### Cluster Analysis with R

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### Outline

Introduction

Data Clustering with R

The Iris Dataset

Partitioning Clustering

Hierarchical Clustering

Density-Based clustering

Cluster Validation

Further Readings and Online Resources

Exercises

## What is Data Clustering?

- ▶ Data clustering is to partition data into groups, where the data in the same group are similar to one another and the data from different groups are dissimilar [Han and Kamber, 2000].
- ► To segment data into clusters so that the *intra-cluster* similarity is maximized and that the *inter-cluster* similarity is minimized.
- The groups obtained are a partition of data, which can be used for customer segmentation, document categorization, etc.

# Data Clustering with R <sup>2</sup>

- Partitioning Methods
  - k-means clustering: stats::kmeans() 1 and fpc::kmeansruns()
  - k-medoids clustering: cluster::pam() and fpc::pamk()
- Hierarchical Methods
  - Divisive hierarchical clustering: DIANA, cluster::diana(),
  - Agglomerative hierarchical clustering: cluster::agnes(),
    stats::hclust()
- Density based Methods
  - DBSCAN: fpc::dbscan()
- Cluster Validation
  - Packages clValid, cclust, NbClust

<sup>&</sup>lt;sup>1</sup>package\_name::function\_name()

<sup>&</sup>lt;sup>2</sup>Chapter 6 - Clustering, in *R* and *Data Mining: Examples and Case Studies*. http://www.rdatamining.com/docs/RDataMining-book.pdf

### The Iris Dataset - I

The iris dataset [Frank and Asuncion, 2010] consists of 50 samples from each of three classes of iris flowers. There are five attributes in the dataset:

- sepal length in cm,
- sepal width in cm,
- petal length in cm,
- petal width in cm, and
- class: Iris Setosa, Iris Versicolour, and Iris Virginica.

Detailed desription of the dataset can be found at the UCI Machine Learning Repository  $^3$ .

<sup>3</sup>https://archive.ics.uci.edu/ml/datasets/Iris

### The Iris Dataset - II

Below we have a look at the structure of the dataset with str().

```
## 'data.frame': 150 obs. of 5 variables:
## $ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9...
## $ Sepal.Width : num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3...
## $ Petal.Length: num 1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4...
## $ Petal.Width : num 0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2...
## $ Species : Factor w/ 3 levels "setosa", "versicolor"...
```

- ▶ 150 observations (records, or rows) and 5 variables (or columns)
- ▶ The first four variables are numeric.
- ► The last one, Species, is categoric (called as "factor" in R) and has three levels of values.

### The Iris Dataset - III

```
summary(iris)
##
    Sepal.Length
                Sepal.Width Petal.Length Petal.W...
   Min. :4.300
                Min.
                        :2.000
                                       :1.000
##
                                Min.
                                               Min. :...
   1st Qu.:5.100 1st Qu.:2.800
                               1st Qu.:1.600
##
                                               1st Qu.:...
##
   Median :5.800
                Median :3.000
                                Median :4.350
                                               Median :...
##
   Mean :5.843 Mean :3.057
                                Mean :3.758
                                               Mean :...
##
   3rd Qu.:6.400 3rd Qu.:3.300
                                3rd Qu.:5.100
                                               3rd Qu.:...
##
   Max. :7.900 Max. :4.400
                                Max. :6.900
                                               Max. :...
##
         Species
##
   setosa
          :50
##
   versicolor:50
##
   virginica:50
##
##
##
```

### Outline

Introduction

Partitioning Clustering
The k-Means Clustering
The k-Medoids Clustering

Hierarchical Clustering

Density-Based clustering

Cluster Validation

Further Readings and Online Resources

Exercises

### Partitioning clustering - I

- Partitioning the data into k groups first and then trying to improve the quality of clustering by moving objects from one group to another
- ▶ k-means [Alsabti et al., 1998, Macqueen, 1967]: randomly selects k objects as cluster centers and assigns other objects to the nearest cluster centers, and then improves the clustering by iteratively updating the cluster centers and reassigning the objects to the new centers.
- ▶ k-medoids [Huang, 1998]: a variation of k-means for categorical data, where the medoid (i.e., the object closest to the center), instead of the centroid, is used to represent a cluster.
- ▶ PAM and CLARA [Kaufman and Rousseeuw, 1990]
- CLARANS [Ng and Han, 1994]

### Partitioning clustering - II

- ▶ The result of partitioning clustering is dependent on the selection of initial cluster centers and it may result in a local optimum instead of a global one. (Improvement: run k-means multiple times with different initial centers and then choose the best clustering result.)
- ► Tends to result in sphere-shaped clusters with similar sizes
- Sentitive to outliers
- ▶ Non-trivial to choose an appropriate value for k

### k-Means Algorithm

- ▶ k-means: a classic partitioning method for clustering
- ► First, it selects *k* objects from the dataset, each of which initially represents a cluster center.
- Each object is assigned to the cluster to which it is most similar, based on the distance between the object and the cluster center.
- ➤ The means of clusters are computed as the new cluster centers.
- The process iterates until the criterion function converges.

### k-Means Algorithm - Criterion Function

A typical criterion function is the squared-error criterion, defined as

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} \|p - m_i\|^2, \tag{1}$$

where E is the sum of square-error, p is a point, and  $m_i$  is the center of cluster  $C_i$ .

### k-means clustering

```
## set a seed for random number generation to make the results
## reproducible
set.seed(8953)
## make a copy of iris data
iris2 <- iris
## remove the class label, Species
iris2$Species <- NULL
## run kmeans clustering to find 3 clusters
kmeans.result <- kmeans(iris2, 3)</pre>
```

```
## print the clusterng result
kmeans.result
```

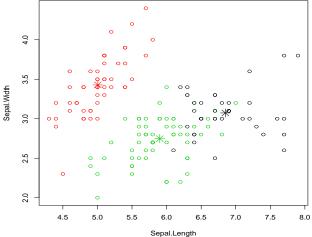
```
## K-means clustering with 3 clusters of sizes 38, 50, 62
##
## Cluster means:
##
   Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1
     6.850000 3.073684 5.742105 2.071053
## 2 5.006000 3.428000 1.462000 0.246000
## 3 5.901613 2.748387 4.393548 1.433871
##
## Clustering vector:
##
  ##
  [91] 3 3 3 3 3 3 3 3 3 3 3 1 3 1 1 1 1 3 1 1 1 1 1 1 3 3 1...
##
##
## Within cluster sum of squares by cluster:
## [1] 23.87947 15.15100 39.82097
##
  (between_SS / total_SS = 88.4 %)
##
## Available components:
##
## [1] "cluster" "centers" "totss" "withins...
## [5] "tot.withinss" "betweenss" "size"
                                  "iter" ...
## [9] "ifault"
                                            14 / 61
```

# Results of k-Means Clustering

### Check clustering result against class labels (Species)

- ▶ Class "setosa" can be easily separated from the other clusters
- ► Classes "versicolor" and "virginica" are to a small degree overlapped with each other.

```
plot(iris2[, c("Sepal.Length", "Sepal.Width")],
      col = kmeans.result$cluster)
points(kmeans.result$centers[, c("Sepal.Length", "Sepal.Width")],
      col = 1:3, pch = 8, cex=2) # plot cluster centers
```



## k-means clustering with estimating k and initialisations

- kmeansruns() in package fpc [Hennig, 2014]
- calls kmeans() to perform k-means clustering
- initializes the k-means algorithm several times with random points from the data set as means
- estimates the number of clusters by Calinski Harabasz index or average silhouette width

```
library(fpc)
kmeansruns.result <- kmeansruns(iris2)</pre>
kmeansruns.result
## K-means clustering with 3 clusters of sizes 62, 50, 38
##
## Cluster means:
##
   Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1 5.901613 2.748387 4.393548 1.433871
## 2 5.006000 3.428000 1.462000 0.246000
## 3 6.850000 3.073684 5.742105 2.071053
##
## Clustering vector:
##
  ##
## [91] 1 1 1 1 1 1 1 1 1 1 3 1 3 3 3 3 1 3 3 3 3 3 1 1 3...
##
## Within cluster sum of squares by cluster:
## [1] 39.82097 15.15100 23.87947
##
  (between_SS / total_SS = 88.4 %)
##
                                            18 / 61
## Available components:
```

## The *k*-Medoids Clustering

- ▶ Difference from *k*-means: a cluster is represented with its center in the *k*-means algorithm, but with the object closest to the center of the cluster in the *k*-medoids clustering.
- ▶ more robust than *k*-means in presence of outliers
- PAM (Partitioning Around Medoids) is a classic algorithm for k-medoids clustering.
- ► The CLARA algorithm is an enhanced technique of PAM by drawing multiple samples of data, applying PAM on each sample and then returning the best clustering. It performs better than PAM on larger data.
- ► Functions pam() and clara() in package *cluster* [Maechler et al., 2016]
- ► Function pamk() in package fpc does not require a user to choose k.

# Clustering with pam()

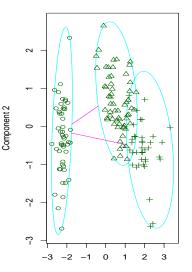
```
library(cluster)
# group into 3 clusters
pam.result <- pam(iris2, 3)
# check against actual class label
table(pam.result$clustering, iris$Species)

##
## setosa versicolor virginica
## 1 50 0 0
## 2 0 48 14
## 3 0 2 36</pre>
```

#### Three clusters:

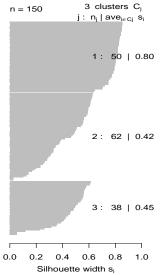
- Cluster 1 is species "setosa" and is well separated from the other two.
- Cluster 2 is mainly composed of "versicolor", plus some cases from "virginica".
- ► The majority of cluster 3 are "virginica", with two cases from "versicolor".

#### clusplot(pam(x = iris2, k = 3))



Component 1
These two components explain 95.8

#### Silhouette plot of pam(x = iris



Average silhouette width: 0.55

£ 990

- ▶ The left chart is a 2-dimensional "clusplot" (clustering plot) of the three clusters and the lines show the distance between clusters.
- ▶ The right chart shows their silhouettes. A large  $s_i$  (almost 1) suggests that the corresponding observations are very well clustered, a small  $s_i$  (around 0) means that the observation lies between two clusters, and observations with a negative  $s_i$  are probably placed in the wrong cluster.
- ▶ Silhouette width of cluster 1 is 0.80, which means it is well clustered and seperated from other clusters. The other two are of relatively low silhouette width (0.42 and 0.45), and they are somewhat overlapped with each other.

# Clustering with pamk()

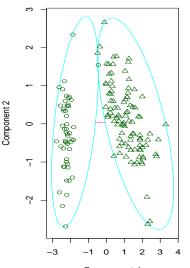
```
library(fpc)
pamk.result <- pamk(iris2)</pre>
# number of clusters
pamk.result$nc
## [1] 2
# check clustering against actual class label
table(pamk.result$pamobject$clustering, iris$Species)
##
##
       setosa versicolor virginica
           50
##
                                  50
##
                       49
```

#### Two clusters:

- "setosa"
- a mixture of "versicolor" and "virginica"

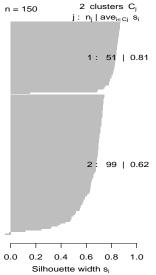
### plot(pamk.result)

#### clusplot(pam(x = sdata, k = k, diss = d)



Component 1
These two components explain 95.8

#### Silhouette plot of pam(x = sd:



Average silhouette width: 0.69

# Results of Clustering

▶ In this example, the result of pam() seems better, because it identifies three clusters, corresponding to three species.

## Results of Clustering

- ▶ In this example, the result of pam() seems better, because it identifies three clusters, corresponding to three species.
- Note that we cheated by setting k = 3 when using pam(), which is already known to us as the number of species.

### Outline

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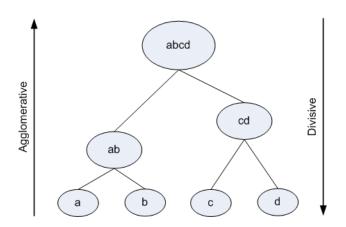
Further Readings and Online Resources

Exercises

## Hierarchical Clustering - I

- With hierarchical clustering approach, a hierarchical decomposition of data is built in either bottom-up (agglomerative) or top-down (divisive) way.
- ► Generally a dendrogram is generated and a user may select to cut it at a certain level to get the clusters.

# Hierarchical Clustering - II



# Hierarchical Clustering Algorithms

- With agglomerative clustering, every single object is taken as a cluster and then iteratively the two nearest clusters are merged to build bigger clusters until the expected number of clusters is obtained or when only one cluster is left.
  - AGENS [Kaufman and Rousseeuw, 1990]
- Divisive clustering works in an opposite way, which puts all objects in a single cluster and then divides the cluster into smaller and smaller ones.
  - DIANA [Kaufman and Rousseeuw, 1990]
  - ▶ BIRCH [Zhang et al., 1996]
  - CURE [Guha et al., 1998]
  - ROCK [Guha et al., 1999]
  - ► Chameleon [Karypis et al., 1999]

### Hierarchical Clustering - Distance Between Clusters

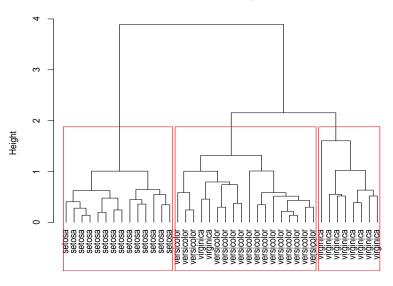
In hierarchical clustering, there are four different methods to measure the distance between clusters:

- Centroid distance is the distance between the centroids of two clusters.
- Average distance is the average of the distances between every pair of objects from two clusters.
- ► Single-link distance, a.k.a. minimum distance, is the distance between the two nearest objects from two clusters.
- ► Complete-link distance, a.k.a. maximum distance, is the distance between the two objects which are the farthest from each other from two clusters.

### Hierarchical Clustering of the iris Data

```
set.seed(2835)
# draw a sample of 40 records from the iris data, so that the
# clustering plot will not be over crowded
idx <- sample(1:dim(iris)[1], 40)</pre>
iris3 <- iris[idx, ]</pre>
# remove class label
iris3$Species <- NULL
# hierarchical clustering
hc <- hclust(dist(iris3), method = "ave")</pre>
# plot clusters
plot(hc, hang = -1, labels = iris$Species[idx])
# cut tree into 3 clusters
rect.hclust(hc, k = 3)
# get cluster IDs
groups <- cutree(hc, k = 3)
```

#### **Cluster Dendrogram**



### Agglomeration Methods of hclust

```
hclust(d, method = "complete", members = NULL)
```

- method = "ward.D" or "ward.D2": Ward's minimum variance method aims at finding compact, spherical clusters [R Core Team, 2015].
- method = "complete": complete-link distance; finds similar clusters.
- method = "single": single-link distance; adopts a "friends of friends" clustering strategy.
- method = "average": average distance
- method = "centroid": centroid distance
- method = "median":
- method = "mcquitty":

### DIANA

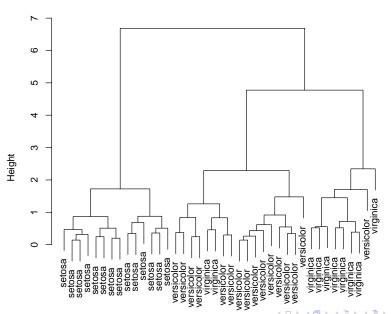
- ▶ DIANA [Kaufman and Rousseeuw, 1990]: divisive hierarchical clustering
- Constructs a hierarchy of clusterings, starting with one large cluster containing all observations.
- Divides clusters until each cluster contains only a single observation.
- ▶ At each stage, the cluster with the largest diameter is selected. (The diameter of a cluster is the largest dissimilarity between any two of its observations.)
- ► To divide the selected cluster, the algorithm first looks for its most disparate observation (i.e., which has the largest average dissimilarity to other observations in the selected cluster). This observation initiates the "splinter group". In subsequent steps, the algorithm reassigns observations that are closer to the "splinter group" than to the "old party". The result is a division of the selected cluster into two new clusters.

### DIANA

```
library(cluster)
diana.result <- diana(iris3)</pre>
```

```
plot(diana.result, which.plots = 2, labels = iris$Species[idx])
```

#### Dendrogram of diana(x = iris3)



## Outline

Introduction

Partitioning Clustering

Hierarchical Clustering

Density-Based clustering

Cluster Validation

Further Readings and Online Resources

Exercises

## **Density-Based Clustering**

- The rationale of density-based clustering is that a cluster is composed of well-connected dense region, while objects in sparse areas are removed as noises.
- DBSCAN is a typical density-based clustering algorithm, which works by expanding clusters to their dense neighborhood [Ester et al., 1996].
- Other density-based clustering techniques: OPTICS [Ankerst et al., 1999] and DENCLUE [Hinneburg and Keim, 1998]
- ► The advantage of density-based clustering is that it can filter out noise and find clusters of arbitrary shapes (as long as they are composed of connected dense regions).

# DBSCAN [Ester et al., 1996]

- Group objects into one cluster if they are connected to one another by densely populated area
- ► The DBSCAN algorithm from package *fpc* provides a density-based clustering for numeric data.
- Two key parameters in DBSCAN:
  - eps: reachability distance, which defines the size of neighborhood; and
  - MinPts: minimum number of points.
- If the number of points in the neighborhood of point  $\alpha$  is no less than MinPts, then  $\alpha$  is a *dense point*. All the points in its neighborhood are *density-reachable* from  $\alpha$  and are put into the same cluster as  $\alpha$ .
- Can discover clusters with various shapes and sizes
- Insensitive to noise

## Density-based Clustering of the iris data

```
library(fpc)
iris2 <- iris[-5] # remove class tags
ds <- dbscan(iris2, eps = 0.42, MinPts = 5)
ds

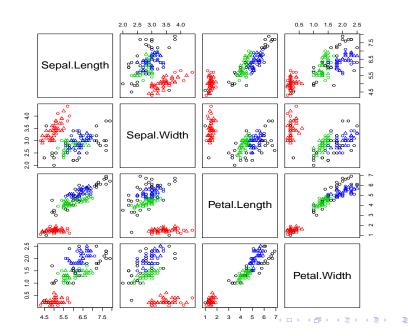
## dbscan Pts=150 MinPts=5 eps=0.42
## 0 1 2 3
## border 29 6 10 12
## seed 0 42 27 24
## total 29 48 37 36</pre>
```

## Density-based Clustering of the iris data

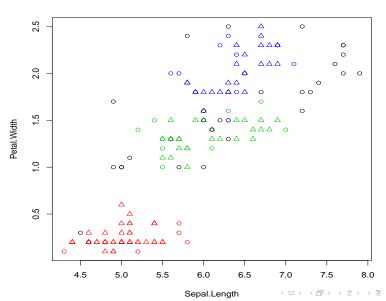
```
# compare clusters with actual class labels
table(ds$cluster, iris$Species)

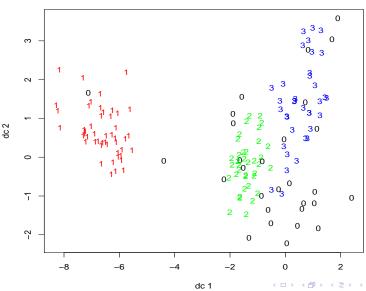
##
## setosa versicolor virginica
## 0 2 10 17
## 1 48 0 0
## 2 0 37 0
## 3 0 3 33
```

- 1 to 3: identified clusters
- ▶ 0: noises or outliers, i.e., objects that are not assigned to any clusters



plot(ds, iris2[, c(1, 4)])





## Prediction with Clustering Model

- Label new data, based on their similarity with the clusters
- Draw a sample of 10 objects from iris and add small noises to them to make a new dataset for labeling
- Random noises are generated with a uniform distribution using function runif().

### Results of Prediction

```
##
## pred setosa versicolor virginica
## 1 3 0 0
## 2 0 3 0
## 3 0 1 2
```

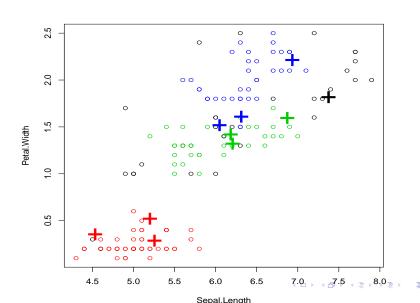
#### Results of Prediction

```
table(pred, iris$Species[idx]) # check cluster labels

##
## pred setosa versicolor virginica
## 0 0 0 1
## 1 3 0 0
## 2 0 3 0
## 3 0 1 2
```

Eight(=3+3+2) out of 10 objects are assigned with correct class labels.

```
plot(iris2[, c(1, 4)], col = 1 + ds$cluster)
points(new.data[, c(1, 4)], pch = "+", col = 1 + pred, cex = 3)
```



47 / 61

## Outline

Introduction

Partitioning Clustering

Hierarchical Clustering

Density-Based clustering

Cluster Validation

Further Readings and Online Resources

Exercises

## Cluster Validation

- silhouette() compute or extract silhouette information
  (cluster)
- cluster.stats() compute several cluster validity statistics from a clustering and a dissimilarity matrix (fpc)
- clValid() calculate validation measures for a given set of clustering algorithms and number of clusters (clValid)
- clustIndex() calculate the values of several clustering indexes, which can be independently used to determine the number of clusters existing in a data set (cclust)
- ▶ NbClust() provide 30 indices for cluster validation and determining the number of clusters (*NbClust*)

## Outline

Introduction

Partitioning Clustering

Hierarchical Clustering

Density-Based clustering

Cluster Validation

Further Readings and Online Resources

Exercises

## Further Readings - Clustering

- ➤ A breif overview of various apporaches for clustering
  Yanchang Zhao, et al. "Data Clustering." In Ferraggine et al. (Eds.), Handbook
  of Research on Innovations in Database Technologies and Applications, Feb
  2009. http://yanchang.rdatamining.com/publications/
  Overview-of-Data-Clustering.pdf
- Cluster Analysis & Evaluation Measures https://en.wikipedia.org/wiki/Cluster\_analysis
- ▶ Detailed review of algorithms for data clustering
  Jain, A. K., Murty, M. N., Flynn, P. J. (1999). Data clustering: a review. ACM
  Computing Surveys, 31(3), 264-323.
  Berkhin, P. (2002). Survey of Clustering Data Mining Techniques. Accrue
  Software, San Jose, CA, USA.
  - http://citeseer.ist.psu.edu/berkhin02survey.html.
- ► A comprehensive textbook on data mining Han, J., Kamber, M. (2000). Data mining: concepts and techniques. San Francisco, CA, USA: Morgan Kaufmann Publishers Inc.

## Further Readings - Clustering with R

- ► Data Mining Algorithms In R: Clustering https:
  - //en.wikibooks.org/wiki/Data\_Mining\_Algorithms\_In\_R/Clustering
- ▶ Data Mining Algorithms In R: k-Means Clustering https://en.wikibooks.org/wiki/Data\_Mining\_Algorithms\_In\_R/ Clustering/K-Means
- Data Mining Algorithms In R: k-Medoids Clustering https://en.wikibooks.org/wiki/Data\_Mining\_Algorithms\_In\_R/ Clustering/Partitioning\_Around\_Medoids\_(PAM)
- ▶ Data Mining Algorithms In R: Hierarchical Clustering https://en.wikibooks.org/wiki/Data\_Mining\_Algorithms\_In\_R/ Clustering/Hierarchical\_Clustering
- ▶ Data Mining Algorithms In R: Density-Based Clustering https://en.wikibooks.org/wiki/Data\_Mining\_Algorithms\_In\_R/ Clustering/Density-Based\_Clustering

#### Online Resources

- Chapter 6 Clustering, in book R and Data Mining: Examples and Case Studies http://www.rdatamining.com/docs/RDataMining-book.pdf
- RDataMining Reference Card
   http://www.rdatamining.com/docs/RDataMining-reference-card.pdf
- ► Free online courses and documents http://www.rdatamining.com/resources/
- ► RDataMining Group on LinkedIn (20,000+ members)
  http://group.rdatamining.com
- Twitter (2,500+ followers)@RDataMining

## Outline

Introduction

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Further Readings and Online Resources

Exercises

#### Exercise - I

### Clustering cars based on road test data

- mtcars: the Motor Trend Car Road Tests data, comprising fuel consumption and 10 aspects of automobile design and performance for 32 automobiles (1973–74 models) [R Core Team, 2015]
- ▶ A data frame with 32 observations on 11 variables:
  - 1. mpg: fuel consumption (Miles/gallon)
  - 2. cyl: Number of cylinders
  - 3. disp: Displacement (cu.in.)
  - 4. hp: Gross horsepower
  - 5. drat: Rear axle ratio
  - 6. wt: Weight (lb/1000)
  - 7. qsec: 1/4 mile time
  - 8. vs: V engine or straight engine
  - 9. am: Transmission (0 = automatic, 1 = manual)
  - 10. gear: Number of forward gears
  - 11. carb: Number of carburetors

#### Exercise - II

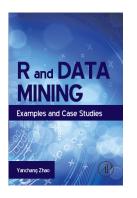
#### To cluster states of US

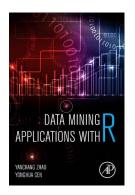
- state.x77: statistics of the 50 states of US [R Core Team, 2015]
- ▶ a matrix with 50 rows and 8 columns
  - 1. Population: population estimate as of July 1, 1975
  - 2. Income: per capita income (1974)
  - 3. Illiteracy: illiteracy (1970, percent of population)
  - 4. Life Exp: life expectancy in years (1969–71)
  - 5. Murder: murder and non-negligent manslaughter rate per 100,000 population (1976)
  - 6. HS Grad: percent high-school graduates (1970)
  - 7. Frost: mean number of days with minimum temperature below freezing (1931–1960) in capital or large city
  - 8. Area: land area in square miles

## Exercise - Questions

- Which attributes to use?
- Are the attributes at the same scale?
- Which clustering techniques to use?
- Which clustering algorithms to use?
- How many clusters to find?
- Are the clustering results good or not?

## The End





#### Thanks!

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