

Module 10: Unsupervised learning

TMA4268 Statistical Learning V2023

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Supervised vs Unsupervised Learning

- **Supervised Learning**

- For each observation $i = 1, \dots, N$ we record:
 - p features X_{i1}, \dots, X_{ip} AND one response variable Y_i
- **Main Interest:**
 - Prediction or inference

- **Unsupervised Learning**

- For each observation $i = 1, \dots, N$ we record:
 - p features X_{i1}, \dots, 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:

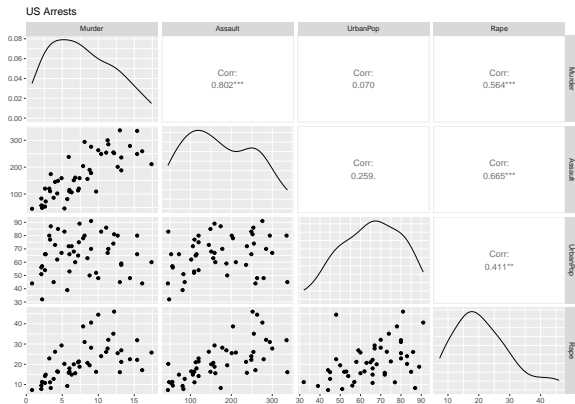
- **PCA (Principal Component Analysis)**
 - Data Visualization
 - Data pre-processing
- • *Clustering**
 - Discovering unknown subgroups in the data
 - 1. k-means clustering
 - 2. Hierarchical clustering

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 Analysis (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 m th 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

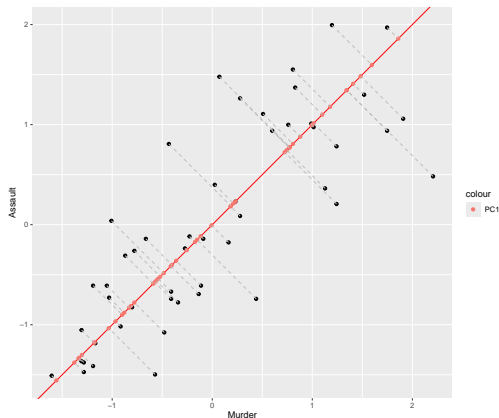
$$\max_{\phi_{11}, \dots, \phi_{p1}} (\text{Var}(z_1)) = \max_{\phi_{11}, \dots, \phi_{p1}} \left(\frac{1}{n} \sum_i \left(\sum_{j=1}^p \phi_{j1} x_{ij} \right)^2 \right)$$

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

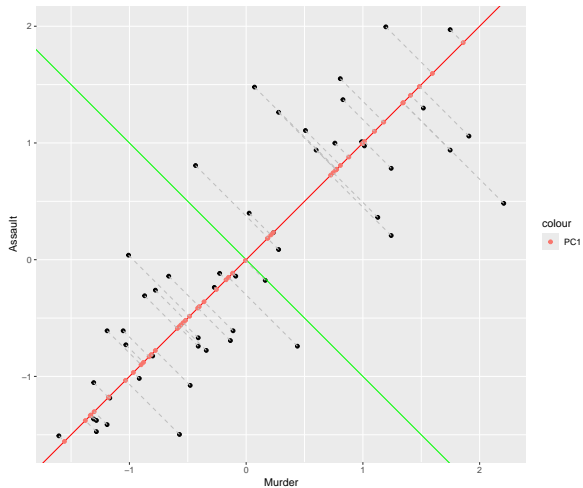
- The loading vector $\phi_1 = (\phi_{11}, \dots, \phi_{p1})$ defines the direction along which the data vary most



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

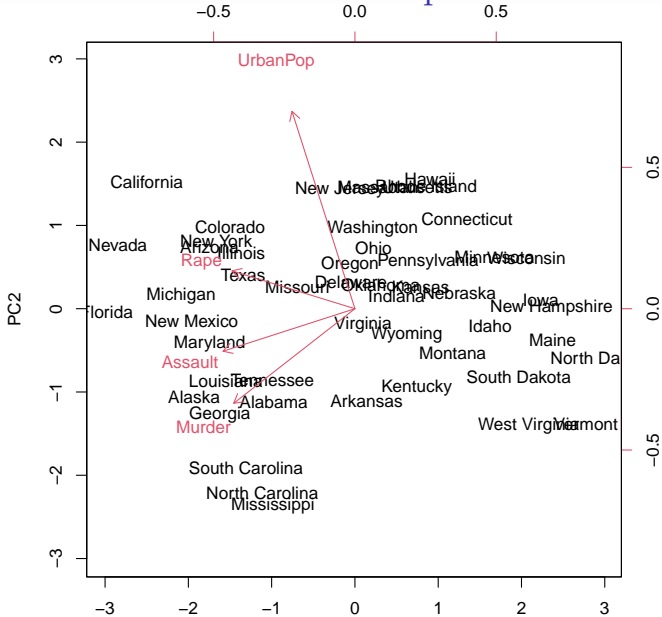


Example 2

```
## [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



PCA - General setup

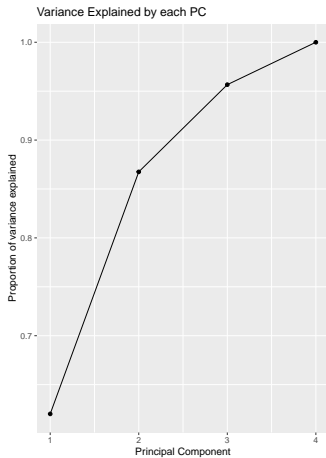
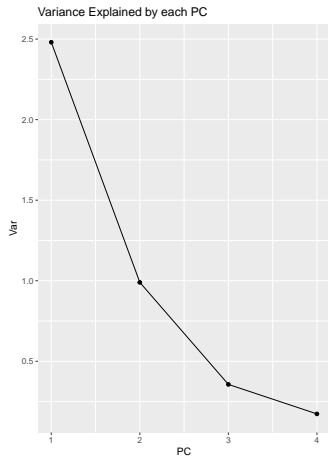
- Let X be a (standardized) matrix with dimension $n \times p$.
- Assume Σ to be the covariance matrix associated with X .
- Σ is non-negative, therefore:

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

- $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$ 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



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.

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, \dots, C_k : Sets containing indices of observations in each cluster.
 - These sets satisfy two properties:
 - $C_1 \cup C_2 \cup \dots \cup C_k = \{1, \dots, n\}$
 - $C_k \cap C_{k'} = \emptyset$ 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

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

- Squared Euclidean distance is the most common

K-means algorithm

- Find algorithm to solve:

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

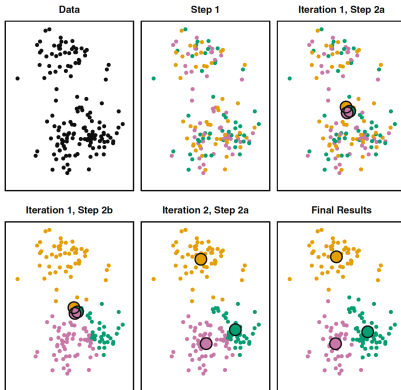
- Difficult problem: K^n ways to partition n observations into K clusters.
- Fortunately, there is a simple algorithm that can provide a local optimum

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 k th cluster centroid is the vector of the p feature means for the observations in the k th 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

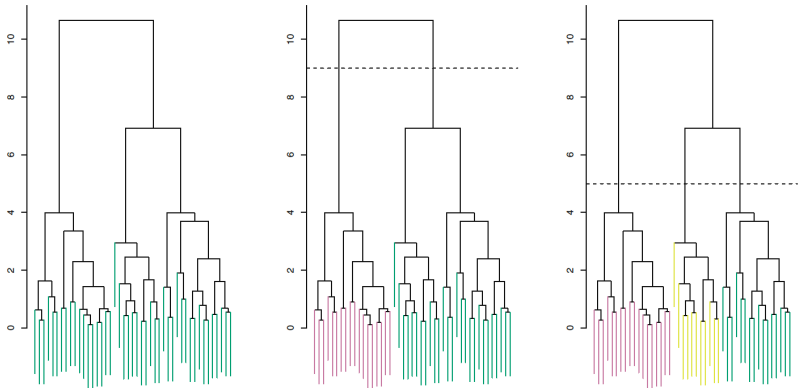
K-means algorithm

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

Hierarchical Clustering

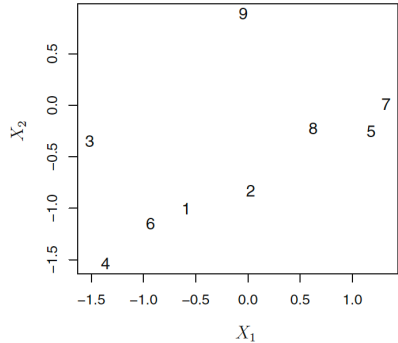
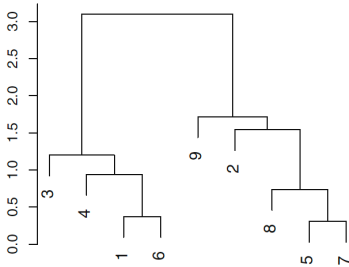
- Does not require us to commit to a particular choice of K in advance
- Produces an attractive tree-based representation called *dendogram*
- We will describe bottom-up or agglomerative clustering
 - Most common type of hierarchical clustering
- Other approach available is called Divisive or “top down”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

Interpreting a dendrogram



- The height of the cut in the dendrogram 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 \rightarrow 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.

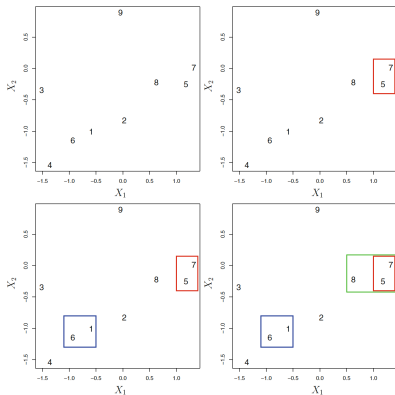
Hierarchical structure

- 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 bottom of the dendrogram
 - 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

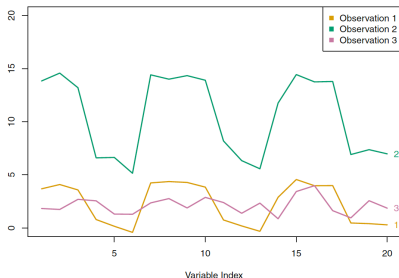


- First few steps of the hierarchical clustering algorithm
 - Euclidean distance
 - Complete linkage
- 5 and 7
- 6 and 1

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 \rightarrow large correlation-based distance
- Observations 1 and 2
 - Different values for each variable \rightarrow large euclidean distance
 - Strongly correlated

Online retailer example

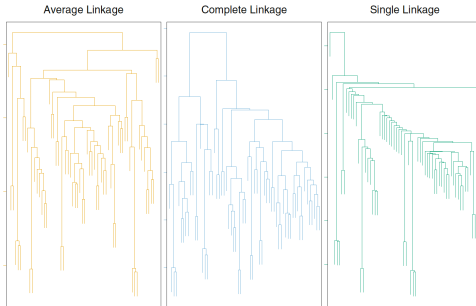
- Online retailer example
 - Identify subgroups of similar shoppers
 - Matrix with shoppers (rows) and items (columns)
 - Value indicate number of times a shopper bought an item
- Euclidean distance
 - Infrequent shoppers will be clustered together
 - The amount of items bought matters
- Correlation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

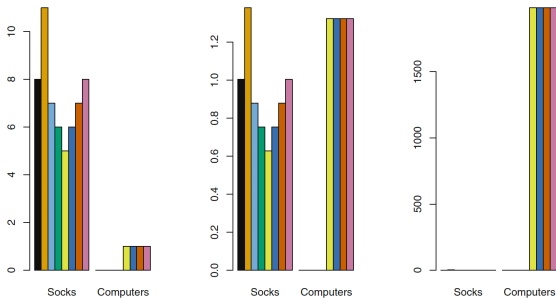
- Dendrogram depends strongly on the type of linkage used



- 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 items, 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 dendrogram?
- 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/>