Clustering algorithms (*Algorithmes de partitionnement*)

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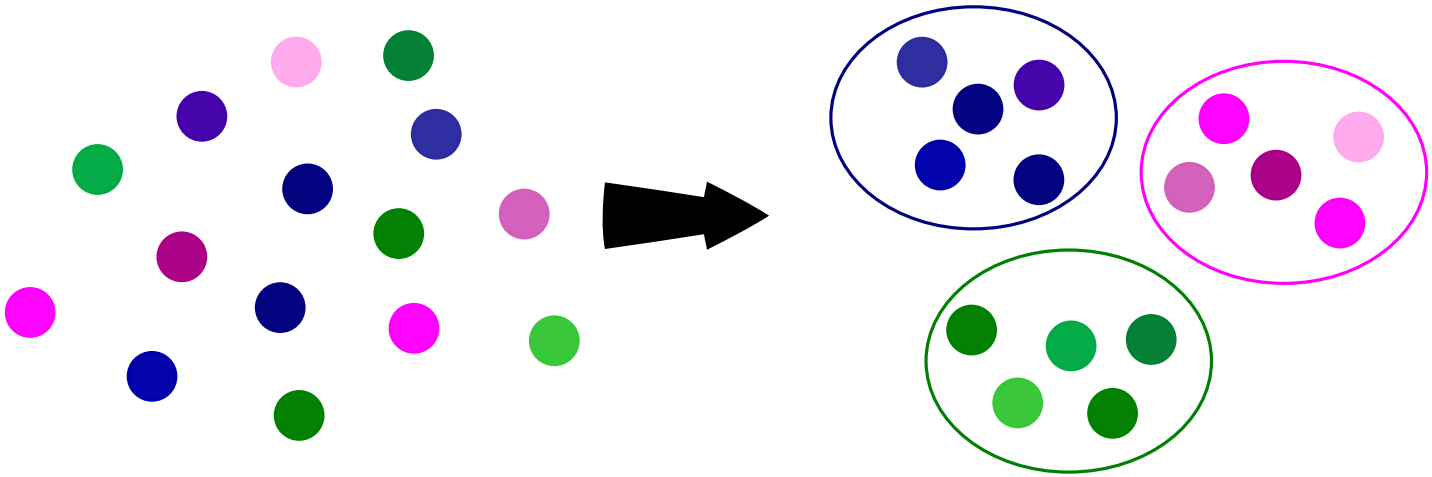
- **Unsupervised learning :** no class label needed.
- Find the class labels directly from the data.



- Cluster : a collection of data objects
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters
  - Need a way to calculate object similarity/distance
- Typical applications :
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Examples of Clustering Applications

- Marketing : Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Land use : Identification of areas of similar land use in an earth observation database
- Insurance : Identifying groups of motor insurance policy holders with a high average claim cost
- City-planning : Identifying groups of houses according to their house type, value, and geographical location
- web : Cluster Web log data to discover groups of similar access patterns
- Earth-quake studies : Observed earth quake epicenters should be clustered along continent faults

What Is Good Clustering ?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

Outline

Similarity : an example

- images from six classes :
  - muffin,
  - bagel,
  - fried chicken,
  - chihuahua,
  - labradoodle and
  - puppy
- How would you do a binary clustering of theses images ?

Similarity : an example

- images from six classes :
  - muffin,
  - bagel,
  - fried chicken,
  - chihuahua,
  - labradoodle and
  - puppy
- How would you do a binary clustering of theses images ?
  - food : muffin, bagel and fried chicken
  - pet : chihuahua, labradoodle and puppy

Similarity : an example

- food : muffin, bagel and fried chicken
- pet : chihuahua, labradoodle and puppy

Similarity / dissimilarity : distance

The distance measures the similarity between data.

- Types of Data in Clustering :
  - Interval-scaled variables
  - Binary variables
  - Nominal, ordinal, and ratio variables
  - Variables of mixed types

Interval-scaled variables

- Standardize data
  - Calculate the mean absolute deviation : $s_j = \frac{1}{n} \sum_{i=1}^{n} |x_{ij} - \mu_j|$ where

$$\mu_j = \frac{1}{n} \sum_{i=1}^{n} x_{ij}$$

  - Calculate the standardized measurement (z-score) : $z_{ij} = \frac{x_{ij} - \mu_j}{s_j}$
- Using mean absolute deviation is more robust than using standard deviation
- A classical example ($\mu_{age} = 60$; $\mu_{salary} = 11074$; $s_{age} = 5$; $s_{salary} = 37$) :

	age	salary
alice	50	11000
bob	70	11100
charly	60	11122
dany	60	11074

$\Rightarrow$

	age	salary
alice	-2	-2
bob	2	0.7
charly	0	1.3
dany	0	0

Why standardizing data ?

	age	salary
alice	50	11000
bob	70	11100
charly	60	11122
dany	60	11074

Manhattan distance	alice	bob	charly	dany
alice	0	120	132	84
bob	120	0	32	36
charly	132	32	0	48
dany	84	36	48	0

Why standardizing data ?

	age	salary
alice	-2	-2
bob	2	0.7
charly	0	1.3
dany	0	0

Manhattan distance	alice	bob	charly	dany
alice	0	6.7	5.3	4
bob	6.7	0	2.6	2.7
charly	5.3	2.6	0	1.3
dany	4	2.7	1.3	0

- Minkowski distance

$$d_q(i,j) = \sqrt[q]{\sum_{k=1}^{m} |x_{ik} - x_{jk}|^q}$$

- if $q = 1$: Manhattan distance

$$d_1(i,j) = \sum_{k=1}^{m} |x_{ik} - x_{jk}|$$

- if $q = 2$: Euclidean distance

$$d_2(i,j) = \sqrt{\sum_{k=1}^{m} |x_{ik} - x_{jk}|^2}$$

- if $q = \infty$: Max. distance

binary variables

- A contingency table for binary data :

		Obj. j	
		0	1
Obj. i	0	a	b
	1	c	d

- Example : $x_i = (0, 1, 1, 0, 0, 1)$ and $x_j = (0, 0, 1, 1, 1, 0)$.
  $a = 1, b = 2, c = 2, d = 1$
- distance for symmetric binary variables (e.g. male/female) :

$$d(i,j) = \frac{b + c}{a + b + c + d}$$

- distance for asymmetric binary variables (1 assigned to less frequent class, e.g. Nobel prize laureate) :

$$d(i,j) = \frac{b + c}{a + b + c}$$

binary variables : an example

Name	Gender	Fever	Cough	Test 1	Test 2	Test 3	Test 4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	Y	N	N	N	N

- Gender is a symmetric attribute
- For assymetric attributes, let Y and P be set to 1, N set to 0
- Lets compute the distance on asymmetric values :
  - $d(Jack, Mary) = \frac{0+1}{2+0+1} = 0.33$
  - $d(Jack, Jim) = \frac{1+1}{1+1+1} = 0.67$
  - $d(Jim, Mary) = \frac{1+2}{1+1+2} = 0.75$
  - Jack and Mary may have similar illness

Nominal variables

- generalisation of binary variables (more than 2 values)
  - e.g. : flavour $\in$ vanilla, strawberry, chocolate
- Two methods :
  - Simple matching : h : number of matches, m : total number of variables

$$d(i,j) = \frac{m-h}{m}$$

  - Use binary variables : create a new binary variable for each of the nominal states
    - flavour==’vanilla’
    - flavour==’strawberry’
    - flavour==’chocolate’

Ordinal variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank
- Can be treated like interval-scaled
  - replace x_{ik} by their rank $r_{ik} \in 1 \dots M_k$
  - map the range of each variable onto [0, 1] by replacing i-th object in the f-th variable by

$$z_{ik} = \frac{r_{ik} - 1}{M_k - 1}$$

  - compute the dissimilarity using methods for interval-scaled variables

Variables of mixed types

- A database may contain all the types of variables
- One may use a weighted formula to combine their effects :

$$d(i,j) = \frac{\sum_{k=1}^{m} \delta_{ij}^{(k)} d_{ij}^{(k)}}{\sum_{k=1}^{m} \delta_{ij}^{(k)}}$$

  - Column k is binary or nominal : $d_{ij}(k) = 0$ if $x_{ik} = x_{jk}$, $d_{ij}(k) = 1$ otherwise
  - Column k is interval-based : use the normalized distance
  - Column k is ordinal or ratio-scaled
    - compute ranks r_{ik} and
    - and treat z_{ik} as interval-scaled

$$z_{ik} = \frac{r_{ik} - 1}{M_k - 1}$$

Edit distance or transformation distance

- Distance = effort needed for the transformation of one sample to another one

Substitution: hat, hair, mouth
Insertion: flowers

distance = 4

Deletion: hair
Substitution: hat
Insertion: shoes

distance = 3

Deletion: shoes
Substitution: mouth
Insertion: flowers, hair

distance = 4

Edit distance (for text)

- Transformation of strings using only Substitution, Insertion and Deletion
  - Eg : Bad - Gad - Gaod - Good (2 substitutions and 1 insertion)
- Similarity between 2 strings : the cost of the cheapest transformation
  - Eg : 3 for 'Bad' and 'Good'
  - Eg : Piotr, Pyotr, Petros, Pietro, Pedro, Pierre, Piero, Peter
- How to find the cheapest ?

Typical alternatives for the Distance between clusters

- Single linkage : smallest distance between an element in one cluster and an element in the other, i.e., $d(K_p, K_q) = \min_{x_i \in K_p, x_j \in K_q} d(x_i, x_j)$
- Complete linkage : largest distance between an element in one cluster and an element in the other, i.e., $d(K_p, K_q) = \max_{x_i \in K_p, x_j \in K_q} d(x_i, x_j)$
- Average linkage : average distance between an element in one cluster and an element in the other
- Centroid : distance between the centroids of two clusters, i.e., $d(K_p, K_q) = d(C_p, C_q)$
- Medoid : distance between the medoids of two clusters, i.e., $d(K_p, K_q) = d(M_p, M_q)$
  - Medoid : one chosen, centrally located object in the cluster

Centroid, Radius and Diameter

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Centroid : the "midpoint" of a cluster

$$C_p = \frac{1}{N_p} \sum_{i=1}^{N_p} x_i^{(p)}$$

Radius : square root of average distance from any point of the cluster to its centroid

$$R_p = \sqrt{\frac{1}{N_p} \sum_{i=1}^{N_p} (x_i^{(p)} - C_p)^2}$$

Diameter : square root of average mean squared distance between all pairs of points in the cluster

$$D_p = \sqrt{\frac{1}{N_p(N_p-1)} \sum_{i=1}^{N_p} \sum_{j \neq i} (x_i^{(p)} - x_j^{(p)})^2}$$

Major Clustering Approaches

- Partitioning (iterative construction of partitions)
  - K-Means, k-Medoids, etc.
- Hierarchical (construct a dendrogram of instances)
  - Diana, Agnes, BIRCH, ROCK, CAMELEON
- Density-Based (based on connectivity and density function)
  - DBSCAN, OPTICS, DenClue
- Grid-Based
  - STING, WaveCluster, CLIQUE
- Model-Based
  - Expectation Maximization
  - Self-organizing maps (SOM)
- Spectral clustering
- Frequent-Pattern-Based

Outline

- Partitioning method : Construct a partition of a dataset D of n objects into a set of k clusters, minimizing the sum of squared distances :

$$\sum_{p=1}^{k}\sum_{i=1}^{N_p}(x_i^{(p)} - C_p)^2$$

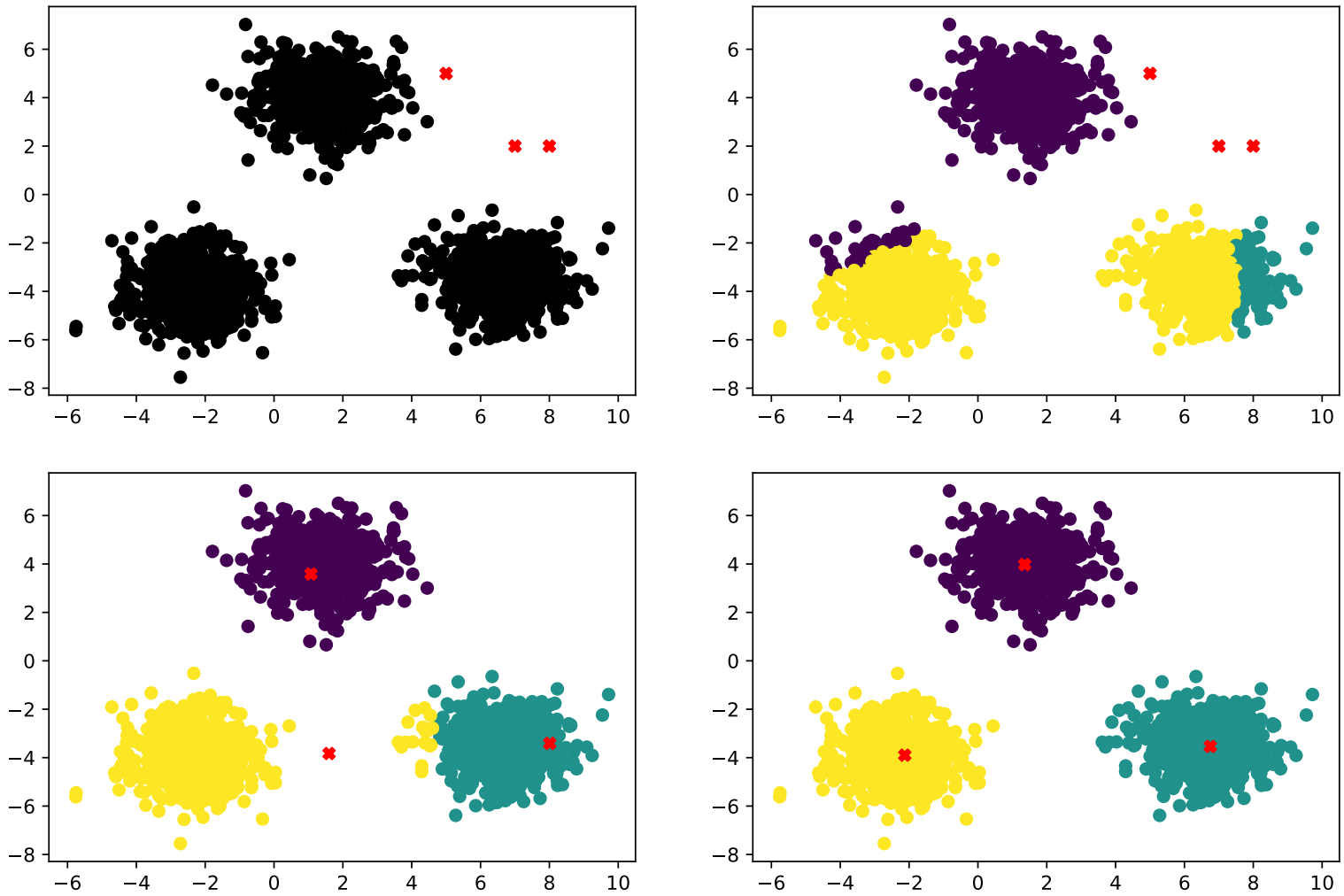
- Given a k, find a partition of k clusters that optimizes the chosen partitioning criterion
  - Global optimal : exhaustively enumerate all partitions
  - Heuristic methods : k-means and k-medoids algorithms
    - k-means (MacQueen '67) : Each cluster is represented by the centroid of the cluster
    - k-medoids or PAM (Partition around medoids) (Kaufman and Rousseeuw '87) : Each cluster is represented by one of the objects in the cluster

The k-means clustering algorithm

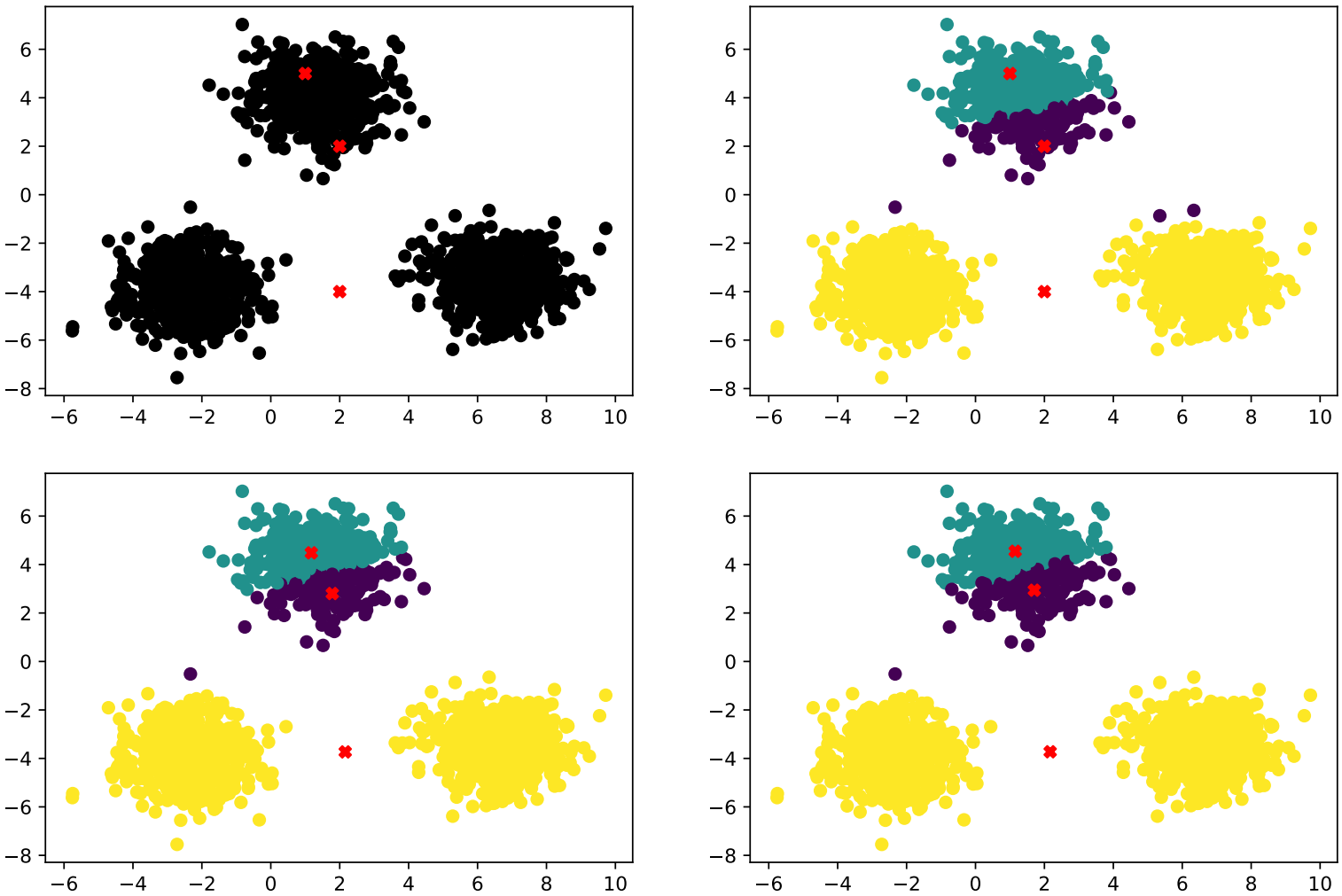
Given k, the k-means algorithm is implemented in four steps :

1. Choose k initial centroids (could be samples), each labeled as k
2. Assign each object to the cluster having the nearest centroid point
3. Compute centroids of the clusters of the current partition (the centroid is the center, i.e., mean point, of the cluster)
4. Go back to Step 2, stop when no more change

Example of k-means



Example of k-means : bad initialisation

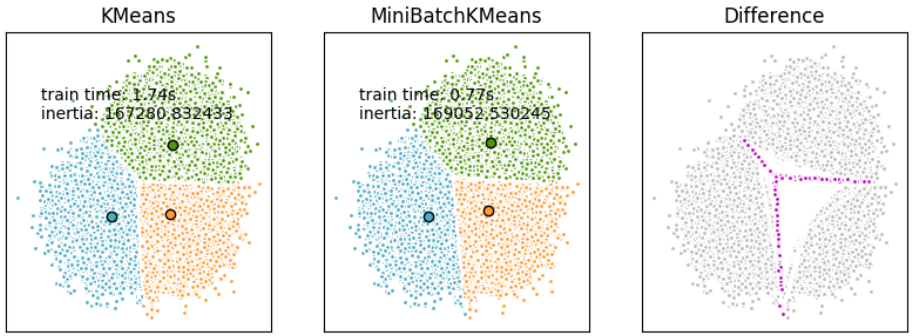


k-mean advantages and drawbacks

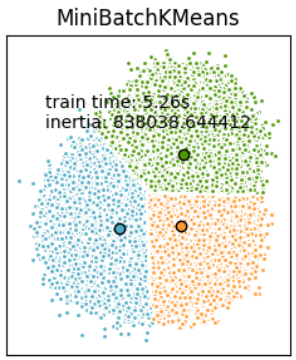
- Strength : Relatively efficient : $O(tkn)$, where n nb. of objects, k nb. of clusters, and t nb. of iterations. Normally, $k, t << n$.
  - For comparison : PAM : $O(k(n–k)^2)$, CLARA : $O(ks^2 + k(n–k))$
- Comment : Often terminates at a local optimum.
  - The global optimum may be found using optimization methods such as : simulated annealing and evolutionary algorithms.
  - In practice : several trials using aleatory initialisations and some heuristics.
- Weaknesses :
  - Applicable only when mean is defined, then what about categorical data ?
  - Need to specify k, the number of clusters, in advance
    - or use the Elbow method
  - Unable to handle noisy data and outliers
  - Not suitable to discover clusters with non-convex shapes

mini-batch k-mean

- a variant of k-mean for scalability improving
- mini-batch = subset of dataset
  - randomly sampled at each iteration of the training process
- results almost as good as the standard algorithm
  - code from `https://scikit-learn.org/stable/auto_examples/cluster/plot_mini_batch_kmeans.html#sphx-glr-auto-examples-cluster-plot-mini-batch-kmeans-py` with modification of the number of data to 200000 (upper limit to have k-means running).

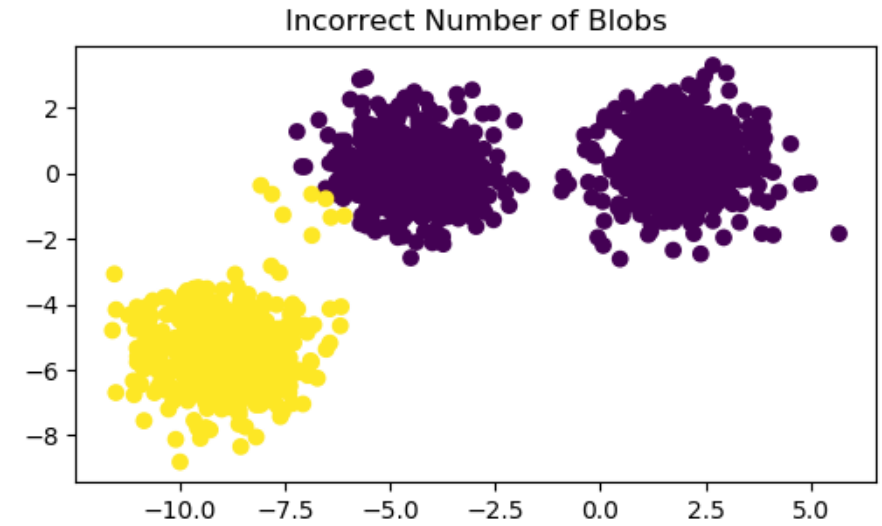


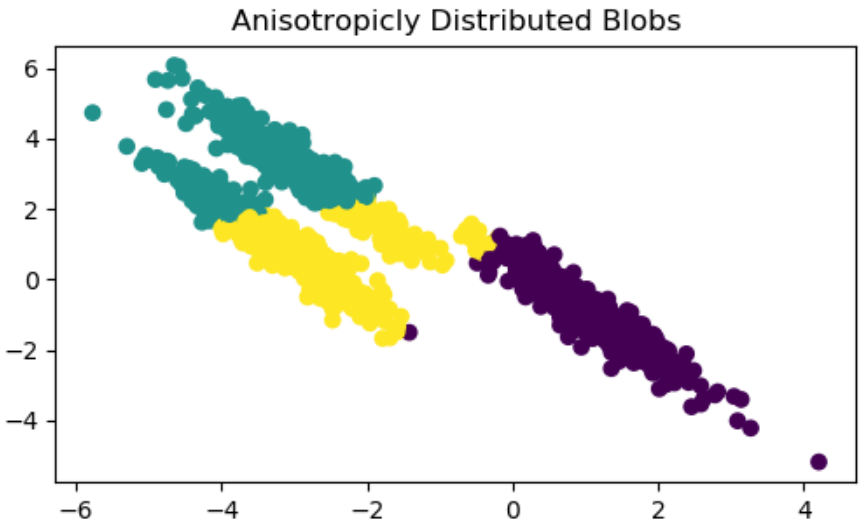
  - Only with mini-batch and using 1 million of data :

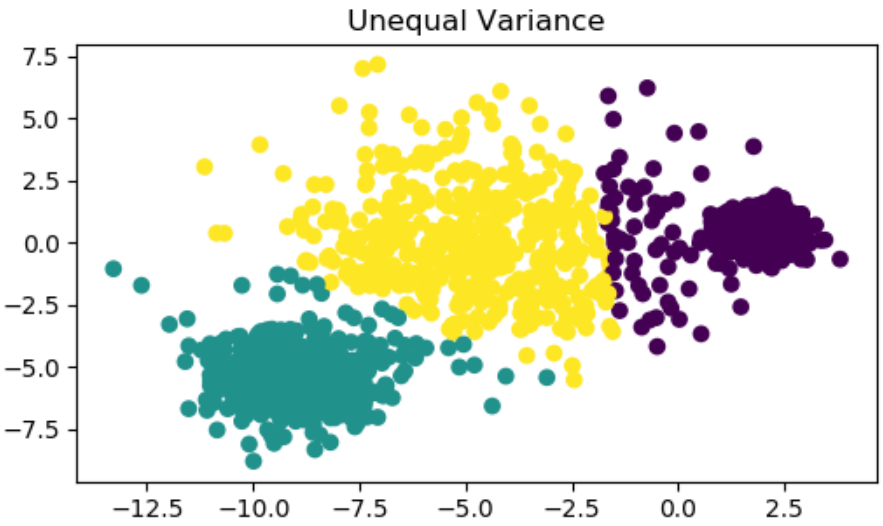


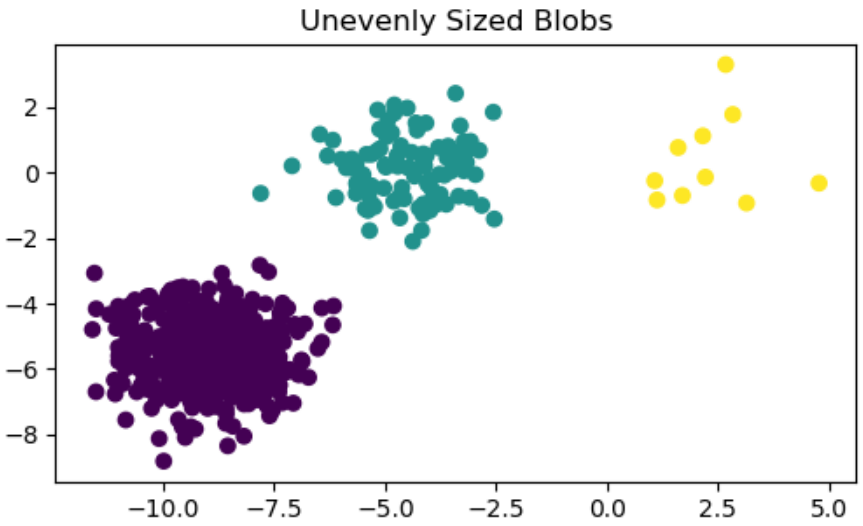
Demonstration of k-means assumptions

https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_assumptions.html





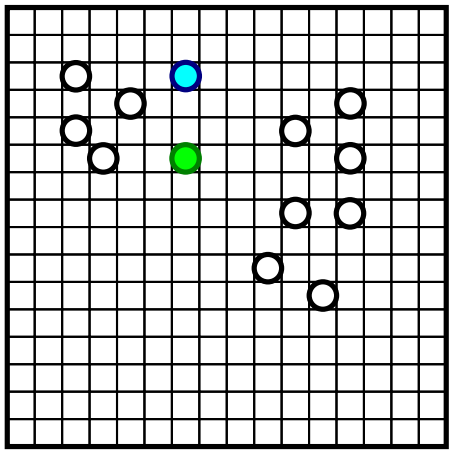




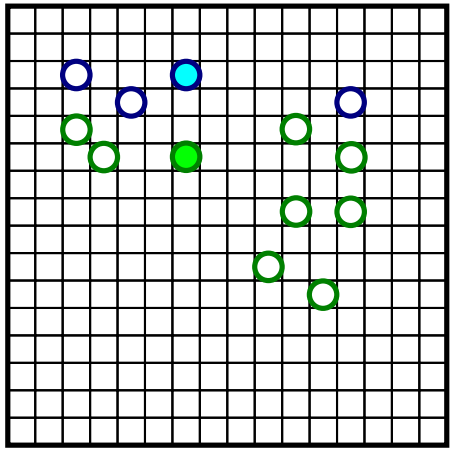
The k-Medoids Clustering Method

- Find representative objects, called medoids, in clusters
- PAM (Partitioning Around Medoids, 1987)
  - starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering
  - less sensitive to outliers than k-mean
  - PAM works effectively for small data sets, but does not scale well for large data sets
- CLARA (Clustering LARge Applications, Kaufmann & Rousseeuw, 1990) : PAM on several subsets of samples (take the best clustering)
- CLARANS (Clustering Large Applications based upon RANdomized Search, Ng & Han, 1994) : Randomized sampling. Graph of solutions (=set of centroids).

k-medoids : an example

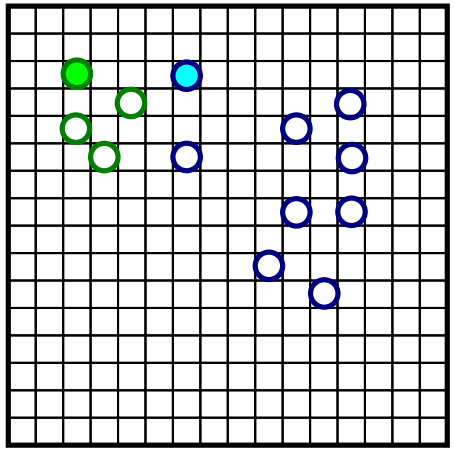


initialisation
choose 2 samples



label all data
compute the cost:
14+50=64

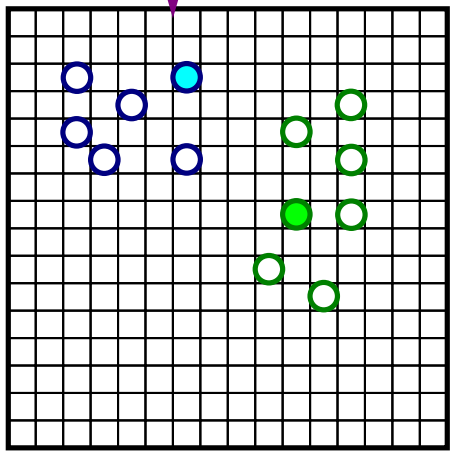
try to change
a medoid



new cost: 9+68=77 > 64

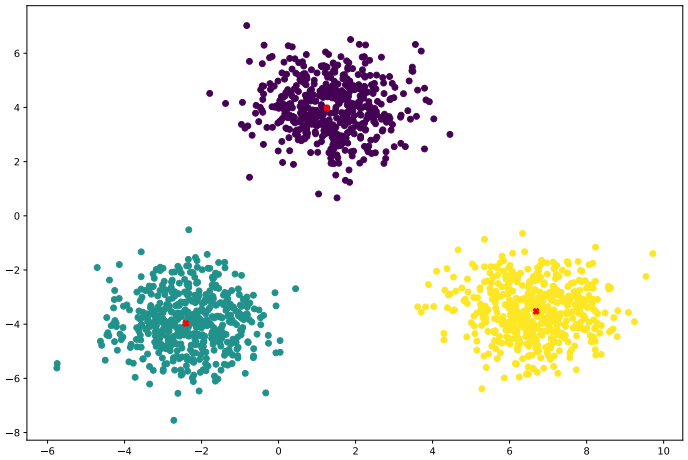
another try

keep this change
and try other changes
until no possible change

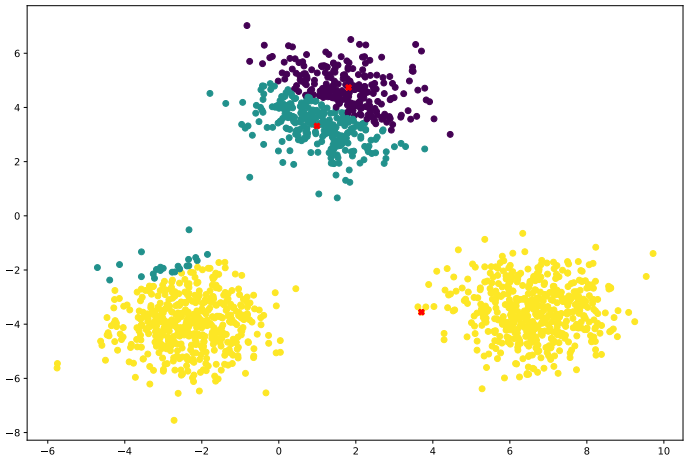


new cost: 22 + 22 = 44 < 64

k-medoids : previous example



good initialization



bad initialization

C-mean clustering method

- A fuzzy extension of the k-means algorithm
- A record can belong to more than one cluster to a degree (soft vs hard assignment) :
  - how much x_i belongs to cluster k : $0 \leq \mu_k(x_i) \leq 1$
  - constraint (c the nb. of clusters) : $\sum_{k=1}^{c} \mu_k(x_i) = 1$
  - objective function (v_k represents the cluster k) :

$$\min \sum_{k=1}^{c} \sum_{i=1}^{N} \mu_k(x_i) d(x_i, v_k)$$

Practice (1)

- play with simple data (slides 25 or 26)

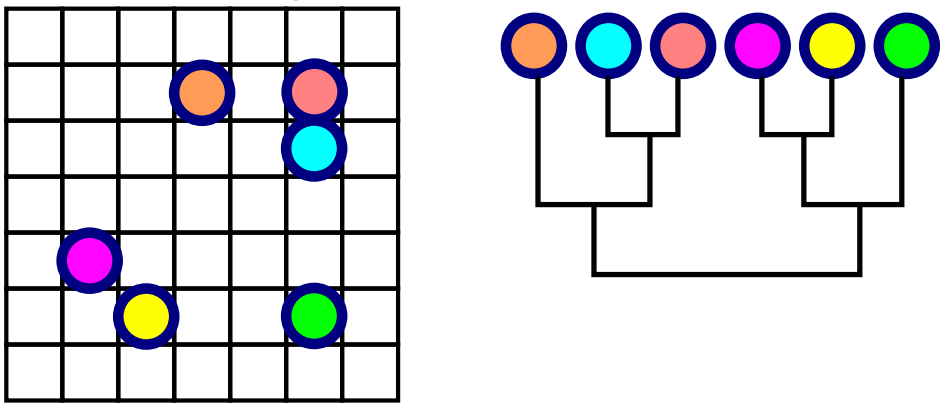
```
from sklearn.datasets import make_blobs
n_samples = 1500
random_state = 160
nb = 3 # number of blobs
X, y = make_blobs(n_samples=n_samples, centers=nb, random_state=random_state)
```

  - try different initialisations, number of points, ...
- play in higher dimension
  - choose a dataset of higher dimension : Iris (4) or MNIST/FMNIST (784)
  - test different algorithms from the family of k-means
  - visualize the results using dimension reduction to 2 (t-SNE)

Outline

Hierarchical clustering methods

- Input : distance matrix - Output : a dendrogram (tree of clusters)
- This method does not require the number of clusters k as an input, but may need a termination condition
- Two approches :
  - Bottom up approach = agglomerative
    - Example using Manhattan distance and complete linkage



  - Top down approach (DIANA = DIvide ANAlysis)
    - start with all samples in one cluster. Hierarchical division of clusters related to a dispersion criterion (divide into clusters where closest samples are the more distant ones).

Agglomerative hierarchical clustering methods

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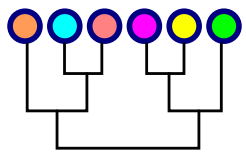
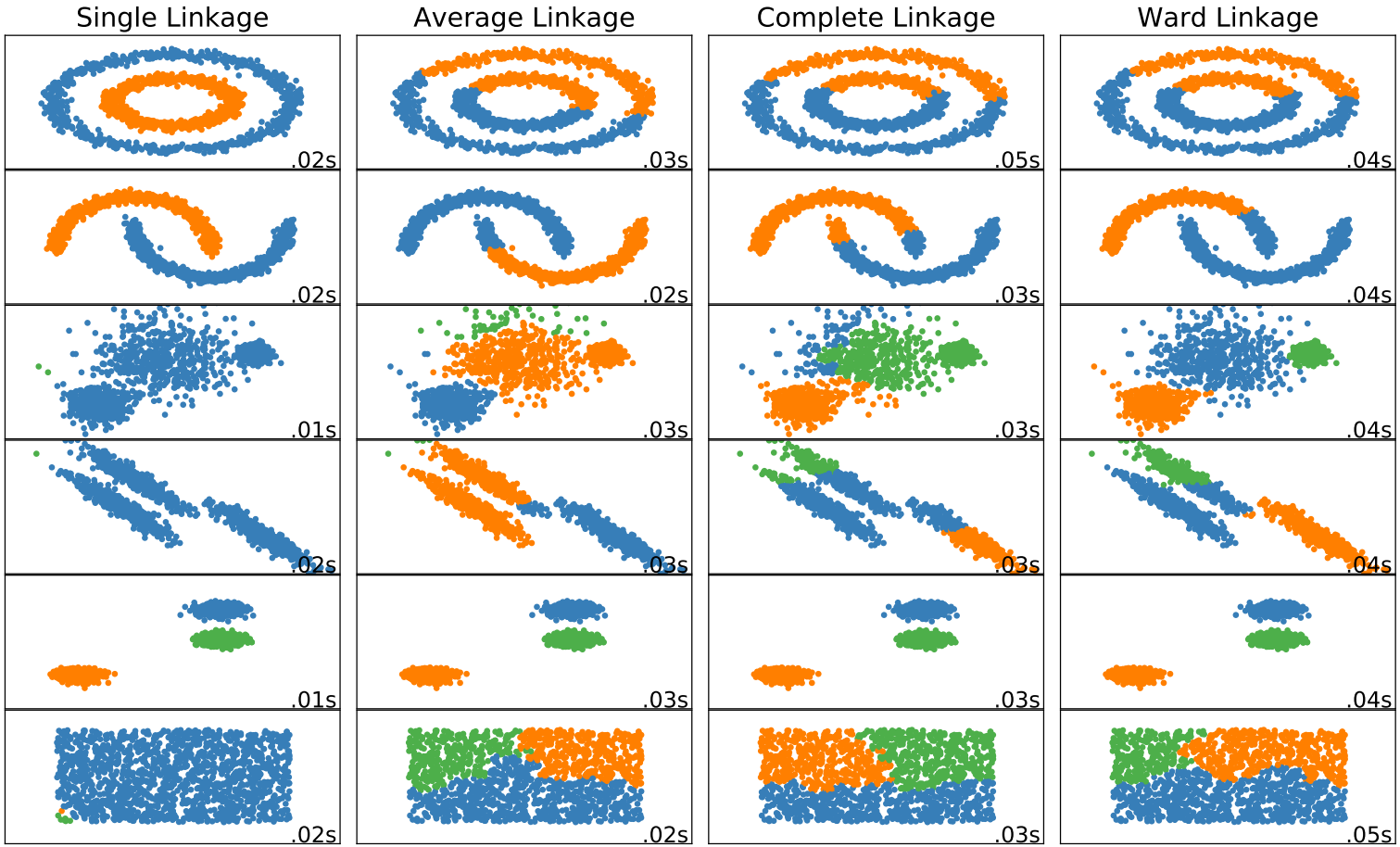
- Algorithm :
  - starts with all single data as their own cluster
  - merged clusters together according to a linkage criteria
  - ends when all data are in the same cluster
- The linkage criteria determines the metric used for the merge strategy : (from `https://scikit-learn.org/stable/modules/clustering.html#hierarchical-clustering`)
  - **Ward** minimizes the sum of squared differences within all clusters. It is a variance-minimizing approach and in this sense is similar to the k-means objective function but tackled with an agglomerative hierarchical approach.
  - **Maximum or complete linkage** minimizes the maximum distance between observations of pairs of clusters.
  - **Average linkage** minimizes the average of the distances between all observations of pairs of clusters.
  - **Single linkage** minimizes the distance between the closest observations of pairs of clusters.



Impact of the linkage criteria

From `https://scikit-learn.org/stable/modules/clustering.html#different-linkage-type-ward-complete-average-and-single-linkage.`



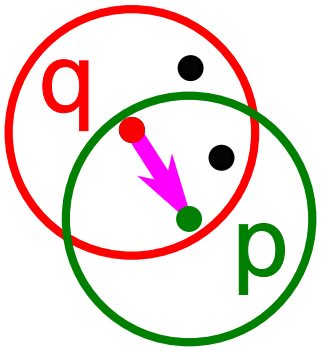
Outline

Density based clustering methods

- Clusters : areas of high density separated by areas of low density
- Clustering based on density (local cluster criterion), such as density-connected points
- Major features :
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Examples of density-based methods :
  - DBSCAN, OPTICS, DENCLUE, CLIQUE

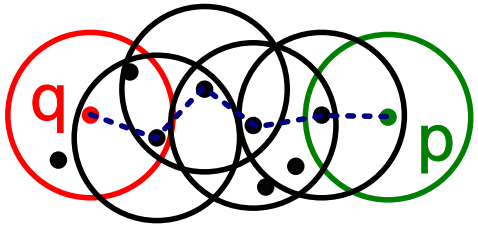
Density-Based Clustering : Basic Concepts

- Two parameters :
  - ϵ : Maximum radius of the neighbourhood
  - MinPts : Minimum number of points in an ϵ-neighbourhood of that point
- Neighborhood : $N_\epsilon(p) = \{q \in D | d(p,q) \leq \epsilon\}$
- Core point : if at least MinPts points are within distance ϵ of p (including p).
- Directly density-reachable : A point p is directly density-reachable from a point q w.r.t. ϵ, MinPts if :
  - p belongs to $N_\epsilon(q)$
  - core point condition : $|N_\epsilon(q)| \geq MinPts$

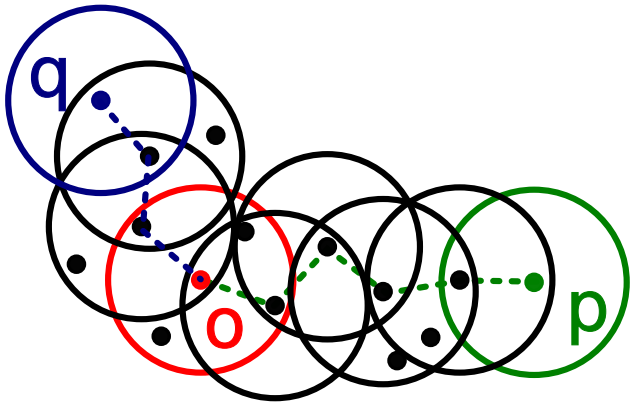


Density-Reachable and Density-Connected

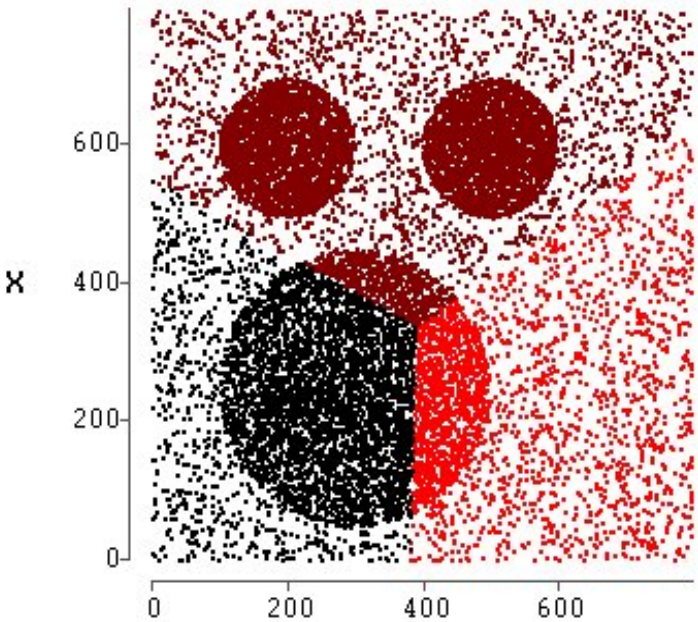
- Density-Reachable :
  - A point p is density-reachable from a point q w.r.t. ϵ, MinPts if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i



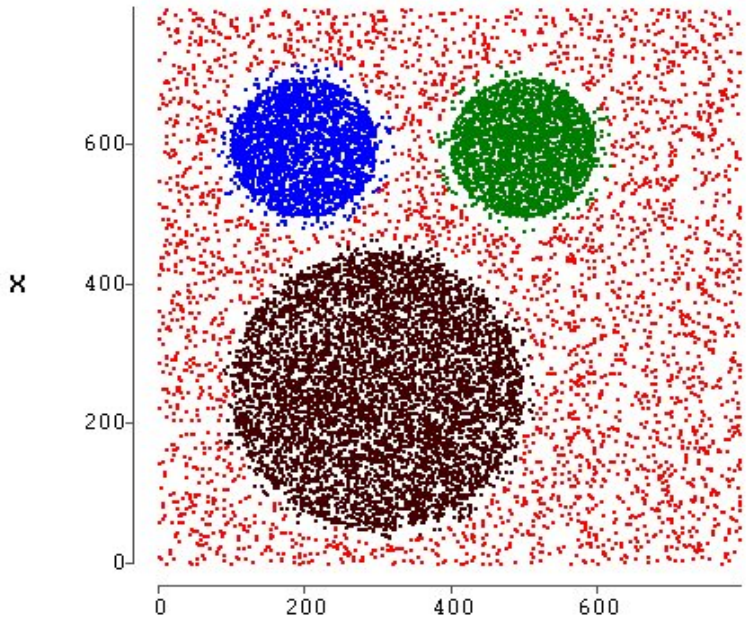
- Density-Connected :
  - A point p is density-connected to a point q w.r.t. ϵ, MinPts if there is a point o such that both, p and q are density-reachable from o w.r.t. ϵ and MinPts



- choose a core point p, not already assigned to a cluster
- add all density-reachable points from p to this cluster
- go back to step 1 until no more points without a cluster
- all points not reachable from any other point are outliers or noise points



using k-means

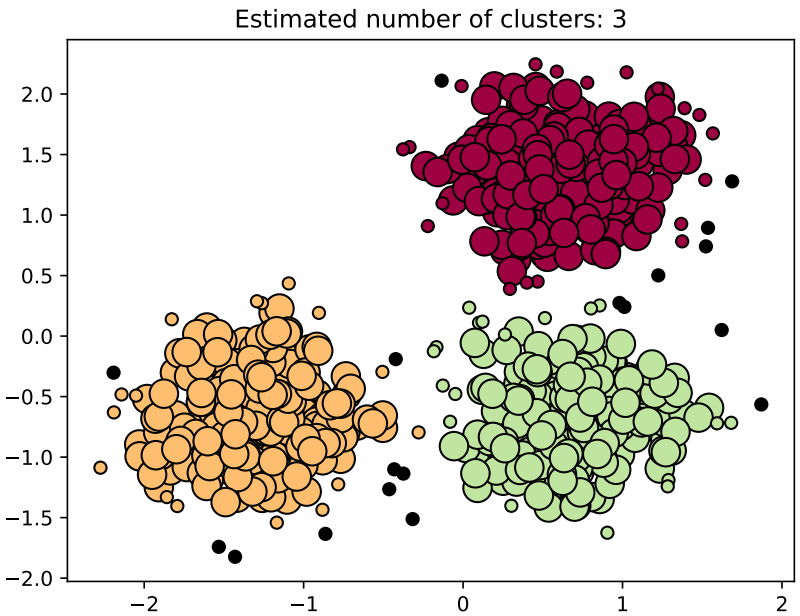


using DBSCAN

DBSCAN in scikit-learn

from `https://scikit-learn.org/stable/auto_examples/cluster/plot_dbscan.html#`

`sphx-glr-download-auto-examples-cluster-plot-dbscan-py`




```
from sklearn.cluster import DBSCAN
db = DBSCAN(eps=0.3, min_samples=10)
```

Outline

- A popular probability-based iterative refinement algorithm
- Based on the assumption that the distribution of samples is a mixture of gaussians (GMM)
  - likelihood of x knowing its gaussian distribution $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$:

$$p(\mathrm{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\mathrm{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathrm{x}-\boldsymbol{\mu})\right\}$$

  - likelihood of x knowing the GMM (the K, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$ and w_k) with $\forall k\ w_k > 0$ and $\sum_{k=1}^{K} w_k = 1$:

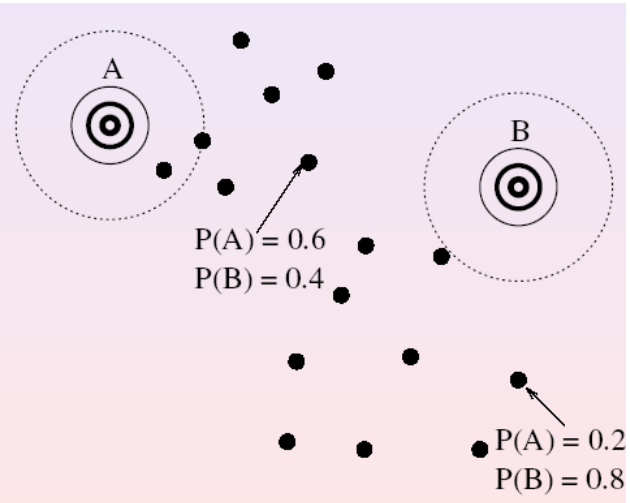
$$p(\mathrm{x}) = \sum_{k=1}^{K} w_k p(\mathrm{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \sum_{k=1}^{K} p(k)p(\mathrm{x}|k)$$

- Learning the GMM : Expectation Maximisation
- sklearn : `mixture.GaussianMixture`

- A 3 steps algorithm :
  - step 1 : Initialization
  - step 2 : Expectation (compute probability for each sample of belonging to each gaussian)
  - step 3 : Maximisation (compute parameters of the GMM using result of step 2)
- Loop steps 2 and 3 until convergence
- The larger the log likelihood, the better the model fits the data

- estimate the posterior probability of cluster k for each x_i
- for each x_i estimate the probability of belonging to each gaussian : $p(k|x_i)$:

$$p(k|x_i) = \frac{p(x_i|k)p(k)}{p(x_i)}$$



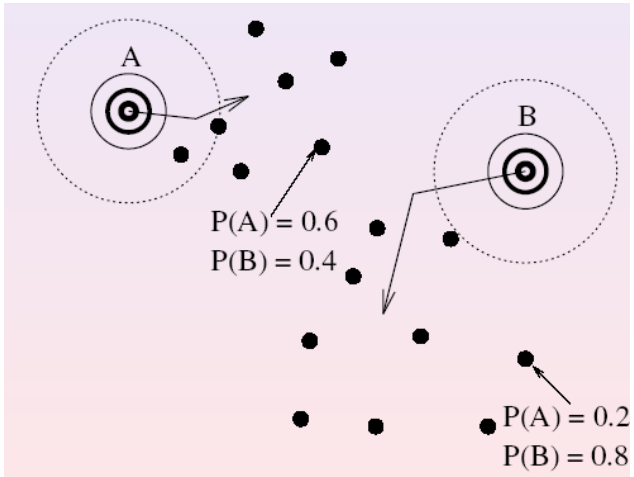
Maximisation

- maximisation of the log of likelihood (partial derivatives equal to 0)
- update of the parameters $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$ and w_k :

$$\boldsymbol{\mu}_k = \frac{\sum_{i=1}^{n} p(k|x_i)x_i}{\sum_{i=1}^{n} p(k|x_i)}$$

$$\boldsymbol{\Sigma}_k^2 = \frac{\sum_{i=1}^{n} p(k|x_i)(x_i - \boldsymbol{\mu}_k)^2}{\sum_{i=1}^{n} p(k|x_i)}$$

$$w_k = \frac{1}{n}\sum_{i=1}^{n} p(k|x_i)$$



Outline

Spectral clustering

- Affinity matrix representation of samples : A_{ij} is high if samples x_i and x_j are close.
  - could be measured using troncated gaussian :
    - if $\|x_j - x_i\| > R$: $A_{ij} = 0$
    - else $A_{ij} = \exp(-\alpha \|x_j - x_i\|^2)$
- Eigenvalues and eigenvectors decomposition $\Rightarrow$ space reduction using eigenvectors corresponding to highest eigenvalues
- Clustering of points in new dimension
- only for small number of clusters

Outline

Huge number of data

- use a canopy clustering as pre-clustering
  - algorithm using 2 thresholds : T_1 and T_2, a set of samples S

take one element e of S and starts a new canopy
for *all element s of* S **do**
  if $d(e, s) < T_1$ **then**
    assign s to the current canopy
  end
  if $d(e, s) < T_2$ **then**
    remove s from S
  end
end
repeat until S empty

  - one sample may belongs to several canopies
  - refine the results using a clustering algorithm
- sample the data
- mini batch

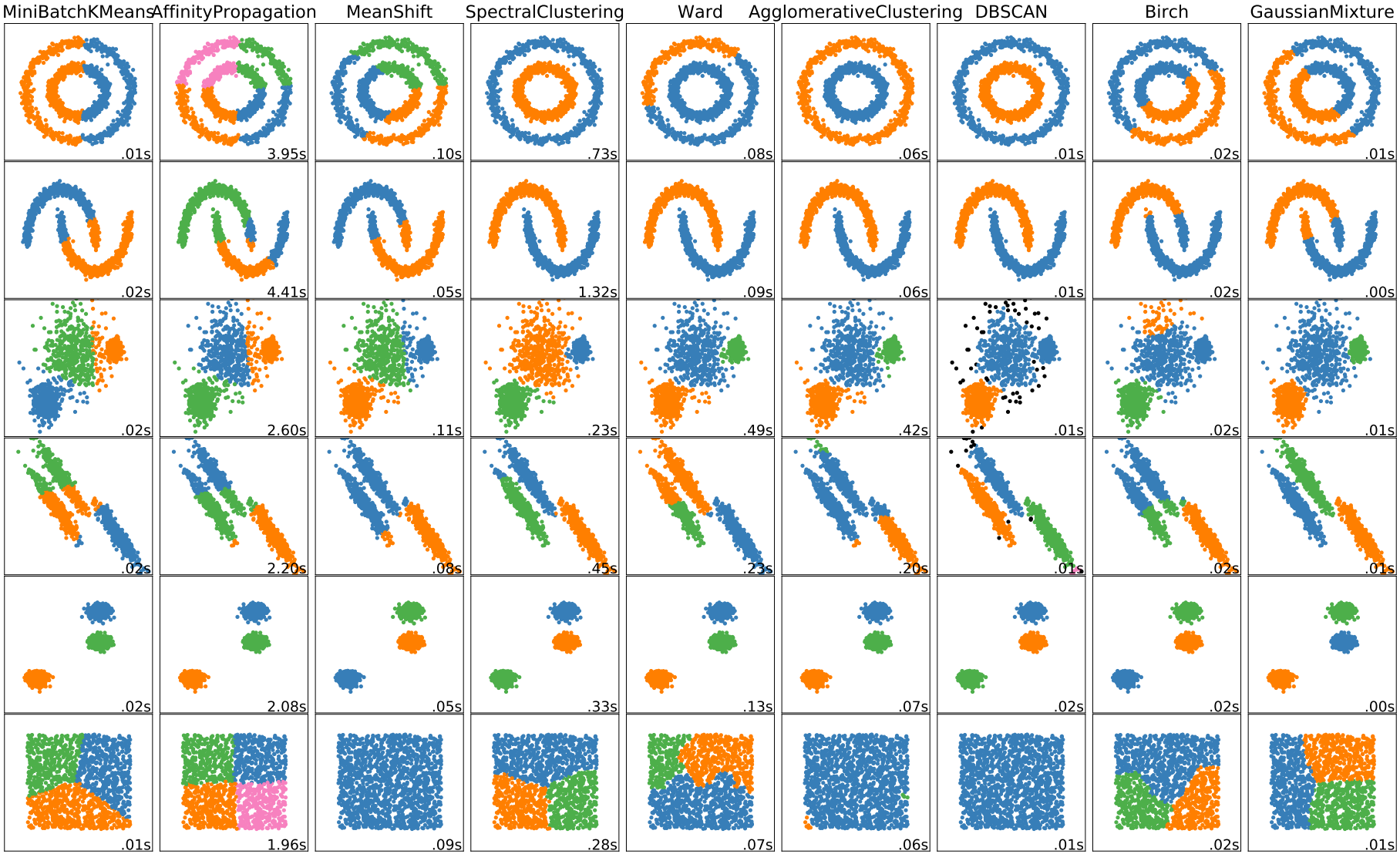
High dimension of data

- curse of dimensionality
  - volume of hypersphere $<<$ volume of hypercube
  - distance from center to corner of hyper cube grows without limit
- reducing the dimension
  - PCA, ...

Practice (2)

- Example : k-means and GMM
- Comparison between k-means and GMM
  - increase the size of the dataset
  - increase the dimension of the data
  - increase the number of clusters
  - change the shape of clusters
- try initialisation with k-means and refinement with GMM

Outline


MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
Birch
GaussianMixture
.01s
3.95s
.10s
.73s
.08s
.06s
.01s
.02s
.01s
.02s
4.41s
.05s
1.32s
.09s
.06s
.01s
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.00s
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.28s
.07s
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.02s
.01s

Evaluation of clustering

- ground truth known
  - ARI (Adjusted Rand Index)
  - MI (Mutual Information)
  - V-measure
- ground truth not known
  - Davies-Bouldin index
  - Dunn index
  - Calinkski-Harabaz
  - silhouette

Adjusted Rand Index (ARI)

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- value in $[-1 \ +1]$
  - good : $+1$
  - bad : negative or close to 0
  - random label assignments : value close to 0
- no assumption on the data stucture
- Rand Index :
  - n : number of data samples
  - a : number of pairs of samples in the same set in C and in K
  - b : number of pairs of samples in different sets in C and in K
  - C_2^n : total number of pairs of samples

$$RI = \frac{a+b}{C_2^n}$$

- Adjusted Rand Index :
  - $E[RI]$ is computed from random clusterings

$$ARI = \frac{RI - E[RI]}{\max(RI) - E[RI]}$$

- can be used to measure similarity between 2 clustering results
- sklearn : `metrics.adjusted_rand_score`

V-measure

- quality of clustering :
  - homegeneity : each cluster contains only samples of a single class
  - completeness : all members of a given class are assigned to the same cluster
- V-measure represents the (weighted) harmonic mean of these 2 quantities
- value in $[0 \ +1]$
  - random clustering : be careful if small dataset, high number of clusters
- no assumption on the data stucture
- sklearn :
  - `metrics.homogeneity_score`
  - `metrics.completeness_score`
  - `metrics.v_measure_score`

- Internal validation : Separation ? Compactness ?
  - E.g. Dunn, Davies-Bouldin, Calinski-Harabaz, and Silhouette indexes.
  - Problems :
    - Different performance WRT existence of noise, variable densities, and non well-separated clusters.
    - Overrate the algorithm that uses the same clustering model.

number of clusters	average silhouette score	Calinski Harabaz score
2	0.71	1604
3	0.59	1810
4	0.65	2704
5	0.56	2263
6	0.45	2043

Davies-Bouldin score

- average similarity between each cluster C_i and its most similar one C_j. In the context of this index, similarity is defined as a measure R_{ij} that trades off :
  - s_i the average distance between each point of cluster i and the centroid of that cluster
  - d_{ij} the distance between cluster centroids c_i and c_j

$$R_{ij} = \frac{s_i + s_j}{d_{ij}}$$

- Davies-Bouldin score :

$$DB = \frac{1}{k} \sum_{i=1}^{k} \max_{i \neq j} R_{ij}$$

- Zero is the lowest possible score. Values closer to zero indicate a better partition.
- sklearn : `davies_bouldin_score`

Calinski-Harabaz score

For k clusters, the Calinski-Harabaz score s is given as the ratio of the between-clusters dispersion mean and the within-cluster dispersion (N is the size of the dataset) :

$$s(k) = \frac{Tr(B_k)}{Tr(W_k)} \frac{N-k}{k-1}$$

with :

$$W_k = \sum_{q=1}^{k} \sum_{x \in C_q} (x - c_q)(x - c_q)^T$$

and

$$B_k = \sum_{q} n_q (c_q - c)(c_q - c)^T$$

c_q is the centroid of cluster C_q containing n_q samples. c is the centroid of the dataset

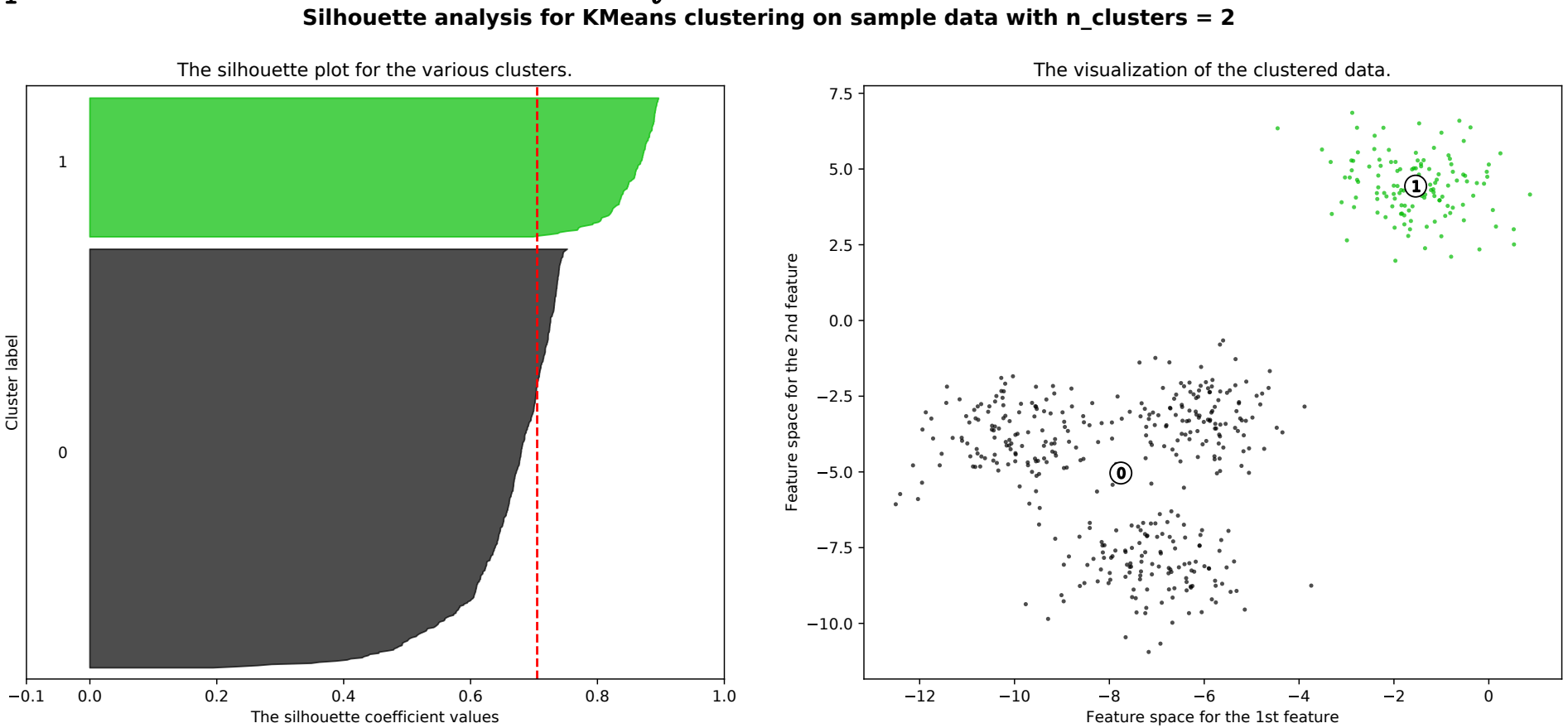
in sklearn : `metrics.calinski_harabasz_score`

Silhouette coefficients

- for a single sample : Silhouette coefficient $s = \frac{b-a}{\max(a,b)}$ with
  - a : mean distance between a sample and all other samples from the same cluster
  - b : mean distance between a sample and all other samples in the next nearest cluster
- for a dataset : mean of Silhouette coefficients for each sample
- sklearn : `metrics.silhouette_score`

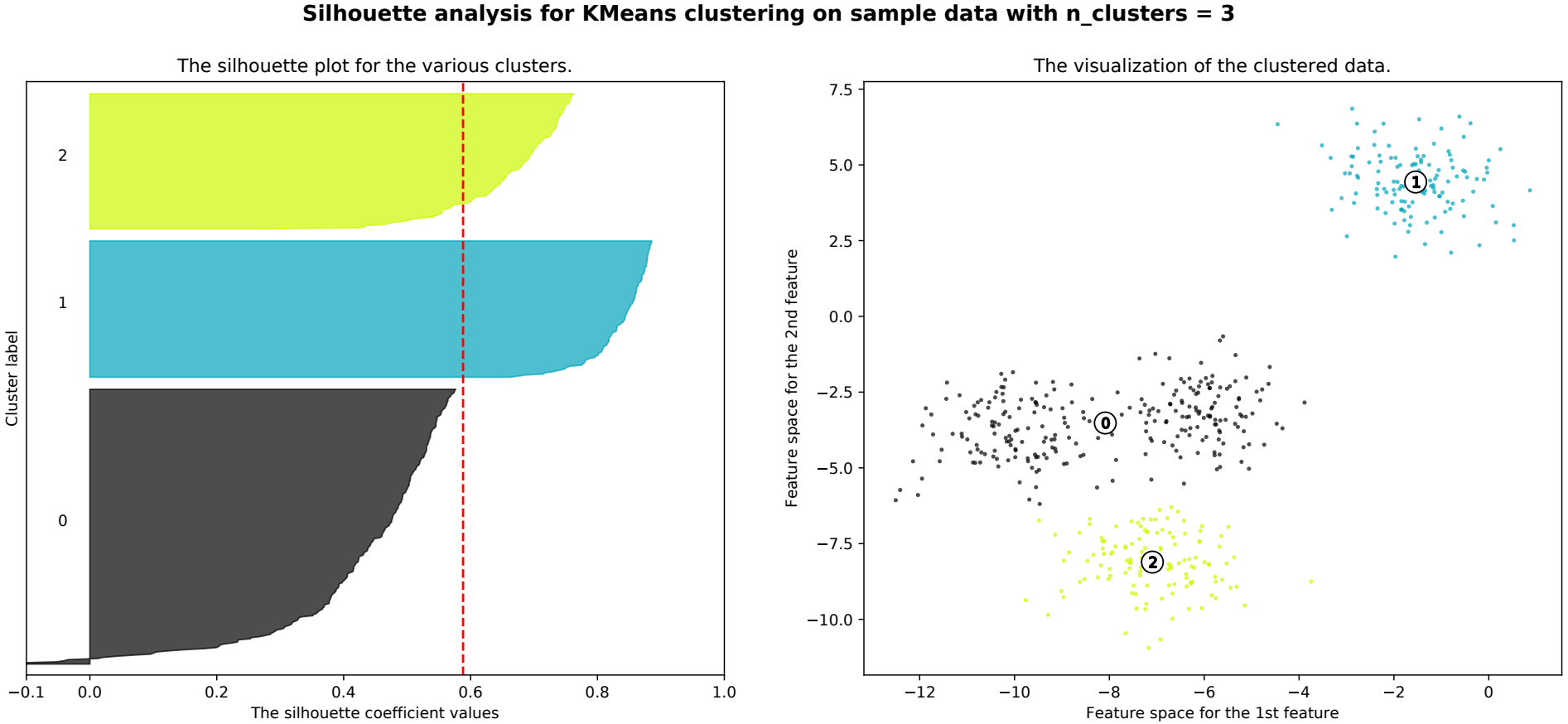
k-means with $k = 2$ and silhouette profiles

inspired by `https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html`



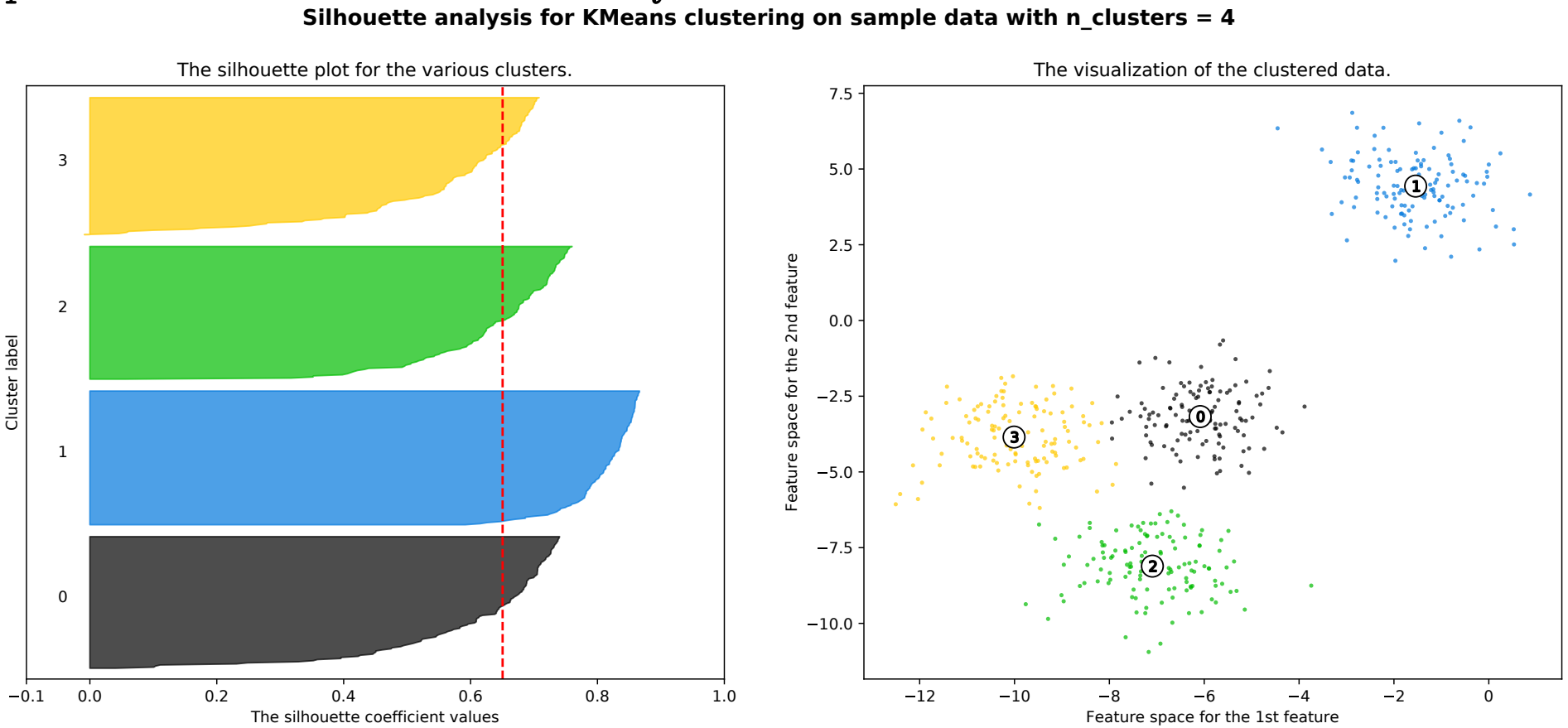
k-means with $k = 3$ and silhouette profiles

inspired by `https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html`



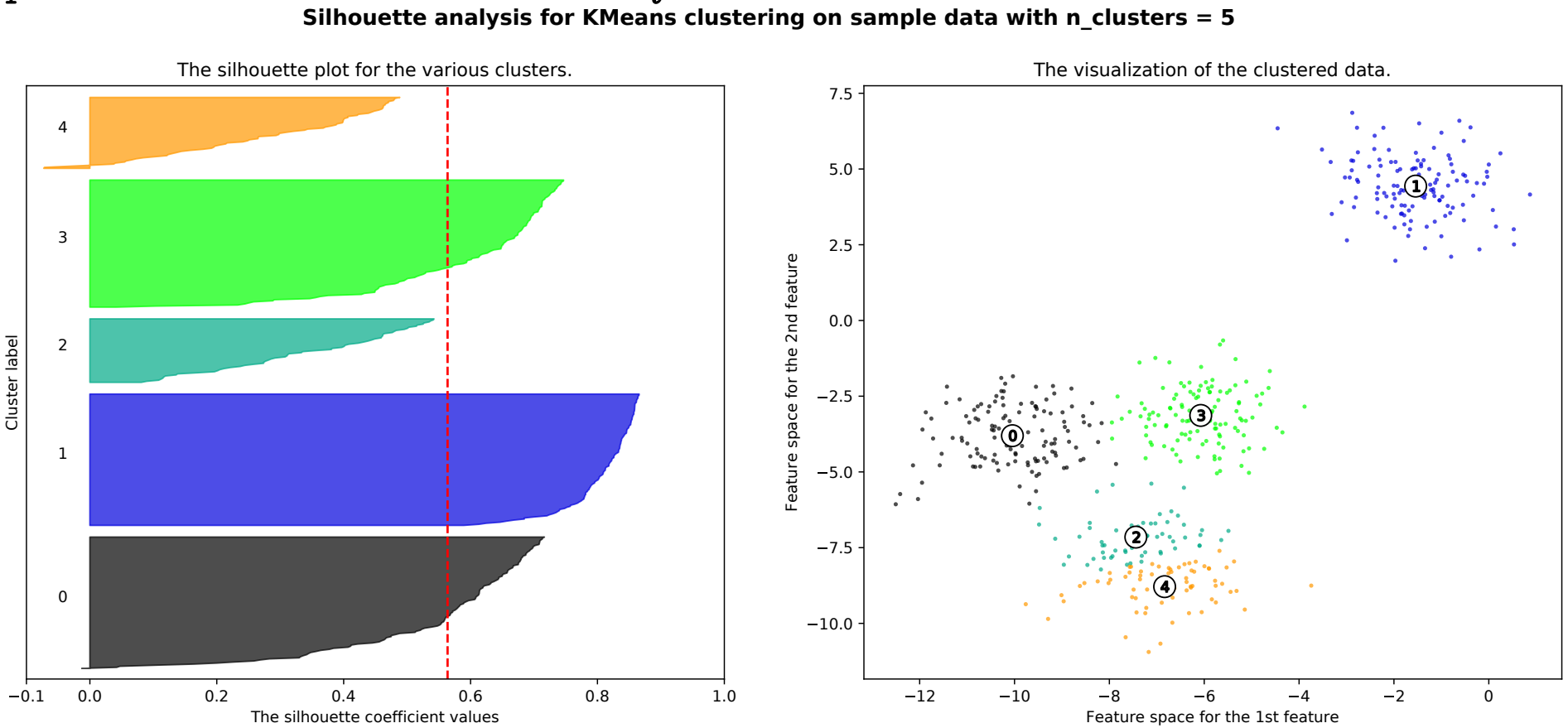
k-means with $k = 4$ and silhouette profiles

inspired by `https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html`



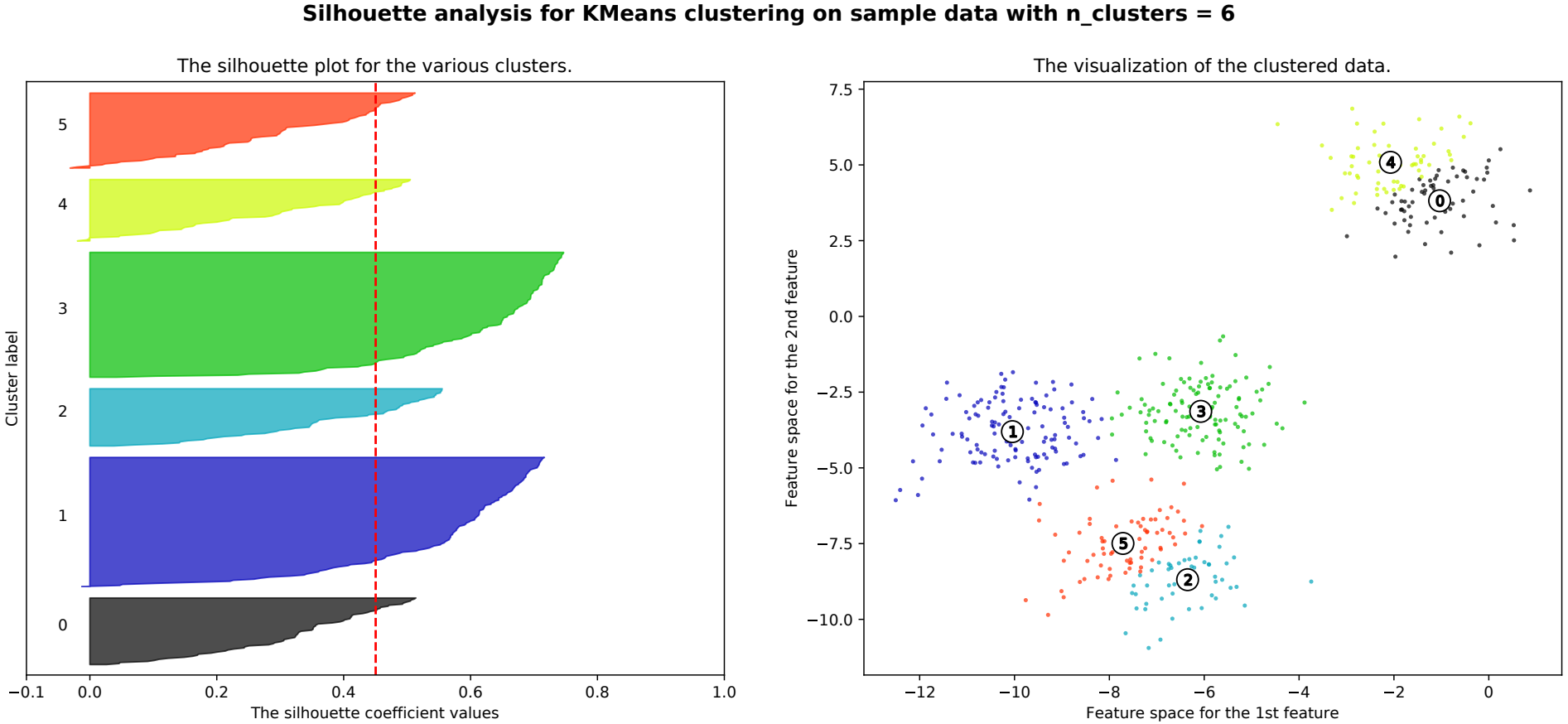
k-means with $k = 5$ and silhouette profiles

inspired by `https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html`

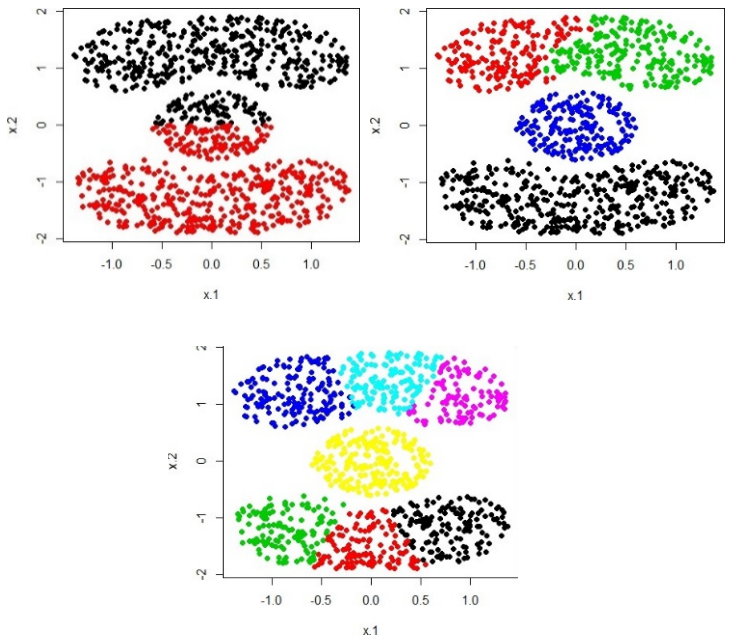


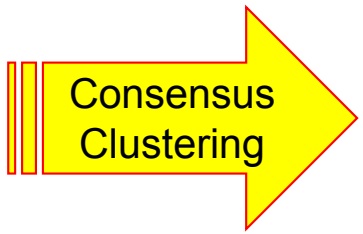
k-means with $k = 6$ and silhouette profiles

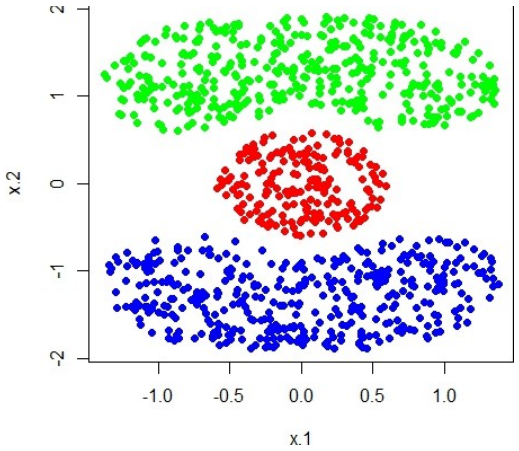
inspired by `https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html`



Consensus clustering







Ensemble of 3 base clusterings

Consensus solution