M.D. & A.G. 2021

11. Clustering

Network Data Analysis - NDA'21
M. Danisch and A. Giovanidis

Sorbonne-LIP6

Decembre 08, 2021

Bibliography

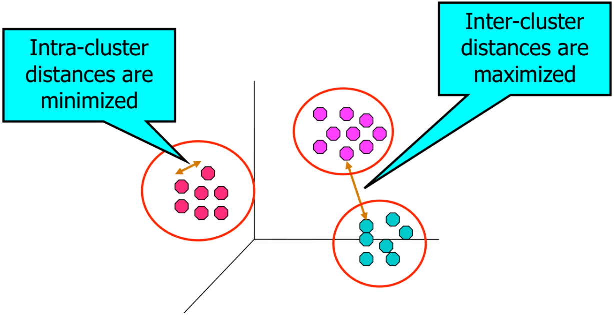
M.D. & A.G. 2021

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

What is clustering?

M.D. & A.G. 2021

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?

M.D. & A.G. 2021

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

Why is it useful?

M.D. & A.G. 2021

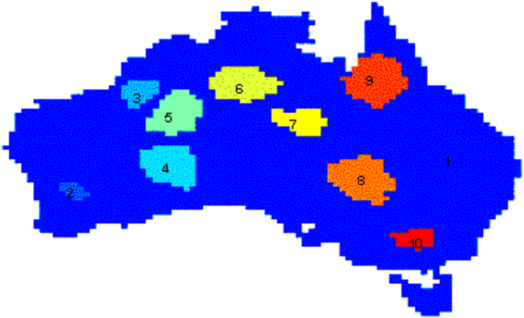
Understanding the data / get insights on the data:

- 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

M.D. & A.G. 2021

Why is it usefull (applications of cluster analysis)?

Summarization: Reduce the size of large data sets

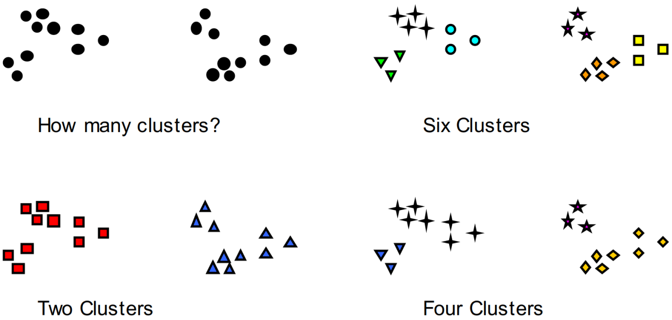


Clustering precipitation in Australia

Custering is an ill-defined problem

M.D. & A.G. 2021

How many clusters?



- An Impossibility Theorem for Clustering, Jon Kleinberg, NeurIPS 2015.

Several types of clusters

M.D. & A.G. 2021

1. **Well-separated:** any point in a cluster is closer to every other point in this cluster than to any point not in this cluster.
2. **Center-based:** any point in a cluster is closer to the center of this cluster, than to the center of any other cluster.
3. **Contiguous:** any point in a cluster is closer to one or more other points in the cluster than to any point not in the cluster.
4. **Density-based:** a cluster is a dense region of points, separated by low-density regions from other regions of high density (other clusters).

Several types of clusterings

M.D. & A.G. 2021

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

- **Partitional clustering:** A partition (split/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

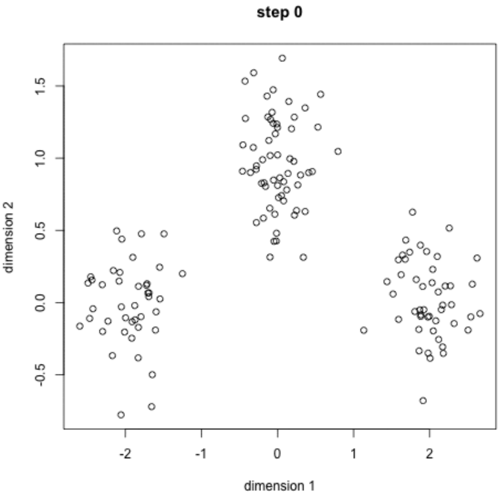
M.D. & A.G. 2021

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.

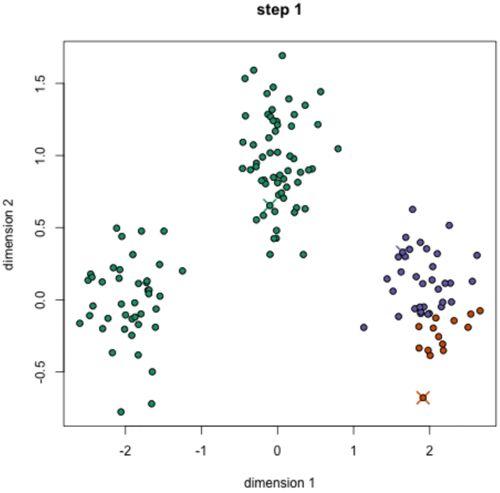
k-means

M.D. & A.G. 2021



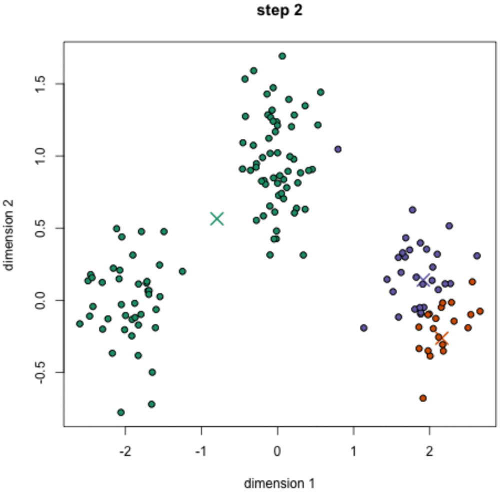
k-means

M.D. & A.G. 2021



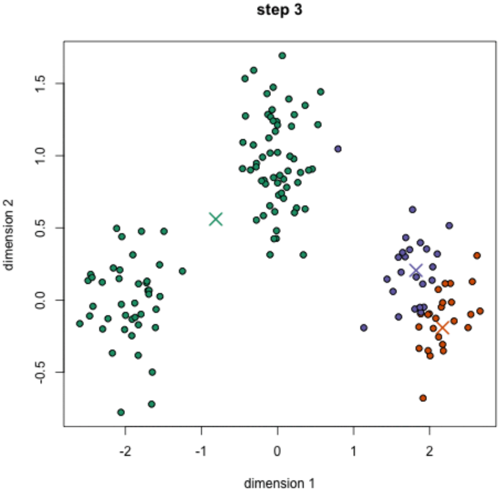
k-means

M.D. & A.G. 2021



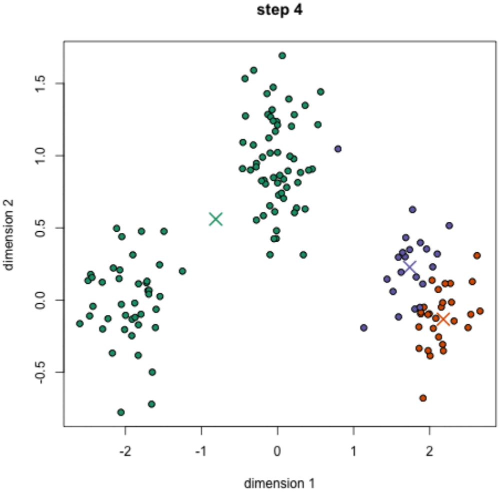
M.D. & A.G. 2021

k-means



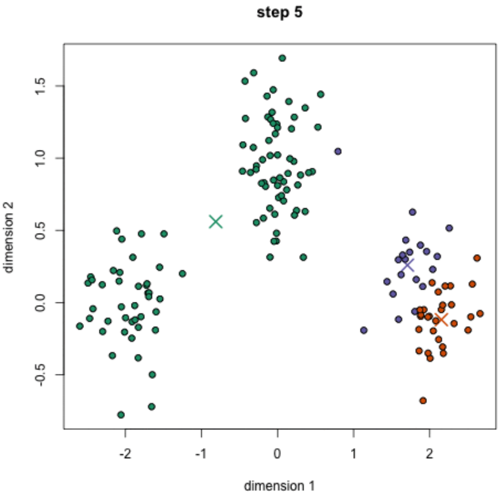
M.D. & A.G. 2021

k-means



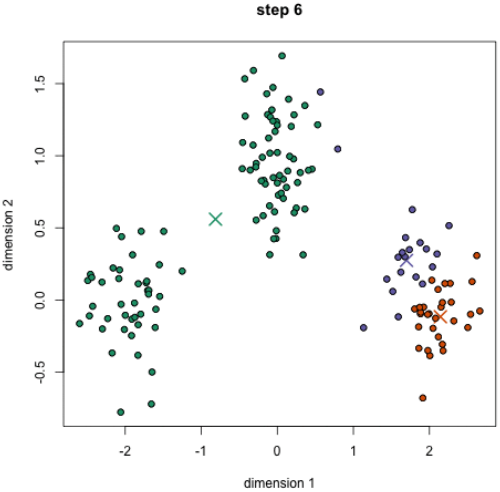
k-means

M.D. & A.G. 2021



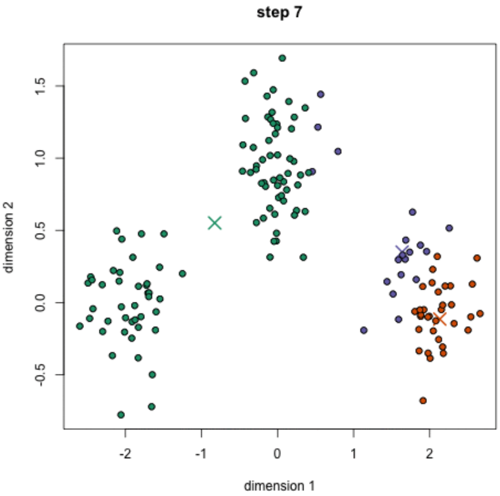
M.D. & A.G. 2021

k-means



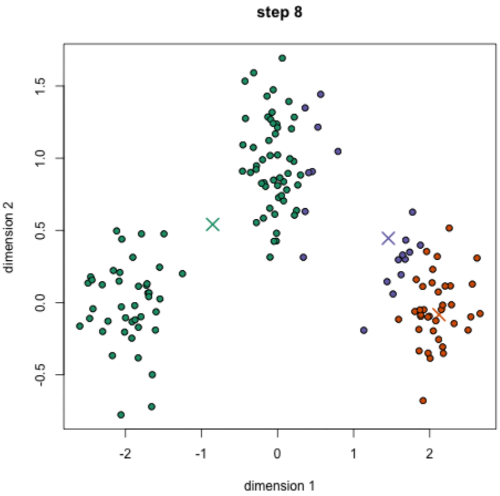
k-means

M.D. & A.G. 2021



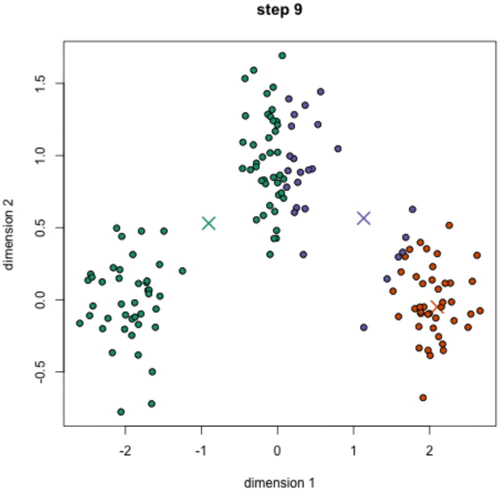
k-means

M.D. & A.G. 2021



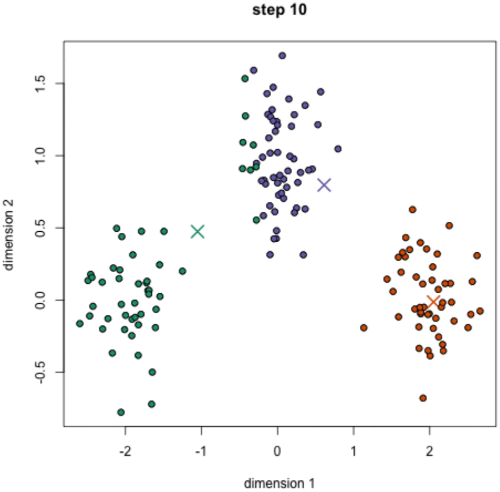
k-means

M.D. & A.G. 2021



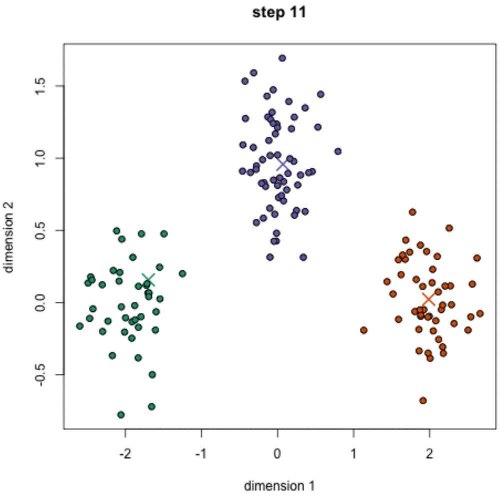
k-means

M.D. & A.G. 2021



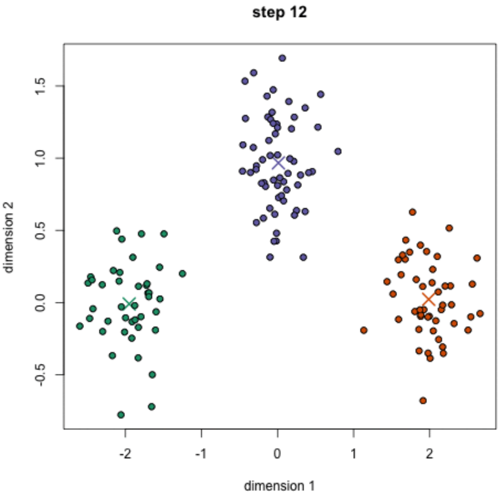
k-means

M.D. & A.G. 2021



k-means

M.D. & A.G. 2021



k-means

M.D. & A.G. 2021

- 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

M.D. & A.G. 2021

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

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

$$\text{distortion} = \sum_{j=1}^{k} \sum_{i=1}^{n} \delta_{i,j} ||\mathbf{x}_i - \mu_j||_2^2$$

or SSD: Sum-of-Square-Deviations, with

- μ_j the vector of centroid j and
- $\delta_{i,j} = 1$ if the sample $\mathbf{x}_i$ is in cluster j and 0 otherwise.

☞ $||\mathbf{x}_i - \mu_j||_2^2 = \sum_{p=1}^{P} (x_{i,p} - \mu_{j,p})^2$ is the **Euclidean distance**.

✂ An exact solution to the above problem would be NP-hard.

Limitation of k-means: clusters

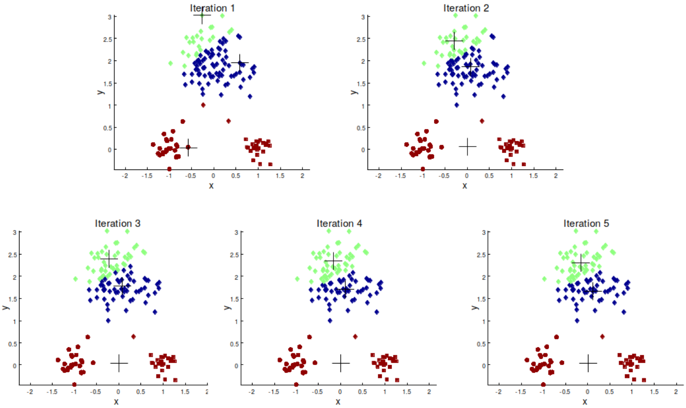
M.D. & A.G. 2021

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

Normalising the data and removing outliers can help!

M.D. & A.G. 2021

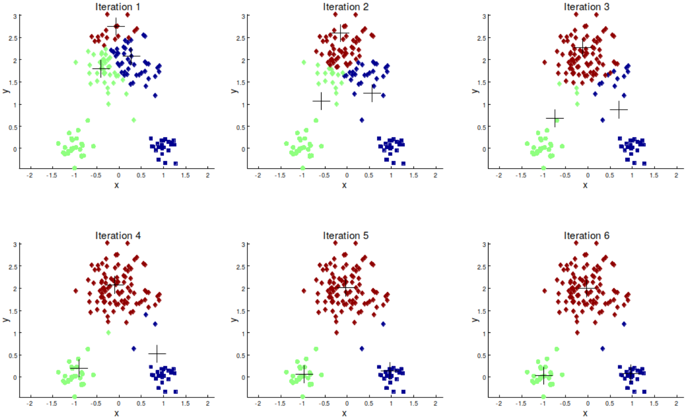
Limitation of k-means: initialisation



Using multiple runs or kmeans++ can help!

M.D. & A.G. 2021

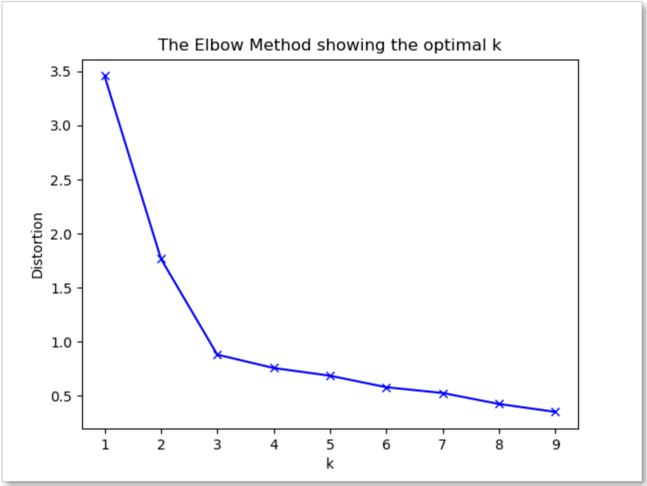
Limitation of k-means: initialisation



Using multiple runs or kmeans++ can help!

Limitation of k-means: How to choose k?

M.D. & A.G. 2021



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

Limitation of k-means: How to choose k? M.D. & A.G. 2021

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**

Distance choice

M.D. & A.G. 2021

The Euclidean distance creates ball-shaped clusters:

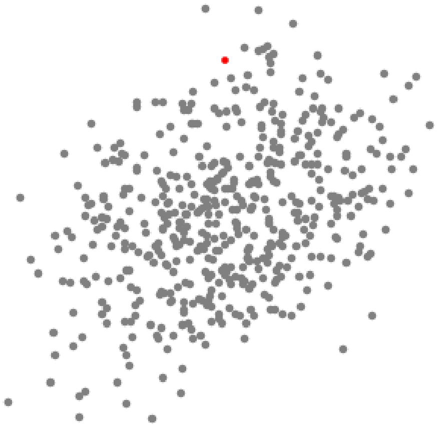
$$d_E\left(\mathbf{x}_i,\ \mu_j\right) = ||\mathbf{x}_i - \mu_j||_2 = \sqrt{\sum_{p=1}^{P} \left(x_{i,p} - \mu_{j,p}\right)^2}$$

☞ Alternative distance metrics for other shapes

- Mahalanobis: $d_M\left(\mathbf{x}_i,\ \mu_j\right) = \sqrt{\left(\mathbf{x}_i - \mu_j\right)^T \mathbf{S}^{-1} \left(\mathbf{x}_i - \mu_j\right)}$
- norm-1: $d_{L1}\left(\mathbf{x}_i,\ \mu_j\right) = \sum_{p=1}^{P} |x_{i,p} - \mu_{j,p}|$
- Hyperbolic: $d_H\left(\mathbf{x}_i,\ \mu_j\right) = arcosh\left(1 + 2\frac{||\mathbf{x}_i - \mu_j||_2^2}{\left(1 - ||\mathbf{x}_i||_2^2\right)\left(1 - ||\mu_j||_2^2\right)}\right)$

Mean-shift (with one centroid)

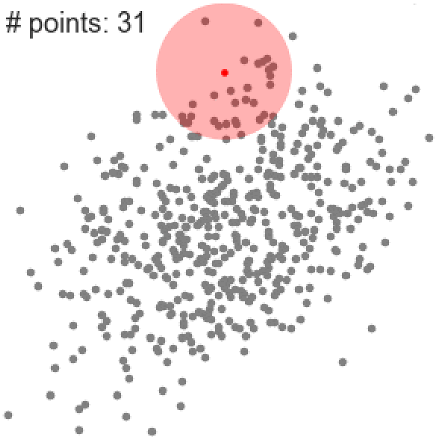
M.D. & A.G. 2021



The centroid moves towards a higher density region

Mean-shift (with one centroid)

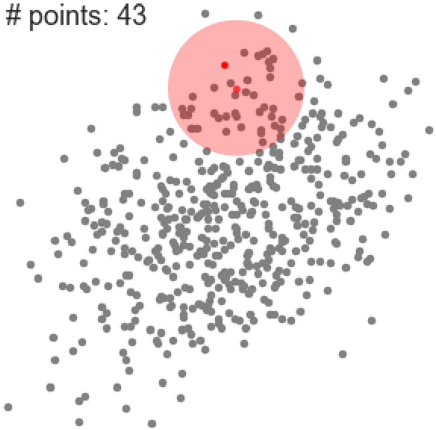
M.D. & A.G. 2021



The centroid moves towards a higher density region

Mean-shift (with one centroid)

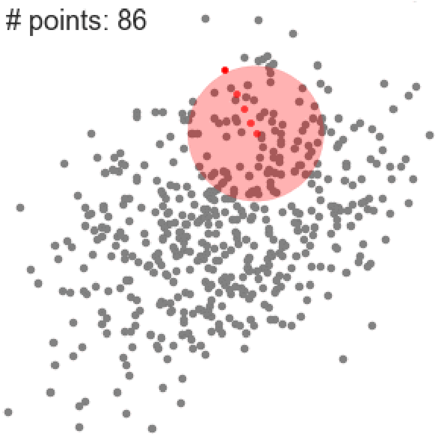
M.D. & A.G. 2021



The centroid moves towards a higher density region

M.D. & A.G. 2021

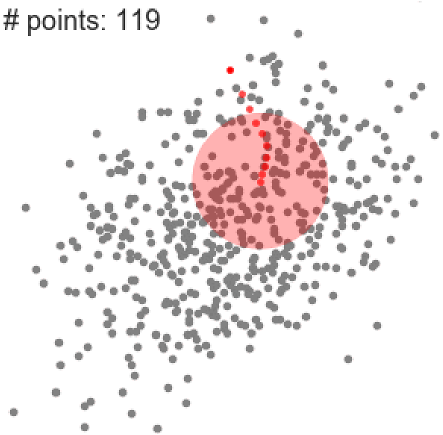
Mean-shift (with one centroid)



The centroid moves towards a higher density region

M.D. & A.G. 2021

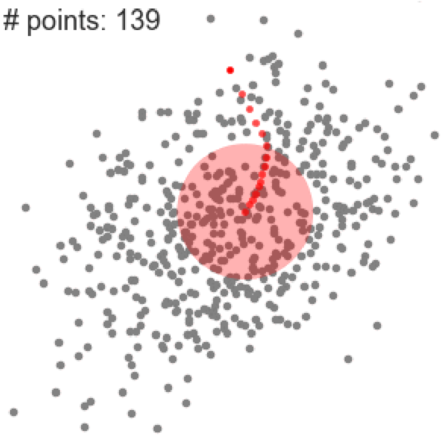
Mean-shift (with one centroid)



The centroid moves towards a higher density region

M.D. & A.G. 2021

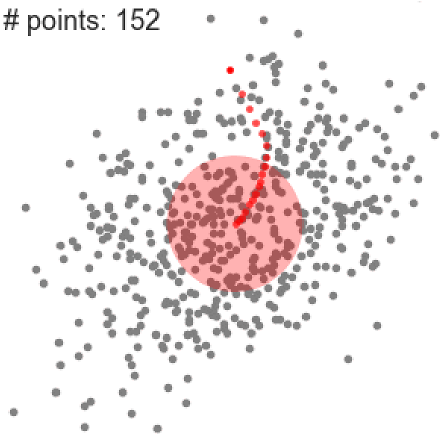
Mean-shift (with one centroid)



The centroid moves towards a higher density region

Mean-shift (with one centroid)

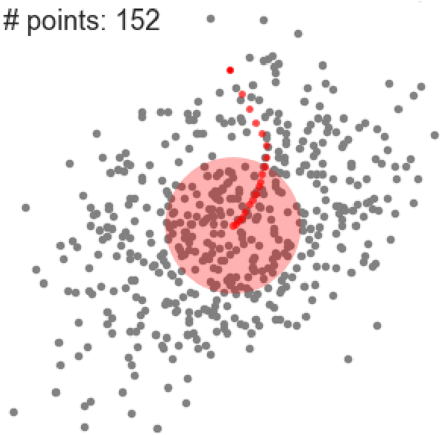
M.D. & A.G. 2021



The centroid moves towards a higher density region

M.D. & A.G. 2021

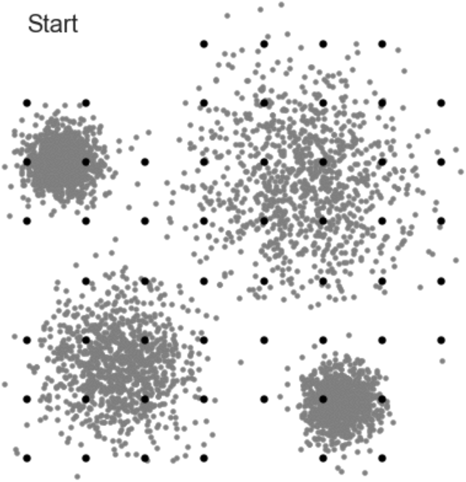
Mean-shift (with one centroid)



The centroid moves towards a higher density region

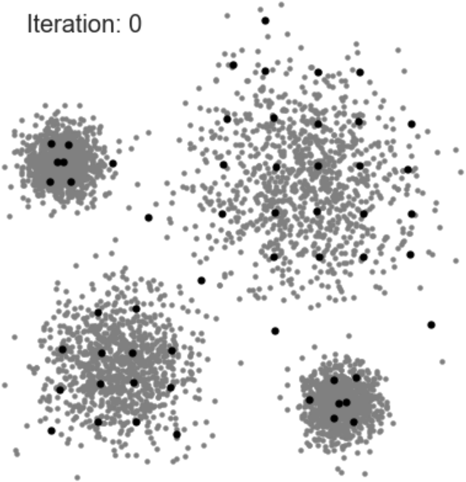
Mean-shift

M.D. & A.G. 2021



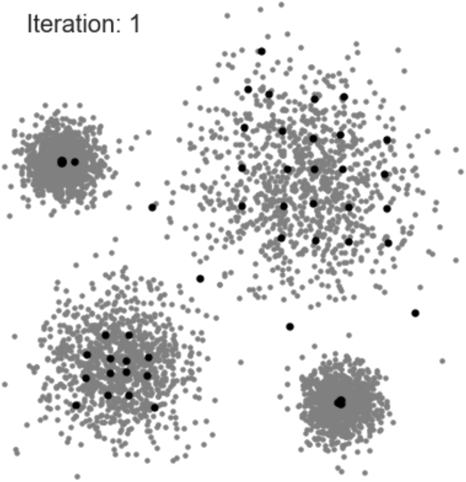
Mean-shift

M.D. & A.G. 2021



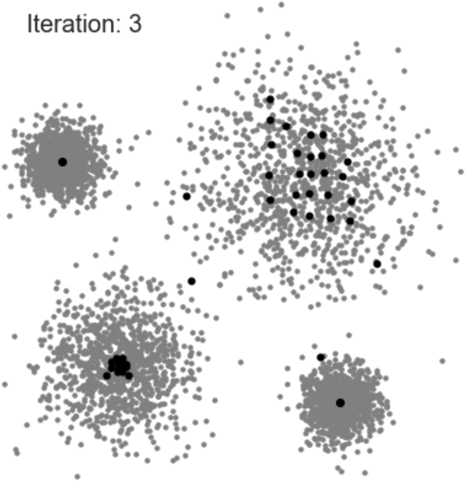
Mean-shift

M.D. & A.G. 2021



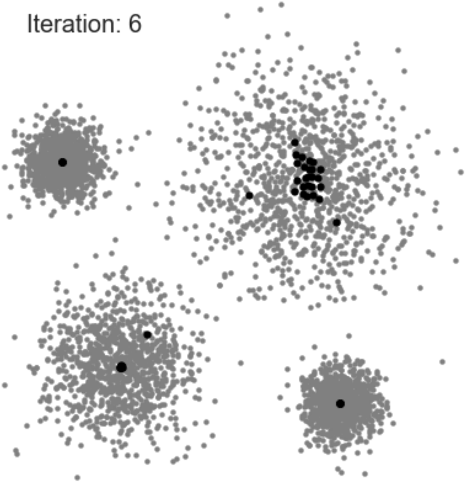
Mean-shift

M.D. & A.G. 2021



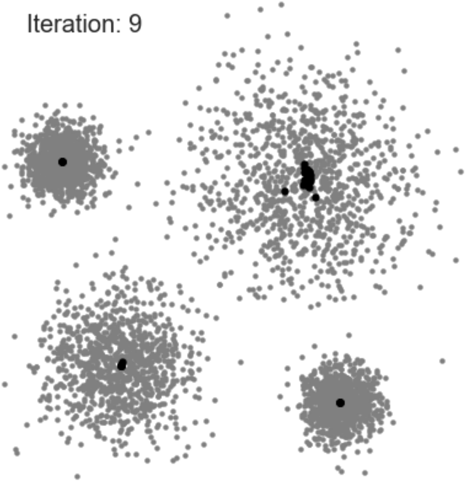
M.D. & A.G. 2021

Mean-shift



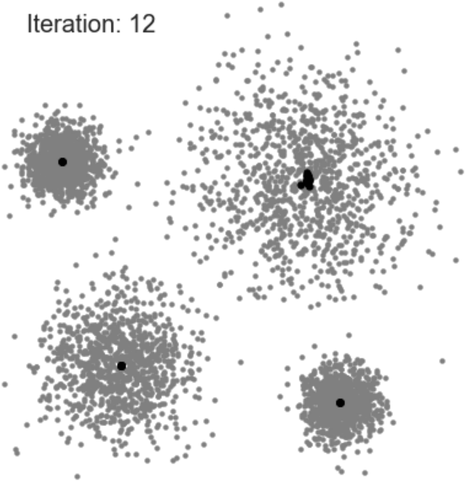
Mean-shift

M.D. & A.G. 2021



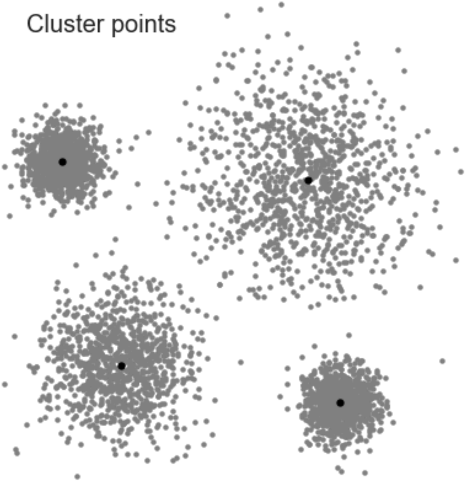
Mean-shift

M.D. & A.G. 2021



Mean-shift

M.D. & A.G. 2021



Mean-shift

M.D. & A.G. 2021

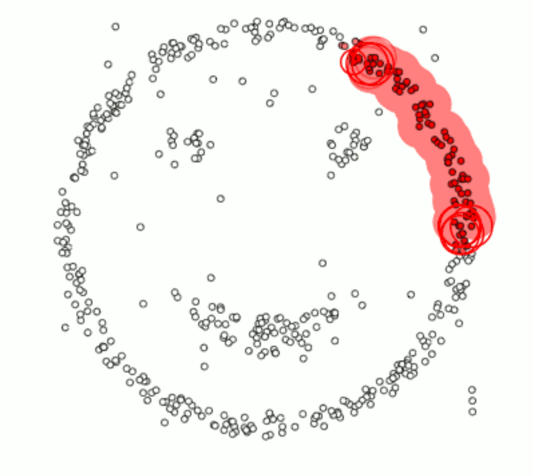
Mean-shift

M.D. & A.G. 2021

- 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.

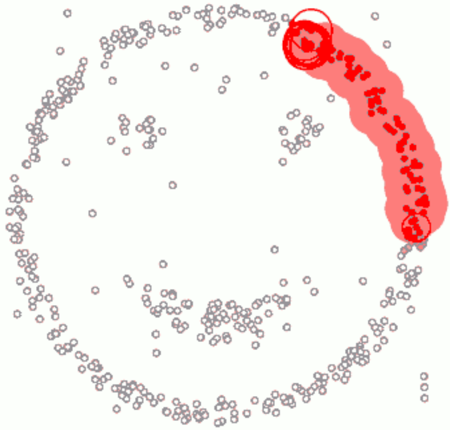
DBSCAN

M.D. & A.G. 2021



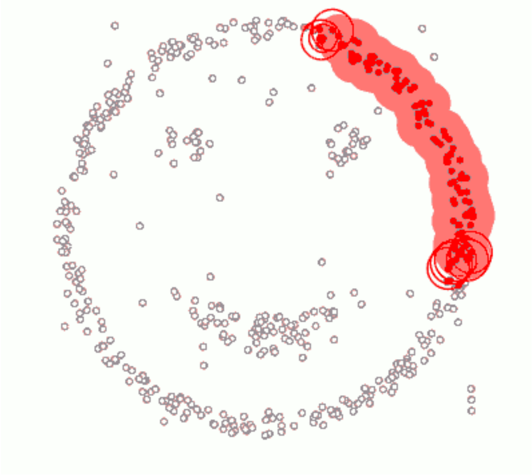
DBSCAN

M.D. & A.G. 2021



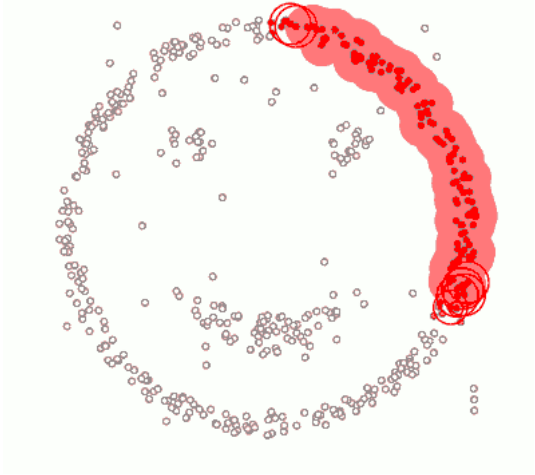
DBSCAN

M.D. & A.G. 2021



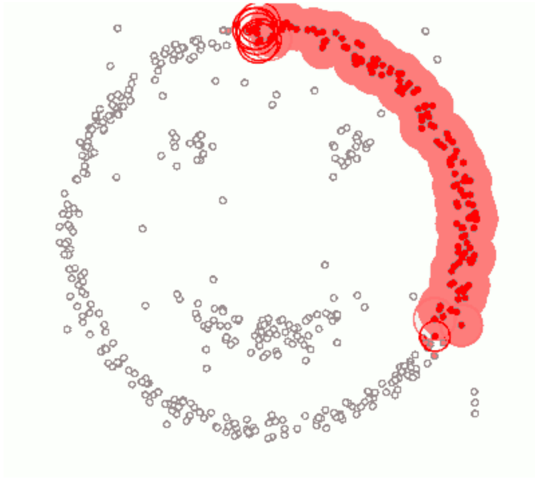
DBSCAN

M.D. & A.G. 2021



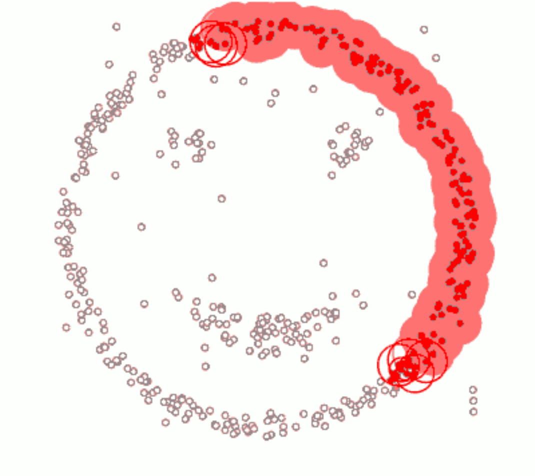
DBSCAN

M.D. & A.G. 2021



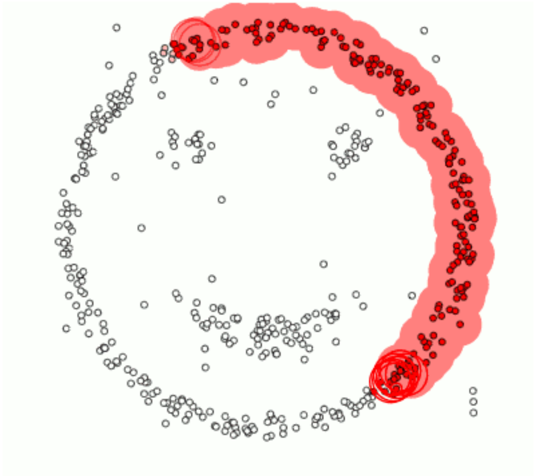
DBSCAN

M.D. & A.G. 2021



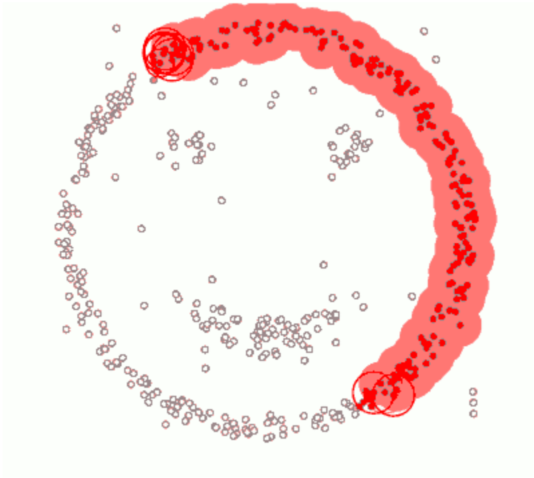
DBSCAN

M.D. & A.G. 2021



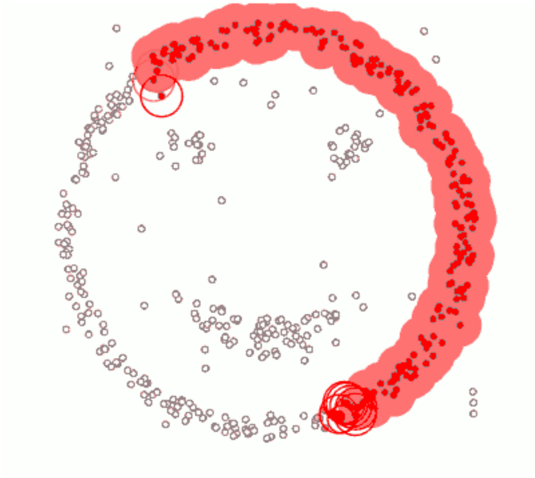
DBSCAN

M.D. & A.G. 2021



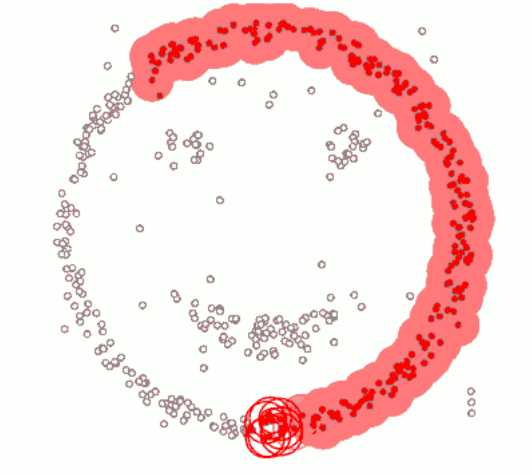
DBSCAN

M.D. & A.G. 2021



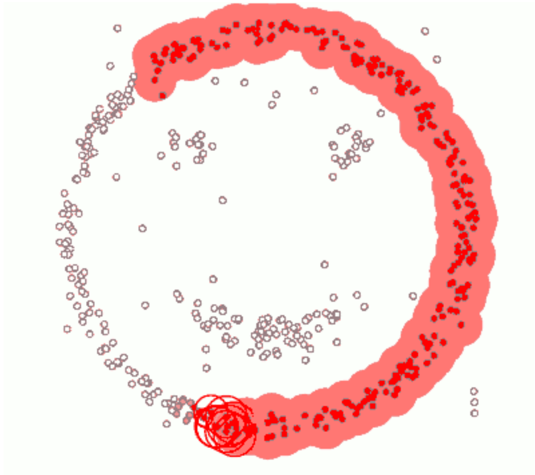
DBSCAN

M.D. & A.G. 2021



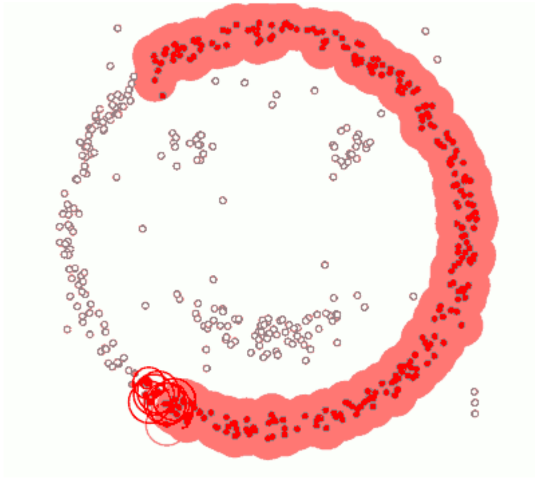
DBSCAN

M.D. & A.G. 2021



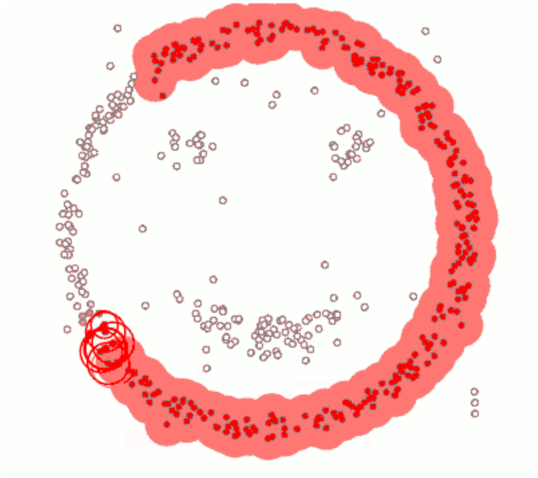
DBSCAN

M.D. & A.G. 2021



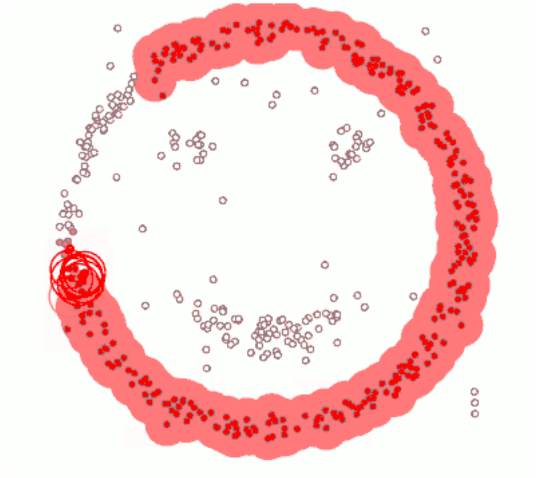
DBSCAN

M.D. & A.G. 2021



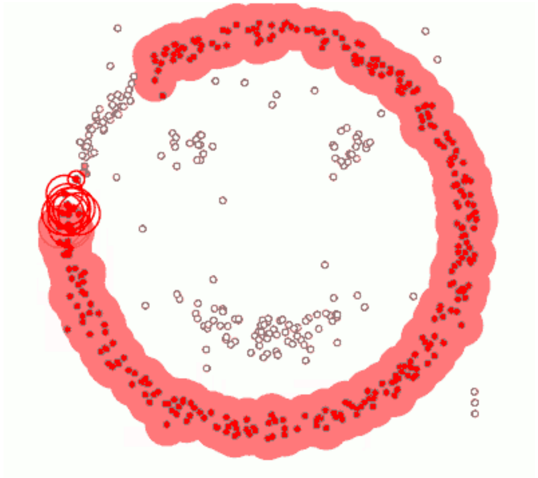
DBSCAN

M.D. & A.G. 2021



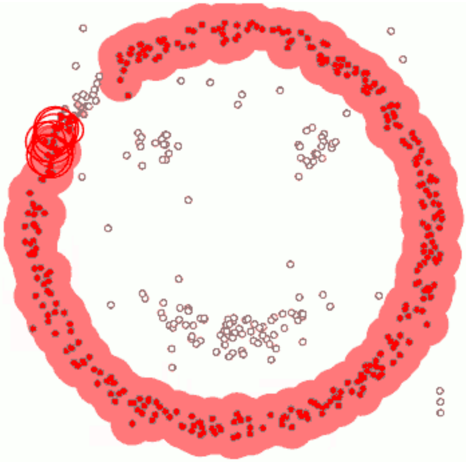
DBSCAN

M.D. & A.G. 2021



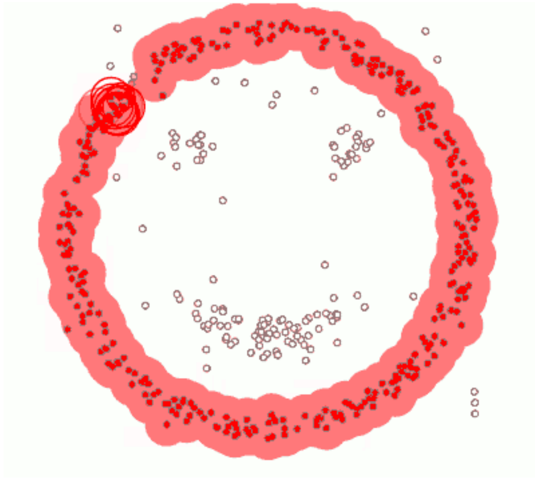
M.D. & A.G. 2021

DBSCAN



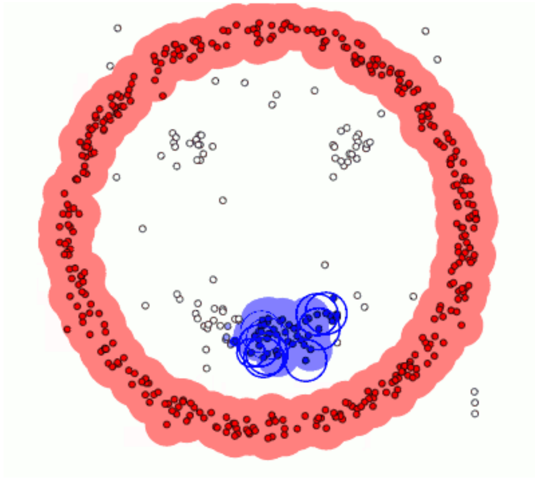
DBSCAN

M.D. & A.G. 2021



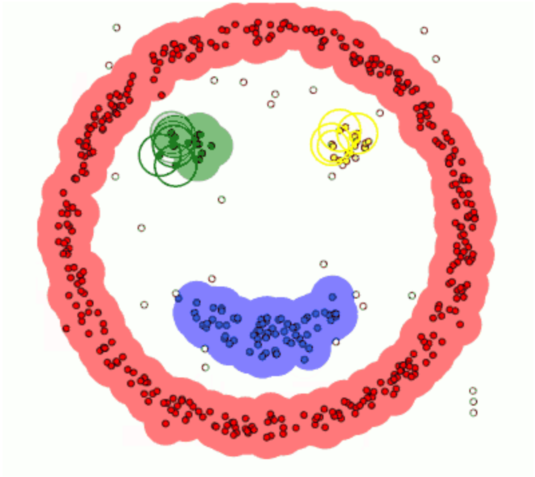
DBSCAN

M.D. & A.G. 2021



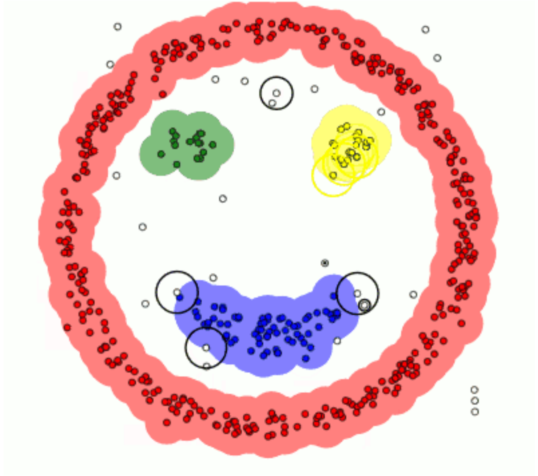
DBSCAN

M.D. & A.G. 2021



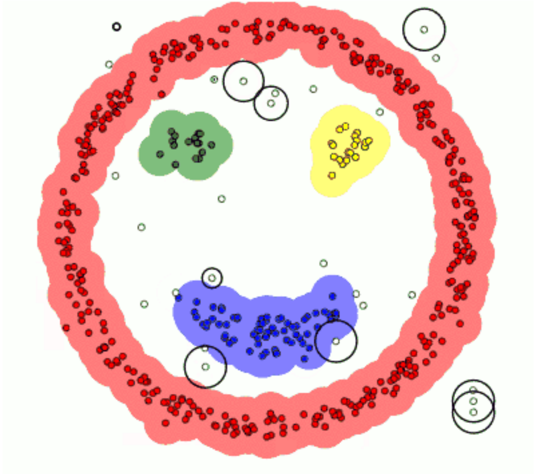
DBSCAN

M.D. & A.G. 2021



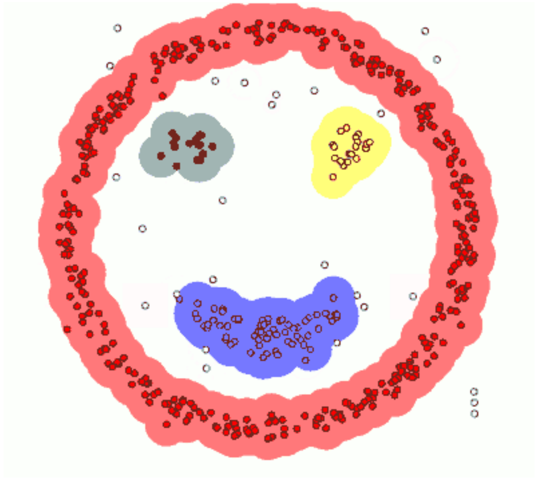
DBSCAN

M.D. & A.G. 2021



DBSCAN

M.D. & A.G. 2021



DBSCAN

M.D. & A.G. 2021

It groups together points that are closely packed together (=points with many nearby neighbours)

2 parameters: ϵ (=radius) and *minPts*.
3 types of points: • core points, • reachable points, • outliers

- 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 (outlier).

DBSCAN

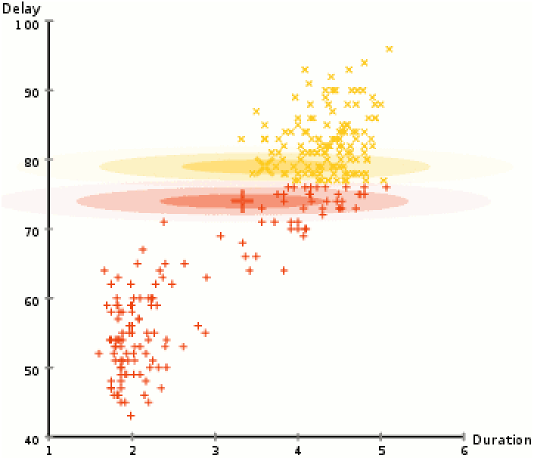
M.D. & A.G. 2021

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

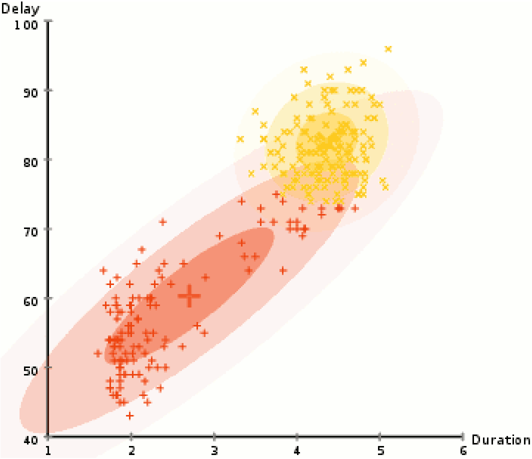
M.D. & A.G. 2021

GMM: Gaussian Mixture Model



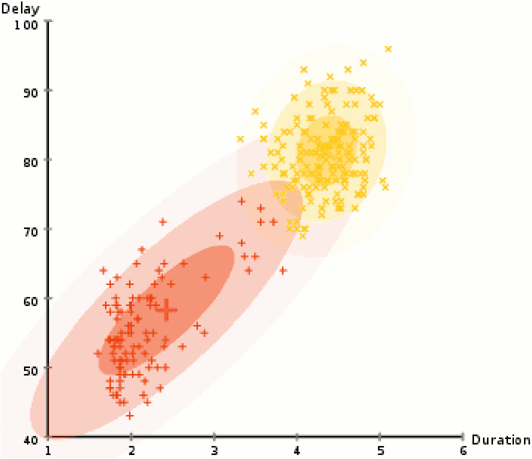
GMM: Gaussian Mixture Model

M.D. & A.G. 2021



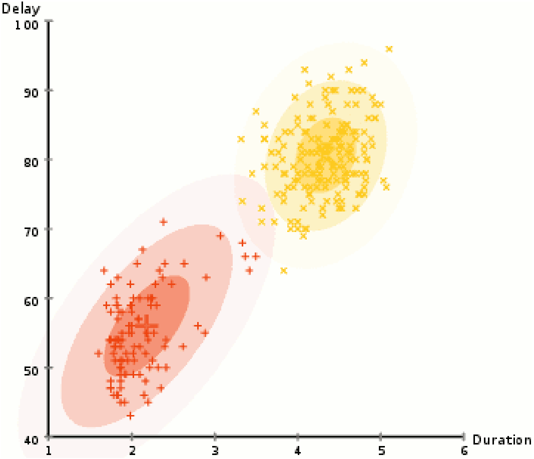
GMM: Gaussian Mixture Model

M.D. & A.G. 2021



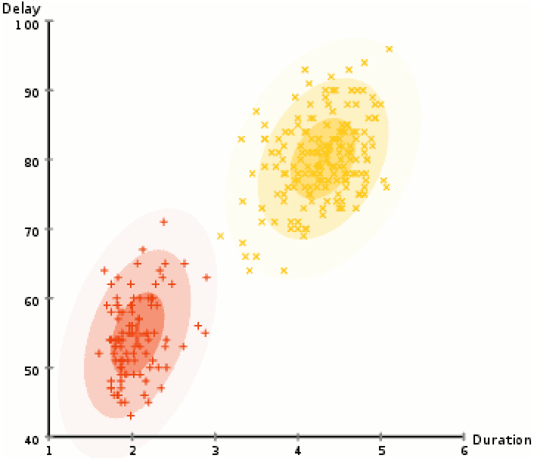
GMM: Gaussian Mixture Model

M.D. & A.G. 2021



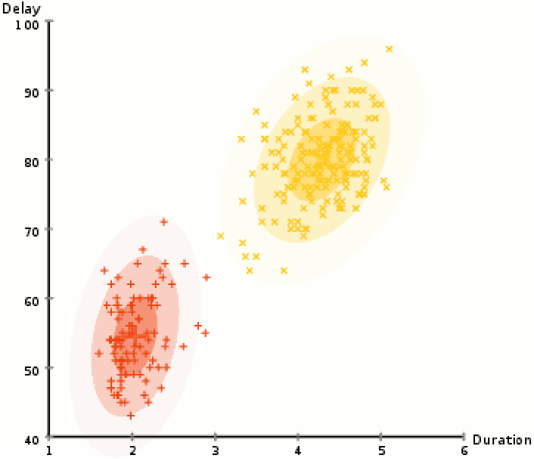
GMM: Gaussian Mixture Model

M.D. & A.G. 2021



GMM: Gaussian Mixture Model

M.D. & A.G. 2021



GMM: Gaussian Mixture Model

M.D. & A.G. 2021

- Model: K gaussians (e.g. in one-dimension/feature):
  - $p(x) = \sum_{k=1}^{K} \Phi_k N(x|\mu_k, \sigma_k)$
  - $N(x|\mu_k, \sigma_k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$
  - $\sum_{k=1}^{K} \Phi_k = 1$
- Want to maximize likelihood $\prod_{i=1}^{n} p(x_i)$
- 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

M.D. & A.G. 2021

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

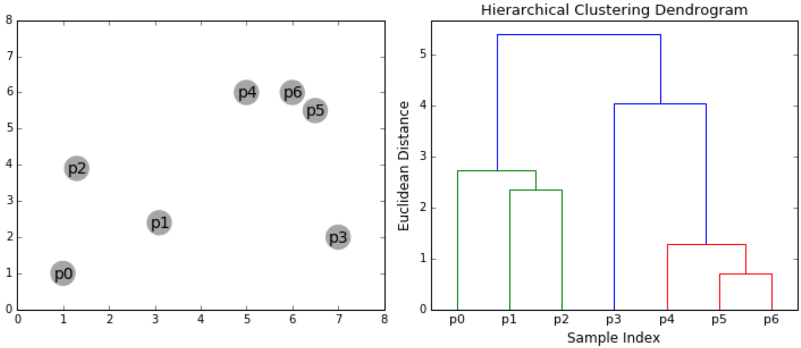
$$\gamma_{i,k} = \frac{\Phi_k \mathcal{N}(x|\mu_k,\sigma_k)}{\sum_{k=1}^{K} \Phi_k \mathcal{N}(x|\mu_k,\sigma_k)}$$

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

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

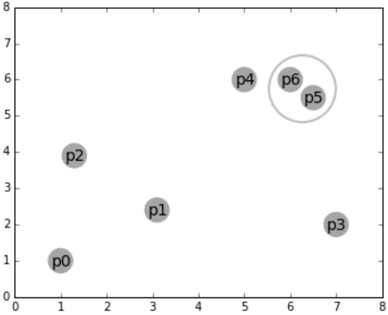
Hierarchical clustering

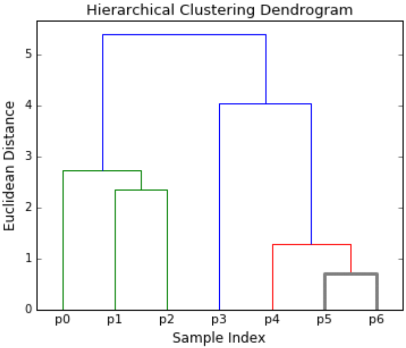
M.D. & A.G. 2021



Hierarchical clustering

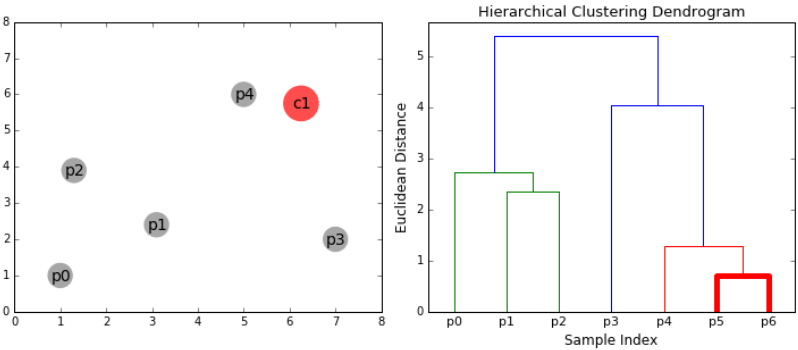
M.D. & A.G. 2021





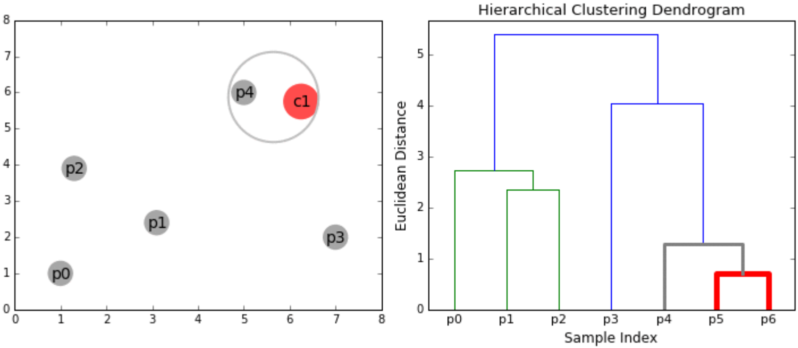
Hierarchical clustering

M.D. & A.G. 2021



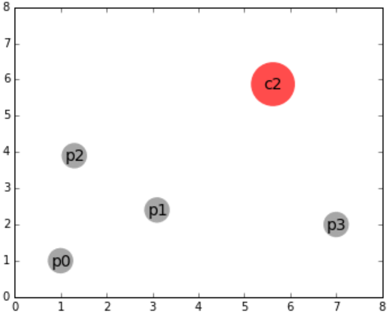
Hierarchical clustering

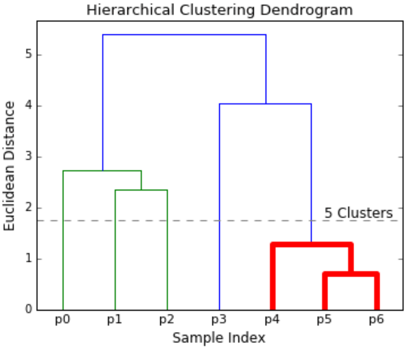
M.D. & A.G. 2021



Hierarchical clustering

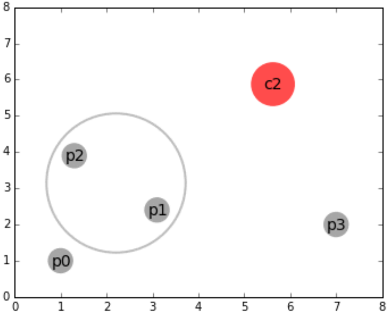
M.D. & A.G. 2021

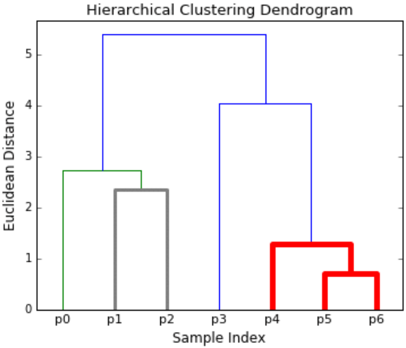




Hierarchical clustering

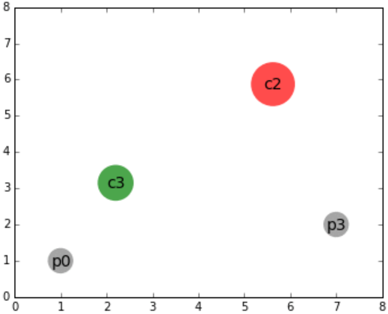
M.D. & A.G. 2021

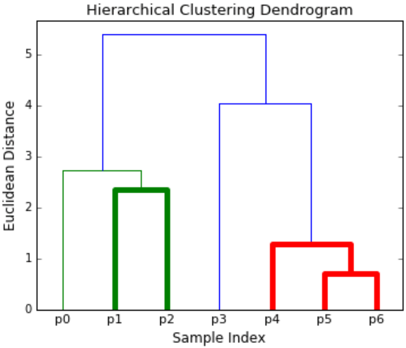




Hierarchical clustering

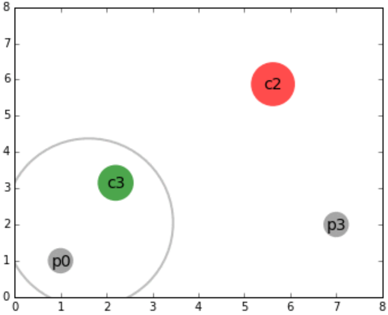
M.D. & A.G. 2021

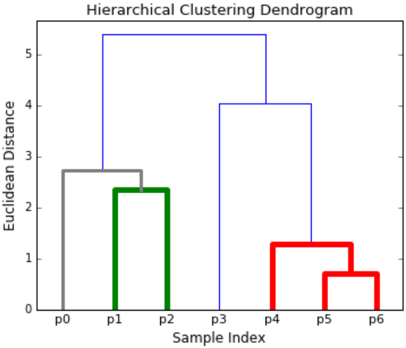




Hierarchical clustering

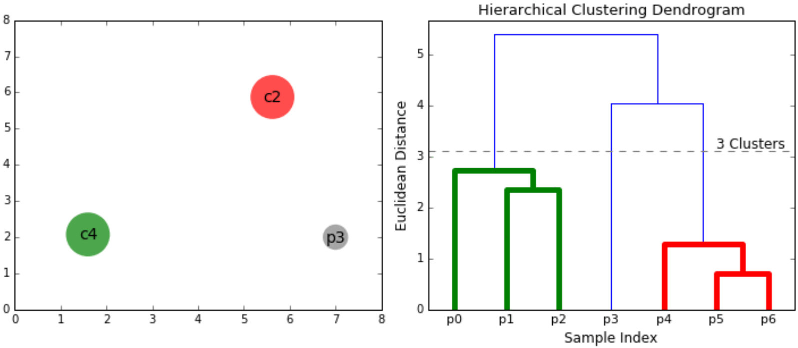
M.D. & A.G. 2021





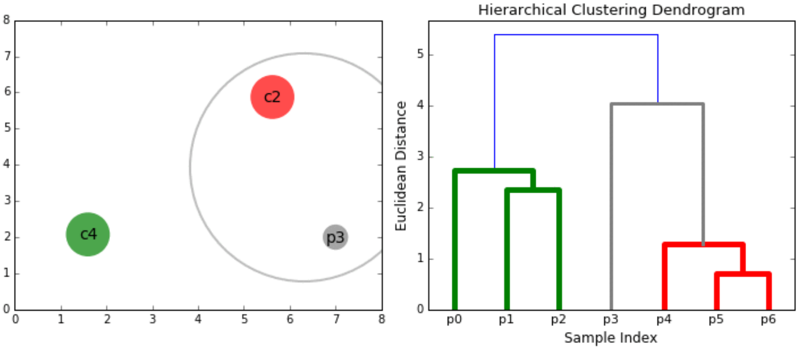
Hierarchical clustering

M.D. & A.G. 2021



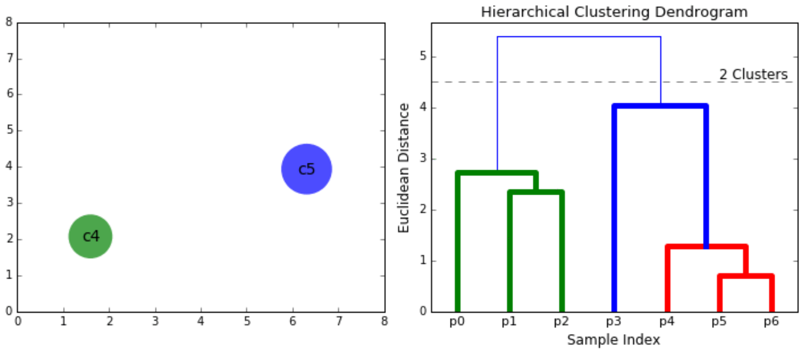
M.D. & A.G. 2021

Hierarchical clustering



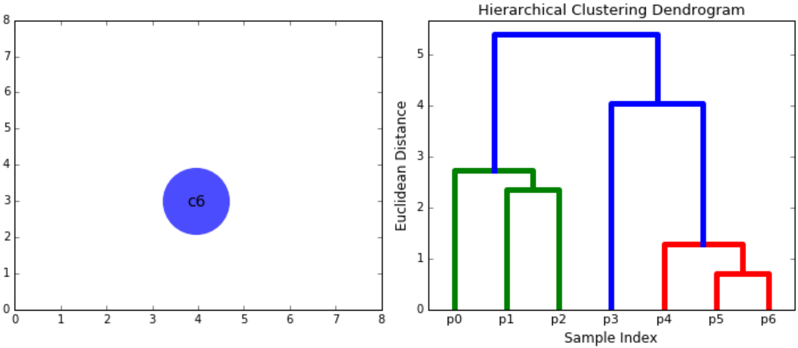
Hierarchical clustering

M.D. & A.G. 2021



Hierarchical clustering

M.D. & A.G. 2021



Hierarchical clustering

M.D. & A.G. 2021

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

M.D. & A.G. 2021

- 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:

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

Validation

M.D. & A.G. 2021

- 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 avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Validation

M.D. & A.G. 2021

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, Adjusted Rand Index)

Entropy

M.D. & A.G. 2021

1. Given a discrete random variable X with possible value $\{1, .., n\}$, 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

M.D. & A.G. 2021

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