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MACHINE LEARNING, R

How to determine the number of Clusters for K-Means in R

A walk-through example of how you can determine the number of Clusters for K-Means

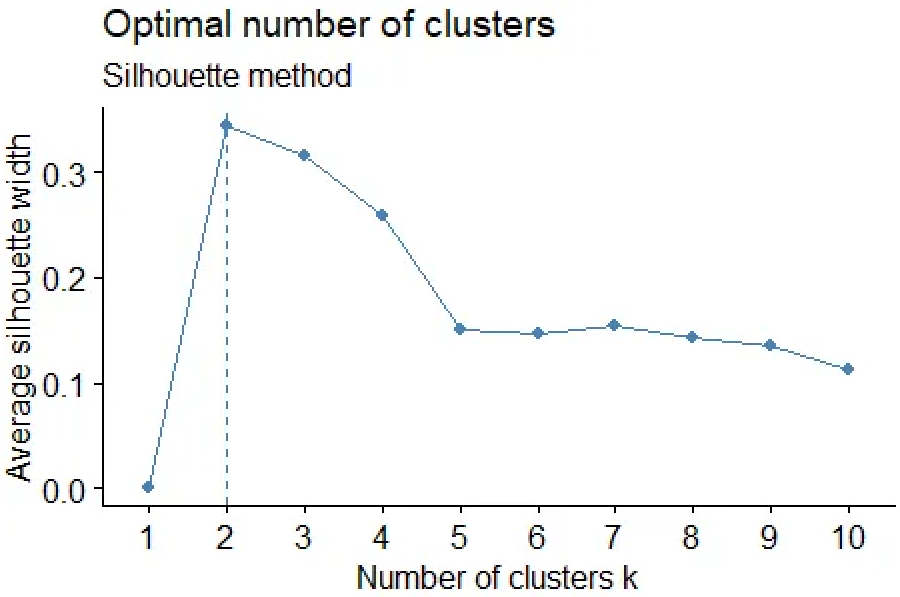


Image by the Author

We will work with the Breast Cancer Wisconsin dataset, where we will apply the K-Means algorithm to the individual's features ignoring the dependent variable `diagnosis`. Notice that all the features are numeric.

```
library(tidyverse)
# the column names of the dataset

names <- c('id_number', 'diagnosis', 'radius_mean', 'texture_mean',
'perimeter_mean', 'area_mean', 'smoothness_mean', 'compactness_mean',
'concavity_mean','concave_points_mean', 'symmetry_mean',
'fractal_dimension_mean', 'radius_se', 'texture_se', 'perimeter_se',
'area_se', 'smoothness_se', 'compactness_se', 'concavity_se',
'concave_points_se', 'symmetry_se', 'fractal_dimension_se',
'radius_worst', 'texture_worst', 'perimeter_worst', 'area_worst',
'smoothness_worst', 'compactness_worst', 'concavity_worst',
'concave_points_worst', 'symmetry_worst', 'fractal_dimension_worst')

# get the data from the URL and assign the column names
df<-read.csv(url("https://archive.ics.uci.edu/ml/machine-learning-
databases/breast-cancer-wisconsin/wdbc.data"), col.names=names)
```

Scale your Data

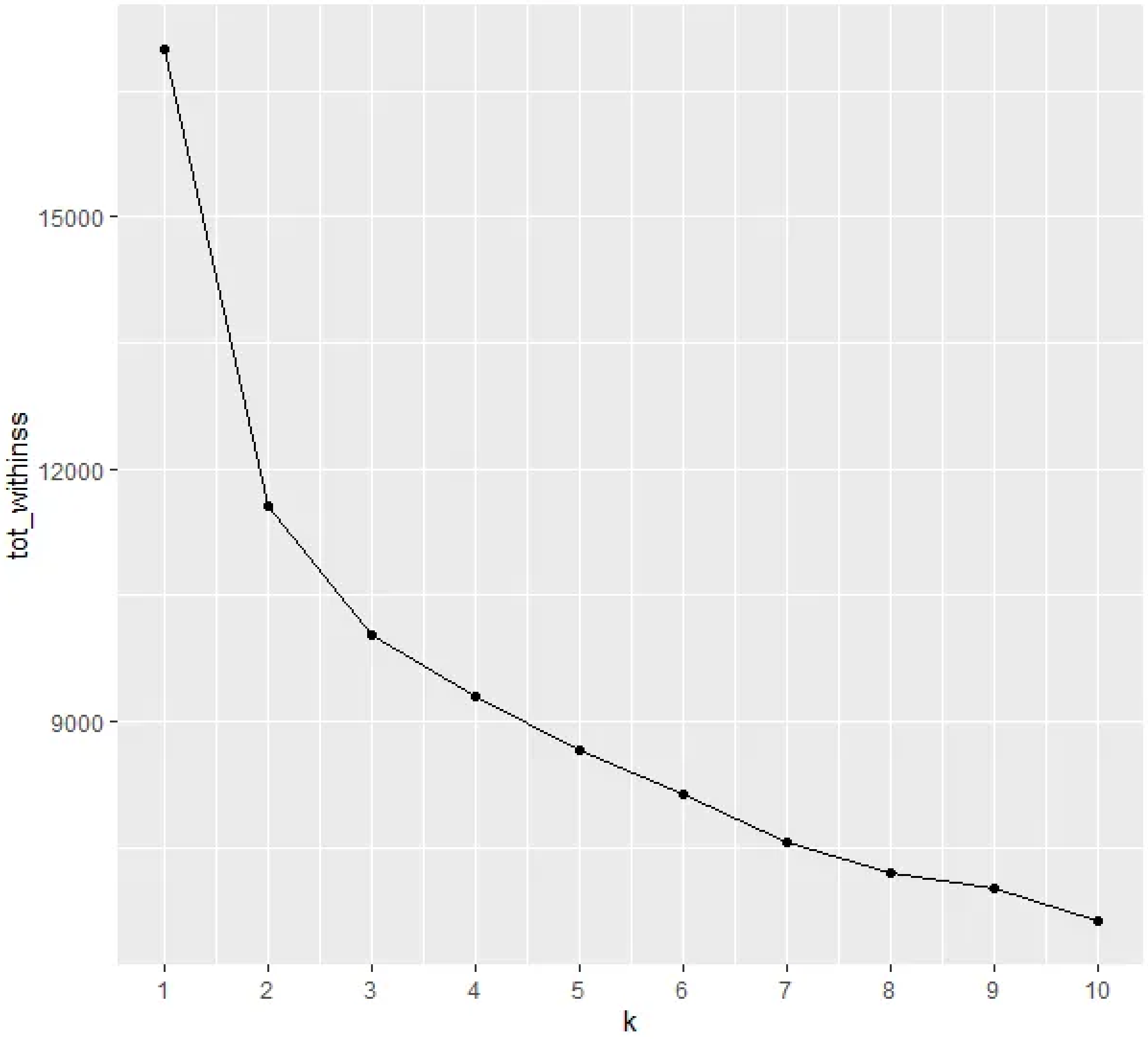
Before we apply any cluster analysis, we should scale our data. We will remove the `id_number` and the `diagnosis`

```
scaled_data<-as.data.frame(scale(df%>%select(-id_number, -diagnosis)))
```

Elbow Method

In a previous post, we explained how we can apply the Elbow Method in Python. Here, we will use the `map_dbl` to run `kmeans` using the `scaled_data` for `k` values ranging from 1 to 10 and extract the total **within-cluster sum of squares** value from each model. Then we can visualize the relationship using a line plot to create the elbow plot where we are looking for a sharp decline from one k to another followed by a more gradual decrease in slope. The last value of k before the slope of the plot levels off suggests a "good" value of k.

```
# Use map_dbl to run many models with varying value of k (centers)

tot_withinss <- map_dbl(1:10,  function(k){

model <- kmeans(x = scaled_data, centers = k)
model$tot.withinss
})

# Generate a data frame containing both k and tot_withinss

elbow_df <- data.frame(k = 1:10,
tot_withinss = tot_withinss)

# Plot the elbow plot

ggplot(elbow_df, aes(x = k, y = tot_withinss)) +
geom_line() + geom_point()+scale_x_continuous(breaks = 1:10)
```



According to the Elbow Method, we can argue that the number of suggested K Clusters are **2**.

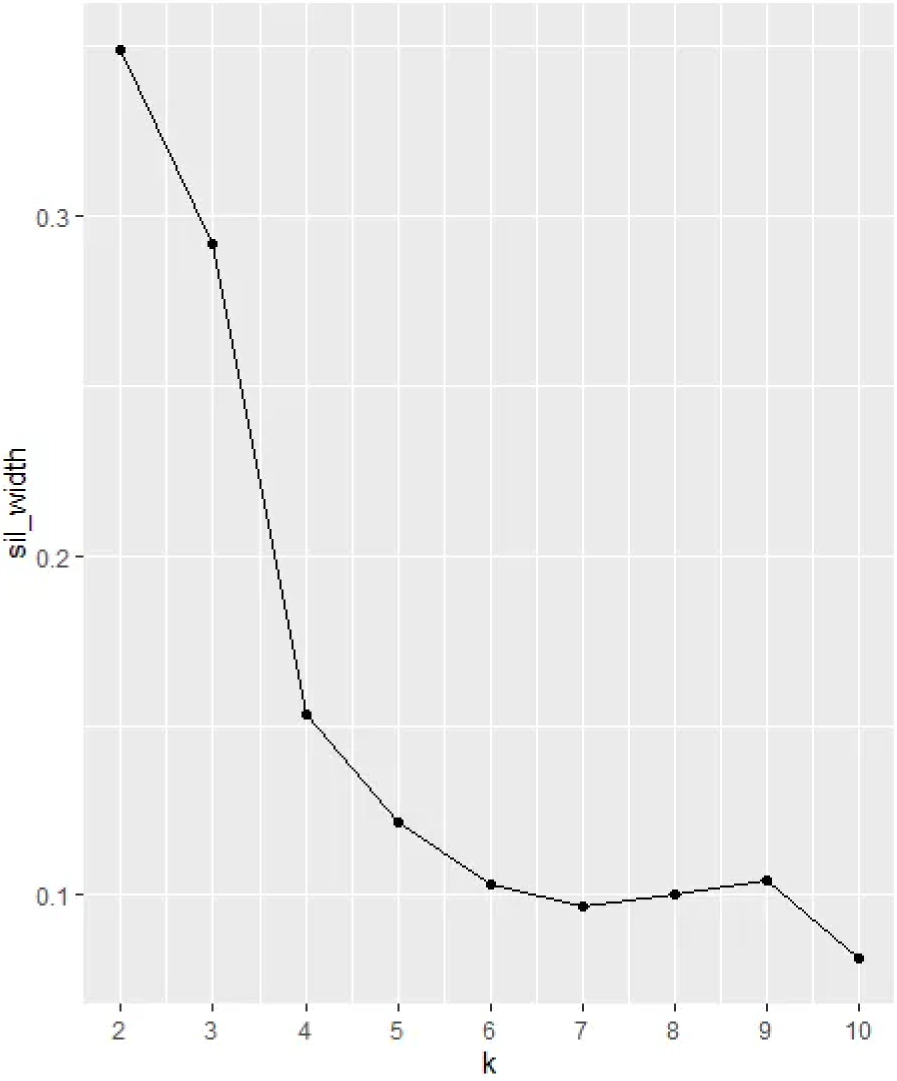
Silhouette Analysis

Silhouette analysis allows you to calculate how similar each observation is with the cluster it is assigned relative to other clusters. This metric ranges from **-1** to **1** for each observation in your data and can be interpreted as follows:

- Values close to **1** suggest that the observation is well matched to the assigned cluster
- Values close to **0** suggest that the observation is borderline matched between two clusters
- Values close to **-1** suggest that the observations may be assigned to the wrong cluster

We can determine the number of clusters K using the average silhouette width. We pick the K which maximizes that score.

```
# Use map_dbl to run many models with varying value of k
sil_width <- map_dbl(2:10,  function(k){
model <- pam(x = scaled_data, k = k)
model$silinfo$avg.width
})
# Generate a data frame containing both k and sil_width
sil_df <- data.frame(
k = 2:10,
sil_width = sil_width
)
# Plot the relationship between k and sil_width
ggplot(sil_df, aes(x = k, y = sil_width)) +
geom_line() + geom_point() +
  scale_x_continuous(breaks = 2:10)
```



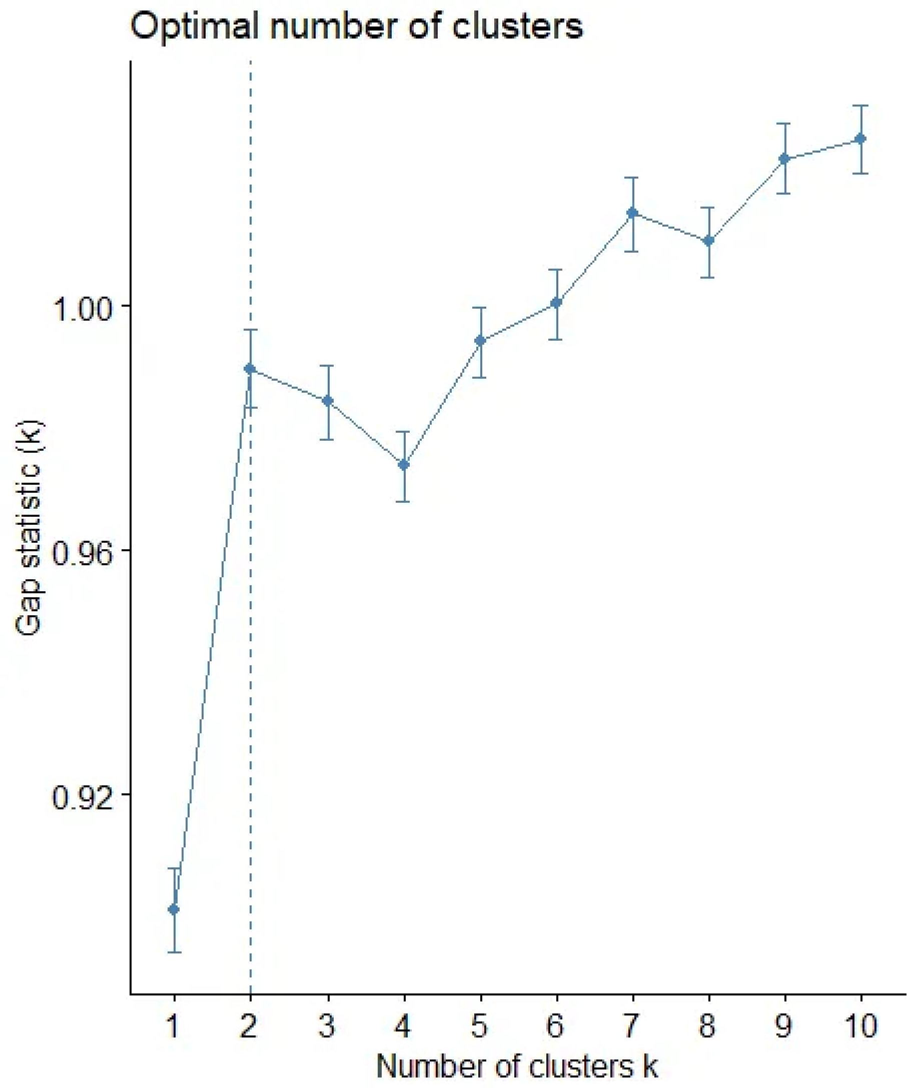
As we can see from the plot above, the **"Best" k is 2**

Gap Statistic

The gap statistic compares the total intracluster variation for different values of k with their expected values under null reference distribution of the data (i.e. a distribution with no obvious clustering). The reference dataset is generated using Monte Carlo simulations of the sampling process

```
library(factoextra)
library(cluster)
```

```
# compute gap statistic set.seed(123)
gap_stat <- clusGap(scaled_data, FUN = kmeans, nstart = 25, K.max =
10, B = 50) fviz_gap_stat(gap_stat)
```



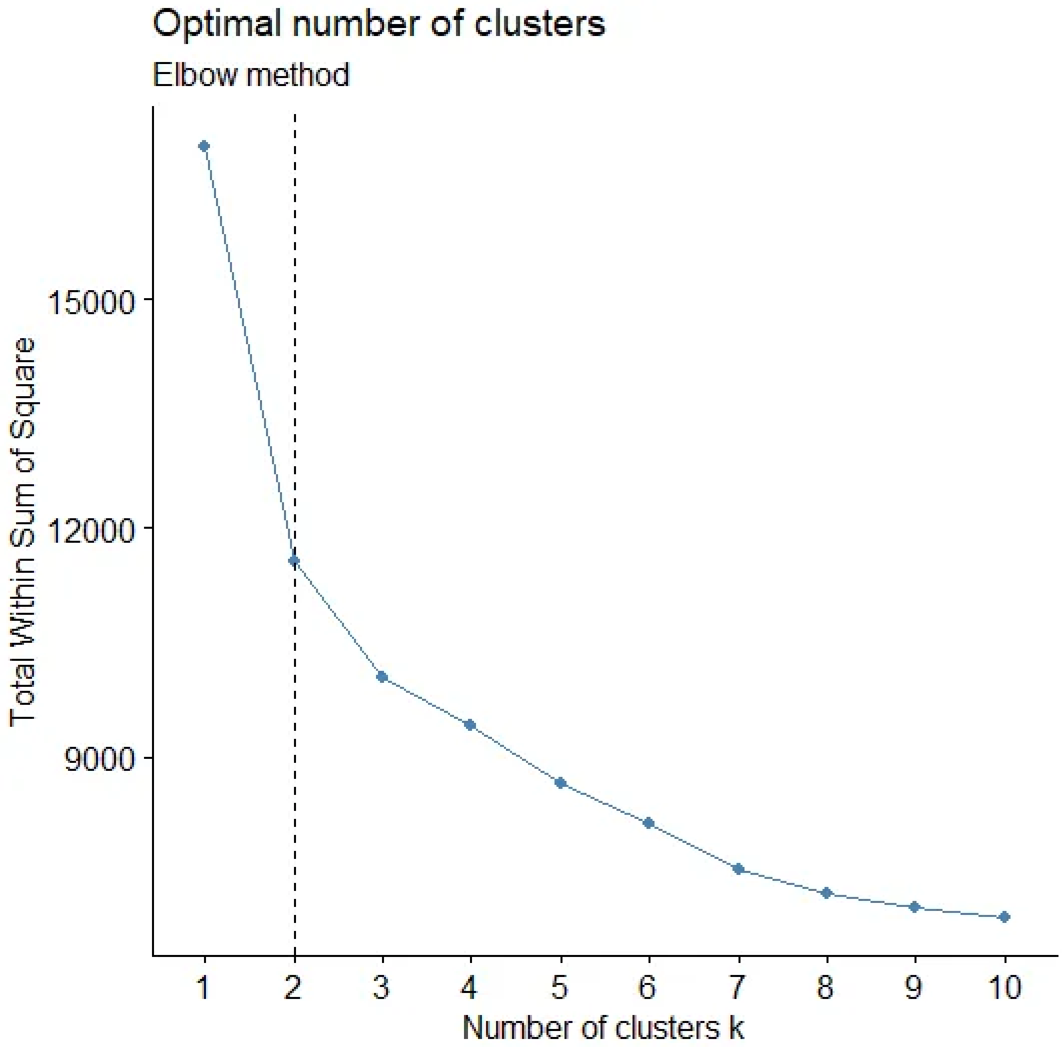
Again, according to the **Gap Statistic**, the optimum number of clusters is the **k=2.**

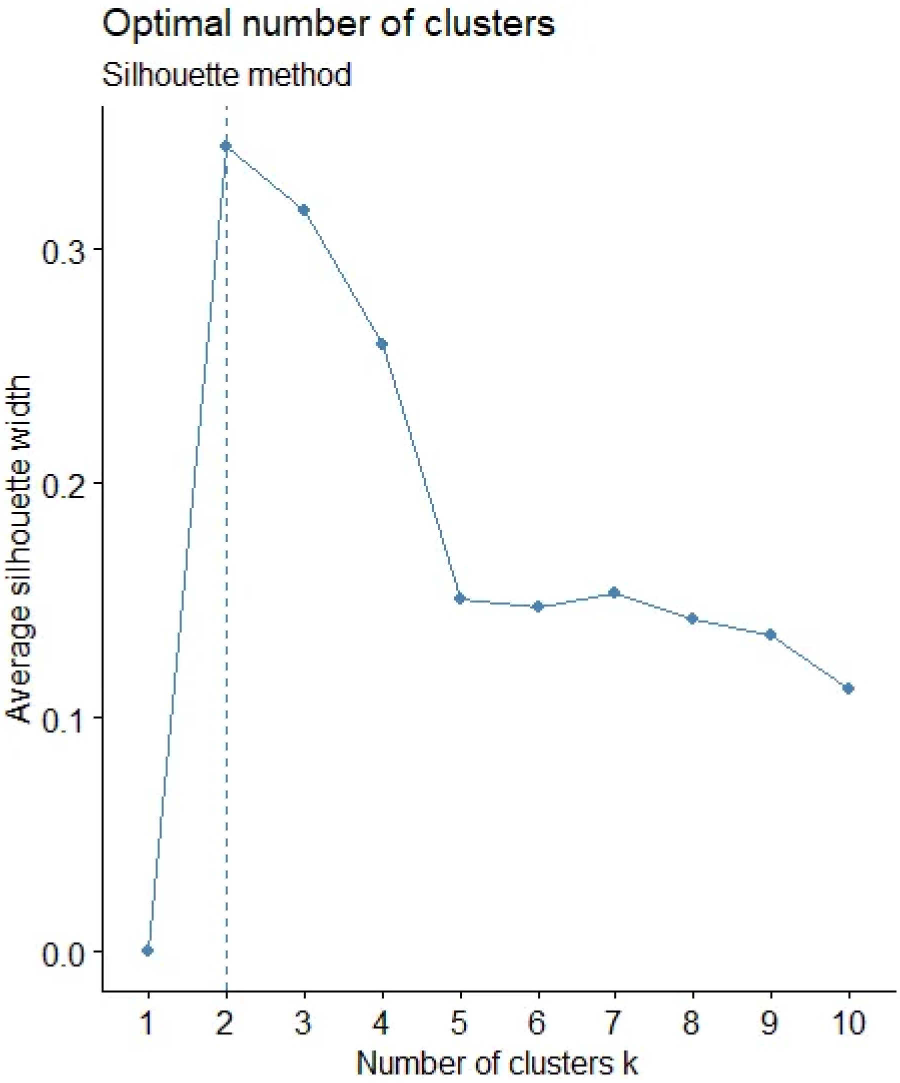
All 3 methods in one package

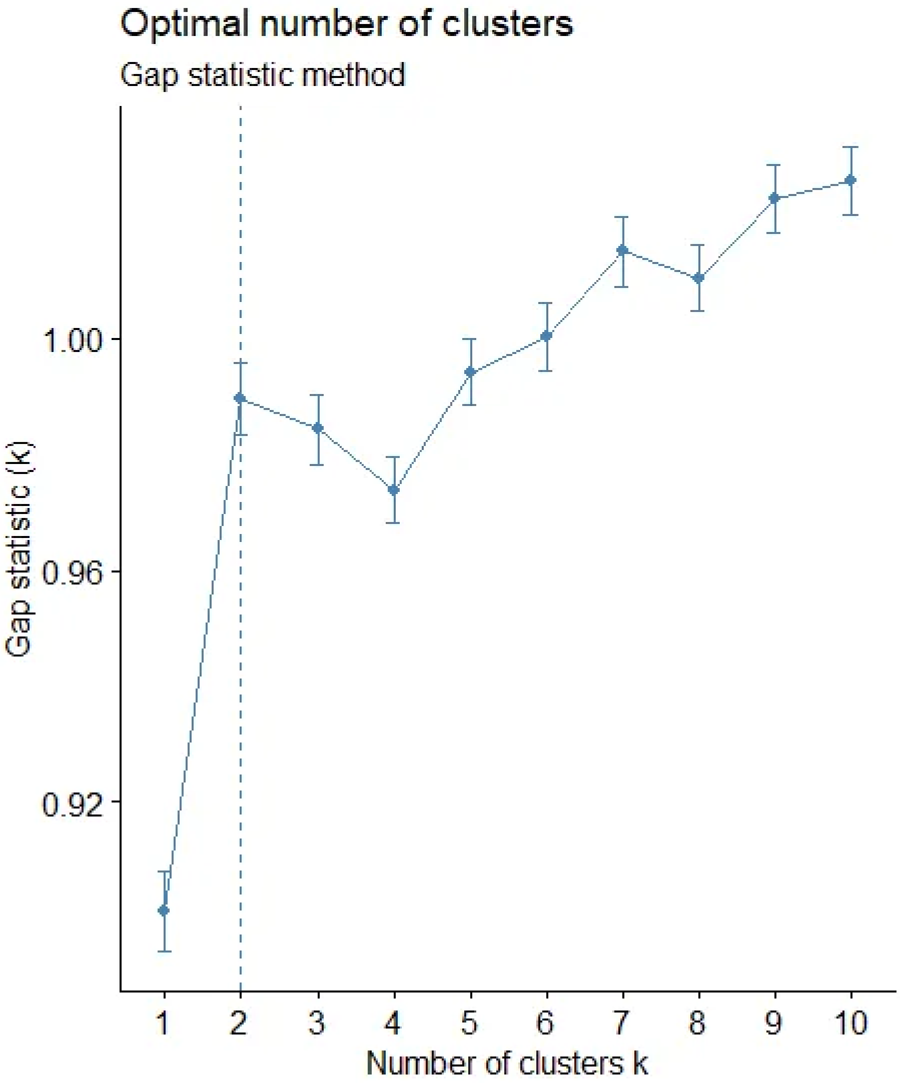
Let's see how we can produce the same analysis for the three methods above with a few lines of coding!

```
library(factoextra)

library(NbClust)

# Elbow method
```

```
fviz_nbclust(scaled_data, kmeans, method = "wss") +

geom_vline(xintercept = 2, linetype = 2)+

labs(subtitle = "Elbow method")

# Silhouette method

fviz_nbclust(scaled_data, kmeans, method = "silhouette")+

labs(subtitle = "Silhouette method")

# Gap statistic

# nboot = 50 to keep the function speedy.

# recommended value: nboot= 500 for your analysis.

# Use verbose = FALSE to hide computing progression.

set.seed(123)

fviz_nbclust(scaled_data, kmeans, nstart = 25,  method = "gap_stat",
nboot = 50)+

labs(subtitle = "Gap statistic method")
```


Optimal number of clusters
Elbow method
Total Within Sum of Square
15000
12000
9000
1
2
3
4
5
6
7
8
9
10
Number of clusters k

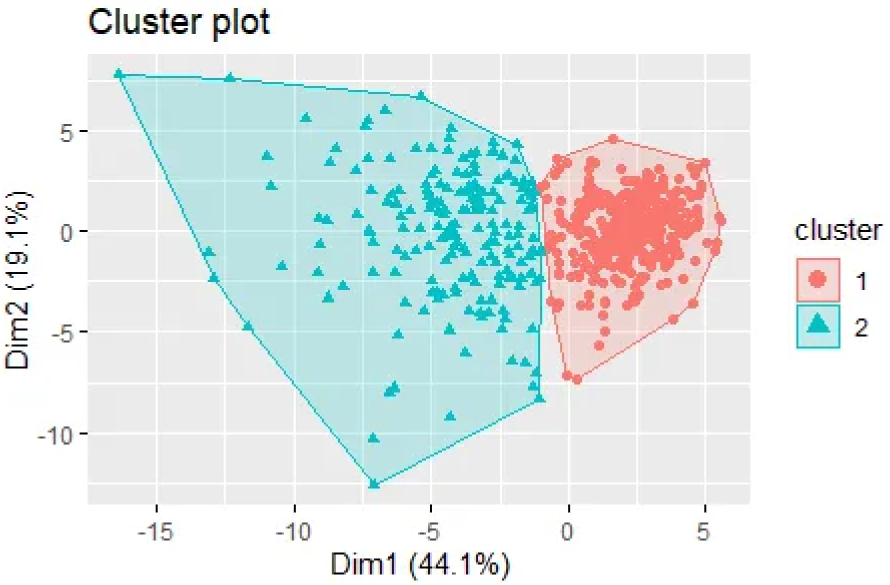

Optimal number of clusters
Silhouette method
Average silhouette width
0.0
0.1
0.2
0.3
1
2
3
4
5
6
7
8
9
10
Number of clusters k



Visualize the K-Means

Since we determined that the number of clusters should be 2, then we can run the k-means algorithm with k=2. Let’s visualize our data into two dimensions.

```
fviz_cluster(kmeans(scaled_data, centers = 2), geom = "point", data =
scaled_date)
```

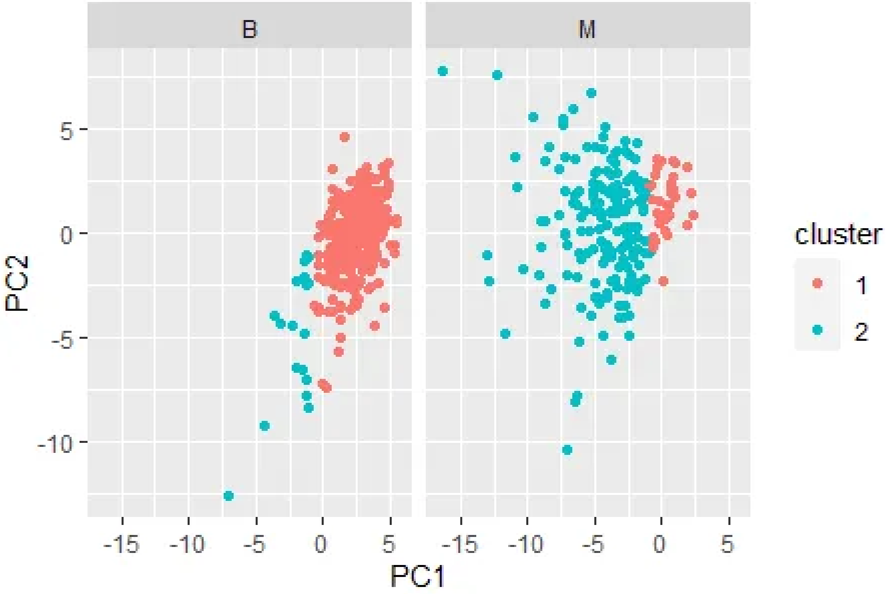


Clusters and Classes in the same plot

Based on the analysis above, the suggested number of clusters in K-means was 2. Bear in mind that in our dataset we have also the dependent variable `diagnosis` which takes values `B` and `M`. Let's represent at the same plot the `Clusters (k=2)` and the `Classes (B,M)`.

We will apply **PCA** by keeping the first two PCs.

```
# get the PCA of the scaled data

pca_res <- prcomp(scaled_data)

# add the Cluster to the original data frame

df$cluster<-as.factor(kmeans(scaled_date, centers = 2)$cluster)

# add the PC1 and PC2 to the original data frame

df$PC1<-pca_res$x[,1]

df$PC2<-pca_res$x[,2]

# do a scatter plot of PC1, PC2 with a color of cluster on a separate
graph

# for diagnosis is M and B

ggplot(aes(x=PC1, y=PC2, col=cluster),
data=df)+geom_point()+facet_grid(.~diagnosis)
```



As we can see the majority of patients with a “Benign” tumor were in the first cluster and the patients with a “Malignant” tumor at the second cluster.

Originally published at https://predictivehacks.com.

R Rstats Clustering K Means Silhouette

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