Not limited to euclidean distance as the similarity metric
- Easy visualized through dendrograms
    - “Height of fusion” on dendrogram quantifies the separation of clusters



Hierarchical clustering algorithm

Algorithm 10.2 *Hierarchical Clustering* *(Agglomerative, bottom up)*

1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster. (singleton clusters)

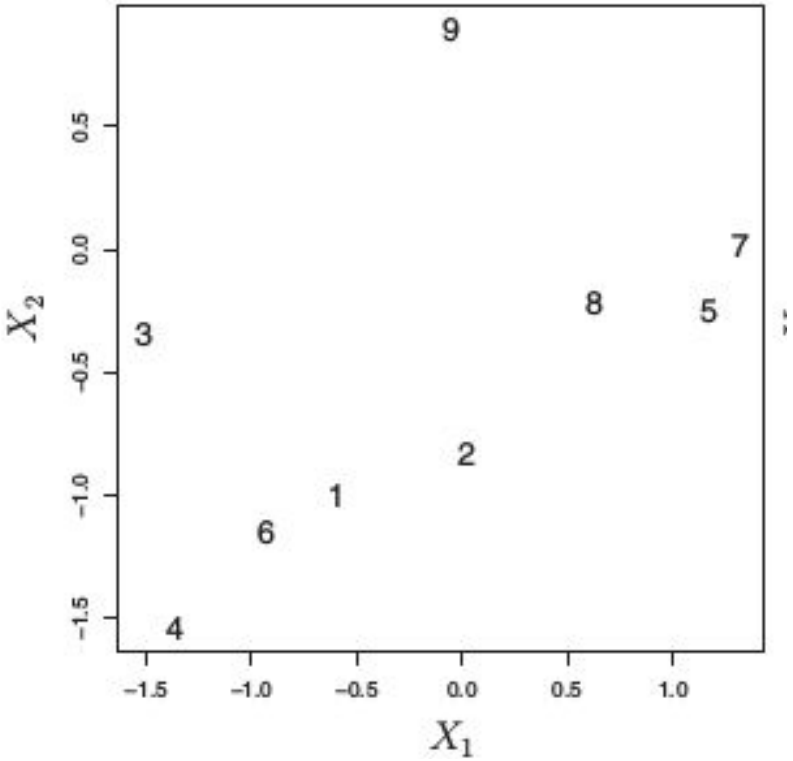
2. For $i = n, n-1, \ldots, 2$:

   (a) Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed. In units of your dissimilarity metric

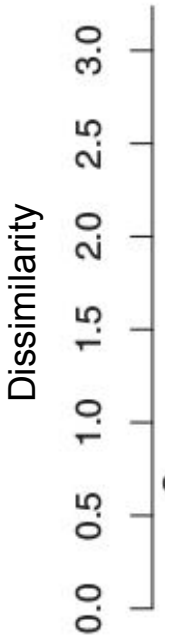
   (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Hierarchical clustering algorithm (visualized)

Data

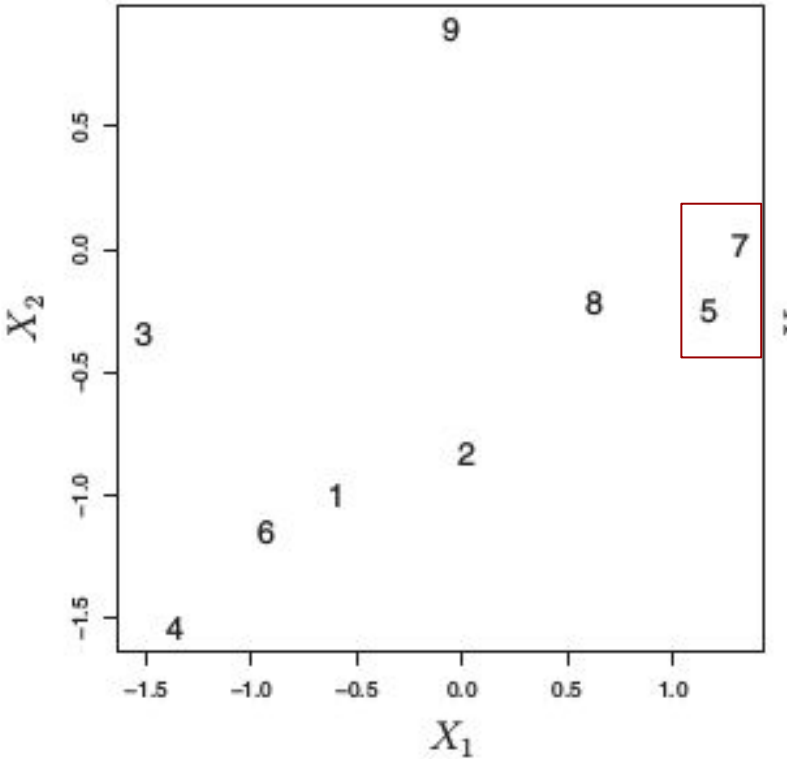


Dendrogram

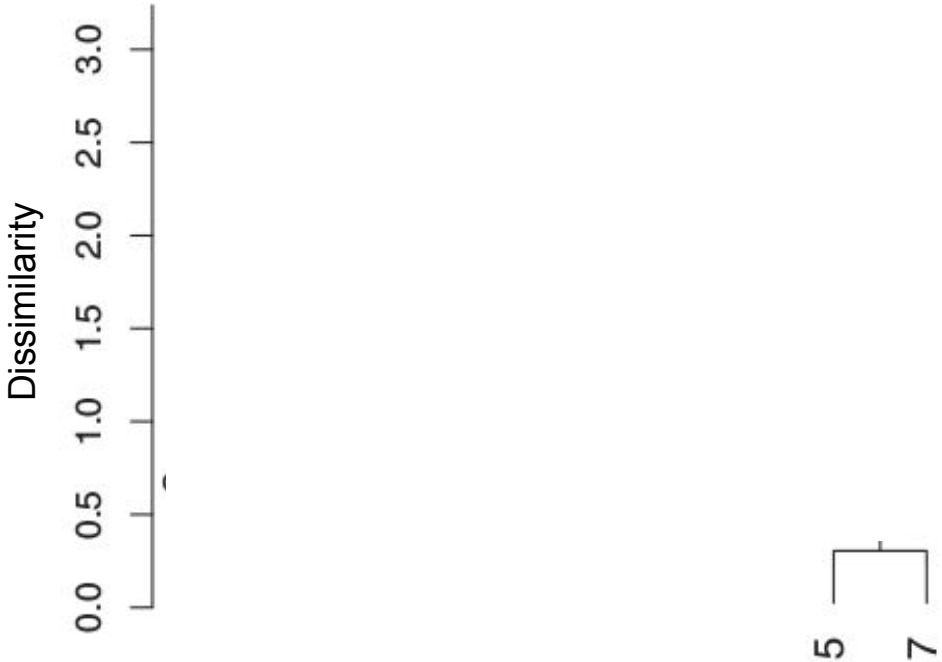


Hierarchical clustering algorithm (visualized)

Data

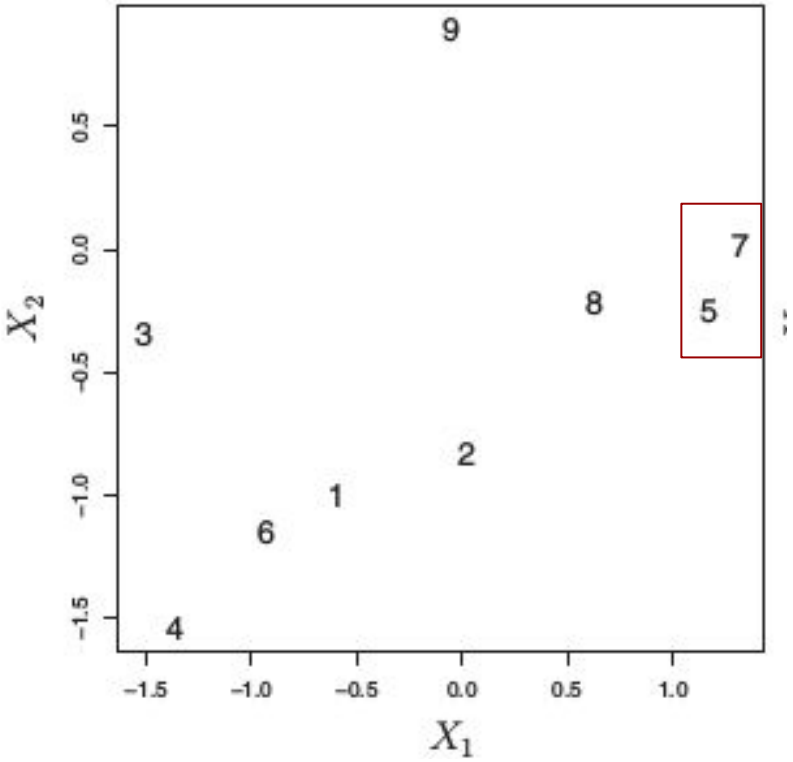


Dendrogram

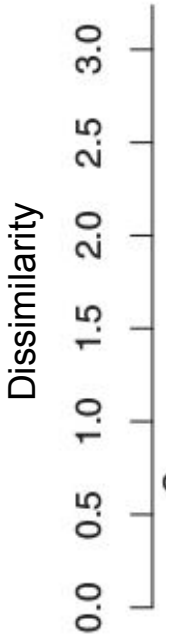


Hierarchical clustering algorithm (visualized)

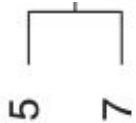
Data



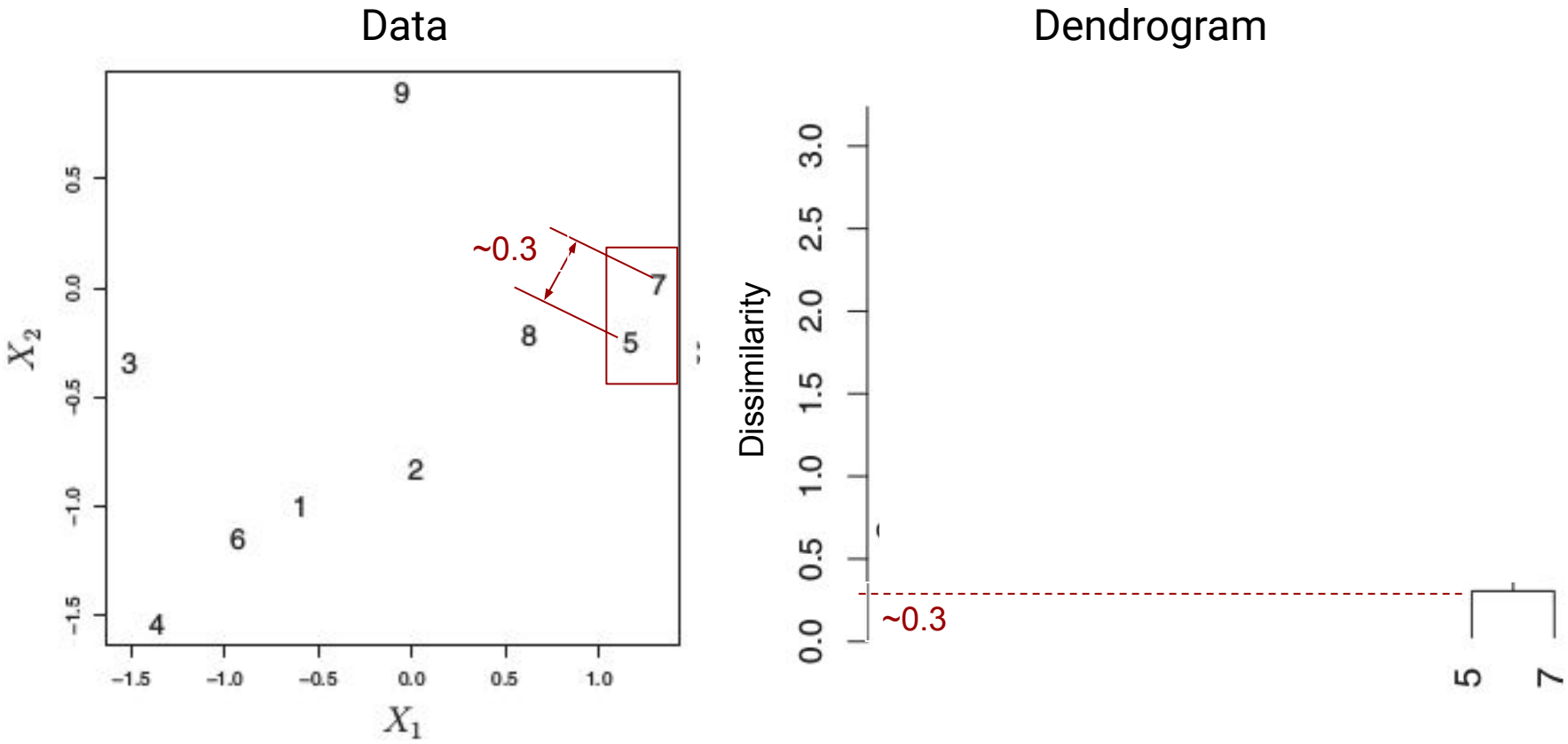
Dendrogram



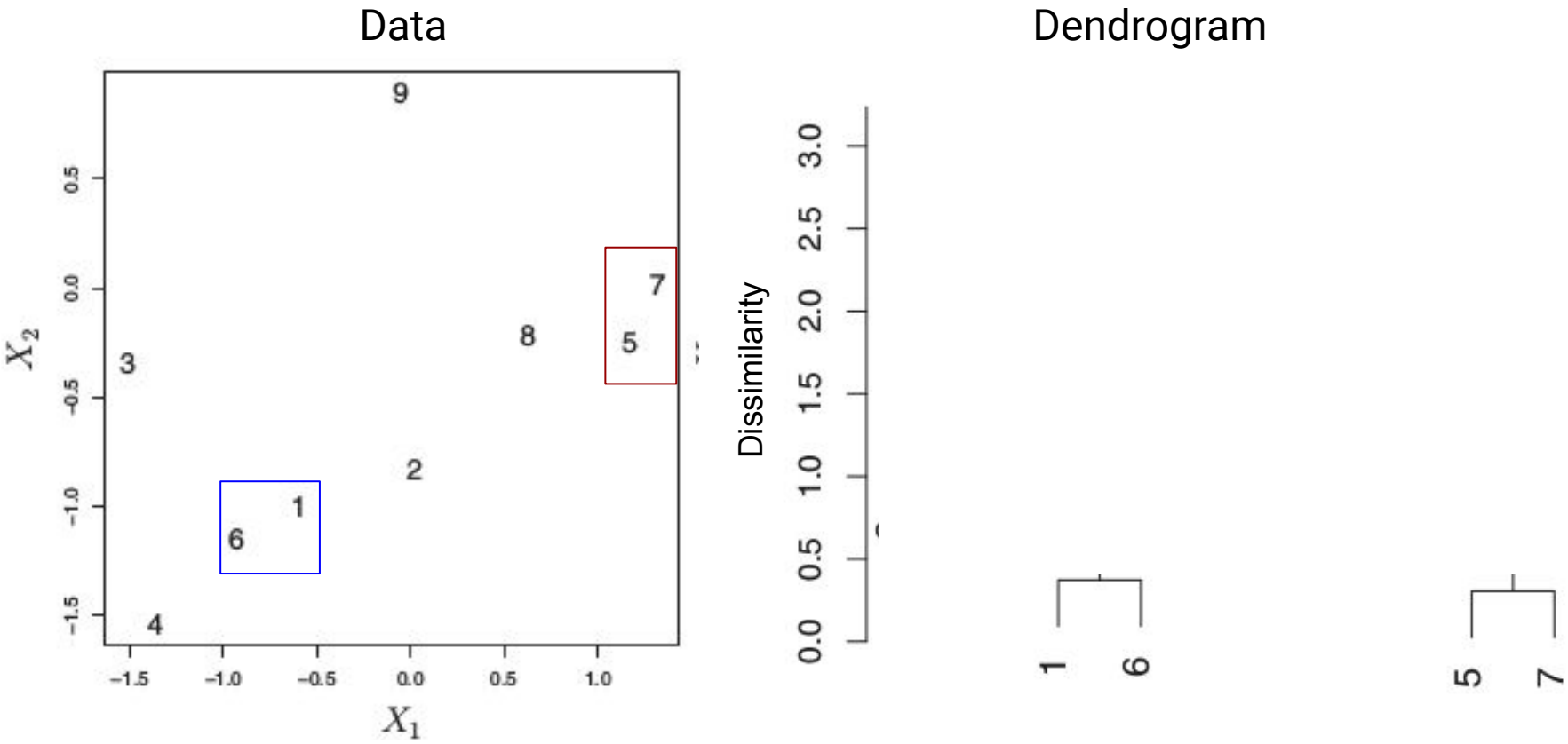
Go through the
pdist_squareform_example.ipynb



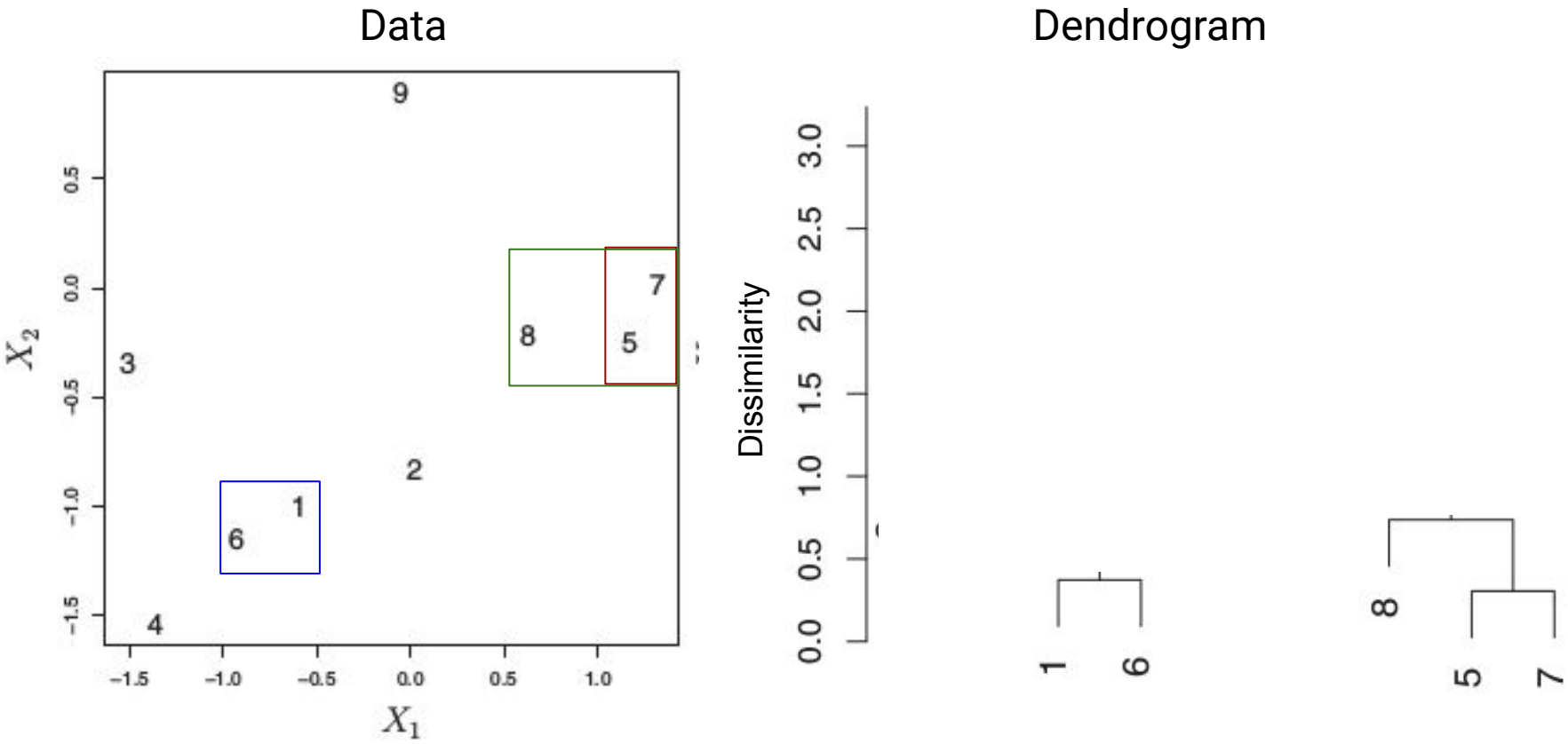
Hierarchical clustering algorithm (visualized)



Hierarchical clustering algorithm (visualized)

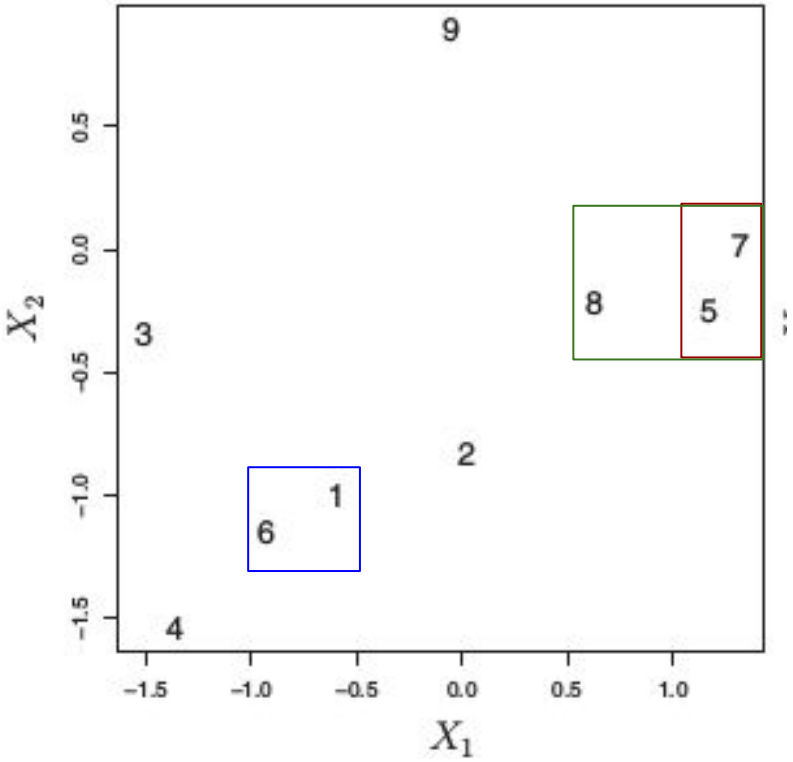


Hierarchical clustering algorithm (visualized)

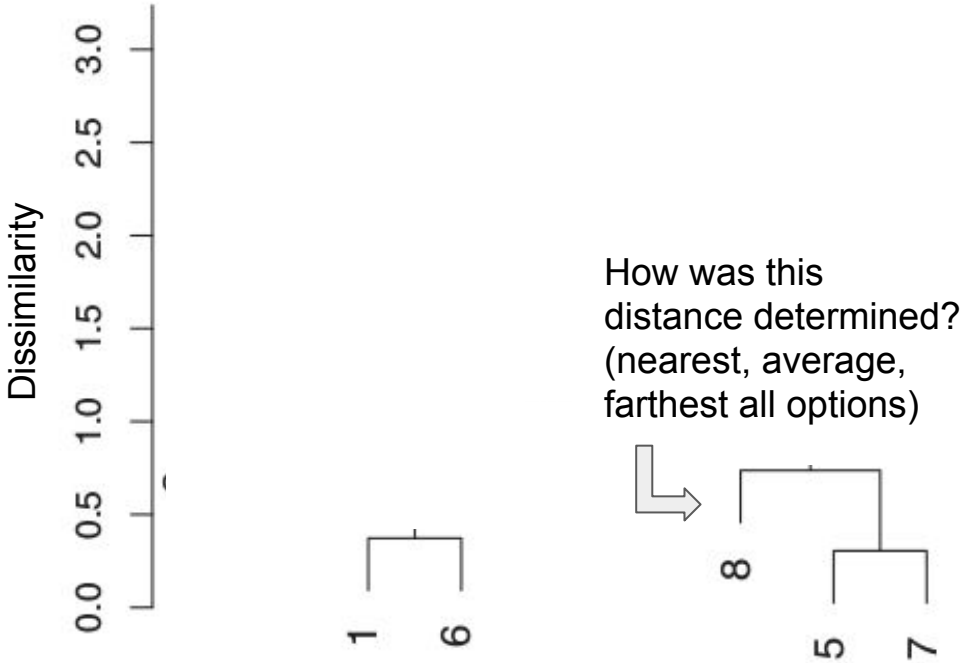


Hierarchical clustering algorithm (visualized)

Data



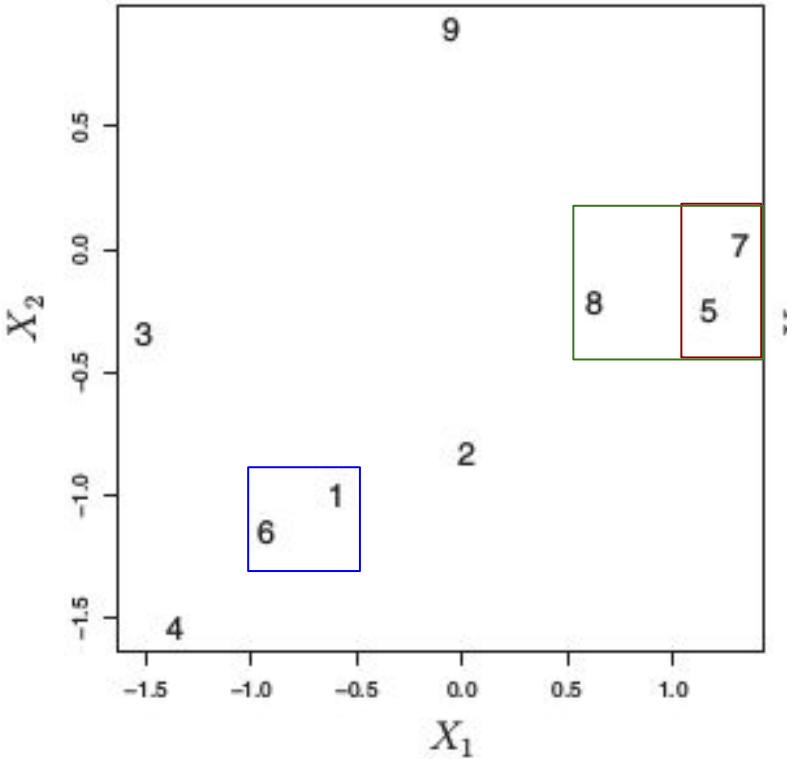
Dendrogram



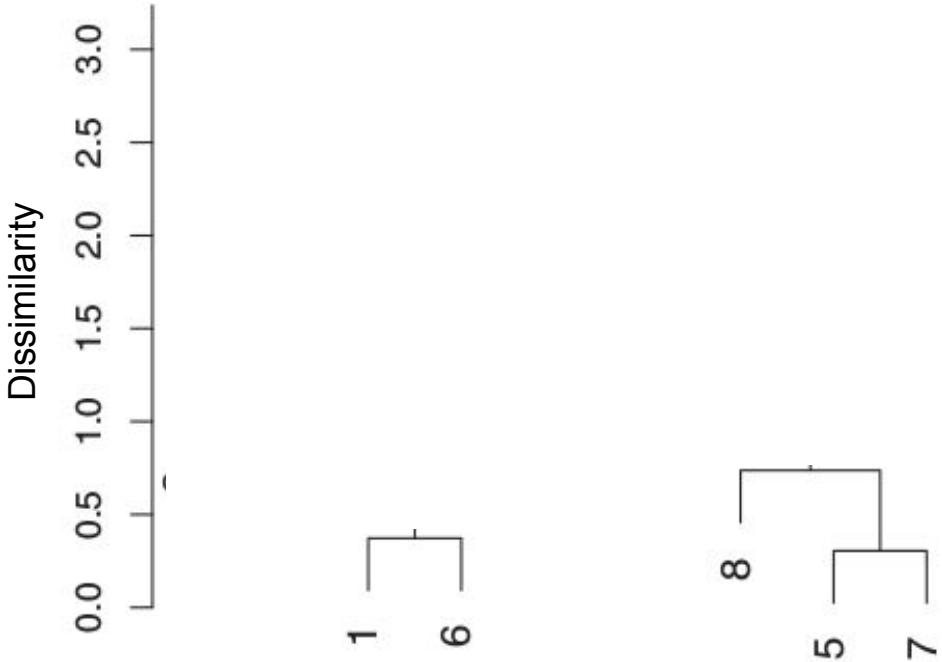
How was this distance determined? (nearest, average, farthest all options)

Breakout: complete the dendrogram

Data



Dendrogram



Breakout: complete the dendrogram

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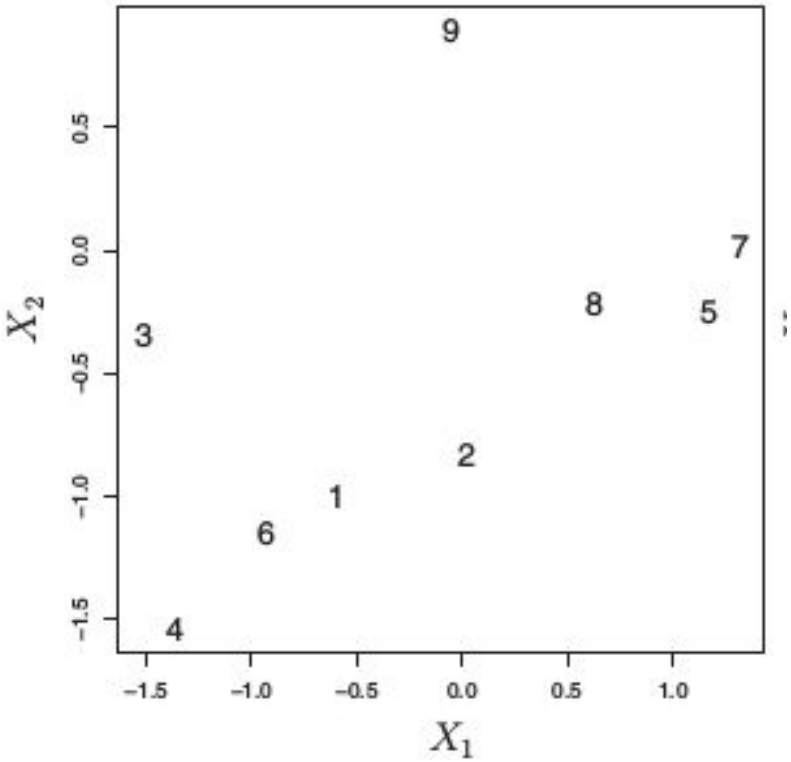
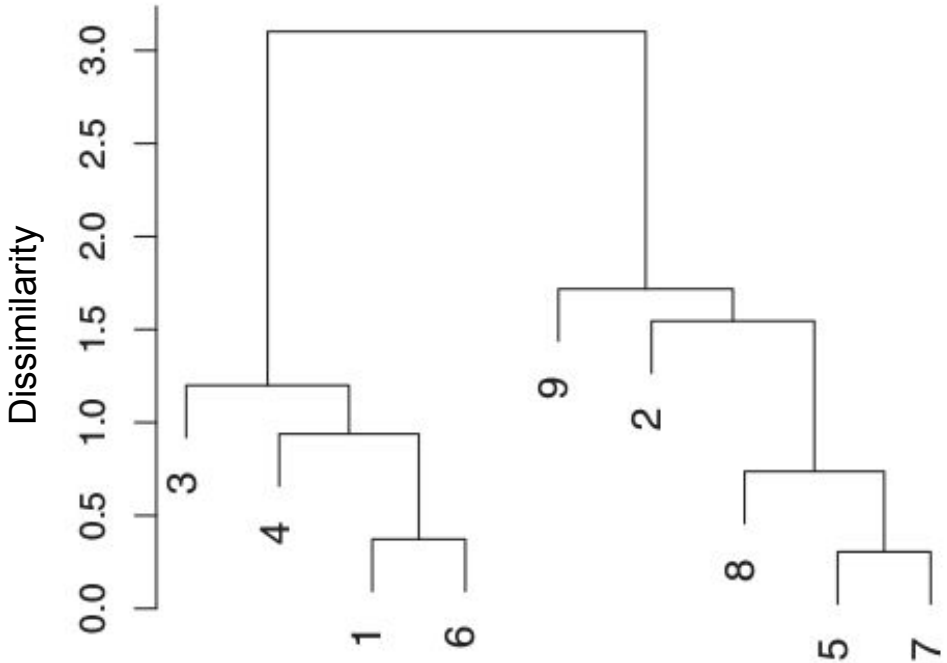


Dendrogram

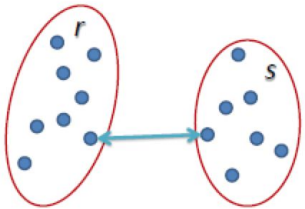


Measures of similarity/dissimilarity between groups

Single Linkage In single linkage hierarchical clustering, the distance between two clusters is defined as the *shortest* distance between two points in each cluster.

"Nearest neighbor"

Drawback: Chaining - several clusters may be joined to just because of a few close cases

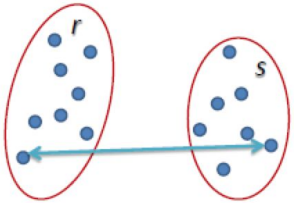


$$L(r,s) = \min(D(x_{ri}, x_{sj}))$$

Complete Linkage In complete linkage hierarchical clustering, the distance between two clusters is defined as the *longest* distance between two points in each cluster.

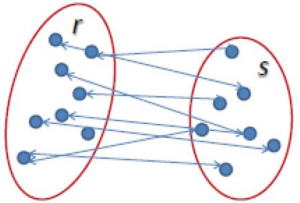
"Farthest neighbor"

Drawback: Cluster outliers prevent otherwise close clusters from merging.



$$L(r,s) = \max(D(x_{ri}, x_{sj}))$$

Average Linkage In average linkage hierarchical clustering, the distance between two clusters is defined as the average distance between each point in one cluster to every point in the other cluster.



$$L(r,s) = \frac{1}{n_r n_s} \sum_{i=1}^{n_r} \sum_{j=1}^{n_s} D(x_{ri}, x_{sj})$$

Average and complete are most common

http://www.saedsayad.com/clustering_hierarchical.htm

Choice of linkage matters

(clusters based on same data)

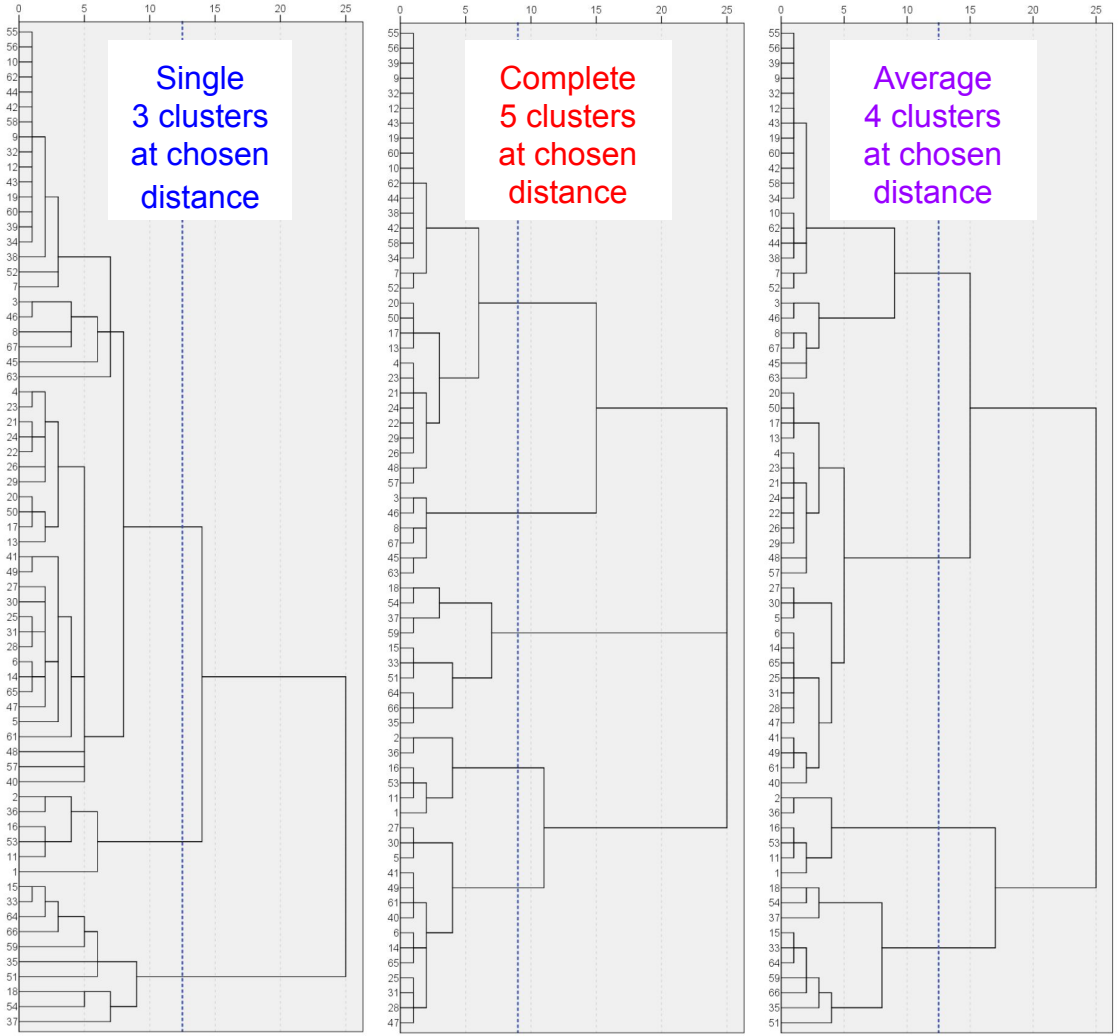
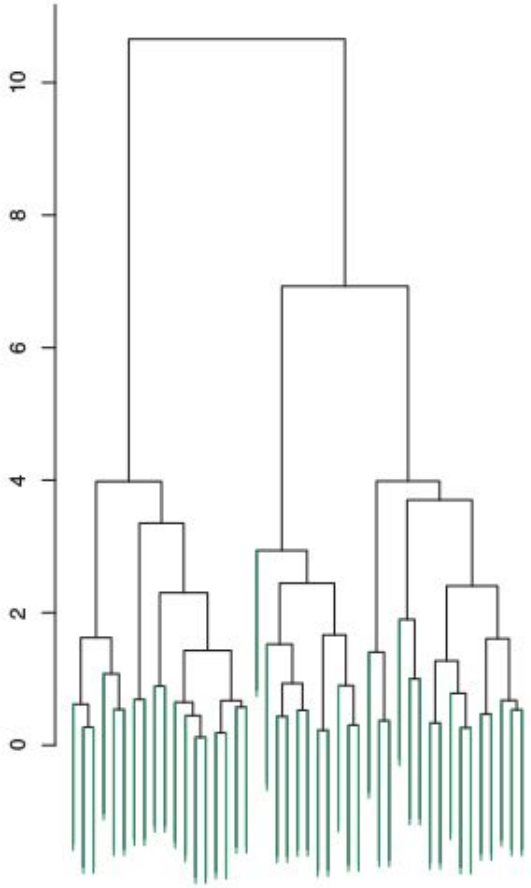
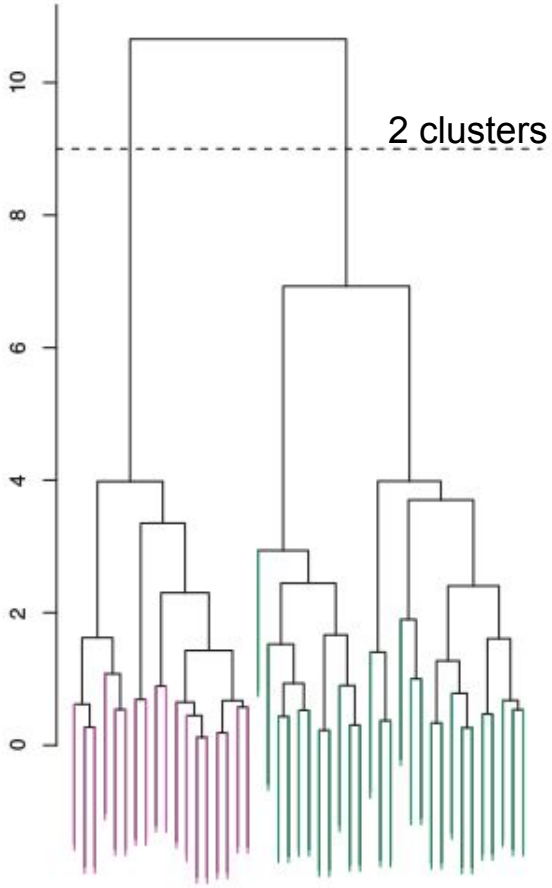


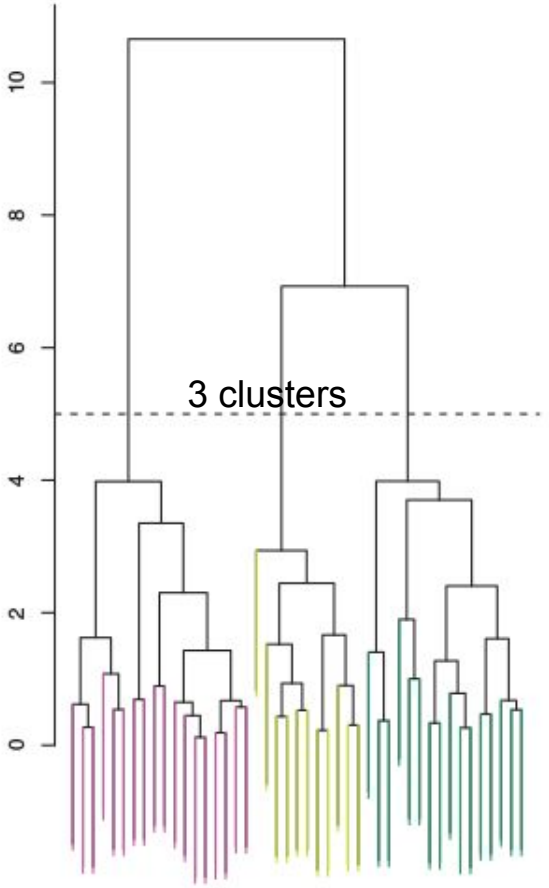
Chart from :

Yim, O. and K.T. Ramdeen, “Hierarchical Cluster Analysis: Comparison of Three Linkage Measures and Application to Psychological Data” The Quantitative Methods for Psychology, vol. 11, no. 1, 2015.

Choice of clusters - where you make the cut







Go through hierarchical clustering example

`hierarchical_clustering_example.ipynb`

Objectives

- Explain how agglomerative clustering works
- Differentiate hierarchical, agglomerative clustering from Kmeans
- Explain what is shown in a dendrogram
- Be able to perform hierarchical clustering in sklearn