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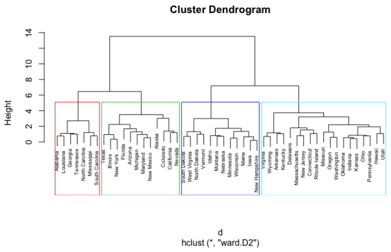
Hierarchical Cluster Analysis



In the k-means cluster analysis tutorial I provided a solid introduction to one of the most popular clustering methods. Hierarchical clustering is an alternative approach to k-means clustering for identifying groups in the dataset. It does not require us to pre-specify the number of clusters to be generated as is required by the k-means approach. Furthermore, hierarchical clustering has an added advantage over K-means clustering in that it results in an attractive tree-based representation of the observations, called a dendrogram.

tl;dr

This tutorial serves as an introduction to the hierarchical clustering method.

1. R Package Requirements: Packages you’ll need to reproduce the analysis in this tutorial
2. Hierarchical Clustering Algorithms: A description of the different types of hierarchical clustering algorithms
3. Data Preparation: Preparing our data for hierarchical cluster analysis
4. Hierarchical Clustering with R: Computing hierarchical clustering with R
5. Working with Dendrograms: Understanding and managing dendrograms
6. Determining Optimal Clusters: Identifying the right number of clusters to group your data

R Package Requirements

The required packages for this tutorial are:

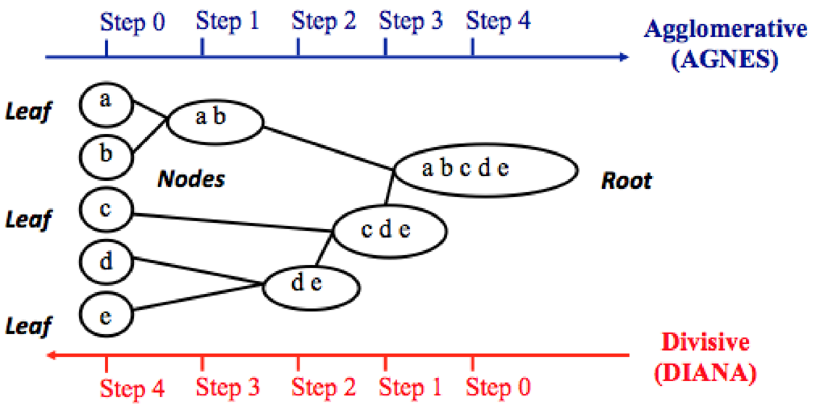
```
library(tidyverse)  # data manipulation
library(cluster)    # clustering algorithms
library(factoextra) # clustering visualization
library(dendextend) # for comparing two dendrograms
```

Hierarchical Clustering Algorithms

Hierarchical clustering can be divided into two main types: *agglomerative* and *divisive*.

1. **Agglomerative clustering:** It's also known as AGNES (Agglomerative Nesting). It works in a bottom-up manner. That is, each object is initially considered as a single-element cluster (leaf). At each step of the algorithm, the two clusters that are the most similar are combined into a new bigger cluster (nodes). This procedure is iterated until all points are member of just one single big cluster (root) (see figure below). The result is a tree which can be plotted as a dendrogram.
2. **Divisive hierarchical clustering:** It's also known as DIANA (Divise Analysis) and it works in a top-down manner. The algorithm is an inverse order of AGNES. It begins with the root, in which all objects are included in a single cluster. At each step of iteration, the most heterogeneous cluster is divided into two. The process is iterated until all objects are in their own cluster (see figure below).

Note that agglomerative clustering is good at identifying small clusters. Divisive hierarchical clustering is good at identifying large clusters.

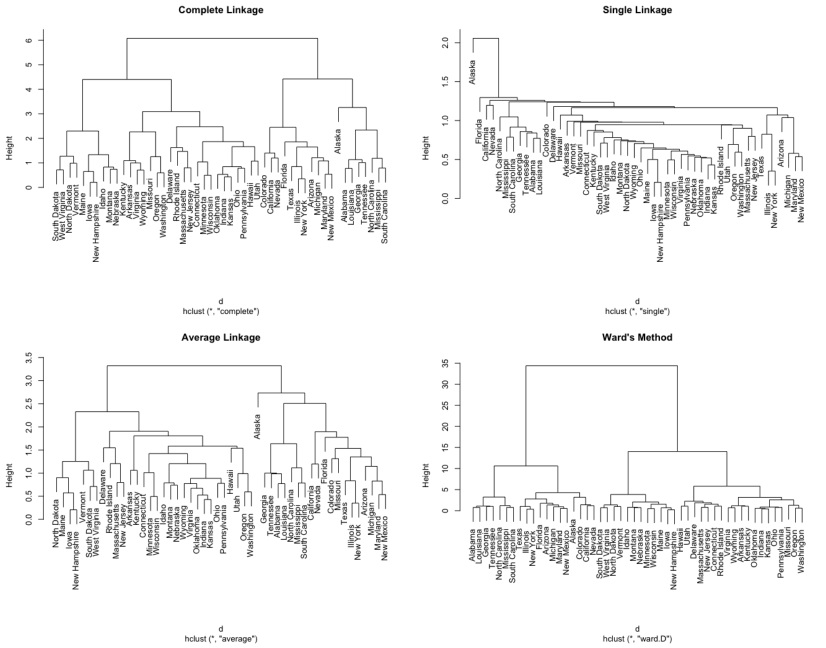


As we learned in the k-means tutorial, we measure the (dis)similarity of observations using distance measures (i.e. Euclidean distance, Manhattan distance, etc.) In R, the Euclidean distance is used by default to measure the dissimilarity between each pair of observations. As we already know, it's easy to compute the dissimilarity measure between two pairs of observations with the `get_dist` function.

However, a bigger question is: *How do we measure the dissimilarity between two clusters of observations?* A number of different cluster agglomeration methods (i.e, linkage methods) have been developed to answer to this question. The most common types methods are:

- **Maximum or complete linkage clustering:** It computes all pairwise dissimilarities between the elements in cluster 1 and the elements in cluster 2, and considers the largest value (i.e., maximum value) of these dissimilarities as the distance between the two clusters. It tends to produce more compact clusters.
- **Minimum or single linkage clustering:** It computes all pairwise dissimilarities between the elements in cluster 1 and the elements in cluster 2, and considers the smallest of these dissimilarities as a linkage criterion. It tends to produce long, "loose" clusters.
- **Mean or average linkage clustering:** It computes all pairwise dissimilarities between the elements in cluster 1 and the elements in cluster 2, and considers the average of these dissimilarities as the distance between the two clusters.
- **Centroid linkage clustering:** It computes the dissimilarity between the centroid for cluster 1 (a mean vector of length p variables) and the centroid for cluster 2.
- **Ward's minimum variance method:** It minimizes the total within-cluster variance. At each step the pair of clusters with minimum between-cluster distance are merged.

We can see the differences these approaches in the following dendrograms:



Data Preparation

To perform a cluster analysis in R, generally, the data should be prepared as follows:

1. Rows are observations (individuals) and columns are variables
2. Any missing value in the data must be removed or estimated.
3. The data must be standardized (i.e., scaled) to make variables comparable. Recall that, standardization consists of transforming the variables such that they have mean zero and standard deviation one.[^scale]

Here, we'll use the built-in R data set `USArrests`, which contains statistics in arrests per 100,000 residents for assault, murder, and rape in each of the 50 US states in 1973. It includes also the percent of the population living in urban areas

```
df <- USArrests
```

To remove any missing value that might be present in the data, type this:

```
df <- na.omit(df)
```

As we don't want the clustering algorithm to depend to an arbitrary variable unit, we start by scaling/standardizing the data using the R function `scale` :

```
df <- scale(df)
head(df)
##                 Murder   Assault   UrbanPop
## Alabama    1.24256408 0.7828393 -0.5209066 -0.003
## Alaska     0.50786248 1.1068225 -1.2117642  2.484
## Arizona    0.07163341 1.4788032  0.9989801  1.042
## Arkansas   0.23234938 0.2308680 -1.0735927 -0.184
## California 0.27826823 1.2628144  1.7589234  2.067
## Colorado   0.02571456 0.3988593  0.8608085  1.864
```

Hierarchical Clustering with R

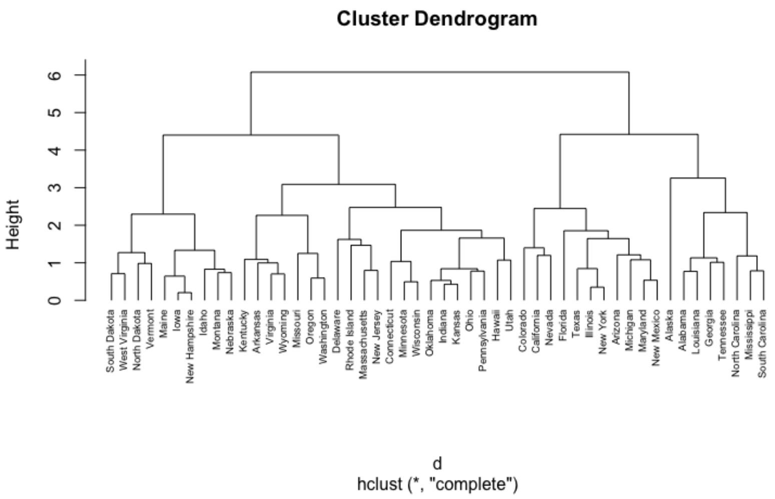
There are different functions available in R for computing hierarchical clustering. The commonly used functions are:

- `hclust` [in stats package] and `agnes` [in cluster package] for agglomerative hierarchical clustering (HC)
- `diana` [in cluster package] for divisive HC

Agglomerative Hierarchical Clustering

We can perform agglomerative HC with `hclust` . First we compute the dissimilarity values with `dist` and then feed these values into `hclust` and specify the agglomeration method to be used (i.e. “complete”, “average”, “single”, “ward.D”). We can then plot the dendrogram.

```
# Dissimilarity matrix
d <- dist(df, method = "euclidean")

# Hierarchical clustering using Complete Linkage
hc1 <- hclust(d, method = "complete" )

# Plot the obtained dendrogram
plot(hc1, cex = 0.6, hang = -1)
```



Alternatively, we can use the `agnes` function. These functions behave very similarly; however, with the `agnes` function you can also get the agglomerative coefficient, which measures the amount of clustering structure found (values closer to 1 suggest strong clustering structure).

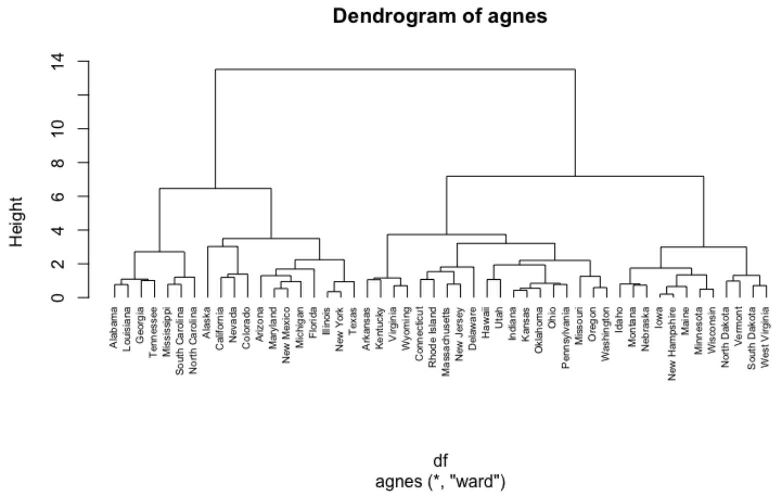
```
# Compute with agnes
hc2 <- agnes(df, method = "complete")

# Agglomerative coefficient
hc2$ac
## [1] 0.8531583
```

This allows us to find certain hierarchical clustering methods that can identify stronger clustering structures. Here we see that Ward's method identifies the strongest clustering structure of the four methods assessed.

```
# methods to assess
m <- c( "average", "single", "complete", "ward")
names(m) <- c( "average", "single", "complete", "war

# function to compute coefficient
ac <- function(x) {
  agnes(df, method = x)$ac
}

map_dbl(m, ac)
##   average    single  complete      ward
## 0.7379371 0.6276128 0.8531583 0.9346210
```

Similar to before we can visualize the dendrogram:

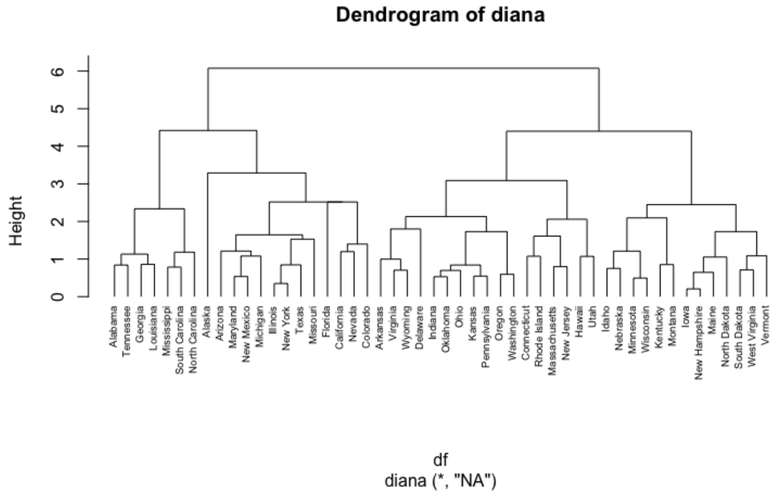
```
hc3 <- agnes(df, method = "ward")
pltree(hc3, cex = 0.6, hang = -1, main = "Dendrogram
```



Divisive Hierarchical Clustering

The R function `diana` provided by the cluster package allows us to perform divisive hierarchical clustering. `diana` works similar to `agnes`; however, there is no method to provide.

```
# compute divisive hierarchical clustering
hc4 <- diana(df)

# Divise coefficient; amount of clustering structure
hc4$dc
## [1] 0.8514345

# plot dendrogram
pltree(hc4, cex = 0.6, hang = -1, main = "Dendrogram
```



Working with Dendrograms

In the dendrogram displayed above, each leaf corresponds to one observation. As we move up the tree, observations that are similar to each other are combined into branches, which are themselves fused at a higher height.

The height of the fusion, provided on the vertical axis, indicates the (dis)similarity between two observations. The higher the height of the fusion, the less similar the observations are. ***Note that, conclusions about the proximity of two observations can be drawn only based on the height where branches containing those two observations first are fused. We cannot use the proximity of two observations along the horizontal axis as a criteria of their similarity.***

The height of the cut to the dendrogram controls the number of clusters obtained. It plays the same role as the k in k-means clustering. In order to identify sub-groups (i.e. clusters), we can cut the dendrogram with `cutree` :

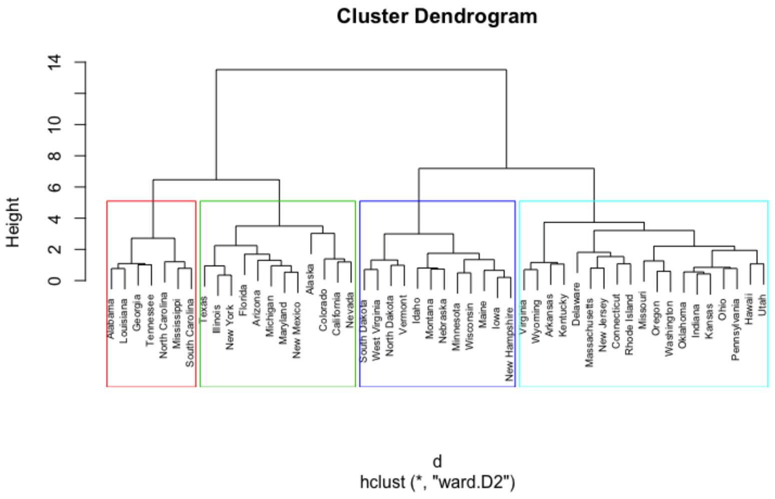
```
# Ward's method
hc5 <- hclust(d, method = "ward.D2" )

# Cut tree into 4 groups
sub_grp <- cutree(hc5, k = 4)

# Number of members in each cluster
table(sub_grp)
## sub_grp
##  1  2  3  4
##  7 12 19 12
```

We can also use the `cutree` output to add the the cluster each observation belongs to to our original data.

```
USArrests %>%
  mutate(cluster = sub_grp) %>%
  head
##   Murder Assault UrbanPop Rape cluster
## 1   13.2     236       58 21.2       1
## 2   10.0     263       48 44.5       2
## 3    8.1     294       80 31.0       2
## 4    8.8     190       50 19.5       3
## 5    9.0     276       91 40.6       2
## 6    7.9     204       78 38.7       2
```

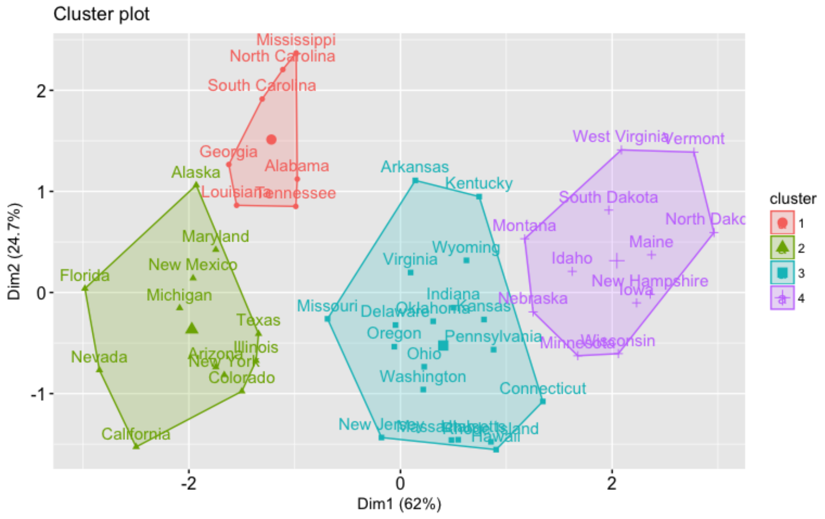
It's also possible to draw the dendrogram with a border around the 4 clusters. The argument border is used to specify the border colors for the rectangles:

```
plot(hc5, cex = 0.6)
rect.hclust(hc5, k = 4, border = 2:5)
```



As we saw in the k-means tutorial, we can also use the `fviz_cluster` function from the `factoextra` package to visualize the result in a scatter plot.

```
fviz_cluster(list(data = df, cluster = sub_grp))
```

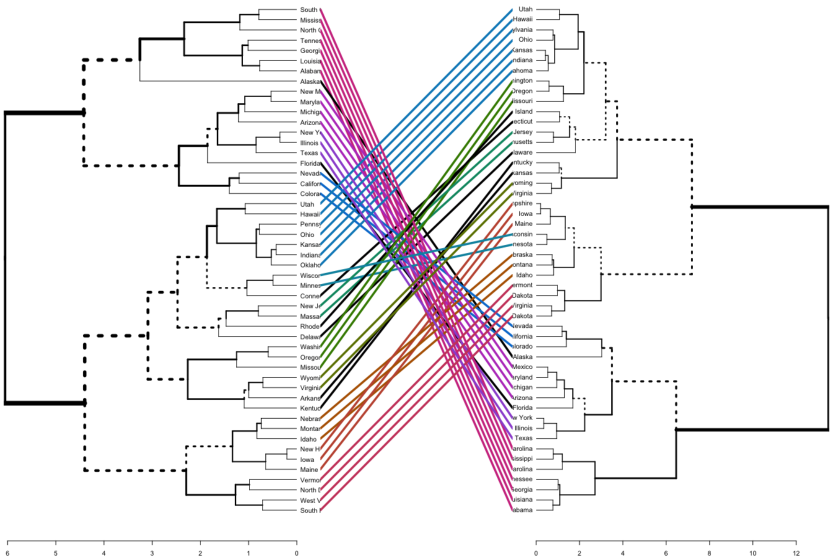


To use `cutree` with `agnes` and `diana` you can perform the following:

```
# Cut agnes() tree into 4 groups
hc_a <- agnes(df, method = "ward")
cutree(as.hclust(hc_a), k = 4)

# Cut diana() tree into 4 groups
hc_d <- diana(df)
cutree(as.hclust(hc_d), k = 4)
```

Lastly, we can also compare two dendrograms. Here we compare hierarchical clustering with complete linkage versus Ward's method. The function `tanglegram` plots two dendrograms, side by side, with their labels connected by lines.

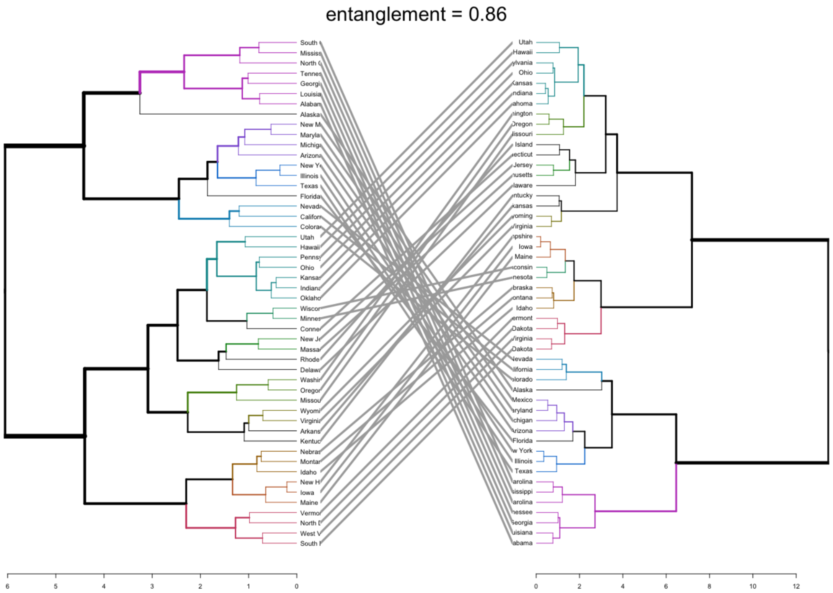
```
# Compute distance matrix
res.dist <- dist(df, method = "euclidean")

# Compute 2 hierarchical clusterings
hc1 <- hclust(res.dist, method = "complete")
hc2 <- hclust(res.dist, method = "ward.D2")

# Create two dendrograms
dend1 <- as.dendrogram (hc1)
dend2 <- as.dendrogram (hc2)

tanglegram(dend1, dend2)
```



The output displays "unique" nodes, with a combination of labels/items not present in the other tree, highlighted with dashed lines. The quality of the alignment of the two trees can be measured using the function `entanglement`. Entanglement is a measure between 1 (full entanglement) and 0 (no entanglement). A lower entanglement coefficient corresponds to a good alignment. The output of `tanglegram` can be customized using many other options as follow:

```
dend_list <- dendlist(dend1, dend2)

tanglegram(dend1, dend2,
  highlight_distinct_edges = FALSE, # Turn-off dashe
  common_subtrees_color_lines = FALSE, # Turn-off li
```

```
    common_subtrees_color_branches = TRUE, # Color comm
    main = paste("entanglement =", round(entanglement(
    )
```



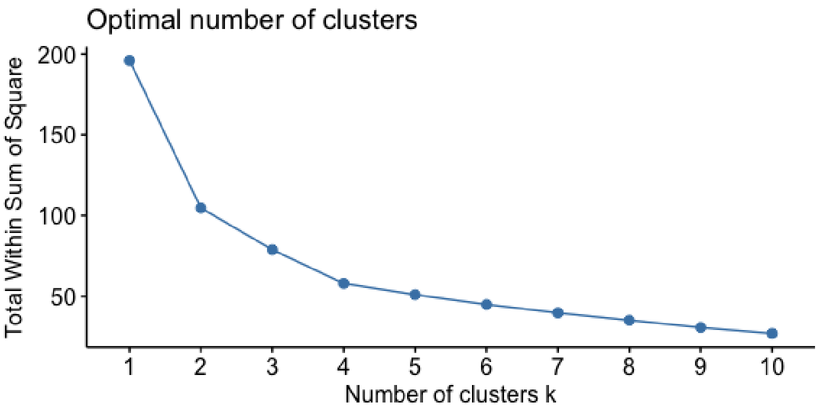
Determining Optimal Clusters

Similar to how we determined optimal clusters with k-means clustering, we can execute similar approaches for hierarchical clustering:

Elbow Method

To perform the elbow method we just need to change the second argument in `fviz_nbclust` to `FUN = hcut`.

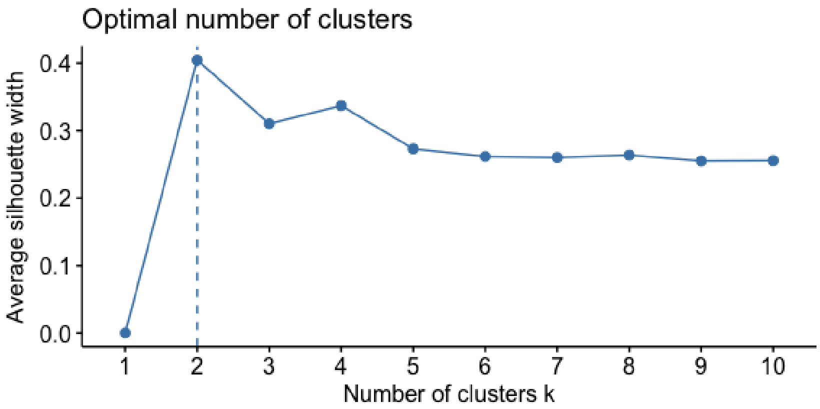
```
fviz_nbclust(df, FUN = hcut, method = "wss")
```



Average Silhouette Method

To perform the average silhouette method we follow a similar process.

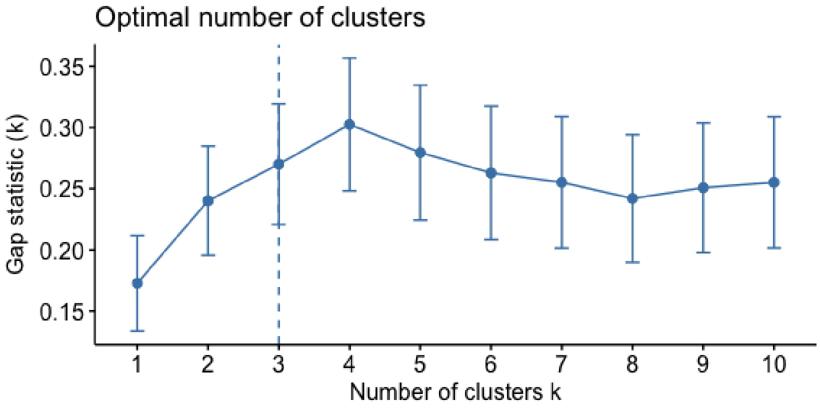
```
fviz_nbclust(df, FUN = hcut, method = "silhouette")
```



Gap Statistic Method

And the process is quite similar to perform the gap statistic method.

```
gap_stat <- clusGap(df, FUN = hcut, nstart = 25, K.m
fviz_gap_stat(gap_stat)
```



Additional Comments

Clustering can be a very useful tool for data analysis in the unsupervised setting. However, there are a number of issues that arise in performing clustering. In the case of hierarchical clustering, we need to be concerned about:

- What dissimilarity measure should be used?
- What type of linkage should be used?
- Where should we cut the dendrogram in order to obtain clusters?

Each of these decisions can have a strong impact on the results obtained. In practice, we try several different choices, and look for the one with the most useful or interpretable solution. With these methods, there is no single right answer - any solution that exposes some interesting aspects of the data should be considered.

So, keep in mind that although hierarchical clustering can be performed quickly in R, there are many important variables to consider. However, this tutorial gets you started performing the hierarchical clustering approach and you can learn more with:

- An Introduction to Statistical Learning
- Applied Predictive Modeling
- Elements of Statistical Learning
- A Practical Guide to Cluster Analysis in R