

Lecture 5: Clustering

Reading: Chapter 10, Sections 3.1-2

STATS 202: Data mining and analysis

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Slide credits: Sergio Bacallado

Clustering

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We will discuss 2 algorithms:

- ▶ K -means clustering
- ▶ Hierarchical clustering

K -means clustering

- K is the number of clusters and must be fixed in advance.

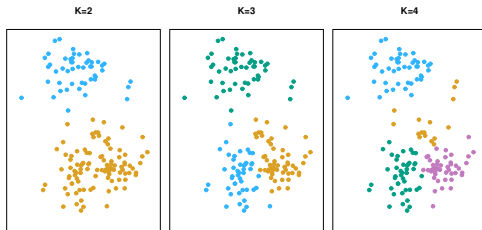


Figure 10.5

K -means clustering

- ▶ K is the number of clusters and must be fixed in advance.
- ▶ The goal of this method is to maximize the similarity of samples within each cluster:

$$\min_{C_1, \dots, C_K} \sum_{\ell=1}^K W(C_\ell)$$

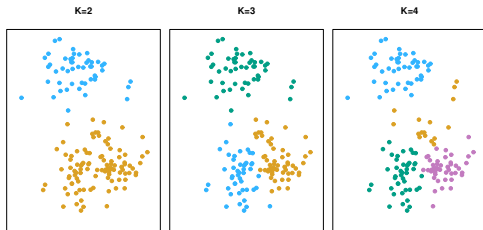


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$$\min_{C_1, \dots, C_K} \sum_{\ell=1}^K W(C_\ell) \quad ; \quad W(C_\ell) = \frac{1}{|C_\ell|} \sum_{i,j \in C_\ell} \text{Distance}^2(x_{i,:}, x_{j,:}).$$

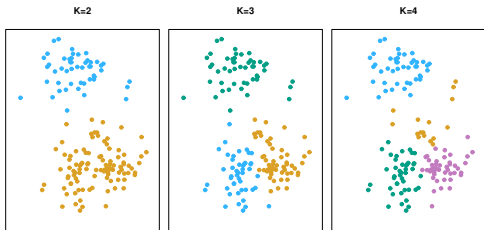


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- ▶ Reassign each sample to the nearest centroid.

K -means clustering algorithm

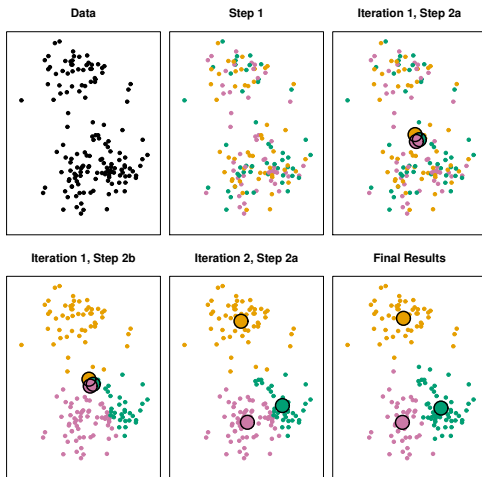


Figure 10.6

Properties of K -means clustering

- ▶ The algorithm always converges to a local minimum of

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- Each initialization could yield a different minimum.

Example: K -means output with different initializations

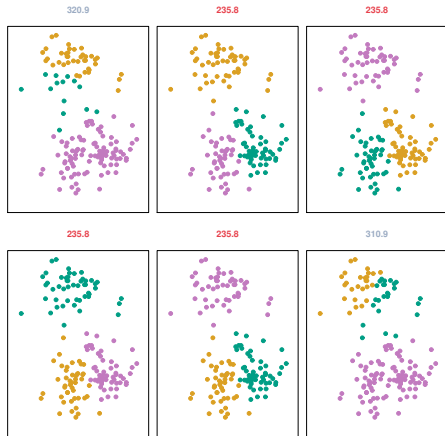
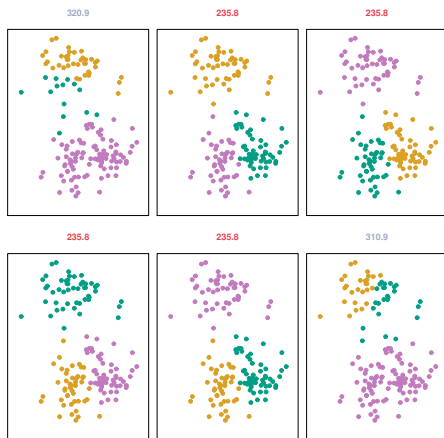


Figure 10.7

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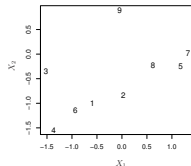
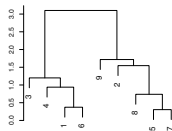
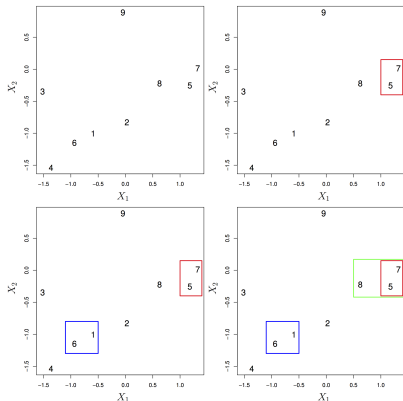
In practice, we start from many random initializations and choose the output which minimizes the objective function.

Figure 10.7

Hierarchical clustering

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Most algorithms for hierarchical clustering are *agglomerative*.

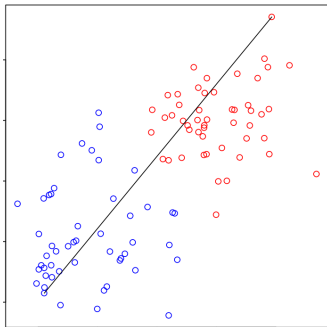


The output of the algorithm is a *dendrogram*. We must be careful about how we interpret the dendrogram.

Notion of distance between clusters

At each step, we link the 2 clusters that are “closest” to each other.

Hierarchical clustering algorithms are classified according to the notion of distance between clusters.



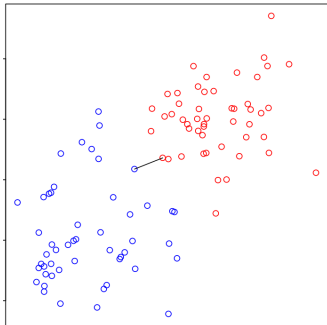
Complete linkage:

The distance between 2 clusters is the *maximum* distance between any pair of samples, one in each cluster.

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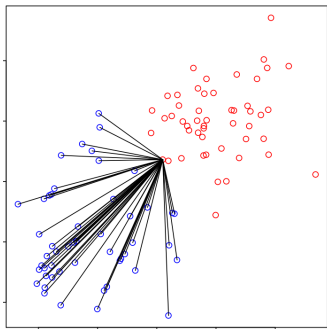
Single linkage:

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Average linkage:

The distance between 2 clusters is the average of all pairwise distances.

Example

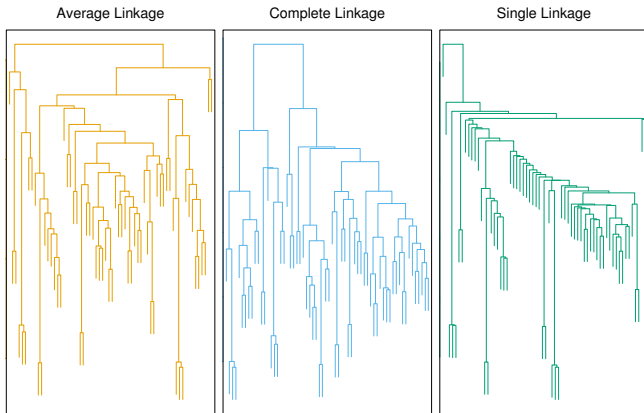


Figure 10.12

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 - ▶ Most important: temper your conclusions.

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 - ▶ Variables with larger variance have a larger effect on the Euclidean distance between two samples.

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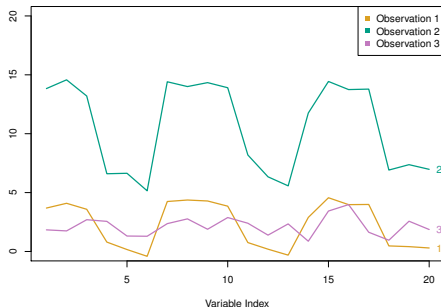
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- ▶ Does Euclidean distance capture dissimilarity between samples?

Correlation distance

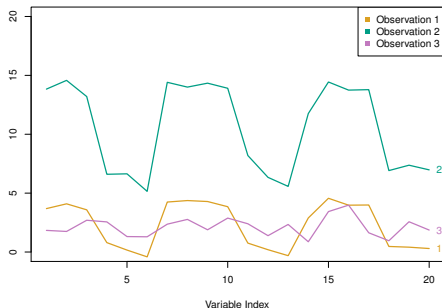
Example: Suppose that we want to cluster customers at a store for market segmentation.

- ▶ Samples are customers
- ▶ Each variable corresponds to a specific product and measures the number of items bought by the customer during a year.



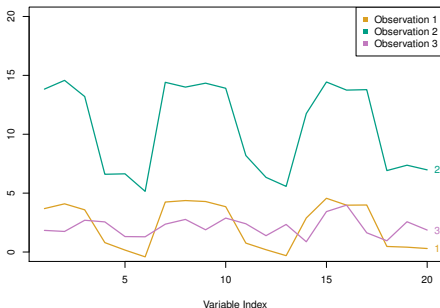
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- ▶ Euclidean distance would cluster all customers who purchase few things (orange and purple).
- ▶ Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- ▶ Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.

