Unsupervised learning

Clustering and Dimensionality Reduction

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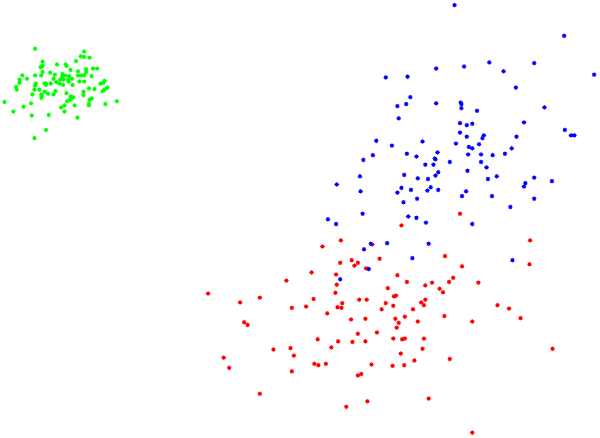
- Mètodes
  - Supervised
    - classificació
    - regressió
  - Unsupervised
    - agrupant (clustering)
    - reducció de dimensions

Clustering

Partition input examples into *similar* subsets

Clustering

Partition input examples into *similar* subsets



Clustering

Main challenges

- How to measure similarity?
- How many clusters?
- How do we evaluate the clusters?

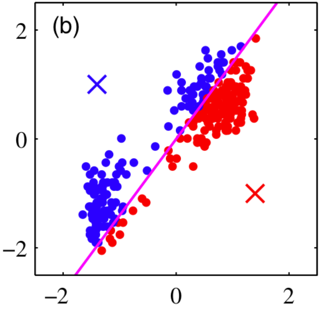
Algorithms we will cover

- K-means
- Hierarchical clustering

K-means clustering

Intuition

- Input data are:
  - m examples $\mathrm{x}^1, .., \mathrm{x}^m$, and
  - K, the number of desired clusters
- Clusters represented by cluster centers $\mu_1, .., \mu_K$
- Given centers $\mu_1, .., \mu_K$, each center defines a cluster: the subset of inputs x^i that are closer to it than to other centers



K-means clustering

Intuition

The aim is to find

- cluster centers $\mu_1, .., \mu_K$ and
- a cluster assignment $\mathbf{z} = (z^1, .., z^m)$ where $z^i \in \{1, .., K\}$
  - z^i is the cluster assigned to example $\mathbf{x}^i$

such that $\mu_1, .., \mu_K, \mathbf{z}$ *minimize* the cost function

$$J(\mu_1, .., \mu_K, \mathbf{z}) = \sum_i \|\mathbf{x}^i - \mu_{z^i}\|^2.$$

K-means clustering

Cost function

$$J(\mu_1, .., \mu_K, \mathbf{z}) = \sum_i \|\mathbf{x}^i - \mu_{z^i}\|^2$$

Pseudocode

- Pick initial centers $\mu_1, .., \mu_K$ at random
- Repeat until convergence
  - Optimize $\mathbf{z}$ in $J(\mu_1, .., \mu_K, \mathbf{z})$ keeping $\mu_1, .., \mu_K$ fixed
    - Set z^i to closest center: $z^i = \arg\min_k \|\mathbf{x}^i - \mu_k\|^2$
  - Optimize $\mu_1, .., \mu_K$ in $J(\mu_1, .., \mu_K, \mathbf{z})$ keeping $\mathbf{z}$ fixed
    - For each $k = 1, .., K$, set $\mu_k = \frac{1}{|\{i|z^i = k\}|} \sum_{i:z^i=k} \mathbf{x}^i$

una sola columna

dificultat per minimitzar
- NP-hard = 1D
- Polinòmic > 1D

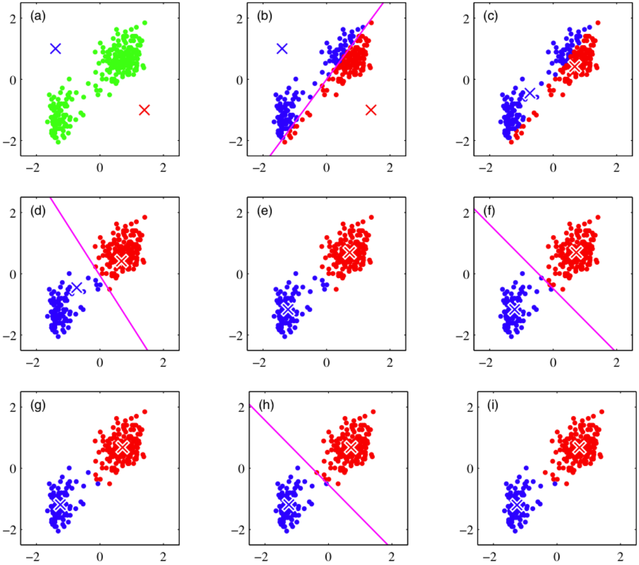
3 grups

x_1 x_2 ... x_n	z

K-Means illustrated

Esperança (expectation) : a, c, e, g, i

Maxim (maximization) : b, d, f, h



Limitations of k-Means

K-Means works well if..

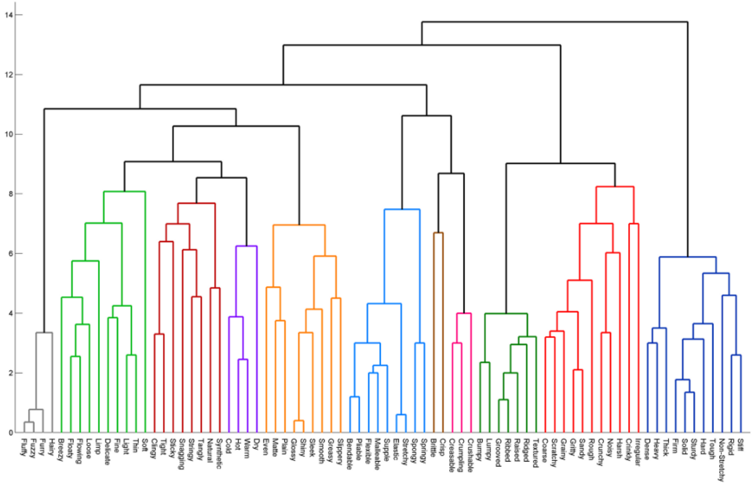
- Clusters are spherical
- Clusters are well separated
- Clusters are of similar volumes
- Clusters have similar number of points

.. so improve it with more general model

- Mixture of Gaussians:
- Learn it using *Expectation Maximization*

Hierarchical clustering

Output is a *dendogram*



Agglomerative hierarchical clustering

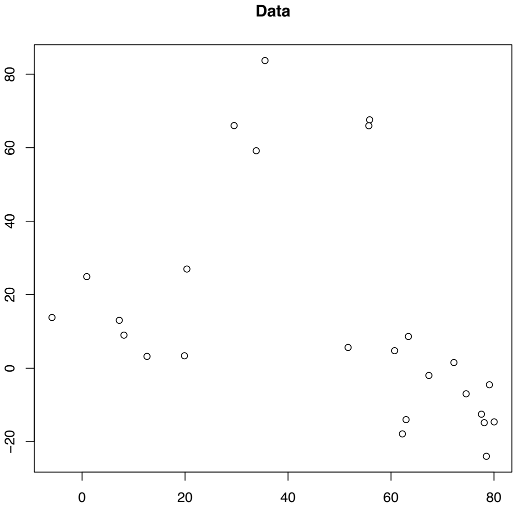
Bottom-up

Pseudocode

1. Start with one cluster per example
2. Repeat until all examples in one cluster
   - merge two closest clusters

(Next example from D. Blei's course at Princeton)

Example



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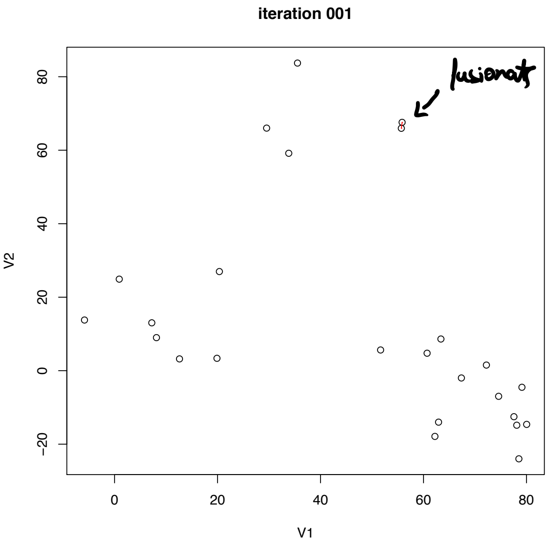
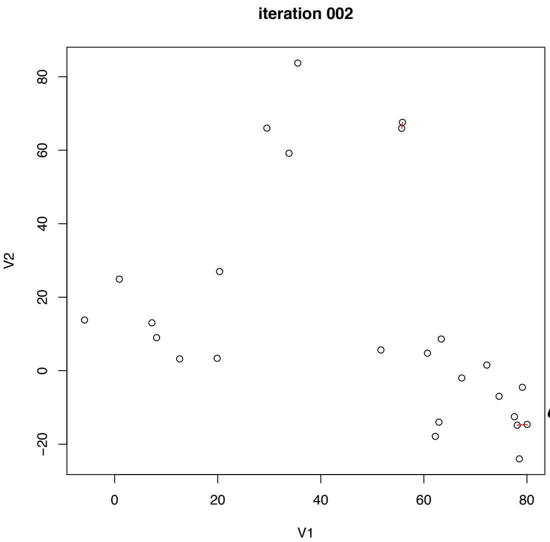
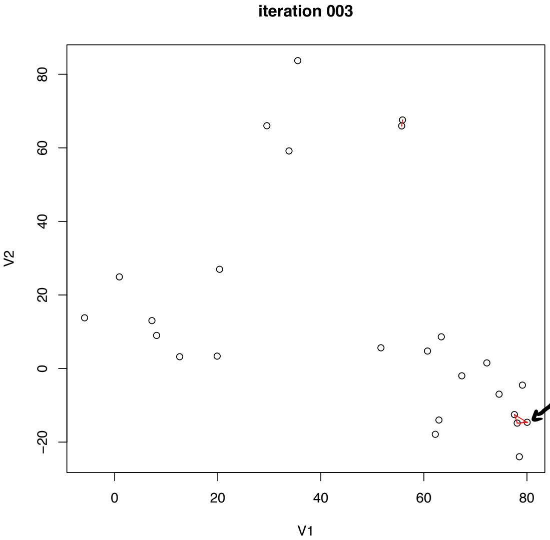


Example



fusionats

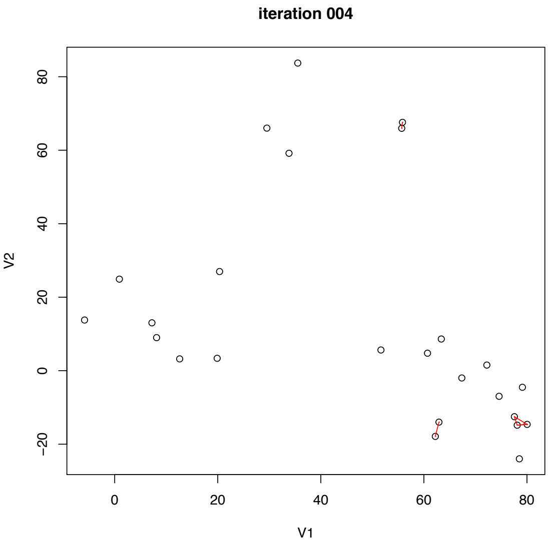
Example



fusionats

Example

I seguim amb el procés...



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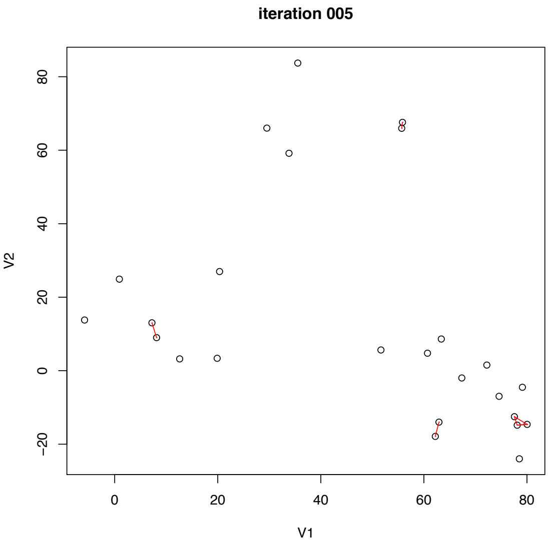
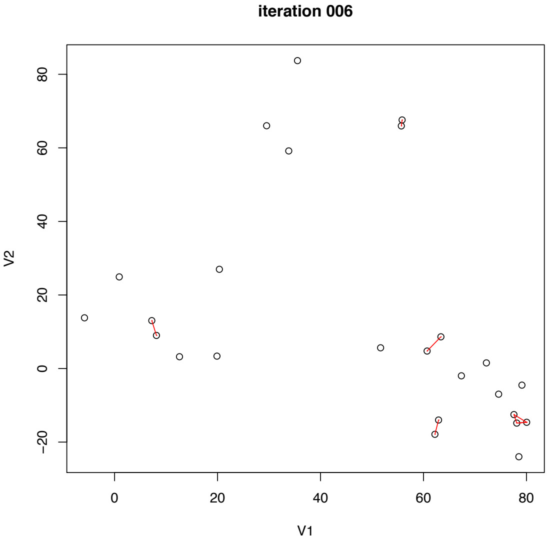
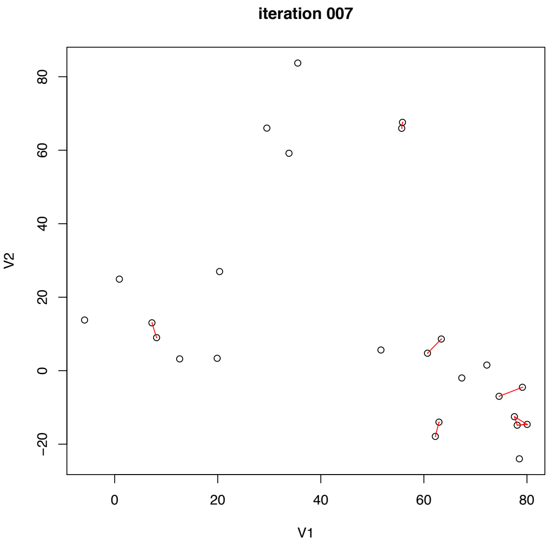


Example



Example



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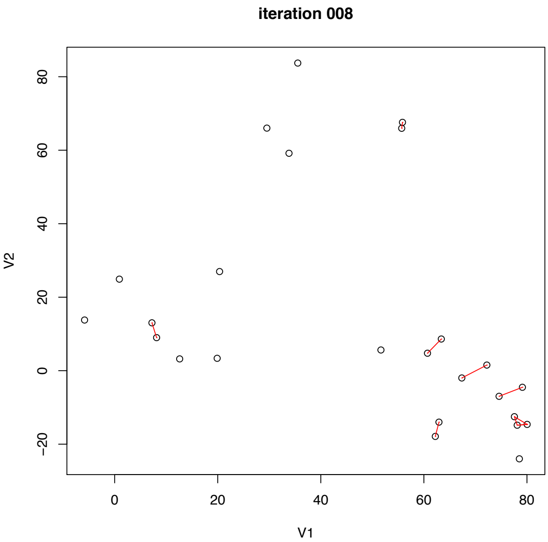

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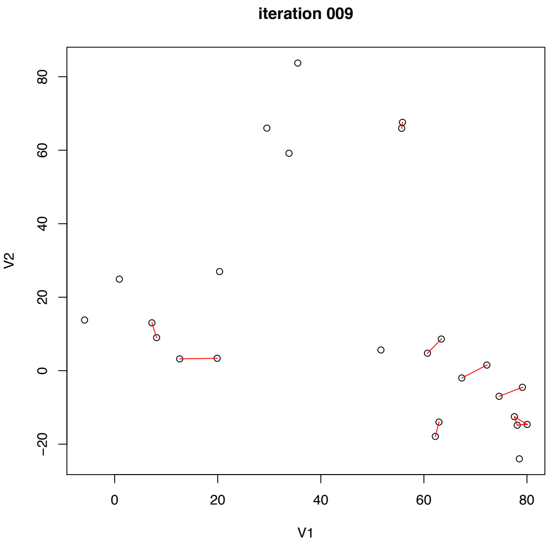

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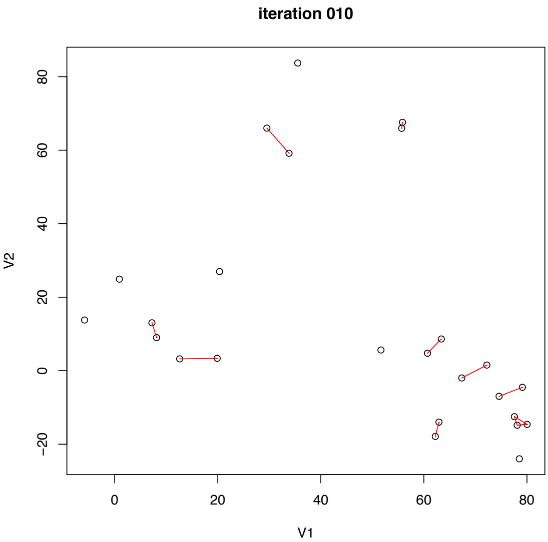

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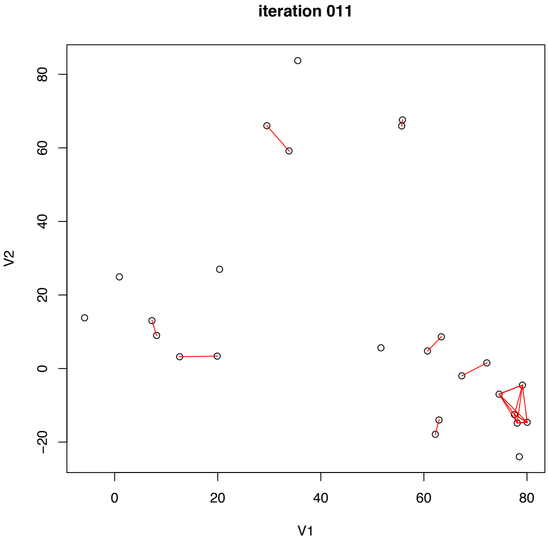

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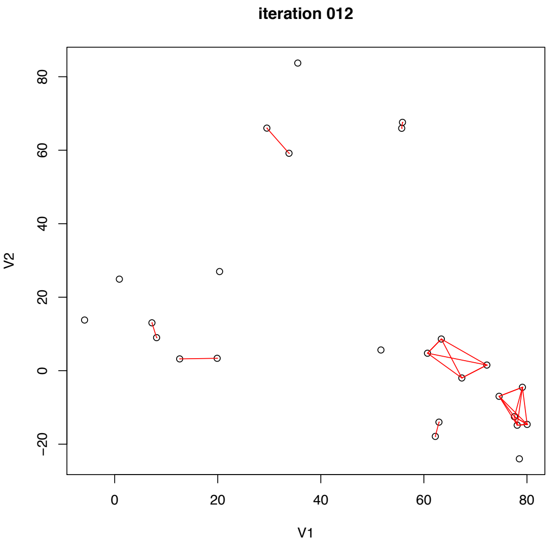

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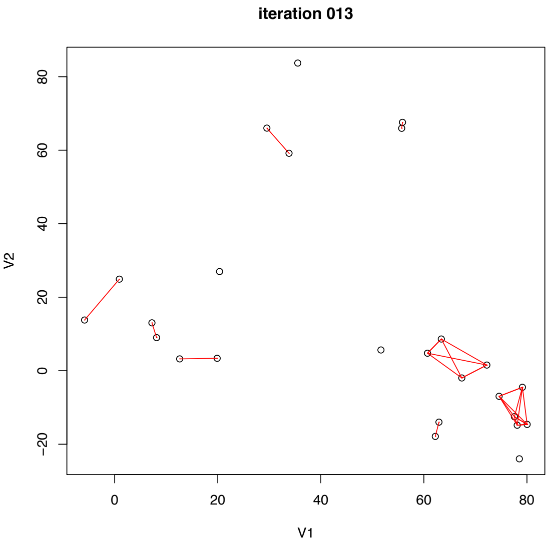

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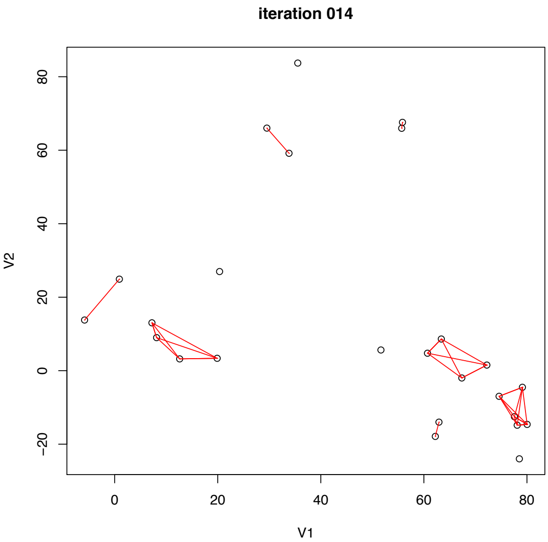

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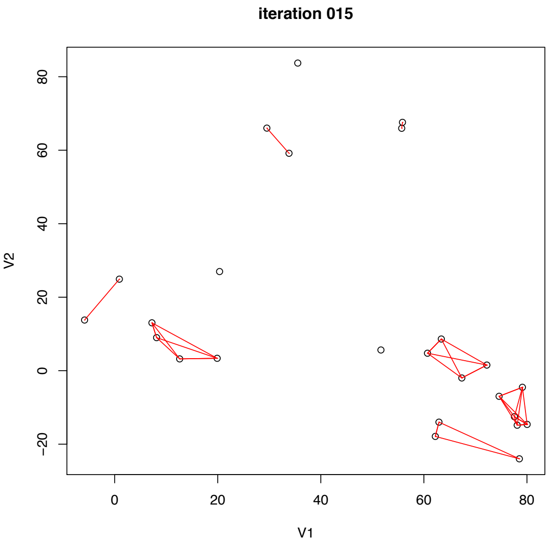

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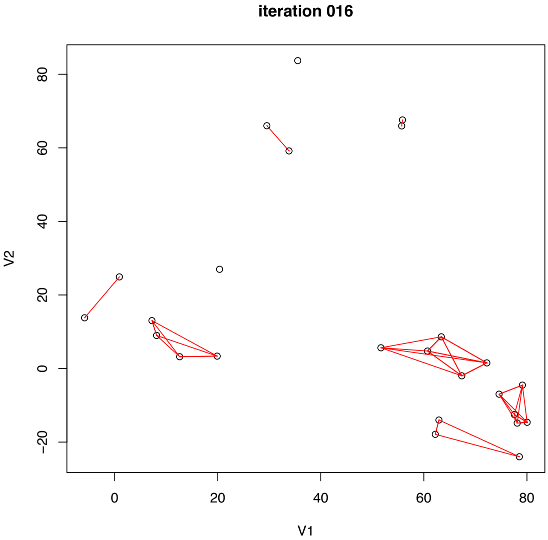

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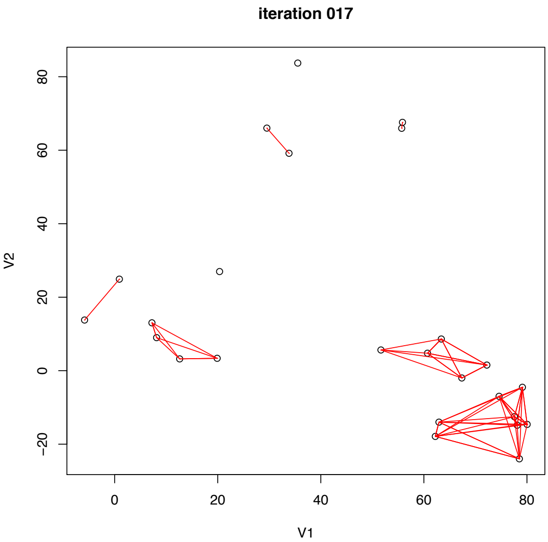

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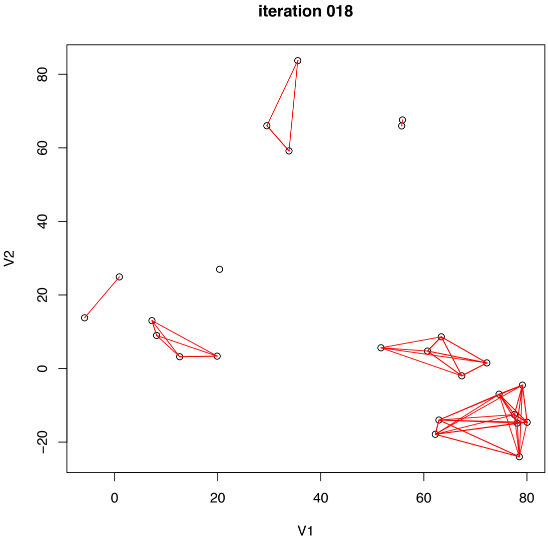

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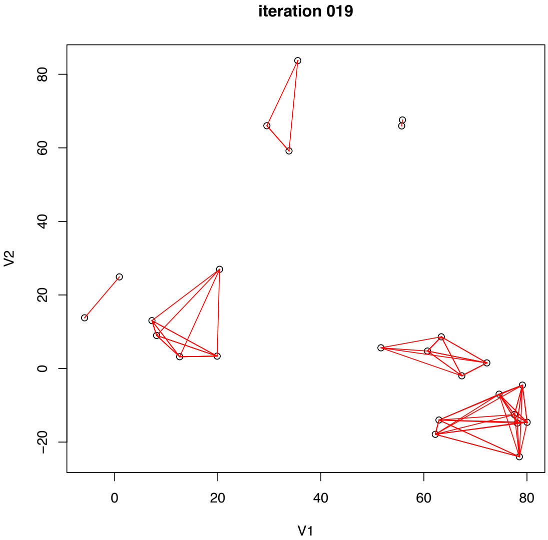

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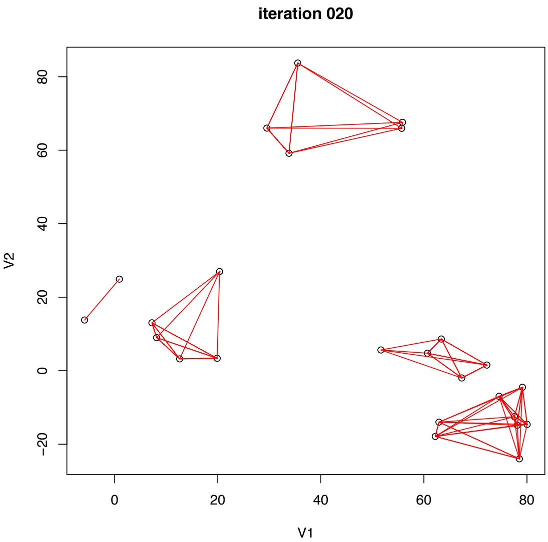

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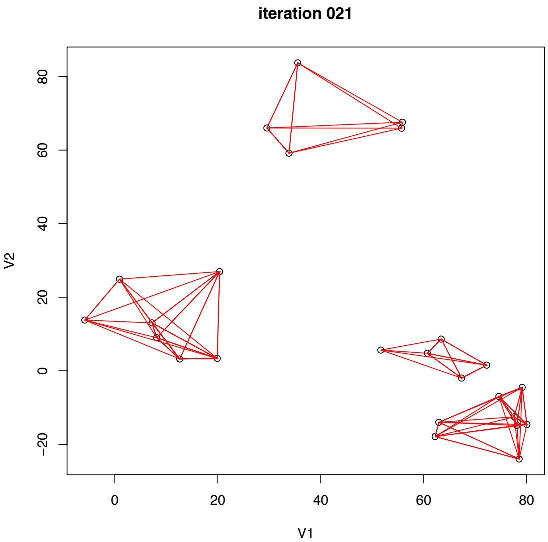

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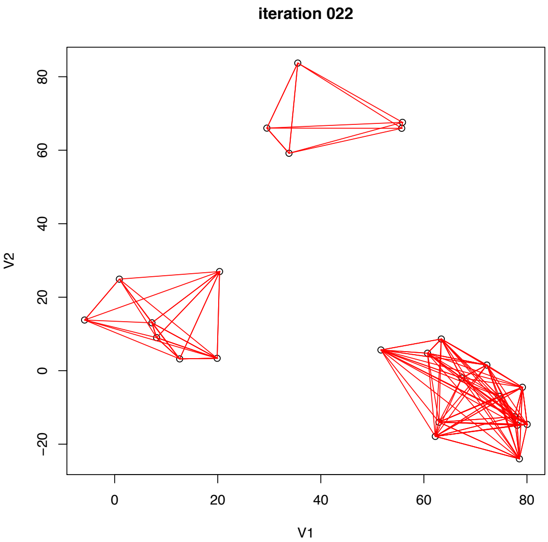
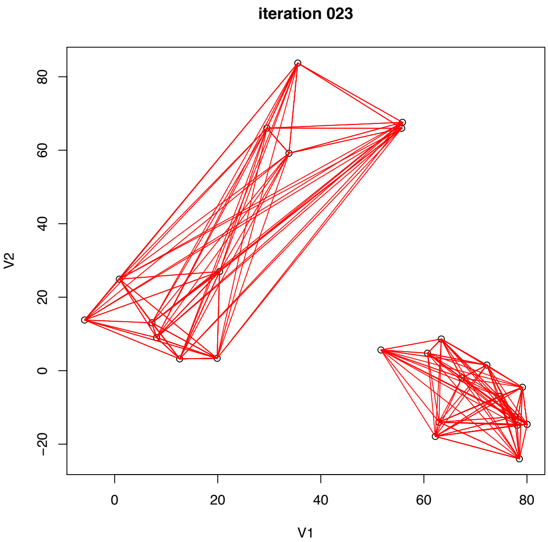
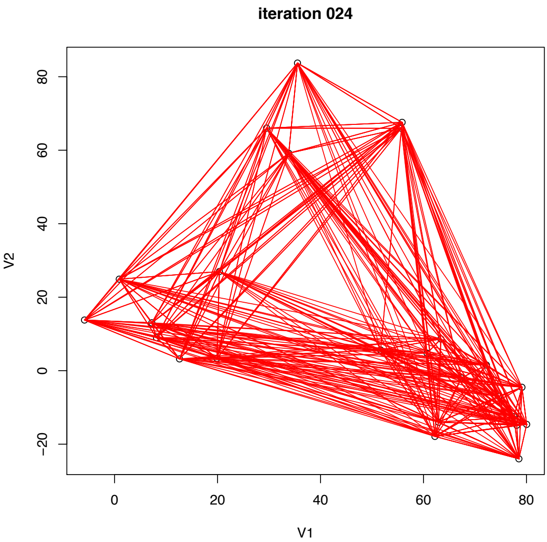


Example



Example



Agglomerative hierarchical clustering

Bottom-up

Pseudocode

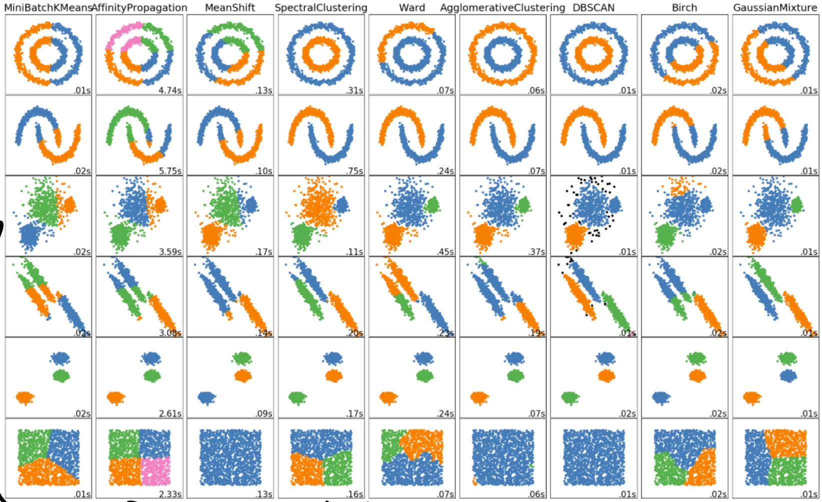
1. Start with one cluster per example
2. Repeat until all examples in one cluster
   - merge two closest clusters

Defining distance between clusters (i.e. *sets* of points)

- Single Linkage: $d(X, Y) = \min_{x \in X, y \in Y} d(x, y)$
- Complete Linkage: $d(X, Y) = \max_{x \in X, y \in Y} d(x, y)$
- (Average Linkage)
  Group Average: $d(X, Y) = \frac{\sum_{x \in X, y \in Y} d(x, y)}{|X| \times |Y|}$ ← # de comparacions total
- Centroid Distance: $d(X, Y) = d\left(\frac{1}{|X|} \sum_{x \in X} x, \frac{1}{|Y|} \sum_{y \in Y} y\right)$

Many, many, many other algorithms available ..

busca formes esfèriques, per això surt malament



li costa perquè assumeix que hi havia fronteres ben delimitades

Clustering with *scikit-learn* I

K-means: an example with the Iris dataset

In [33]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt

from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs, load_iris

iris = load_iris()
kmeans = KMeans(n_clusters = 3)
kmeans.fit(iris.data)

kmeans.cluster_centers_
```

Out[33]:
```
array([[5.006     , 3.428     , 1.462     , 0.246     ],
       [5.9016129 , 2.7483871 , 4.39354839, 1.43387097],
       [6.85      , 3.07368421, 5.74210526, 2.07105263]])
```

In [34]:
```
kmeans.labels_
```

Out[34]:
```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 2, 2, 2, 2, 1, 2, 2, 2,
       2, 2, 2, 1, 1, 2, 2, 2, 2, 1, 2, 1, 2, 1, 2, 2, 1, 1, 2, 2, 2, 2,
       2, 1, 2, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2, 1], dtype=int32)
```

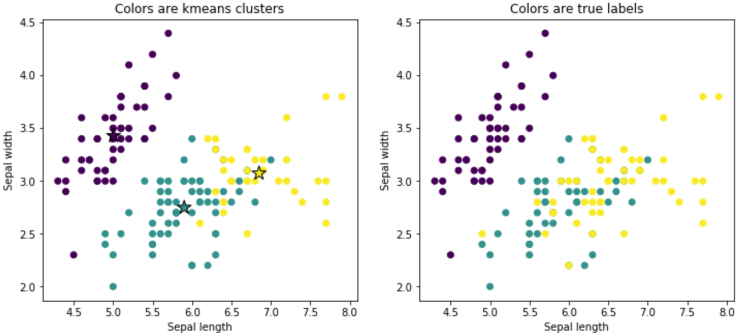
In [35]:
```
import pandas as pd
pd.crosstab(iris.target, kmeans.labels_)
```

Out[35]:

col_0	0	1	2
row_0			
0	50	0	0
1	0	48	2
2	0	14	36

Clustering with *scikit-learn* II

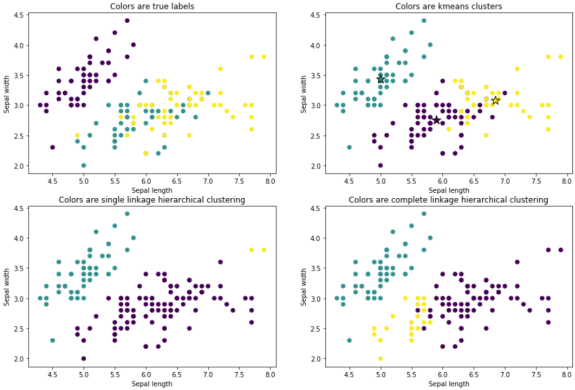
K-means: an example with the `Iris` dataset



Clustering with *scikit-learn* I

Hierarchical clustering: an example with the Iris dataset

```python
from sklearn.cluster import AgglomerativeClustering
clustering1 = AgglomerativeClustering(linkage='single', n_clusters=3)
clustering1.fit(iris.data)
clustering2 = AgglomerativeClustering(linkage='complete', n_clusters=3)
clustering2.fit(iris.data)
```



Dimensionality reduction I

The curse of dimensionality

- When dimensionality increases, data becomes increasingly sparse in the space that it occupies
- Definitions of density and distance between points (critical for many tasks!) become less meaningful
- Visualization and qualitative analysis becomes impossible

Dimensionality reduction II

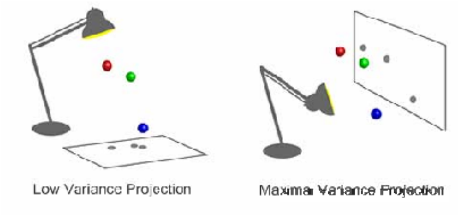
The curse of dimensionality

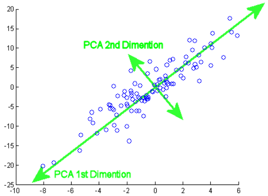
And so dimensionality reduction methods..

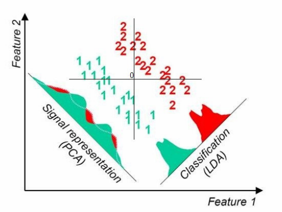
- avoid or at least mitigate the curse of dimensionality
- reduce time and memory required
- allow data to be more easily visualized
- may help eliminate irrelevant features
- may reduce noise

Principal Components Analysis (PCA)

Find linear projections of original coordinates that maximize variance





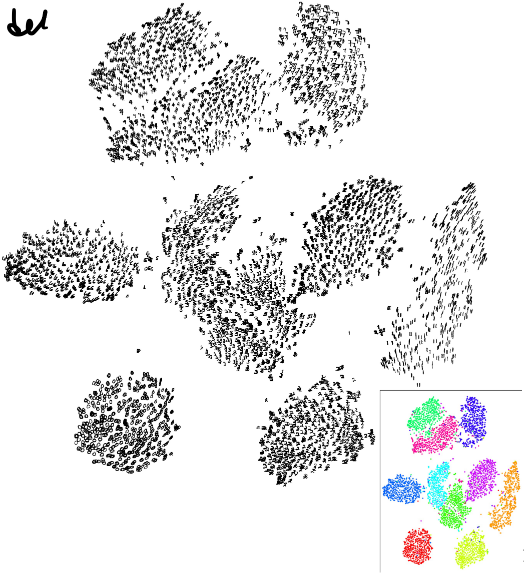


Crear grups d'atributs per a poder ajuntar dimensions properes.
Els atributs d'interès es calculen amb la Maxima Variance Projection.

t-SNE: t-distributed stochastic neighbor embedding (TSNE)

A non-linear distance-preserving method

Mètode potent del seu temps



[1]

[1] From https://lvdmaaten.github.io/tsne/

UMAP: Uniform Manifold Approximation Projection.

- Mètode de projecció de punts.
- L'espai Euclidi és un cas particular d'un espai més gran, Manifold.

Dimensionality reduction with *scikit-learn*

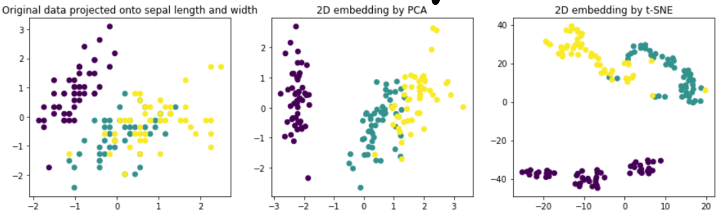
Standard Scaler: mètode per normalitzar $x \rightarrow x' = \frac{x-\mu}{\sigma}$

```python
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
from sklearn.preprocessing import StandardScaler

X_normalized = StandardScaler().fit_transform(iris.data)
X_pca = PCA(n_components=2).fit_transform(X_normalized)
X_tsne = TSNE(n_components=2, perplexity=10).fit_transform(X_normalized)

print(X_pca.shape, X_tsne.shape)
```

2D

defineix com fem les fronteres

```
(150, 2) (150, 2)
```



project data to reduce dimensions

So, we are done for this course

Lots of important things we have left out!

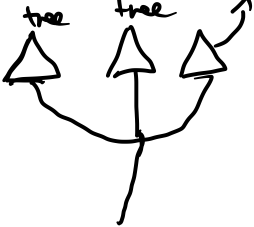
- Online and incremental learning; data mining for streams
- Important models: Support Vector Machines, Neural Nets (and Deep learning)
- Kernel methods and learning from structured objects
- Ensemble methods: random forests, boosting, bagging, etc.
- Spatial and temporal learning
- Feature selection methods
- many many more...

Online learning: fer prediccions a partir d'un mostreig.

Incremental learning: què passa quan venen més dades, has de tornar a entrenar des de 0?

Ensemble methods: aprenentatge amb conjunts de models

- Boosting: models s'encadenen
- Bagging: models en paral·lel (random forest)



Para finalizar

Reading assignment

Article by Pedro Domingos: "*A few useful things to know about machine learning*"

Examen: ver `https://www.cs.upc.edu/~csi/` y aviso correspondiente en Racó.

Será "tipo test". Consistirá en preguntas rápidas de tipo conceptual. No es necesaria calculadora. Sin apuntes. Si se necesita alguna fórmula ya se pondrá en el enunciado.