Chapter 10: Unsupervised Learning

Thiago G. Martins | NTNU & Verizon

Spring 2020

Clustering methods

Clustering methods

- Partition the data into different groups
  - Observations within each group are quite similar
  - Observations in different groups are quite different

Clustering methods

- Partition the data into different groups
  - Observations within each group are quite similar
  - Observations in different groups are quite different
- Must define what it means to be similar or different
  - Domain specific considerations

Clustering methods

- Partition the data into different groups
  - Observations within each group are quite similar
  - Observations in different groups are quite different
- Must define what it means to be similar or different
  - Domain specific considerations
- Examples:
  - Different types of cancer
  - Market segmentation
  - Search Engine

PCA vs. Clustering methods

- Both aim to simplify the data via small number of summaries

PCA vs. Clustering methods

- Both aim to simplify the data via small number of summaries
- PCA looks for a low-dim representation that explains good fraction of variance
    - Principal Components

PCA vs. Clustering methods

- Both aim to simplify the data via small number of summaries
- PCA looks for a low-dim representation that explains good fraction of variance
  - Principal Components
- Clustering looks for homogeneous subgroups among the observations
  - Clusters

Types of clustering

- K-means
- hierarchical clustering

K-means clustering

K-means clustering

- It is an approach for partitioning a dataset into K distinct, non-overlapping clusters.

K-means clustering

- It is an approach for partitioning a dataset into K distinct, non-overlapping clusters.
- $C_1, \ldots, C_k$: Sets containing indices of observations in each cluster.
- This sets satisfy two properties:
  - $C_1 \cup C_2 \cup \ldots \cup C_k = \{1, \ldots, n\}$
  - $C_k \cap C_{k'} = \emptyset$ for all $k \neq k'$

Within-cluster variation

- A good cluster is one for which the **within-cluster variation** is **as small as possible**

Within-cluster variation

- A good cluster is one for which the **within-cluster variation** is **as small as possible**
- Within-cluster variation (squared Euclidean distance)

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

Within-cluster variation

- A good cluster is one for which the **within-cluster variation** is **as small as possible**
- Within-cluster variation (squared Euclidean distance)

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

- As small as possible

$$\underset{C_1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} W(C_k) \right\}$$

K-means algorithm

- Find algorithm to solve:

$$\underset{C_1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

K-means algorithm

- Find algorithm to solve:

$$\underset{C_1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

- Difficult problem: K^n ways to partition n observations into K clusters.

K-means algorithm

- Find algorithm to solve:

$$\underset{C_1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

- Difficult problem: K^n ways to partition n observations into K clusters.
- Fortunately, there is a simple algorithm that can provide a local optimum

K-means algorithm

Algorithm 10.1 *K-Means Clustering*

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).

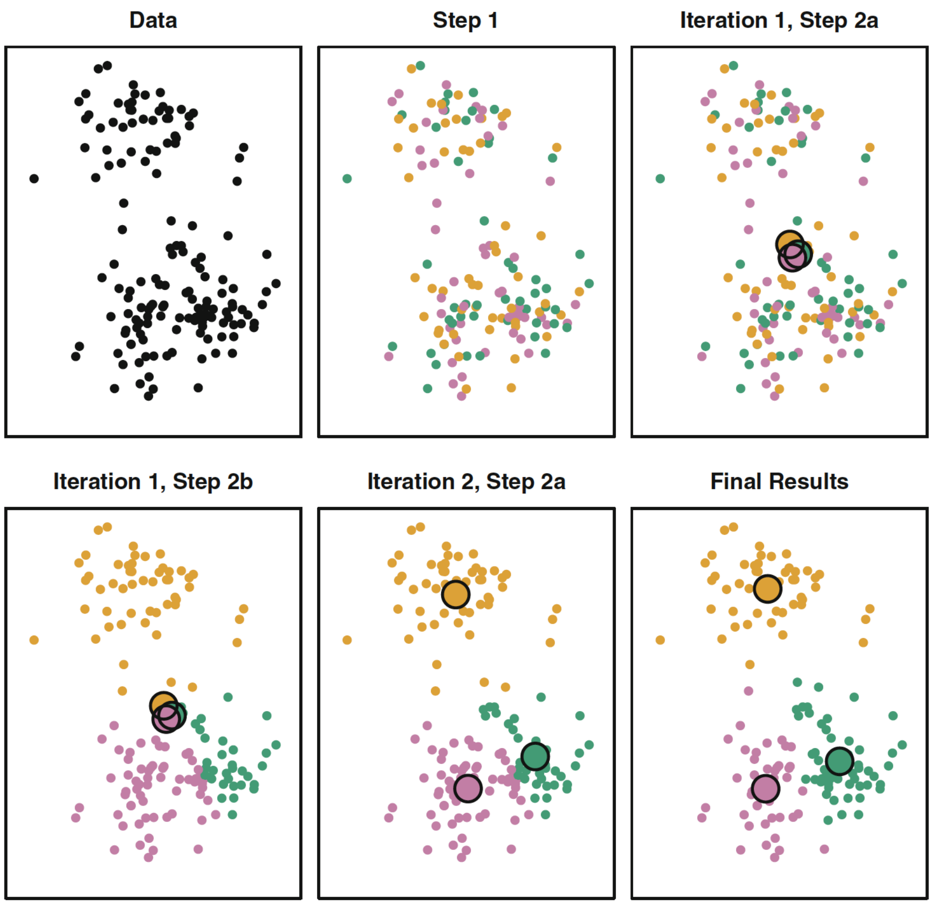
Recommended Exercise 2

Show that the algorithm in the previous slide is guaranteed to decrease the value of the objective

$$\underset{C_1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

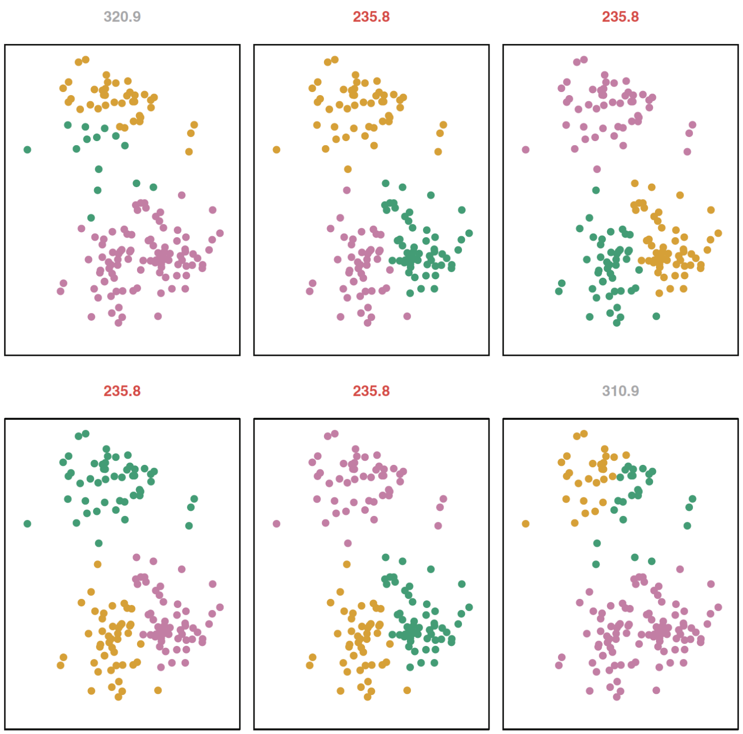
at each step.

K-means algorithm



K-means algorithm

- Depend on random start conditions, need to run multiple times and select the best run



K-means algorithm

- Potential disadvantage of K-means, we need to select K
  - But this is not always a disadvantage, e.g. search engine

Recommended exercise 3

Perform k-means clustering in the New York Times stories dataset.

The pca-examples.rdata can be downloaded from the Blackboard.

Hierarchical Clustering

Hierarchical Clustering

- Does not require us to commit to a particular choice of K in advance

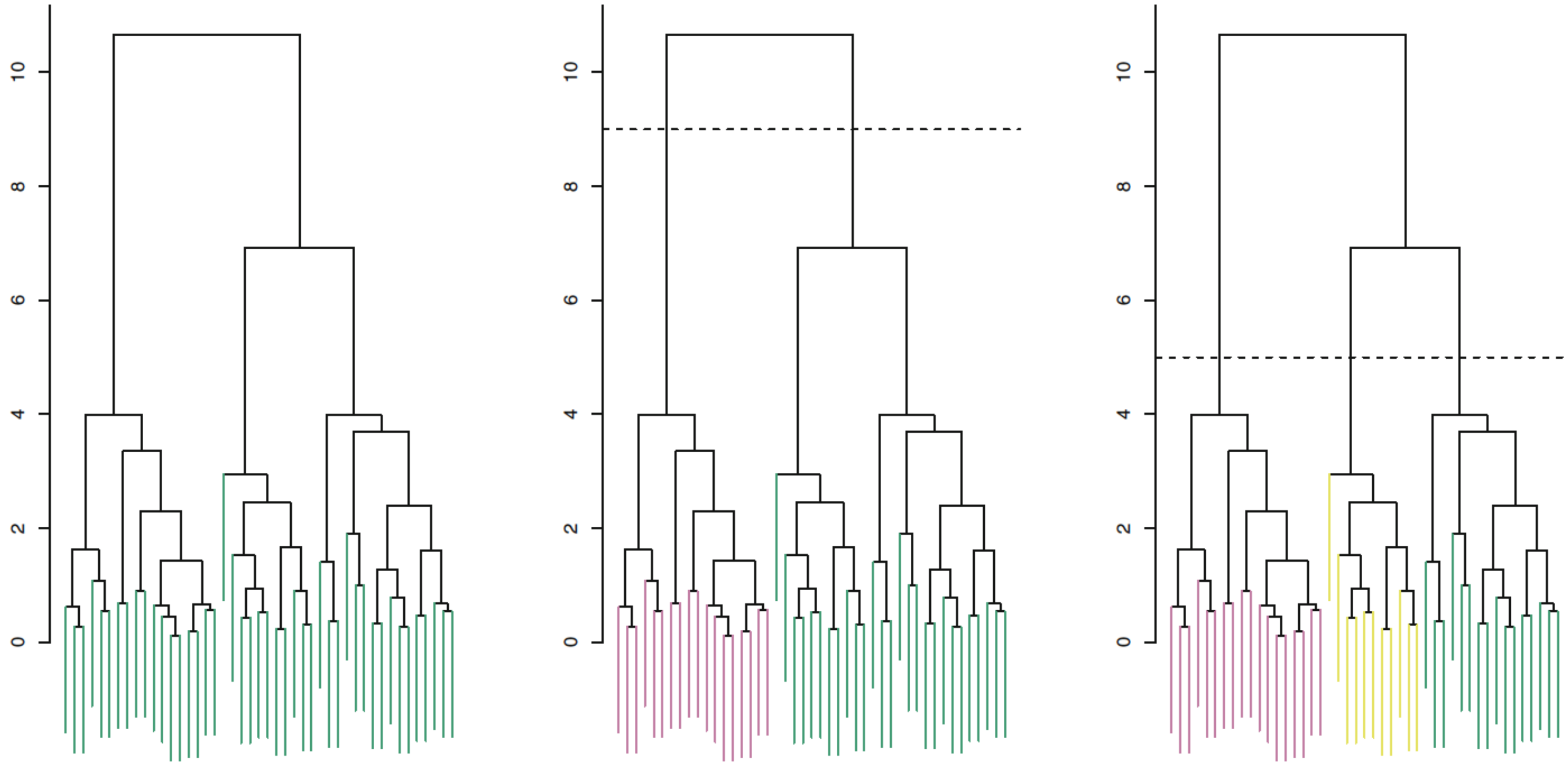
Hierarchical Clustering

- Does not require us to commit to a particular choice of K in advance
- Produces an attractive tree-based representation called dendogram

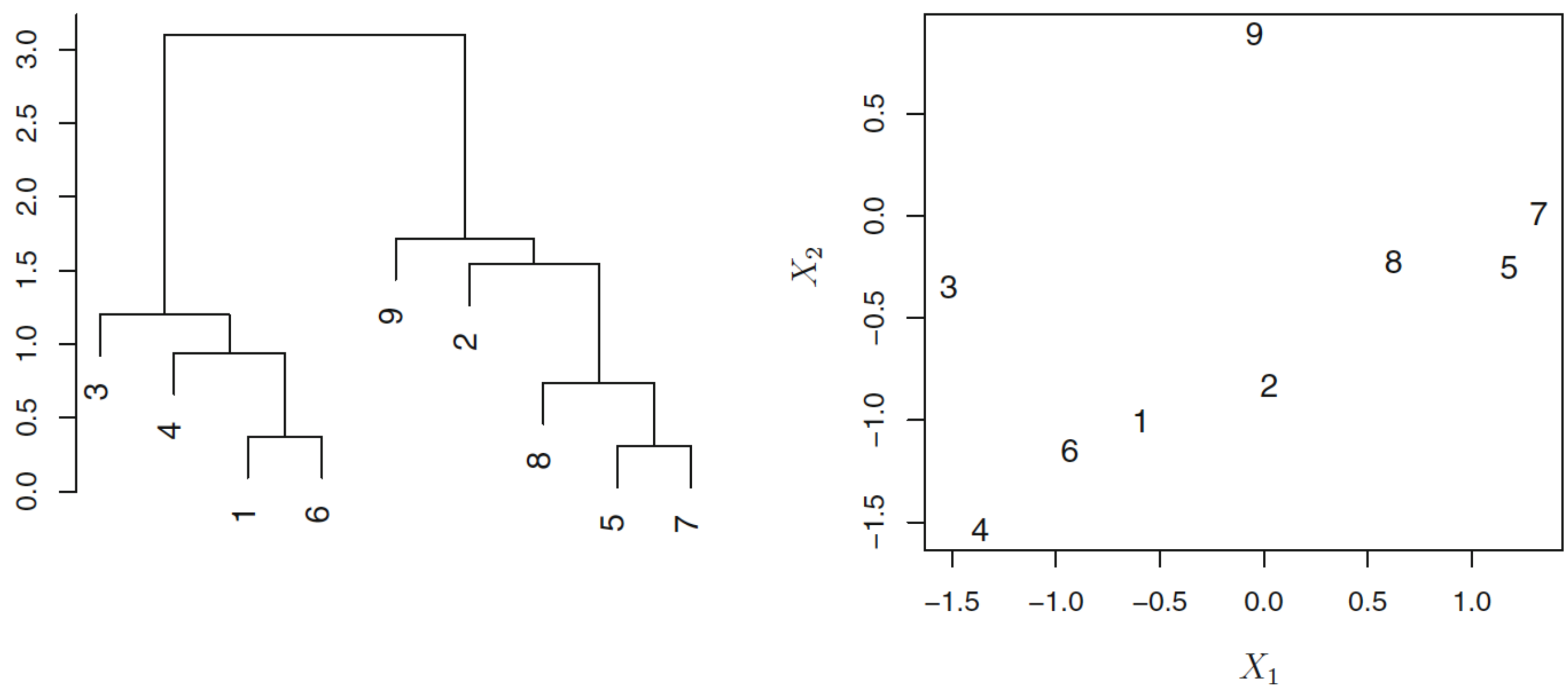
Hierarchical Clustering

- Does not require us to commit to a particular choice of K in advance
- Produces an attractive tree-based representation called dendogram
- We will describe bottom-up or agglomerative clustering
    - Most common type of hierarchical clustering

Interpreting a dendogram



Dendograms can be misleading



Hierarchical structure

- Not always suited for a arbitrary dataset
- Group of people
  - evenly split between male and female
  - evenly split between americans, japanese and french

Hierarchical structure

- Not always suited for a arbitrary dataset
- Group of people
  - evenly split between male and female
  - evenly split between americans, japanese and french
  - best division in two groups -> gender
  - best division in three groups -> nationality

Hierarchical structure

- Not always suited for a arbitrary dataset
- Group of people
  - evenly split between male and female
  - evenly split between americans, japanese and french
  - best division in two groups -> gender
  - best division in three groups -> nationality
  - not nested
- This explains why hierarchical clusters can sometimes yield worse results than K-means for a given number of clusters

The hierarchical clustering algorithm

1. Start at the botton of the dendogram
   - Each of the n observations is treated as its own cluster

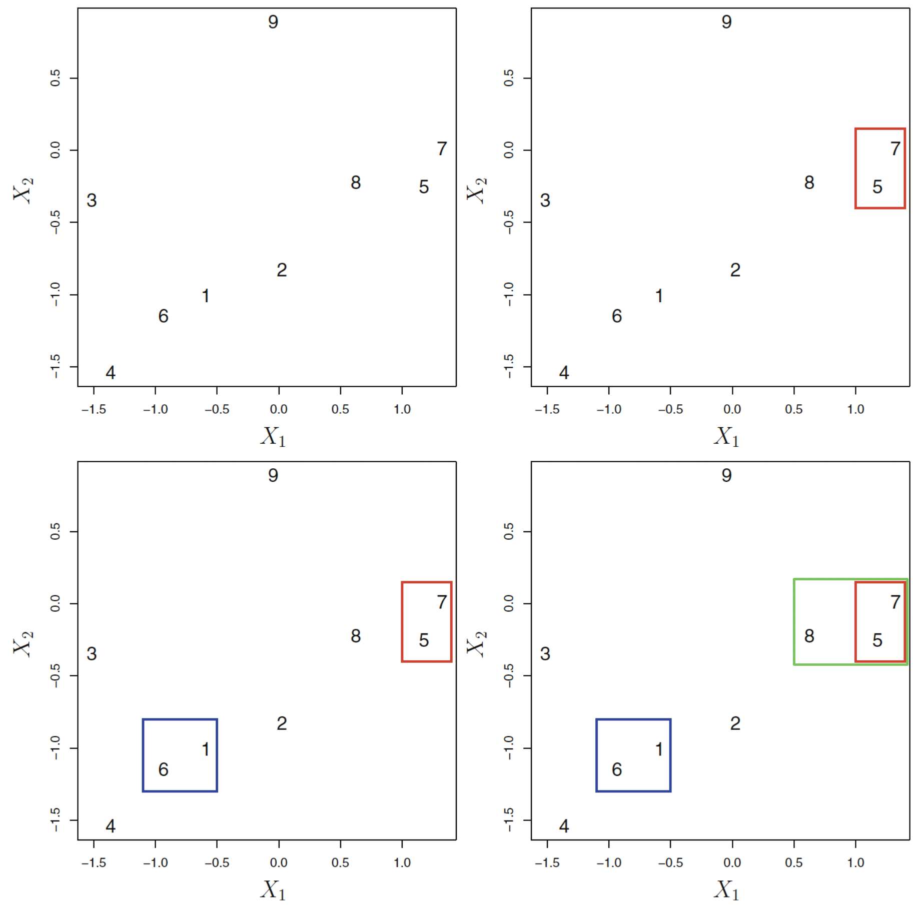
The hierarchical clustering algorithm

1. Start at the botton of the dendogram
    - Each of the n observations is treated as its own cluster
2. Fuse the two clusters that are more similar to each other
    - There are now $n - 1$ clusters

The hierarchical clustering algorithm

1. Start at the botton of the dendogram
    - Each of the n observations is treated as its own cluster
2. Fuse the two clusters that are more similar to each other
    - There are now $n - 1$ clusters
3. Repeat step 2 until there are only one cluster

The hierarchical clustering algorithm



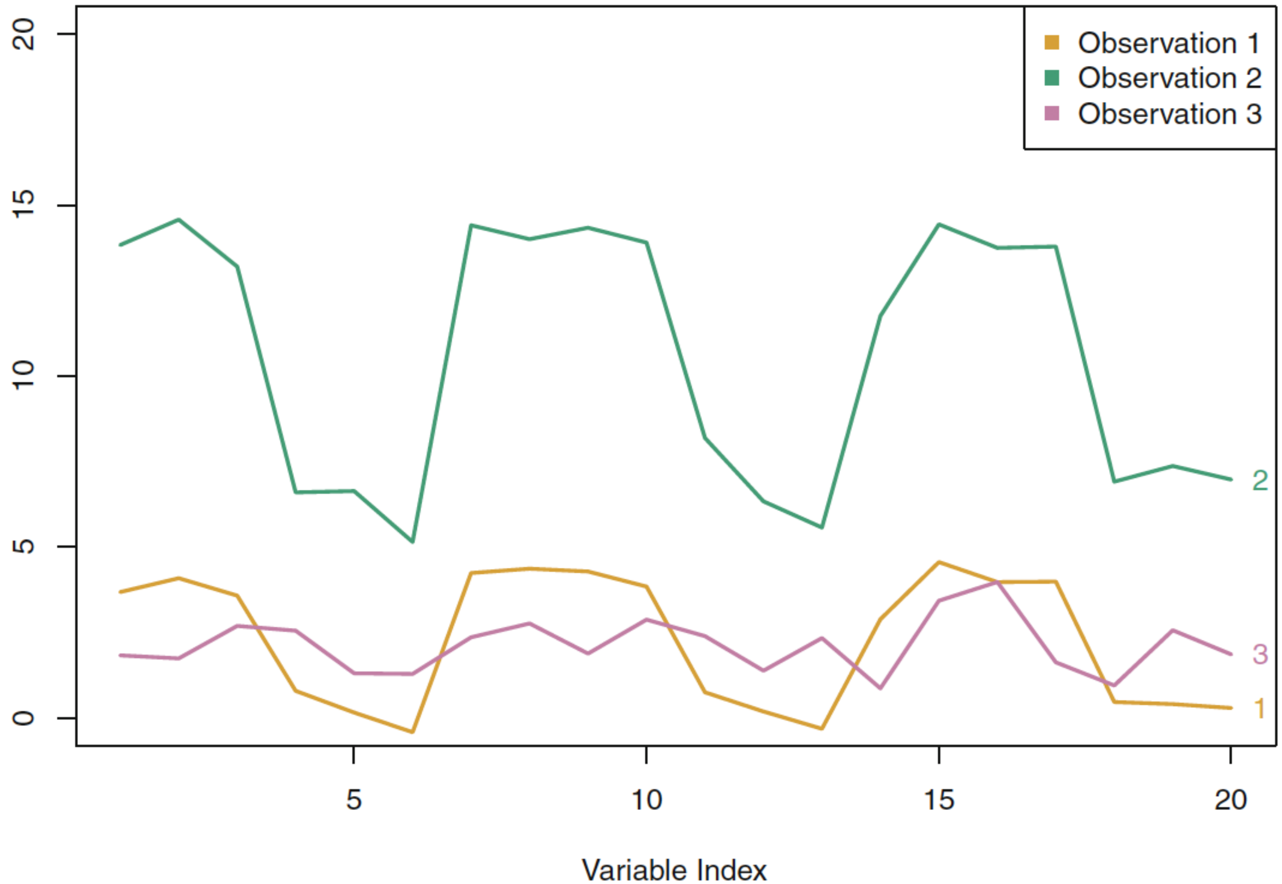
Choice of dissimilarity measure

- Euclidean distance is most common dissimilarity measure to use.
- But there are other options

Choice of dissimilarity measure

- Euclidean distance is most common dissimilarity measure to use.
- But there are other options
- Correlation-based distance
  - Correlation focus on shape of the observation profile rather than their magnitude

Correlation-based distance



Online retailer example

- Online retailer example
    - Identify subgroups of similar shoppers
    - Matrix with shoppers (rows) and items (columns)
    - Value indicate number of times a shopper bought an item

Online retailer example

- Online retailer example
  - Identify subgroups of similar shoppers
  - Matrix with shoppers (rows) and items (columns)
  - Value indicate number of times a shopper bought an item
- Euclidean distance
  - Infrequent shoppers will be clustered together
  - The amount of itens bought matters

Online retailer example

- Online retailer example
  - Identify subgroups of similar shoppers
  - Matrix with shoppers (rows) and items (columns)
  - Value indicate number of times a shopper bought an item
- Euclidean distance
  - Infrequent shoppers will be clustered together
  - The amount of itens bought matters
- Correlation distance
  - Shoppers with similar preference will be clustered together
  - Including both high and low volumes shoppers

Linkage

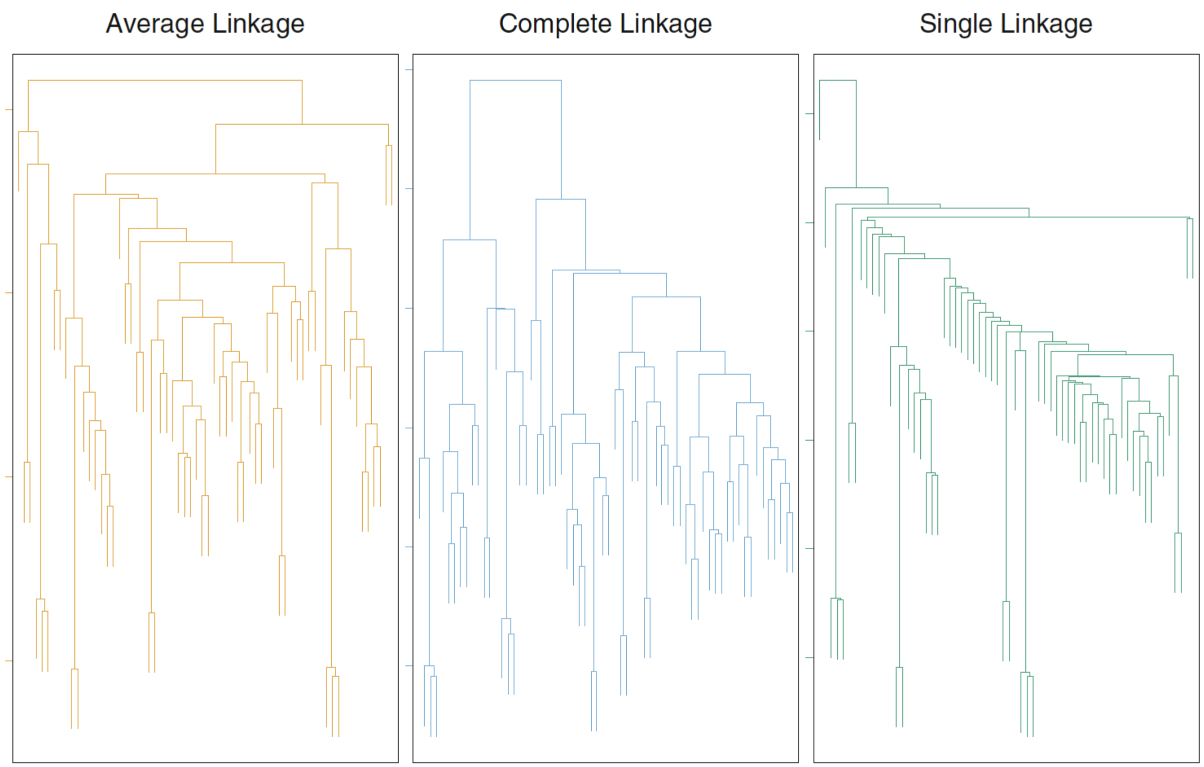
- Need to extend the concept between dissimilarity between pairs of observations to pairs of groups of observations

Linkage

- Need to extend the concept between dissimilarity between pairs of observations to pairs of groups of observations
- Linkages
  - Complete: Maximal intercluster dissimilarity
  - Single: Minimal intercluster dissimilarity
  - Average: Mean intercluster dissimilarity

Linkage

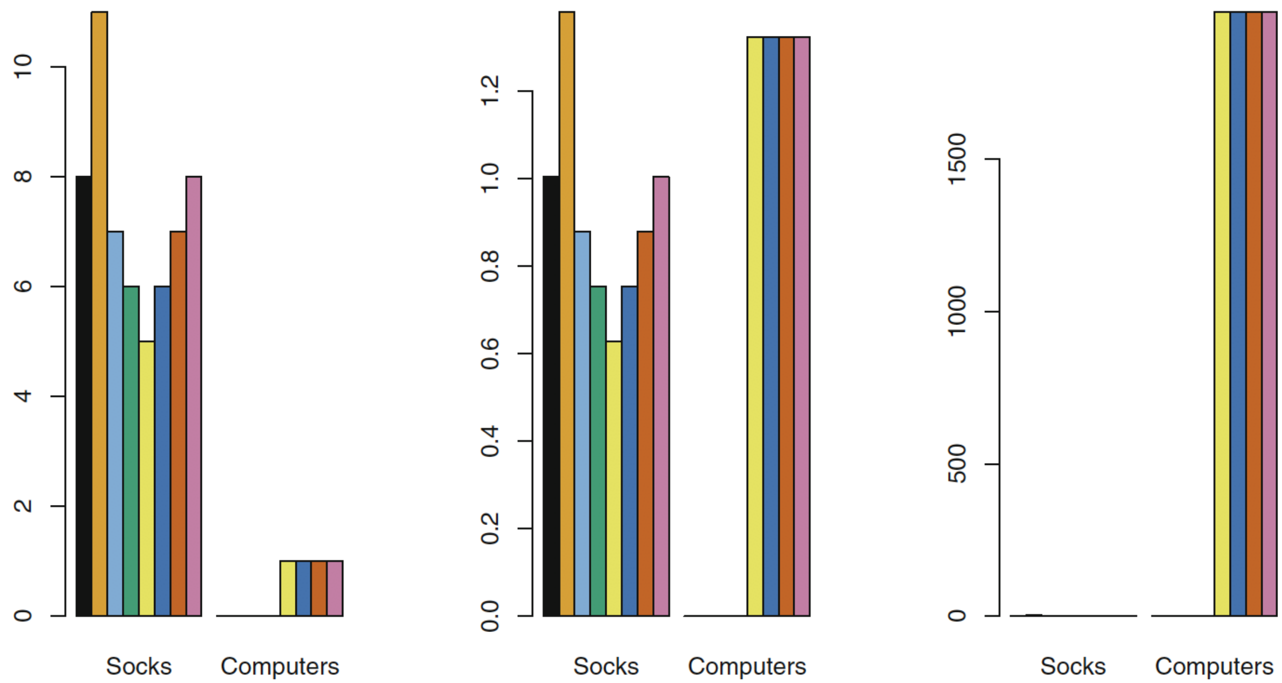
- Dendogram depends strongly on the type of linkage used



- Average and complete linkage tend to yield more balanced clusters.

Scaling variable

- Usually wise to scale the variables



Recommended exercise 4

Perform hierarchical clustering in the New York Times stories dataset.

The pca-examples.rdata can be downloaded from the Blackboard.

Summary of the decisions involved

- Should standardize the variables?
    - Usually yes

Summary of the decisions involved

- Should standardize the variables?
  - Usually yes
- K-means clustering
  - What K?

Summary of the decisions involved

- Should standardize the variables?
  - Usually yes
- K-means clustering
  - What K?
- Hierarchical clustering:
  - dissimilarity measure?
  - Linkage?
  - Where to cut the dendogram?

Summary of the decisions involved

- Should standardize the variables?
  - Usually yes
- K-means clustering
  - What K?
- Hierarchical clustering:
  - dissimilarity measure?
  - Linkage?
  - Where to cut the dendogram?
- With these methods, there is no single right answer—any solution that exposes some interesting aspects of the data should be considered.

Extra slides

- Blog post applying k-means clustering on data from Twitter
  - http://thinktostart.com/cluster-twitter-data-with-r-and-k-means/
- Blog post applying hierarchical clustering on data based on the complete works of william shakespeare
  - https://www.r-bloggers.com/clustering-the-words-of-william-shakespeare/