HUST

ĐẠI HỌC BÁCH KHOA HÀ NỘI

HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

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OF SCIENCE AND TECHNOLOGY

Introduction to
Machine Learning and Data Mining

IT3190

Lecture: Clustering

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Contents

- Lecture 1: Introduction to Machine Learning & Data Mining
- Lecture 2: Data crawling and pre-processing
- Lecture 3: Linear regression
- Lecture 4: Decision tree and Random forest
- Lecture 5: Neural networks
- Lecture 6: Support vector machines
- Lecture 7: Performance evaluation
- **Lecture 8+9: Unsupervised learning - Clustering**
- Lecture 10: Probabilistic models
- Lecture 11: Basics of data mining
- Lecture 12: Association rule mining
- Lecture 13: Regularization and advanced topics

Unsupervised learning (clustering)

- Introduction to Clustering
- K-means
- Hirarchical clustering
- Some practices

Introduction to Clustering

- Overview
  - Basic learning problems
  - Clustering
  - Evaluation of clustering
- Clustering methods
  - Partition method
  - Hierarchical method
  - Density-based method
- Requirements and applications
  - Requirements for clustering methods
  - Applications

Basic learning problems

- Lean a function/model from a given dataset
- Supervised learning
  - $S = \{\{x_1, x_2, \ldots, x_N\}; \{y_1, y_2, \ldots, y_N\}\}$
  - Each training instance has a label/response
  - Target: $y_i \cong f(x_i)$ for every i. Predict classes or values of future data.
- Unsupervised learning
  - $S = \{x_1, x_2, \ldots, x_N\}$
  - No label/response for training instances
  - Target: $y = f(x)$. Detect hidden structures in data.

Clustering

- Clustering problem
  - Unsupervised learning
  - Input: a training set without any label.
  - Output: clusters of the training instances
- A cluster
  - Consists of similar instances in some senses.
  - Two clusters should be different from each other.

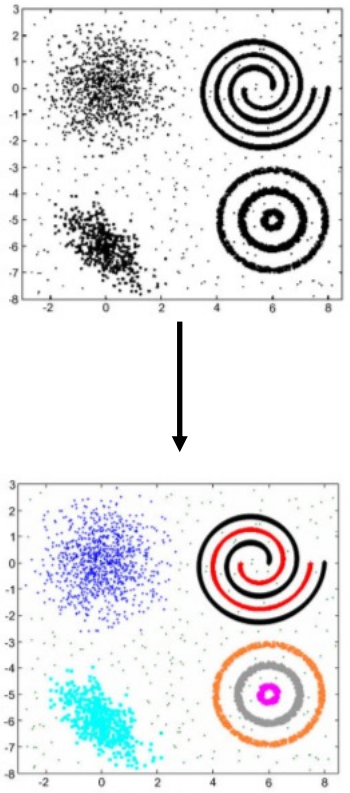
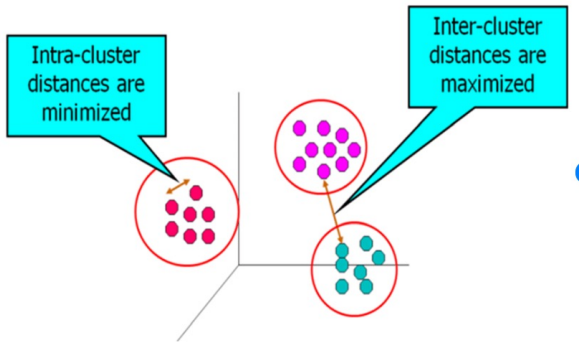


Figure 1: Clustering

Source: *Santosh K., Deepanwita D. and Sanjay K.S.. (2015). Black Hole Algorithm and Its Applications. Studies in CI. 575. 147-170.*

Clustering

- Inter-cluster distance
  - Distance/difference between any two clusters should be large.
- Intra-cluster distance
  - Distance/difference between instances inside a cluster should be small.



Source: *https://www.researchgate.net/figure/Intra-cluster-distances-vs-inter-cluster-distances_fig22_336111538*

- **Evaluation of clustering**
  - Sum-of-Squared error
    - Sum of squared distances between instances and cluster centers

$$E(C) = \sum_{i=1}^{k} \sum_{o \in C_i} d(o, cen_i)^2$$

  - Silhouette value
    - $a(o_i)$: distance $o_i \rightarrow o_j$ same cluster
    - $b(o_i)$: distance $o_i \rightarrow o_j$ different cluster
    - $sil(o_i) \in [-1, 1]$, $sil(o_i) \approx 1$: o_i is well classified

$$a(o_i) = \frac{1}{|C_A| - 1} \sum_{o_j \in C_A, o_j \neq o_i} d(o_i, o_j)$$

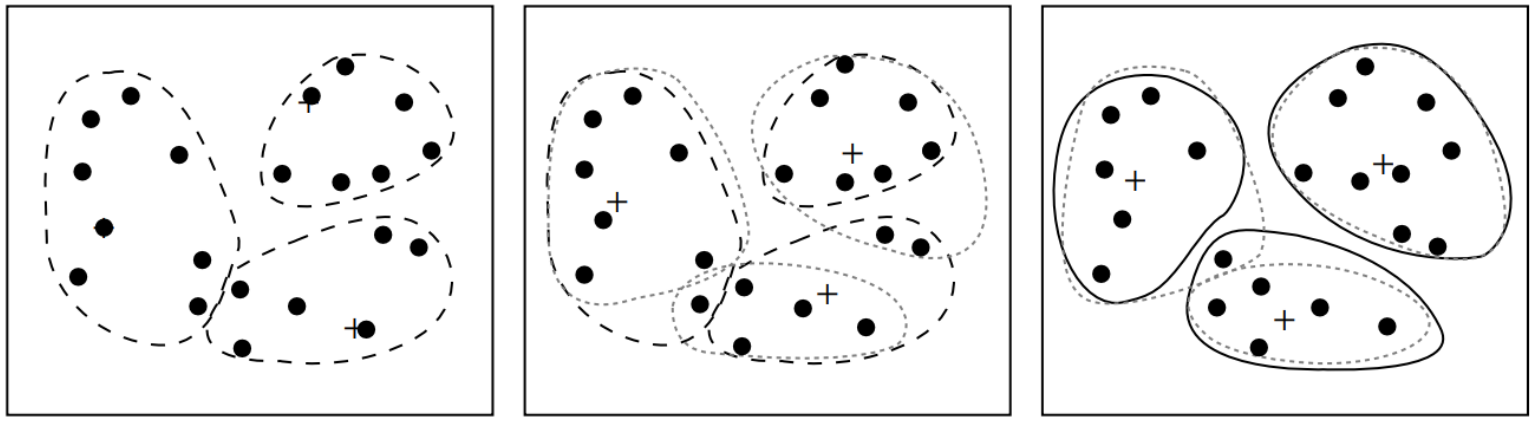
$$b(o_i) = min_{C_B \neq C_A} \frac{1}{|C_B|} \sum_{o_j \in C_B} d(o_i, o_j)$$

$$sil(o_i) = \frac{b(o_i) - a(o_i)}{max\{a(o_i), b(o_i)\}}$$

  - Extrinsic methods:
    - Comparing to a manual clustering (ground of truth)

Partition method (Centroid-based)

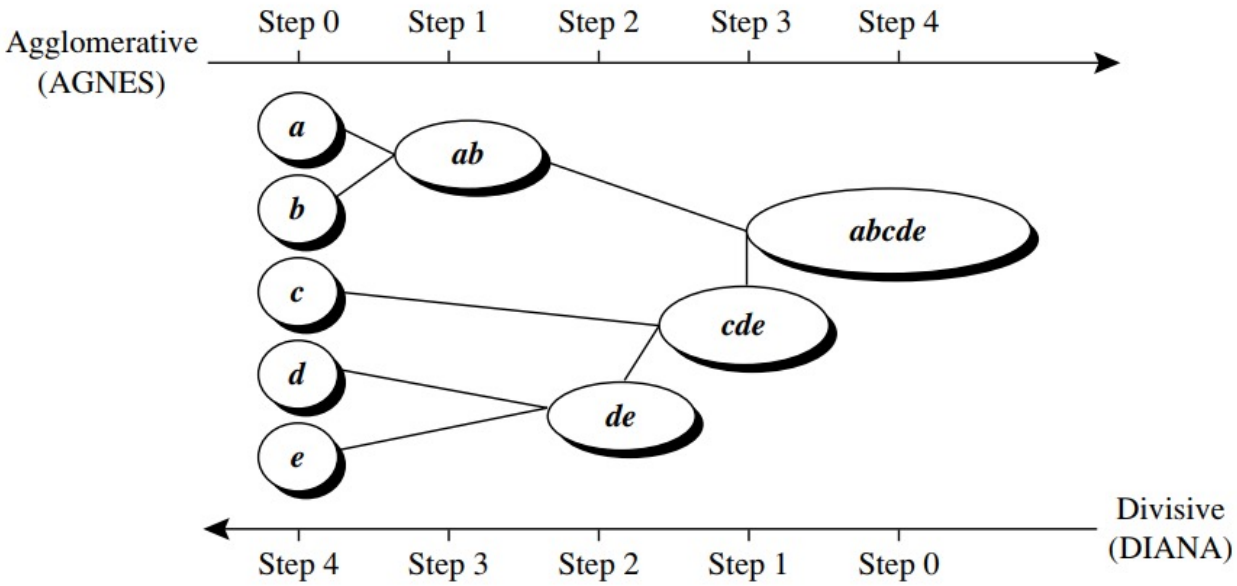
- Example of algorithm: K-means



(a) Initial clustering (b) Iterate (c) Final clustering

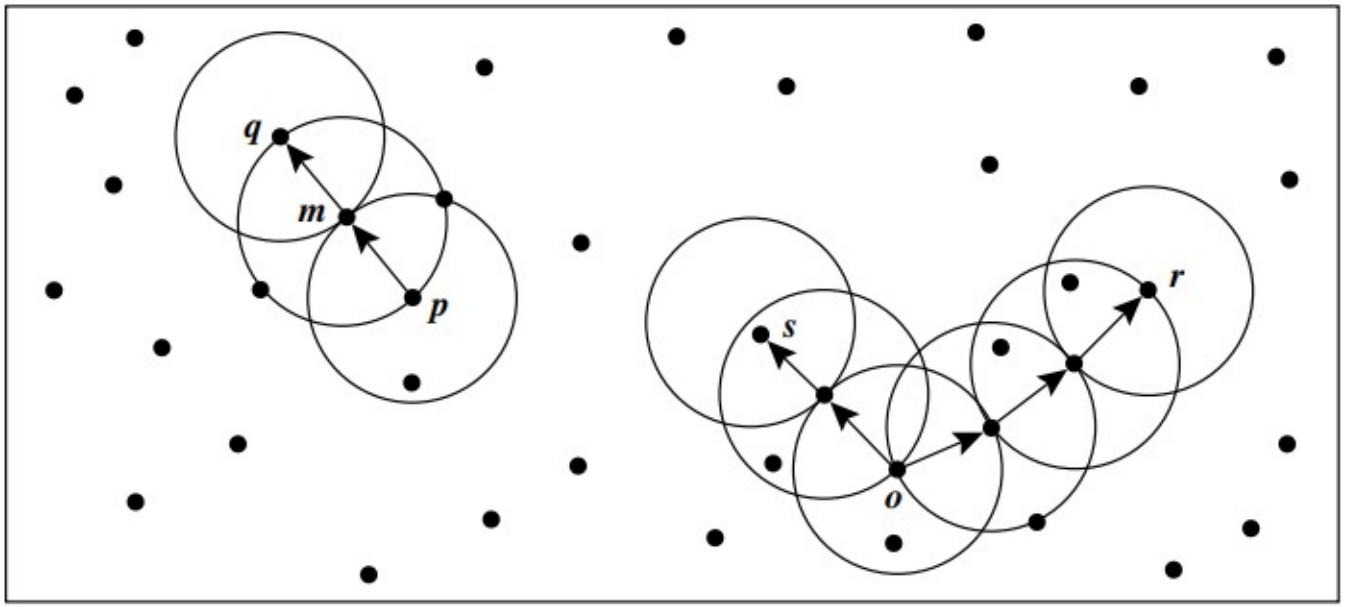
Hierarchical method (Connectivity-based)

- Example of algorithm: BIRCH



Density-based method

- Example of algorithm: DBSCAN



Requirements for clustering methods

- Scalability: Work with small/large databases
- Ability to deal with different types of attributes: Work with numeric, categorical, mixtures or complex data types (graphs, images, text,...).
- Discovery of clusters with arbitrary shape: spherical, not spherical, intersecting data...
- Ability to deal with noisy data: datasets contain outliers, missing, unknown, or erroneous data.

Introduction to Clustering

Applications

- Market segmentation
- Social network analysis
- Wireless network analysis or Network traffic classification
- Image compression
- Data processing and feature weighing
- Life science and healthcare
- …

K-means

- K-means
  - Overview
  - Algorithm
  - Key ingredients
  - Some problems
- K-means++
  - Overview
  - Algorithm
  - Evaluation
- Online K-means
  - Serializing K-means
  - Algorithm

K-means - Overview

- K-means was first introduced by Lloyd in 1957.
- K-means is the most popular method for clustering, which is partition-based.
- Data representation:
  - $D = \{x_1, x_2, \ldots, x_r\}$, each instance x_i is a vector in the n-dimensional Euclidean space.
- K-means partitions D into k clusters:
  - Each cluster has a central point which is called centroid.
  - K is a pre-specified constant.

K-means - Algorithmn

- Input: training data *D*, number of clusters *k*, distance measure *dist*(x,y).

1. Initialization: select randomly *k* initial centroids $C = \{c_1, \ldots, c_k\}$
2. For each instance $x \in D$
   - Assign *x* to the cluster with nearest centroid
3. For each cluster $i \in \{1, \ldots, k\}$:
   - Recompute the centroid of cluster *i* from its instances
4. Repeat Steps 2 and 3 until *C* no longer changes.

K-means - Algorithmn

- Assign *x* to the cluster with nearest centroid
  - Compute distance from *x* to each centroid: $dist(x, cen_i)$
  - Assign *x* to cluster of closest centroid (C_i):

$$\text{j} = \underset{i \in \{1,2,\ldots k\}}{arg\,min}\, dist(x, cen_i)$$

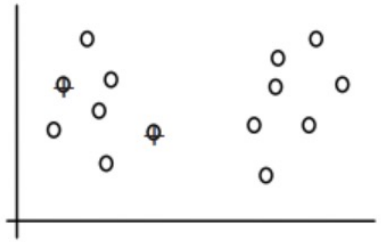
$$C_j \leftarrow x$$

- Recompute the centroid of cluster *i* from its instances

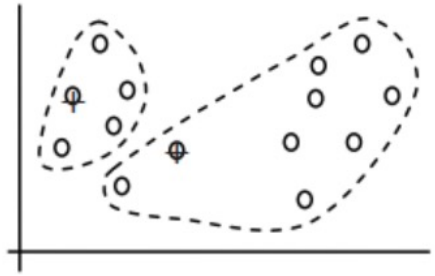
$$cen_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$$

  - Sum of instances: adding the corresponding dimensions of the vectors (vector addition)

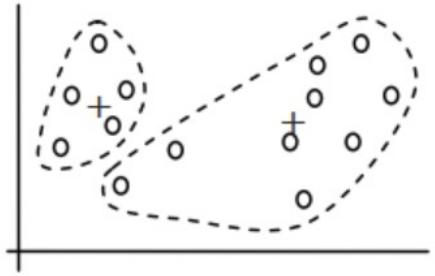
K-means - Algorithmn



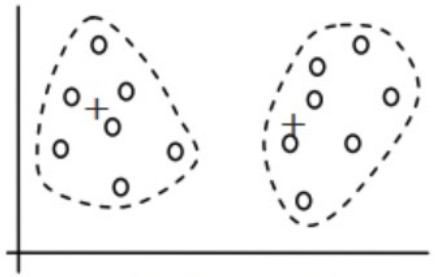
(A). Random selection of k seeds (or centroids)



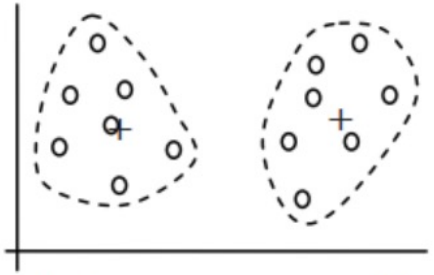
Iteration 1: (B). Cluster assignment



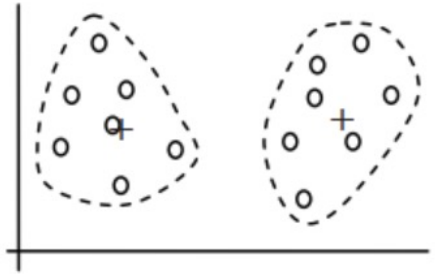
(C). Re-compute centroids



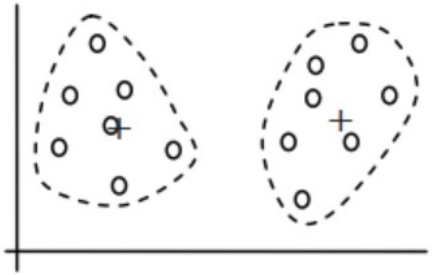
Iteration 2: (D). Cluster assignment



(E). Re-compute centroids



Iteration 3: (F). Cluster assignment



(G). Re-compute centroids

K-means - Key ingredients

- The algorithm converges if:
  - Very few instances are reassigned to new clusters, or
  - The centroids do not change significantly, or
  - The sum of squared error does not change significantly

$$E = \sum_{i=1}^{k} \sum_{x \in C_i} dist(x, cen_i)^2$$

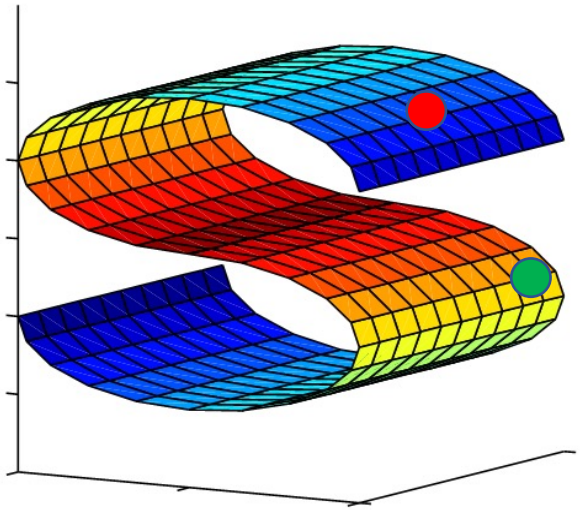
where cen_i is the centroid of cluster C_i.

K-means - Key ingredients

- Distance measures
  - Manhattan (L1-norm): $d(x, z) = \sum_{i=1}^{n} |x_i - z_i|$
  - Euclid (L2-norm): $d(x, z) = \sqrt{\sum_{i=1}^{n} (x_i - z_i)^2}$
  - Hamming distance: $d(x, z) = \sum_{i=1}^{n} Difference\ (x_i, z_i)$
  - Other measures are possible.

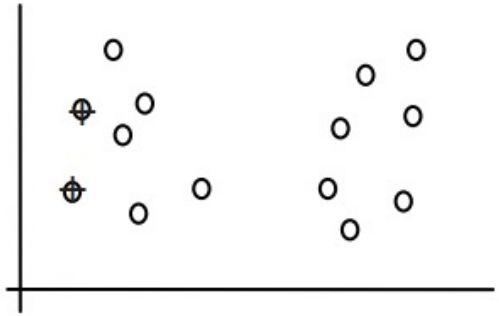
K-means - Key ingredients

- Distance measures
  - Feature
    - Each measure provides a view on data
    - Which distance is good?
  - Similarity measures can be used
    - Similarity between two objects

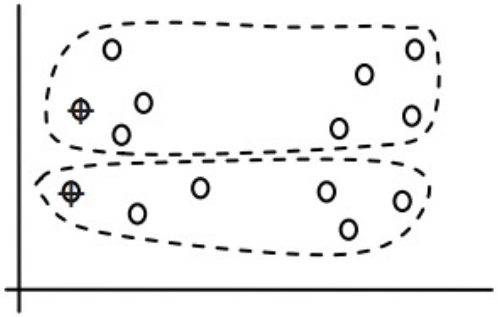


K-means – Some problems

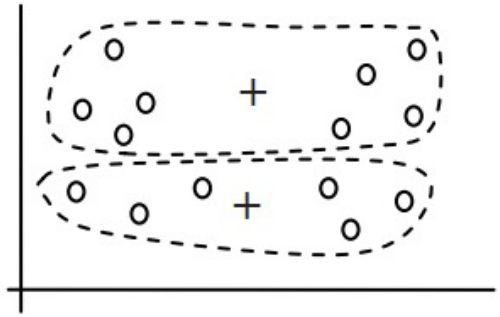
- Quality of K-means depends much on the initial centroids



(A). Random selection of seeds (centroids)



(B). Iteration 1



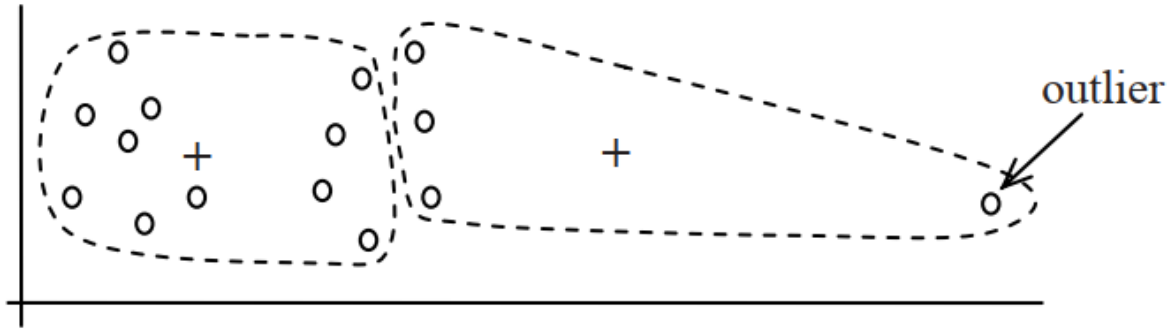
(C). Iteration 2

K-means – Some problems

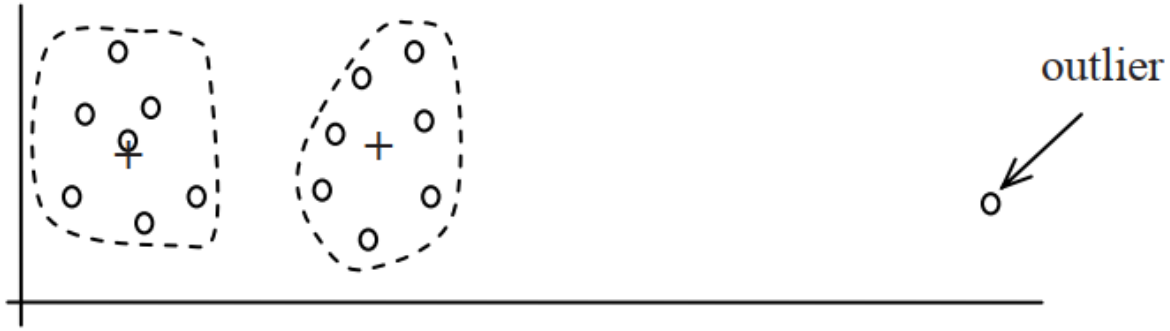
- **Solutions**
  - Repeat K-means many times. Each time initialize a different set of centroids.
  - After learning, we combine results from those runs to obtain a unified clustering.
  - K-means++ (next session)

K-means – Some problems

- Some outliers in data can affect quality of K-means



(A): Undesirable clusters



(B): Ideal clusters

K-means – Some problems

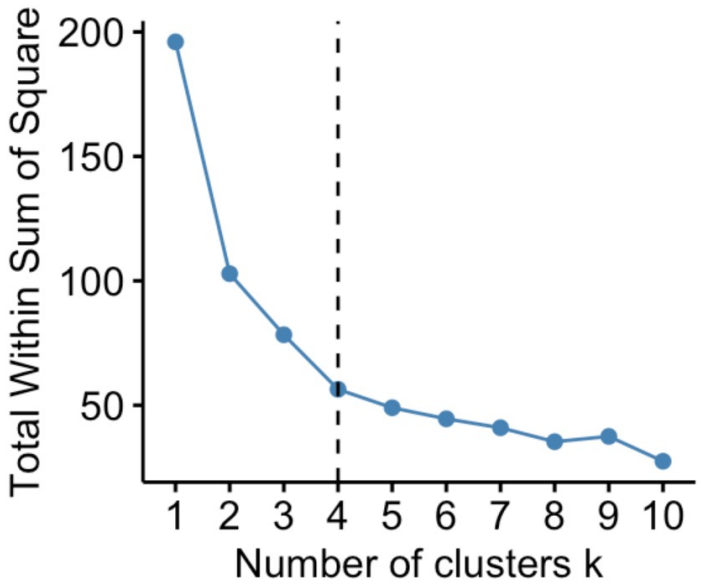
- **2.2. Solutions**
  - Outlier removal
    - Remove instances that are far from the centroids
    - Removal can be done a priori or when learning clusters.
  - Random sampling
    - Cluster a random sample *S* instead of the whole training data
    - *S* contains fewer noises/outliers than the original training data.
    - After learning, the remaining data will be assigned to the learned clusters.

K-means – Some problems

- K-means requires the user to specify the number of clusters
- Optimal number of clusters is subjective and depends on the distance measures

K-means – Some problems

- Elbow method
  - Run K-means different values of k
  - For each k, calculate the total within-cluster sum of square (S).
  - Plot the curve of S according to the number of clusters k.
  - The location of a bend (elbow) in the plot.



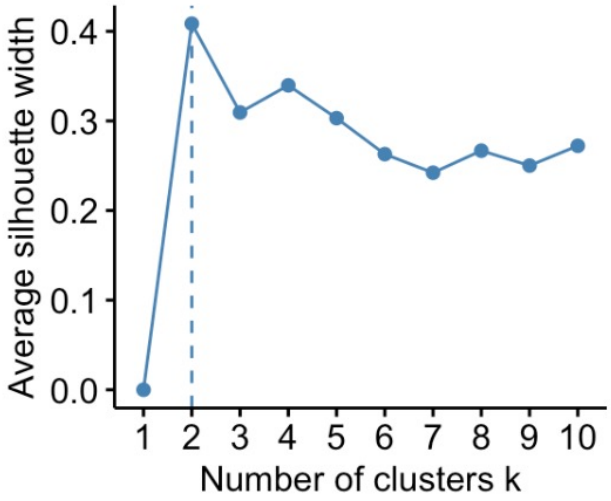
Source: *https://www.datanovia.com/en/lessons/determining-the-optimal-number-of-clusters-3-must-know-methods/*

K-means – Some problems

- Average silhouette method

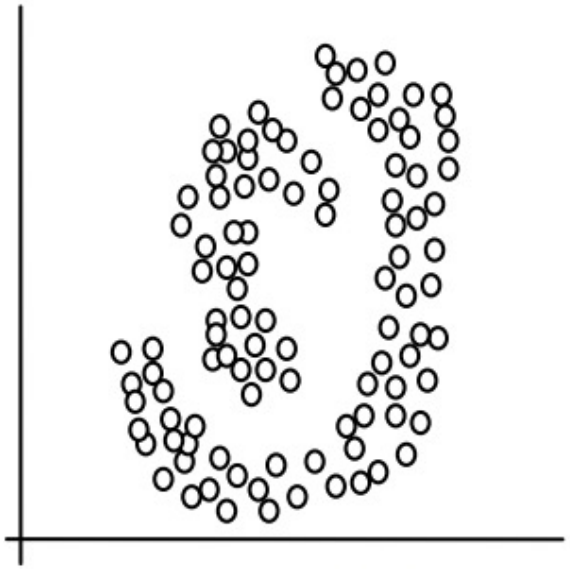
$$SC(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

  - *a(i)*: average distance between sample *i* and other samples in the same cluster.
  - *b(i)*: minimum average distance between sample *i* and samples in other clusters.
  - *SC* $\in$ [-1, 1], *SC* getting closer to 1 indicates good cluster of *i*.

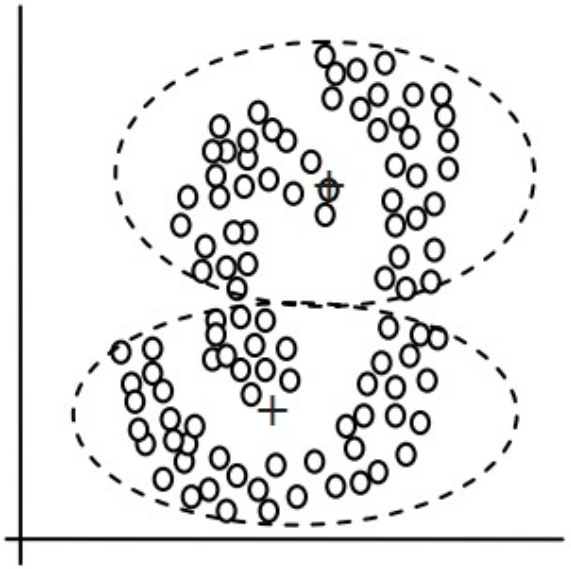


K-means – Some problems

- Data with varying shapes



(A): Two natural clusters



(B): *k*-means clusters

Source: *https://www.datanovia.com/en/lessons/determining-the-optimal-number-of-clusters-3-must-know-methods/*

K-means++

- **K-means++ idea**
  - Problem on K-means initialization: Quality of K-means depends much on the initial centroids
  - Initial centroids that are far away from one another.
    - This increases the chances of centroids that lie in different clusters.
    - Since centroids are picked up from the data points, each centroid has some data points associated with it at the end.

K-means++

Algorithmns

- Update initialization step of K-means:
  - 1. Choose an initial centroid c_1 uniformly at random from X .
  - 2. Choose the next centroid c_i:
    - Select $c_i = x' \in X$ with probability $\frac{D(x')^2}{\sum_{x \in X} D(x)^2}$
    - D(x) denote the shortest distance from x to the closest centroid
  - 3. Repeat Step 2 until a total of k centers has been chosen.

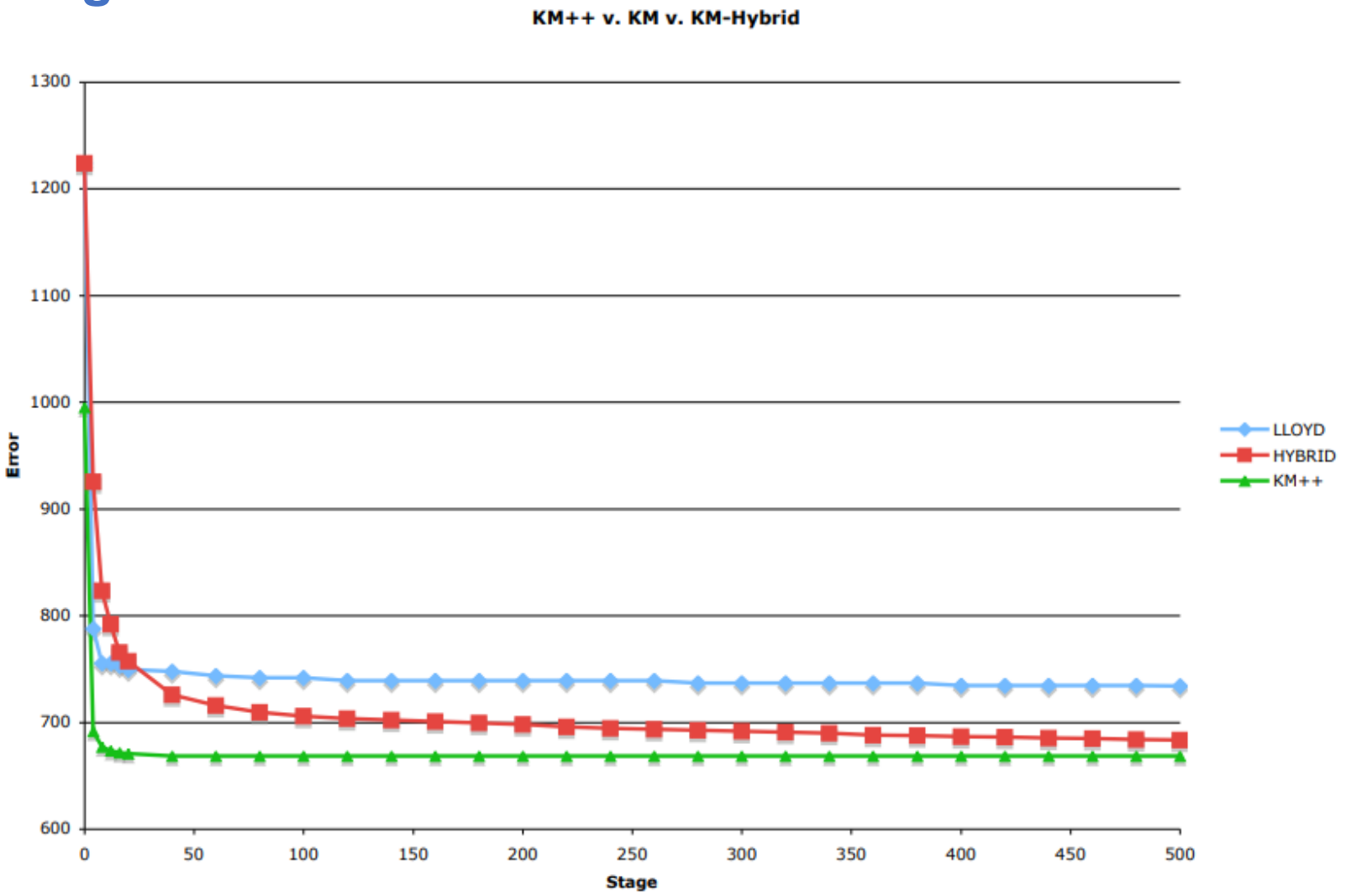
K-means++

Algorithm interpretation

- $\frac{D(x')^2}{\sum_{x \in X} D(x)^2}$ is directly proportional to data point distance to the nearest centroid.
- The point having maximum distance is most likely to be selected
- This increase the chances of picking up centroids that lie in different clusters
- The centroids are selected with some degree of randomness

K-means++

Convergence



Source: *https://theory.stanford.edu/~sergei/slides/BATS-Means.pdf*

Clustering quality

k	Average ϕ		Minimum ϕ		Average T	
	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	$1.365 \cdot 10^5$	8.47%	$1.174 \cdot 10^5$	0.93%	0.12	46.72%
25	$4.233 \cdot 10^4$	99.96%	$1.914 \cdot 10^4$	99.92%	0.90	87.79%
50	$7.750 \cdot 10^3$	99.81%	$1.474 \cdot 10^1$	0.53%	2.04	−1.62%

Experimental results on the Norm25 dataset (n = 1000, d = 15).

k	Average ϕ		Minimum ϕ		Average T	
	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	$3.698 \cdot 10^4$	49.43%	$3.684 \cdot 10^4$	54.59%	2.36	69.00%
25	$3.288 \cdot 10^4$	88.76%	$3.280 \cdot 10^4$	89.58%	7.36	79.84%
50	$3.183 \cdot 10^4$	95.35%	$2.384 \cdot 10^4$	94.30%	12.20	75.76%

Experimental results on the Spam dataset (n = 4601, d = 58).

Source: *Arthur, D.; Vassilvitskii, S. (2007). K-means++: the advantages of careful seeding.*

Online K-means

Idea of serialization

- K-means:
  - K-means requires all training data for each iteration.
  - It cannot work with big datasets.
  - It cannot work with stream data where data come in sequence.
- Sum of squared error function:

$$E = \sum_{i=1}^{k} \sum_{x \in C_i} dist(x, cen_i)^2 = \sum_{x \in D} dist(x, cen(\mathrm{x}))^2$$

  - *cen(x)* is the centroid of cluster containing *x*
  - K-means finds clusters that minimizes error value

Online K-means

- **1.2. Minimizing loss function**
  - K-means is an optimization problem with sum of squared error
    - Rewrite Loss function from Error function:

$$Q_{k-means} = \sum_{i=1}^{M} (x_i - w(x_i))^2$$

    - where $w(x_i)$ is the nearest centroid to x_i, *with M* instances $x_1, x_2, \ldots, x_M$
  - Q can be minimized by using Gradient descent:

$$w_{t+1} = w_t + \gamma_t \sum_{i=1}^{M} [x_t - w_t(x_i)]$$

    - where γ_t is a small constant, often called learning rate.

Online K-means

Stochastic gradient

- Note that each iteration of K-means requires the full gradient:
  - $Q'_t = \sum_{i=1}^{M} [x_i - w_t(x_i)]$
  - Which requires all training data.
- Online K-means minimizes Q using stochastic gradient:
  - Use only information of a traning instance *x* from the whole gradient Q'. $x_t - w_t(x_t)$:
    - $w_{t+1} = w_t + \gamma_t(x_t - w_t(x_t))$

Online K-means

Algorithms

- Initialize *k* centroids randomly.
- Update the centroids as an instance comes
  - At iteration *t*, take an instance x_t.
  - Find the nearest centroid w_t to x_t
  - Update w_t as follows:

$$w_{t+1} = w_t + \gamma_t(x_t - w_t(x_t))$$

Online K-means

Learning rate

- Learning rates are positive constants and satisfy:

$$\sum_{t=1}^{\infty} \gamma_t = \infty; \sum_{t=1}^{\infty} {\gamma_t}^2 < \infty$$

- A popular choice of learning rate:

$$\gamma_t = (t + \tau)^{-\kappa}$$

  - τ, κ are possitive constants.
- $\kappa \in (0.5, 1]$ is called forgeting rate.
  - Large κ means that the algorithm remembers the past longer, and new observation plays less important role as t grows.

Online K-means

Properties

- Online K-means is an online learning version of K-means.
- It follows the methodology from online learning and stochastic gradient.
  - One instance is used to update the available clusters at each iteration.
- Online K-means helps to cluster big/stream data.

Hirarchical clustering

Algorithms

- Two approaches
- Agglomerative algorithm

Cluster distance

- Single-Link Method
- Complete-Link Method
- Other methods

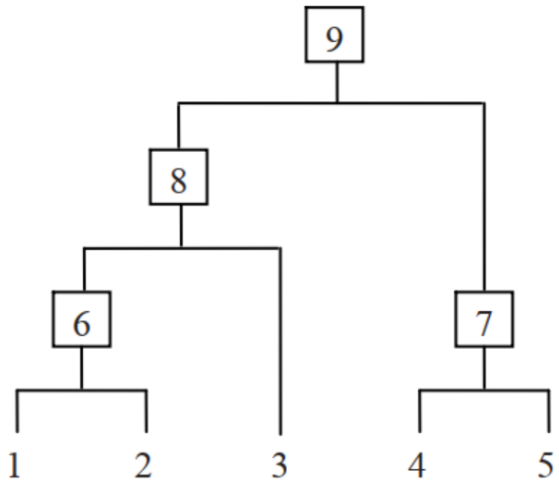
Strengths and Weaknesses

- Strengths
- Weaknesses

Hirarchical clustering

Two approaches

- Agglomerative (bottom up) clustering:
  - Build the dendrogram (tree) from the bottom level
  - Merge the most similar pair of clusters
  - Continue until all points are merged into one cluster
- Divisive (top down) clustering:
  - Start with all data points in one cluster (top level)
  - Split a cluster into smaller ones based on some criterion
  - Continue until each cluster is a single point.



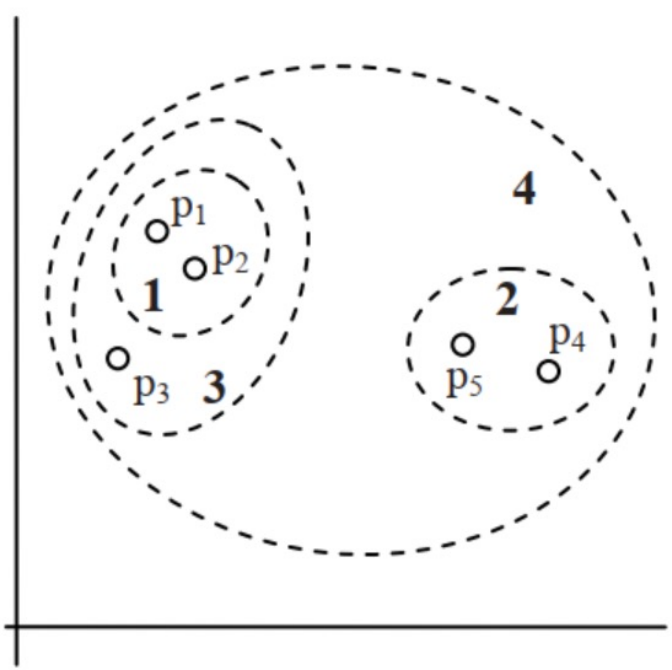
Hirarchical clustering

Agglomerative Algorithm

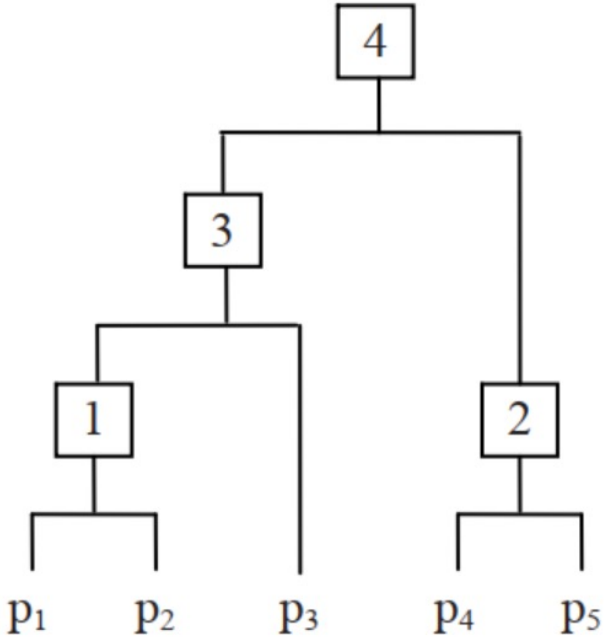
1. Make each data point in the data set D a cluster,
2. Compute all pair-wise distances of $x_1, x_2, \ldots, x_n \in D$
3. Repeat
    4. Find two clusters that are nearest to each other
    5. Merge the two clusters form a new cluster c
    6. Compute the distance from c to all other clusters
7. Until there is only one cluster left

Hirarchical clustering

Agglomerative Algorithm



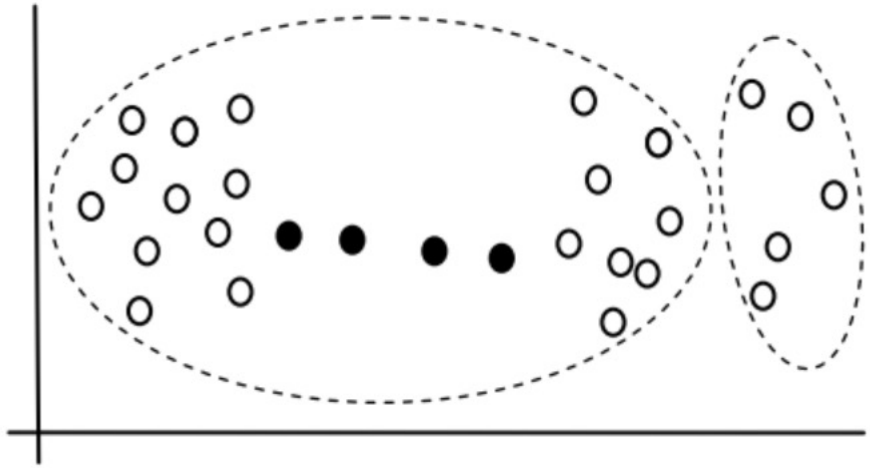
(A). Nested clusters



(B) Dendrogram

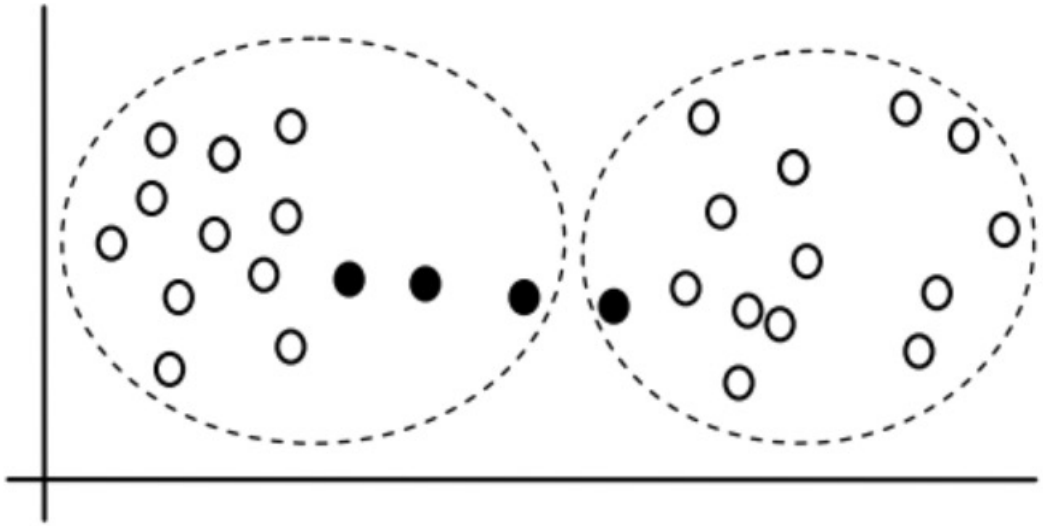
Single-Link Method

- Cluster distance: the distance between two closest points in the two clusters
- Merge the two clusters with the smallest minimum pair-wise distance.
- Can be sensitive to noise in the data (have chain effect)



Complete-Link Method

- Cluster distance: the distance between two furthest points in the two clusters
- Merge the two clusters with the smallest maximum pair-wise distance.
- Can be sensitive to noise (does not have the problem of chain effects)



Other Methods

- Average-Link Method: The distance between two cluster is the average distance of all pair-wise distances between two clusters.
- Centroid method: The distance between two clusters is the distance between their centroids.
- Ward's method: The distance between two clusters is the increase in the sum of squared error (distances) from that of two clusters to that of one merged cluster.

Hirarchical clustering

Strengths

- Can explore clusters at any level of detail
- Resulting hierarchy can be useful
  - Cluster hierarchy may represent a topic hierarchy in the documents.
- It can also find clusters of arbitrary shapes
  - E.g., using the single-link method.

Hirarchical clustering

Weaknesses

- The single-link method may suffer from the chain effect
- The complete-link method is sensitive to outliers
- Computation complexities and space requirements
  - They are at least quadratic

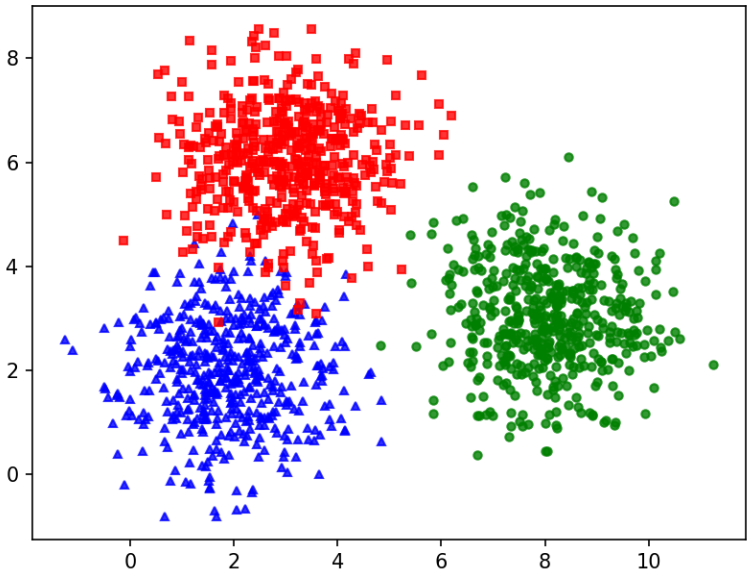
Some practices

Partition clustering (K-means)

Hirarchical clustering

Some practices

- Context
  - Data: synthetic data, 3 clusters, 500 2D points for each cluster
  - Source: https://machinelearningcoban.com/2017/01/01/kmeans/ (data, K-means implementation)
  - Content: Implement K-means using scilearn library and evaluate clustering result



Some practices - K-means

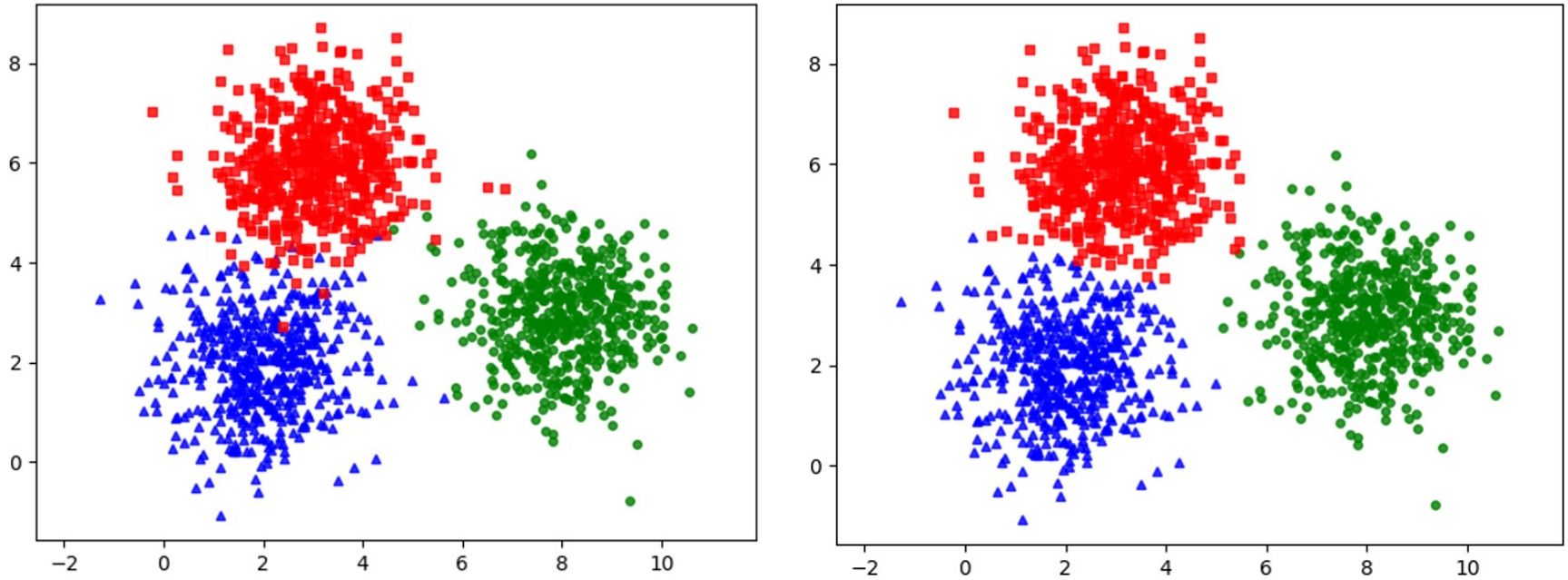
- Using a library to work with K-means

```
from sklearn.cluster import Kmeans

kmeans = KMeans(n_clusters=3)
kmeans.fit(data)
labels = kmeans.predict(data)
kmeans_display(data, labels)
```

Some practices - K-means

- Using a library to work with K-means



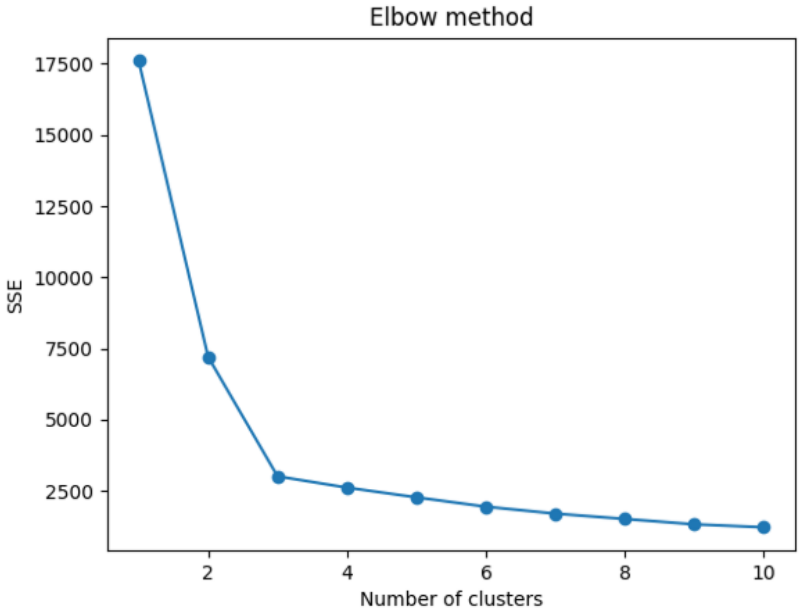
Clusters from original data (left) and found by K-means (right)

Some practices - K-means

- Evaluate clustering result and find number of clusters (SSE)

```
sse = []
for i in range(1,11):
    kmeans = KMeans(n_clusters=i)
    kmeans.fit(data)
    sse.append(kmeans.inertia_)

plt.plot(range(1,11), sse,
marker='o')
plt.title('Elbow method')
plt.xlabel('Number of clusters')
plt.ylabel('SSE')
plt.show()
```



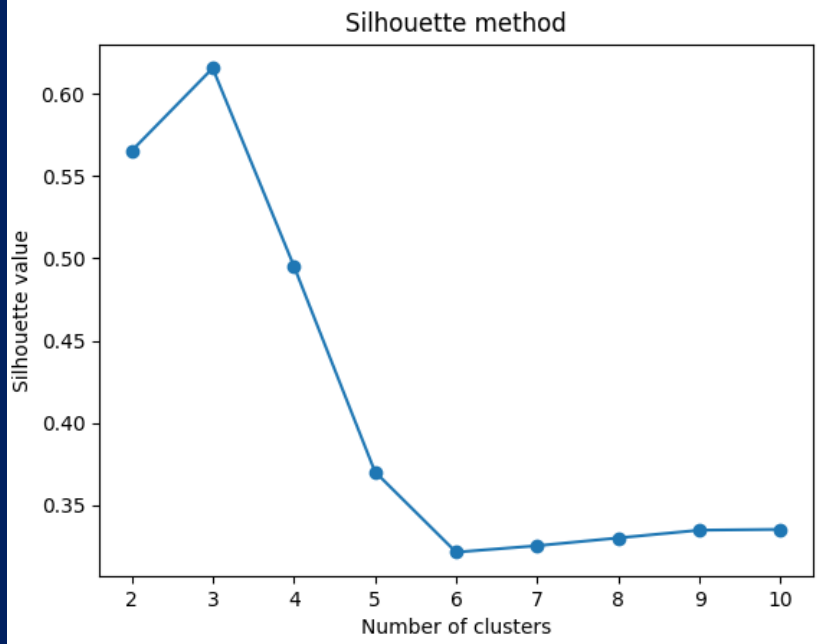
Some practices - K-means

- Evaluate clustering result and find number of clusters (silhouette)

```
from sklearn.metrics import
silhouette_score

silhouette = []
for i in range(2, 11):
    kmeans = KMeans(n_clusters=i,
random_state=0)
    kmeans.fit(data)
    score = silhouette_score(data,
kmeans.labels_)
    silhouette.append(score)

plt.plot(range(2,11), silhouette,
marker='o')
plt.title('Silhouette method')
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette value')
plt.show()
```



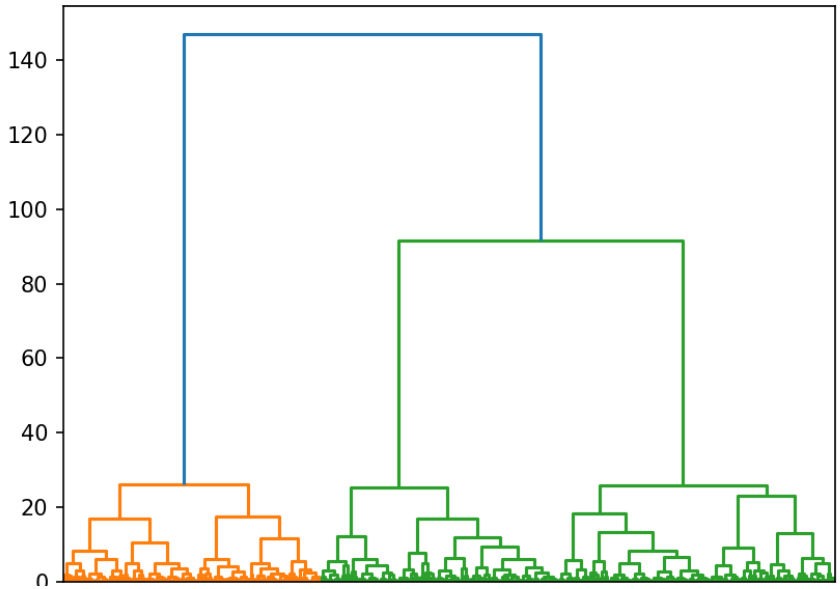
Some practices - Hirarchical clustering

- Evaluate clustering result and find number of clusters

```
from scipy.cluster.hierarchy
import dendrogram, linkage

linkage_data = linkage(data,
method='complete',
metric='euclidean’)

dendrogram(linkage_data)
plt.show()
```



Some practices - Hirarchical clustering

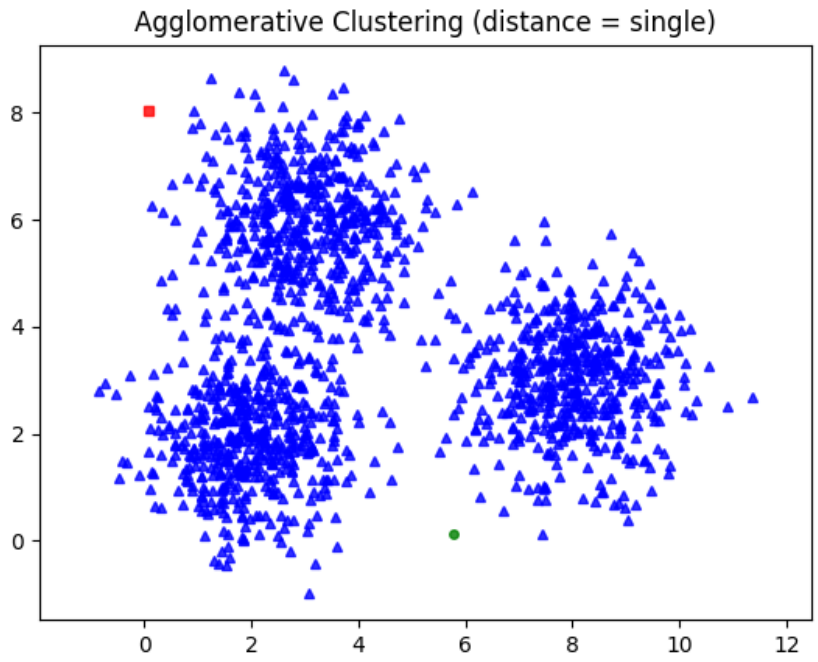
- Implementation of Hirarchical clustering (using library)

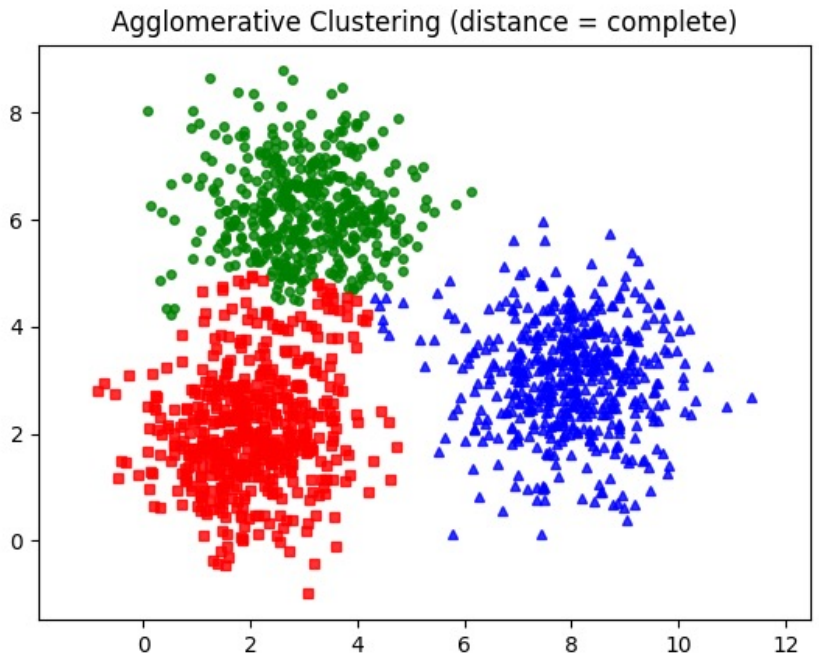
```
from sklearn.cluster import AgglomerativeClustering

for distance in ['single', 'complete', 'average', 'ward']:
    hierarchical_cluster = AgglomerativeClustering(n_clusters=3,\
        affinity='euclidean', linkage=distance)
    labels = hierarchical_cluster.fit_predict(data)
    cluster_display(data, labels, "Agglomerative Clustering \
        (distance = " + distance +')')
```

Some practices - Hirarchical clustering

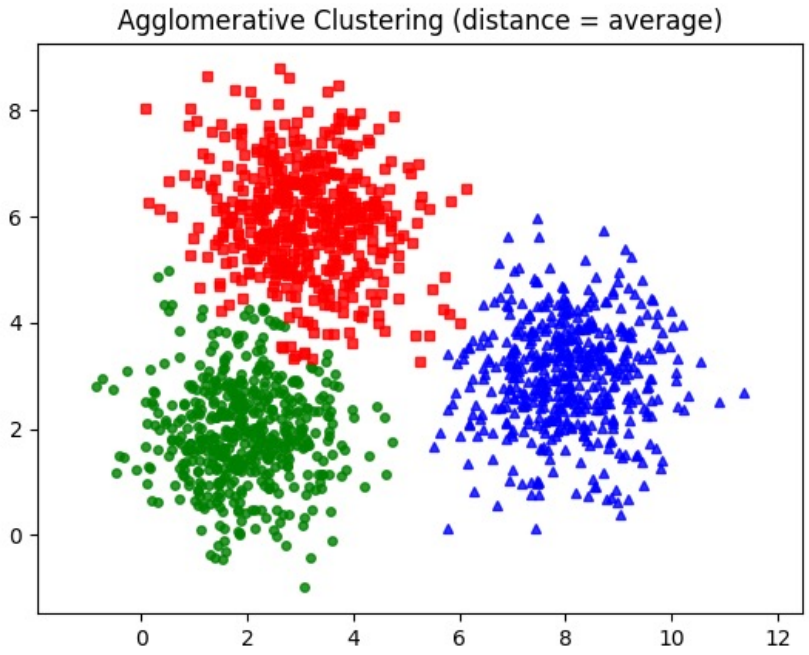
- Implementation of Hirarchical clustering (result)

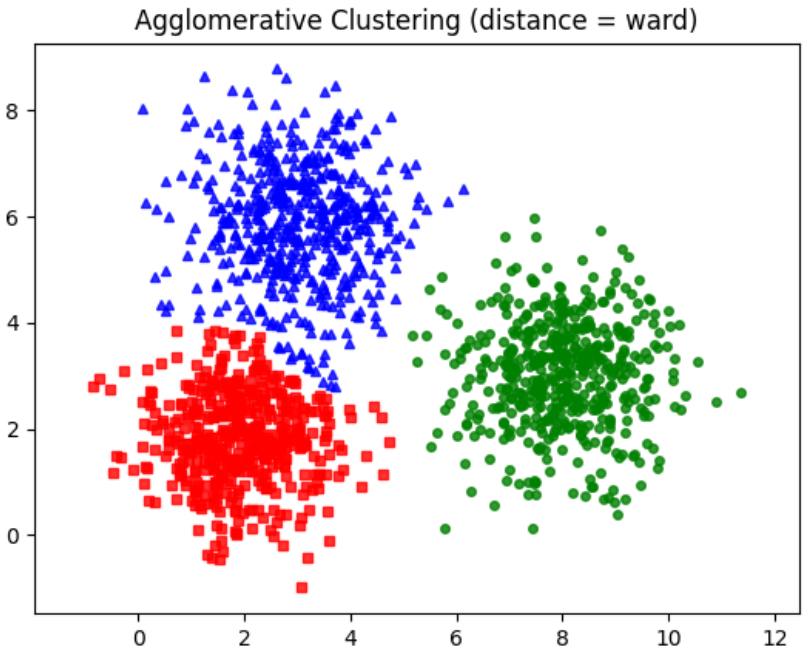




Some practices - Hirarchical clustering

- Implementation of Hirarchical clustering (result)





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THANK YOU !