NDA: Clustering

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Bibliography

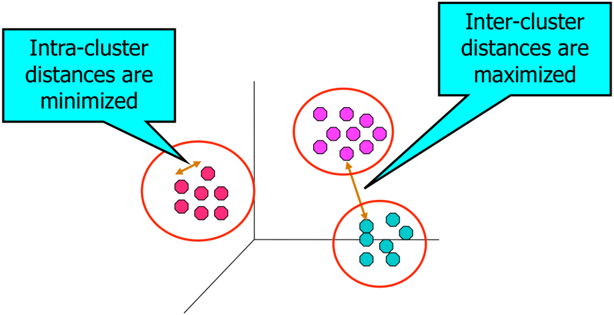
- Introduction to Data Mining, 2nd Edition by Tan, Steinbach, Karpatne, Kumar Chapter 7.

Outline

Outline

What is clustering?

Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



What is clustering?

- Clustering is an unsupervised learning method (i.e. no predefined classes)
- It is different from classification (supervised learning)

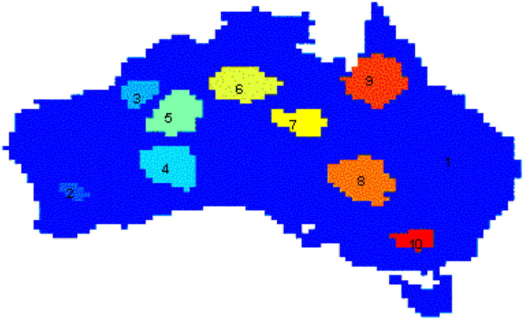
Why is it usefull (applications of cluster analysis)?

Understanding the data / get insights on the data:

- Group related documents for browsing
- Group genes and proteins that have similar functionality
- Group people sharing similar interest
- Group movies with similar genres or actors

Why is it usefull (applications of cluster analysis)?

Summarization: Reduce the size of large data sets



Clustering precipitation in Australia

Custering is an ill-defined problem

How many clusters?

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- An Impossibility Theorem for Clustering, Jon Kleinberg, NIPS2003.

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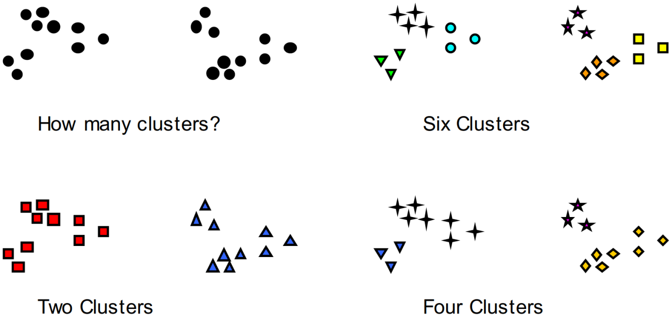

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Several types of clusterings

A clustering is a set of clusters. Important distinction between hierarchical and partitional sets of clusters.

- **Partitional clustering:** A division of data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- **Hierarchical clustering:** A set of nested clusters organized as a hierarchical tree

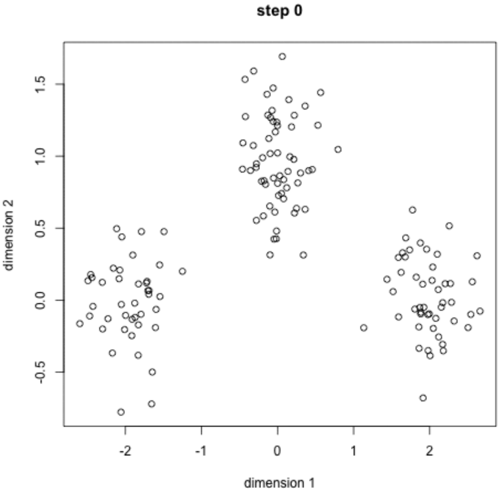
Several types of clusterings

Other distinctions:

- **Exclusive versus non-exclusive:** In non-exclusive clusterings, points may belong to multiple clusters. Can represent multiple classes or ‘border’ points
- **Fuzzy versus non-fuzzy:** In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1. Weights must sum to 1
- **Partial versus complete:** In some cases, we only want to cluster some of the data
- **Heterogeneous versus homogeneous:** Clusters of widely different sizes, shapes, and densities

Outline

k-means



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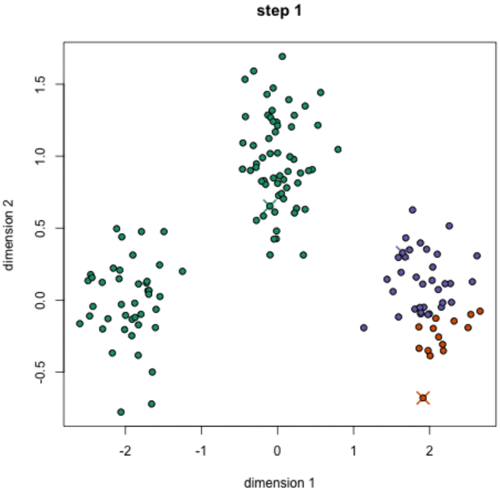

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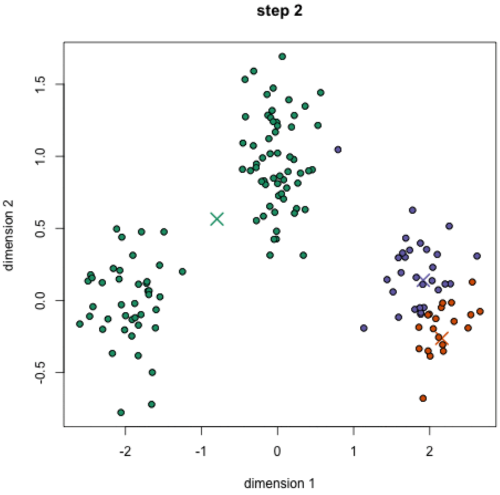

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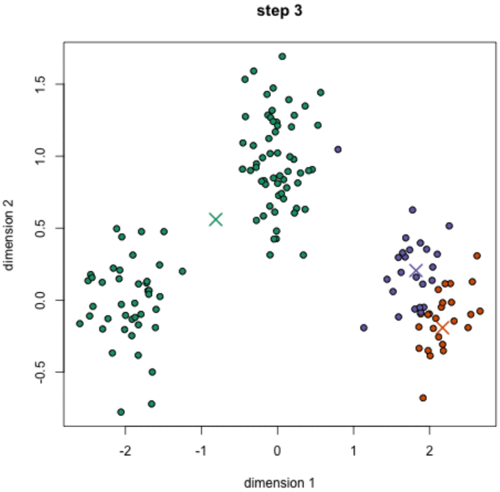

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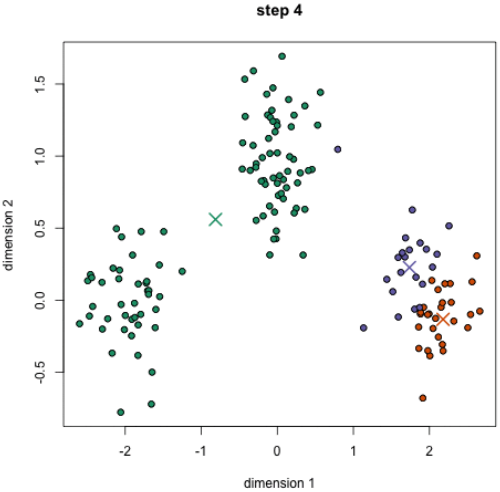

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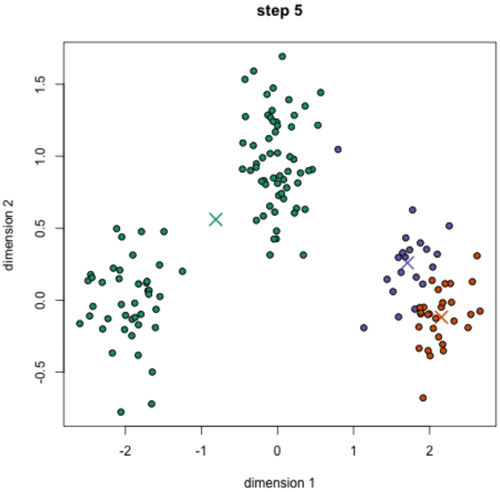

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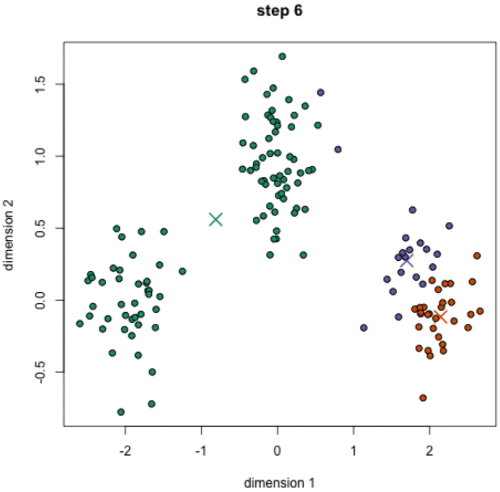

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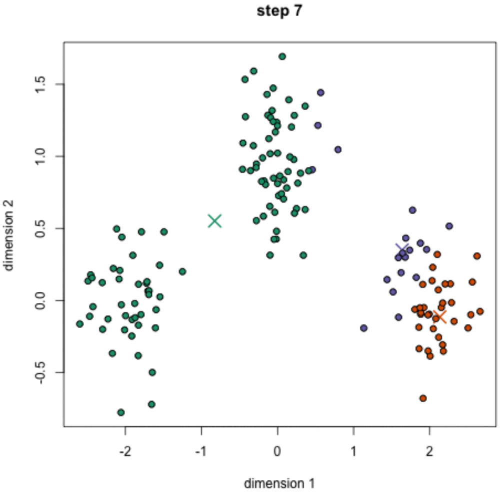

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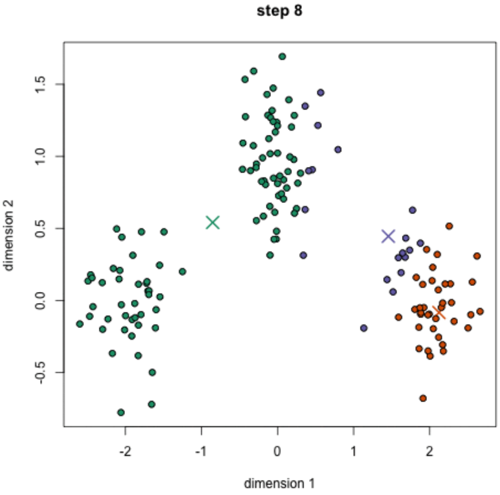

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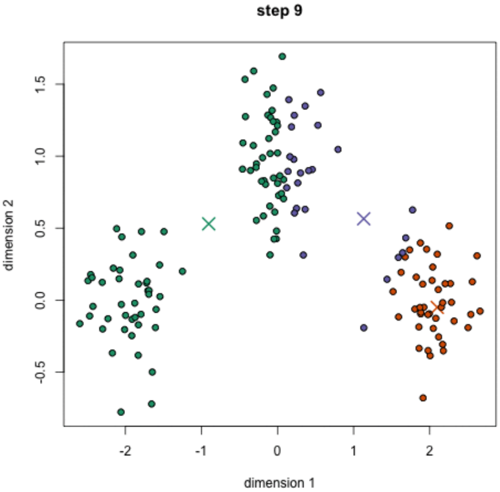

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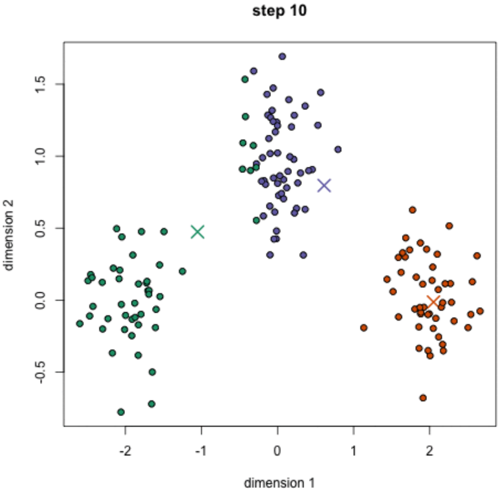

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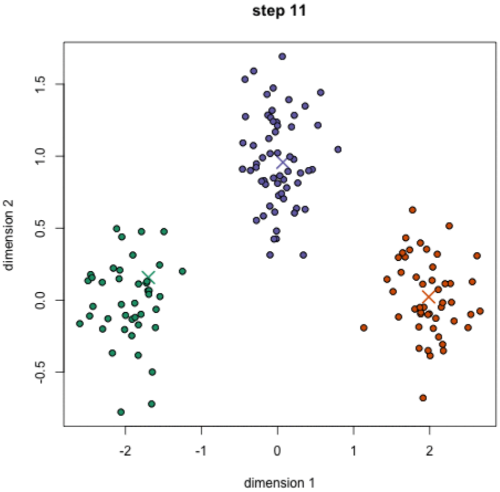

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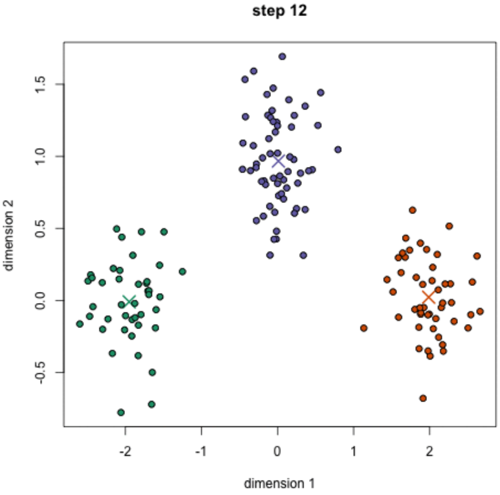
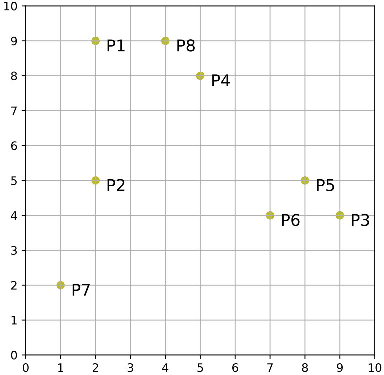


k-means

- Randomly chose k initial centroids
- While True:
  - Create k clusters by assigning each point to closest centroid
  - Compute k new centroids by averaging points in each clustering
  - If centroids don't change:
    - Break

k-means

Exercice: simulate some executions of kmeans wth $k = 3$ on the following set of points



k-means: distortion (a.k.a. SSE or SSD)

k-means can be seen as a heuristic to minimize the distortion:

$$\text{distortion} = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{i,j} ||x_i - \mu_j||_2^2$$

with

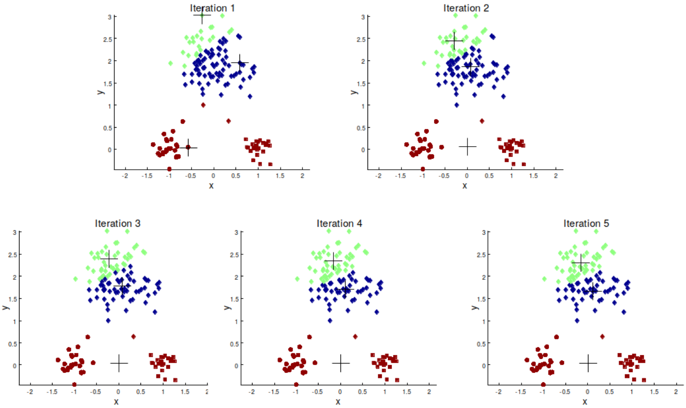
- μ_j the vector of centroid j and
- $w_{i,j} = 1$ if the sample x_i is in cluster j and 0 otherwise.

Limitation of k-means: clusters

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- K-means has problems when the data contains outliers.

Normalising the data and removing outliers can help!

Limitation of k-means: initialisation



Using multiple runs or kmeans++ can help!

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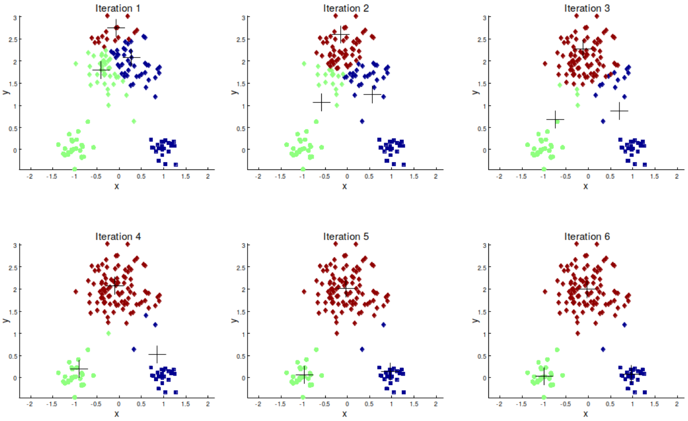

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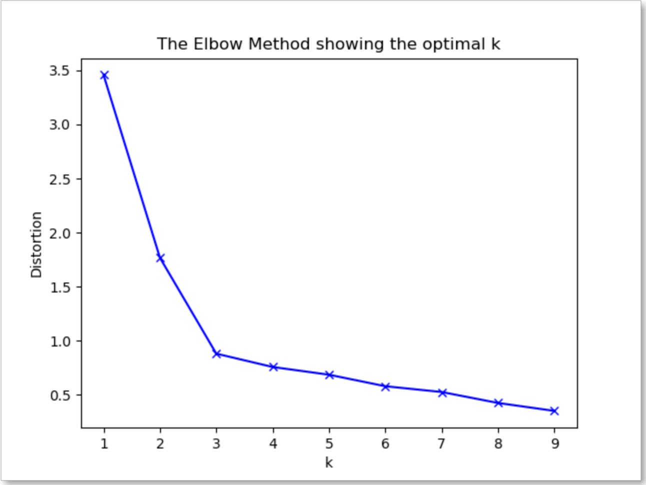
Limitation of k-means: How to choose k?



The elbow method: choose k=3, where the elbow is located

Limitation of k-means: How to choose k?

Silhouette value. A measure of how similar an object is to its own cluster (cohesion) compared to other clusters (separation).

For data point i in cluster C_k, let

$$a(i) = \frac{1}{|C_k| - 1} \sum_{j \in C_k, i \neq j} d(i,j) \quad \text{and} \quad b(i) = \min_{l \neq k} \frac{1}{|C_l|} \sum_{j \in C_l} d(i,j)$$

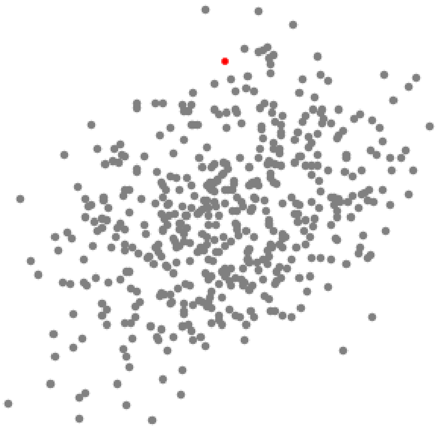
The silhouette score of one data point i: $s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$

Silouette score of a partition = average of the $s(i)$'s.

- **Elbow method with silhouette score instead of distortion**

Outline

Mean-shift (with one centroid)



The centroid moves towards a higher density region

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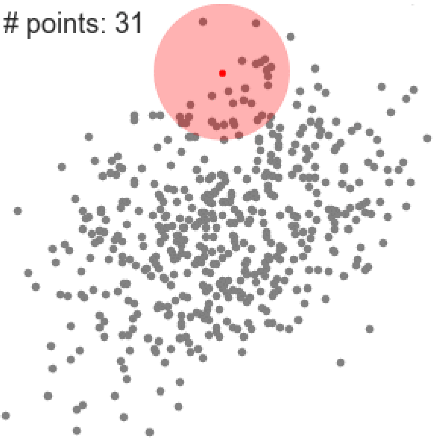

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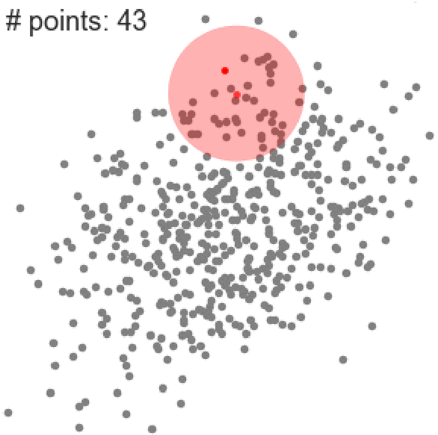

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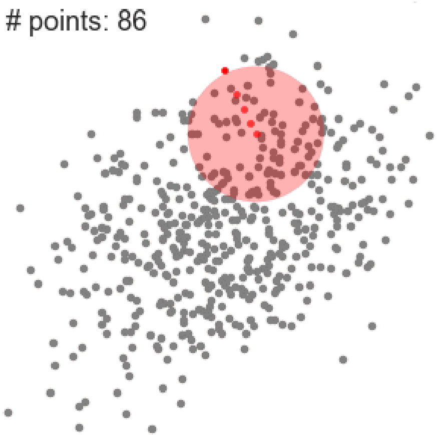

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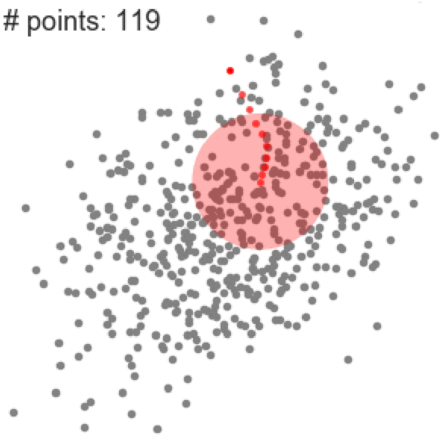

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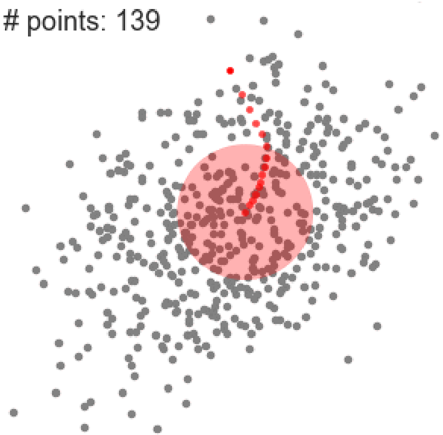

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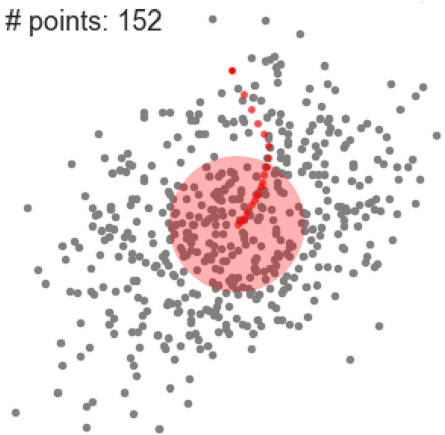

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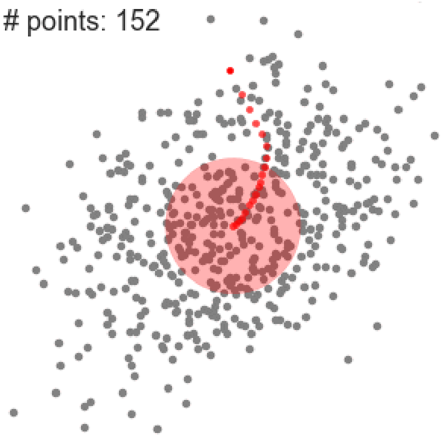

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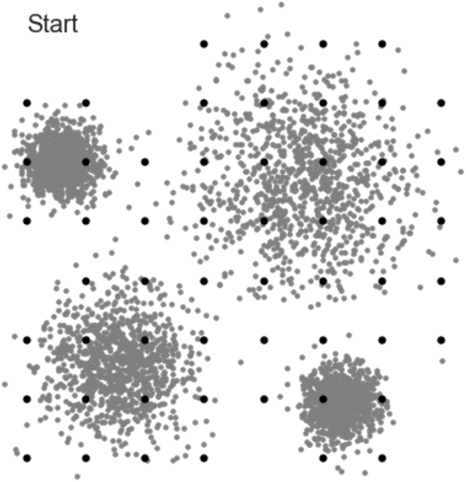

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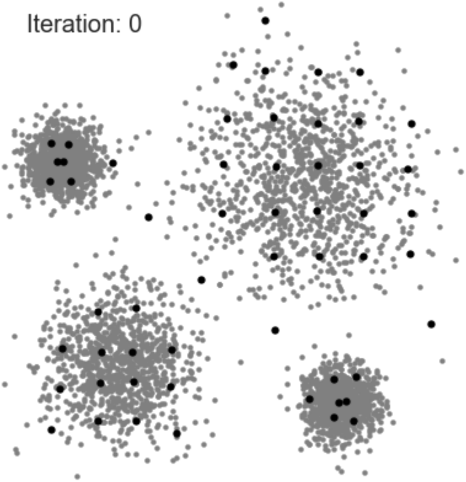

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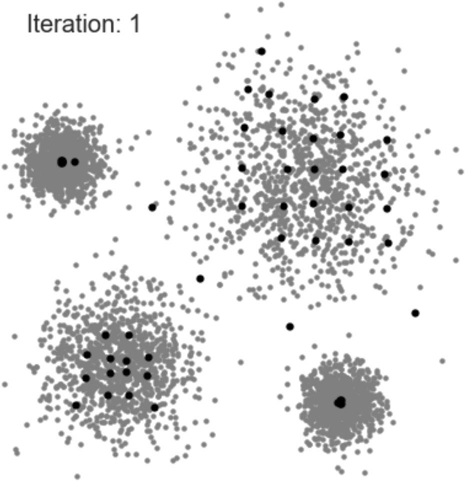

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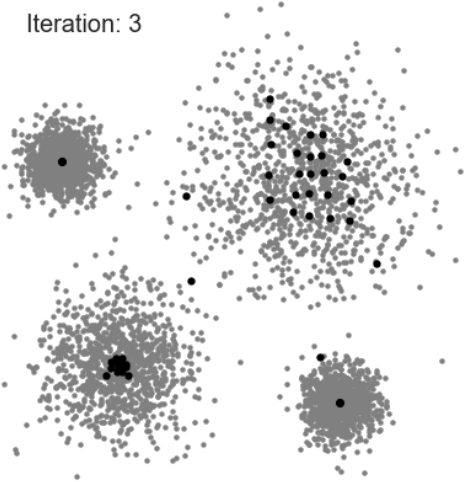

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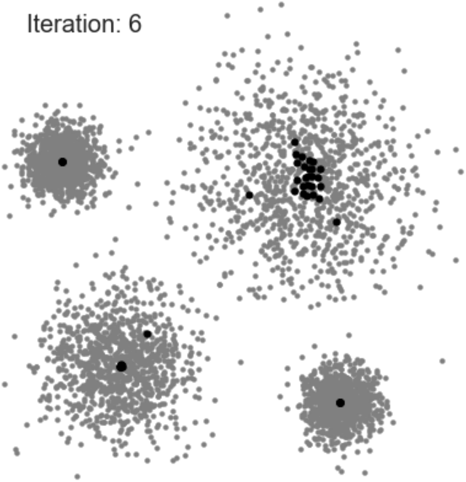

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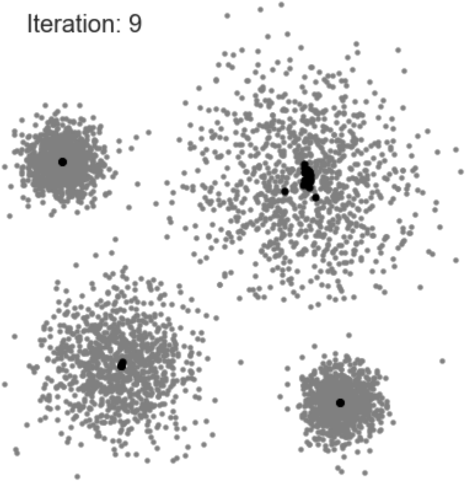

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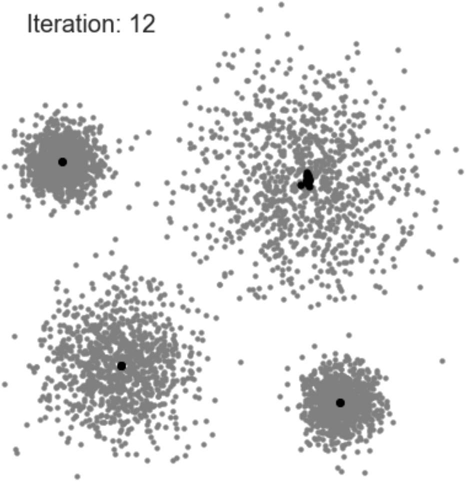

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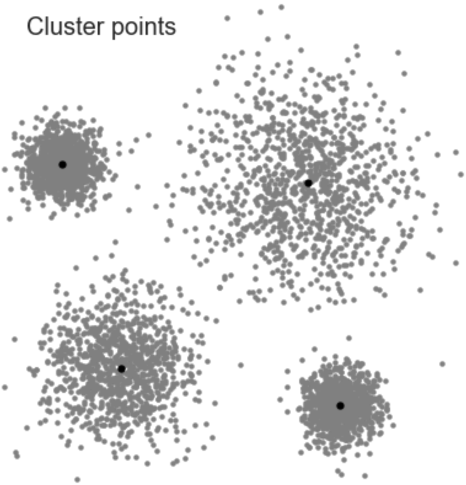
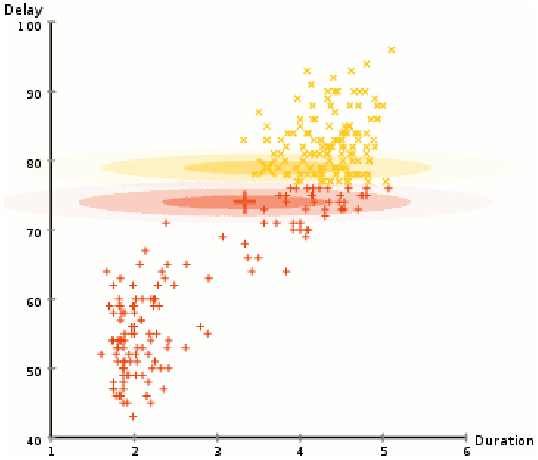


Mean-shift

Mean-shift

- Start with a given (large) number of circular sliding windows centered at randomly selected centroids and having radius *r*.
- While True;
  - Compute k new centroids by averaging examples in each sliding windows (the centroids are shifted towards regions of higher density)
  - If centroids don't change:
    - Break
- If multiple sliding windows overlap, then only the window containing the most points is preserved.
- Each data point is assigned to the nearest centroid.

GMM: Gaussian Mixture Model



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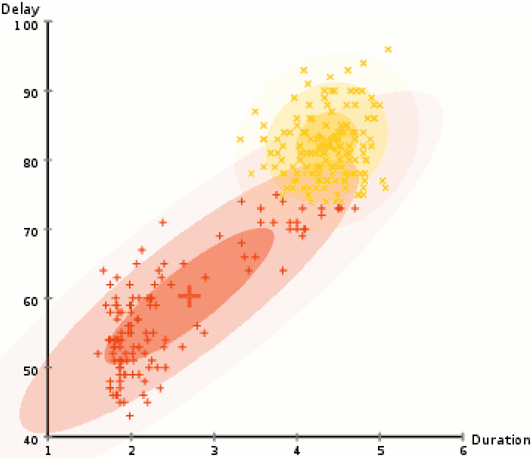

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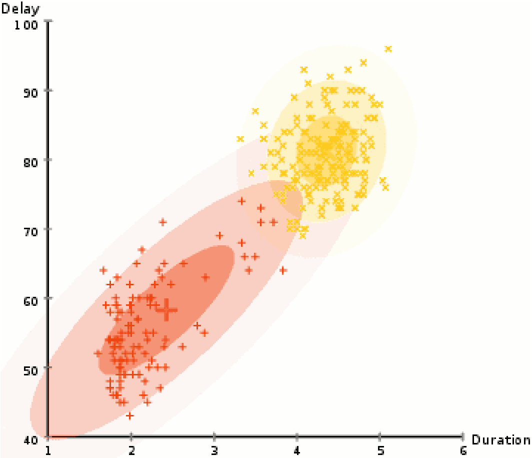

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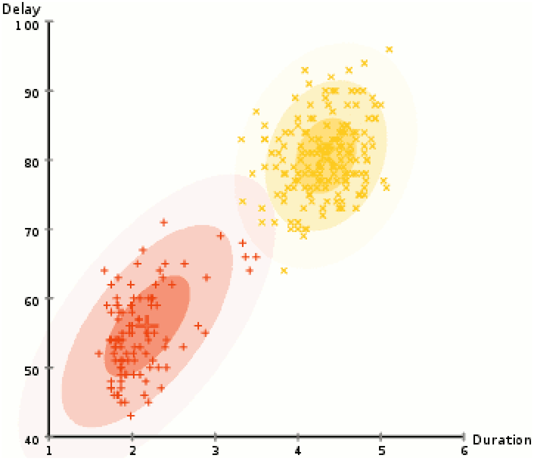

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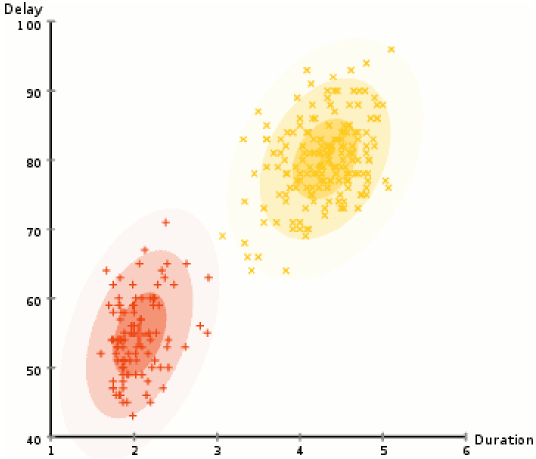

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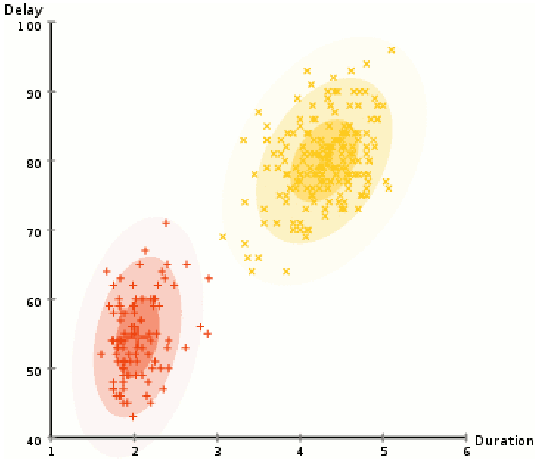


GMM: Gaussian Mixture Model

- Model: K gaussians (one-dimentional):
  - $p(x) = \sum_{k=1}^{K} \Phi_k N(x|\mu_k, \sigma_k)$
  - $N(x|\mu_k, \sigma_k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$
  - $\sum_{k=1}^{K} \Phi_k = 1$
- Want to find $(\Phi_k, \mu_k, \sigma_k)$ for all k maximizing $\prod_{i=1}^{n} p(x_i)$
- Chicken and egg problem:
  - need $(\Phi_k, \mu_k, \sigma_k)$ for all k to guess source of points
  - need to know source to estimate $(\Phi_k, \mu_k, \sigma_k)$

GMM: Gaussian Mixture Model

Expectation-Maximization algorithm:

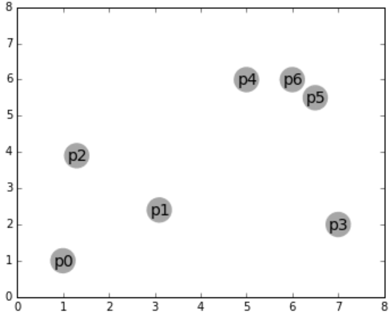
- start with randomly placed Gaussians $(\Phi_k, \mu_k, \sigma_k)$
- (E-step) for each i, k compute $\gamma_{i,k} \sim$ did x_i came from k?
- (M-step) adjust $(\Phi_k, \mu_k, \sigma_k)$ to fit points assigned to them
- iterate until convergence

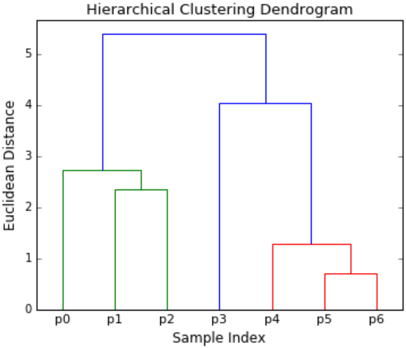
$$\Phi_k = \sum_{i=1}^{N} \frac{\gamma_{i,k}}{N}$$

$$\gamma_{i,k} = \frac{\Phi_k \mathcal{N}(x_i|\mu_k,\sigma_k)}{\sum_{k=1}^{K} \Phi_k(x|\mu_k,\sigma_k)}$$

$$\mu_k = \frac{\sum_{i=1}^{N} \gamma_{i,k} x_i}{\sum_{i=1}^{N} \gamma_{i,k}} \qquad \sigma_k^2 = \frac{\sum_{i=1}^{N} \gamma_{i,k}(x_i-\mu_k)^2}{\sum_{i=1}^{N} \gamma_{i,k}}$$

Hierarchical clustering





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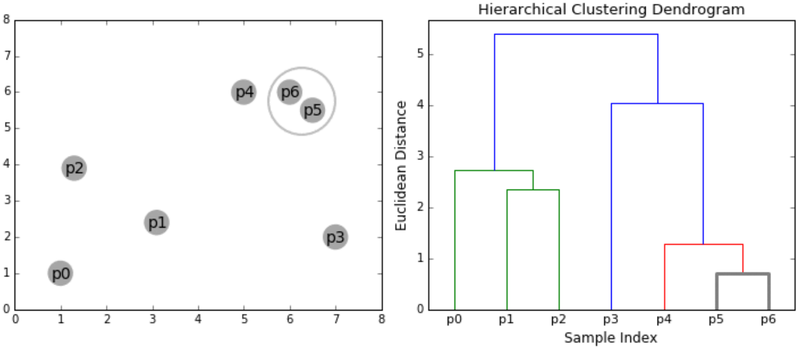

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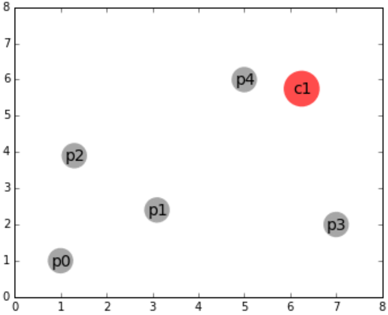

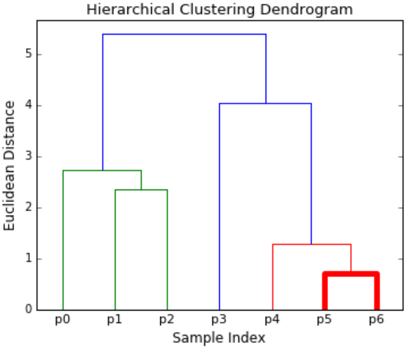

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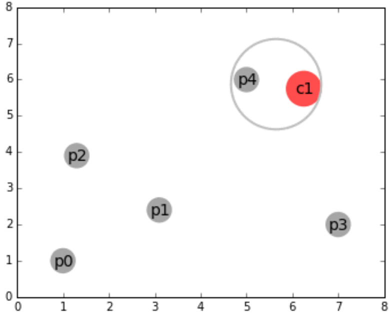

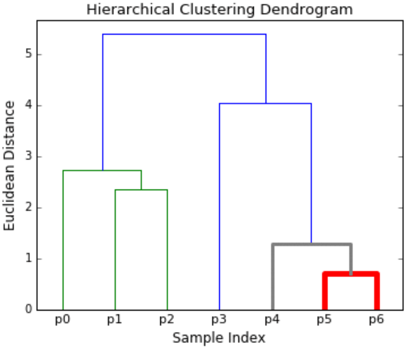

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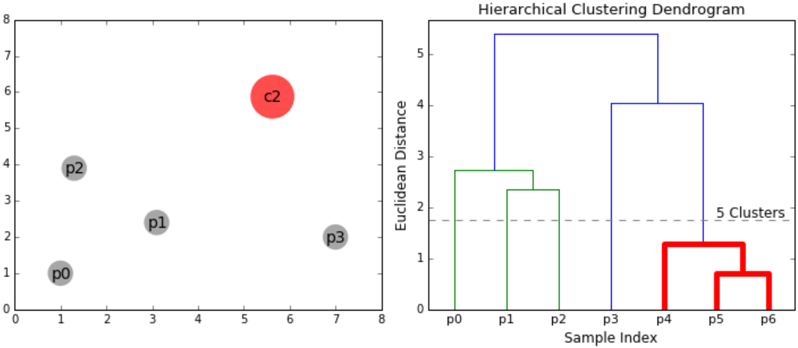

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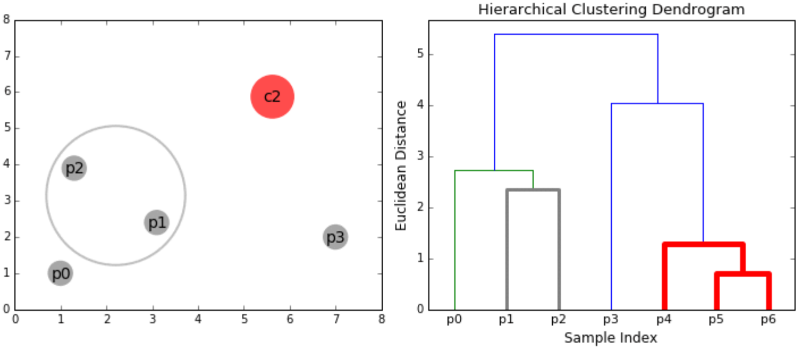

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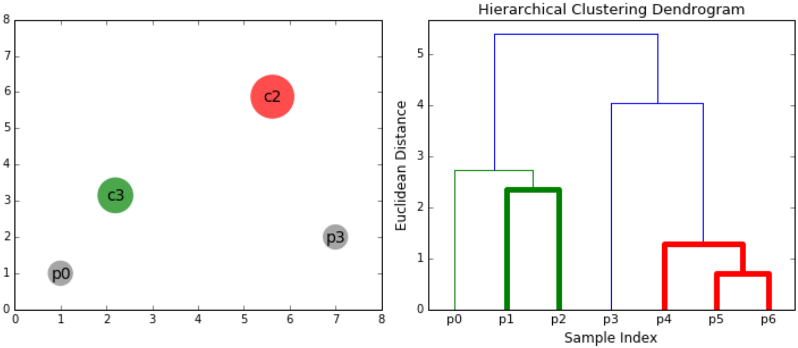

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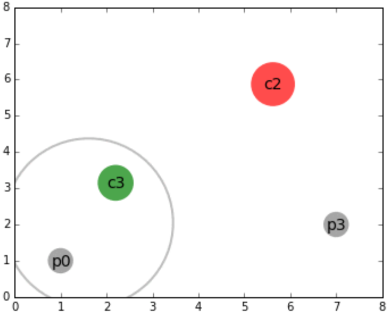

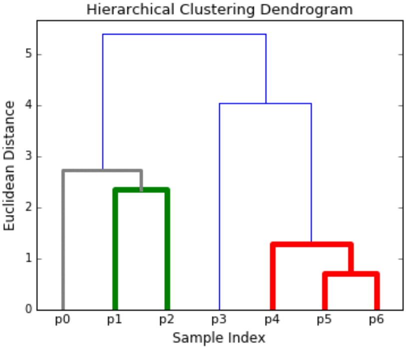

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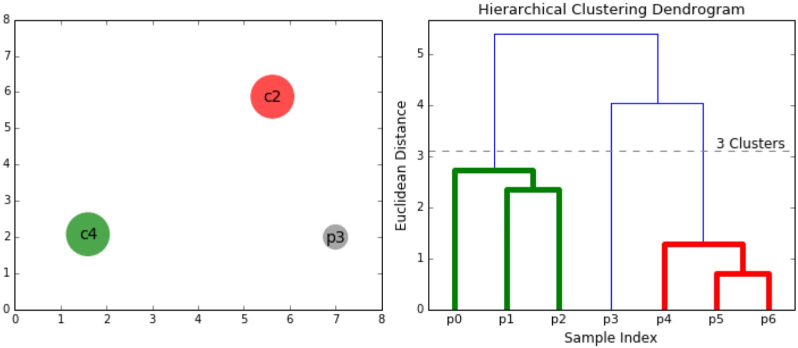

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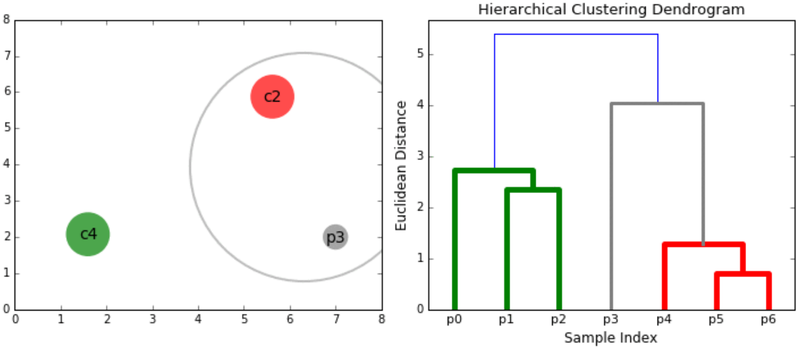
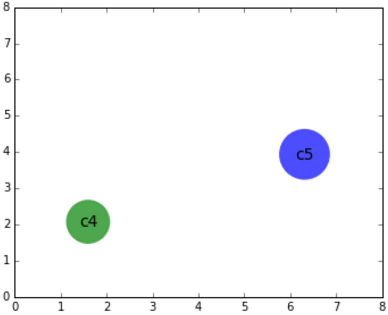
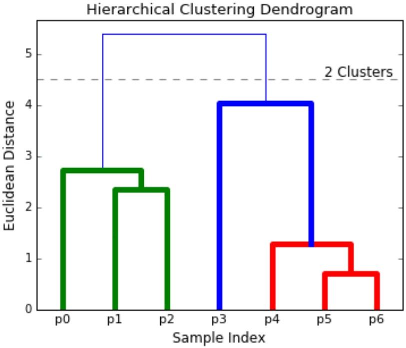
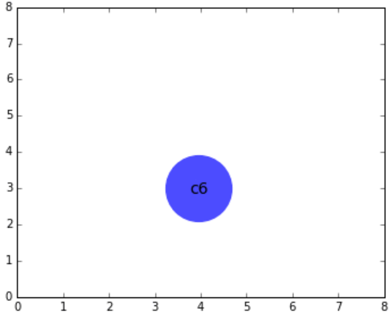


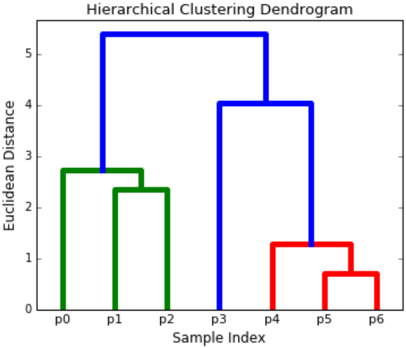
Hierarchical clustering





Hierarchical clustering





Hierarchical clustering

Two types of hierarchical clustering:

1. **Agglomerative.** This is a "bottom-up" approach: each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.
2. **Divisive.** This is a "top-down" approach: all observations start in one cluster, and splits are performed recursively as one moves down the hierarchy.

Aglomerative hierarchical clustering

- Maximum (or complete) linkage clustering:

$$d(A, B) = \max\{d(a, b) : a \in A, b \in B\}$$

- Minimum (or single) linkage clustering:

$$d(A, B) = \min\{d(a, b) : a \in A, b \in B\}$$

- Average linkage clustering:

$$d(A, B) = \frac{1}{|A| \cdot |B|} \sum_{a \in A} \sum_{b \in B} d(a, b)$$

Divisive hierarchical clustering

Dasgupta's objective and algorithm: Repeatedly subdivides the elements using an approximation algorithm for the sparsest cut problem.

Outline

1. What is clustering? Motivation?
2. k-means
3. Other clustering algorithms
   - Mean-shift
   - GMM: Gaussian Mixture Model
   - Hierarchical clustering
4. Validation

Validation

- For supervised classification we have a variety of measures to evaluate how good our model is: Accuracy, precision, recall
- For clustering, the analogous question is how to evaluate the “goodness” of the resulting clusters?
- "Clusters are in the eye of the beholder"!
- We still want some tools to:
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Validation

Two types of numerical measures to judge cluster validity:

1. Internal Index: Used to measure the goodness of a clustering structure without respect to external information. (e.g. distortion, silhoutte score)
2. External Index: Used to measure the extent to which cluster labels match externally supplied class labels. (e.g. Entropy, Purity, Adjusted Rand Index)

Validation: External Index

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

m_j = size of cluster j, m = number of documents
p_{ij} = probability that a random document of cluster j belongs to topic i. For example, $p_{13} = 1/685$.

- Entropy of a cluster:

$$e_j = -\sum_{i=1}^{n} p_{ij} \log_2(p_{ij})$$

- Entropy of a clustering:

$$\sum_j \frac{m_j}{m} e_j$$

- Purity of a cluster:

$$purity_j = max_i(p_{ij})$$

- Purity of a clustering:

$$\sum_j \frac{m_j}{m} purity_j$$