Lecture 25 Cluster Analysis II

ECE 625: Data Analysis and Knowledge Discovery

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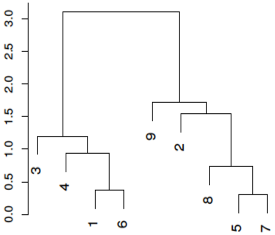
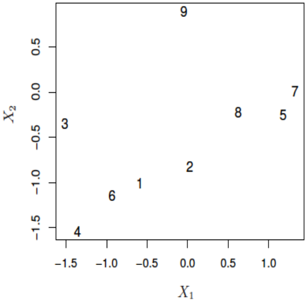
Outline

Another Example

- An illustration of how to properly interpret a dendrogram with nine observations in two-dimensional space. The raw data on the right was used to generate the dendrogram on the left.



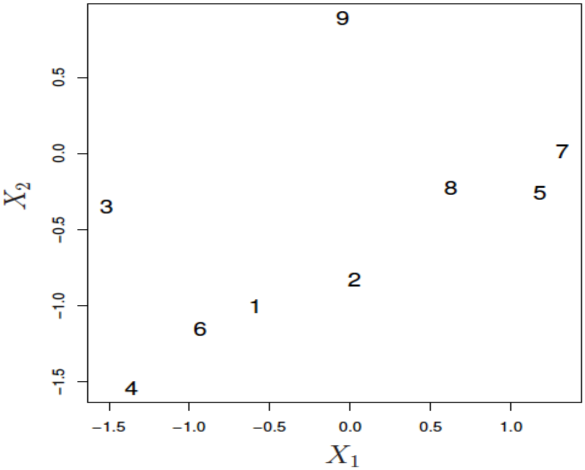


Another Example

- Observations 5 and 7 are quite similar to each other, as are observations 1 and 6.
- However, observation 9 is no more similar to observation 2 than it is to observations 8, 5, and 7, even though observations 9 and 2 are close together in terms of horizontal distance.
- This is because observations 2, 8, 5, and 7 all fuse with observation 9 at the same height, approximately 1.8.

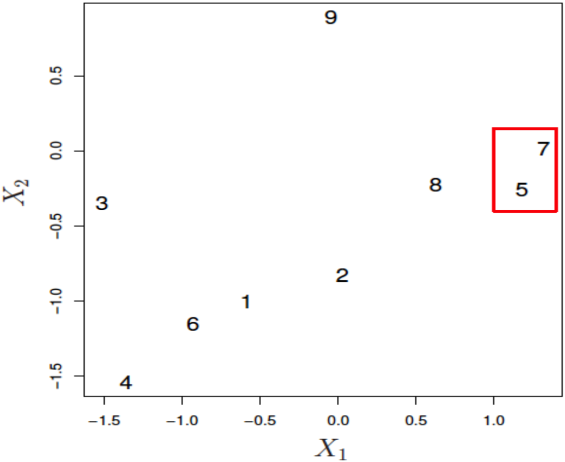
Another Example

Merges in previous example



Another Example

Merges in previous example



Another Example

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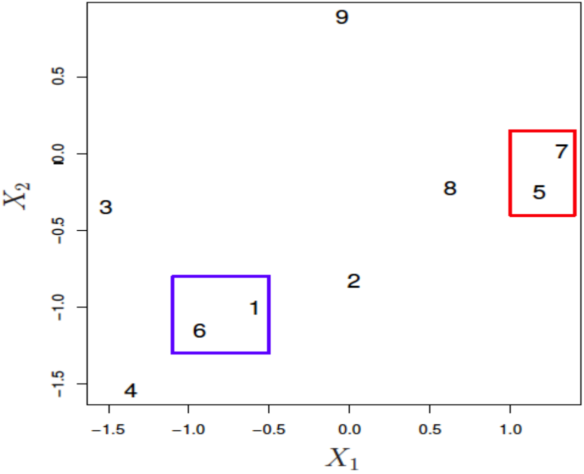

Another Example

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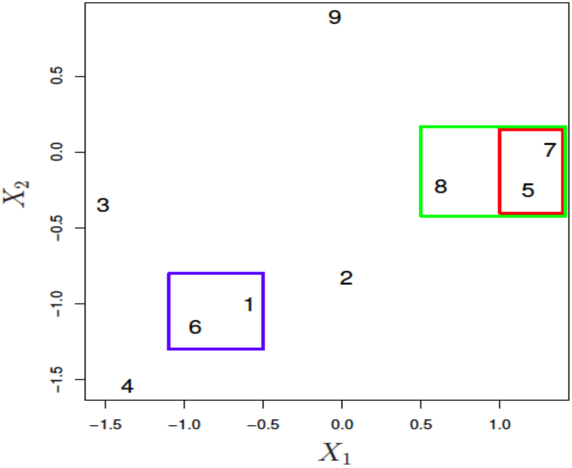
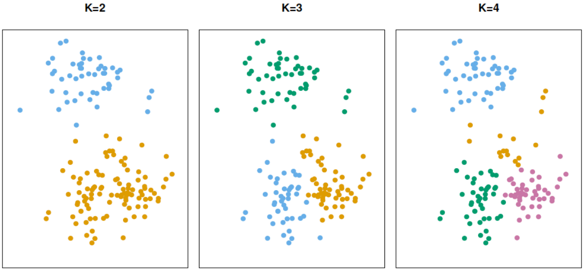


Types of Linkage

- Complete Linkage: Maximal inter-cluster 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 Linkage: Minimal inter-cluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the smallest of these dissimilarities.
- Average Linkage: Mean inter-cluster 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 Linkage: Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B.

K-means Clustering

- In K-means clustering, we seek to partition the observations into a pre-specified number of clusters.
- A simulated data set with 150 observations in 2-dimensional space.



K-means Clustering

- Panels show the results of applying K-means clustering with different values of K, the number of clusters.
- The color of each observation indicates the cluster to which it was assigned using the K-means clustering algorithm.
- Note that there is no ordering of the clusters, so the cluster coloring is arbitrary.
- These cluster labels were not used in clustering; instead, they are the outputs of the clustering procedure.

K-means Clustering

- Let $C_1, \cdots, C_K$ denote sets containing the indices of the observations in each cluster. Theses satisfy two properties:
- 1. $C_1 \cup \cdots \cup C_K = \{1, \cdots, n\}$. In other words, each observation belongs to at least one of the K clusters.
- 2. $C_k \cap C_{k'} = \emptyset$ for all $k \neq k'$. In other words, the clusters are non-overlapping: no observation belongs to more than one cluster.
- For instance, if the ith observation is in the kth cluster, then $i \in C_k$.

K-means Clustering

- The idea behind K-means clustering is that a good clustering is one for which the within-cluster variation is as small as possible.
- The within-cluster variation for cluster C_k is a measure $\mathrm{WCV}(C_k)$ of the amount by which the observations within a cluster differ from each other.
- Hence we want to solve the problem

$$\min_{C_1,\cdots,C_K} \sum_{k=1}^{K} \{WCV(C_k)\}.$$

- In words, this formula says that we want to partition the observations into K clusters such that the total within-cluster variation, summed over all K clusters, is as small as possible.

Within-cluster variation

- Typically we use Euclidean distance

$$WCV(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2,$$

where $|C_k|$ denotes the number of observations in the kth cluster.

- The optimization problem that defines K-means clustering is of the form

$$\min_{C_1,\cdots,C_K} \sum_{k=1}^{K} \left\{ \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}.$$

K-Means Clustering Algorithm

- 1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
- 2. Iterate until the cluster assignments stop changing:
- a) For each of the K clusters, compute the cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
- b) Assign each observation to the cluster whose centroid is closest (where closest is defined using Euclidean distance).

K-Means Clustering Algorithm

- This algorithm is guaranteed to decrease the value of the objective at each step. Why?
- Note that

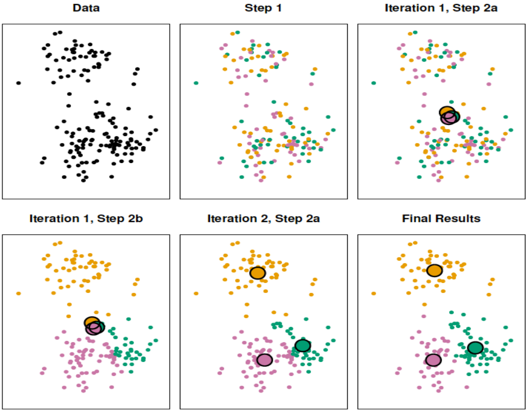
$$\frac{1}{|C_k|}\sum_{i,i'\in C_k}\sum_{j=1}^{p}(x_{ij}-x_{i'j})^2 = 2\sum_{i\in C_k}\sum_{j=1}^{p}(x_{ij}-\bar{x}_{kj})^2,$$

where $\bar{x}_{kj} = \frac{1}{|C_k|}\sum_{i\in C_k} x_{ij}$ is the mean for feature j in cluster C_k.

- In Step 2(a) the cluster means for each feature are the constants that minimize the sum-of-squared deviations.
- In Step 2(b), reallocating the observations can only reduce the objective value.
- However, K-Means is not guaranteed to produce the global minimum. Why not?

Example

The progress of the K-means algorithm with $K = 3$ with 10 iterations.



Example

Different starting values and above each plot is the value of the objective. Three different local optima were obtained, one of which resulted in a smaller value of the objective and provides better separation.

Practical issues

- Should the observations or features first be standardized in some way? For instance, maybe the variables should be centered to have mean zero and scaled to have standard deviation one.
- In the case of hierarchical clustering, What dissimilarity measure should be used? What type of linkage should be used?
- How many clusters to choose? (in both K-means or hierarchical clustering). Difficult problem. No agreed-upon method.

Summary and Remark

- Hierarchical clustering
- K-means clustering
- Read textbook Chapter 14 and R code
- Do R lab