Module 10: Unsupervised learning

TMA4268 Statistical Learning V2023

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Supervised vs Unsuperviser Learning

- **Supervised Learning**
  - For each observation $i = 1, ... N$ we record:
    - p features $X_{i1}, ..., X_{ip}$ AND one response variable Y_i
  - **Main Interest:**
    - Prediction or inference
- **Unsupervised Learning**
  - For each observation $i = 1, ... N$ we record:
    - p features $X_{i1}, ..., X_{ip}$
  - **Main Interest:**
    - Better data visualization, discover interesting patterns, exploratory analysis, clustering

Applications of Unsupervised Learning (Examples)

- Cancer research: Look for subgroups within the patients or within the genes in order to better understand the disease
- Online shopping site: Identify groups of shoppers as well as groups of items within each of those shoppers groups.
- Search engine: Search only a subset of the documents in order to find the best one for retrieval.
- +++

General Challenges of Unsupervised Learning

- In general, unsupervised learning methods are
  - more subjective
  - hard to assess results
- There is usually no obvious ground-truth to compare to

General Challenges of Unsupervised Learning

- In general, unsupervised learning methods are
  - more subjective
  - hard to assess results
- There is usually no obvious ground-truth to compare to
- Remedy:
  - Unsupervised methods are usually part of a bigger goal
  - Evaluate them as how they contribute to such bigger goal
- Examples:
  - How clustering shoppers improved your recommendation algorithm?
  - How clustering documents reduced computational complexity and what was the cost involved?

Unsupervised Learning techniques

Covered in this module:

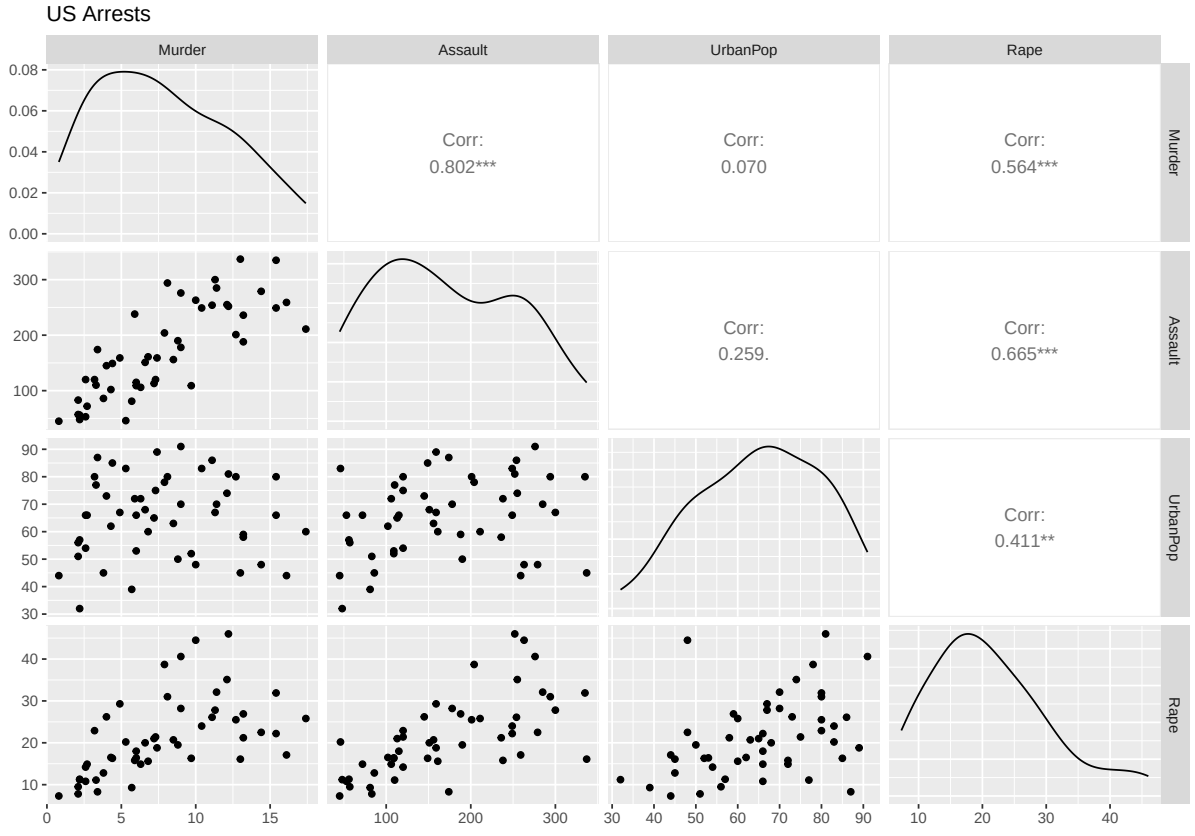
- **PCA (Principal Component Analysis)**
  - Data Visualization
  - Data pre-processing
- **Clustering**
  - Discovering unknown subgroups in the data
  - 1. k-means clustering
  - 2. Hierarchical clustering

Data Visualization

```
##            Murder Assault UrbanPop Rape
## Alabama      13.2     236       58 21.2
## Alaska       10.0     263       48 44.5
## Arizona       8.1     294       80 31.0
## Arkansas      8.8     190       50 19.5
## California    9.0     276       91 40.6
## Colorado      7.9     204       78 38.7
```

Number of arrest per 100 000 inhabitants, Percent of population living in urban areas.

Data Visualization



- Many plots to look at $(p(p-1))$
- Each contains only a small part of the information

We want to find low dimensional representation of the data that captures most of the info as possible: **Principal Components Analysis (PCA)** is a way to obtain that !

Principal Components Analisis (I)

- We have a $n \times p$ matrix X (mean centered)
- We want to create a $n \times M$ matrix Z, with $M < p$ such that the mth column is:

$$Z_m = \sum_{j=1}^{p} \phi_{jm} X_j \quad \text{subject to} \quad \sum_{j=1}^{p} \phi_{jm}^2 = 1$$

- Why do we have the constrain $\sum_{j=1}^{p} \phi_{jm}^2 = 1$?

The first principal component Z_1

- We look for linear combinations of the form

$$z_{i1} = \sum_{j=1}^{p} \phi_{j1} x_{ij} = \phi_{11} x_{i1} + \phi_{21} x_{i1} + \cdots + \phi_{p1} x_{ip}$$

that have largest variance subject to $\sum |\phi_{j1}^2| = 1$

- The sample variance of z_1 is $\frac{1}{n} \sum_i z_{i1}^2 = \frac{1}{n} \sum_i \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2$

The first principal component Z_1 - Maximization problem

We want to find

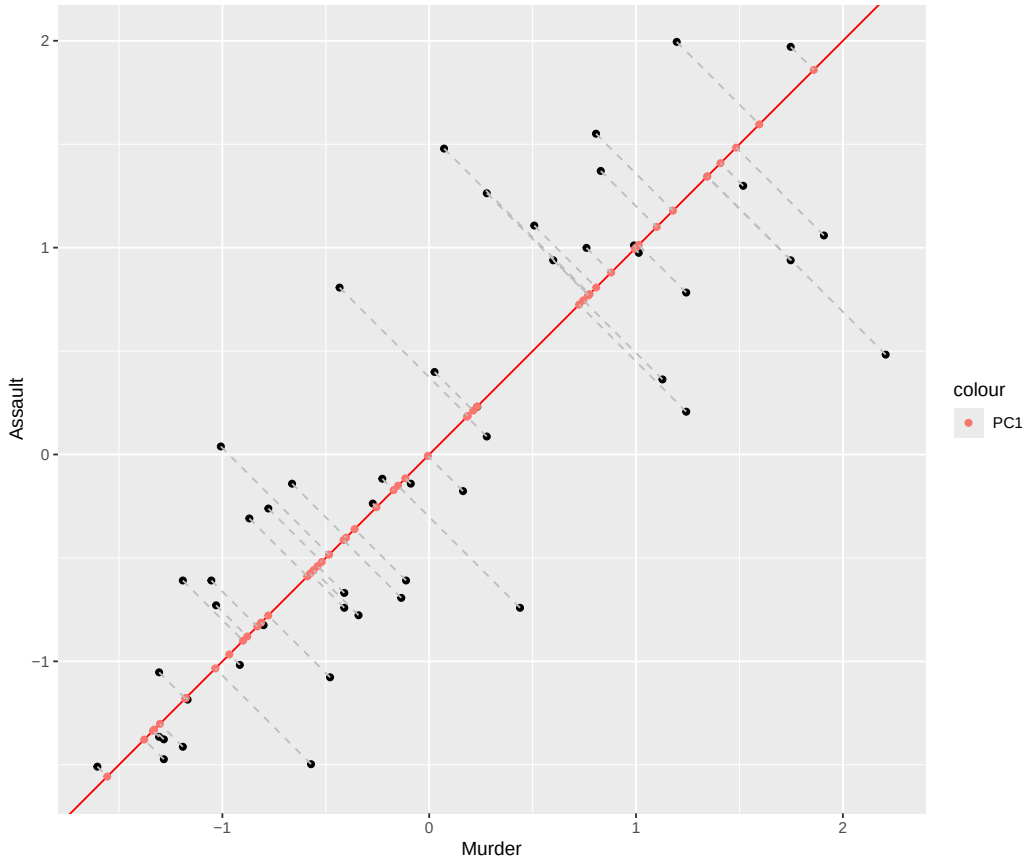
$$\max_{\phi_{11},\ldots,\phi_{p1}}(\mathrm{Var}(z_1)) = \max_{\phi_{11},\ldots,\phi_{p1}}\left(\frac{1}{n}\sum_i\left(\sum_{j=1}^{p}\phi_{j1}x_{ij}\right)^2\right)$$

given $\sum|\phi_{j1}^2| = 1$

- This is a standard problem in linear algebra solved via singular-value decomposition of $\mathbf{X}$

The first principal component Z_1 - Geometric interpretation

- The loading vector $\phi_1 = (\phi_{11}, \ldots, \phi_{p1})$ defines the direction along with the data vary most

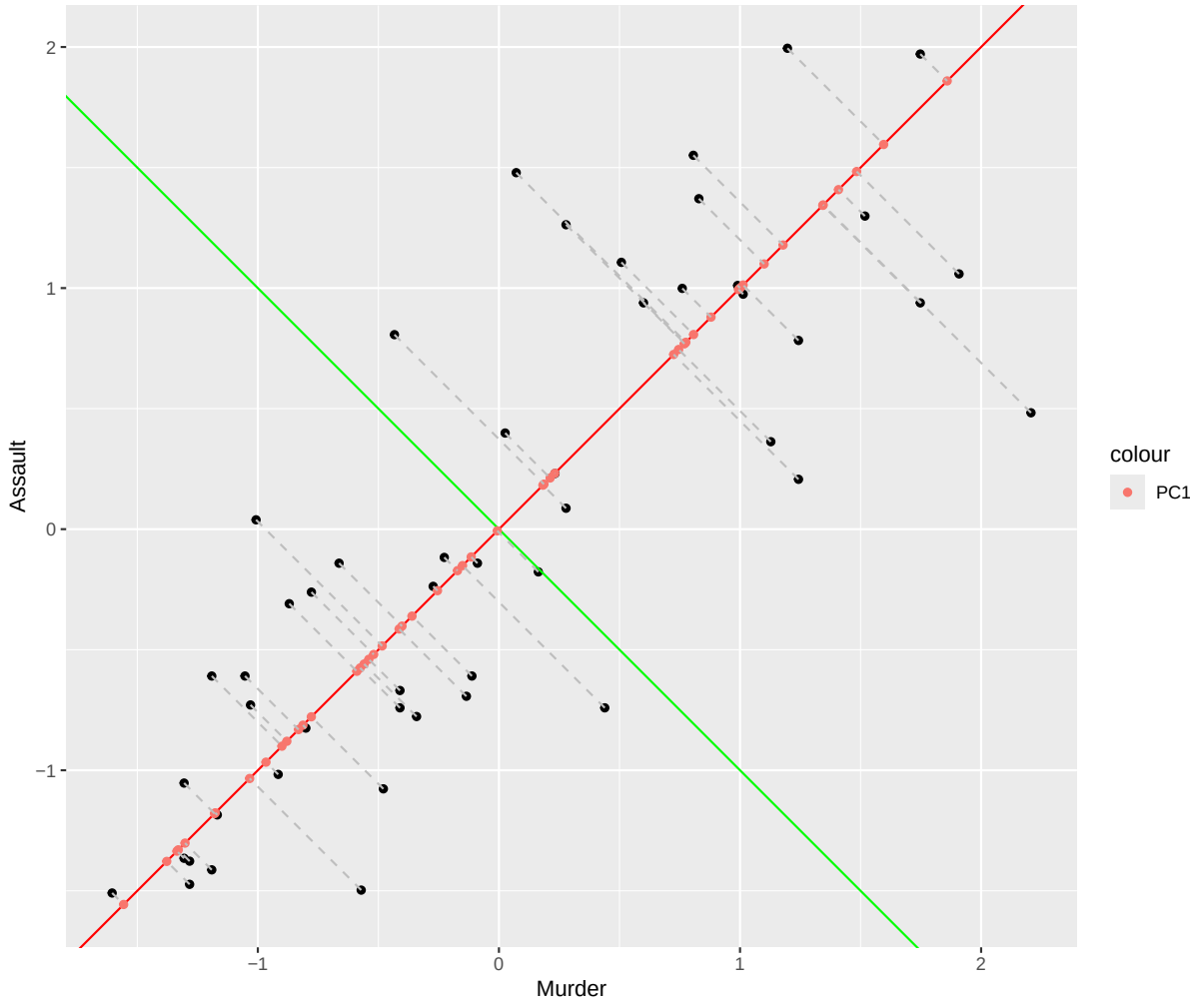


The second principal component Z_2

- Once we have Z_1:
- Z_2 should be uncorrelated to Z_1, and have the highest variance, subject to this constrain.
  - The direction of Z_1 must be perpendicular (or orthogonal) to the direction of Z_2
- And so on ...

- We can construct up to p PCs that way.
- In which case we have:
  - Captured all the variability contained in the data
  - Created a set of orthogonal predictors
  - But **not** accomplished dimensionality reduction

Example 1

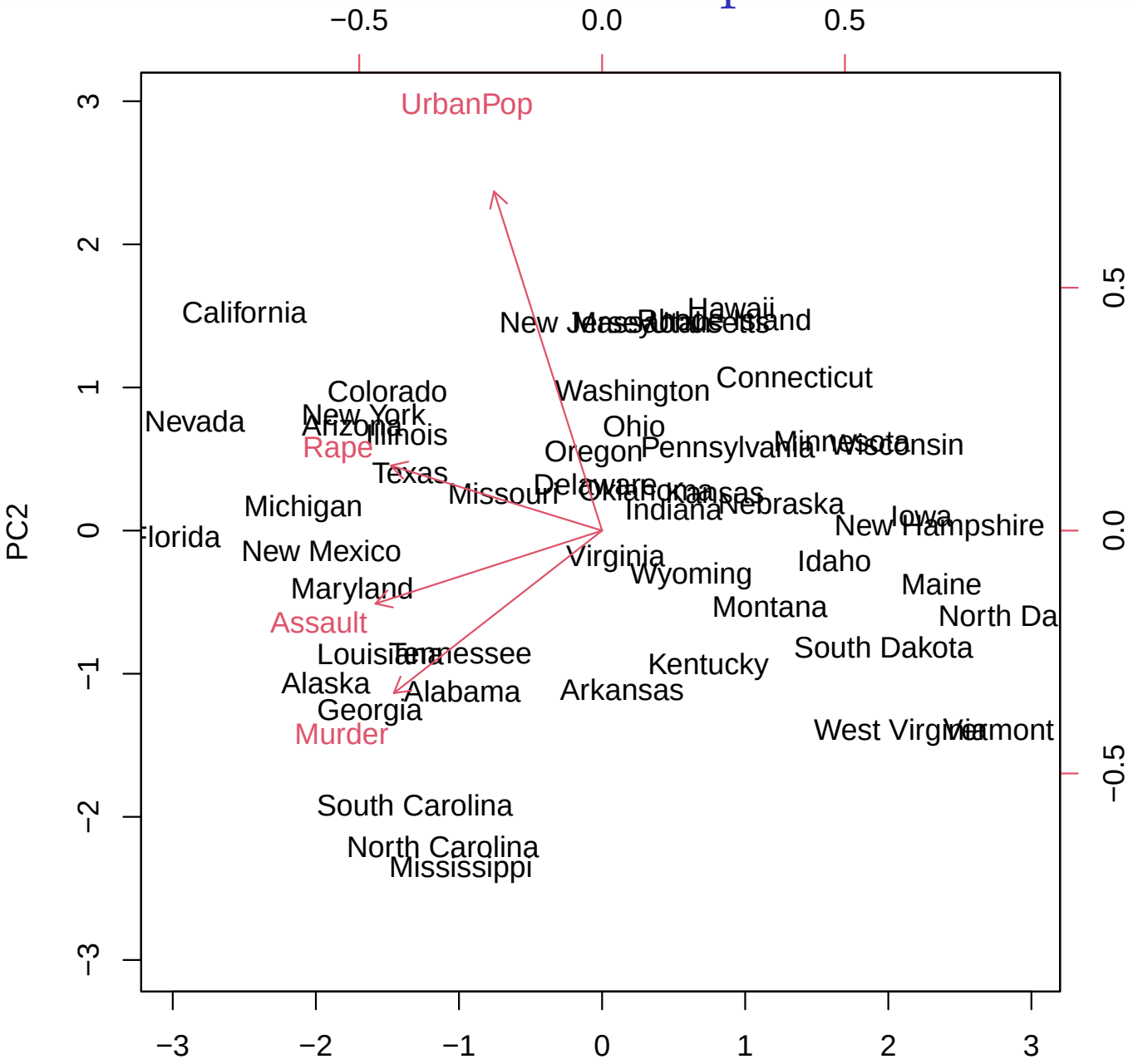


Example 2

```
## [1] "Loadings"
```

```
##                 PC1        PC2        PC3         PC4
## Murder   -0.5358995 -0.4181809  0.3412327  0.64922780
## Assault  -0.5831836 -0.1879856  0.2681484 -0.74340748
## UrbanPop -0.2781909  0.8728062  0.3780158  0.13387773
## Rape     -0.5434321  0.1673186 -0.8177779  0.08902432
```

Example 2


−0.5
0.0
0.5
UrbanPop
3
2
1
0
−1
−2
−3
PC2
0.5
0.0
−0.5
California
Hawaii
Connecticut
Washington
Colorado
Nevada
New York
Arizona
Illinois
Ohio
Rape
Oregon
Pennsylvania
Texas
Michigan
Indiana
Nebraska
Iowa
New Hampshire
New Mexico
Virginia
Idaho
Wyoming
Maine
Maryland
Montana
Assault
South Dakota
Louisiana
Tennessee
Kentucky
Alaska
Alabama
Arkansas
Georgia
Murder
West Virginia
Vermont
South Carolina
North Carolina
Mississippi
−3
−2
−1
0
1
2
3

PCA - General setup

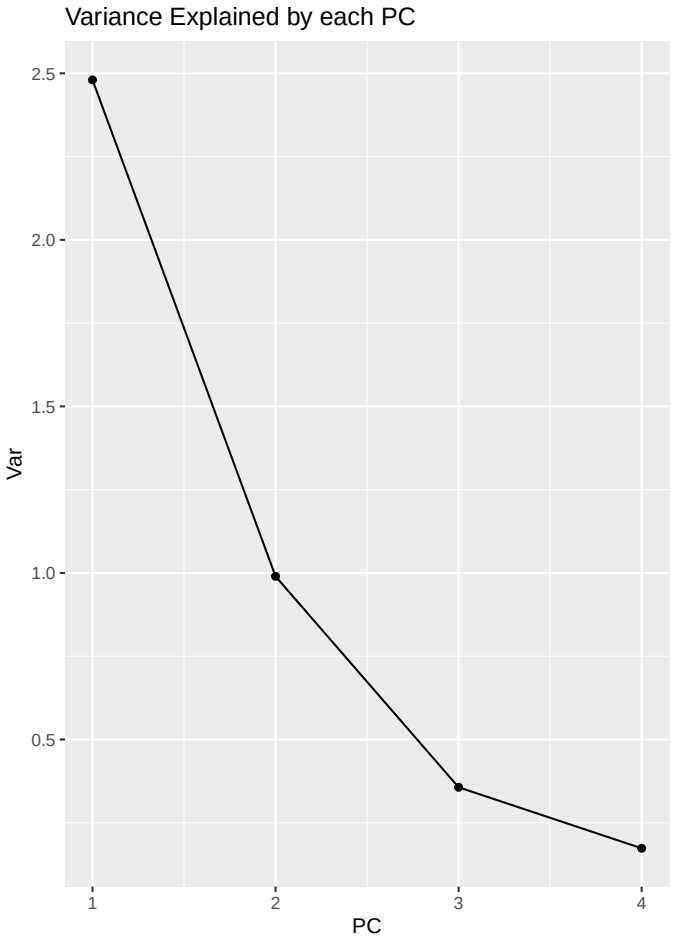
- Let X be a (standardized) matrix with dimension $n \times p$.
- Assume Σ to be the covariance matrix associated with X.
- Σ is non-negative, therefore:

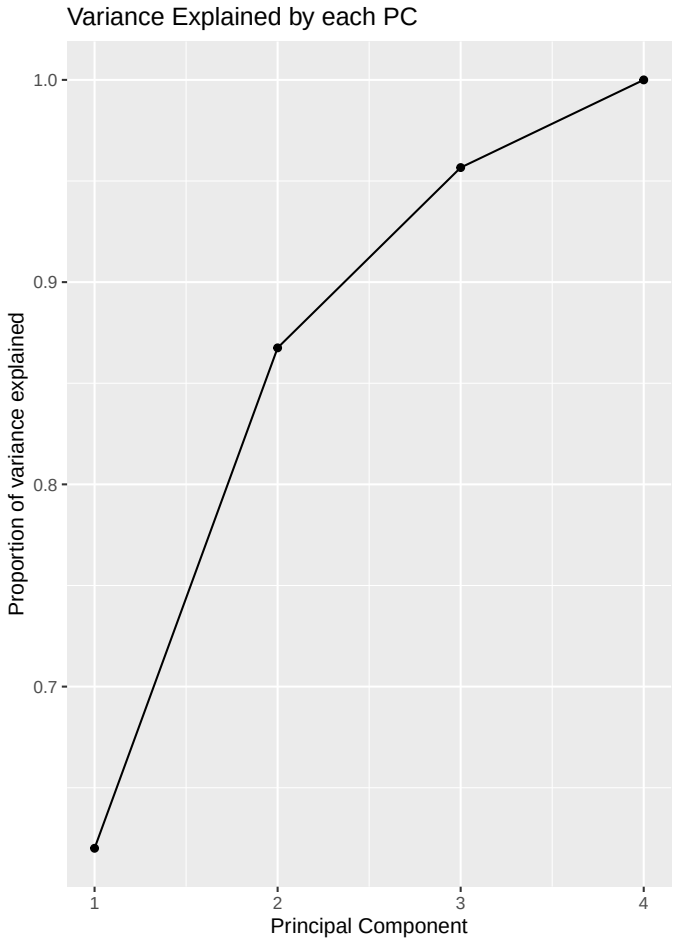
$$\Sigma = C\Lambda C^{-1}$$

- $\Lambda = diag(\lambda_1, ..., \lambda_p)$ is a diagonal matrix of ordered eigenvalues
- C is a matrix of eigenvectors of Σ.
- We want $Z_1 = \phi_1 X$, subject to $||\phi_1||_2 = 1$ so that the variance $V(Z_1) = \phi_1^T \Sigma \phi_1$ is maximised
  - ϕ_1 is the eigenvector corresponding to the largest eigenvalue of Σ
  - The fraction of the original variance kept by the first M principal component

$$R^2 = \frac{\sum_{i=1}^{M} \lambda_i}{\sum_{j=1}^{p} \lambda_j}$$

Example 2


Variance Explained by each PC
Var
PC
2.5
2.0
1.5
1.0
0.5
1
2
3
4


Variance Explained by each PC
Proportion of variance explained
Principal Component
1.0
0.9
0.8
0.7
1
2
3
4

Notes about PCA

- PCA is dependent on the scaling of the variables involved....why?
- Each Principal Component loading vector is unique, up to a sign flip.
- Flipping the sign has no effect as the direction of the PC does not change.

PCA for face recognition

PCA for face recognition

- The data set consist of 400 faces from 10 different persons.
- Each picture has 64×64 grey-scale pixels

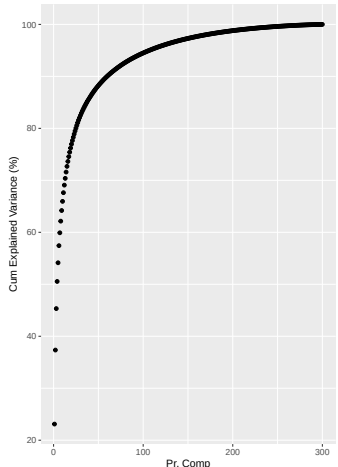
We want to use PCA to recognize faces.

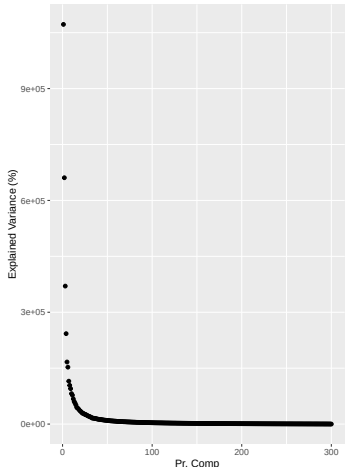
- Training set 300 pictures
- Test set 100 pictures
- Our training set is 300×4096 matrix

PCA analysis

```r
face_matrix <- t(sapply(faces, function(x) as.vector(x)))
# set labels
labels = rep(1:40, each = 10)
# create test and training set
train_indices = sort(sample(1:400, 300))
train_data = face_matrix[train_indices,]
test_data = face_matrix[-train_indices,]

train_labels <- labels[train_indices]
test_labels <- labels[-c(train_indices)]
# Perform PCA
pca_result <- prcomp(train_data, center = T, scale. = FALSE)
```





Eigenfaces

PCA for face recognition

Run the code

`face_recognition.R`

Clustering methods

- **Goal**: 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 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

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

  1. Each observation belongs to one of the K clusters.
  2. No observation belongs to more than one cluster.

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

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

- Squared Euclidean distance is the most common

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*

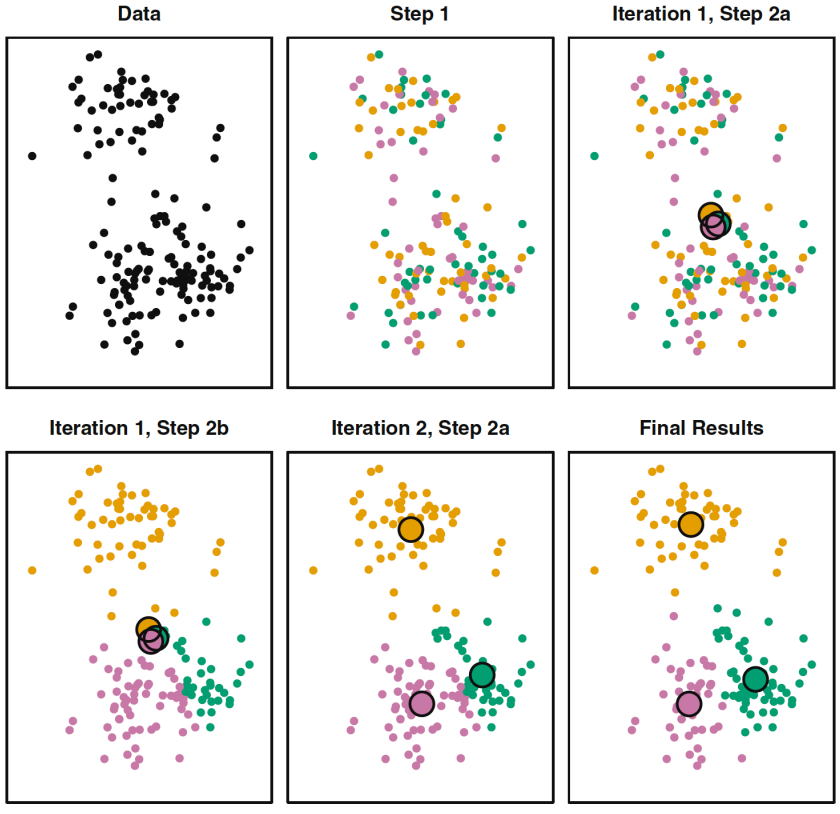
1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.

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.

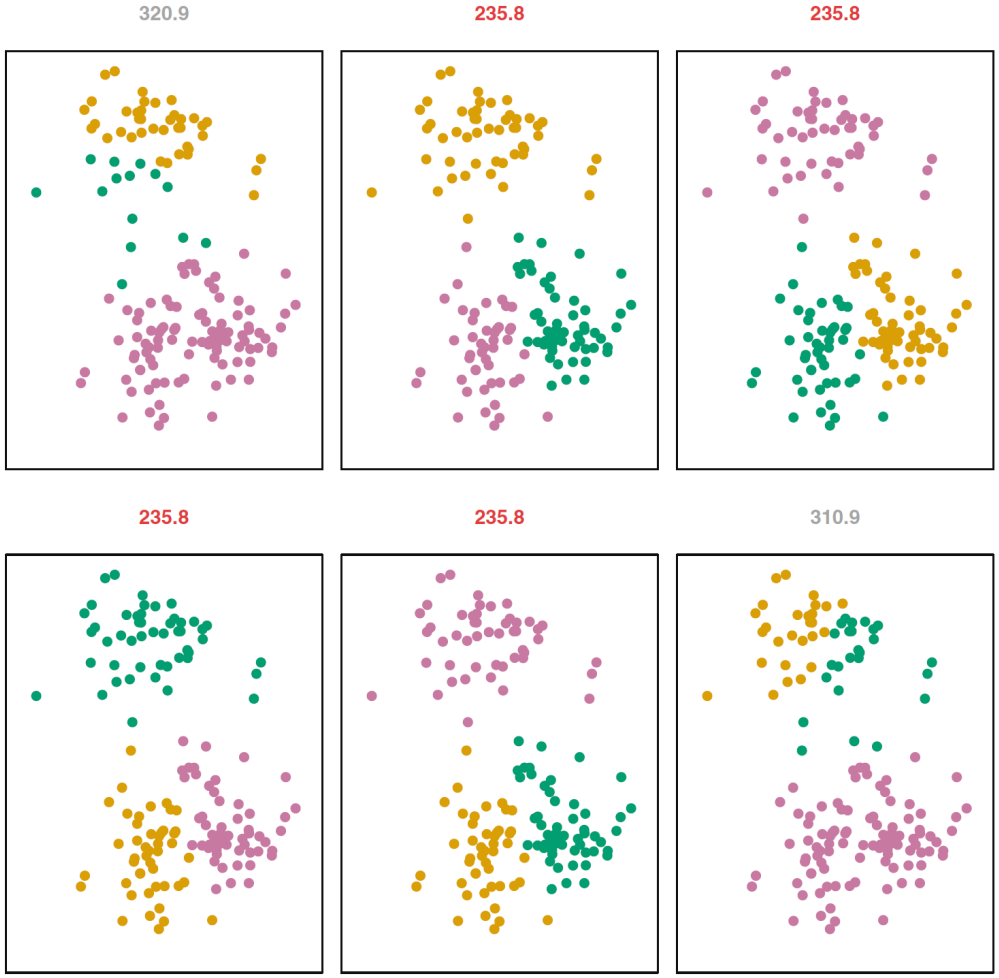
   (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).

K-means algorithm



- A simulated data set with 150 observations in two-dimensional space.
- K = 3
- Final result is obtained after 10 iterations

K-means algorithm (stating conditions)



- K-means performed six times with random initial conditions
- K = 3
- Above is the value of objective function

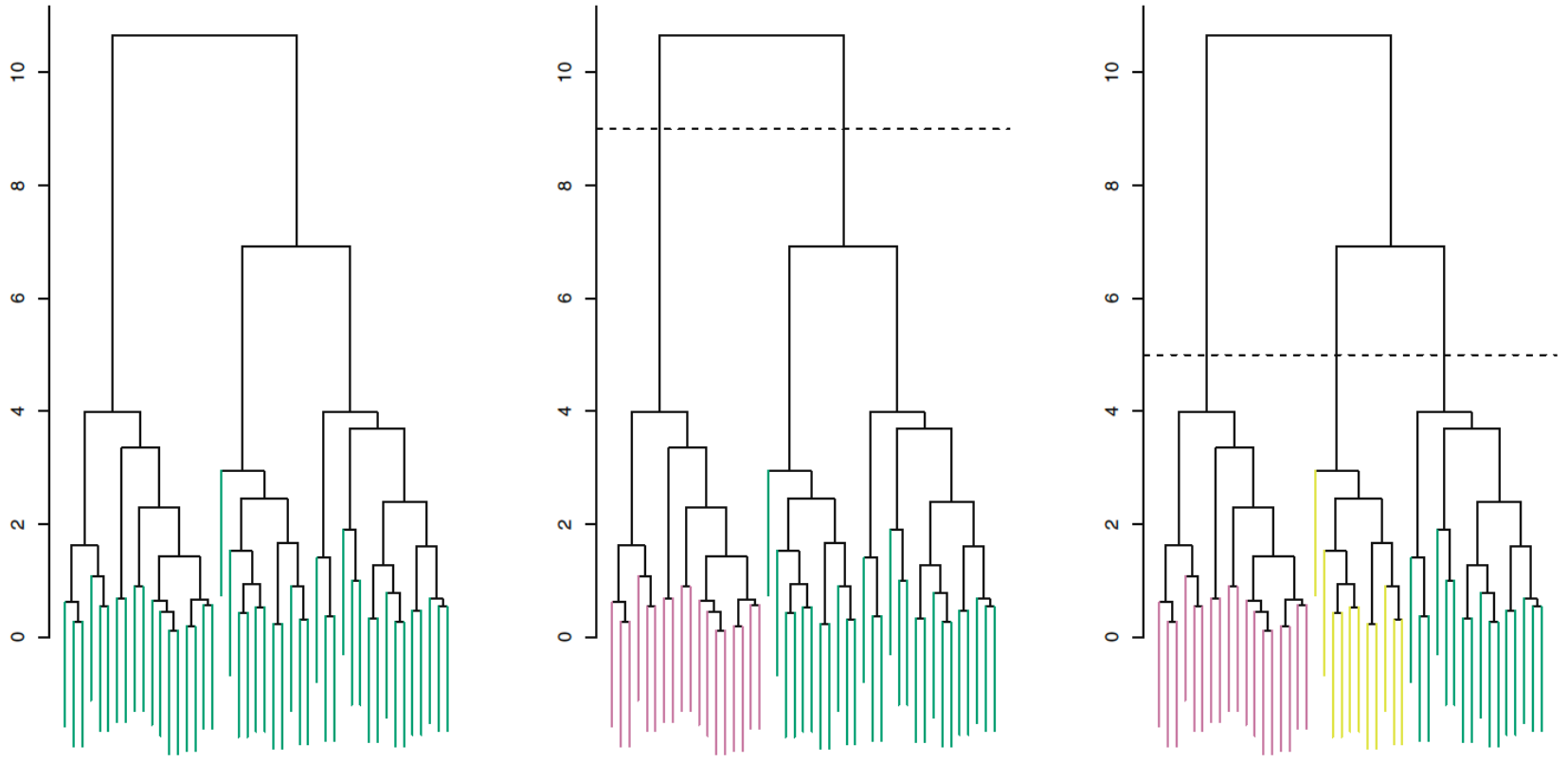
K-means algorithm

- Potential disadvantage of K-means, we need to select K
- This is not always a disadvantage

Hierarchical Clustering

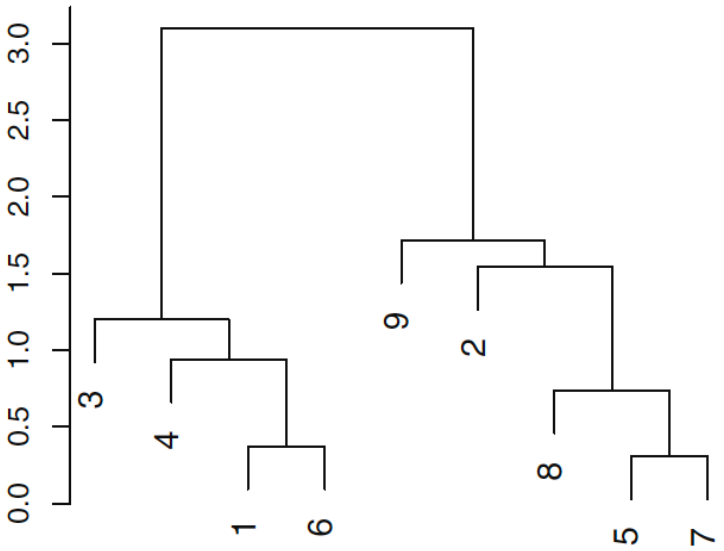
- Does not require us to commit to a particular choice of K in advance
- Produces an attractive tree-based representation called *dendogram*
- We will describe bottom-up or agglomerative clustering
  - Most common type of hierarchical clustering
- Other approach available is called Divisive or "top down" approach

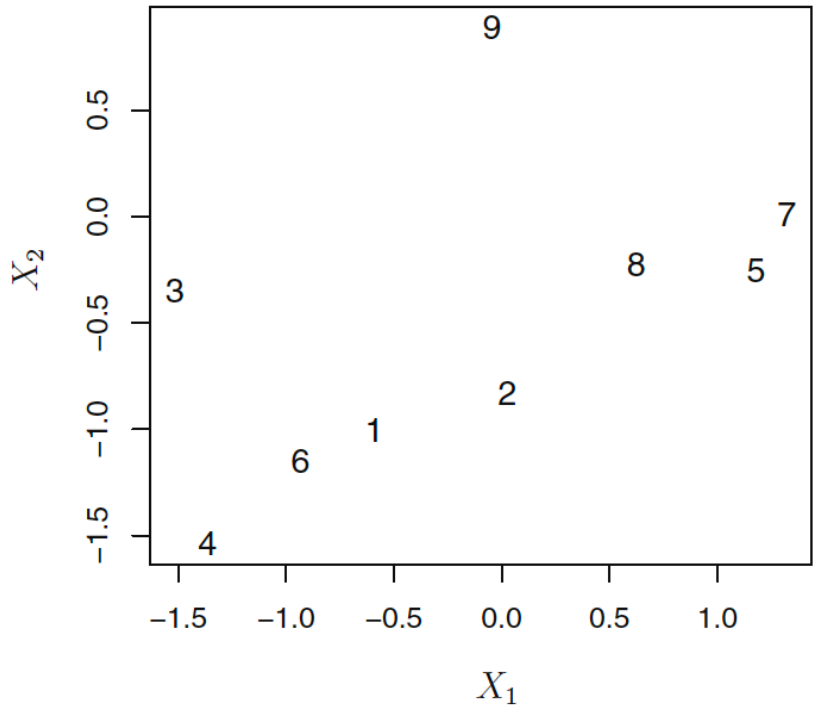
Interpreting a dendogram



- The height of the cut in the dendogram serves the same role as K in K-means clustering
  - Not always clear where to make the cut
- Clusters obtained by cutting the vertical axis at a lower level are always nested within clusters obtained by cutting at a higher level.

Dendograms can be misleading





- The lower in the tree fusions occur -> more similar
- The height of the fusion, as measured on the vertical axis, indicates how different the two observations are.
  - We should not draw conclusions based on the horizontal axis
- It is tempting but incorrect to conclude that observations 9 and 2 are quite similar to each other.

Hierarchical structure

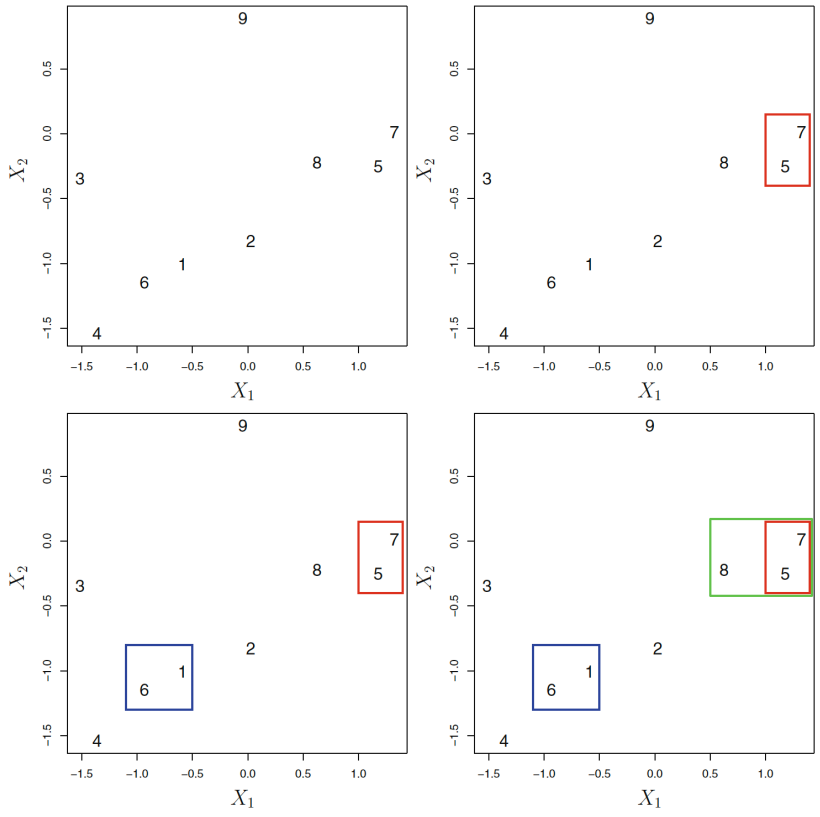
- Not always suited for a arbitrary dataset
- Group of people
  - evenly split between male and female
  - evenly split between americans, japanese and french
  - best division in two groups -> gender
  - best division in three groups -> nationality
  - not nested
- This explains why hierarchical clusters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

- Dissimilarity measure
  - We need to chose a dissimilarity measure
- Linkage
  - Extend the concept of dissimilarity from a pair of observation to a pair of groups of observations

The hierarchical clustering algorithm

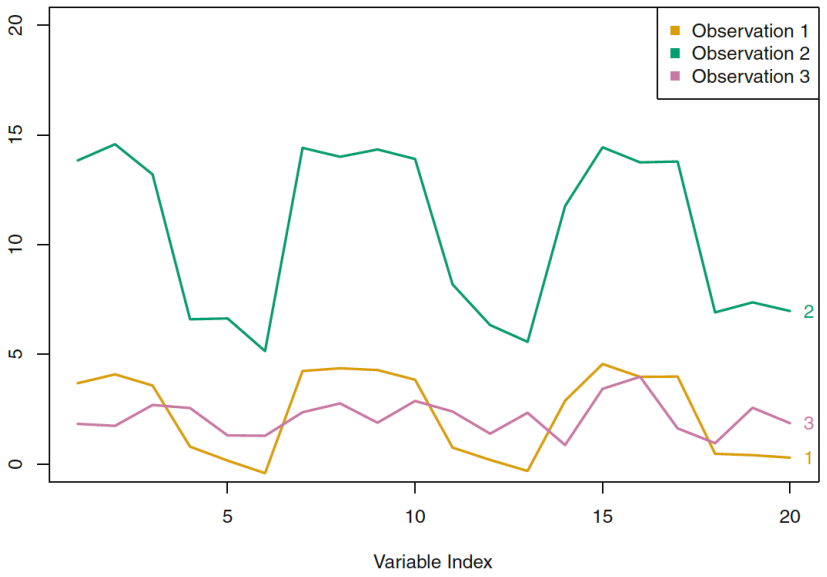


- First few steps of the hierarchical clustering algorithm
  - Euclidean distance
  - Complete linkage
- 5 and 7
- 6 and 1

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:
  - Two observations are similar if their features are highly correlated
  - Even though observed values might be far apart according to Euclidean distance

Correlation-based distance



- Three observations with measure on 20 variables
- Observations 1 and 3
  - close to each other in Euclidean distance
  - weakly correlated -> large correlation-based distance
- Observations 1 and 2
  - Different values for each variable -> large euclidean distance
  - Strongly correlated

Online retailer example

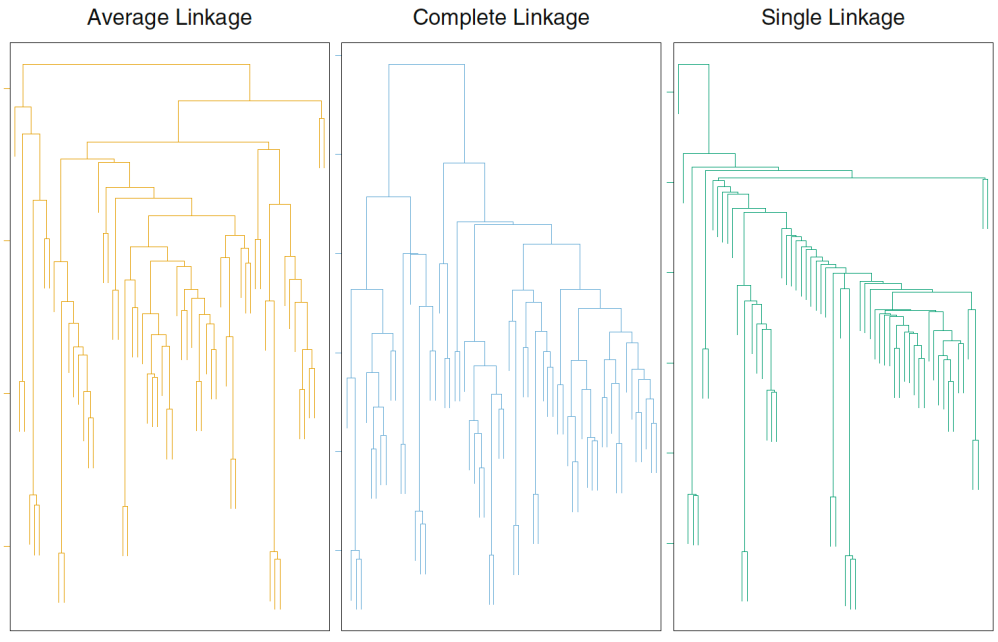
- Online retailer example
  - Identify subgroups of similar shoppers
  - Matrix with shoppers (rows) and items (columns)
  - Value indicate number of times a shopper bought an item
- Euclidean distance
  - Infrequent shoppers will be clustered together
  - The amount of itens bought matters
- Correlation 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
- Linkages
  - Complete: Maximal intercluster dissimilarity
  - Single: Minimal intercluster dissimilarity
  - Average: Mean intercluster dissimilarity
- Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B.
- Then apply the appropriate function to compute either Complete, Single and Average linkage

Linkage

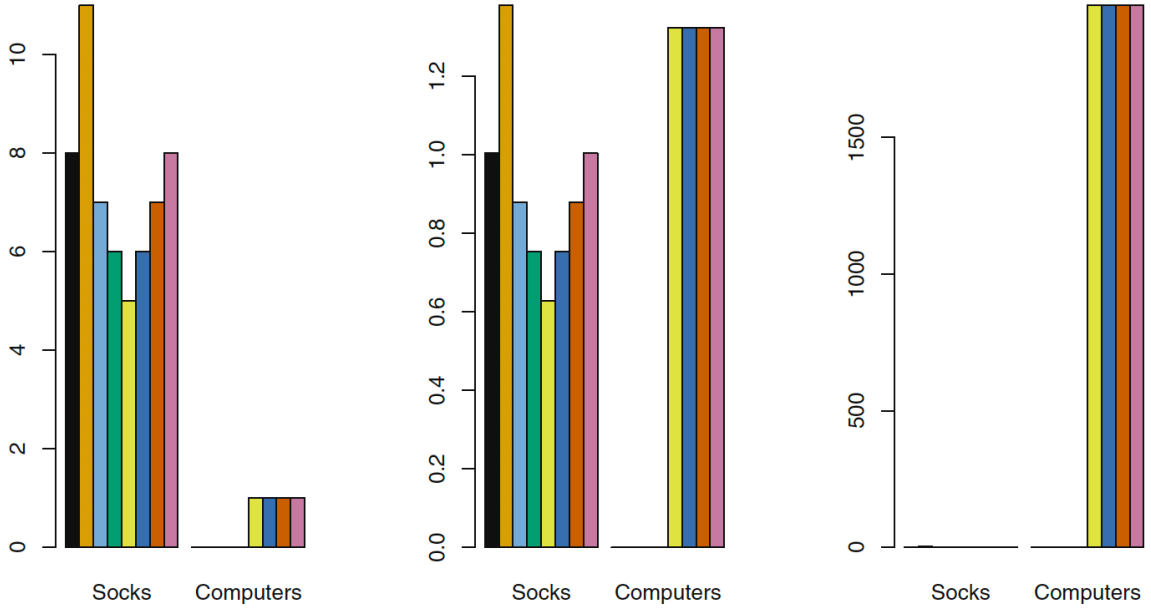
- Dendogram depends strongly on the type of linkage used



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

Scaling variable

- Usually wise to scale the variables



- Eight online shoppers (each with one color)
- (Left) Number of pairs of socks, and computers -> Socks will dominate
- (Center) Number of itens, scaled -> The weight of computer increase
- (Right) Number of dollar spent -> Computers will dominate

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/