

NDA: Clustering

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Bibliography

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

Outline

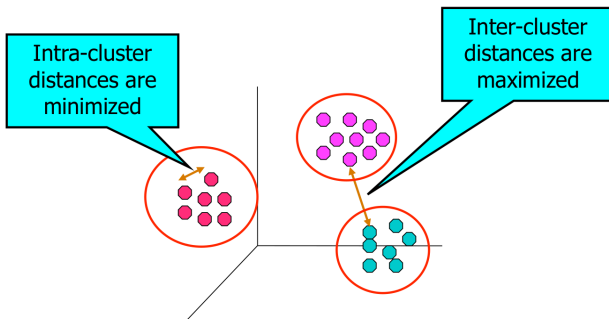
- 1 What is clustering? Motivation?
- 2 k-means
- 3 Other clustering algorithms
 - Mean-shift
 - DBSCAN
 - GMM: Gaussian Mixture Model
- 4 Hierarchical clustering
- 5 Validation

Outline

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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)

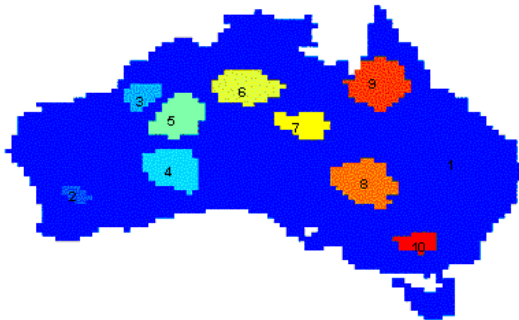
Why is it useful (applications of cluster analysis)?

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 useful (applications of cluster analysis)?

Summarization: Reduce the size of large data sets



Clustering precipitation in Australia

Clustering is an ill-defined problem

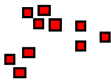
How many clusters?



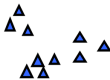
How many clusters?



Six Clusters



Two Clusters



Four Clusters



► An Impossibility Theorem for Clustering, Jon Kleinberg, NIPS2015.

Several types of clusters

- 1 A well-separated cluster is a set of points such that any point in a cluster is closer to every other point in the cluster than to any point not in the cluster.
- 2 A center-based cluster is a set of objects such that an object in a cluster is closer to the “center” of a cluster, than to the center of any other cluster
- 3 A contiguous cluster is a set of points such that a point in a cluster is closer to one or more other points in the cluster than to any point not in the cluster.
- 4 A density-based cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.

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

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What is clustering? Motivation?

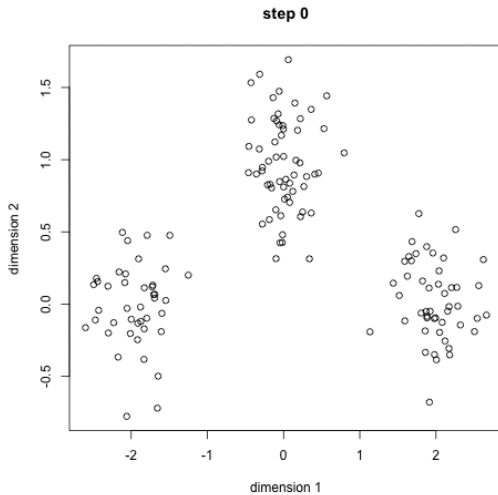
k-means

Other clustering algorithms

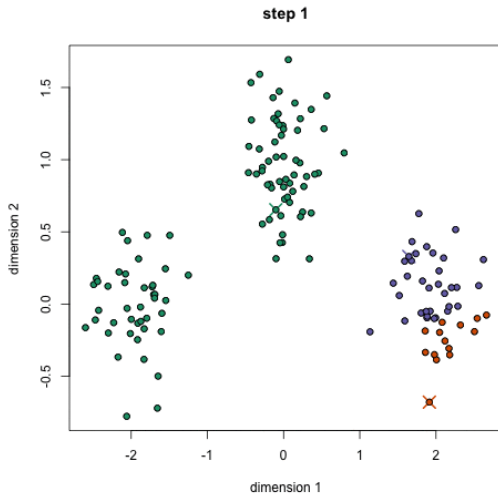
Hierarchical clustering

Validation

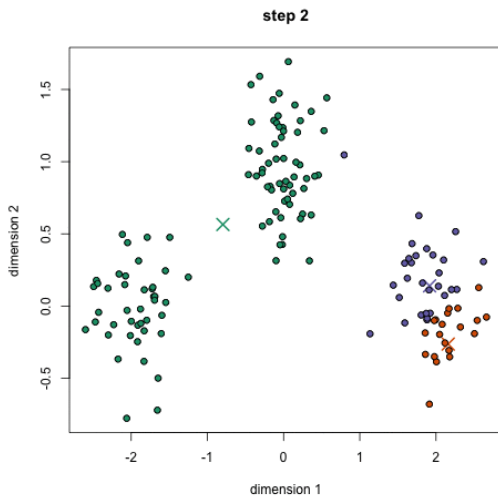
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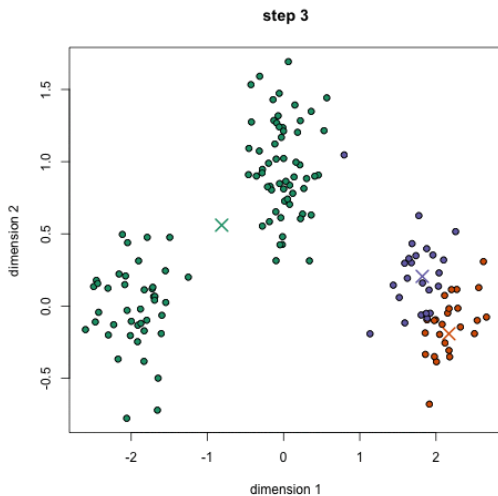
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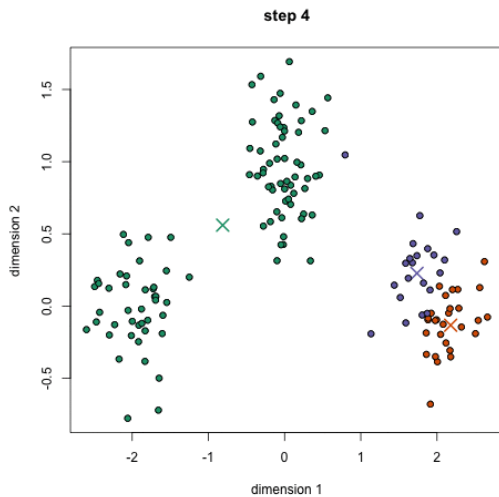
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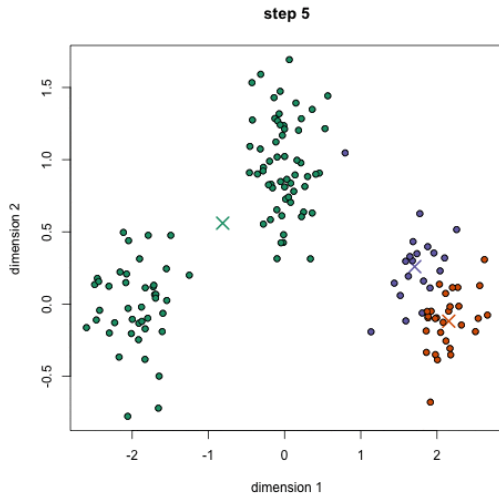
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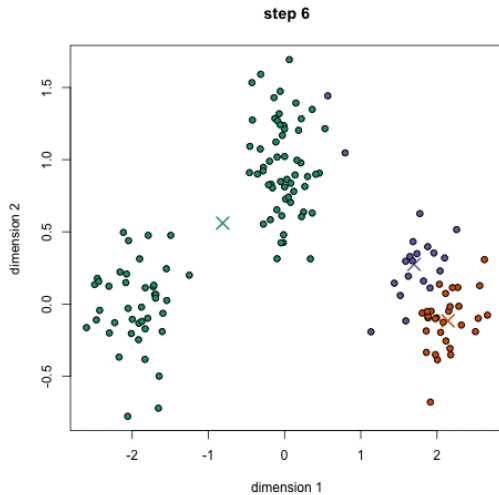
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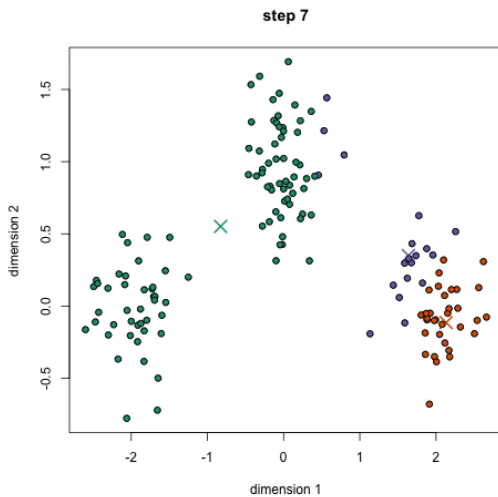
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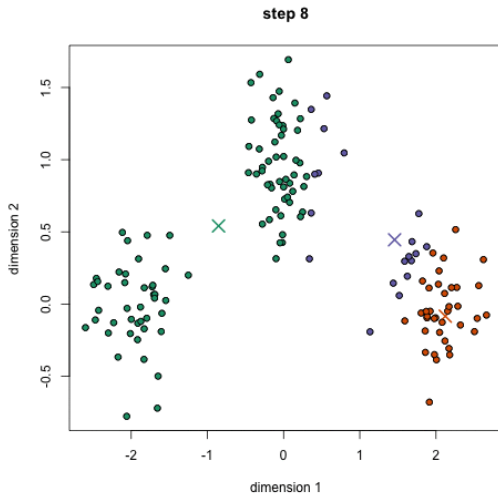
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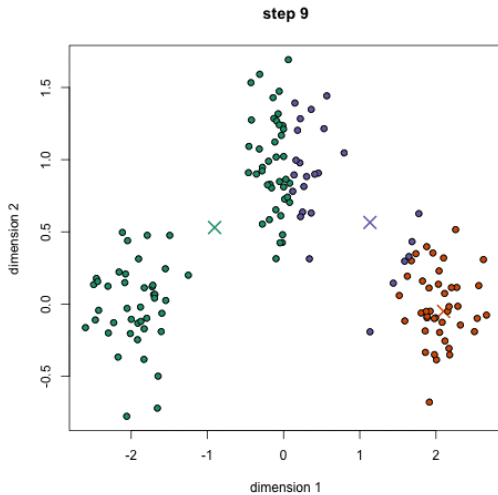
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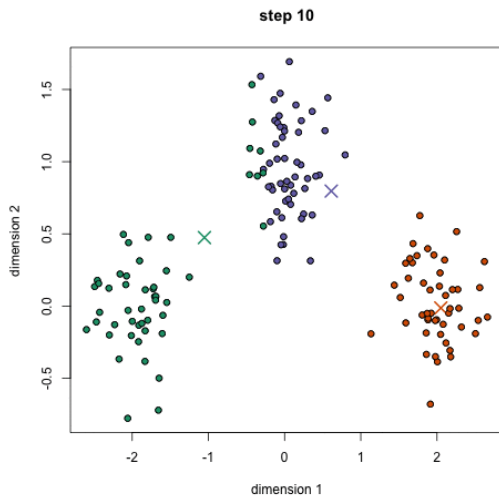
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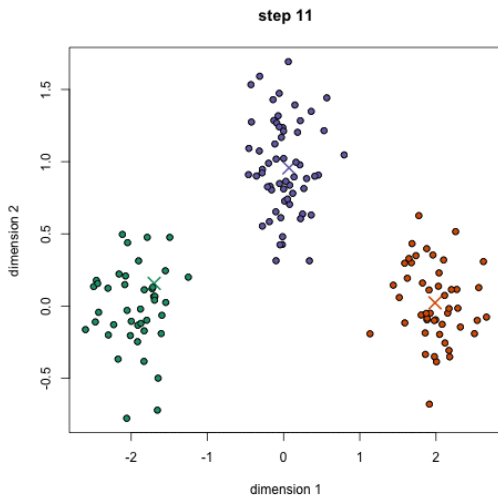
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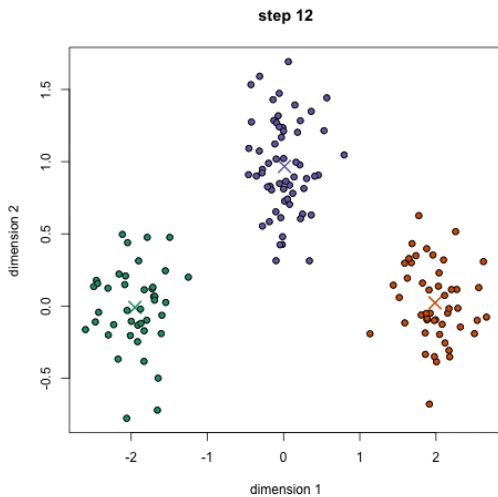
k-means



k-means



k-means



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: 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!

What is clustering? Motivation?

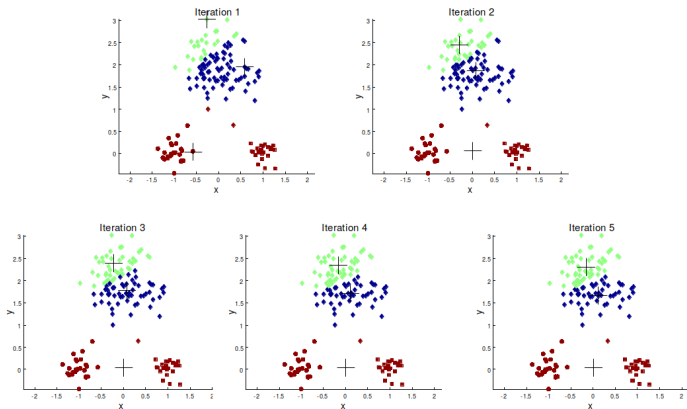
k-means

Other clustering algorithms

Hierarchical clustering

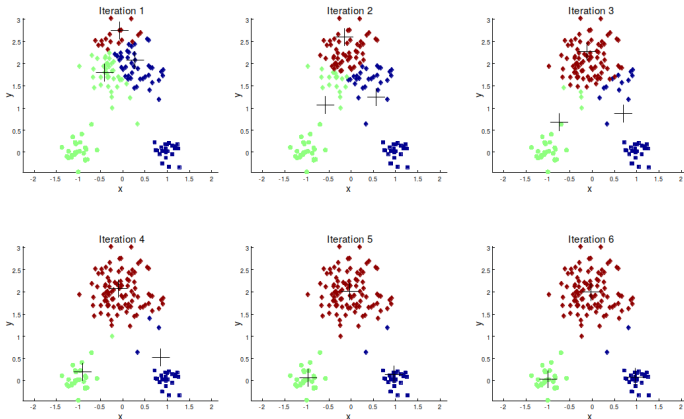
Validation

Limitation of k-means: initialisation



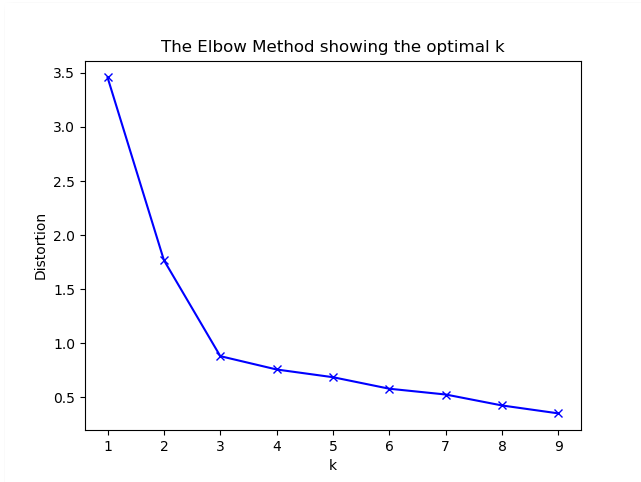
Using multiple runs or kmeans++ can help!

Limitation of k-means: initialisation



Using multiple runs or `kmeans++` can help!

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 : $s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$

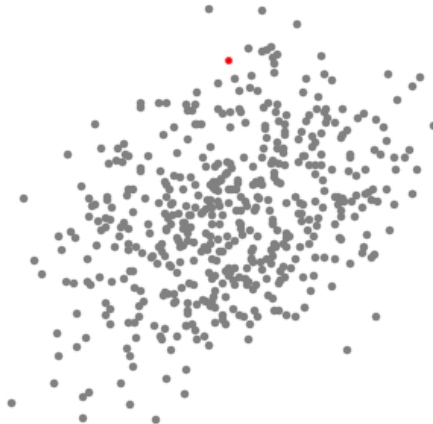
Silhouette score of a partition = average of the $s(i)$'s.

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

Outline

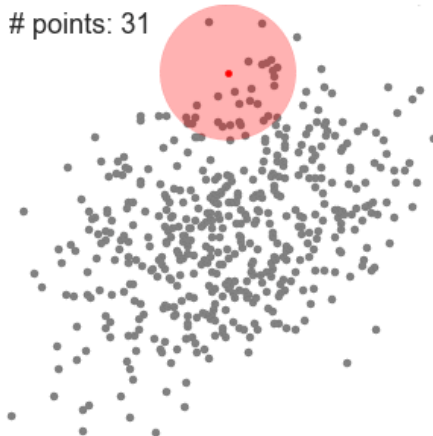
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Mean-shift (with one centroid)



The centroid moves towards a higher density region

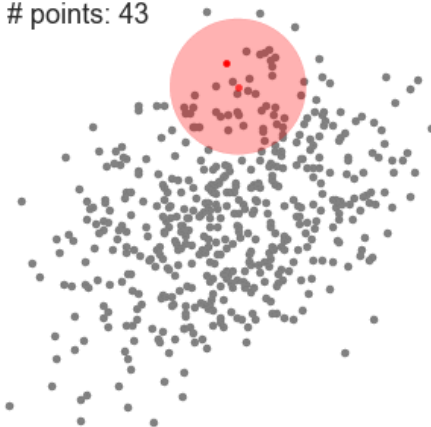
Mean-shift (with one centroid)



The centroid moves towards a higher density region

Mean-shift (with one centroid)

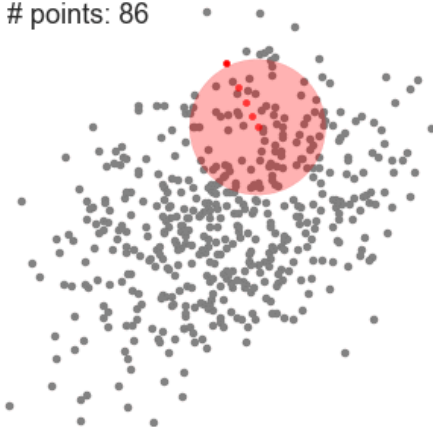
points: 43



The centroid moves towards a higher density region

Mean-shift (with one centroid)

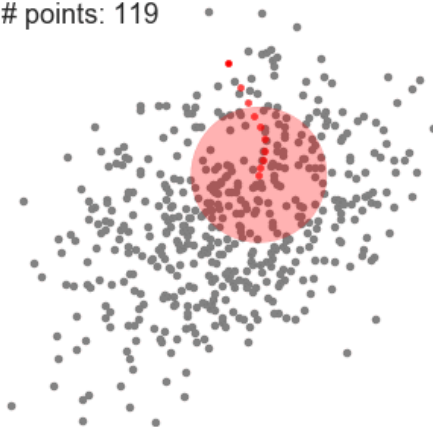
points: 86



The centroid moves towards a higher density region

Mean-shift (with one centroid)

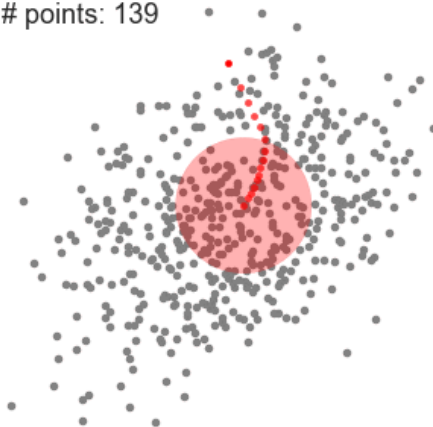
points: 119



The centroid moves towards a higher density region

Mean-shift (with one centroid)

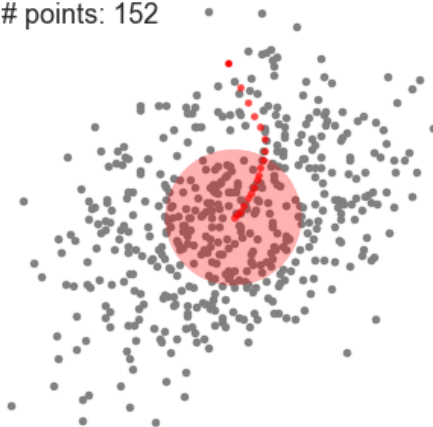
points: 139



The centroid moves towards a higher density region

Mean-shift (with one centroid)

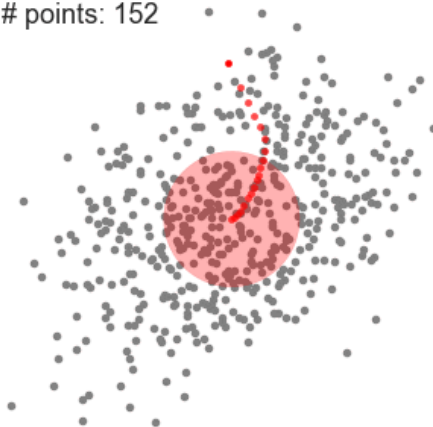
points: 152



The centroid moves towards a higher density region

Mean-shift (with one centroid)

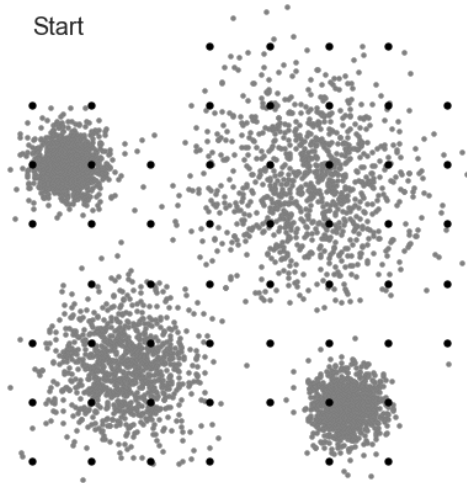
points: 152



The centroid moves towards a higher density region

Mean-shift

Start



What is clustering? Motivation?

k-means

Other clustering algorithms

Hierarchical clustering

Validation

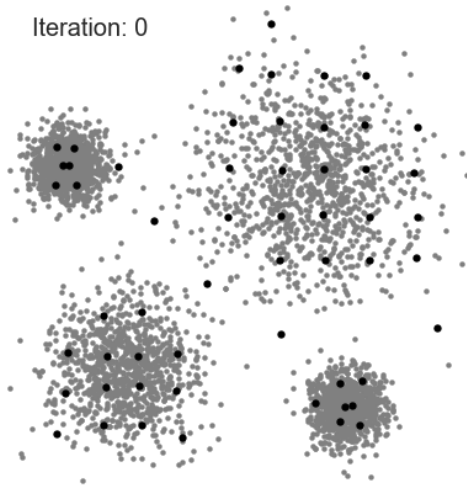
Mean-shift

DBSCAN

GMM: Gaussian Mixture Model

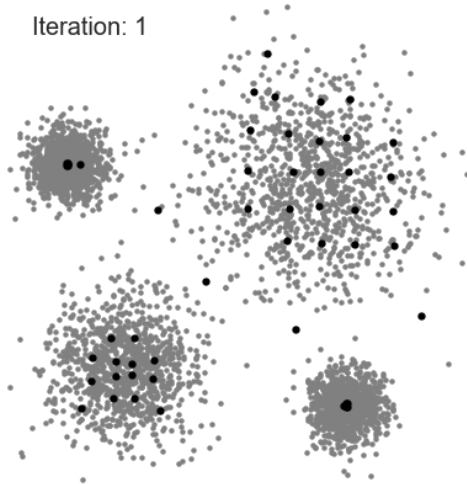
Mean-shift

Iteration: 0



Mean-shift

Iteration: 1



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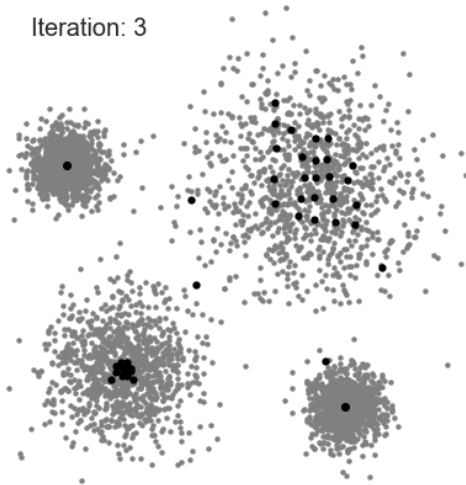
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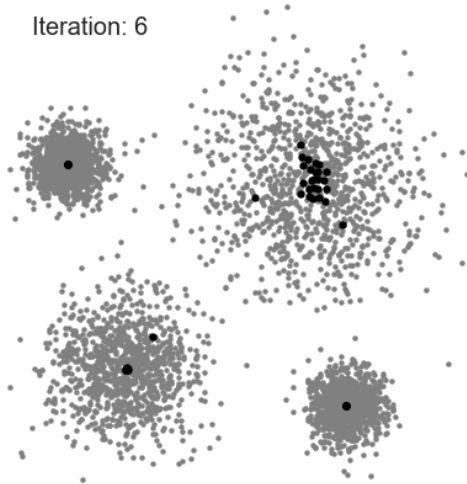
Mean-shift

Iteration: 3



Mean-shift

Iteration: 6



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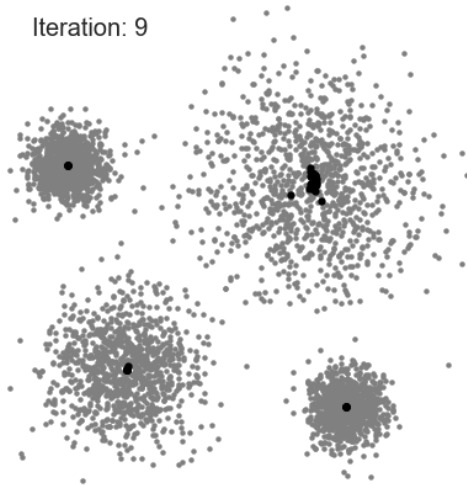
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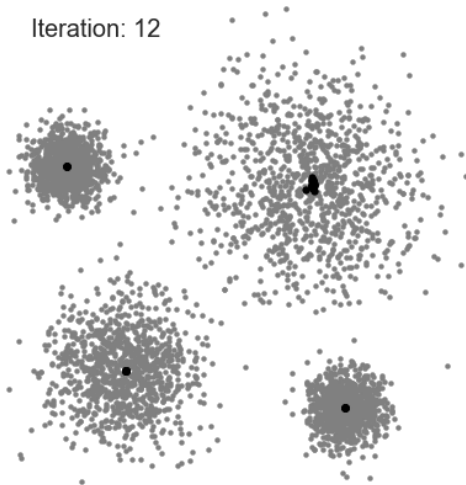
Mean-shift

Iteration: 9



Mean-shift

Iteration: 12



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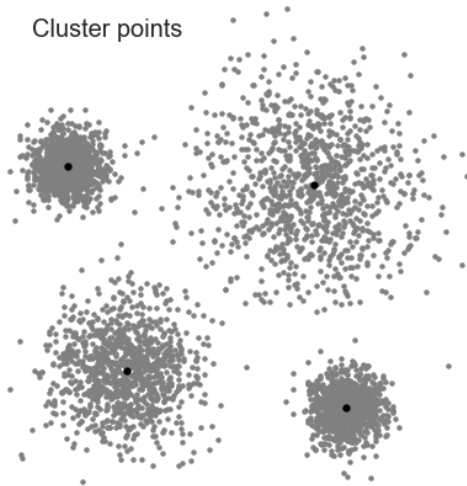
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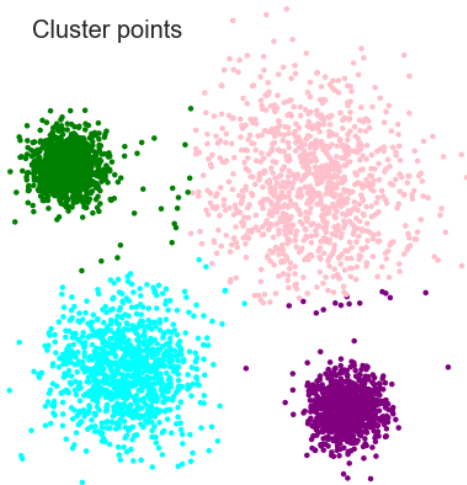
Mean-shift

Cluster points



Mean-shift

Cluster points



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.

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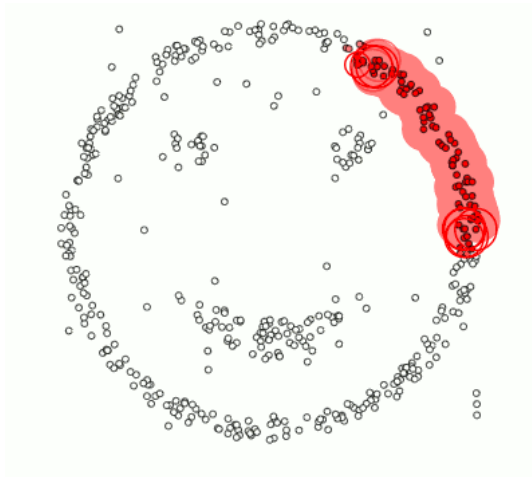
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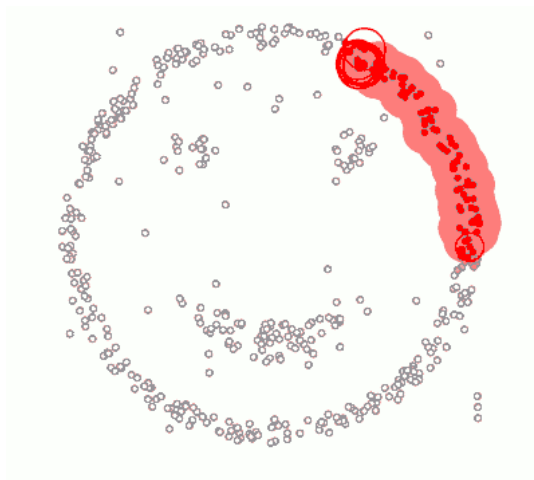
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DBSCAN



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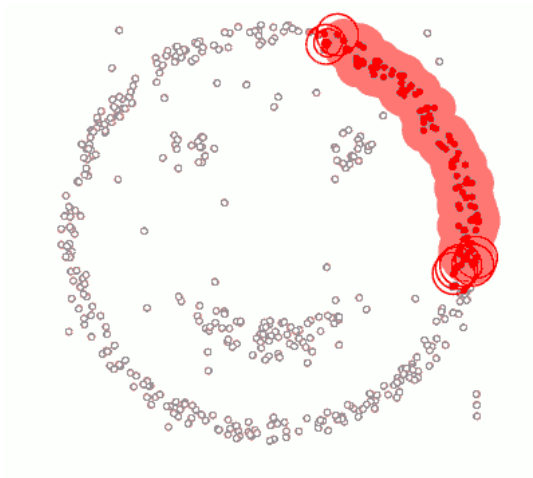
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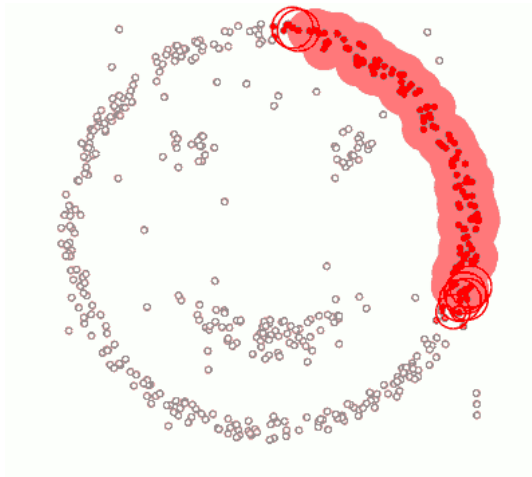
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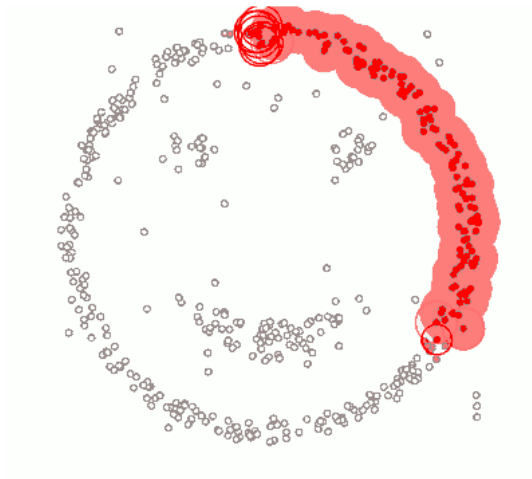
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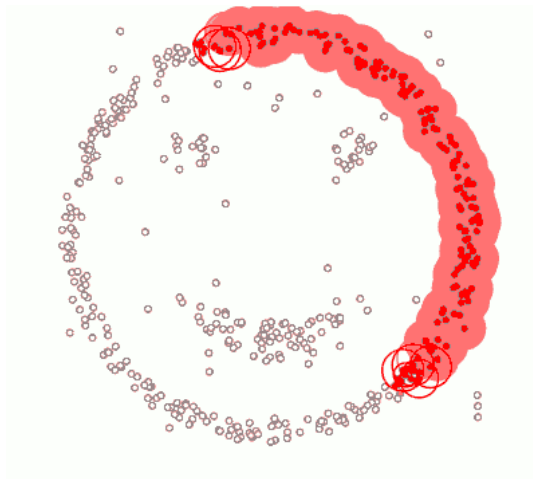
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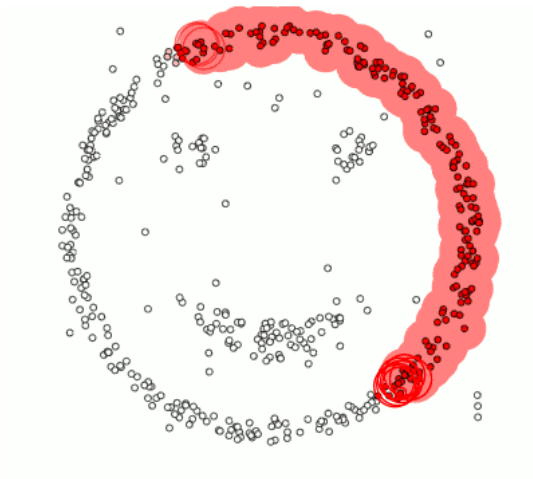
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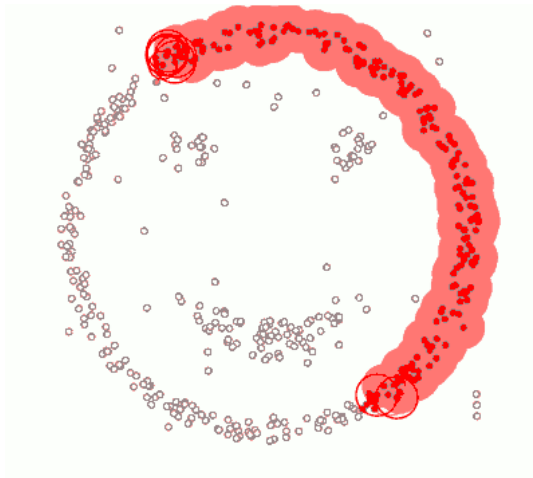
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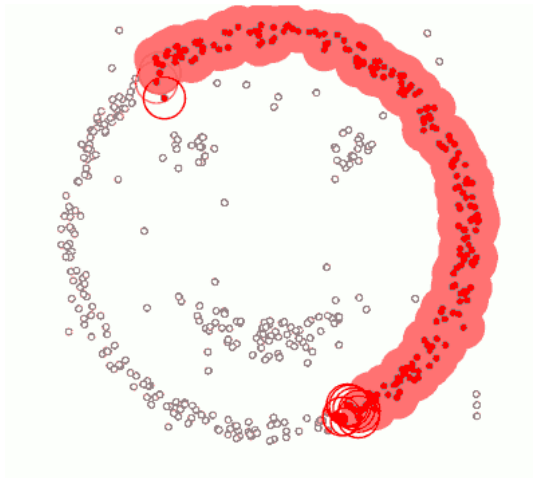
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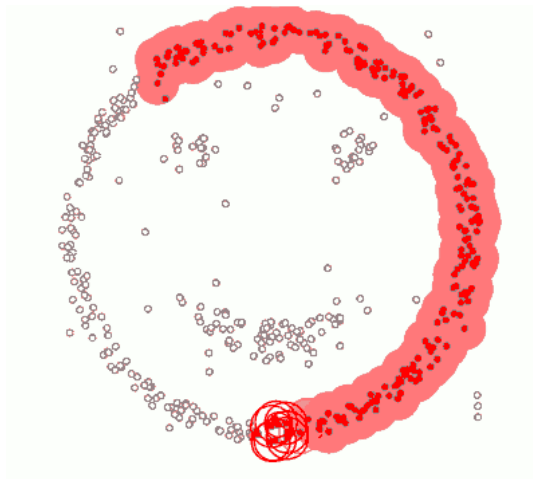
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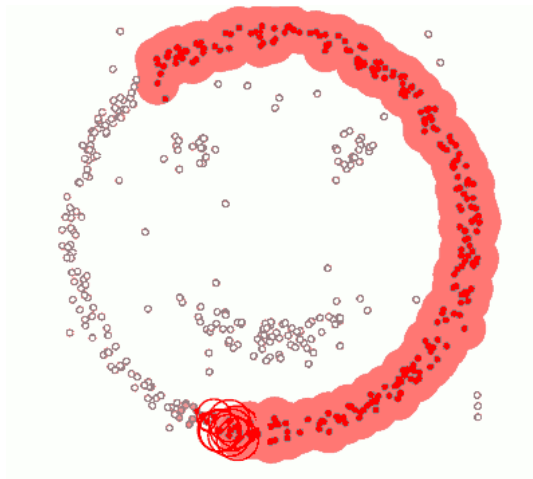
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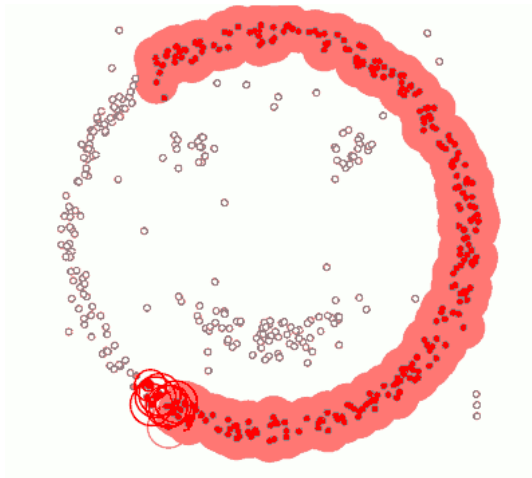
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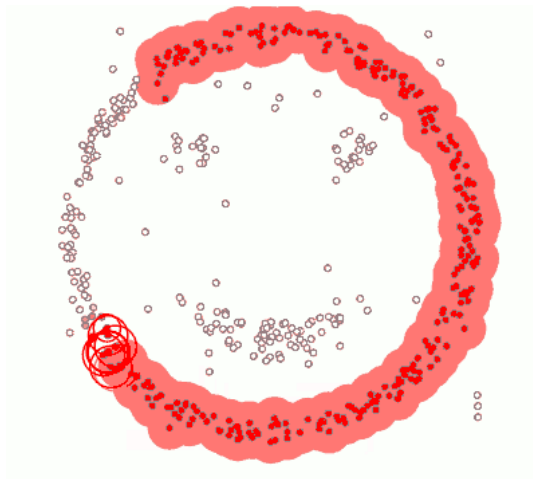
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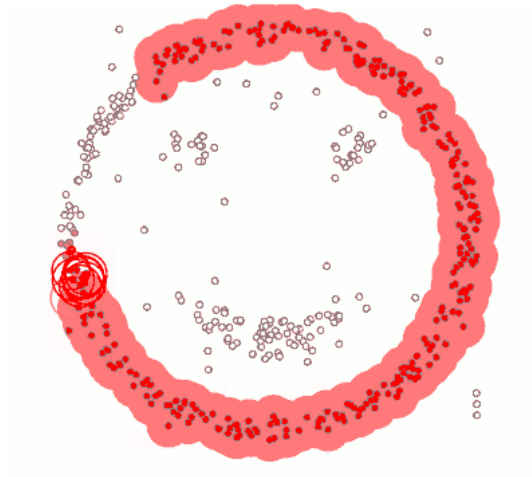
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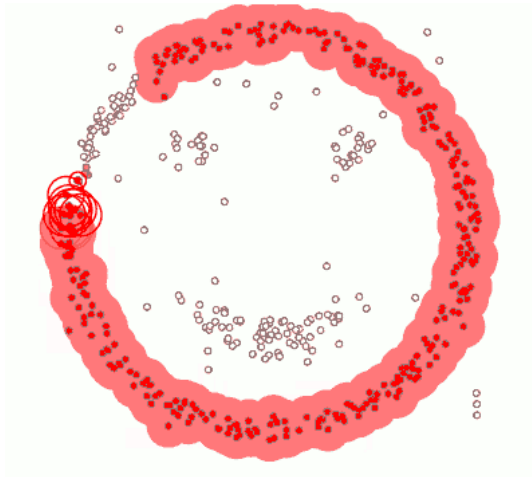
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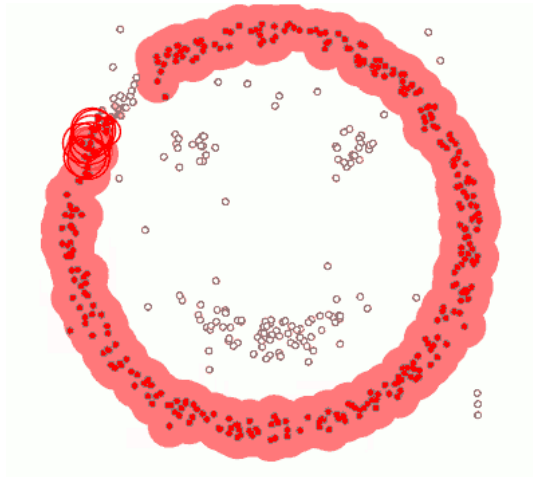
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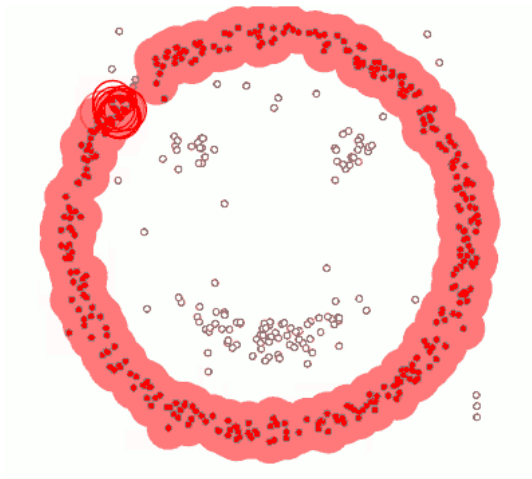
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k-means
Other clustering algorithms
Hierarchical clustering
Validation

Mean-shift
DBSCAN
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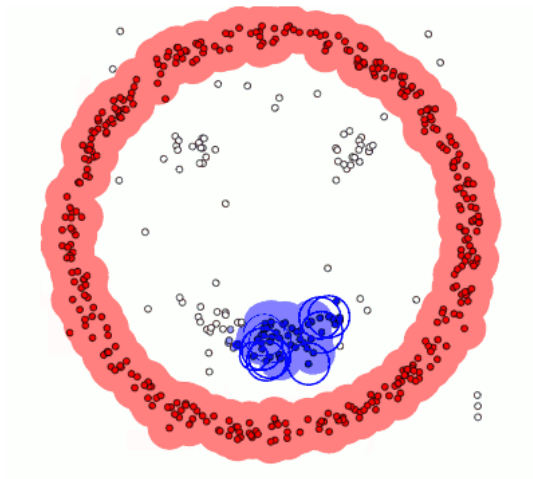
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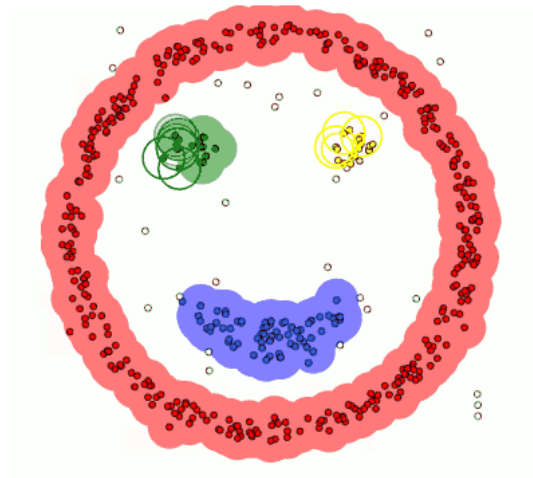
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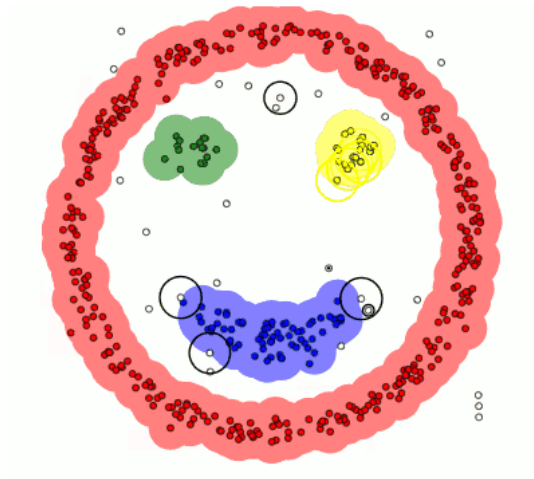
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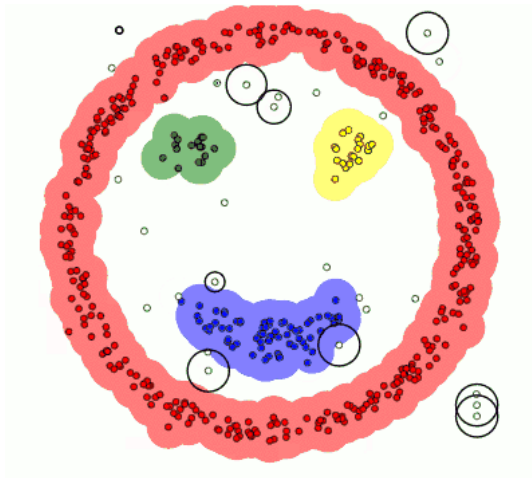
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What is clustering? Motivation?
k-means
Other clustering algorithms
Hierarchical clustering
Validation

Mean-shift
DBSCAN
GMM: Gaussian Mixture Model

DBSCAN



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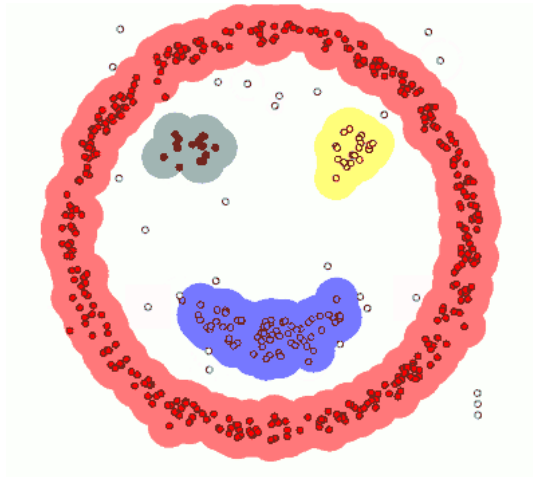
Validation

Mean-shift

DBSCAN

GMM: Gaussian Mixture Model

DBSCAN



DBSCAN

2 parameters: ϵ and *minPts*.

- Find the points in the ϵ -neighborhood of every point, and identify the core points with more than *minPts* neighbors.
- Find the connected components of core points on the neighbor graph, ignoring all non-core points.
- Assign each non-core point to a nearby cluster if the cluster is an ϵ -neighbor (call it a border point), otherwise assign it to noise.

DBSCAN

Choosing ϵ and $minPts$?

- The idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor

What is clustering? Motivation?

k-means

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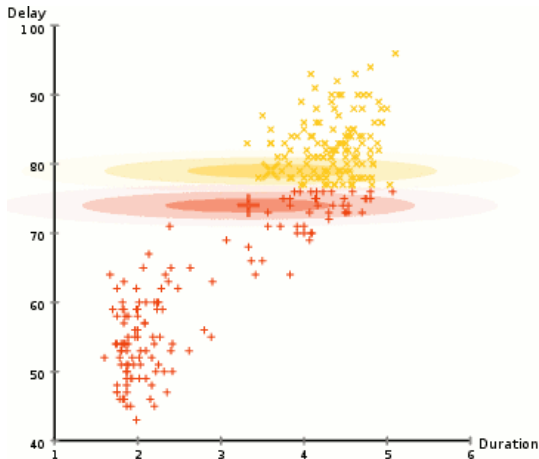
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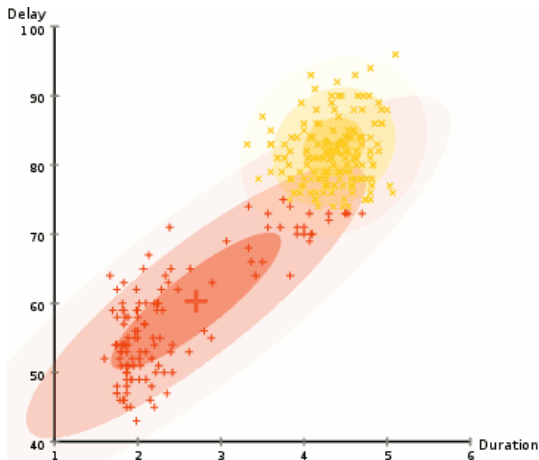
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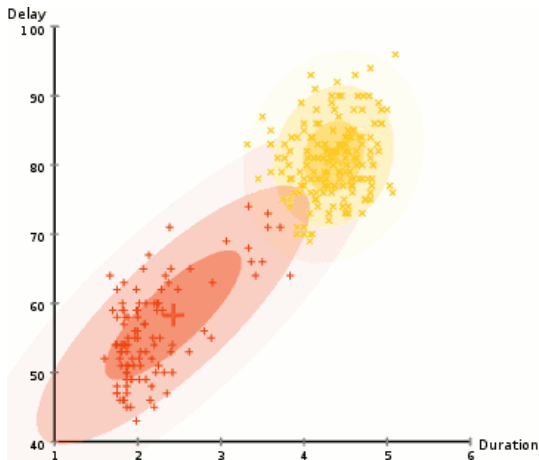
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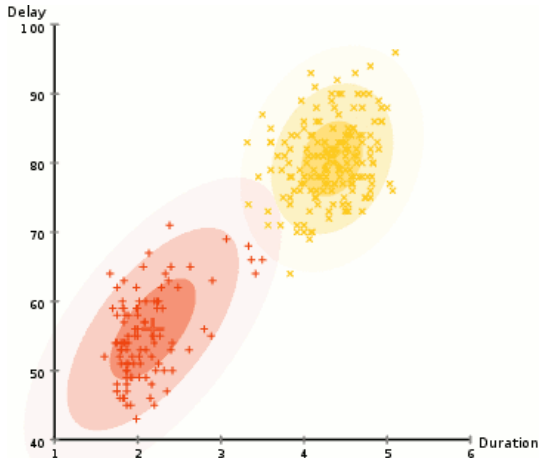
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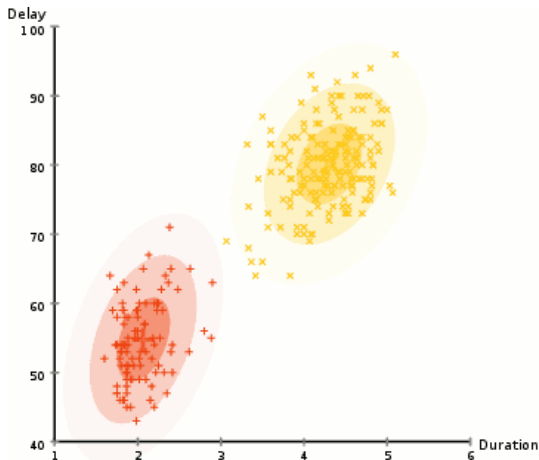
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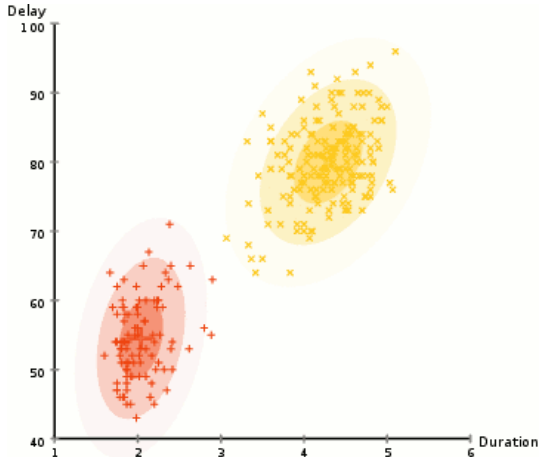
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Mean-shift

DBSCAN

GMM: Gaussian Mixture Model

GMM: Gaussian Mixture Model



GMM: Gaussian Mixture Model

- Model: K gaussians (one-dimensional):

- $p(x) = \sum_{k=1}^K \Phi_k N(x|\mu_k, \sigma_k)$
- $N(x|\mu_k, \sigma_k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$
- $\sum_{k=1}^K \Phi_k = 1$

- Want to maximize $\prod_{i=1}^n p(x_i)$

- 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 (Φ_k, μ_k, σ_k)
- (E-step) for each i, k compute $\gamma_{i,k} \sim$ did x_i came from k ?
- (M-step) adjust (Φ_k, μ_k, σ_k) to fit points assigned to them
- iterate until convergence

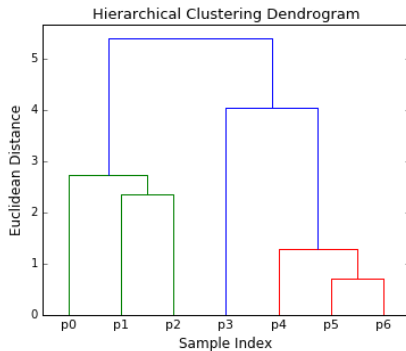
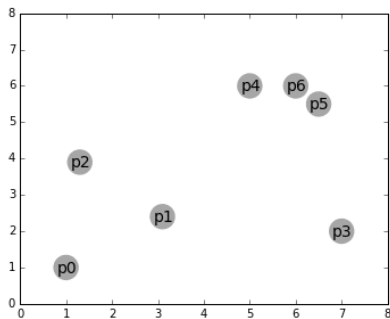
$$\gamma_{i,k} = \frac{\Phi_k \mathcal{N}(x_i | \mu_k, \sigma_k)}{\sum_{k=1}^K \Phi_k \mathcal{N}(x_i | \mu_k, \sigma_k)}$$

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

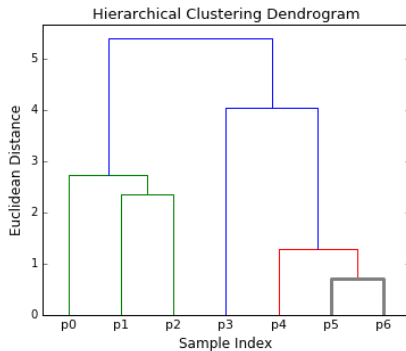
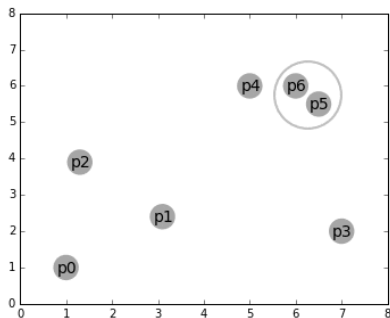
Outline

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

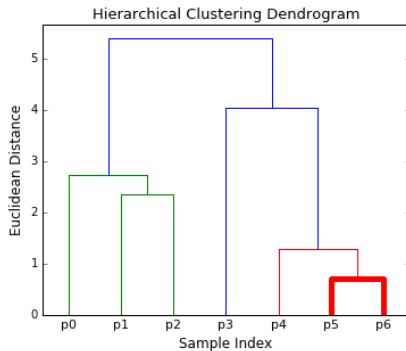
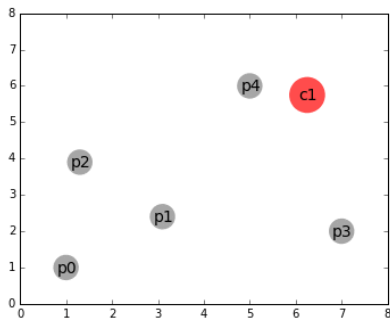
Hierarchical clustering



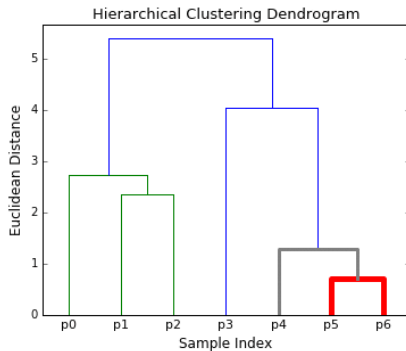
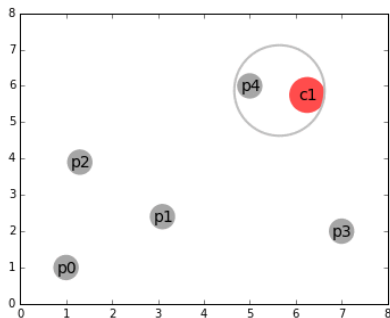
Hierarchical clustering



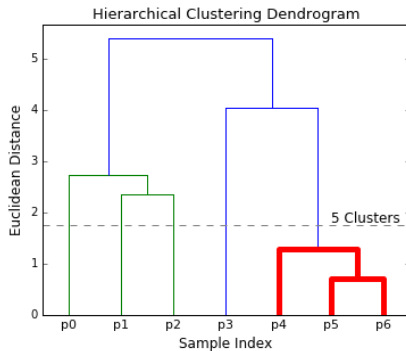
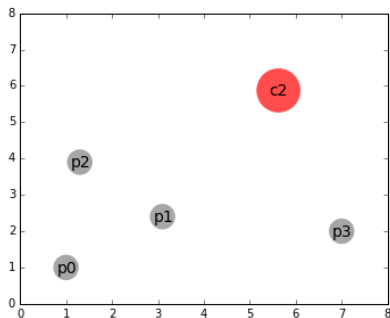
Hierarchical clustering



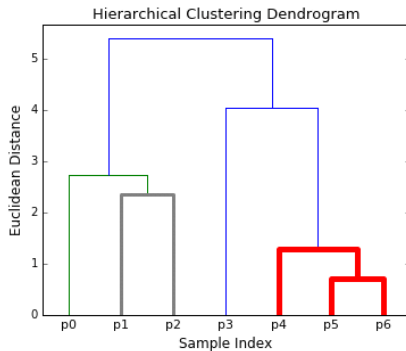
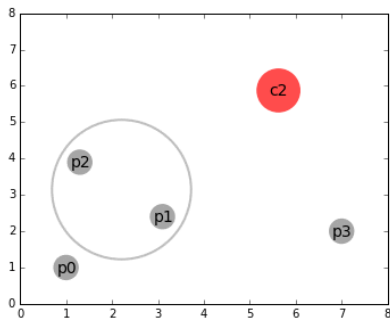
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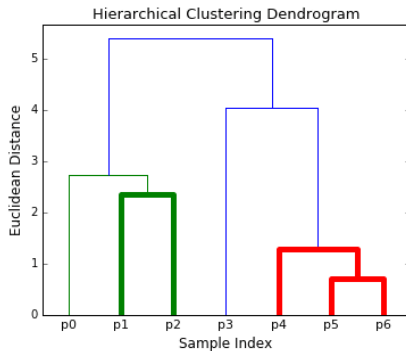
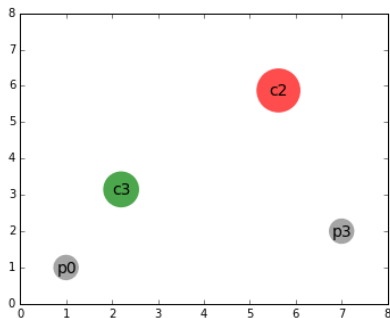
Hierarchical clustering



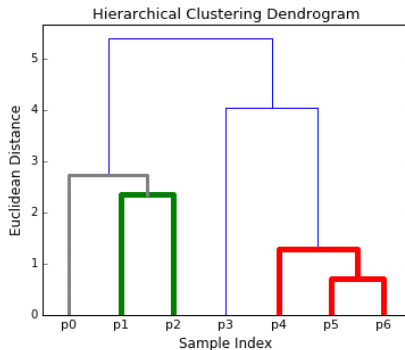
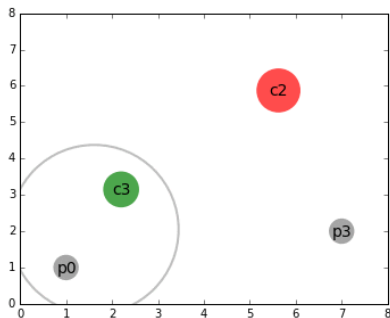
Hierarchical clustering



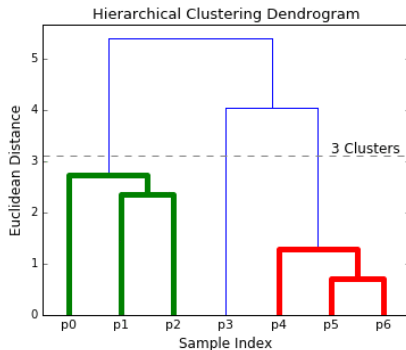
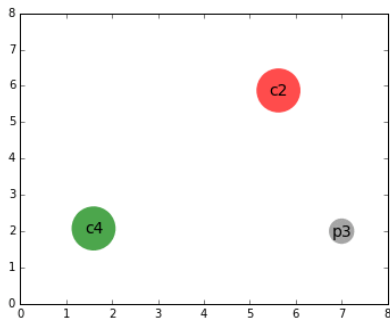
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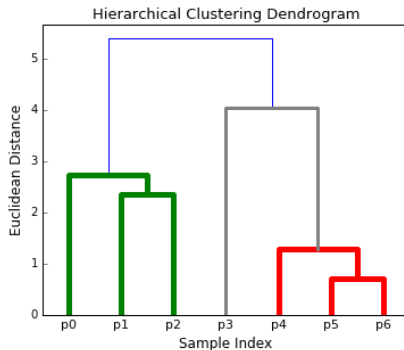
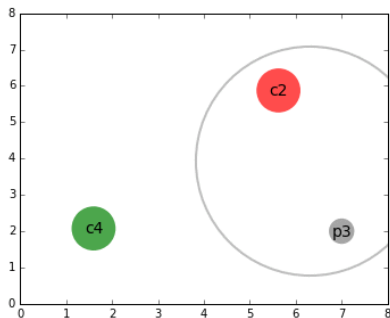
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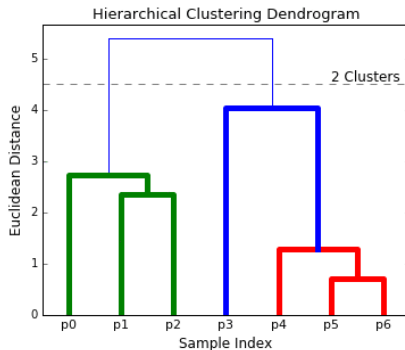
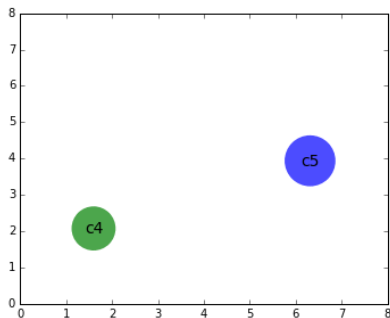
Hierarchical clustering



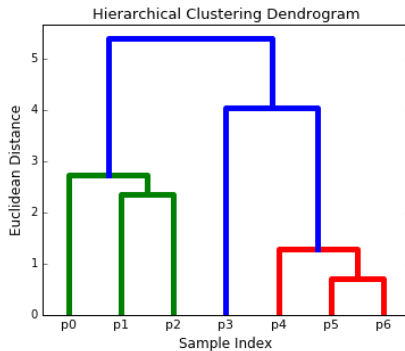
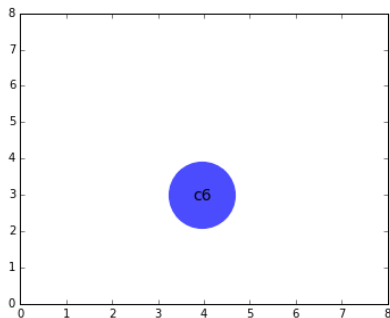
Hierarchical clustering



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:

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

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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, silhouette score)
- 2 External Index: Used to measure the extent to which cluster labels match externally supplied class labels. (e.g. Entropy, Adjusted Rand Index)

Entropy

- 1 Given a discrete random variable X with possible value $\{1, \dots, n\}$, entropy is defined as

$$H(X) = - \sum_{i=1}^n P(X = i) \log_2(P(X = i))$$

- 2 Entropy measures how uncertain is an event, the larger the entropy the more uncertain is the event.

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:

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

Principal Component Analysis (PCA)

- PCA is a method to reduce the number of dimensions of the data.
- If the number of dimensions is reduced to 2 or 3 then the data points can be visualised/plotted. For high dimensional data, it can be used to fasten downstream ML tasks.
- PCA can be thought of as fitting a p -dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component.
- If some axis of the ellipsoid is small, then the variance along that axis is also small, and we can omitting it.