Clustering algorithms

K-means and DBSCAN

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Aims of this lesson

- Introduce you to the clustering algorithms and evaluation

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- Give some application examples

Introduction

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- Extract abnormal observations

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- Model based clustering: In this technique, the probability or likelihood of an observation being partitioned into a cluster is calculated.
- Non-parametric clustering: an observation is partitioned into exactly one cluster (no probability is calculated).

Distance calculation for clustering

1. Distance calculations for quantitative variables are highly influenced by variable units and magnitude. Standardize!

Suppose, we are given a 2-dimensional data with

$$X = (x_1, x_2, \cdots, x_p)$$

and

$$Y = (y_1, y_2, \cdots, y_p)$$

We can calculate various distances as follows:

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2. Use of a particular distance measure depends on the variable types.

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Numeric variables

- Euclidean Distance: $d(X, Y) = \sum(x_i - y_i)^2$

Catergorical variables

Hamming Distance: $d(x, y) = \sum(x_i \neq y_i)$

Mixed variables

Distance calculation for clustering

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- Manhattan Distance: $d(X, Y) = \sum |x_i - y_i|$

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Mixed variables

- Gower Distance
- Cosine Similarity

Distance calculation for clustering

1. Julie loves me more than Linda loves me

List of the words from both texts

me Julie loves Linda than more likes Jane

words	frequency 1	frequency 2
me	2	2
Jane	0	1
Jullie	1	0
Linda	0	1
likes	0	1
loves	2	1
more	1	1
than	1	1

Distance calculation for clustering

1. `Julie loves me more than Linda loves me`
2. `Jane likes me more than Julie loves me`

List of the words from both texts

`me Julie loves Linda than more likes Jane`

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Distance calculation for clustering

Cosine Similarity

The two vectors are, again:

```
a: [2, 1, 0, 2, 0, 1, 1, 1]

b: [2, 1, 1, 1, 1, 0, 1, 1]
```

$$\text{cos-similarity}(X, Y) = \cos(X, Y) = \frac{X.Y}{||X||.||Y||}$$

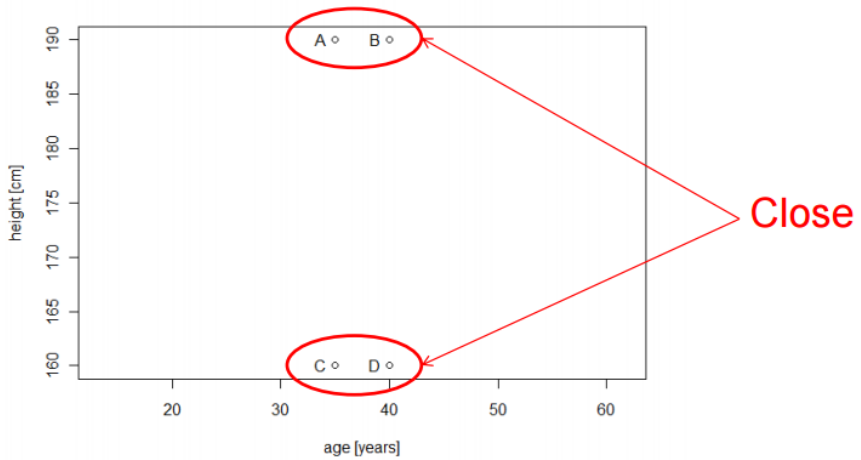
The cosine of the angle between a and b is about 0.822.

Why Standardization?

Person	Age [years]	Height [cm]
A	35	190
B	40	190
C	35	160
D	40	160

Example 1: cm

- 4 persons

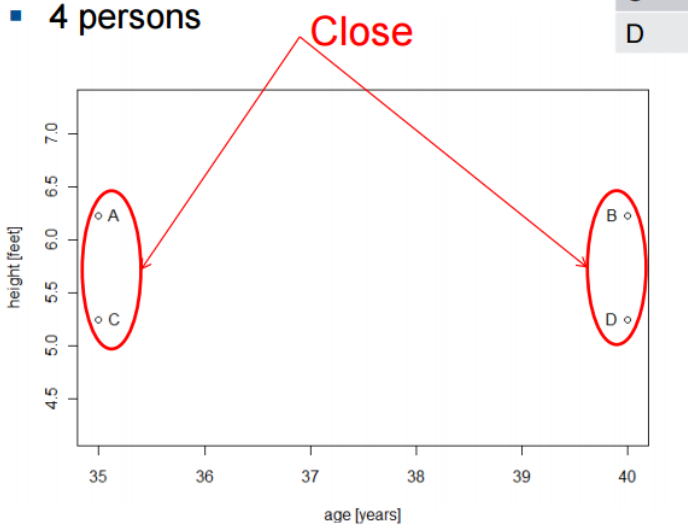


Why Standardization?

Person	Age [years]	Height [feet]
A	35	6.232
B	40	6.232
C	35	5.248
D	40	5.248

Example 1: feet

- 4 persons

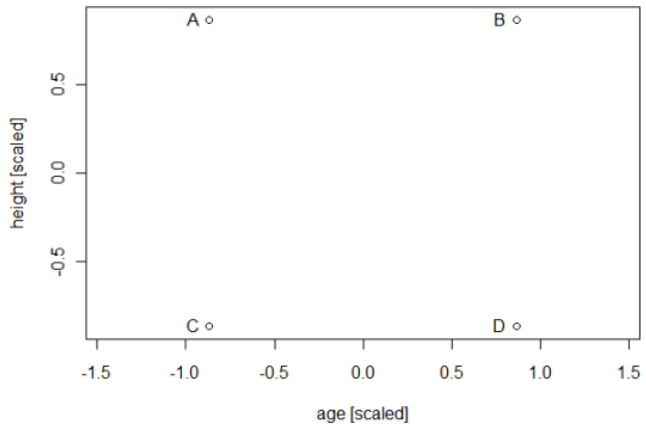


Why Standardization?

Example 1: scaled

- 4 persons

Person	Age [scaled]	Height [scaled]
A	-0.87	0.87
B	0.87	0.87
C	-0.87	-0.87
D	0.87	-0.87



No subgroups anymore

K-means clustering

K-means clustering: How does it work ?

- Input: K, set pf points $x_1, \cdots, x_n$

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- Stop when none of the cluster assignments change

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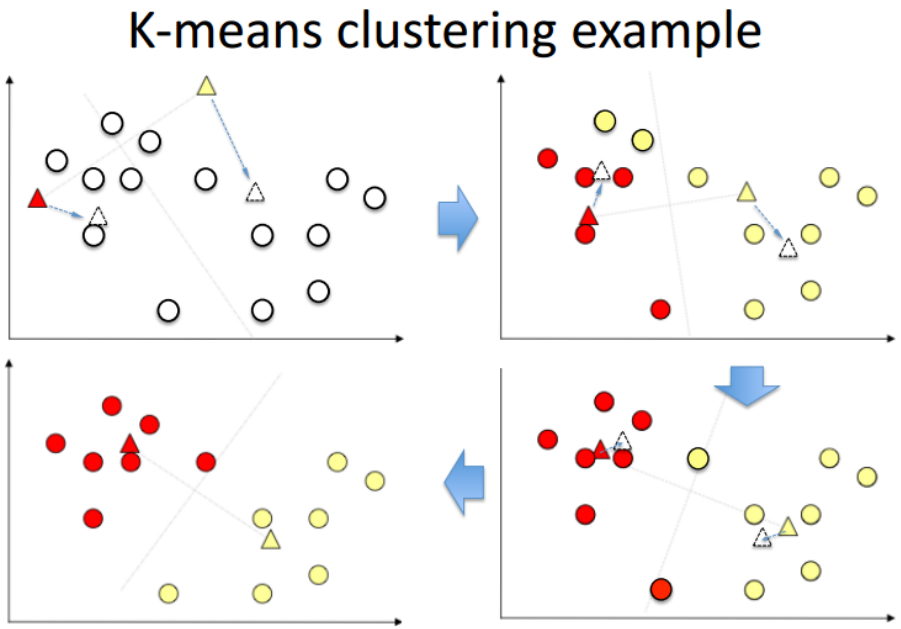

K-means clustering in R

Function `kmeans` from package `kmeans`

```
kmeans(x, centers, iter.max = 10, nstart = 1)
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- *x*: numeric matrix, numeric data frame or a numeric vector

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- *centers:* Possible values are the number of clusters (k) or a set of initial cluster centers.
- *iter.max:* The maximum number of iterations allowed. Default value is 10.
- *nstart:* The number of random starting partitions when centers is a number.

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`kmeans()` from package `kmeans` function returns a list including:

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- *withinss:* vector of within-cluster sum of squares, one component per cluster.
- *tot.withinss:* total within-cluster sum of squares. That is, `sum(withinss)`.
- *size:* the number of points in each cluster.

K-means clustering in R

```
set.seed(123)
# Two-dimensional data format
df <- rbind(matrix(rnorm(100, sd = 0.3), ncol = 2),
            matrix(rnorm(100, mean = 1, sd = 0.3),
            ncol = 2))
colnames(df) <- c("x", "y")
head(df,5)
```

```
##                   x            y
## [1,] -0.16814269  0.075995554
## [2,] -0.06905325 -0.008564027
## [3,]  0.46761249 -0.012861137
## [4,]  0.02115252  0.410580685
## [5,]  0.03878632 -0.067731296
```

K-means clustering in R

The R code below performs k-means clustering with k = 2:

```
# Compute k-means
set.seed(123)
km.res <- kmeans(df, 2, nstart = 25)
# Cluster number for each of the observations
km.res$cluster
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2
##  [71] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

K-means clustering in R

```
# Cluster size
km.res$size
```

```
## [1] 50 50
```

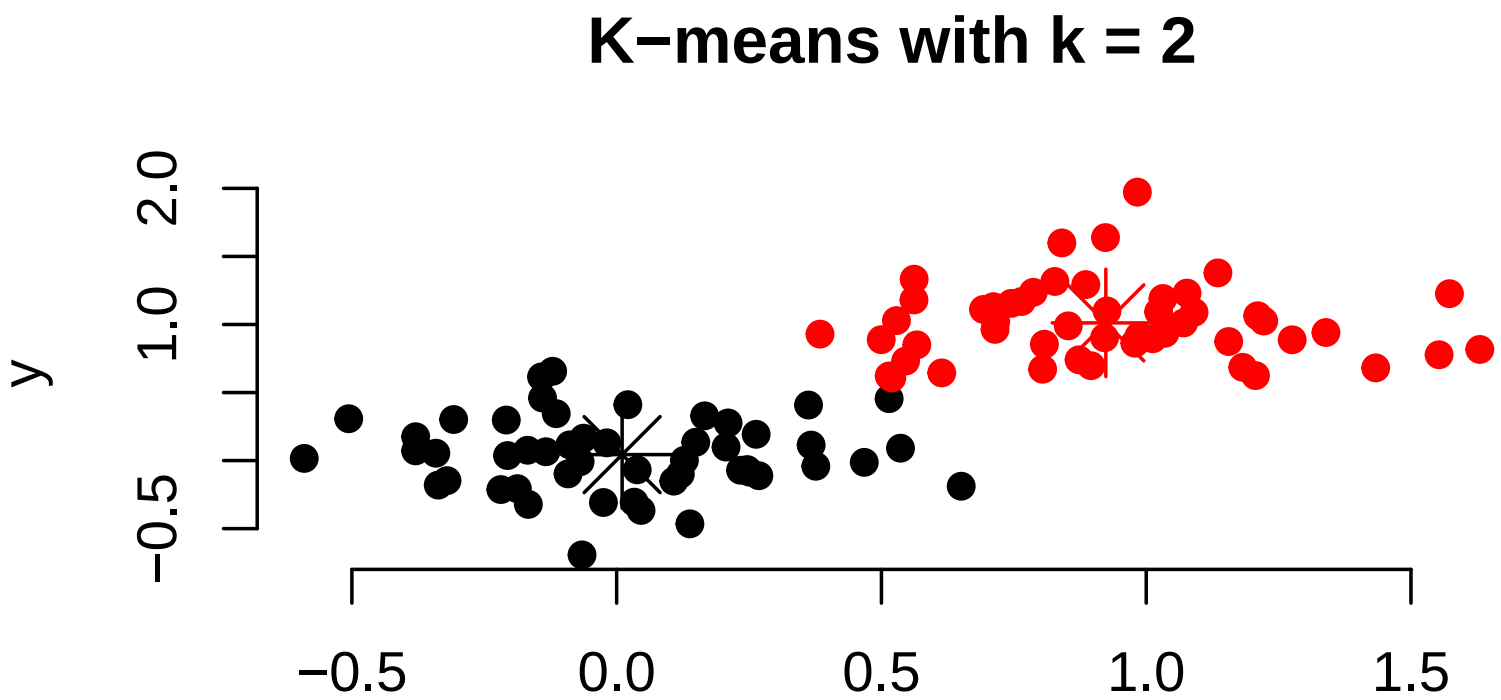
```
# Cluster means
km.res$centers
```

```
##           x          y
## 1 0.01032106 0.04392248
## 2 0.92382987 1.01164205
```

It's possible to plot the data with coloring each data point according to its cluster assignment. The cluster centers are specified using "big stars":

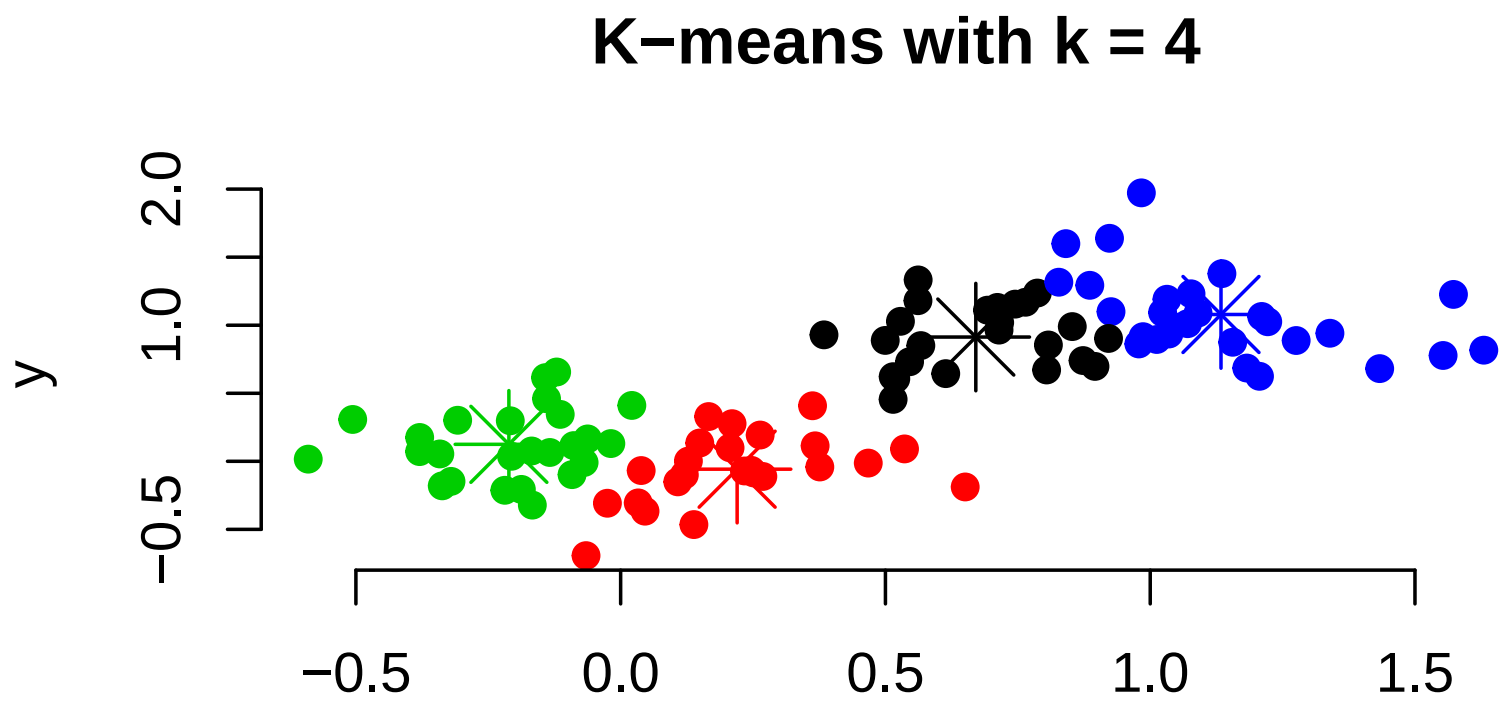
K-means clustering in R

```
plot(df, col = km.res$cluster, pch = 19, frame = FALSE,
     main = "K-means with k = 2")
points(km.res$centers, col = 1:2, pch = 8, cex = 3)
```



K-means clustering in R

```
km.res <- kmeans(df, 4, nstart = 25)
plot(df, col = km.res$cluster, pch = 19, frame = FALSE,
     main = "K-means with k = 4")
points(km.res$centers, col = 1:4, pch = 8, cex = 3)
```



K-means clustering in R

```
# Print the result
km.res
```

```
## K-means clustering with 4 clusters of sizes 24, 24, 25,
##
## Cluster means:
##             x           y
## 1  0.6706931  0.91293798
## 2  0.2199345 -0.05766457
## 3 -0.2110757  0.12500530
## 4  1.1336807  1.07876045
##
## Clustering vector:
##   [1] 3 3 2 3 2 1 2 3 3 3 2 2 2 2 3 2 2 3 2 3 3 2 3 3 3
##  [36] 2 2 3 3 3 3 3 3 2 2 3 3 3 2 2 1 4 4 1 1 4 1 1 4 4
##  [71] 4 1 1 4 4 1 4 4 1 4 4 4 4 1 1 4 1 4 4 1 4 1 1 1 1
```

K-means clustering in R

```
set.seed(123)
# K-means with nstart = 1
km.res <- kmeans(df, 4, nstart = 1)
km.res$tot.withinss
```

```
## [1] 10.13198
```

```
# K-means with nstart = 25
km.res <- kmeans(df, 4, nstart = 25)
km.res$tot.withinss
```

```
## [1] 9.814517
```

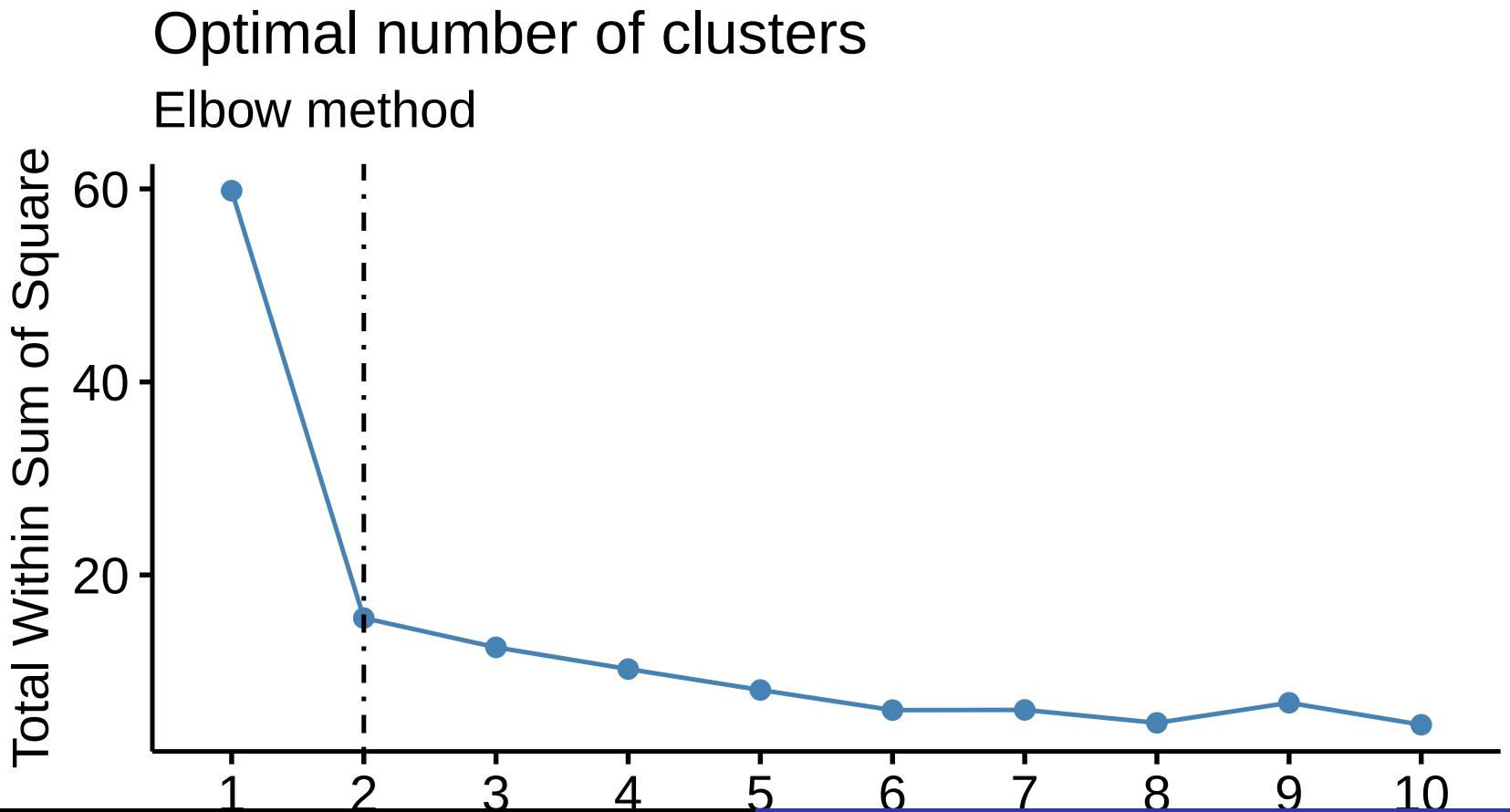
Predict memberships

```r
#load the libeary clue and use the function cl_predict
library(clue)
nr  <- nrow(df)
#choose a random 90% sample
ind <- sample(nr, 0.9 * nr, replace = FALSE)
km.res <- kmeans(df[ind, ], 2, nstart = 25)
cl_predict(km.res, df[-ind, ])
```

```
## Class ids:
##  [1] 1 1 1 1 1 1 2 2 2 2
```

How to choose k

```
fviz_nbclust(df, kmeans, method = "wss") +
  geom_vline(xintercept = 2, linetype = 4) +
  labs(subtitle = "Elbow method")
```



Drawbacks of K-means

1. Need to choose the right `k`

Pleae complete clustering_algorithms_lab.Rmd (kmeans section)

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Drawbacks of K-means

1. Need to choose the right `k`
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3. Cannot Handle Non-spherical Data

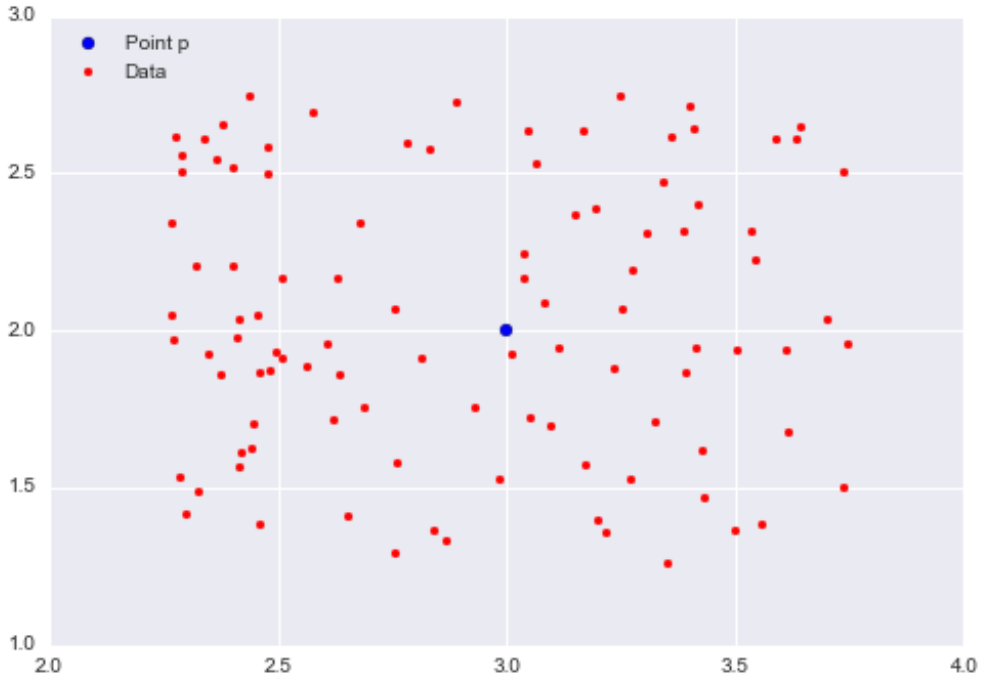
Pleae complete clustering_algorithms_lab.Rmd (kmeans section)

DBSCAN: Density-Based Spatial Clustering Algorithm with Noise

Preliminary: ϵ-Balls and neighborhood density

For some $\epsilon > 0$ and some point p, the ϵ-neighborhood of p is defined as the set of points that are at most distance ϵ away from p.

Preliminary: ϵ-Balls and neighborhood density



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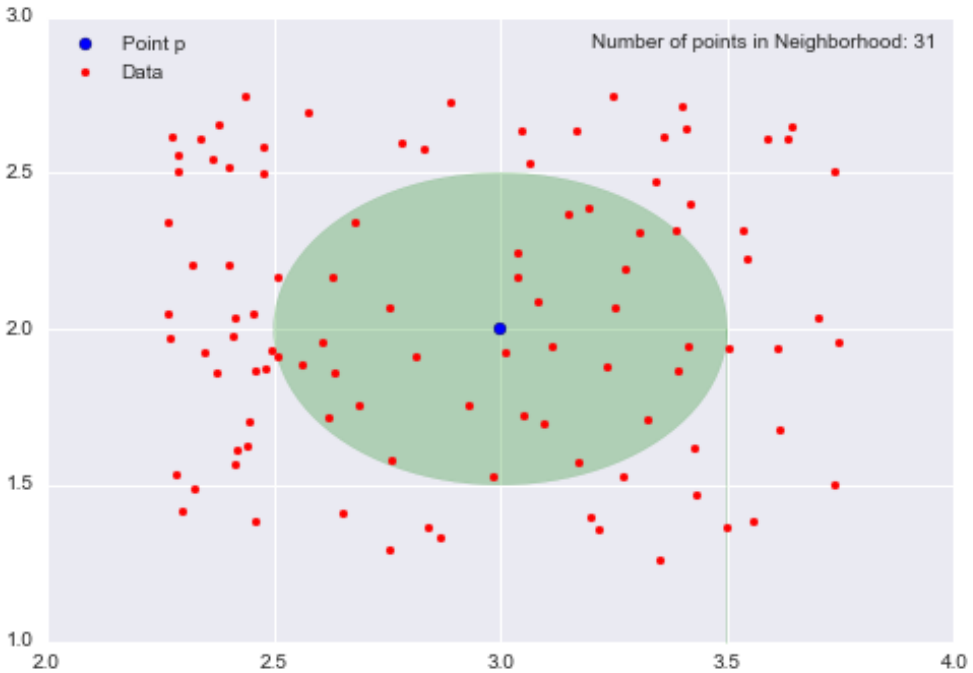

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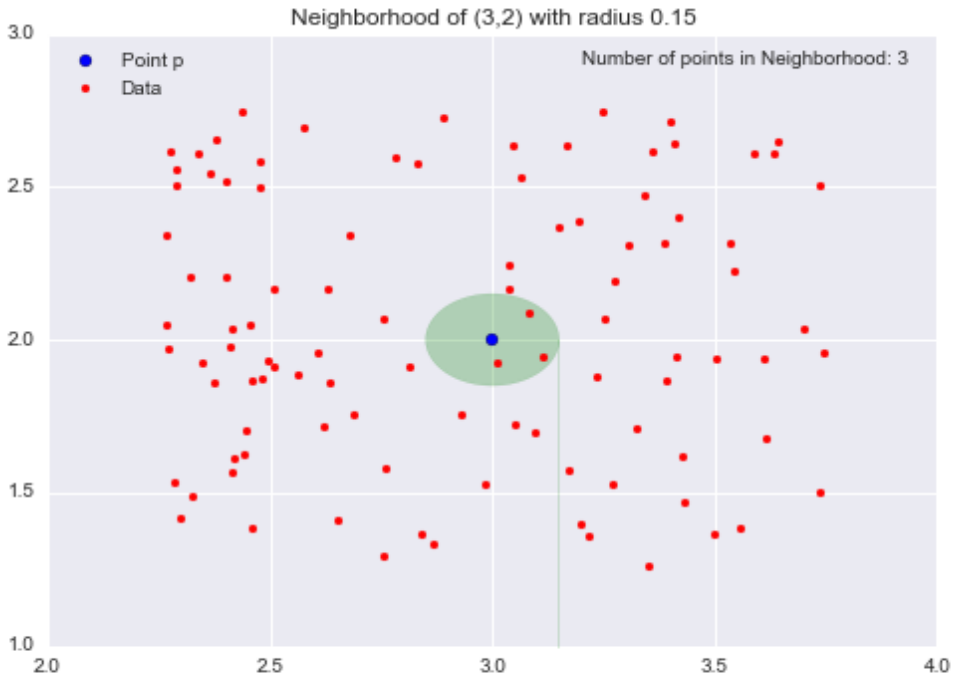

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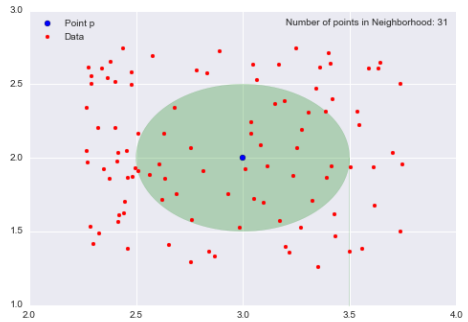

$$density = \frac{mass}{volume}$$

$mass = 31.$

$volume = \pi \times 0.5^2 = \frac{\pi}{4}$

Therefore, our local density approximation at $p = (3, 2)$ is calculated as $density = mass/volume = 31/\frac{\pi}{4} = 124/\pi \ = 39.5.$

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- This value is meaningless by itself, but if we calculate the local density approximation for all points in our dataset

While this is not exactly what DBSCAN does, it forms the general intuition behind density-based clustering.

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- we could cluster our points by saying that points that are nearby (contained in the same neighborhood) and have similar local density approximations belong in the same cluster.If we decrease the value of ϵ we can construct smaller neighborhoods (less volume) that would also contain fewer data points.

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- we could cluster our points by saying that points that are nearby (contained in the same neighborhood) and have similar local density approximations belong in the same cluster.If we decrease the value of ϵ we can construct smaller neighborhoods (less volume) that would also contain fewer data points.
- Ideally, we want to identify highly dense neighborhoods where most of the data points are contained in these neighborhoods, but the volume of each of these neighborhoods is relatively small.

While this is not exactly what DBSCAN does, it forms the general intuition behind density-based clustering.

DBSCAN

The ϵ-neighborhood is fundamental to DBSCAN to approximate local density, so the algorithm has two parameters:

- ϵ: The radius of our neighborhoods around a data point p. minPts: The minimum number of data points we want in a neighborhood to define a cluster.

Using these two parameters, DBSCAN categories the data points into three categories:

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- *Core Points*: A data point p is a core point if **Nbhd**(p, ϵ) [$\epsilon-$neighborhood of p] contains at least minPts ; **Nbhd**(p, ϵ) $>=$ *minPts*.

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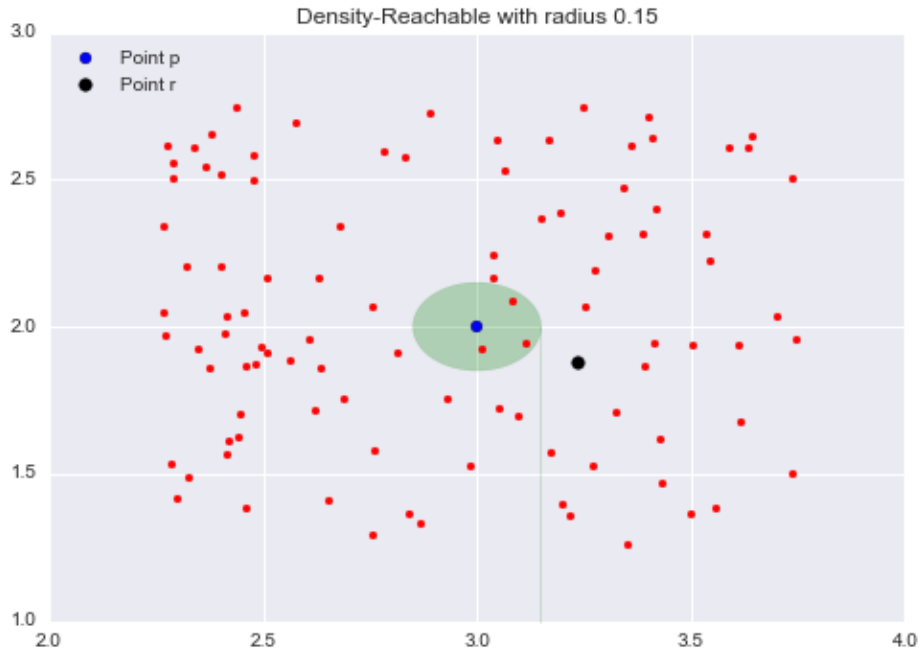
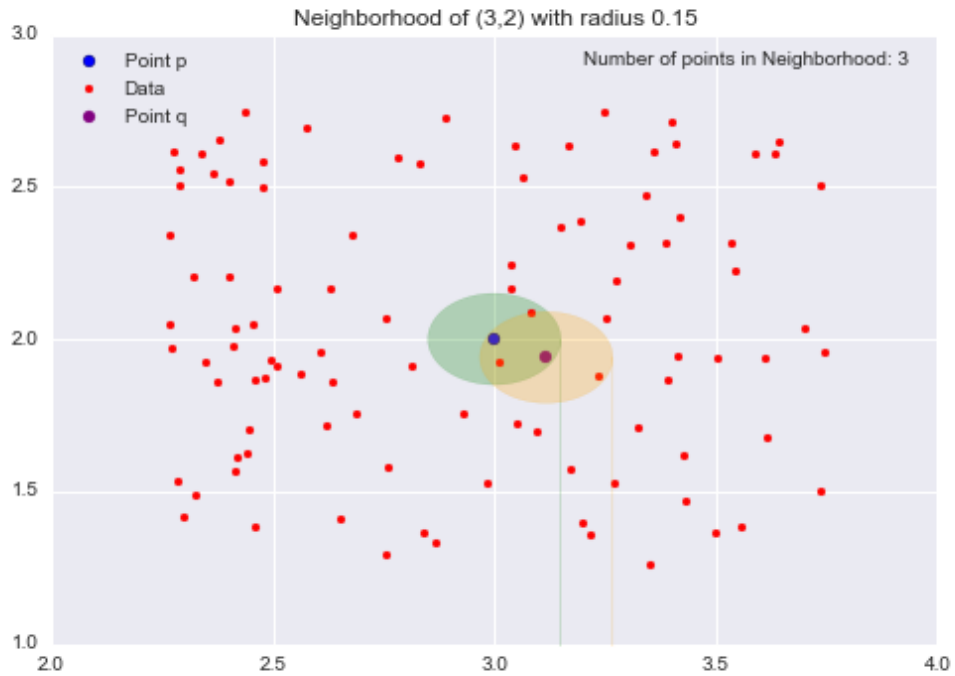
- *Outlier*: A data point O is an outlier if it is neither a *core point* nor a *border point*. Essentially, this is the "other" class.

DBSCAN: Border Points



The three points in **Nbhd**(p, ϵ) are said to be directly reachable from p

DBSCAN: Border Points



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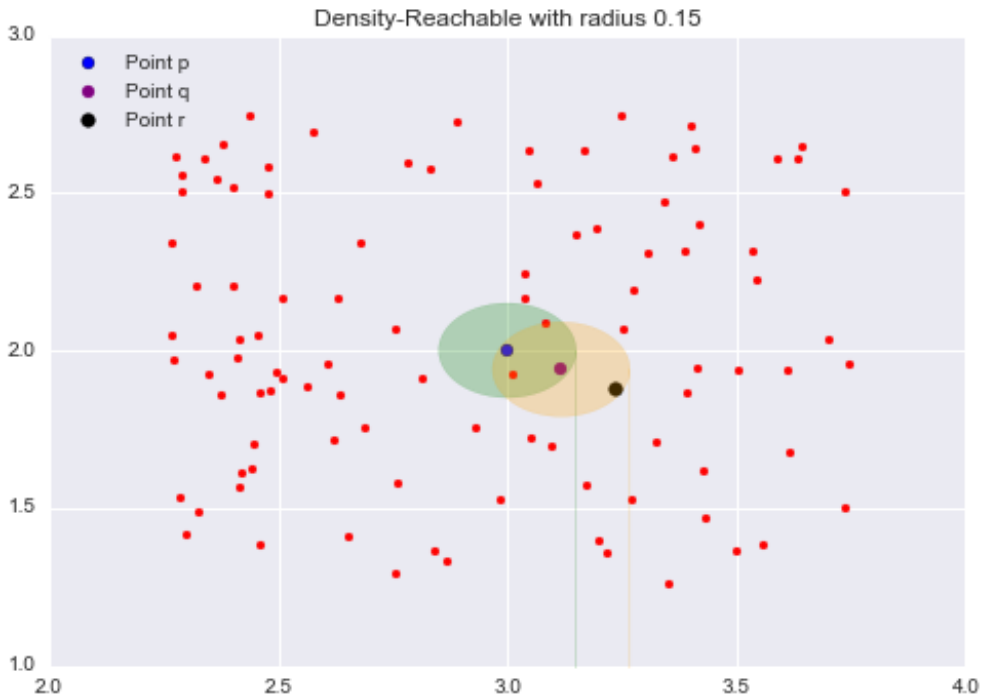

If I can get to the point *r* by jumping from neighborhood to neighborhood, starting at a point *p*, then the point r is *density-reachable* from the point *p*.

DBSCAN: Outliers

Outliers are points that are neither core points nor are they close enough to a cluster to be *density-reachable* from a core point. Outliers are not assigned to any cluster and, depending on the context, may be considered anomalous points.

Now that I have covered all the preliminaries, we can finally talk about how the algorithm works in practice.

DBSCAN algorithm

- Pick a point at random that has not been assigned to a cluster or been designated as an outlier. Compute its neighborhood to determine if it's a core point. If yes, start a cluster around this point. If no, label the point as an outlier.

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- Repeat these two steps until all points are either assigned to a cluster or designated as an outlier.

DBSCAN R implementation

We need the packages `fpc;dbscan` and `factoextra`

To determine the optimal value of ϵ we use the functionwe use

```
dbscan::kNNdistplot(data, k = minPts)
```

Compute DBSCAN using `fpc::dbscan()` or `dbscan::dbscan()`.

```
# fpc package
res.fpc <- fpc::dbscan(data, eps = espsilon, MinPts = k)
# dbscan package
res.db <- dbscan::dbscan(data, eps = espsilon, MinPts = k)
```

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  - eps: parameter eps
  - MinPts: parameter MinPts
- The result of the function dbscan::dbscan() is an integer vector with cluster assignments. Zero indicates noise points.

DBSCAN R implementation example

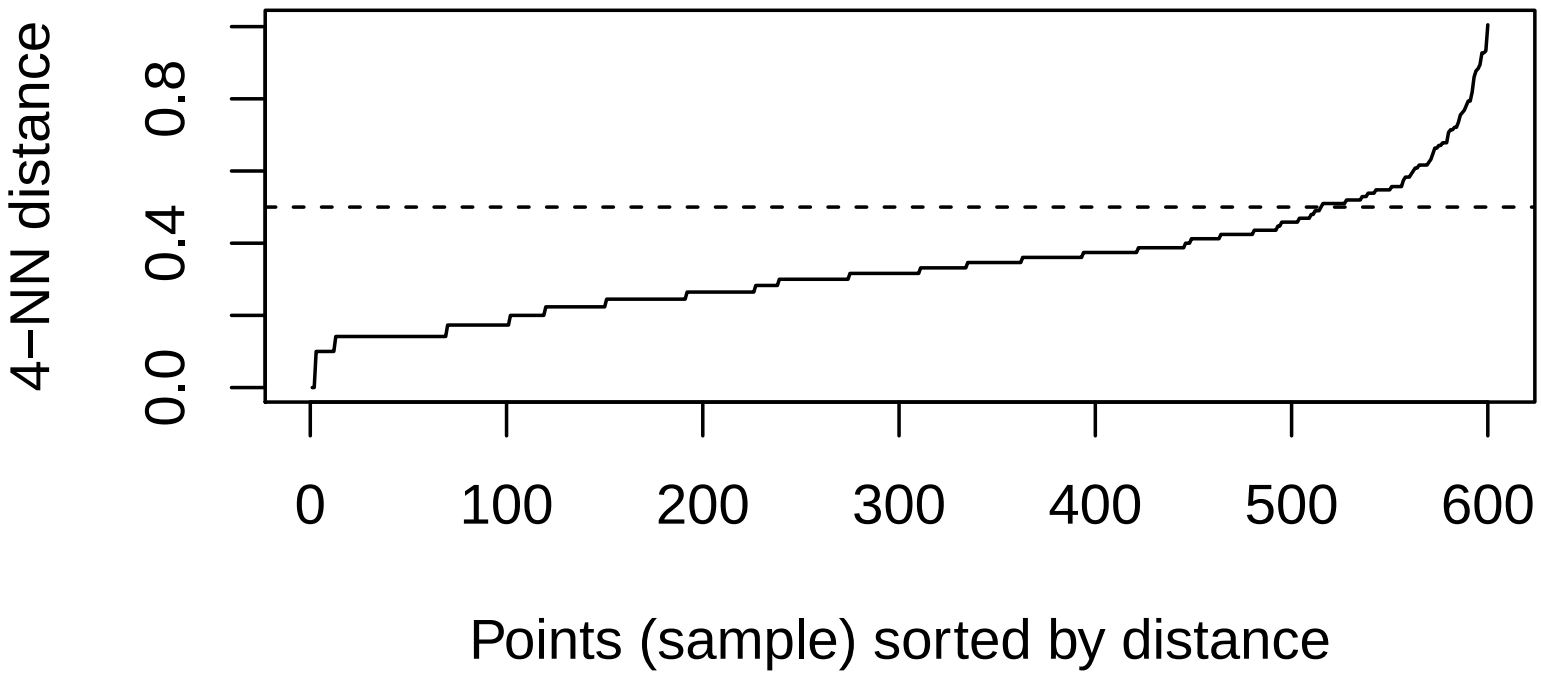
```
# Load the data
data("iris")
iris <- as.matrix(iris[, 1:4])

# The optimal value of "eps" parameter can be determined as

dbscan::kNNdistplot(iris, k =  4)
abline(h = 0.5, lty = 2)
# Compute DBSCAN using fpc::dbscan() and dbscan::dbscan().

set.seed(123)
# fpc package
res.fpc <- fpc::dbscan(iris, eps = 0.4, MinPts = 4)
# dbscan package
res.db <- dbscan::dbscan(iris, 0.4, 4)
```

DBSCAN R implementation example



Pleae complete clustering_algorithms_lab.Rmd (DBSCAN section)