Lecture 5: Clustering

Reading: Chapter 10, Sections 3.1-2

STATS 202: Data mining and analysis

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Clustering

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- K-means clustering
- Hierarchical clustering

K-means clustering

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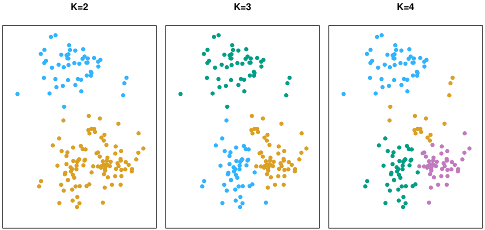
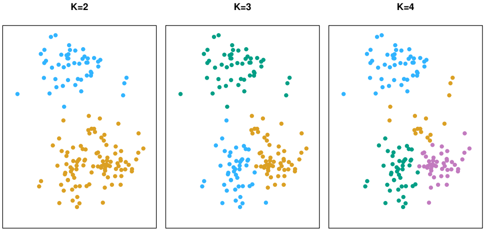


Figure 10.5

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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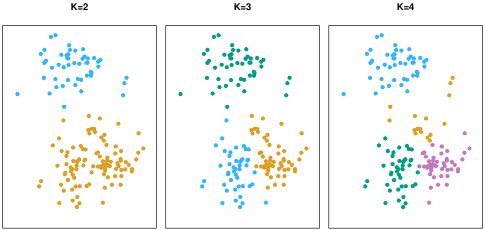

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   - Reassign each sample to the nearest centroid.

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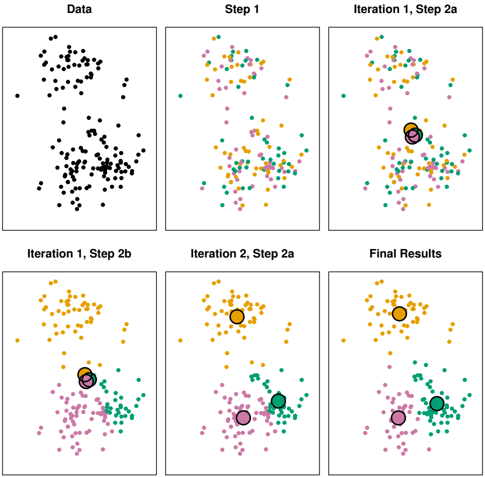

Figure 10.6

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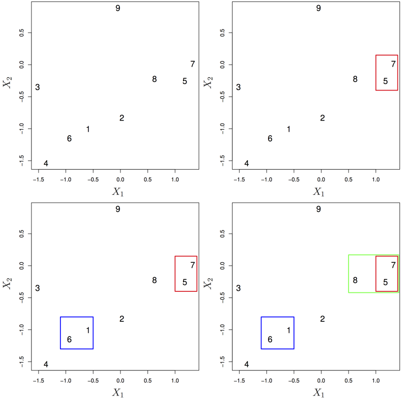
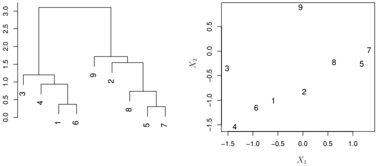
In practice, we start from many random initializations and choose the output which minimizes the objective function.

Hierarchical clustering

Most algorithms for hierarchical clustering are *agglomerative*.



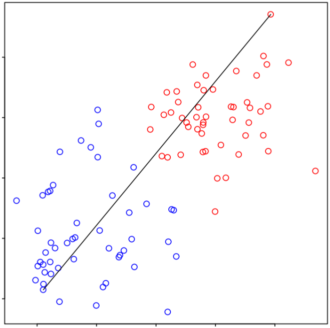


The output of the algorithm is a *dendogram*. We must be careful about how we interpret the dendogram.

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:
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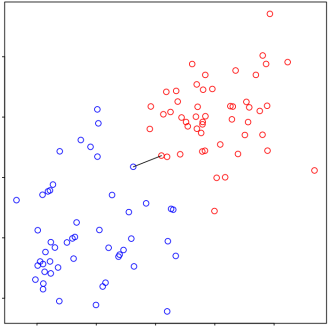

Single linkage:
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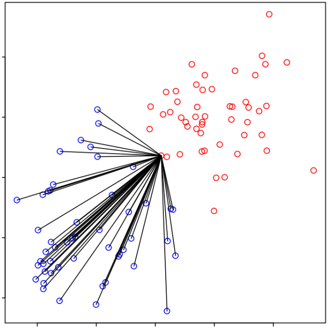

Average linkage:
The distance between 2 clusters is the average of all pairwise distances.

Example

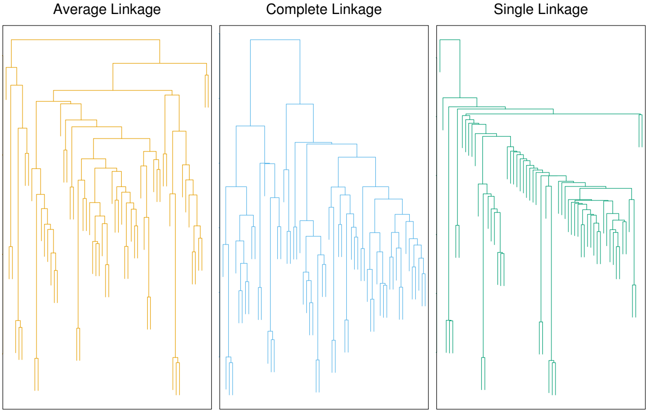

Figure 10.12

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  - Most important: temper your conclusions.

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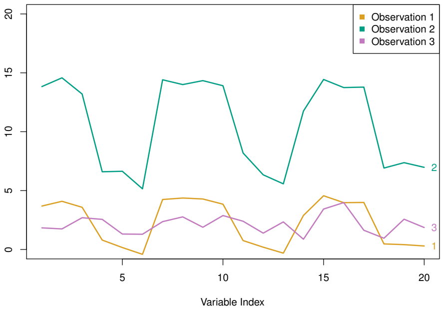
- Does Euclidean distance capture dissimilarity between samples?

Correlation distance

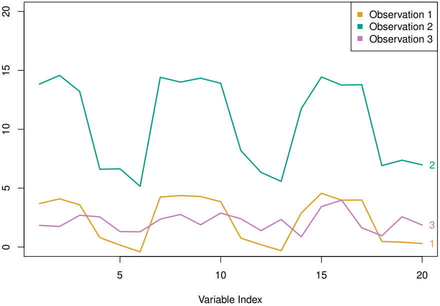
Example: Suppose that we want to cluster customers at a store for market segmentation.

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



Correlation distance

- Euclidean distance would cluster all customers who purchase few things (orange and purple).



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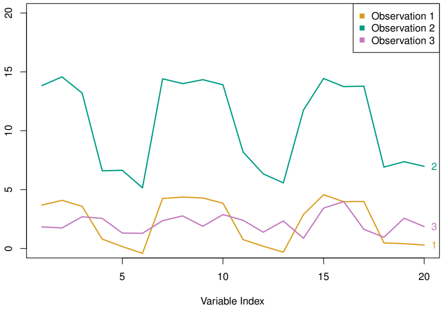

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- Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.