Introduction to Machine Learning

Session 3d: Hierarchical Clustering

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Outline

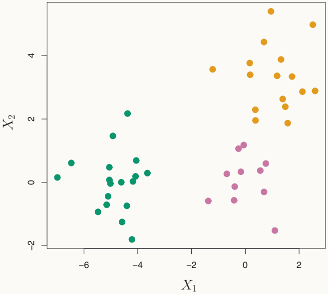
Hierarchical Clustering

Hierarchical Clustering

- A potential disadvantage of K-means clustering is that it requires us to pre-specify the number of clusters K.
- Hierarchical clustering is an alternative approach that does not require us to do that.
- Hierarchical clustering results in a tree-based representation of the observations, called a dendrogram.
- We focus on bottom-up or agglomerative clustering, which is the most common type of hierarchical clustering.

Interpreting a Dendrogram

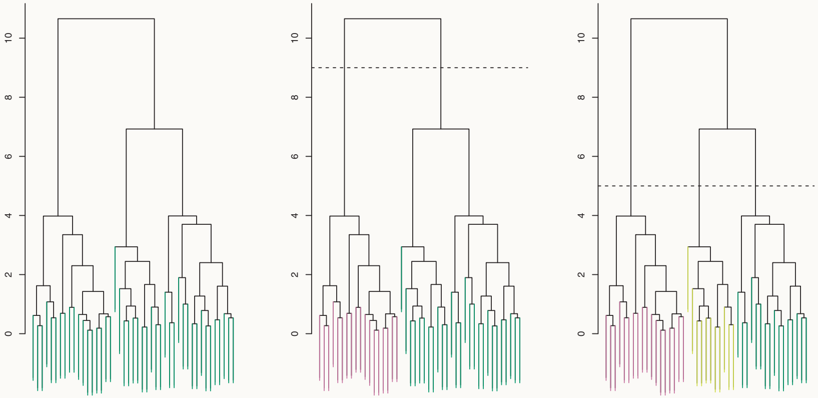
- We have (simulated) data consisting of 45 observations in two-dimensional space.
- The data were generated from a three-class model.
- However, suppose that the data were observed without the class labels and we want to perform hierarchical clustering.



(Source: James et al. 2013, 391)

Interpreting a Dendrogram

Results obtained from hierarchical clustering (with complete linkage)



(Source: James et al. 2013, 392)

Interpreting a Dendrogram

- Each leaf of the dendrogram represents an observation.
- As we move up the tree, leaves fuse into branches and branches into other branches.
- Observations that fuse at the bottom of the tree are similar to each other, whereas observations that fuse close to the top are different.
- We compare the similarity of two observations based on the location on the vertical axis where the branches containing the observations are first fused.
- We cannot compare the similarity of two observations based on their proximity along the horizontal axis.

Interpreting a Dendrogram

- How do we identify clusters on the basis of a dendrogram?
- To do this, we make a horizontal cut across the dendrogram (see center and right panels above).
- The sets of observations beneath the cut can be interpreted as clusters.
- One single dendrogram can be used to obtain any number of clusters.
- The height of the cut to the dendrogram serves the same role as the K in K-means clustering: it controls the number of clusters obtained.

Hierarchical Clustering Versus K-Means Clustering

- Hierarchical clustering is called hierarchical because clusters obtained by a cut at a given height are nested within clusters obtained by cuts at any greater height.
- However, this assumption of hierarchical structure might be unrealistic for a given data set.
- Suppose that we have a group of people with a 50-50 split of males and females, evenly split among Americans, Japanese, and French.

Hierarchical Clustering Versus K-Means Clustering

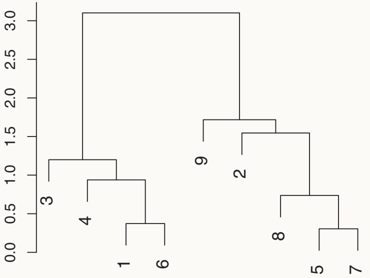
- Suppose further that the best division into two groups splits these people by gender, and the best division into three groups splits them by country.
- In this case, the clusters are not nested.
- Hierarchical clustering might yield worse (less accurate) results than K-means clustering.

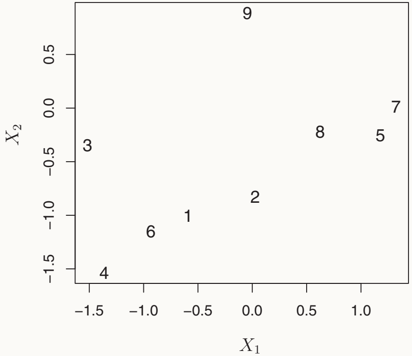
The Hierarchical Clustering Algorithm

- The hierarchical clustering dendrogram is obtained via a simple algorithm.
- We first define a dissimilarity measure between each pair of observations (most often, Euclidean distance is used).
- Starting at the bottom of the dendrogram, each of the n observations is treated as its own cluster.
- The two clusters that are most similar to each other are then fused so that there are now $n-1$ clusters.
- Next the two clusters that are most similar to each other are fused again, leaving us with $n-2$ clusters.
- The algorithm proceeds until all observations belong to one single cluster.

The Hierarchical Clustering Algorithm: Example

Hierarchical clustering dendrogram and initial data

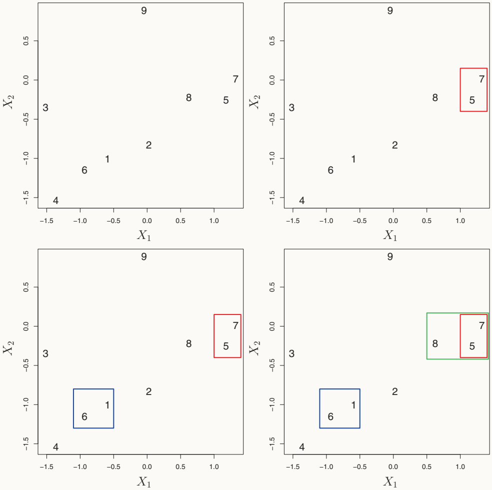




(Source: James et al. 2013, 393)

The Hierarchical Clustering Algorithm: Example

First few steps of the hierarchical clustering algorithm



(Source: James et al. 2013, 396)

The Hierarchical Clustering Algorithm

- In the figure above, how did we determine that the cluster $\{5, 7\}$ should be fused with the cluster $\{8\}$?
- We have a concept of the dissimilarity between pairs of observations, but how do we define the dissimilarity between two clusters if they contain multiple observations?
- We need to extend the concept of dissimilarity between a pair of observations to a pair of groups of observations.
- The linkage defines the dissimilarity between two groups of observations.

Summary of the four most common types of linkage

Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.

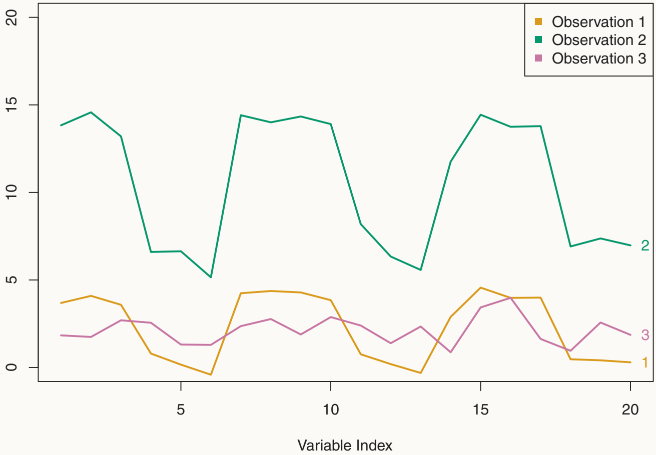
(Source: James et al. 2013, 395)

Choice of Dissimilarity Measure

- So far, we have used Euclidean distance as the dissimilarity measure.
- Sometimes other dissimilarity measures might be preferred.
- An alternative is correlation-based distance which considers two observations to be similar if their features are highly correlated.
- Correlation-based distance focuses on the shapes of observation profiles rather than their magnitudes.

Choice of Dissimilarity Measure

Three observations with measurements on 20 variables



(Source: James et al. 2013, 398)

Practical Issues in Clustering

In order to perform clustering, some decisions must be made.

- Should the observations or features first be standardized in some way?
- In the case of hierarchical clustering:
  - What dissimilarity measure should be used?
  - What type of linkage should be used?
  - Where should we cut the dendrogram in order to obtain clusters?
- In the case of K-means clustering, how many clusters should we look for in the data?