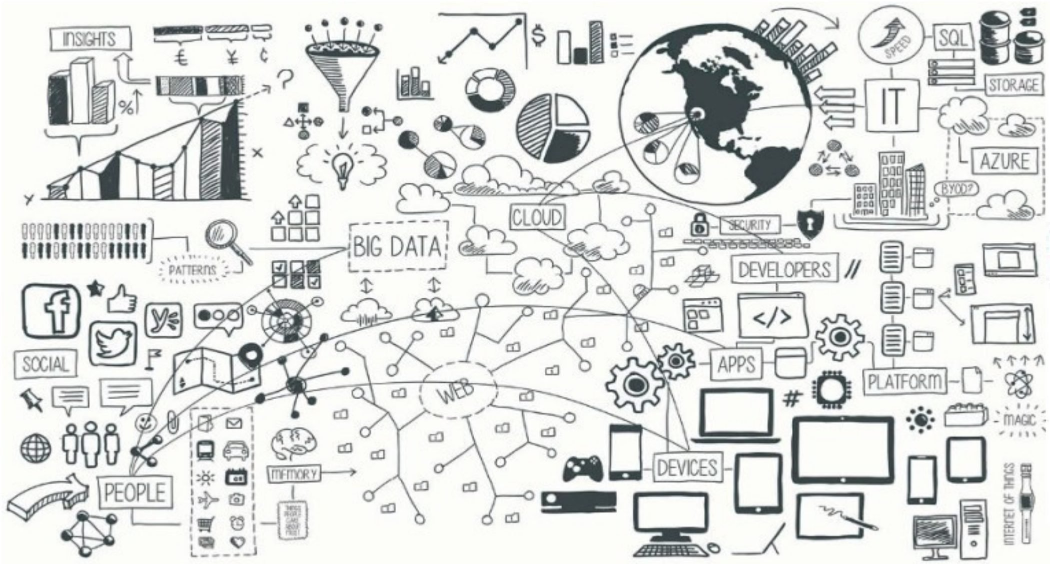
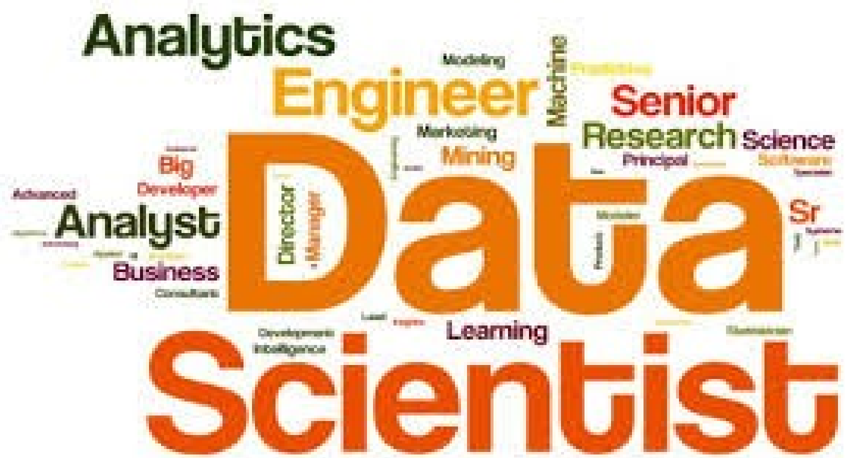
Data Mining (Minería de Datos)

Técnicas de Segmentación: Clustering





Joaquín Bedia
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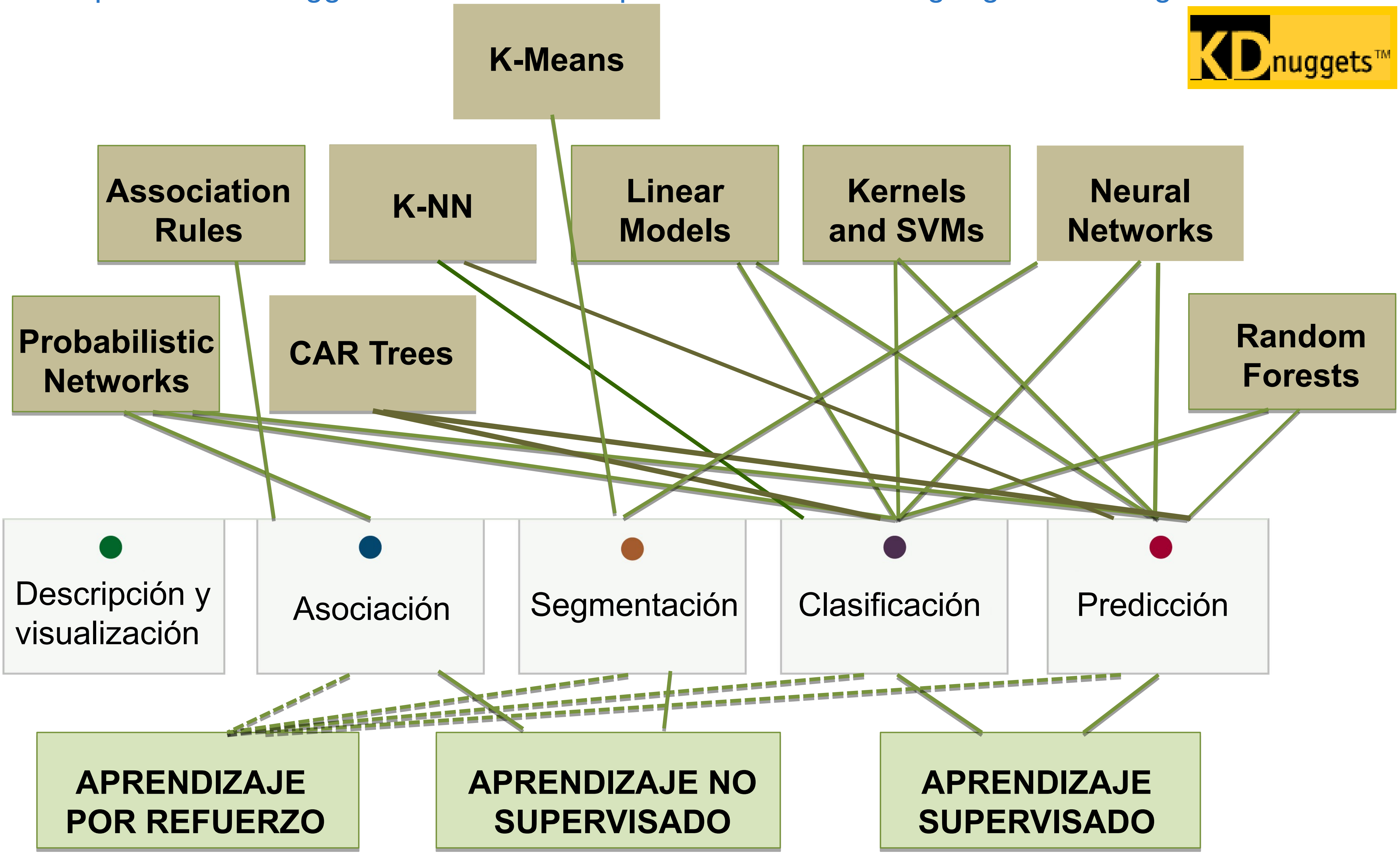
https://www.kdnuggets.com/2015/05/top-10-data-mining-algorithms-explained.html
https://www.kdnuggets.com/2017/10/top-10-machine-learning-algorithms-beginners.html



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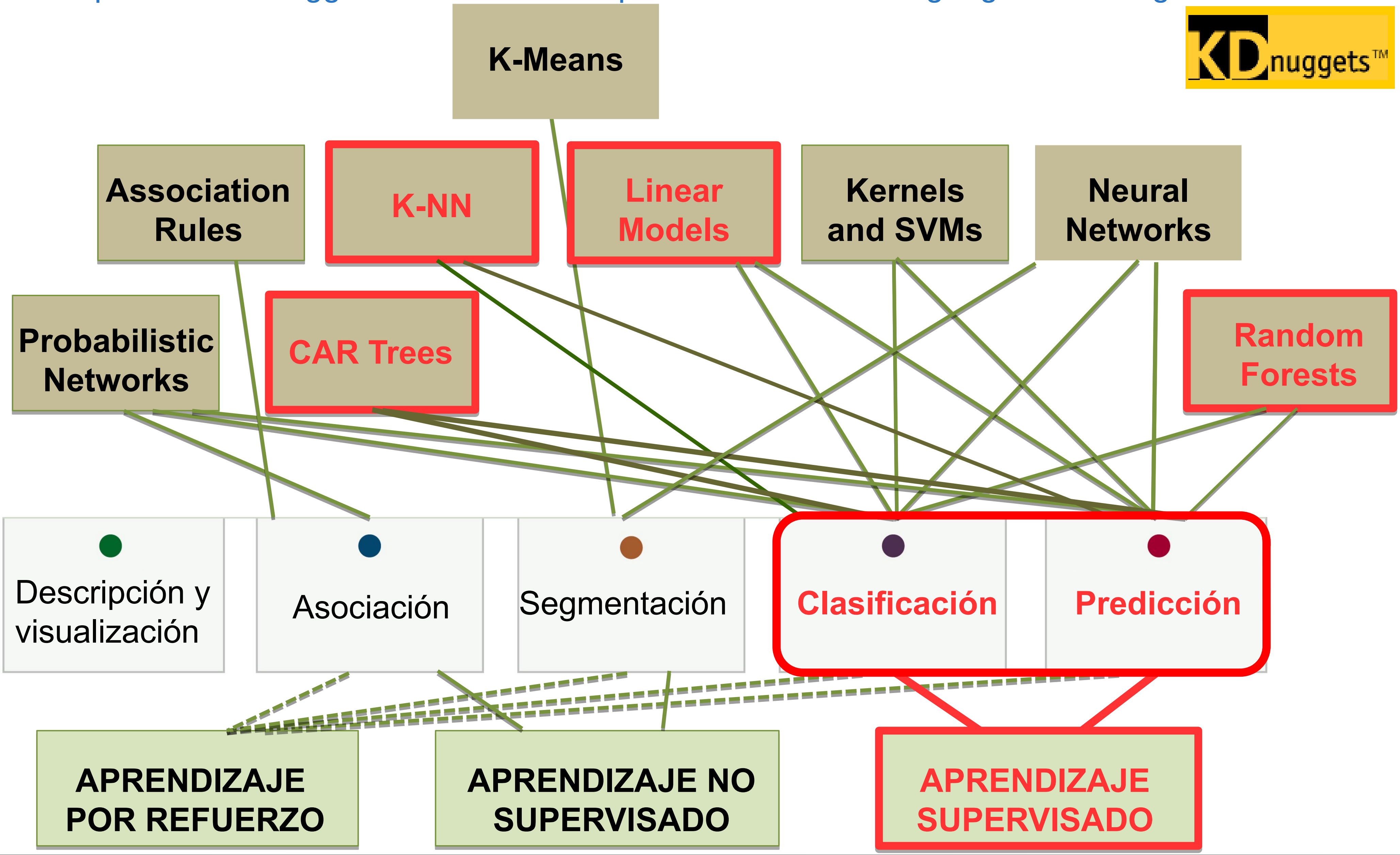

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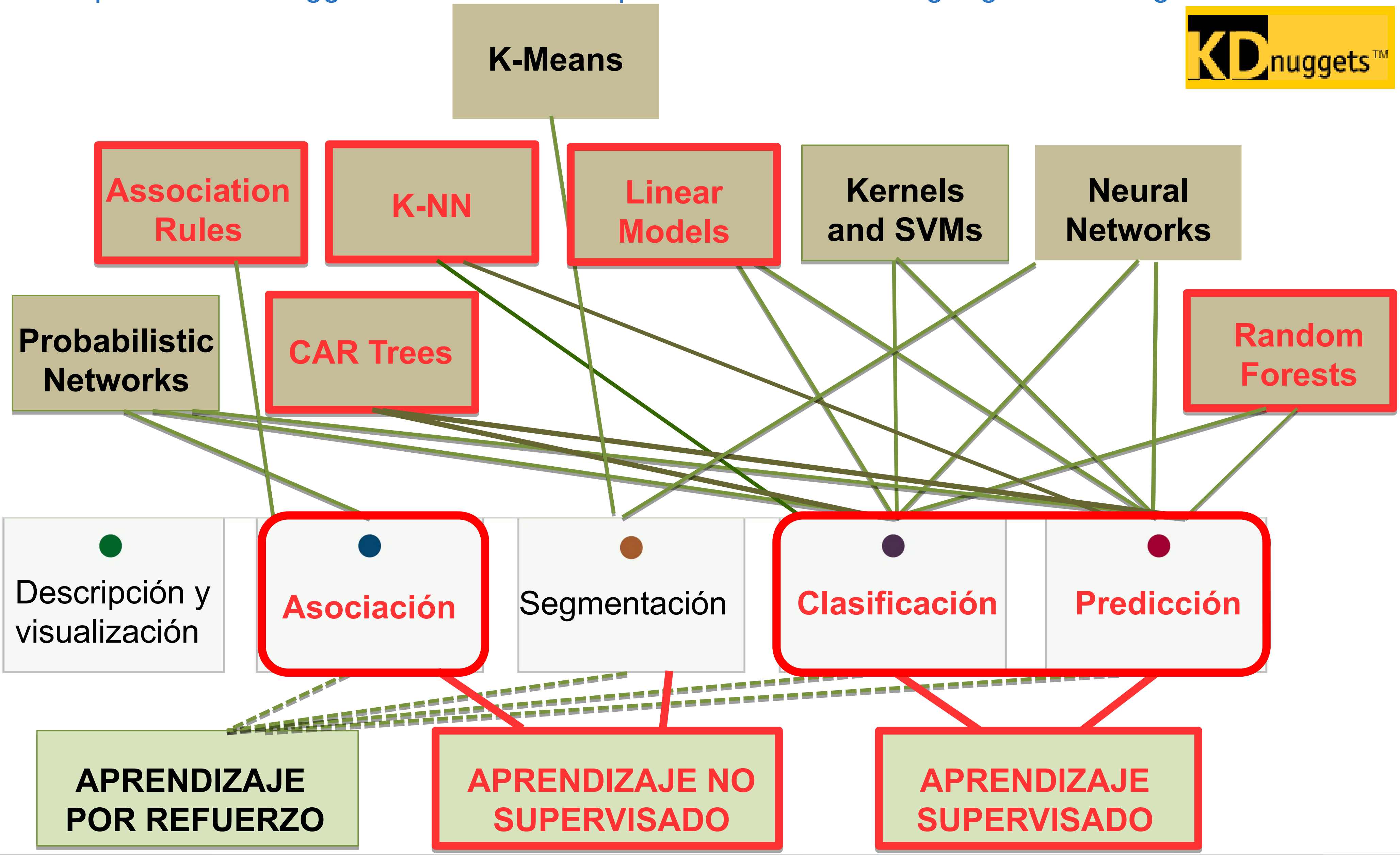

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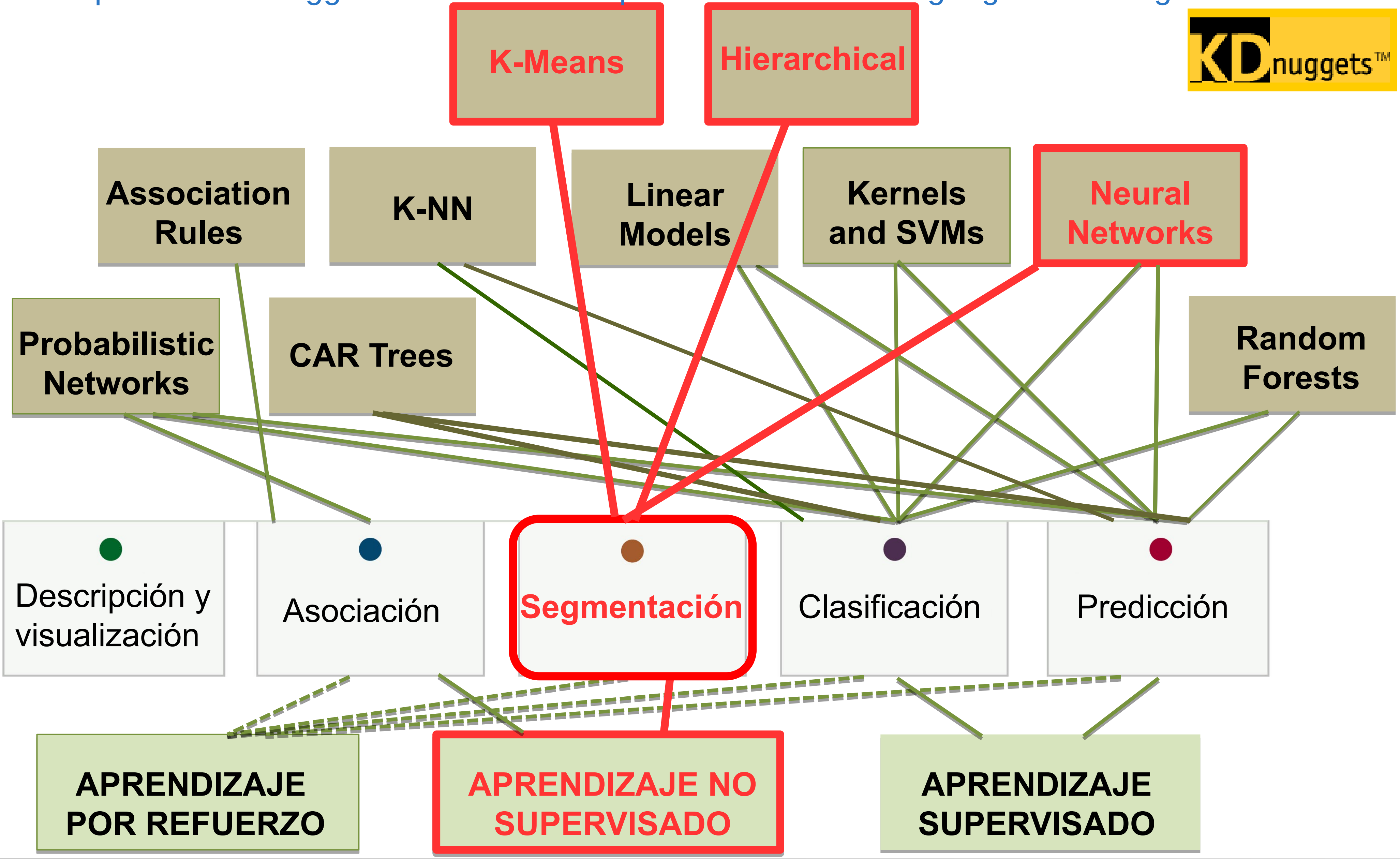

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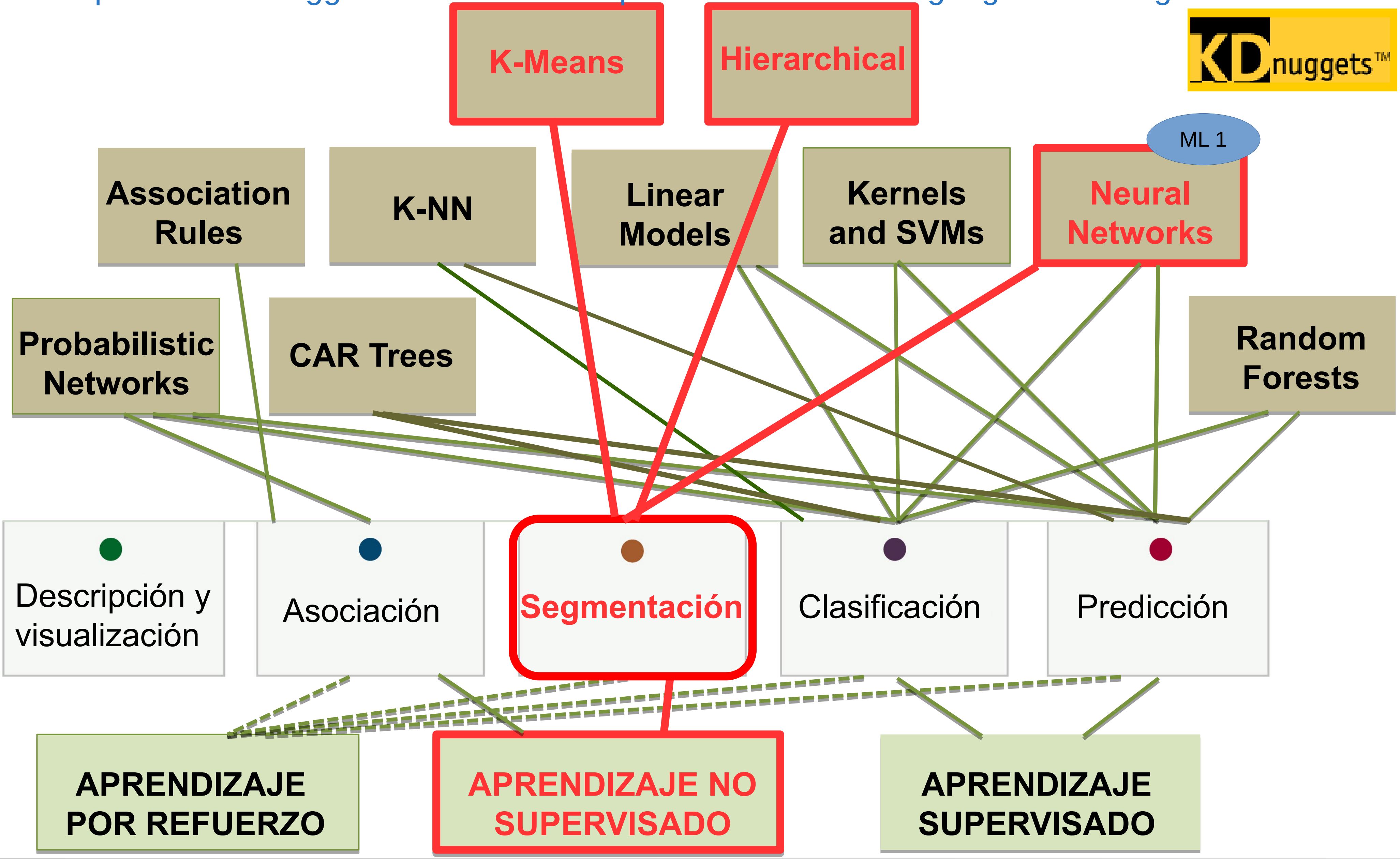
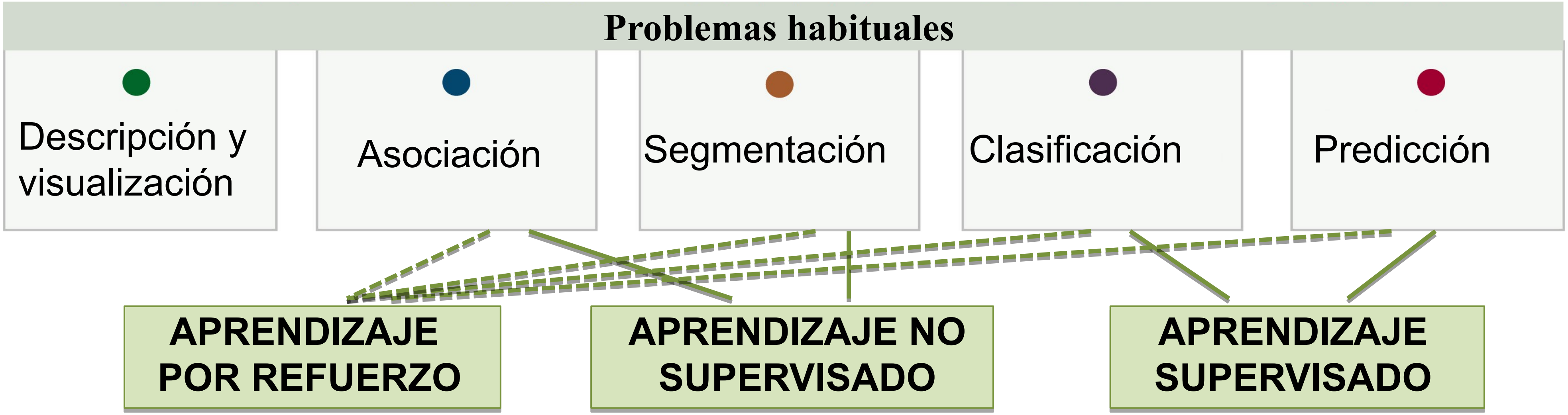


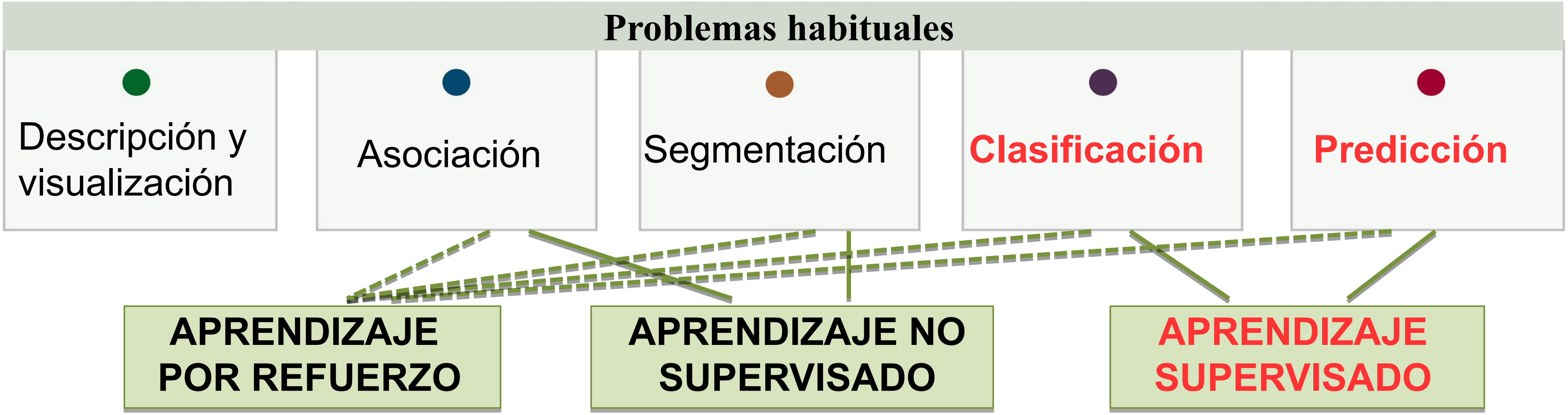


Input data: $x_1, x_2, x_3, x_4, \ldots$

Supervised learning: The machine is also given desired outputs $y_1, y_2, \ldots$, and its goal is to learn to produce the correct output given a new input.

Unsupervised learning: The goal of the machine is to build representations of x that can be used for reasoning, decision making, predicting things, communicating etc.

Reinforcement learning: The machine can also produce actions $a_1, a_2, \ldots$ which affect the state of the world, and receives rewards (or punishments) $r_1, r_2, \ldots$. Its goal is to learn to act in a way that maximises rewards in the long term.



Target Variable: *Y: discrete/factor* or *continuous*

What we are trying to predict.

Predictive Variables: $\{X_1, X_2, \ldots, X_N\}$: *continuous*

"Covariates" used to make predictions.

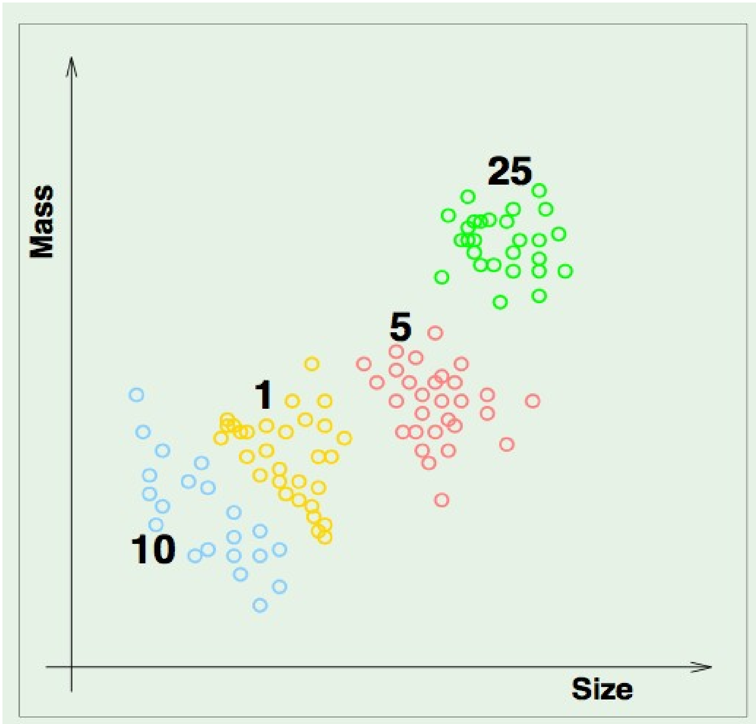
Predictive Model: $Y = f(X_1, X_2, \ldots, X_N)$

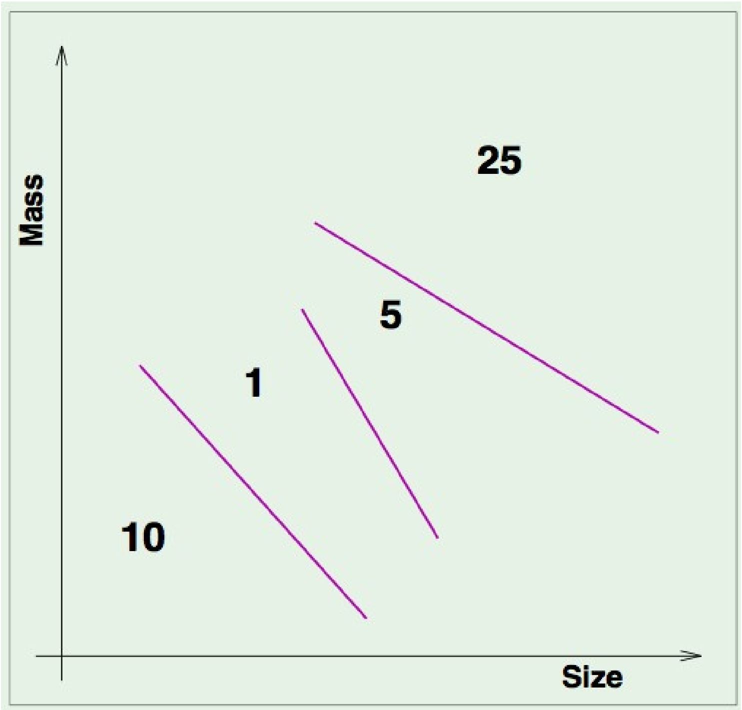
"Learning engine" that estimates the f (or the parameters defining f).

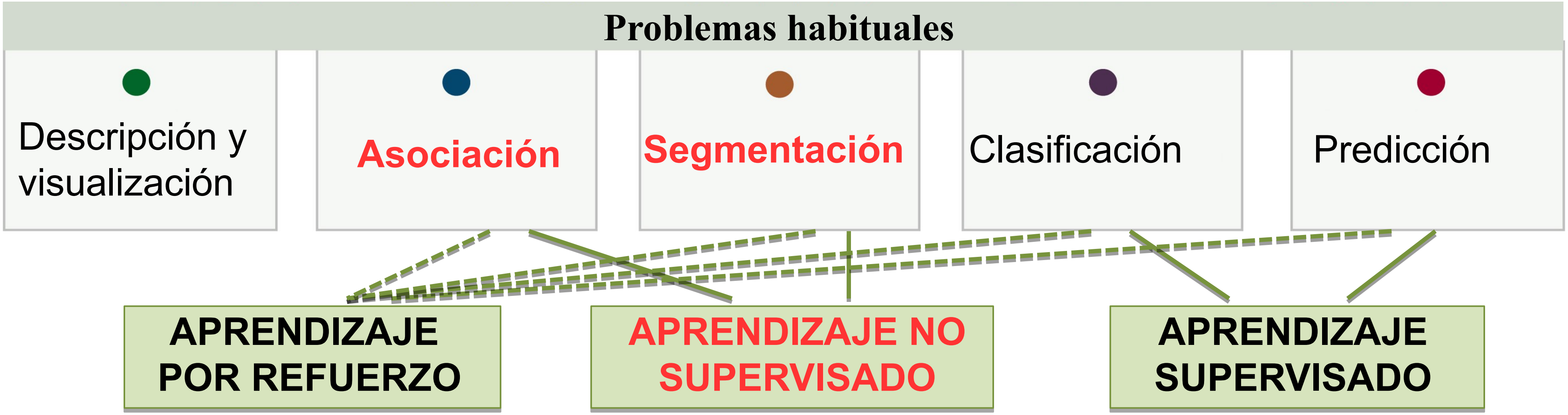
Problemas habituales

Descripción y visualización	Asociación	Segmentación	**Clasificación**	**Predicción**

APRENDIZAJE POR REFUERZO	APRENDIZAJE NO SUPERVISADO	**APRENDIZAJE SUPERVISADO**







Target Variable: *There is no target variable (association)*

K (cluster), discrete: #clusters (segmentation)

Predictive Variables: $\{X_1, X_2, \ldots, X_N\}$: *continuous* or *discrete*

"Covariates" used to make predictions.

Predictive Model: Algorithmic, based on $(X_1, X_2, \ldots, X_N)$.

Ad-hoc "learning" and "prediction" engine.

Problemas habituales

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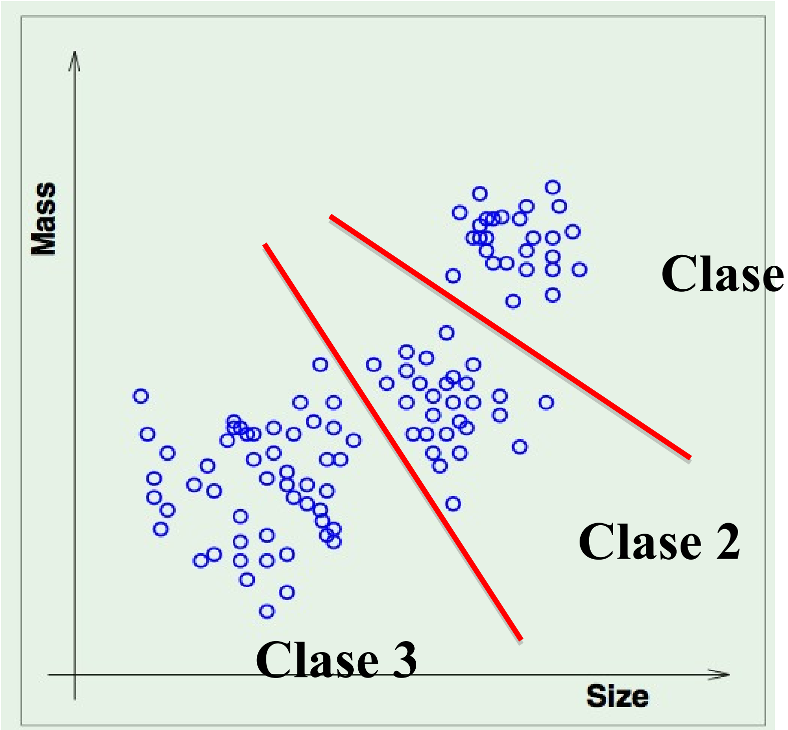

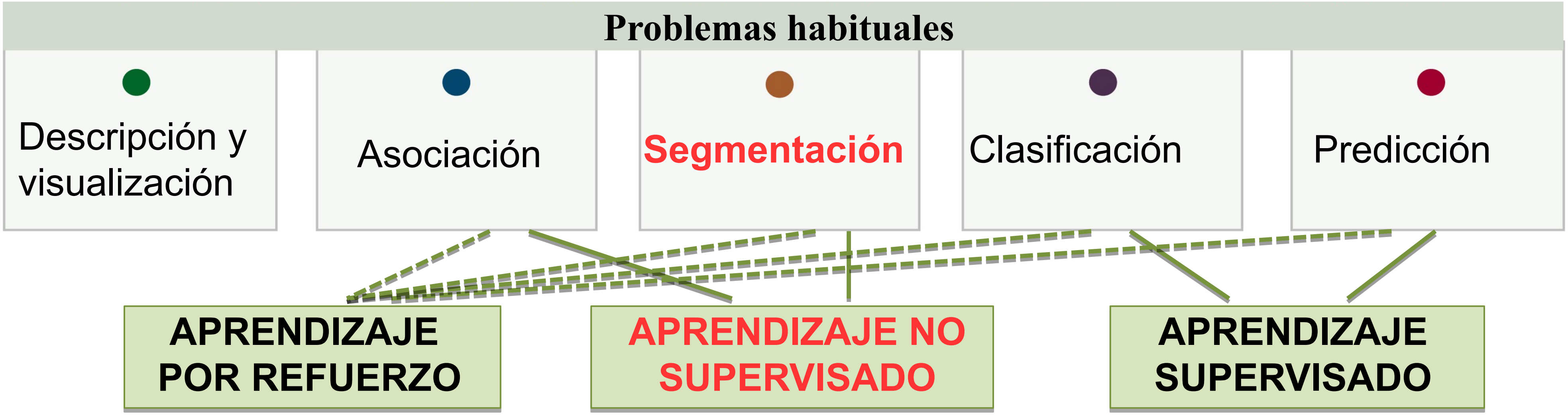

The main objective of the cluster analysis is to group or segmenting a collection of objects, understood as a set of measurements, into subsets or “clusters,” such that those within each cluster are more closely related to one another than objects assigned to different clusters.

Problemas habituales

Descripción y visualización | Asociación | **Segmentación** | Clasificación | Predicción

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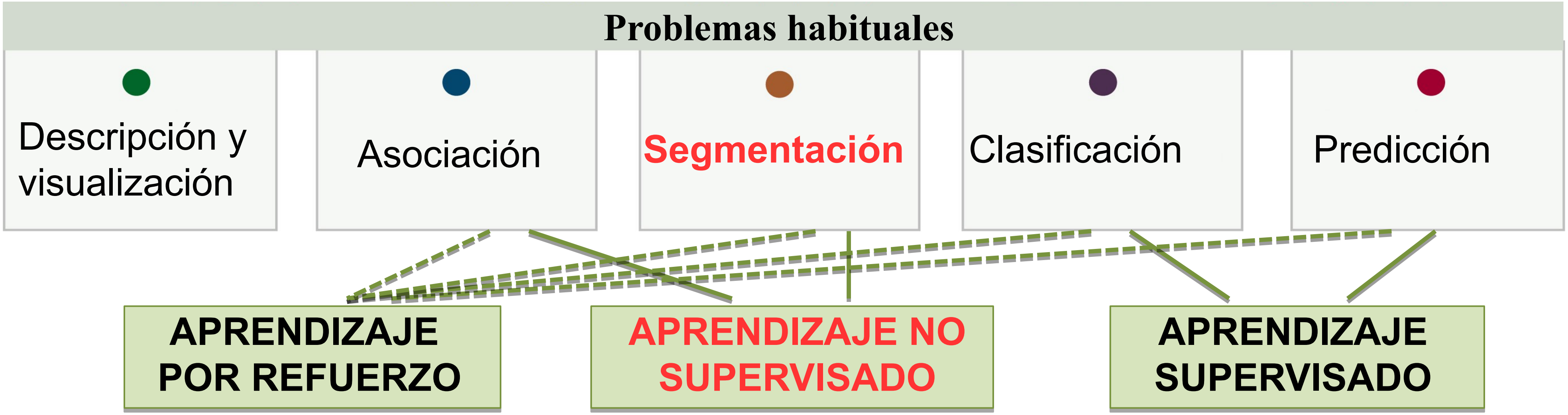
Input

Similarity-based → NxN distance matrix D

Feature-based → NxD feature matrix X



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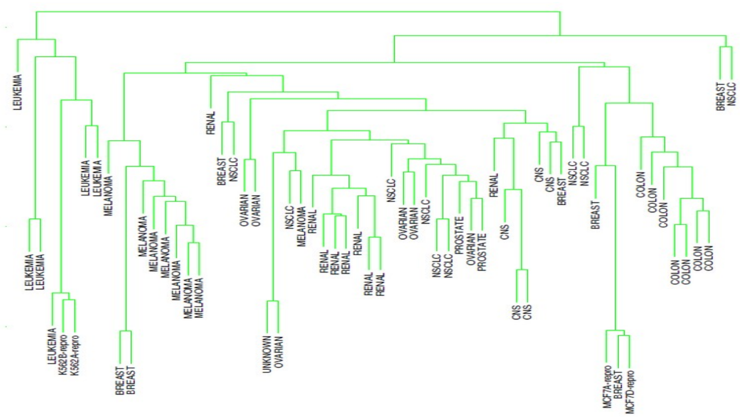
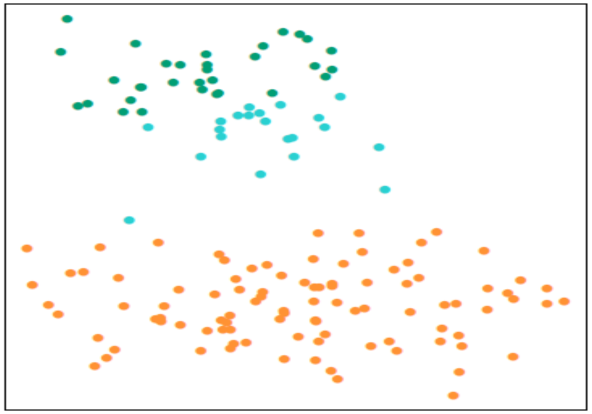


Output

Partitional/Flat

Hierarchical



Problemas habituales

- Descripción y visualización
- Asociación
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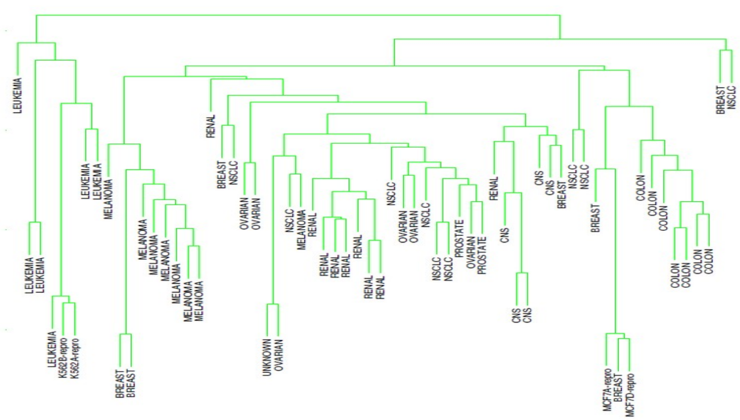
Hierarchical



Complejidad: $O\left(N^2 \log N\right)$

Deterministic

Problemas habituales

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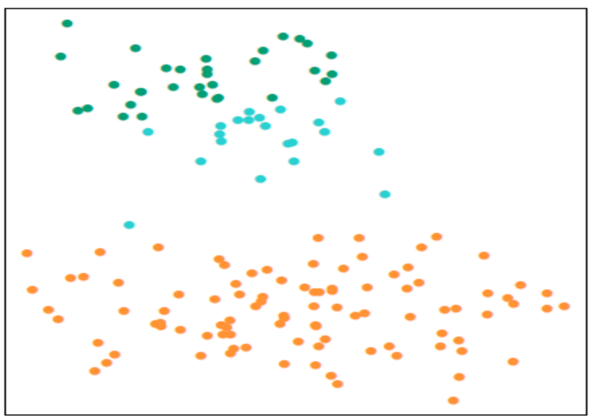
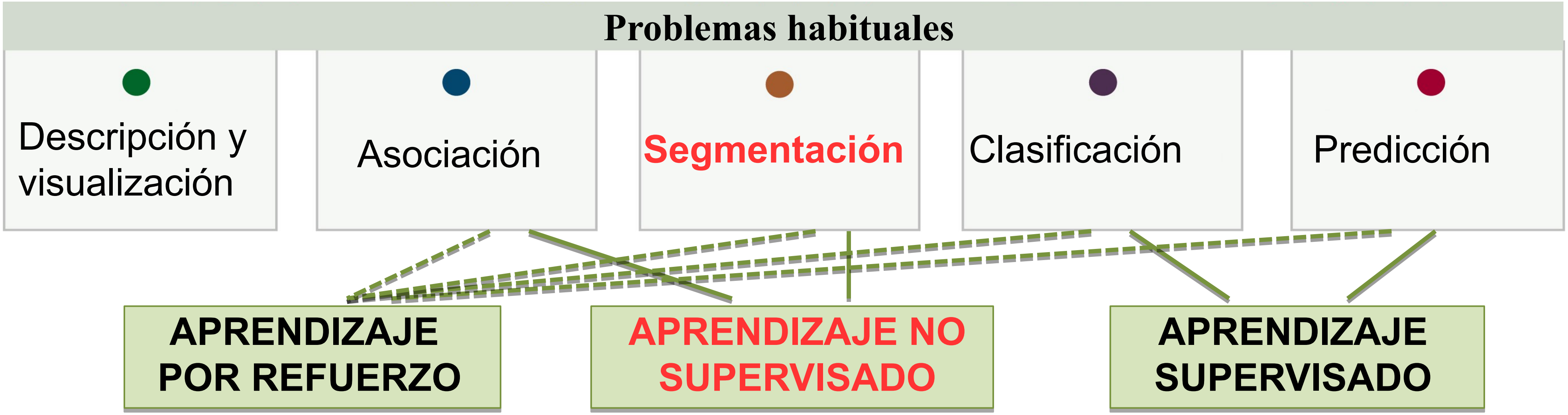
Partitional/Flat



Complejidad: $O(N\,D)$

Depends on the number of clusters

Sensitivity to initial conditions



The main objective of the cluster analysis is to group or segmenting a collection of objects, understood as a set of measurements, into subsets or “clusters,” such that those within each cluster are more closely related to one another than objects assigned to different clusters.

Input	**Output**
Similiraty-based	**Partitional/Flat**
Feature-based	**Hierarchical**

To this aim, an assessment of the **degree of difference (dissimilarity)** between the objects assigned to the respective clusters is required.

Similarity and distance measures are obtained/defined considering the predictors. Therefore, strongly depend on the nature of these variables:

Quantitative
Qualitative
Ordinals
etc...

```
? dist
```

Similarity and distance measures are obtained/defined considering the predictors. Therefore, strongly depend on the nature of these variables:

Quantitative

Minkowsky:

$$D(\boldsymbol{x},\boldsymbol{y}) = \left(\sum_{i=1}^{m} |x_i - y_i|^r\right)^{1/r}$$

Euclidean:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city-block:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

Camberra:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{|x_i - y_i|}{|x_i + y_i|}$$

Chebychev:

$$D(\boldsymbol{x},\boldsymbol{y}) = \max_{i=1}^{m} |x_i - y_i|$$

Quadratic:

$$D(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}-\boldsymbol{y})^T Q(\boldsymbol{x}-\boldsymbol{y}) = \sum_{j=1}^{m}\left(\sum_{i=1}^{m}(x_i - y_i)q_{ji}\right)(x_j - y_j)$$

Q is a problem-specific positive definite $m \times m$ weight matrix

Mahalanobis:

$$D(\boldsymbol{x},\boldsymbol{y}) = [\det V]^{1/m}(\boldsymbol{x}-\boldsymbol{y})^{\mathrm{T}} V^{-1}(\boldsymbol{x}-\boldsymbol{y})$$

V is the covariance matrix of $A_1..A_m$, and A_j is the vector of values for attribute j occuring in the training set instances $1..n$.

Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = \frac{\sum_{i=1}^{m}(x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum_{i=1}^{m}(x_i - \overline{x_i})^2 \sum_{i=1}^{m}(y_i - \overline{y_i})^2}}$$

$\overline{x_i} = \overline{y_i}$ and is the average value for attribute i occuring in the training set.

Chi-square:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{1}{sum_i}\left(\frac{x_i}{size_{\boldsymbol{x}}} - \frac{y_i}{size_{\boldsymbol{y}}}\right)^2$$

sum_i is the sum of all values for attribute i occuring in the training set, and $size_{\boldsymbol{x}}$ is the sum of all values in the vector $\boldsymbol{x}$.

Kendall's Rank Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = 1 - \frac{2}{n(n-1)}\sum_{i=1}^{m}\sum_{j=1}^{i-1}\mathrm{sign}(x_i - x_j)\mathrm{sign}(y_i - y_j)$$

$\mathrm{sign}(x)$=-1, 0 or 1 if $x < 0$, $x = 0$, or $x > 0$, respectively.

```
? dist
dEuc<-dist(iris[,-5],method="euclidean")
dMin<-dist(iris[,-5],method="minkowski",p=4)
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Quantitative

Ordinals → redefine as the rank or the order (e.g. {low, medium, high} → {1/3,2/3,3/3}).

Qualitative – Categorical → assign a distance of 1 if the features are different and 0 otherwise.

$$D(x,y)=\sum_{j=1}^{D} I(x_j \neq y_j)$$

```
? dist
dEuc<-dist(iris[,-5],method="euclidean")
dMin<-dist(iris[,-5],method="minkowski",p=4)
library(cluster)
?daisy
dNom<-daisy(iris,metric="gower")
```

Minkowski:
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$\mathrm{sign}(x)$=-1, 0 or 1 if $x < 0$, $x = 0$, or $x > 0$, respectively.

Defined the distance:

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \cdot d_j(x_{ij}, x_{i'j}); \quad \sum_{j=1}^{p} w_j = 1. \qquad D_I(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \cdot (x_{ij} - x_{i'j})^2$$

The objective of the clustering algorithms is to:

$$T = \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} d_{ii'} = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\left(\sum_{C(i')=k} d_{ii'} + \sum_{C(i')\neq k} d_{ii'}\right),$$

$$T = W(C) + B(C), \begin{cases} W(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k} d(x_i, x_{i'}). \\ B(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')\neq k} d_{ii'} \end{cases}$$

Minimizes the distance intragroup

and

Maximizes the distance between clusters.

```
? kmeans
kmModel<-kmeans(iris[,-5],3,nstart = 1)
kmModel$withinss ## Vector of within-cluster sum of squares, one component per cluster
kmModel$betweenss ## The between-cluster sum of squares
```

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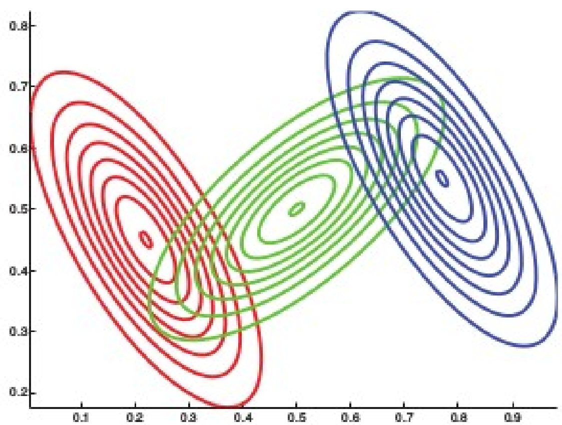
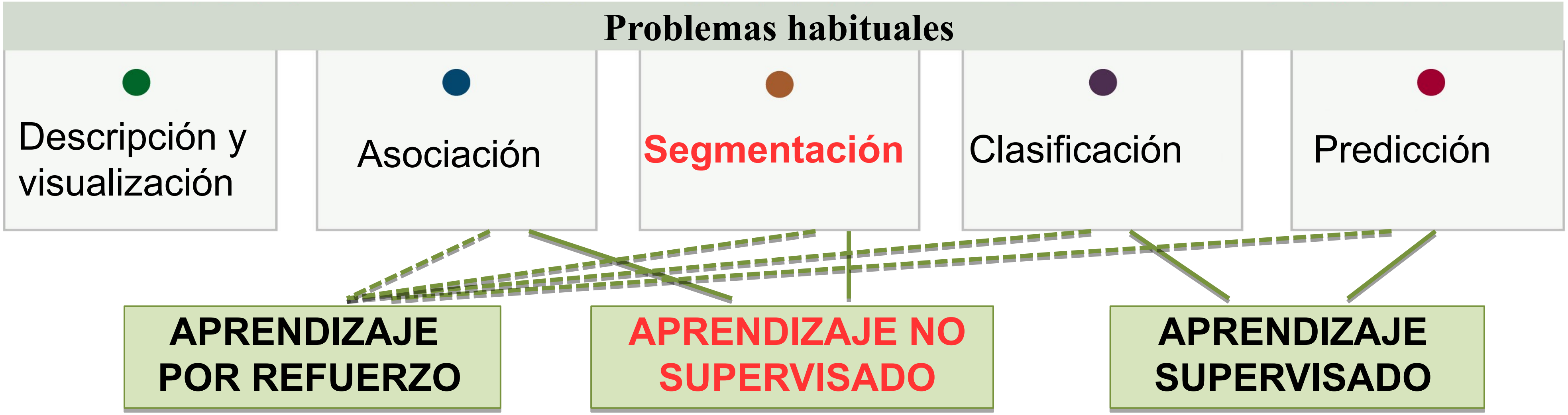
Distribution-based clustering



$$p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p_k(\mathbf{x}_i|\boldsymbol{\theta})$$

π_k satisfy $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1$.

Source: Machine Learning A Probabilistic Perspective, Kevin P. Murphy, The MIT Press, Cambridge, Massachusetts, London, England



Gaussian Mixtures (EM-algorithm)

```r
library(MASS)
library(mclust)
? Mclust
```

$$p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

π_k satisfy $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1.$

- **Expectation step (E):** Calculate the expected value of the log likelihood under the current estimate of the parameters.

$$r_{ik} = \frac{\pi_k p(\mathbf{x}_i|\boldsymbol{\theta}_k^{(t-1)})}{\sum_{k'} \pi_{k'} p(\mathbf{x}_i|\boldsymbol{\theta}_{k'}^{(t-1)})}$$

- **Maximization step (M):** Find the parameters that maximize the log likelihood.

$$\boldsymbol{\mu}_k = \frac{\sum_i r_{ik}\mathbf{x}_i}{r_k}$$

$$\boldsymbol{\Sigma}_k = \frac{\sum_i r_{ik}(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T}{r_k} = \frac{\sum_i r_{ik}\mathbf{x}_i\mathbf{x}_i^T}{r_k} - \boldsymbol{\mu}_k\boldsymbol{\mu}_k^T$$

Iris Data Set

Download: Data Folder, Data Set Description

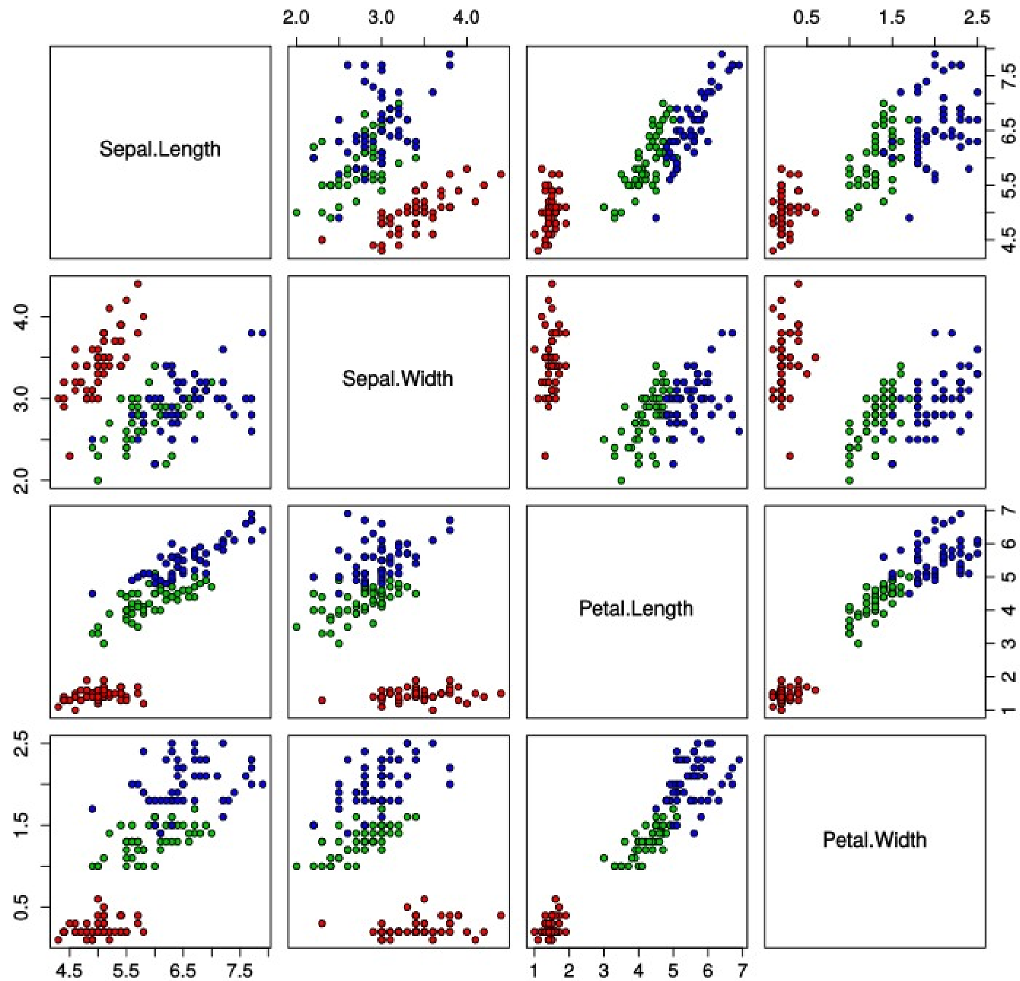
Abstract: Famous database; from Fisher, 1936

Data Set Characteristics:	Multivariate	**Number of Instances:**	150
Attribute Characteristics:	Real	**Number of Attributes:**	4
Associated Tasks:	Classification	**Missing Values?**	No

http://archive.ics.uci.edu/ml/datasets/Iris

```
gmModel<-Mclust(iris[,-5])
summary(gmModel)
Gaussian finite mixture model
fitted by EM algorithm
----------------------------------------
Mclust VEV (ellipsoidal, equal shape)
model with 2 components:
log.likelihood   n df       BIC       ICL
      -215.726 150 26 -561.7285 -561.7289
Clustering table:
  1   2
 50 100
```

Iris Data (red=setosa,green=versicolor,blue=virginica)



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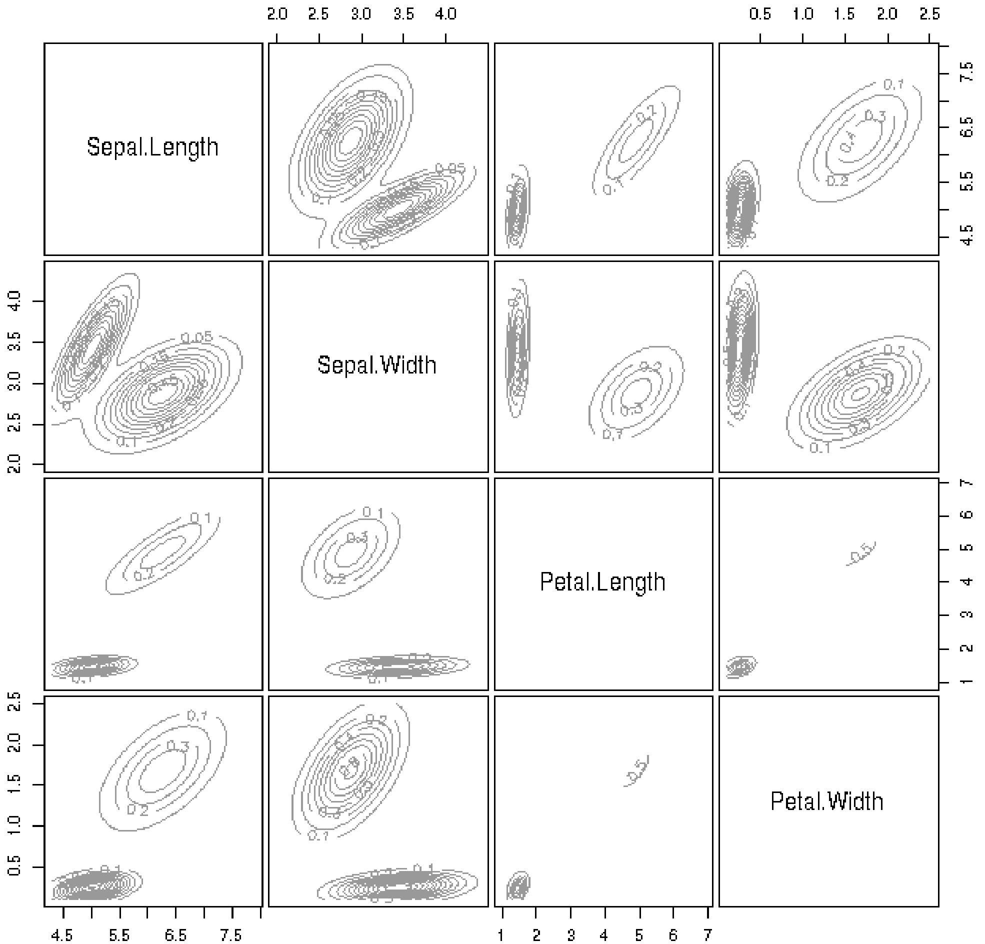
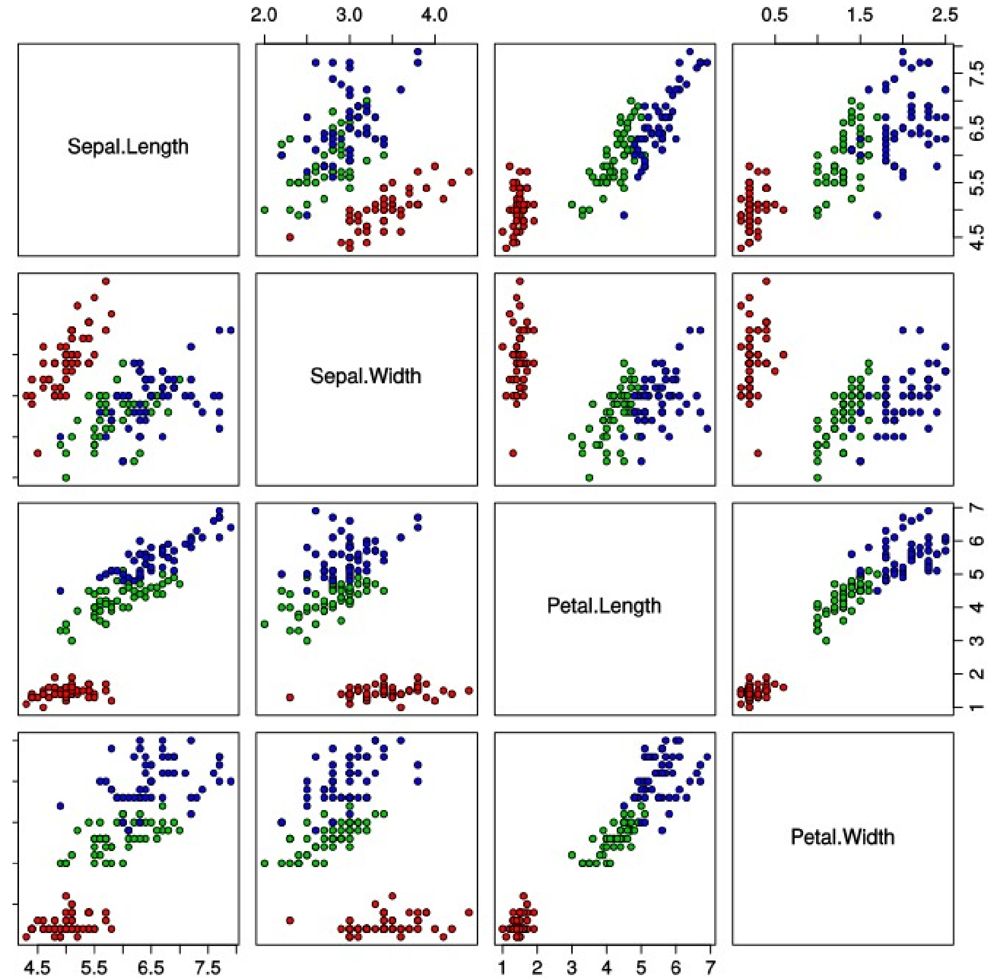
```
plot(gmModel,what="density")
```



Iris Data (red=setosa,green=versicolor,blue=virginica)



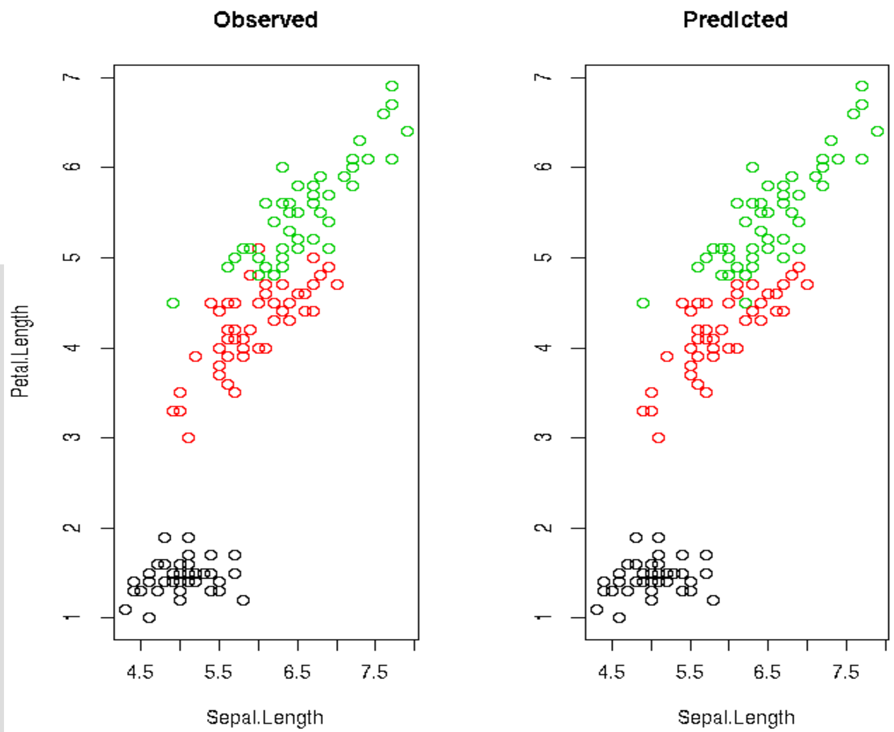
Iris Data Set

Download: Data Folder, Data Set Description

Abstract: Famous database; from Fisher, 1936

http://archive.ics.uci.edu/ml/datasets/Iris

Data Set Characteristics:	Multivariate	**Number of Instances:**	150
Attribute Characteristics:	Real	**Number of Attributes:**	4
Associated Tasks:	Classification	**Missing Values?**	No




```
library(caret)
gmModel<-Mclust(iris[,-5])
summary(gmModel)
plot(gmModel,what="density")
## Defining the number of G-M
gmModel<-Mclust(iris[,-5],G=3)
summary(gmModel)
## Comparing observation and prediction
plot(gmModel,what="density")
par(mfrow=c(1,2))
plot(iris[,c(1,3)],col=iris[,5],main="Observed")
plot(iris[,c(1,3)],col=gmModel$classification,main="Predicted")
confusionMatrix(as.numeric(iris[,5]),gmModel$classification)
```

Problemas habituales

- Descripción y visualización
- Asociación
- **Segmentación**
- Clasificación
- Predicción

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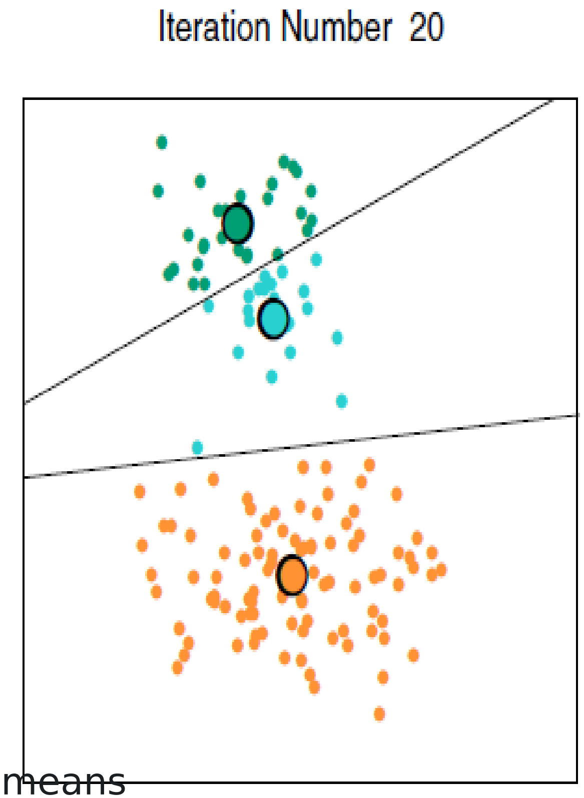
Distribution-based clustering
Centroid-based clustering: Non-overlapping (e.g. K-Means)

```
library(stats)
? kmeans
kmModel<-kmeans(iris[,-5],3,nstart=1)
summary(kmModel)
## Point center of two attributes
plot(iris[,c(1,3)],col=kmModel$cluster,main="K-Means")
points(kmModel$centers[,c(1,3)],col=1:3,pch=8,cex=2)
confusionMatrix(as.numeric(iris[,5]),kmModel$cluster)
```



Example: https://www.kaggle.com/xvivancos/tutorial-clustering-wines-with-k-means

K-Means is one of the most used iterative algorithms. It usually considers the Euclidean distance:

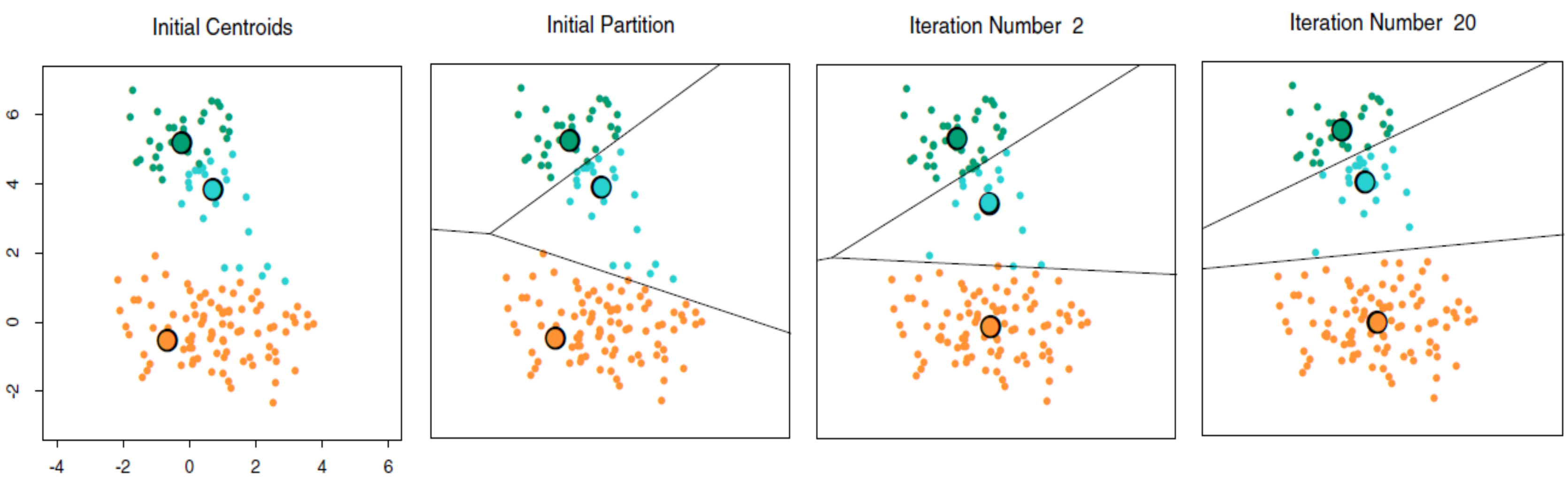
$$d(x_i, x_{i'}) = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = ||x_i - x_{i'}||^2 \Rightarrow W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} ||x_i - x_{i'}||^2 = \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - \bar{x}_k||^2,$$

The objective is to find **K** centroids solution of the following optimization problem:

$$\min_{C, \{m_k\}_1^K} \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - m_k||^2.$$

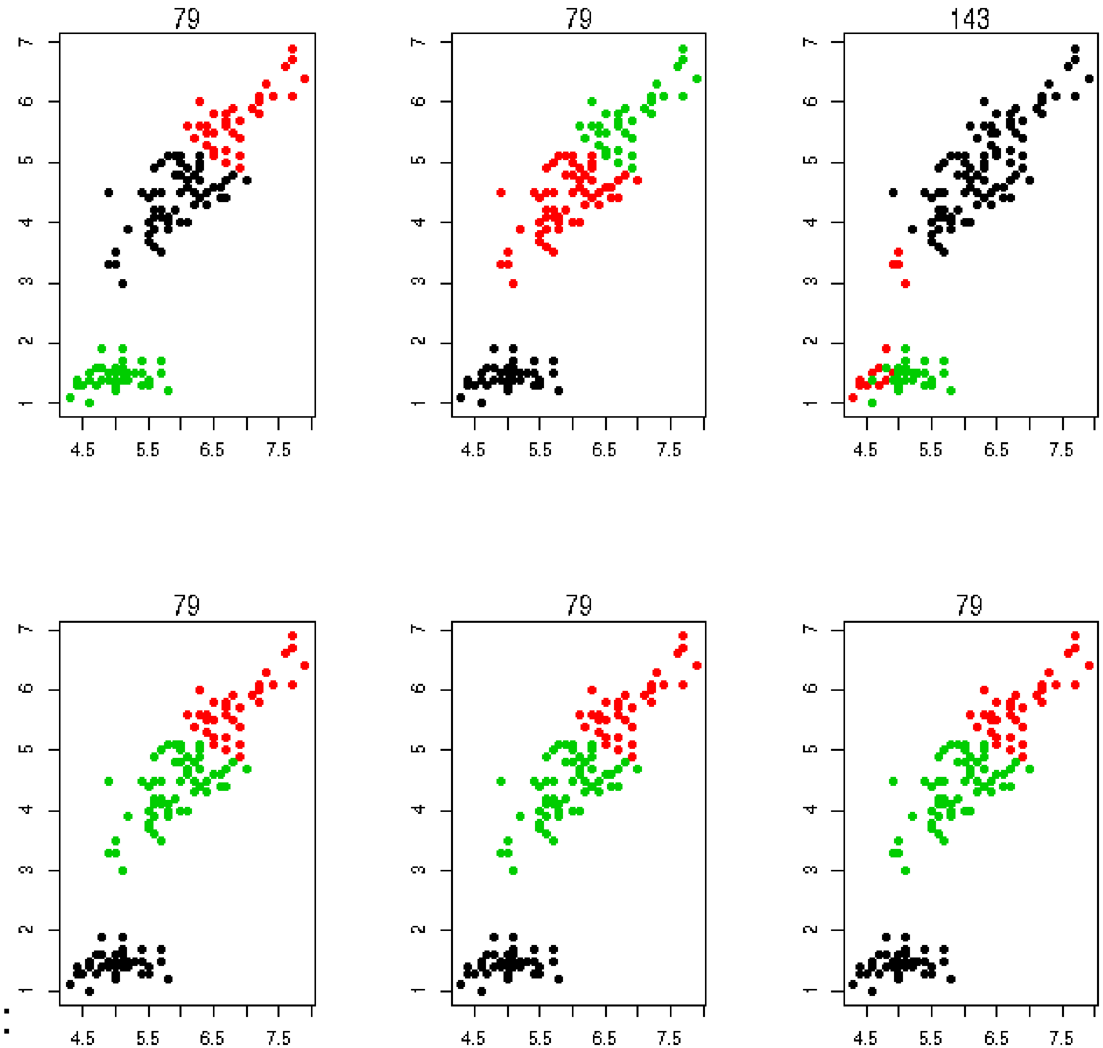
Once the parameter **K** is defined:

- First assignation randomly defined.
- Repeat until converge or reach the maximum number of iterations:
  - Estimate the centroid for each cluster.
  - Re-define the clusters considering the new centroids.



Animated example: https://www.youtube.com/watch?v=5I3Ei69I40s

```
k<-3
par(mfrow=c(2,3))
j<-6
while(j>0){
  set.seed(j)
  j<-j-1
  km<-kmeans(iris[,-5],centers=k)
  plot(iris[,c(1,3)],type="n")
  for(i in 1:k){
    points(iris[km$cluster==i,c(1,3)],
           pch=19,col=i)
  }
  mtext(format(km$tot.withinss,digits=2))
}
```



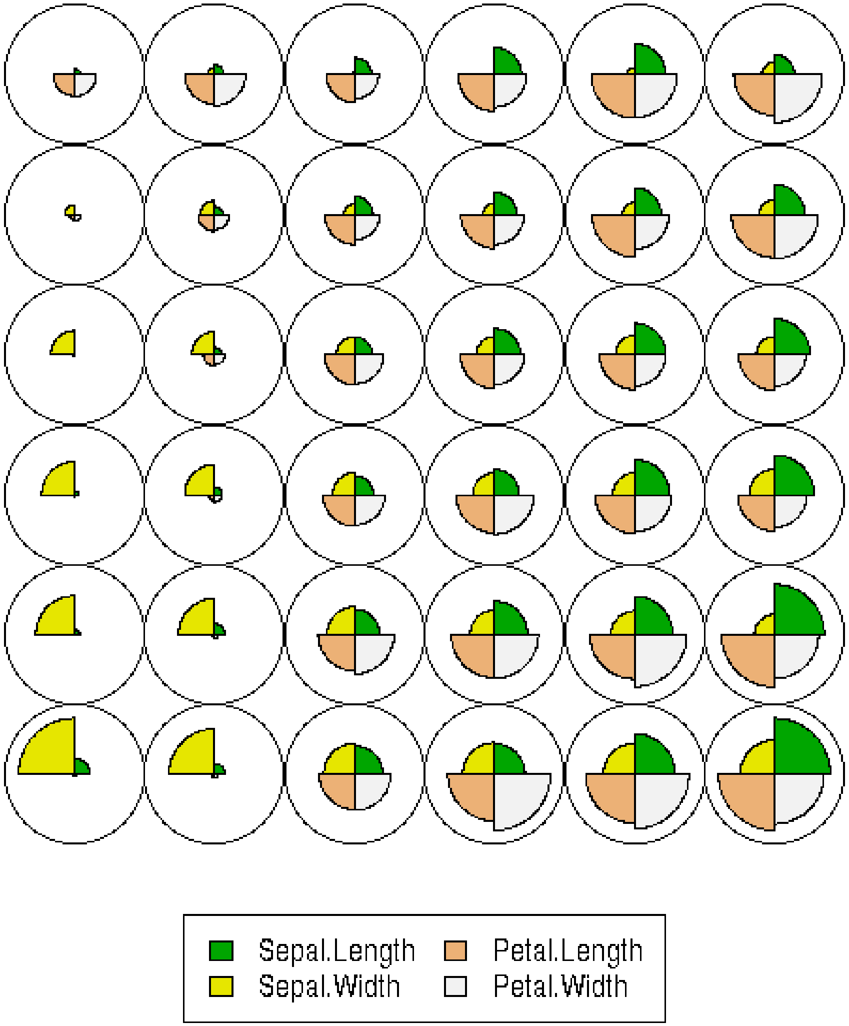
The main problems of this algorithm are:

- How to define the parameter **K**.
- The initialization could lead to different clusters.
- The clusterization is not incremental.

Example: https://www.kaggle.com/xvivancos/tutorial-clustering-wines-with-k-means

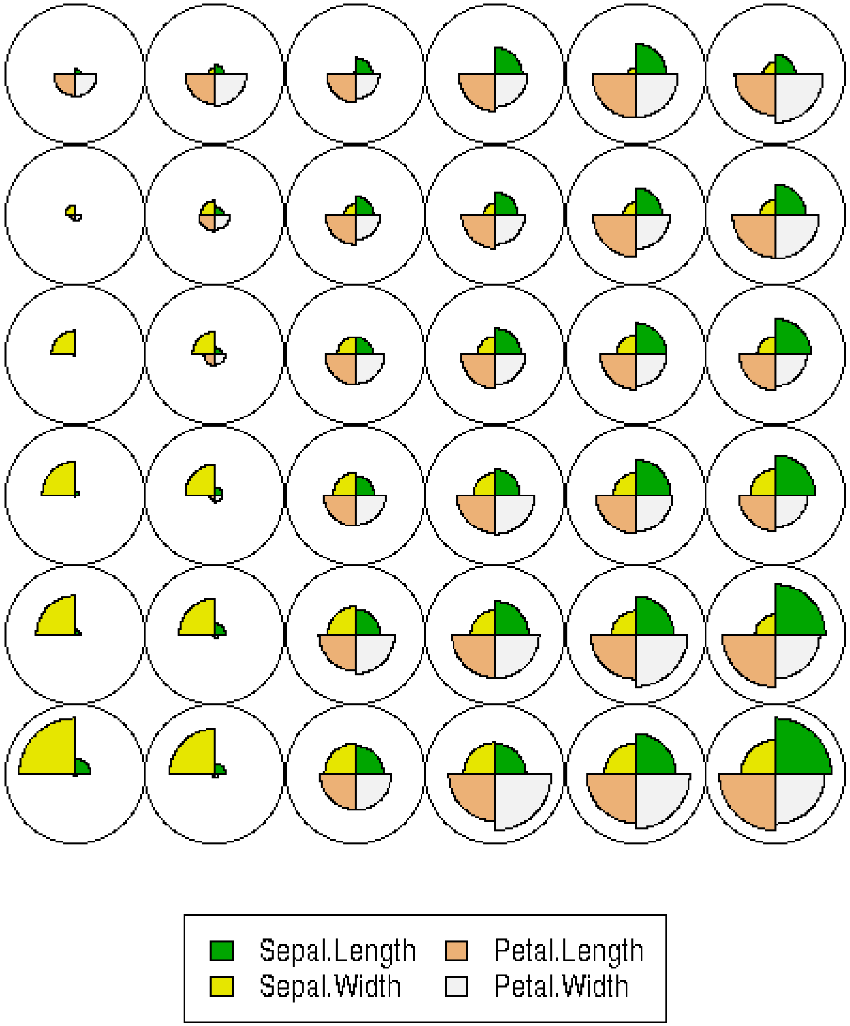
Self-Organising Maps can be considered a modification of the K-means algorithm including **topological constrains**

```r
library(kohonen)
? som ## Clustering function.
? somgrid ## Definition of the topology.
som<-som(as.matrix(scale(iris[,-5])),
  somgrid(xdim=6,ydim=6,topo="rectangular"))
## Should be used to visualize the data:
plot(som)
## Considering 3 classes
somR<-som(as.matrix(scale(iris[,-5])),
  somgrid(xdim=1,ydim=3,topo="rectangular"))
somH<-som(as.matrix(scale(iris[,-5])),
  somgrid(xdim=3,ydim=1,topo="hexagonal"))
plot(somR)
plot(somH)
## We obtain the classification:
confusionMatrix(as.numeric(iris[,5]),
  somH$unit.classif)
```



Self-Organising/Kohonen Maps can be considered a modification of the K-means algorithm including **topological constrains**

Self-Organising/Kohonen Maps is a type of ***artificial neural network (ANN)*** that is trained using unsupervised learning to produce a low-dimensional (typically two-dimensional), discretized representation of the input space of the training samples, called a map, and is therefore a method to do ***dimensionality reduction and/or visualization***.



Self-Organising Maps can be considered a modification of the K-means algorithm including **topological constrains**

Self-Organising/Kohonen Maps is a type of ***artificial neural network (ANN)*** that is trained using unsupervised learning to produce a low-dimensional (typically two-dimensional), discretized representation of the input space of the training samples, called a map, and is therefore a method to do ***dimensionality reduction and/or visualization***.

Self-Organising/Kohonen Maps differ from other artificial neural networks as they apply ***competitive learning*** as opposed to error-correction learning (such as backpropagation with gradient descent), and in the sense that they use a neighborhood function to preserve the topological properties of the input space.

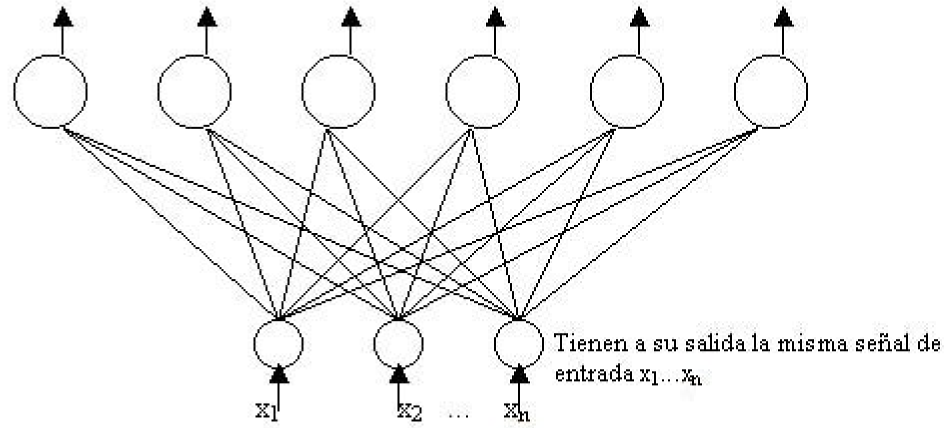


Figura 7: Arquitectura de Red Autoorganizada

1. Initialize weights to some small, random values
2. Repeat until convergence
   - 2a. Select the next input pattern $x^{(n}$ from the database
     - 2a1. Find the unit w_i that best matches the input pattern $x^{(n}$

$$i(x^{(n}) = \underset{j}{\operatorname{argmin}} \left\| x^{(n} - w_j \right\|$$

     - 2a2. Update the weights of the winner w_i and all its neighbors w_k

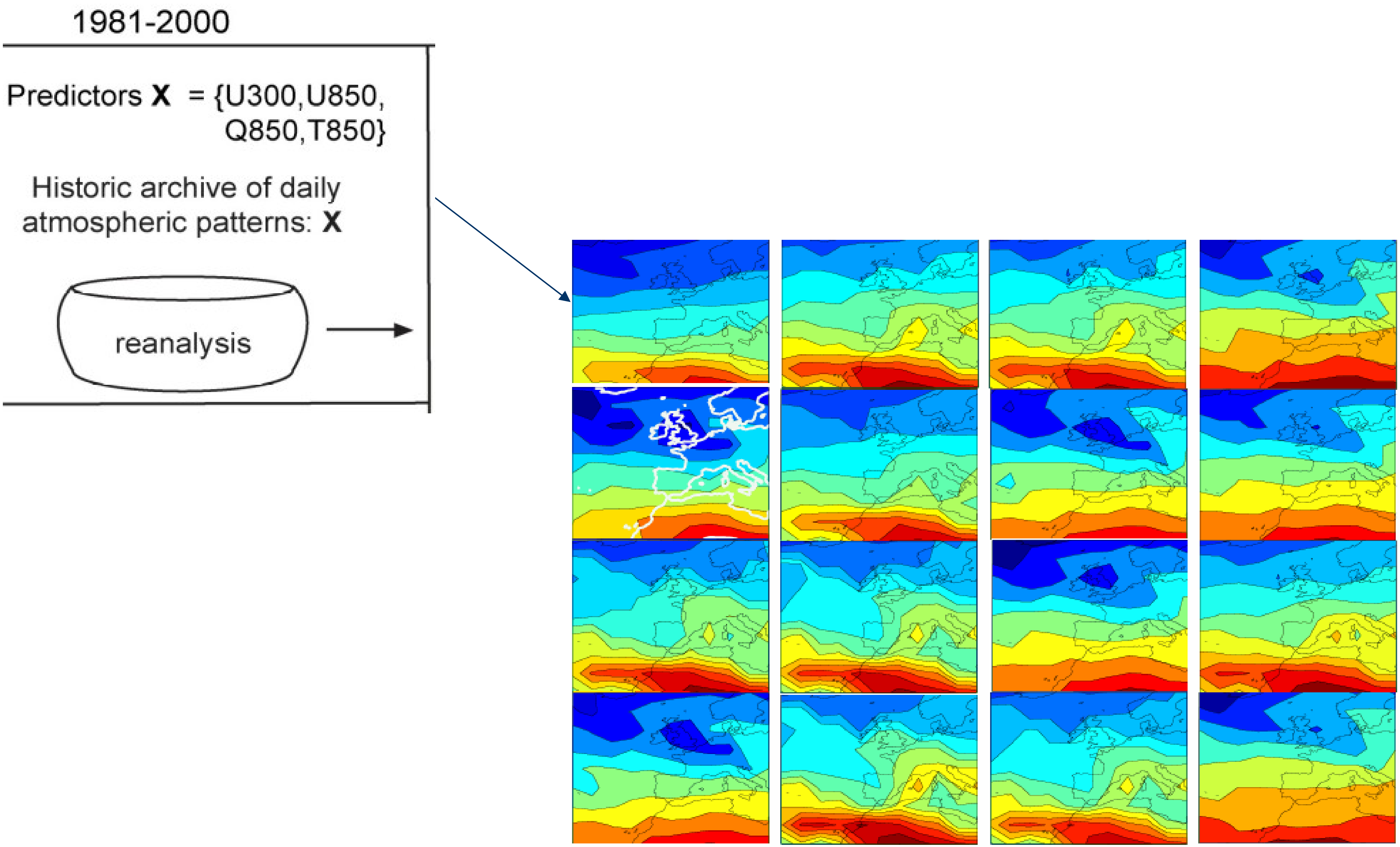
$$w_k = w_k + \eta(t) \cdot h_{ik}(t) \cdot (x^{(n} - w_k)$$

   - 2b. Decrease the learning rate $\eta(t)$
   - 2c. Decrease neighborhood size $\sigma(t)$

https://towardsdatascience.com/self-organizing-maps-1b7d2a84e065

http://avellano.usal.es/~lalonso/RNA/introSOM.htm

Self-Organising Maps can be considered a modification of the K-means algorithm including **topological constrains**



Problemas habituales

- Descripción y visualización
- Asociación
- **Segmentación**
- Clasificación
- Predicción

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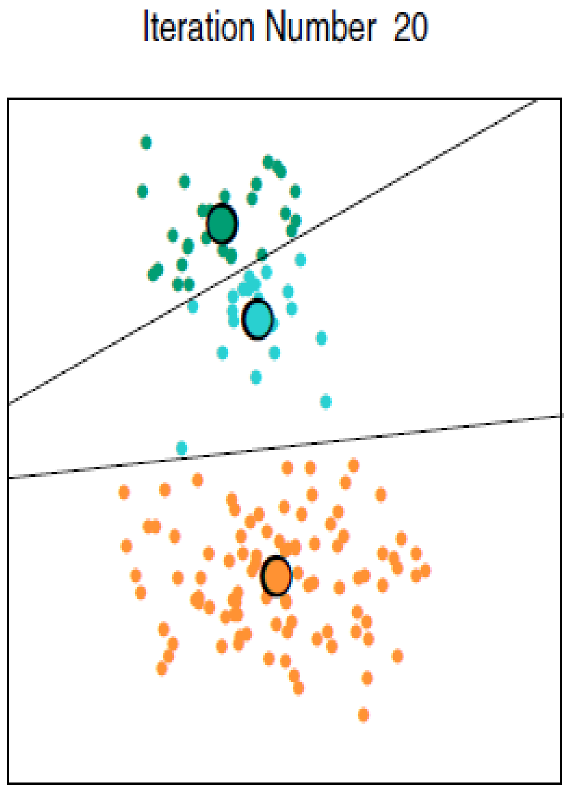
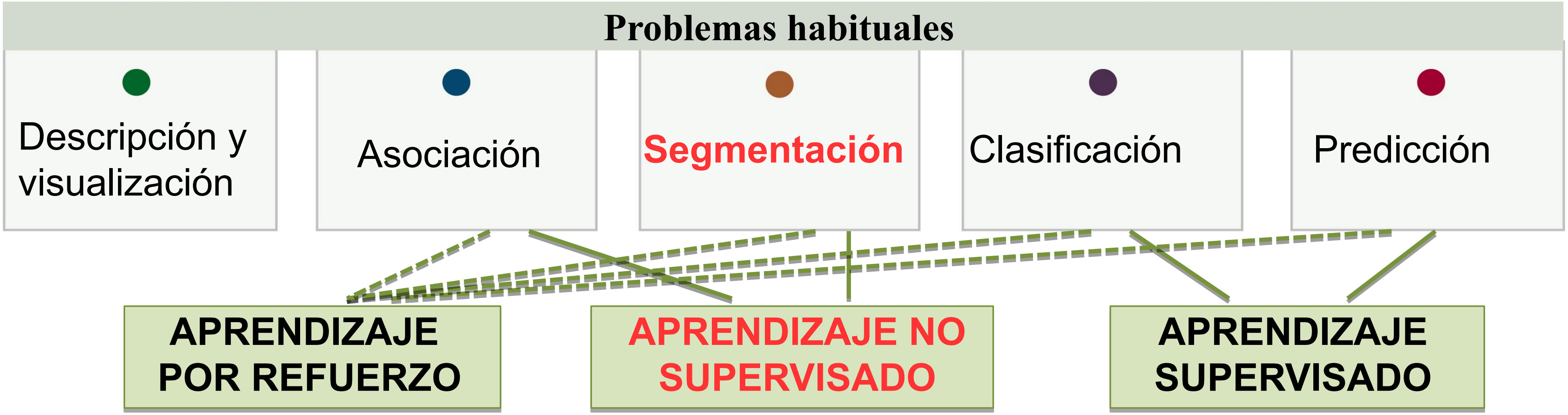
Distribution-based clustering

Centroid-based clustering: Non-overlapping (e.g. K-Means)




```
library(stats)
? kmeans
kmModel<-kmeans(iris[,-5],3,nstart=1)
summary(kmModel)
## Point center of two attributes
plot(iris[,c(1,3)],col=kmModel$cluster,main="K-Means")
points(kmModel$centers[,c(1,3)],col=1:3,pch=8,cex=2)
## How much clusters should we use?
totWithinss<-c(1:15)
for(i in 1:15){
  kmModel<-kmeans(iris[,-5],centers=i,nstart=1)
  totWithinss[i]<-kmModel$tot.withinss
}
plot(x=1:15,y=totWithinss,type="b",
  xlab="N. Of Cluster",ylab="Within groups sum of squares")
```



Distribution-based clustering
Centroid-based clustering: Non-overlapping (e.g. K-Means)
Centroid-based clustering: Fuzzy clustering (e.g. C-Means)

```
library(e1071)
? cmeans
cmModel<-cmeans(iris[,-5],3,iter.max=1,m=2,method="cmeans")
summary(cmModel)
## Point center of two attributes
plot(iris[,c(1,3)],col=cmModel$cluster,main="K-Means")
points(cmModel$centers[,c(1,3)],col=1:3,pch=8,cex=2)
confusionMatrix(as.numeric(iris[,5]),cmModel$cluster)
```

Centroid

$$c_k = \frac{\sum_x w_k(x)^m x}{\sum_x w_k(x)^m}.$$

Weights

$$\arg\min_C \sum_{i=1}^{n} \sum_{j=1}^{c} w_{ij}^m \left\|\mathbf{x}_i - \mathbf{c}_j\right\|^2,$$

$$w_{ij} = \frac{1}{\sum_{k=1}^{c} \left(\frac{\|\mathbf{x}_i - \mathbf{c}_j\|}{\|\mathbf{x}_i - \mathbf{c}_k\|}\right)^{\frac{2}{m-1}}}.$$

Problemas habituales

- Descripción y visualización
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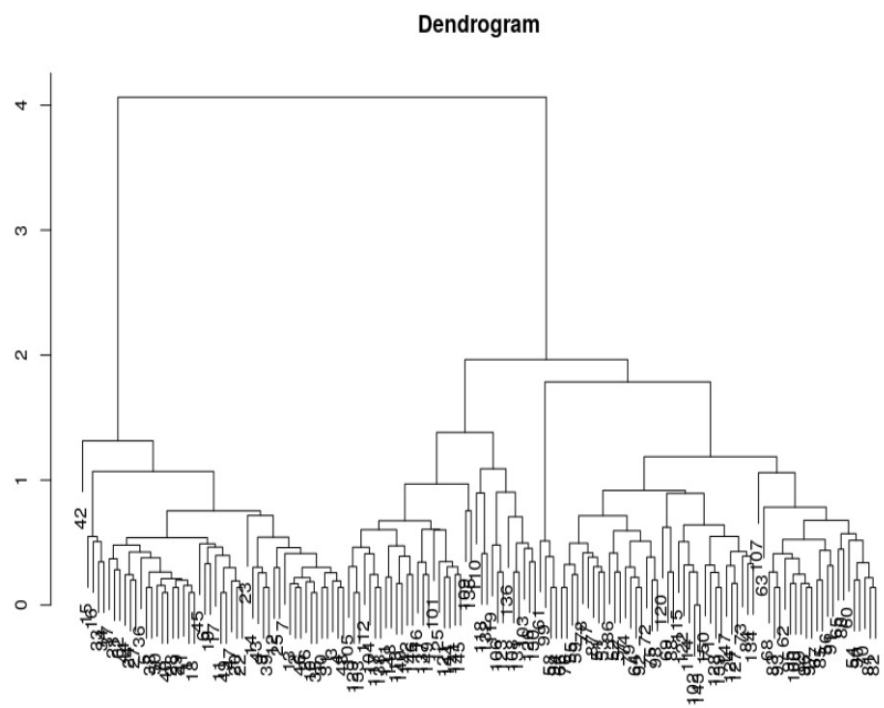
Distribution-based clustering
Centroid-based clustering: Non-overlapping (e.g. K-Means)
Centroid-based clustering: Fuzzy clustering (e.g. C-Means)
Hierarchical clustering

```
library(stats)
require(sparcl)## Include colours for the leaves.
? hclust
d<-dist(iris[,-5],method="euclidean")
hcModel<-hclust(d,method="average")
summary(hcModel)
plot(hcModel,main="Dendrogram")
```



Problemas habituales

- Descripción y visualización
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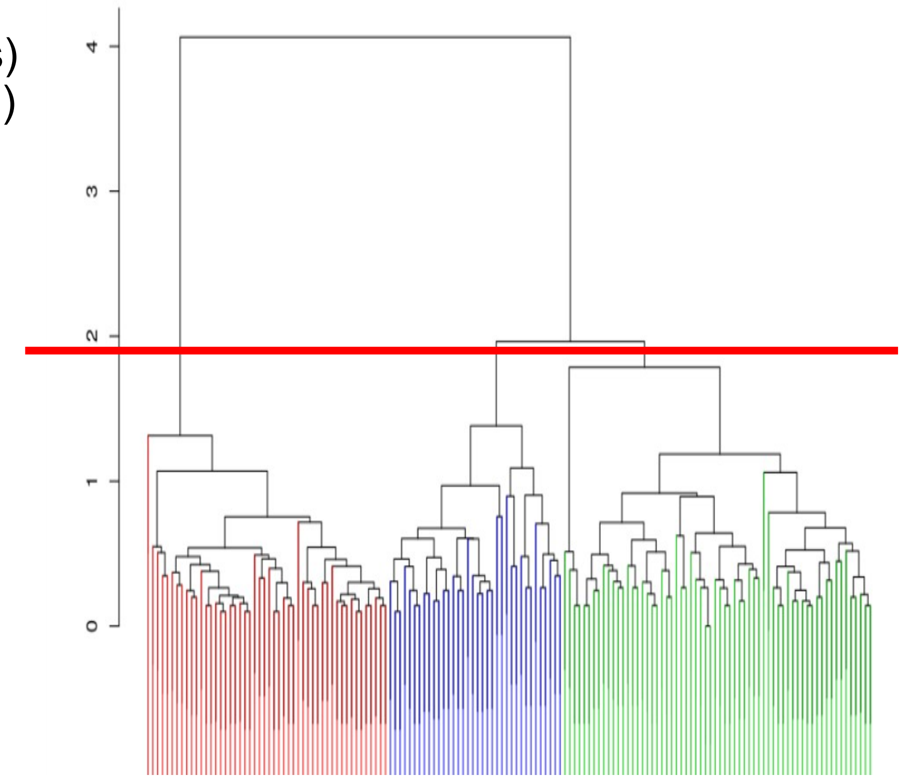
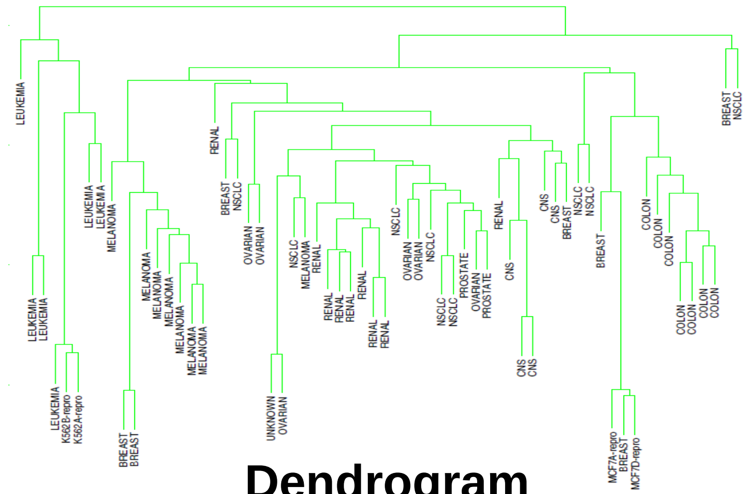
Distribution-based clustering
Centroid-based clustering: Non-overlapping (e.g. K-Means)
Centroid-based clustering: Fuzzy clustering (e.g. C-Means)
Hierarchical clustering

```
library(stats)
require(sparcl)## Include colours for the leaves.
? hclust
d<-dist(iris[,-5],method="euclidean")
hcModel<-hclust(d,method="average")
summary(hcModel)
plot(hcModel,main="Dendrogram")
## To obtain a classification, we should cut the
tree
hc3<-cutree(hcModel,3)## 3 classes
ColorDendrogram(hcModel,y=hc3,branchlength=10)
confusionMatrix(as.numeric(iris[,5]),hc3)
```



Hierarchical clustering is based on the similarity between members of the different groups/clusters to build the **dendrogram**. There are two approaches:

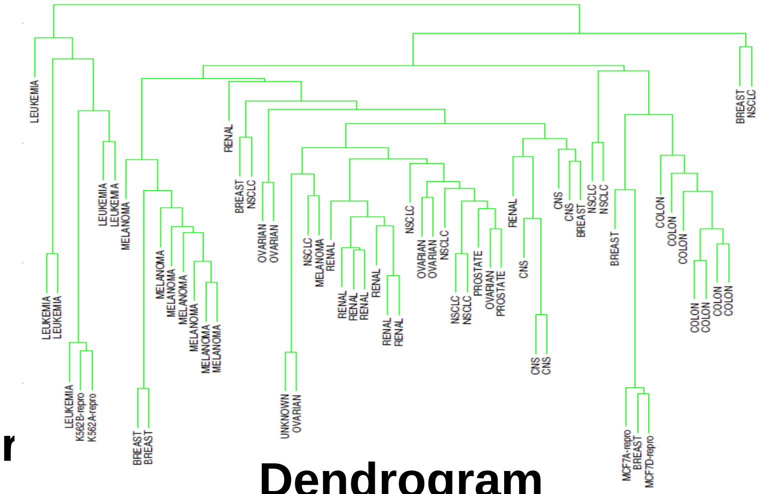
- **Agglomerative:** bottom up approach.
- **Divisive:** top down approach.



Dendrogram

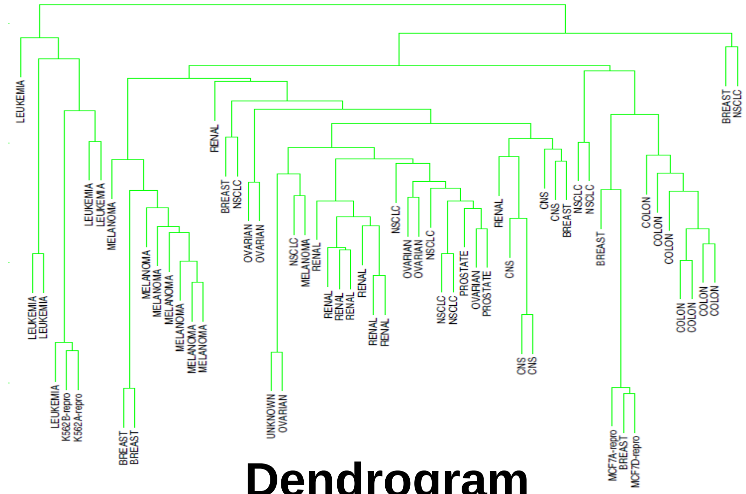
Hierarchical clustering is based on the similarity between members of the different groups/clusters to build the **dendrogram**. There are two approaches:

- **Agglomerative:** bottom up approach.
- **Divisive**: top down approach.
  - Iteratively apply the K-means algorithm with **K=2**.
  - At each stage, the cluster with the **largest diameter** is selected, where the diameter of a cluster is the **largest dissimilarity** between any two of its observations (Macnaughton Smith et al. (1965), Kaufman and Rousseeuw (1990)).



Dendrogram

```r
library(cluster)
? diana ## Divisive clustering algorithm.
d<-dist(iris[,-5],method="euclidean")
diModel<-diana(d,diss=TRUE,metric="euclidean")
plot(diModel)
di3<-cutree(diModel,3)## 3 classes
confusionMatrix(as.numeric(iris[,5]),di3)
confusionMatrix(as.numeric(iris[,5]),hc3)
```



Dendrogram

Hierarchical clustering is based on the similarity between members of the different groups/clusters to build the **dendrogram**. There are two approaches:

- **Agglomerative:** bottom up approach.
- **Divisive:** top down approach.

Linkage criterion determines the distance between the clusters and the agglomeration method:

- **Complete-linkage:** maximum of the distances.
- **Single-linkage:** minimum of the distances.
- **Average-linkage (UPGMA):** mean of the distances.
- **Centroid-linkage (UPGMC):** distances between centroids.
- ...

```r
d<-dist(iris[,-5],method="euclidean")
## Available linkage criterion: "ward.D","ward.D2","single","complete","average",
## "mcquitty","median" or "centroid".
par(mfrow=c(2,2))
plot(hclust(d,method="complete"),main="Complete-Linkage",col="blue",axes=FALSE)
plot(hclust(d,method="single"),main="Single-Linkage",col="red",axes=FALSE)
plot(hclust(d,method="average"),main="Average-Linkage",col="green",axes=FALSE)
plot(hclust(d,method="centroid"),main="Centroid-Linkage",col="black",axes=FALSE)
```

Problemas habituales

- Descripción y visualización
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- **Segmentación**
- Clasificación
- Predicción

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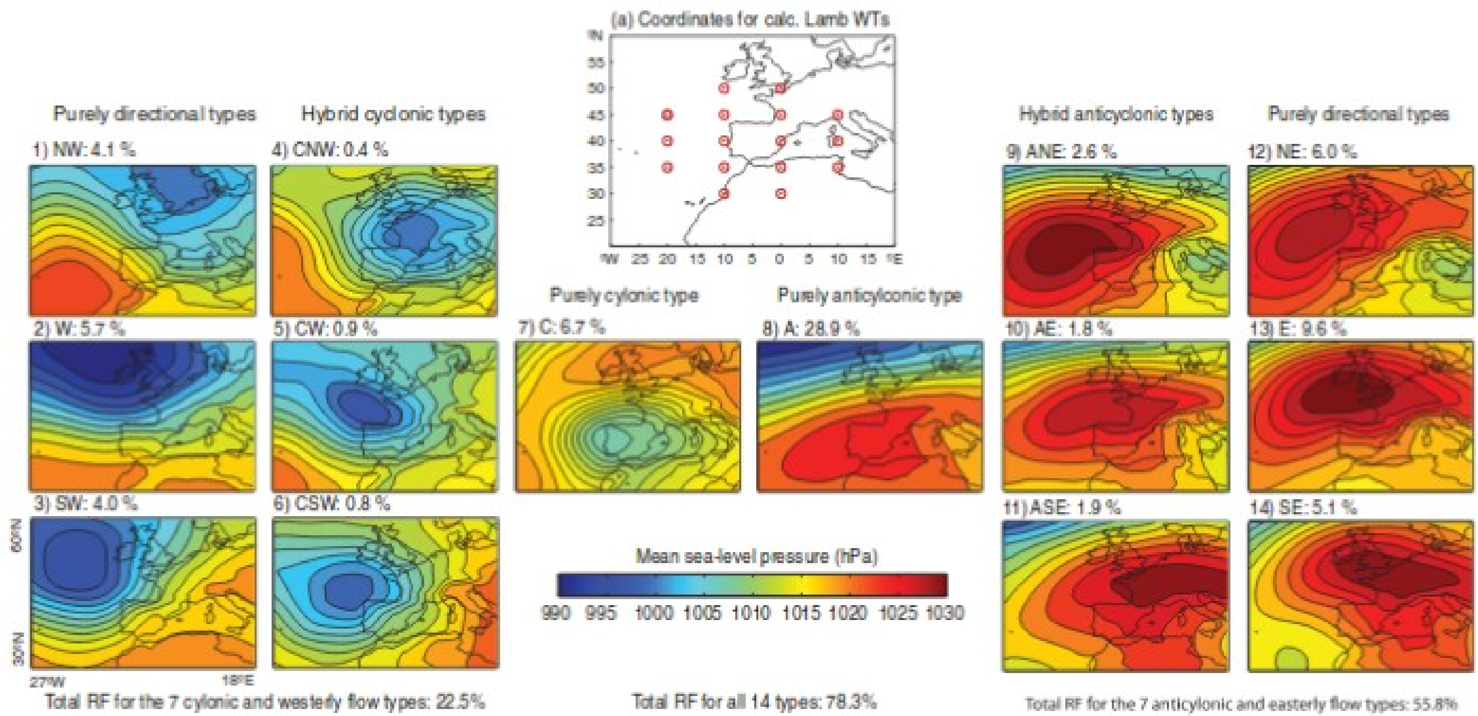
Expert Approach:
Lamb Weather Types



Source: Brands et al. 2014, http://meteo.unican.es/en/node/73157