Homework 2

Pattern Mining and Social Network Analysis

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Contents

Continuous and discrete data sets

Continuous data is data that can take any value while discrete data can take only certain values. with continuous (distance/similarity based) : Silhouette, Dunn, ...

TO D DISCRETE DATA SET

with discrete (binary, graph based) : modularity, C measure, ...

Cluster validation techniques

Clustering Tendency

Why assessing clustering tendency ?

Clustering can create clusters even if there are no meaningful cluster.
Clustering tendency assessment methods are used to evaluate the validity of clustering analysis. It means evaluate if there are meaningful clusters in the data.

Methods

Statistical methods for clustering tendency A method called Hopkins statistic is used to assess the clustering tendency in a data set. It measures the probability for the data set to be generated by an uniform data distribution, it means that this statistic looks at the spatial randomness of the data.

For D, a data set :

Sample n point from D (p_1, ..., p_n)

For all $p_i \in D$, compute the distance to the nearest neighbor $x_i < /li >< li > Generate$(random_D)$fromarandomuniformdi$
q_n) with the same variation as D.

For all $q_i \in random_D$, compute the distance to the nearest neighbor y_i

Calculate the Hopkins statistic (H). It is the mean of the nearest neighbor distances in $random_D$ divided by the sum of the mean nearest neighbor distances in D and $random_D$.

$$H = \frac{\Sigma_i^n y_i}{\Sigma_i^n X_i + \Sigma_i^n y_i}$$

If H is about 0.5, if means that the sum along D and $random_D$ are very close so that the data D is uniformly distributed. It is the null hypothesis, meaning that the data set D is uniformly distributed (no meaningful clusters)

Otherwise we have the Alternative hypothesis: the data set D is not uniformly distributed (contains meaningful clusters).

Visually There is an algorithm of the visual assessment of cluster tendency (VAT) approach (Bezdek and Hathaway, 2002).

Compute the dissimilarity matrix using the Euclidean distance measure

Reorder the DM so that similar objects are close to one another. It is now called the ODM.

Display the ODM as an ordered dissimilarity image (ODI) (with some libraries).

Computing the visual form gives us colored squares along the diagonal. The VAT detects the clustering tendency in a visual form by counting them.

Statistics on a model

Internal measures

Internal cluster validation uses the internal information of the clustering process to evaluate the clustering structure without any external information.

Internal validation measures reflect often the compactness, the connectedness and the separation of the cluster partitions.

Compactness Compactness measures how close are the objects within the same cluster.
We evaluate it with the notion of distance such as the cluster-wise within average/median distances between observations.

Separation Separation measures how well clusters are separated from one another.
We evaluate it by looking at the distances between clusters' centers or with the pairwise minimum distances between objects in different clusters.

Connectivity Connectivity corresponds to what extent items are placed in the same cluster as their nearest neighbors in the data space.

Silhouette coefficient of an observation It measures how well an observation is clustered and it estimates the average distance between clusters.

It is possible to compute this coefficient thanks to the following formula :

$$Silhouette_i = \frac{b_i - a_i}{max(a_i, b_i)}$$

Where :

- a_i is the average distance between the observation i within its cluster
- b_i is the average distance between the observation i and all the observations belonging to another cluster

How to interprete the value of S_i ?

A large S_i, almost 1, means the observation is very well clustered.
A small S_i, close to 0, means that the observation lies between two clusters.
A negative S_i means the observation is probably placed in the wrong cluster.

Dunn index The Dunn index is another internal clustering validation measure.
It is the minimal distance between two clusters (the smallest separation) over the maximal distance between the objects of one clusters (the biggest diameter of a cluster).

$$Dunn\ index = \frac{min.separation}{max.diameter}$$

Compact and well-separated clusters in a data set means a small diameter of the clusters and a large distance between the clusters. Thus, Dunn index should be maximized.

External mesures

External cluster validation compares the results of a cluster analysis with an externally known result. It measures how well a cluster match extern class labels. We know k, the number of clusters, in advance. So we use this validation to choose the correct clustering method.

We compare the identified clusters to an external reference.

Determining the Optimal number of Clusters

Determining the optimal number of clusters in a data set is fundamental because, for example, in partitioning clustering, such as k-means clustering, it requires the user to specify the number of clusters k.

Elbow method

The Elbow method looks at the total within-cluster sum of square as a function of the number of clusters.

Compute the clustering algorithm chosen with k going from 1 to 10 for example.

Calcultate the within-cluster sum of square for each k

Plot the curve of WSS according to k

The location of a bend (knee) in the plot is generally considered as an indicator of the appropriate number of clusters.

An alternative is the Silhouette method.

Average silhouette method

Average silhouette method computes the average silhouette of observations for different values of k. Then k is chosen if it maximizes the average silhouette.

Compute the clustering algorithm chosen with k going from 1 to 10 for example.

Calcultate the average silhouette coeffcients of observations for each k

Plot the curve of AVG.S according to k

The location of the maximum is considered as the appropriate number of clusters.

Gap statistic method

The gap statistic compares the total within intra-cluster variation for different values of k with their expected values under null reference. We choose k when it maximizes the gap statistic so that the clustering structure is far away from the random uniform distribution of points.

Compute the clustering algorithm chosen with k going from 1 to 10 for example.

Calcultate the within-cluster sum of square for each k W_k

Generate B reference data sets with a random uniform distribution.

Compute the clustering algorithm chosen on these reference data sets with k going from 1 to k_max.

Calcultate the within-cluster sum of square for each k W_kb

Compute the gap :

$$Gap(k) = \frac{1}{B}\Sigma_{b=1}^{B} log(W_{kb}) - log(W_k)$$

Compute the standard deviation of the statistics s_k.

Choose the smallest k such that the gap statistic is within one standard deviation of the gap at k+1.

$$Gap(k+1) > Gap(k) - s_{k+1}$$

Principal Components Analysis

The goal of PCA is to identify which features in the dataset explain the most variability.

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Different kinds of PCA

Standard PCA

TO-DO

Incremental PCA

TO-DO

Sparse PCA

TO-DO

Kernel PCA

TO-DO

Proportion of variance explained (PVE)

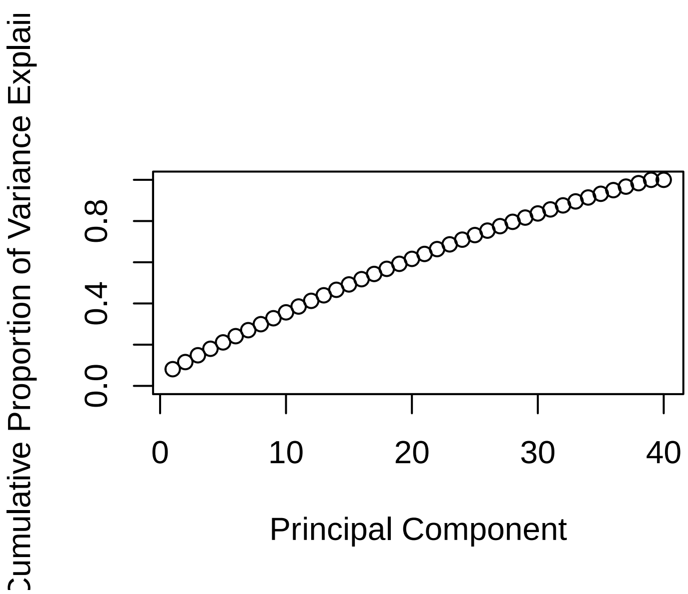
TO-DO

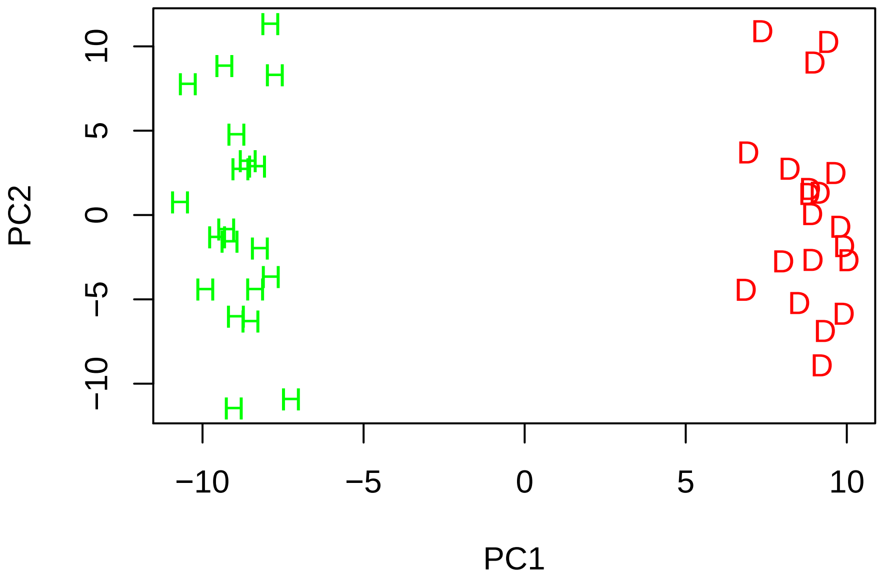
Deciding how many PCs to use

TO-DO

Example

The following dataset consists of 40 tissue samples with measurements of 1,000 genes. The first 20 tissues come from healthy patients (H) and the remaining 20 come from a diseased patient group (D).




PC2
10
5
0
−5
−10
−10
−5
0
5
10
PC1

Clustering

Partitioning Clustering

K-means

The objective of clustering is to distinct groups from the datatest. With k-means we want to distinct k groups. The algorithm will assign each observation to exactly one of the cluster. It optimizes the groups by minimizing the within-cluster variation such that the sum of the with-cluster variations across all the clusters is the smallest possible.

Within-cluster variation (squared Euclidean distance) If μ_k is the center of the cluster k. The total with-cluster variation is TW :

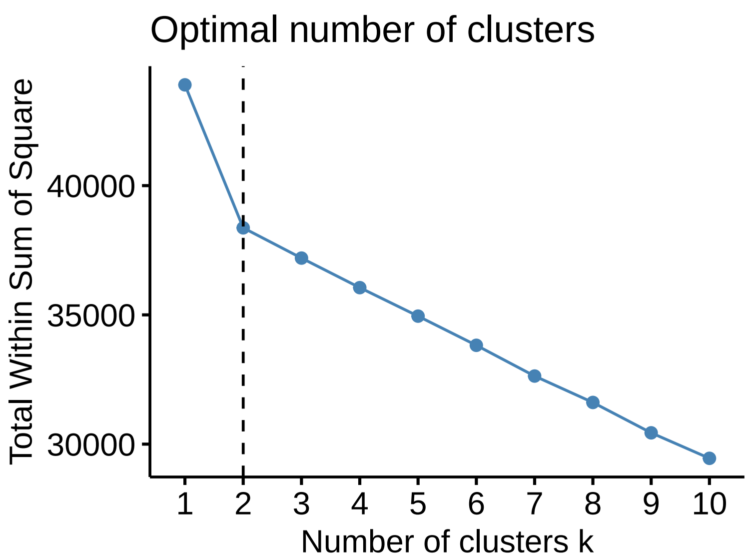
$$TW = \Sigma_{j=1}^{k} W_j = \Sigma_{j=1}^{k} \Sigma_{x_i \in C_j} (x_i - \mu_k)^2$$

K-means algorithm The first step when using k-means clustering is to indicate the number of clusters (k) that will be generated in the final solution. The algorithm starts by randomly selecting k objects from the data set to serve as the initial centers for the clusters. The selected objects are also known as cluster means or centroids.

Choice of k We compute k-means clustering using different k, then we choose the number of cluster according to the location of a bend on the graph representing the Within-cluster variation according to k.

Example

On R According to this graph, we should choose k=2 (it makes sense since we have Healthy and non healthy patients).



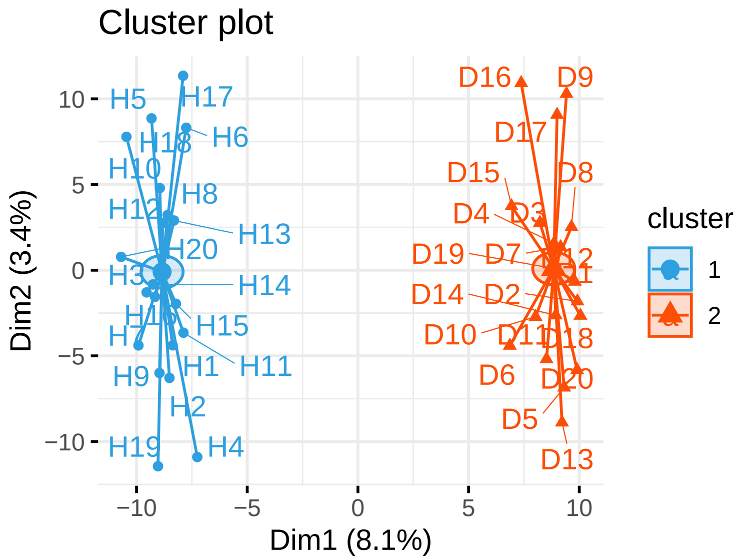
Then applying kmeans with 2 clusters we observe that the 20 first individuals (healthy) are not in the same cluster than the 20 others (non healthy).

```
##  H1  H2  H3  H4  H5  H6  H7  H8  H9 H10 H11 H12 H13 H14 H15 H16 H17 H18 H19 H20
##   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1
##  D1  D2  D3  D4  D5  D6  D7  D8  D9 D10 D11 D12 D13 D14 D15 D16 D17 D18 D19 D20
##   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
```

The following coefficient is the Dunn index.
It is about 1. It means that the separation distance between the two clusters is almost the same as the diameter of the largest cluster.

```
## [1] 0.9744956
```

Since we have a multi-dimensional dataset, we apply dimensionality reduction with the use of PCA to plot the clusters. On the x axis, it is the first PCA, on the y axis, it is the second PCA.



On python with scikit-learn By applying Kmeans (with 2 clusters) from scikit-learn on the gene dataset, we have the following assgnation to clusters. The 20 first individuals (Healthy) are well separated from the 20 last individuals since there are not in the same cluster.

K-medoids algorithm

Principle The k-medoids algorithm is a clustering approach related to k-means clustering. In k-medoids clustering, each cluster is represented by one of the data point in the cluster.

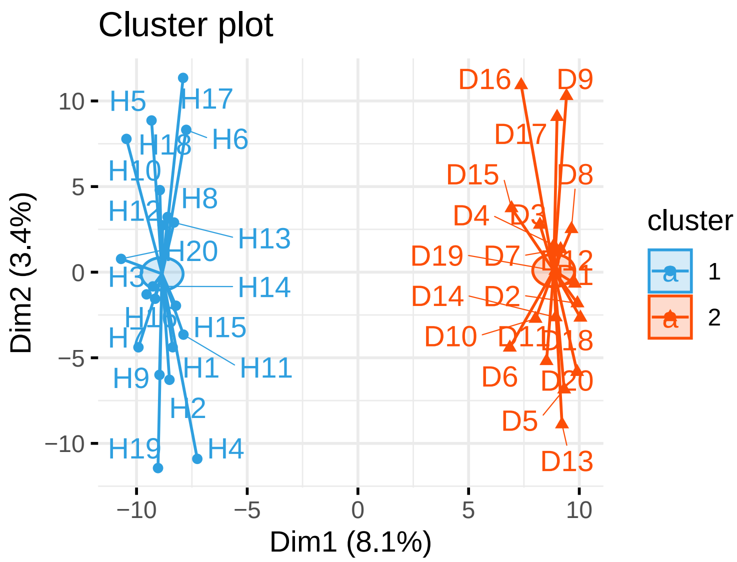
The most common k-medoids clustering methods is the PAM.

PAM algorithm (Partitioning Around Medoids)

```
##  H1  H2  H3  H4  H5  H6  H7  H8  H9 H10 H11 H12 H13 H14 H15 H16 H17 H18 H19 H20
##   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1
##  D1  D2  D3  D4  D5  D6  D7  D8  D9 D10 D11 D12 D13 D14 D15 D16 D17 D18 D19 D20
##   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
```

We have the same Dunn index as with K-means on the same dataset. Both methods perform equally.

```
## [1] 0.9744956
```



CLARA - Clustering Large Applications DEFINITION

TO DO

Hierarchical clustering

Dissimilarity function

Euclidean distance

```
##       H1   H2   H3   H4   H5   H6   H7   H8   H9  H10
## H1   0.0 45.2 44.5 45.6 45.9 45.2 45.0 45.8 45.0 46.0
## H2  45.2  0.0 45.7 44.6 44.4 45.5 44.8 44.6 44.4 44.5
## H3  44.5 45.7  0.0 43.9 46.0 44.9 45.7 45.2 44.1 45.3
## H4  45.6 44.6 43.9  0.0 47.4 45.1 45.6 45.7 44.0 44.4
## H5  45.9 44.4 46.0 47.4  0.0 45.4 44.6 45.6 45.7 44.3
## H6  45.2 45.5 44.9 45.1 45.4  0.0 44.9 43.9 44.7 43.3
## H7  45.0 44.8 45.7 45.6 44.6 44.9  0.0 45.3 43.5 44.4
## H8  45.8 44.6 45.2 45.7 45.6 43.9 45.3  0.0 44.0 44.1
## H9  45.0 44.4 44.1 44.0 45.7 44.7 43.5 44.0  0.0 44.2
## H10 46.0 44.5 45.3 44.4 44.3 43.3 44.4 44.1 44.2  0.0
```

Correlation-based distance Correlation-based distance considers two observations to be similar if their features are highly correlated, even though the observed values may be far apart in terms of Euclidean distance.

```
##      H1 H2  H3  H4  H5  H6  H7  H8  H9 H10
## H1  0.0  1 1.0 1.0 1.0 1.0 1.0 1.1 1.0 1.1
## H2  1.0  0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
## H3  1.0  1 0.0 0.9 1.0 1.0 1.0 1.0 1.0 1.0
## H4  1.0  1 0.9 0.0 1.1 1.0 1.0 1.0 1.0 1.0
## H5  1.0  1 1.0 1.1 0.0 1.0 1.0 1.0 1.0 1.0
## H6  1.0  1 1.0 1.0 1.0 0.0 1.0 1.0 1.0 0.9
## H7  1.0  1 1.0 1.0 1.0 1.0 0.0 1.0 0.9 1.0
## H8  1.1  1 1.0 1.0 1.0 1.0 1.0 0.0 1.0 1.0
## H9  1.0  1 1.0 1.0 1.0 1.0 0.9 1.0 0.0 1.0
## H10 1.1  1 1.0 1.0 1.0 0.9 1.0 1.0 1.0 0.0
```

Linkage

The linkage function takes the distances and groups pairs of objects into clusters based on their similarity. These clusters are then linked to each other to create bigger clusters and the linkage continues until all the data are linked together in a hierarchical tree.

Maximum or complete linkage The distance between two clusters is defined as the maximum value of all pairwise distances between the elements in cluster 1 and the elements in cluster 2. It tends to produce more compact clusters.

Minimum or single linkage The distance between two clusters is defined as the minimum value of all pairwise distances between the elements in cluster 1 and the elements in cluster 2. It tends to produce long, "loose" clusters.

Mean or average linkage The distance between two clusters is defined as the average distance between the elements in cluster 1 and the elements in cluster 2.

Centroid linkage The distance between two clusters is defined as the distance 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 vari- ance. At each step the pair of clusters with minimum between-cluster distance are merged.

P-value

Generate bootstraps samples

Compute hierarchical clustering on each bootstrap copy

Compute for each cluster :

The bootstrap probability (BP) value : frequency that the cluster is identified in bootstrap copies.

The approximately unbiased (AU) probability values (p-values) by multiscale bootstrap resampling. Clusters with p-value above 95% are considered to be strongly supported by data.

Examples

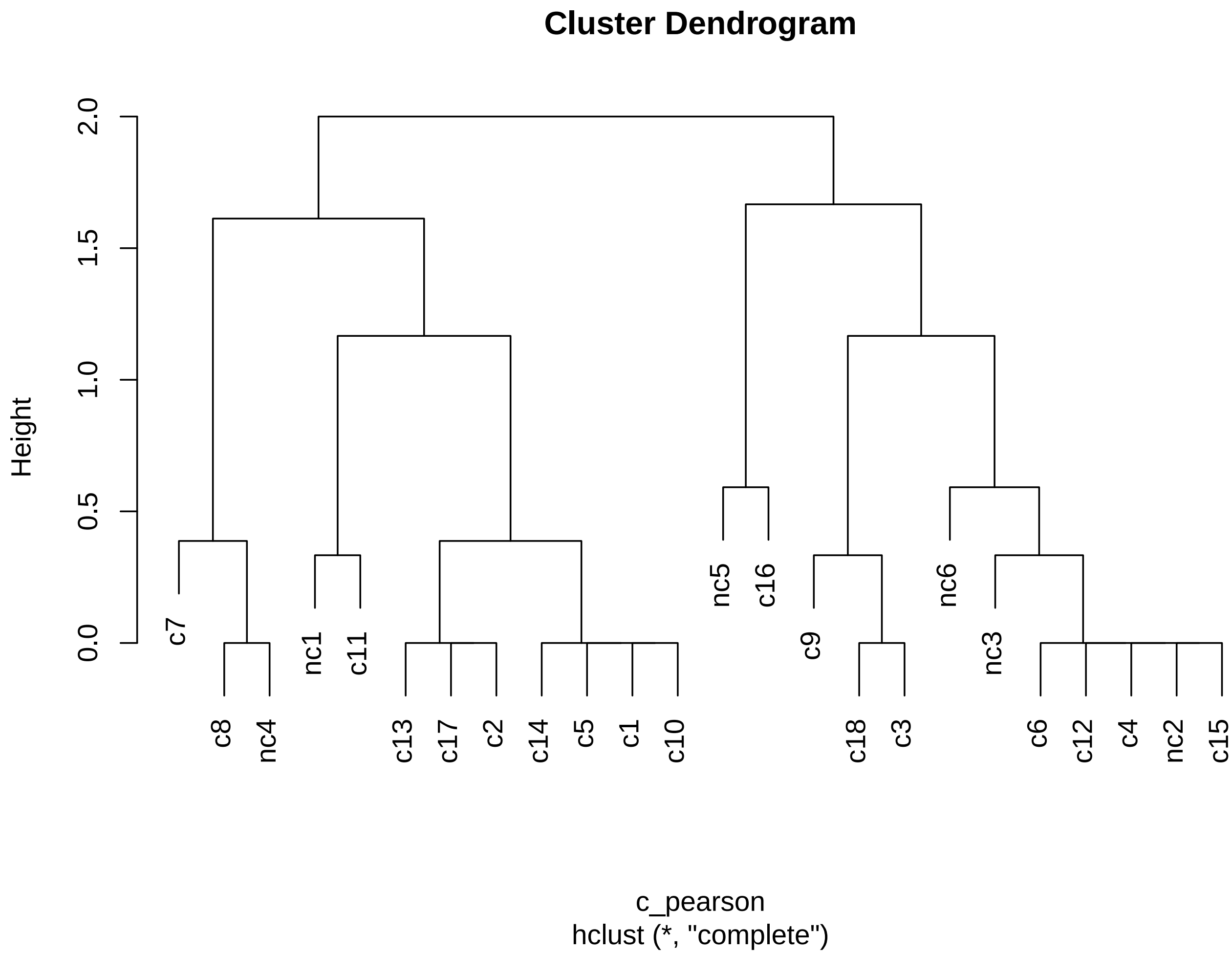
Mushrooms dataset The mushrooms data set contains information about 24 mushrooms. It indicates the smell, form and color but also whether it is possible to eat or not.

The purpous is to see if smell, form and color are enough to cluster the mushrooms into comestible and non-comestible.

n stands for non comestible
c stands for comestible

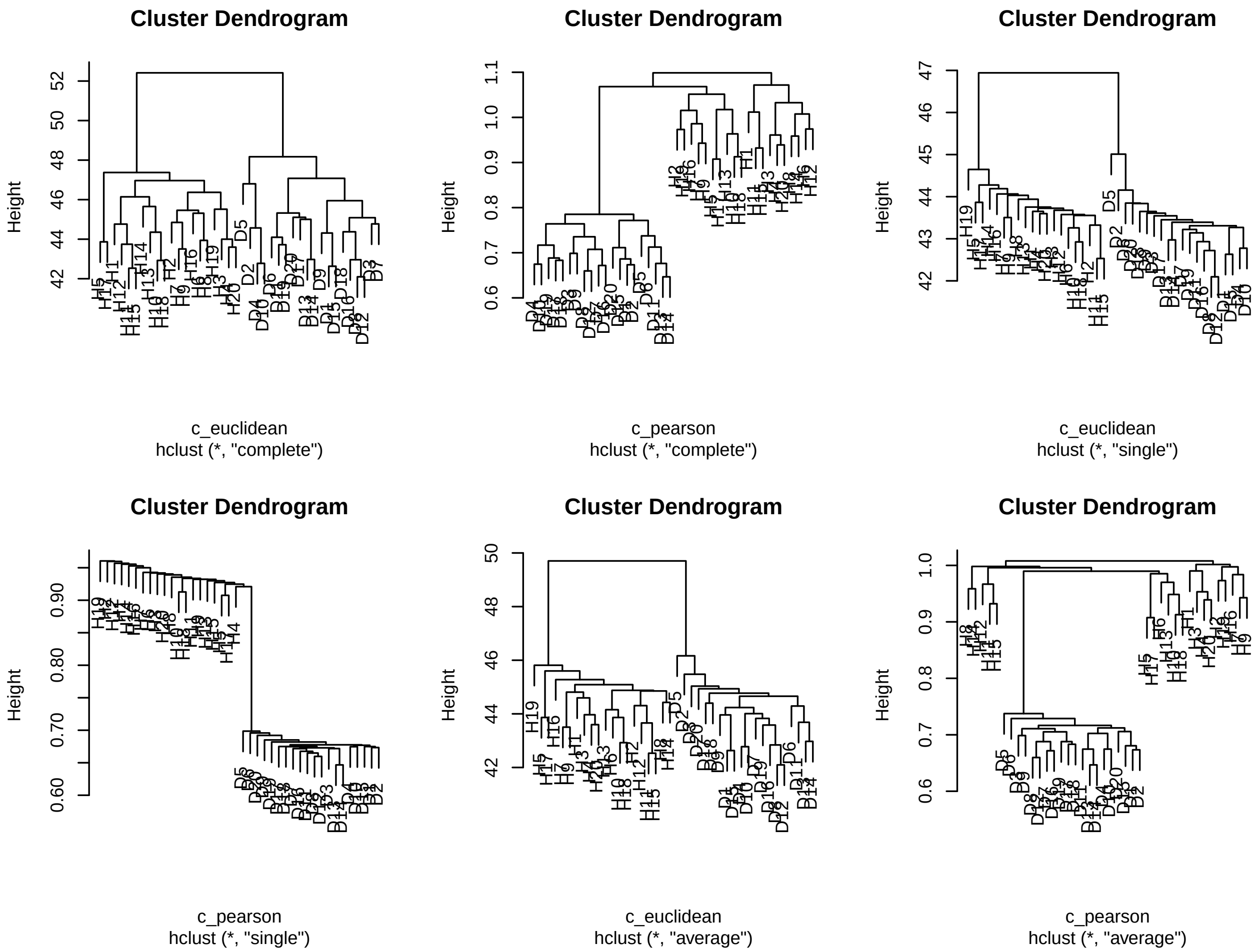
On R

```
##  c8 nc3  c7 nc2 c18 c17  c1  c2 nc5 nc1 c13 nc6 c16  c3 c15 c10  c5 nc4  c4 c12
##   1   2   1   2   2   1   1   1   2   1   1   2   2   2   2   1   1   1   2   2
## c14  c9  c6 c11
##   1   2   2   1
```


Cluster Dendrogram
Height
2.0
1.5
1.0
0.5
0.0
c7
c8
nc4
nc1
c11
c13
c17
c2
c14
c5
c1
c10
nc5
c16
c9
c18
c3
nc6
nc3
c6
c12
c4
nc2
c15
c_pearson
hclust (*, "complete")

Healthy and non-healthy tissues samples Using the tissue and genes data set, we apply hierarchical clustering.

On R



We can see that the use of euclidean distance in the three methods (complete, single, average) gives good results (no missclassification) but the use of correlation-distance gives very bad results.

Furthermore all methods, except Average with correlation-distance, divide the graph in two groups (healthy and non-healthy) which is very good.

We have the same Dunn index as with K-means and PAM on the same dataset (tissues samples). So k-means, PAM and hiearchical clustering (with euclidean distance and complete linkage) methods perform equally.

```
## [1] 0.9744956
```

The cluster average silhouette widths are :

```
##          1          2
## 0.09268309 0.09945822
```

It means that observations are well clustered but the distinction between clusters is not that easy.

On python with scikit-learn

Corona dataset : the problem of over-represented category The corona dataset contains information of patients who have caught Corona. It stores their age, sex and nationality but also if there are dead or not.

The purpous is to use hiearchical clustering to see if the age, sex and nationality is enough to separate the dead from the living patients. H stands for Healthy now and D stands for Deceased.

```
## H446 H447 H448 H449 H450   D1   D2   D3   D4   D5   D6   D7   D8   D9  D10  D11
##    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
##  D12  D13  D14  D15  D16  D17  D18  D19  D20  D21  D22  D23  D24  D25  D26  D27
##    1    1    1    1    1    1    1    1    2    2    2    2    2    2    2    2
##  D28  D29  D30  D31  D32  D33  D34  D35  D36  D37  D38  D39  D40  D41  D42  D43
##    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2
##  D44  D45
##    2    2
```

Looking at the clustering, 1 is the cluster of healthy patients, 2 is the cluster of dead patients.
We can see that it is difficult to cluster the dead patients together because there are only 45 deceased cases against 450 healthy patients. This is a problem of over-represented category.

Fuzzy Clustering

Overall

TO-DO

Examples

The function fanny() computes fuzzy clustering.

We use the tissue dataset.
For the dissimilarity function, the choice was euclidean distance.
2 is for the number of clusters expected.
stand indicates whether variables are standardized before calculating the dissimilarities.

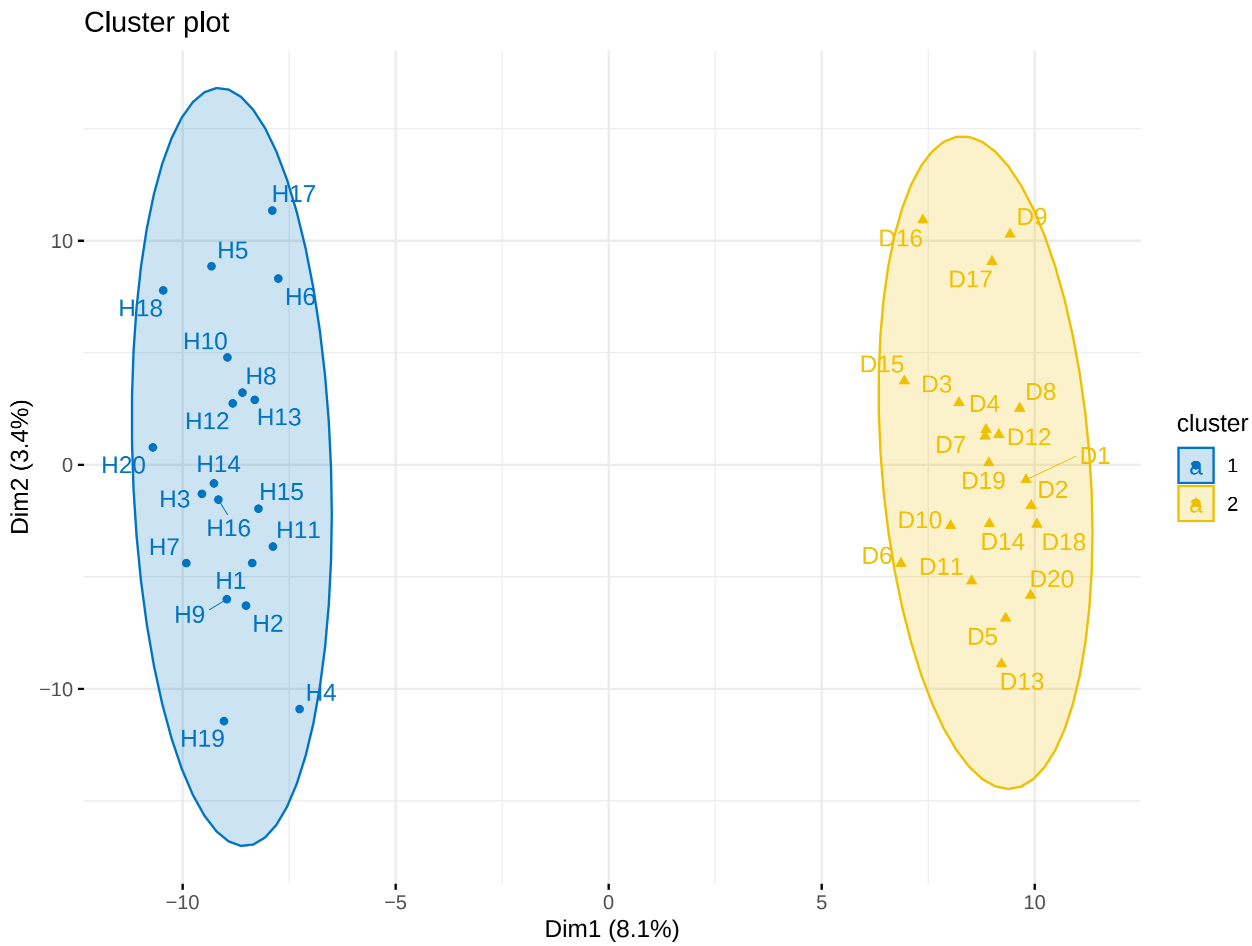
```
##  H1  H2  H3  H4  H5  H6  H7  H8  H9 H10 H11 H12 H13 H14 H15 H16 H17 H18 H19 H20
##   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1
##  D1  D2  D3  D4  D5  D6  D7  D8  D9 D10 D11 D12 D13 D14 D15 D16 D17 D18 D19 D20
##   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
```

We can see that every tissue sample was well clustered.

```
##   dunn_coeff   normalized
## 5.000000e-01 2.220446e-15
```

Looking at the Dunn coefficient, it is about 0.5 meaning that the diameter of one of the cluster is 2 times larger than the minimal separation of two cluster.

This makes sense looking at the following plot.


Cluster plot
Dim2 (3.4%)
10
0
−10
Dim1 (8.1%)
−10
−5
0
5
10
cluster
1
2
H17
H5
H6
H18
H10
H8
H12
H13
H20
H14
H3
H15
H16
H11
H7
H1
H9
H2
H4
H19
D16
D9
D17
D15
D3
D4
D8
D7
D12
D1
D19
D2
D10
D14
D18
D6
D11
D20
D5
D13

Choosing the best algorithm ?

TO-DO