Programa de Verão FGV EMAp 2019

Introduction to Machine Learning with Python

CLUSTERING TECHNIQUES

Prof. Luis Gustavo Nonato

University of São Paulo - São Carlos - SP

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(a) Original points.

(b) Two clusters.

(c) Four clusters.

(d) Six clusters.

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  - Agglomerative
  - Divisive
  - $\vdots$
- Partitional
  - K-means
  - Mixture Resolving
  - Spectral Clustering
  - Density-based
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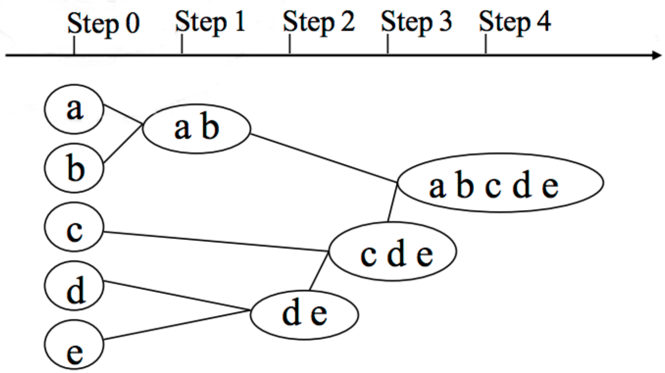

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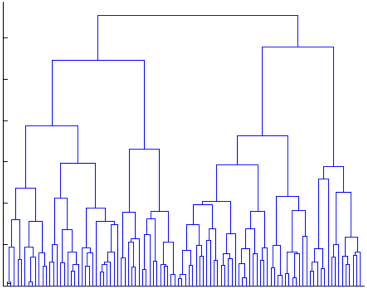
Step 3 can assume different forms:

$$d(C_a, C_b) = \min_{i \in C_a, j \in C_b} \{d(i,j)\} \quad \text{Single Link}$$

$$d(C_a, C_b) = \max_{i \in C_a, j \in C_b} \{d(i,j)\} \quad \text{Complete Link}$$

$$d(C_a, C_b) = \frac{1}{n_a n_b} \sum_{i \in C_a, j \in C_b} \{d(i,j)\} \quad \text{Average Link}$$

Dendogram



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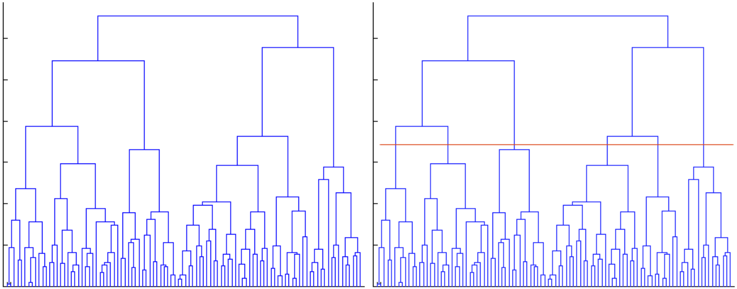

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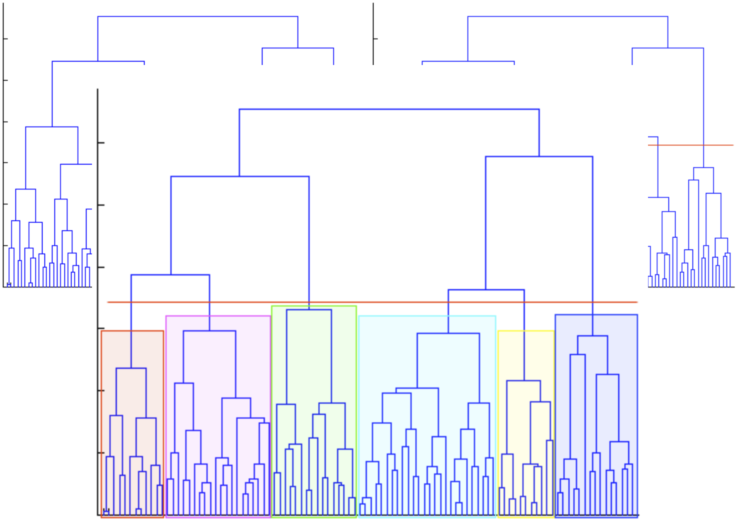

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The goal is to find $\{r_{ij}\}$ and $\{\boldsymbol{\mu}_j\}$ so as to minimize J.

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$\boldsymbol{\mu}_j$ is simply the average of the $\mathbf{x}_i \in cluster_j$.

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4. Repeat 2-3 until there are no changes in the prototypes

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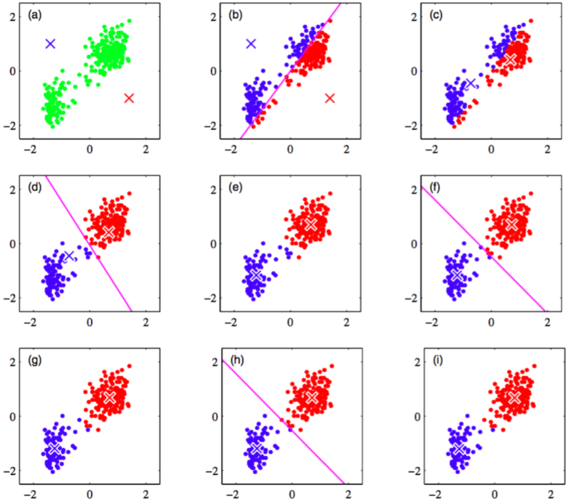

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- K-means is a particular case of a more general method called *Mixture Resolving*

Bisecting K-means

Initialize the list of clusters to contain the cluster consisting of all points.
repeat
    Remove a cluster from the list of clusters.
    {Perform several “trial” bisections of the chosen cluster.}
    for $i = 1$ to *number of trials* **do**
        Bisect the selected cluster using basic K-means.
    end for
    Select the two clusters from the bisection with the lowest total SSE.
    Add these two clusters to the list of clusters.
until Until the list of clusters contains K clusters.

Mixture Resolving

Given a data set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, a mixture solving algorithm aims to find parameters c_i, $\boldsymbol{\mu}_i$, Σ_i and a "responsibility" (membership) function γ_{ij} so as to maximize the likelihood

$$p(\mathbf{X}|\boldsymbol{c}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{i=1}^{n} \left(\sum_{j=1}^{k} c_j N(\mathbf{x}_i | \boldsymbol{\mu}_j, \Sigma_j) \right)$$

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Steps E and M are repeated until convergence.

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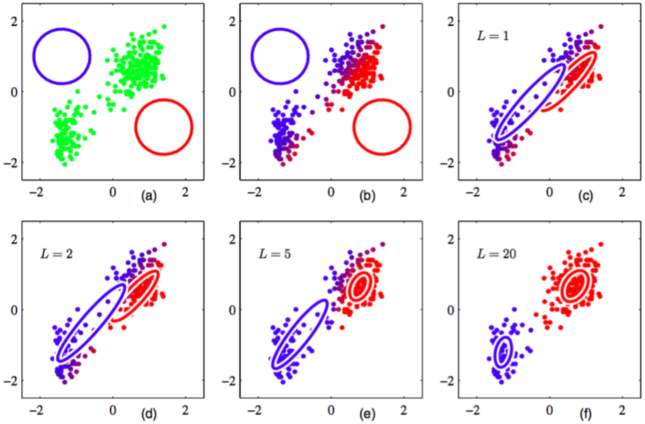

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The convergence of Mixture Resolving is slower than the convergence of K-means.

K-means is typically used to set initial conditions !!

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- The algorithm demands two parameters
  - ϵ: the radius defining the neighbourhood area
  - *npt*: the minimum number of points within in the ϵ-neighbourhood.
- The clustering process is based on the classification of the points as *core points*, *border points*, and *noise points*.

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- **Noisy Point**: a point that is neither a core nor a border point.

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- Find the ϵ-nearest neighbor graph of core points ignoring all non-core points and label each connected component of the graph as being a cluster
- Assign each non-core point to a nearby cluster if the non-core point is in the ϵ-neighbor of a core point of the cluster, otherwise assign it to noise.

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- for $npt \leq 2$ the result tends to be the same as of hierarchical clustering with the single link metric
- there are several methods for estimating ϵ and npt automaticall (for instance, using histograms)