Unsupervised learning

Clustering and Dimensionality Reduction

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Clustering

Partition input examples into *similar* subsets

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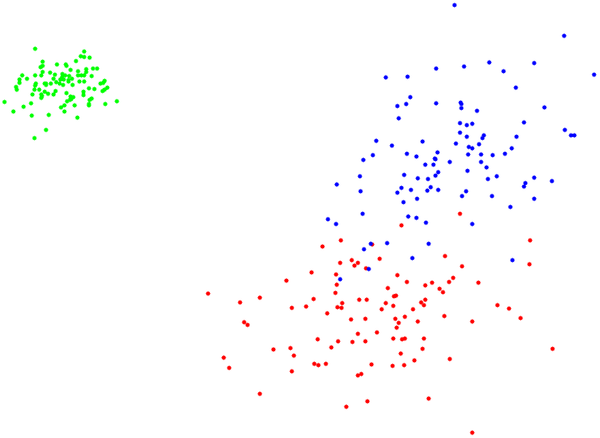


Clustering

Main challenges

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

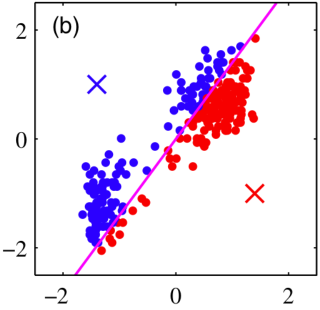
Algorithms we will cover

- K-means
- Hierarchical clustering

K-means clustering

Intuition

- Input data are:
  - m examples $x^1, .., x^m$, 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 x^i

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

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

K-means clustering

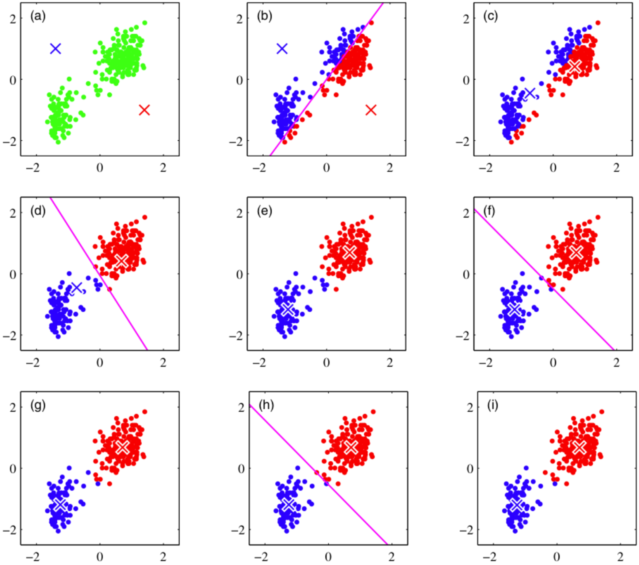
Cost function

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

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 $\mu_k = \frac{1}{|\{i|z^i = k\}|} \sum_{i:z^i=k} \mathbf{x}^i$

K-Means illustrated



Limitations of k-Means

K-Means works well if..

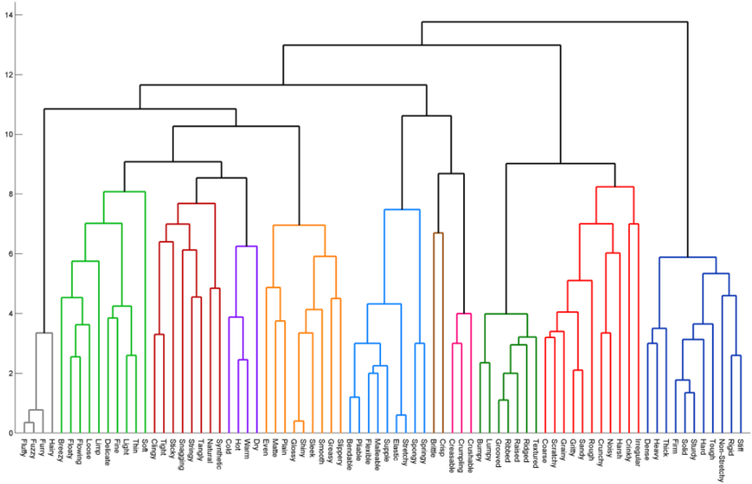
- Clusters are spherical
- Clusters are well separated
- Clusters are of similar volumes
- Clusters have similar number of points

.. so improve it with more general model

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

Hierarchical clustering

Output is a *dendogram*



Agglomerative hierarchical clustering

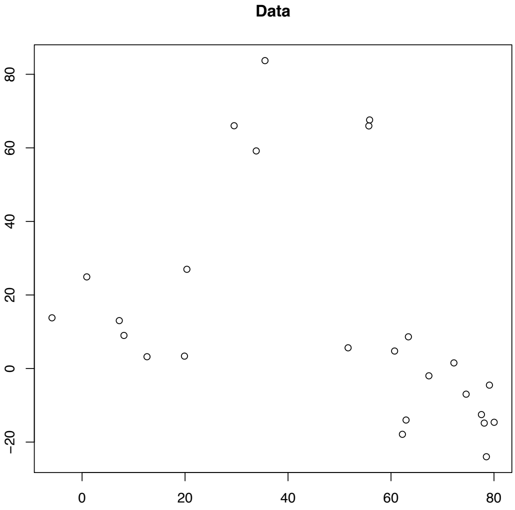
Bottom-up

Pseudocode

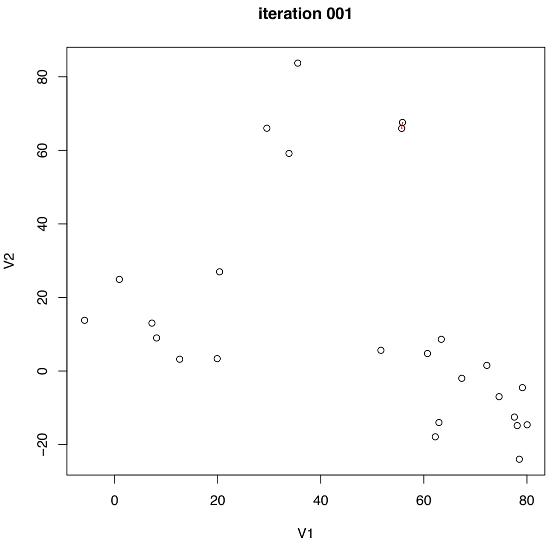
1. Start with one cluster per example
2. Repeat until all examples in one cluster
   - merge two closest clusters

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

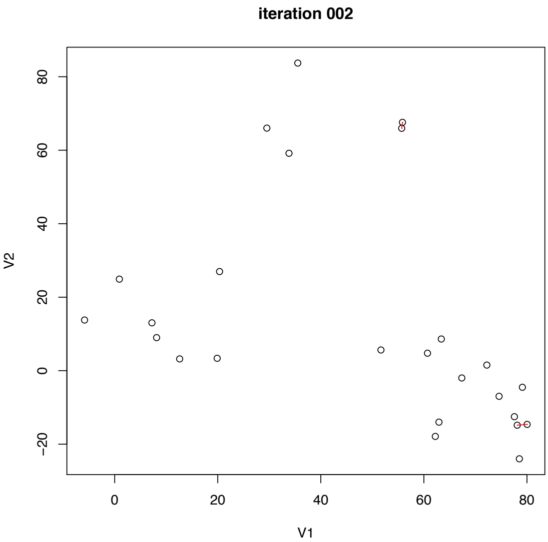
Example



Example



Example



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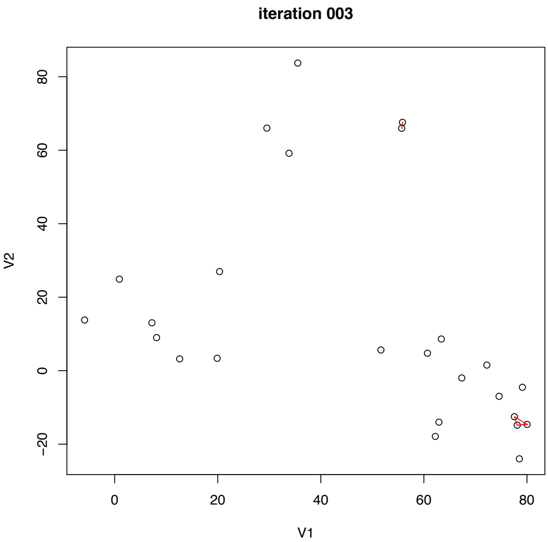

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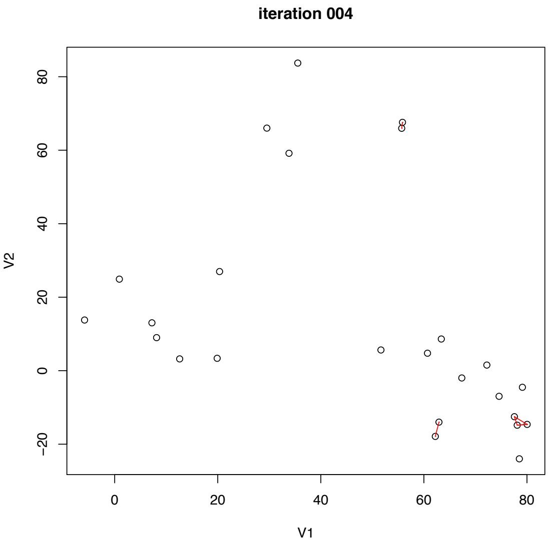
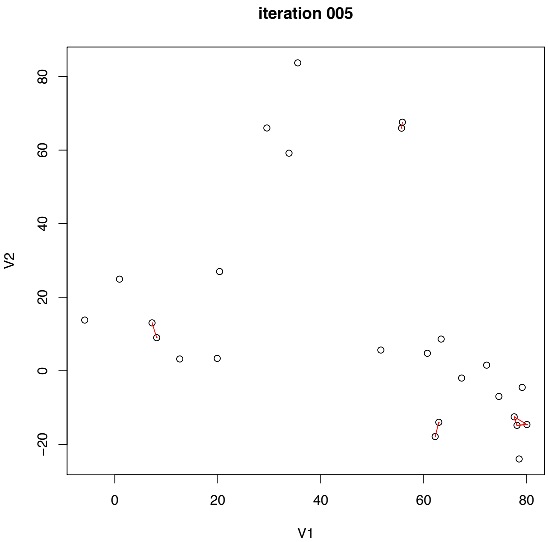
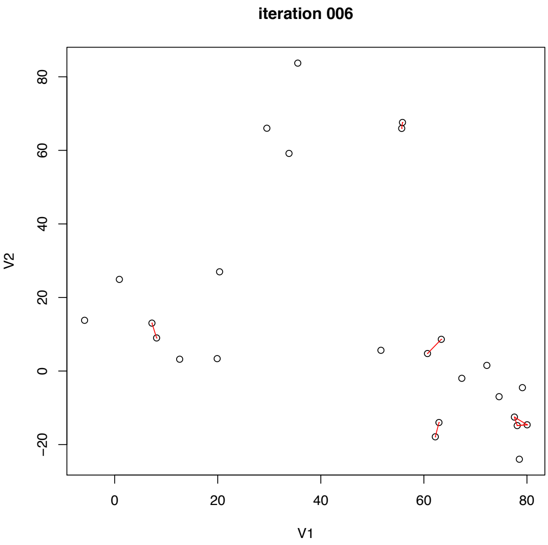


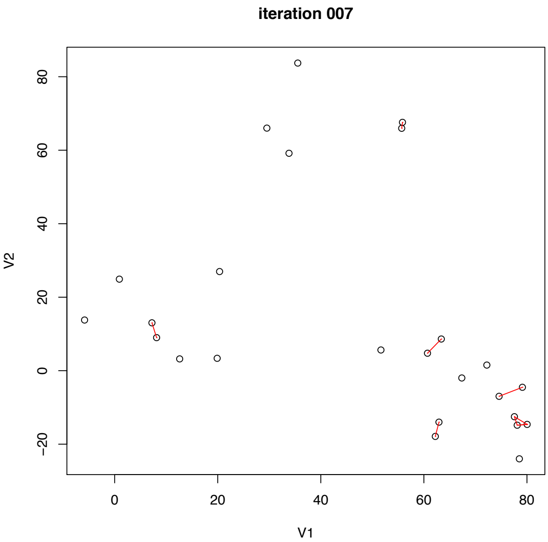
Example



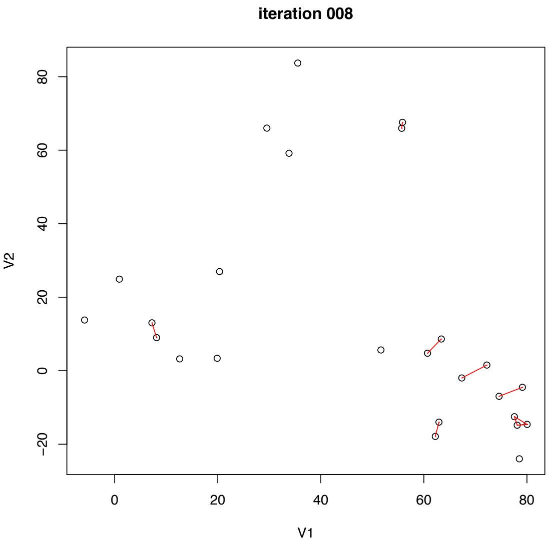
Example



Example



Example



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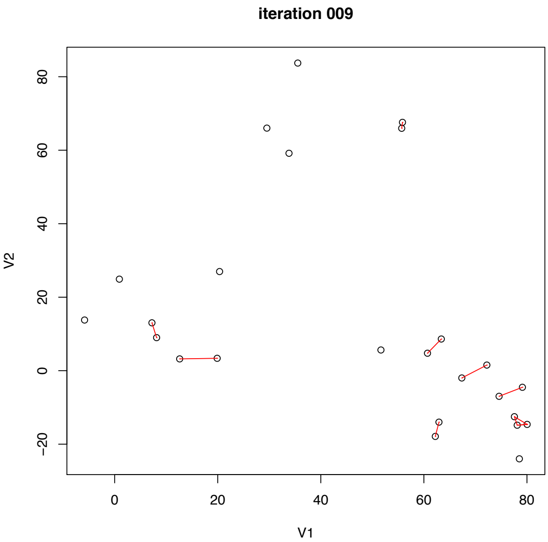
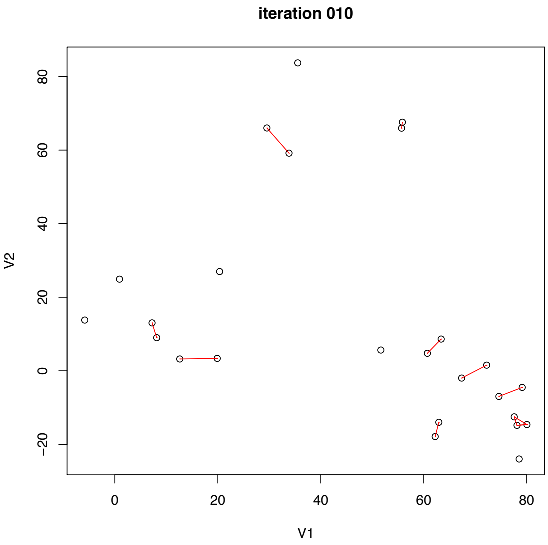
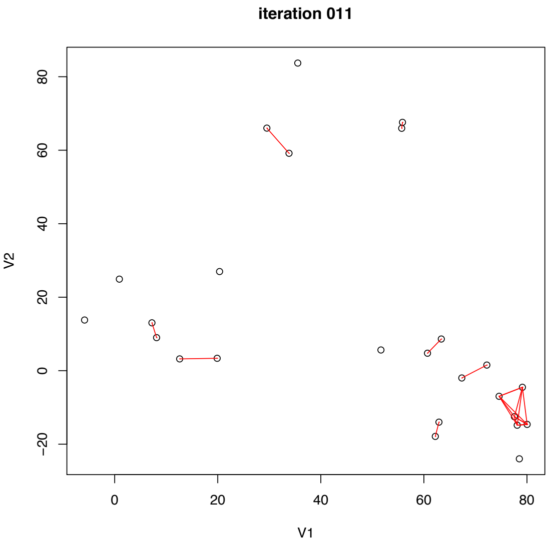


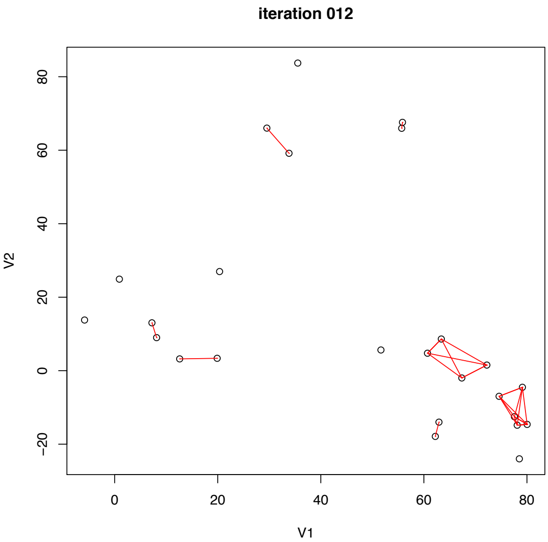
Example



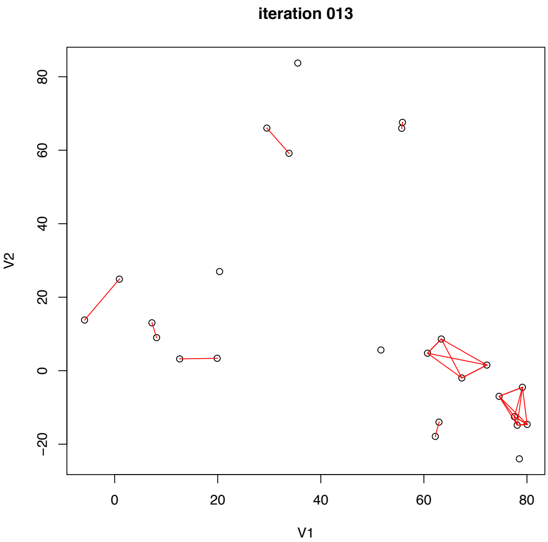
Example



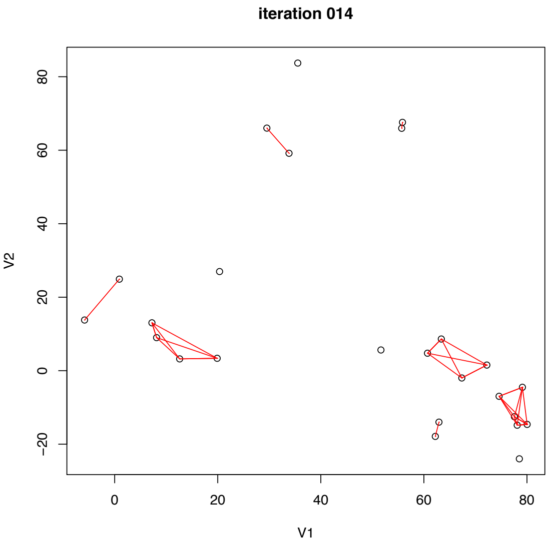
Example



Example



Example



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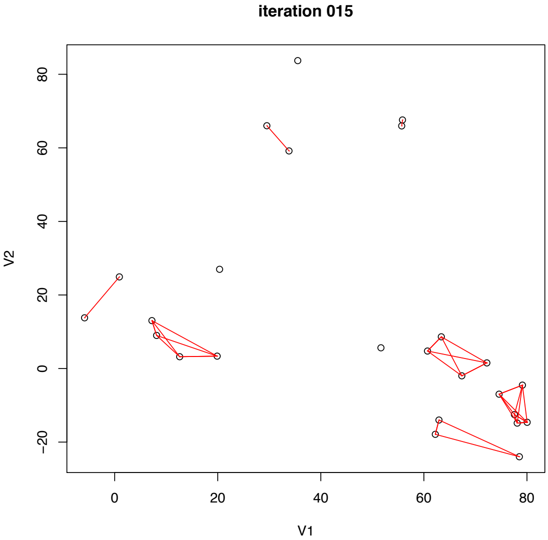

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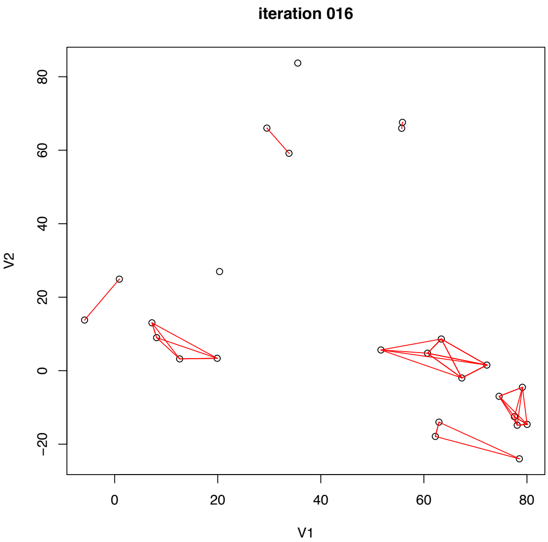

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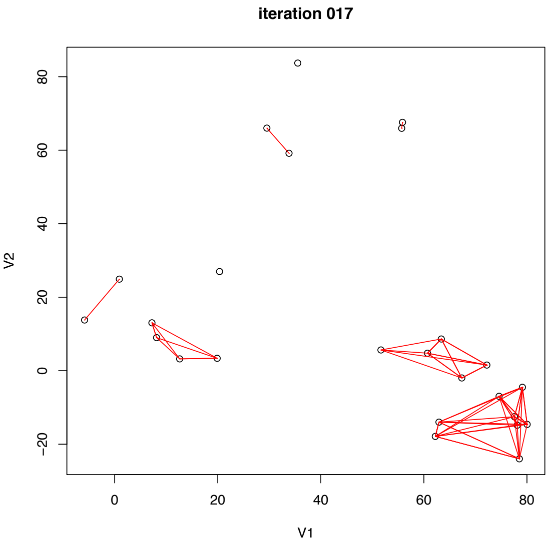

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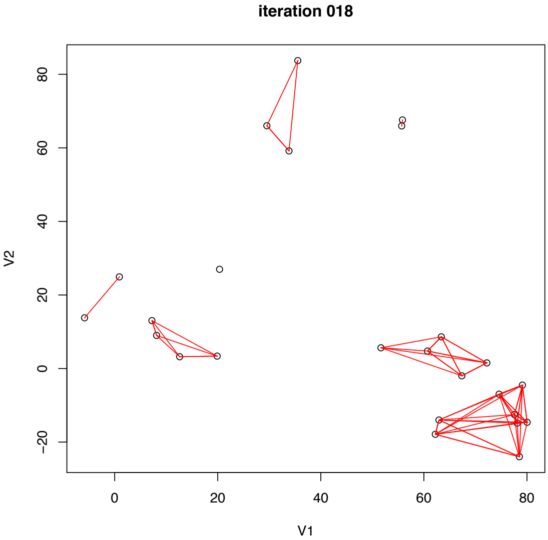
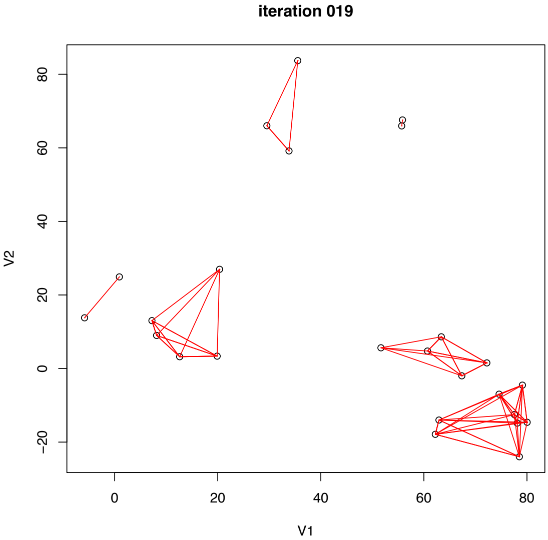
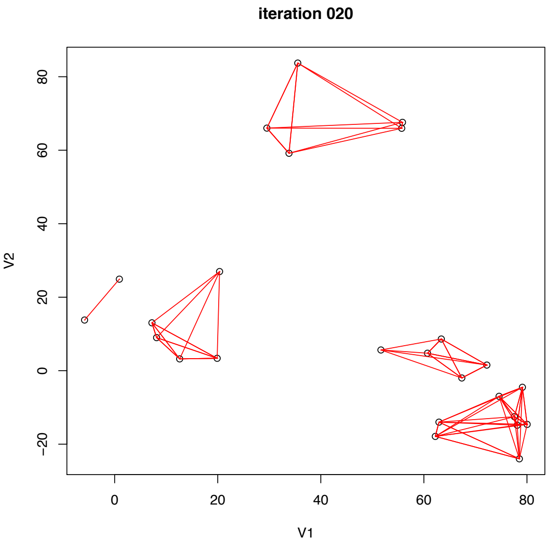


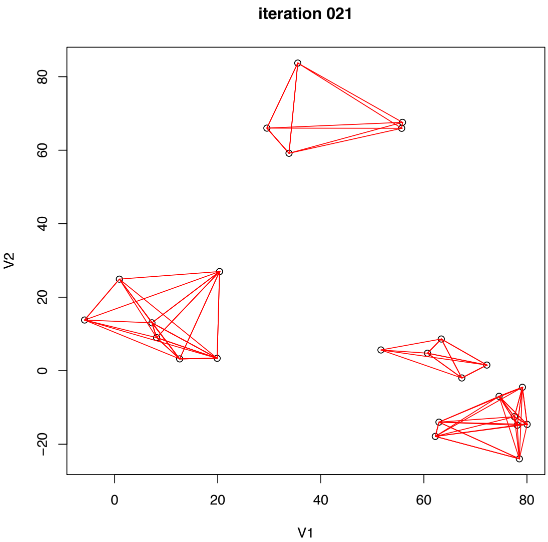
Example



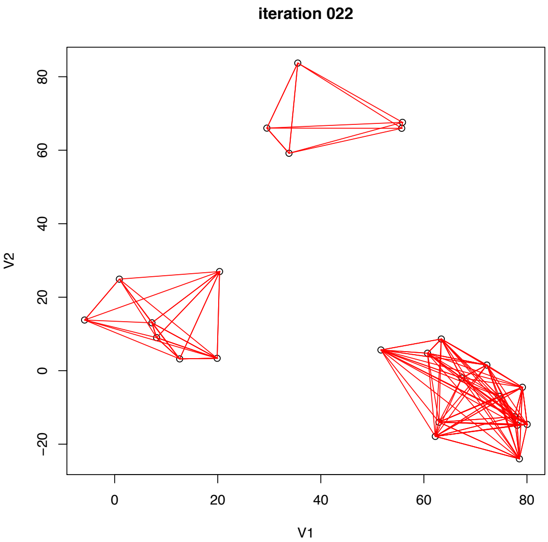
Example



Example



Example



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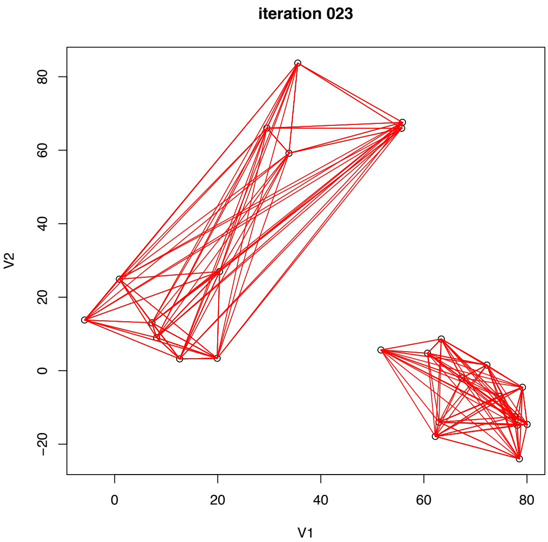
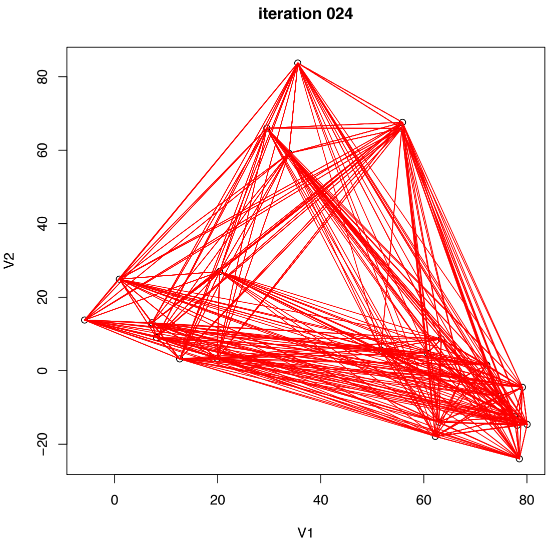


Example



Agglomerative hierarchical clustering

Bottom-up

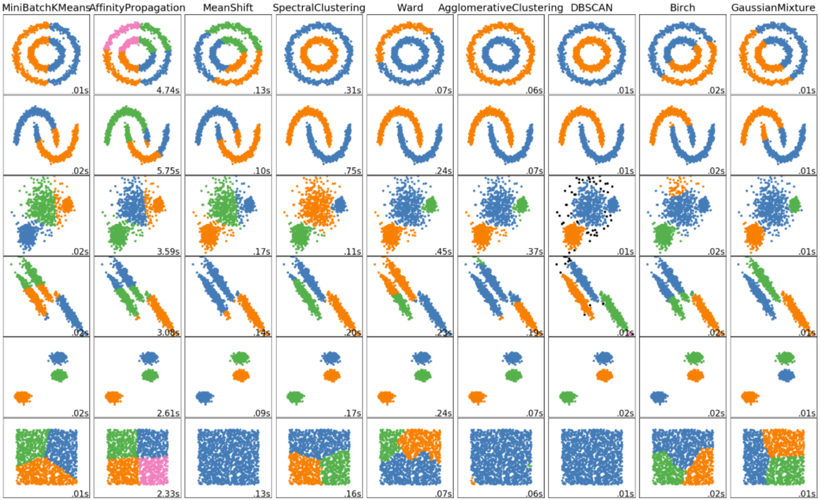
Pseudocode

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: $d(X, Y) = \max_{x \in X, y \in Y} d(x, y)$
- Group Average: $d(X, Y) = \dfrac{\sum_{x \in X, y \in Y} d(x, y)}{|X| \times |Y|}$
- Centroid Distance: $d(X, Y) = d\left(\dfrac{1}{|X|} \sum_{x \in X} x, \dfrac{1}{|Y|} \sum_{y \in Y} y\right)$

Many, many, many other algorithms available ..



Clustering with *scikit-learn* I

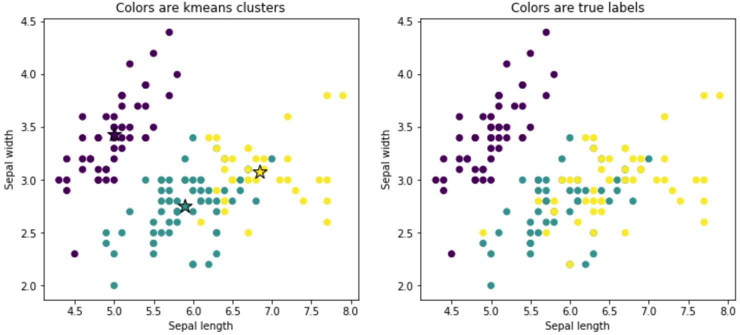
K-means: an example with the Iris dataset

```
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

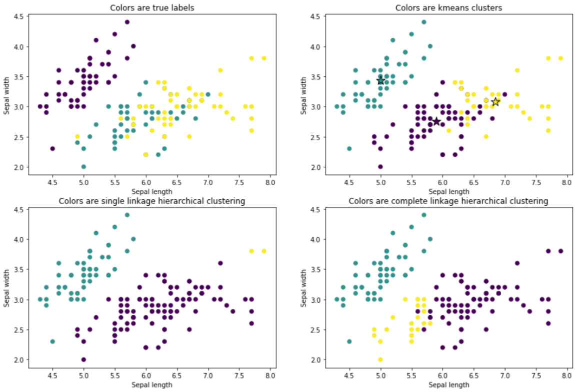
K-means: an example with the Iris dataset



Clustering with *scikit-learn* I

Hierarchical clustering: an example with the Iris dataset

```
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

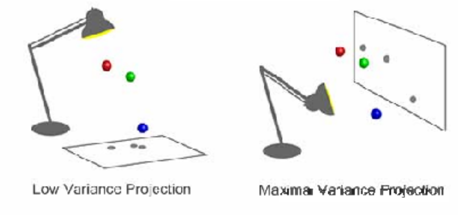
- When dimensionality increases, data becomes increasingly sparse in the space that it occupies
- Definitions of density and distance between points (critical for many tasks!) become less meaningful
- Visualization and qualitative analysis becomes impossible

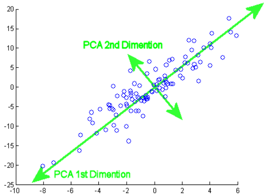
And so dimensionality reduction methods..

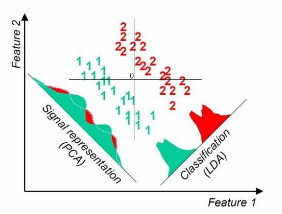
- avoid or at least mitigate the curse of dimensionality
- reduce time and memory required
- allow data to be more easily visualized
- may help eliminate irrelevant features
- may reduce noise

Principal Components Analysis

Find linear projections of original coordinates that maximize variance

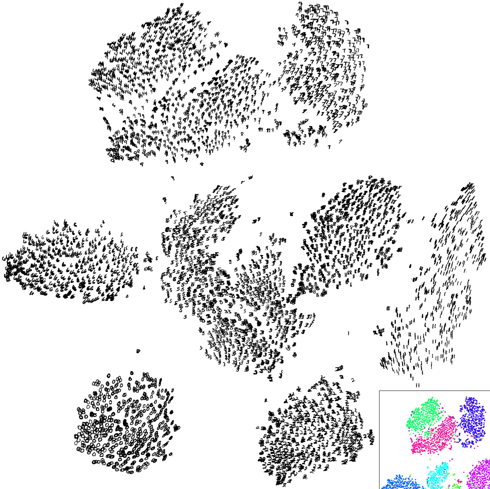


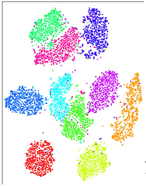




t-SNE: t-distributed stochastic neighbor embedding

A non-linear distance-preserving method



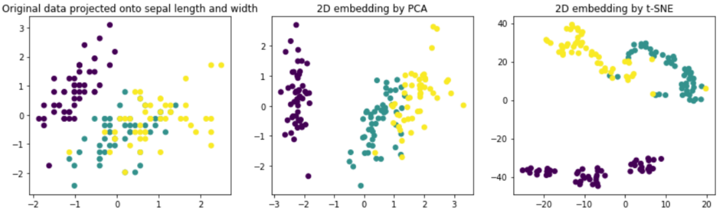

[1]

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

Dimensionality reduction with *scikit-learn*

```
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)
```

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



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...

To finish

Reading assignments: check
https://www.cs.upc.edu/~csi/

Exam: check https://www.cs.upc.edu/~csi/ and
corresponding notice at Racó.