Машинное обучение

Лекция 11

Кластеризация

Михаил Гущин

mhushchyn@hse.ru

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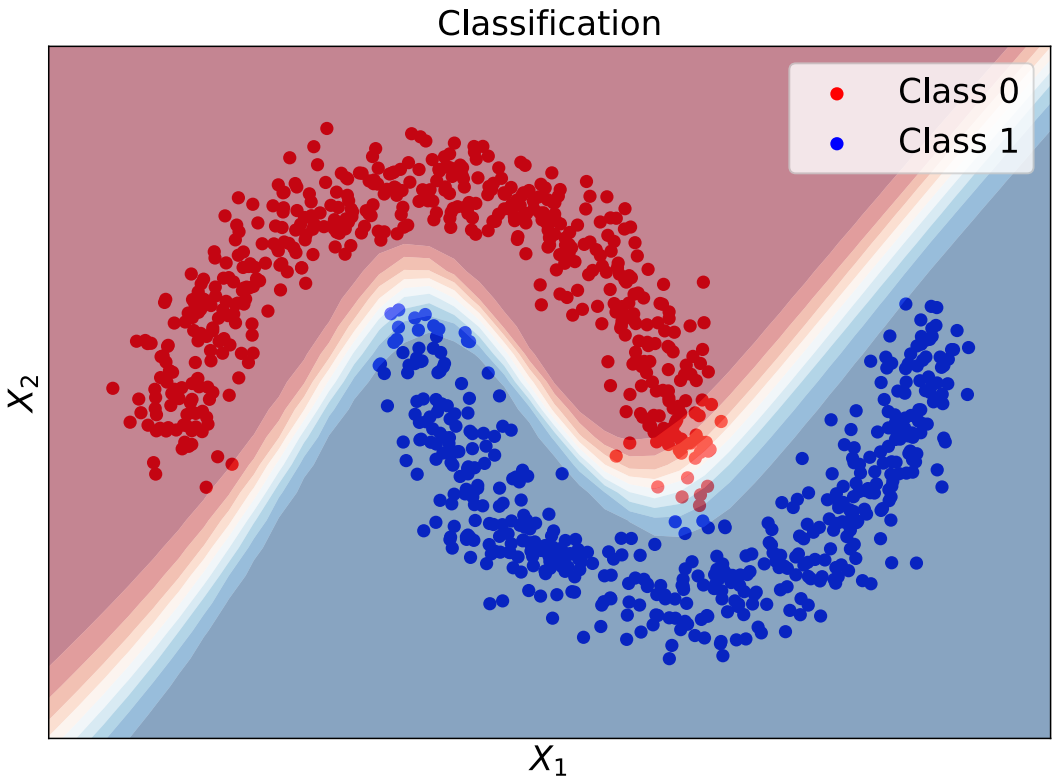
Clustering

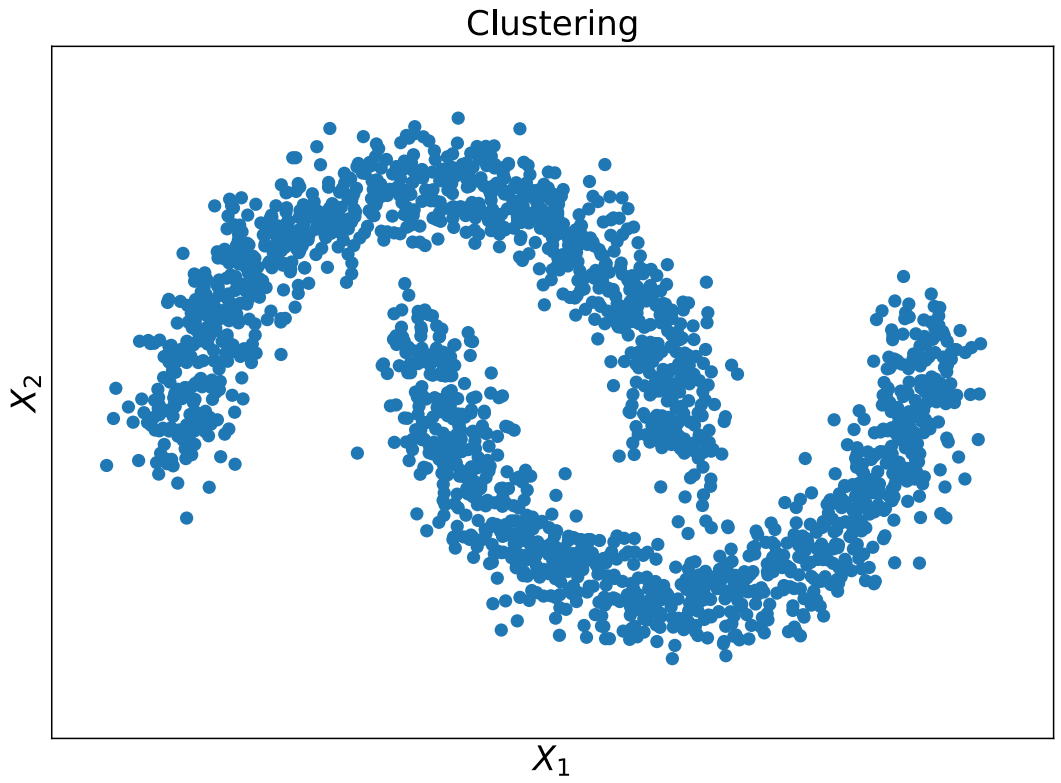
Clustering vs classification

- In classification, we have object features X and class labels $y \in \{0, 1\}$
- A classifier learns decision rule f, so that $f(X) \approx y$
- The trained classifier predicts class labels for new objects

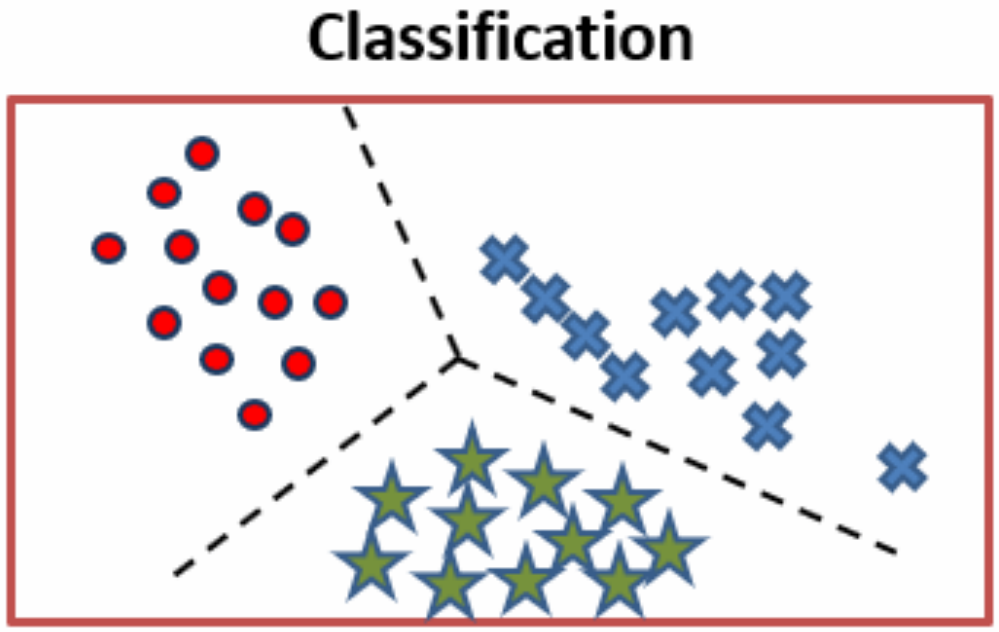


Clustering vs classification

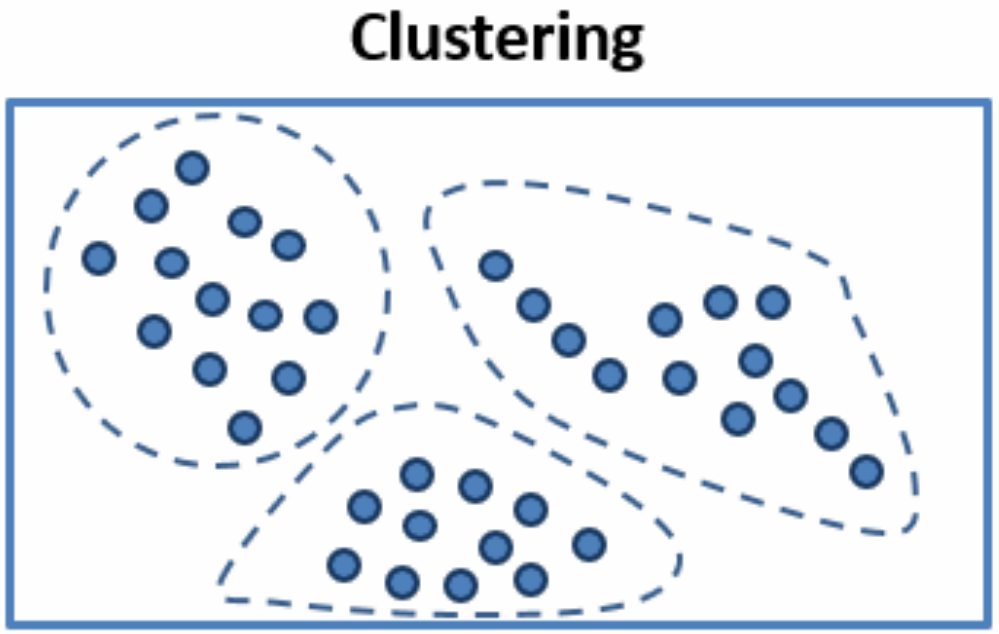
- In clustering, we don't have class labels y
- The goal is to divide all objects into separate groups using only object features X
- Objects inside groups are similar
- Objects from different groups are dissimilar



Clustering vs classification

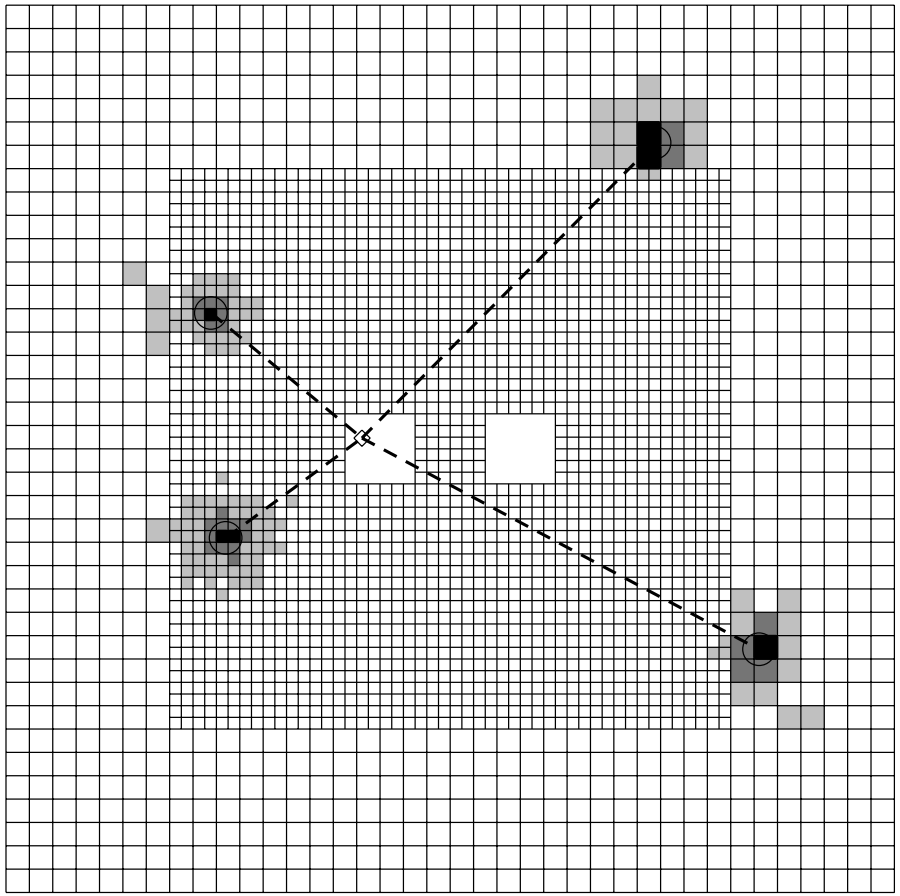


Supervised learning



Unsupervised learning

Example of clustering



Clusters in EM calorimeter of KTEV experiment for $K \to \pi^0\pi^0$ decay.

Clustering assumptions

Most of clustering algorithms are based on the following assumptions:

- Objects form dense clusters
- Objects from one cluster are similar
- Objects from different clusters are dissimilar
- Objects similarity is often based on distance between them
- Distances between neighbors **within one cluster** are smaller than between objects **from different clusters**

Within cluster distance

- Consider a sample with N objects $\{x_n\}_{n=1}^{N}$.
- We will search for K clusters with centers $\{\mu_1, \mu_2, \dots, \mu_K\}$.
- Within-cluster distance:

$$D = \sum_{k=1}^{K} \sum_{i=1}^{N} [a(x_i) = k] \, \rho(x_i, \mu_k)$$

Where $a(x_i)$ denotes the cluster number for x_i

Intercluster distance

- Consider a sample with N objects $\{x_n\}_{n=1}^{N}$.
- We will search for K clusters with centers $\{\mu_1, \mu_2, \dots, \mu_K\}$.
- Intercluster distance:

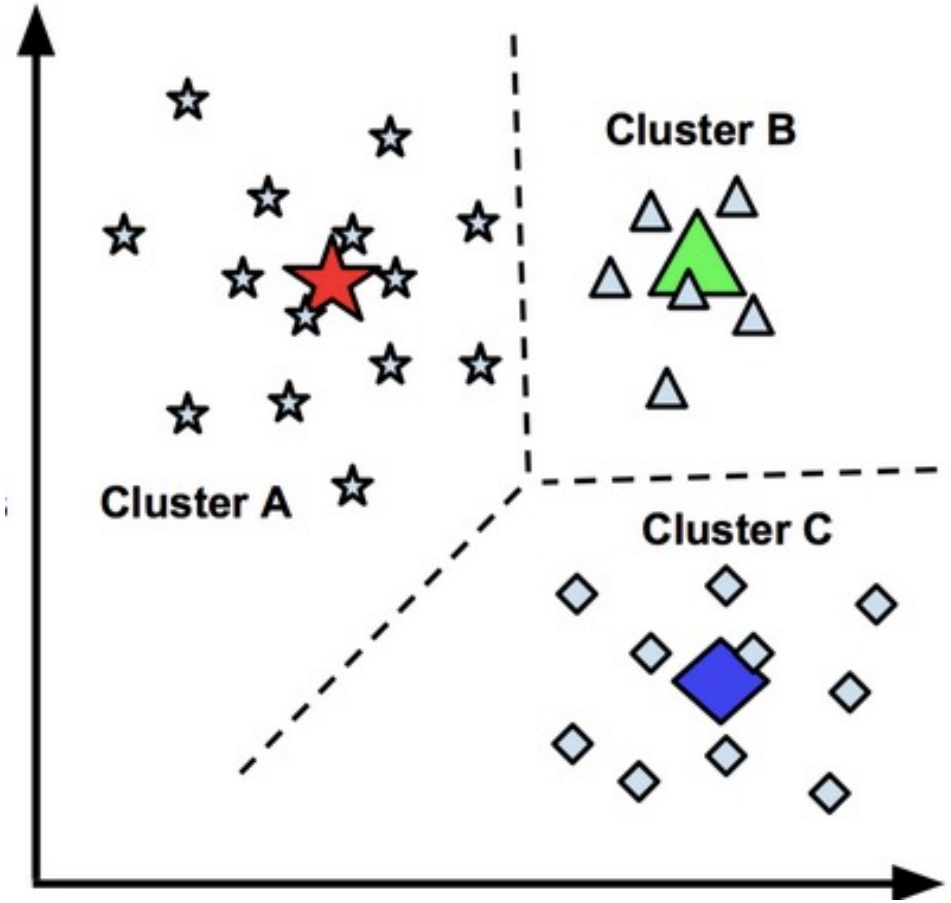
$$D = \sum_{i=1}^{N} \sum_{j=1}^{N} [a(x_i) \neq a(x_j)] \, \rho(x_i, x_j)$$

Where $a(x_i)$ denotes the cluster number for x_i

K-Means

Clustering intuition

- Each cluster is represented by its center
- All objects are assigned to the closest center
- The goal is to find such centers that form the most compact clusters



Link: https://medium.com/@msdasila90/basics-k-means-clustering-algorithm-a77c539c9e00

Notations

- Consider a sample with N objects $\{x_n\}_{n=1}^{N}$.
- We will search for K clusters with centers $\{\mu_1, \mu_2, \dots, \mu_K\}$.
- Criterion to find the best centers is minimum of **within-cluster distance**:

$$Q = \sum_{n=1}^{N} \min_k \rho(x_n, \mu_k) \to \min_{\mu_1,\dots,\mu_K}$$

- Each object x_n is assigned to a cluster $z_n \in \{1, 2, \dots, K\}$ as:

$$z_n = \arg\min_k \rho(x_n, \mu_k)$$

General algorithm

initialize $\mu_1, \ldots \mu_K$ from random training objects

WHILE not converged:

  FOR $n = 1, 2, \ldots N$:

    $z_n = \arg\min_k \rho(x_n, \mu_k)$ ← Assign each object to the nearest center

  FOR $k = 1, 2, \ldots K$:

    $\mu_k = \arg\min_\mu \sum_{n:z_n=k} \rho(x_n, \mu)$ ← Update the centers

RETURN $z_1, \ldots z_N$

Algorithm variations

- Distance $\rho(x_n, \mu_k)$ can be defined in different ways.
- If $\rho(x_n, \mu_k) = \|x_n - \mu_k\|_2^2$, we get **K-Means algorithm**
- If $\rho(x_n, \mu_k) = \|x_n - \mu_k\|_1$, we get **K-Medians algorithm**

K-Means algorithm

Initialize μ_j, $j = 1, 2, \ldots K$.

WHILE not converged:

FOR $i = 1, 2, \ldots N$:

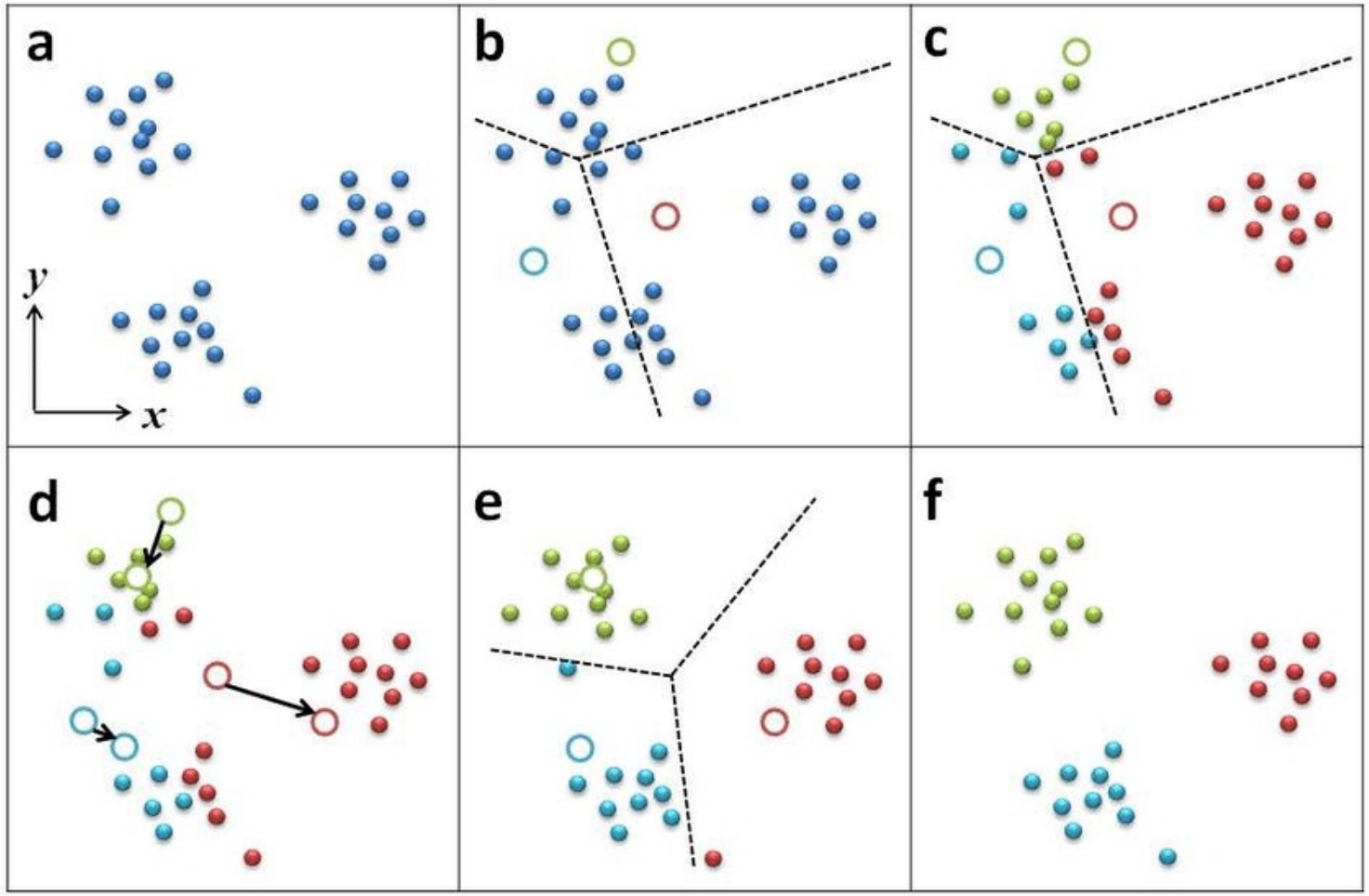
find cluster number of x_i:

$z_i = \arg\min_{j \in \{1,2,\ldots K\}} ||x_i - \mu_j||_2^2$

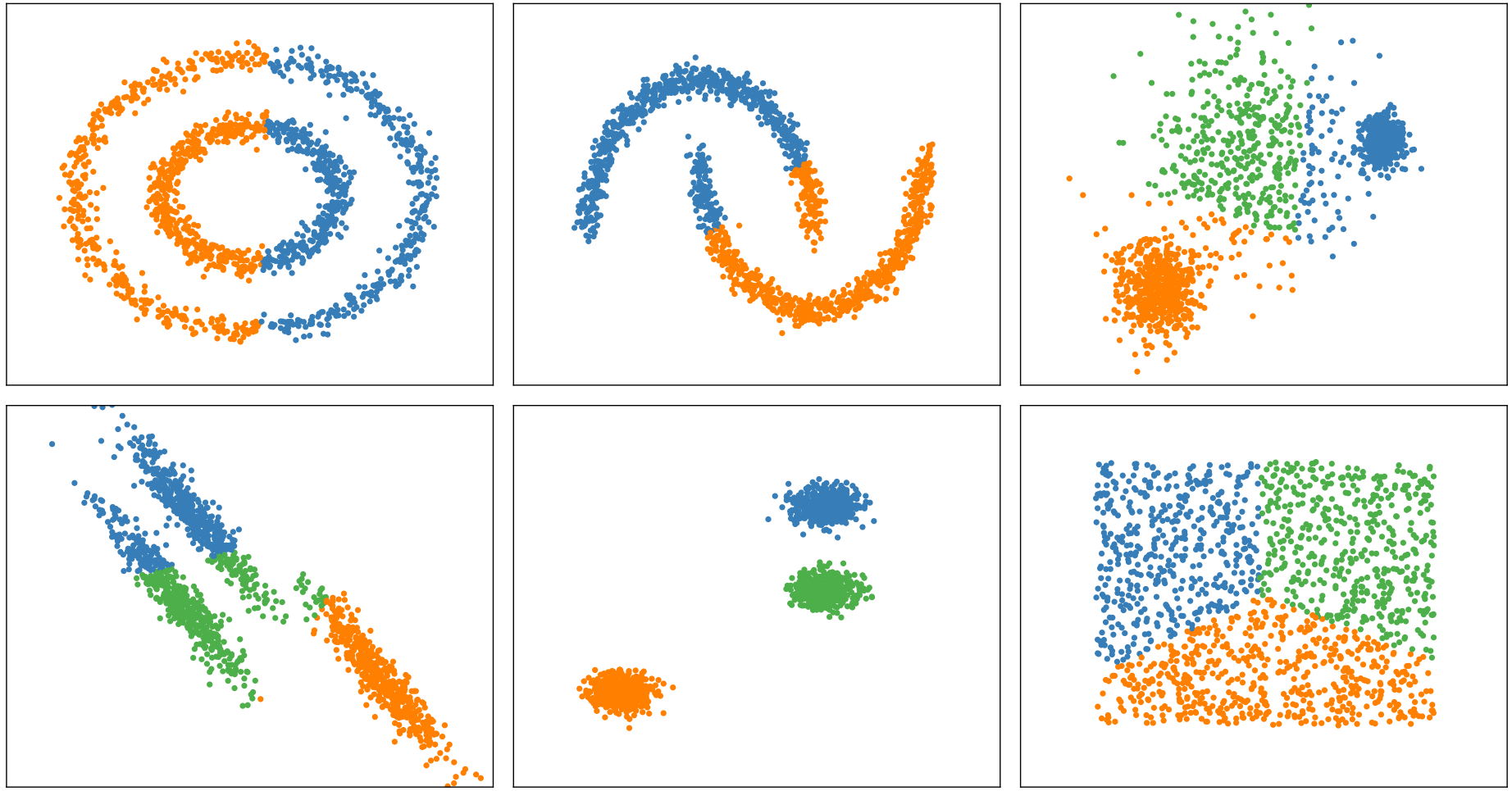
FOR $j = 1, 2, \ldots K$:

$\mu_j = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n = j]} \sum_{n=1}^{N} \mathbb{I}[z_n = j] x_i$

K-Means demonstration



K-Means examples



Properties #1

- Initializaion:
  - Centers $\{\mu_k\}_{k=1}^K$ are usually initialized randomly from training objects
  - Number of clusters (and centers) K is fixed
- Convergence criteria:
  - Iterations limit is reached
  - Centers stop changing significantly
  - Cluster assignments $\{z_n\}_{n=1}^N$ stop changing

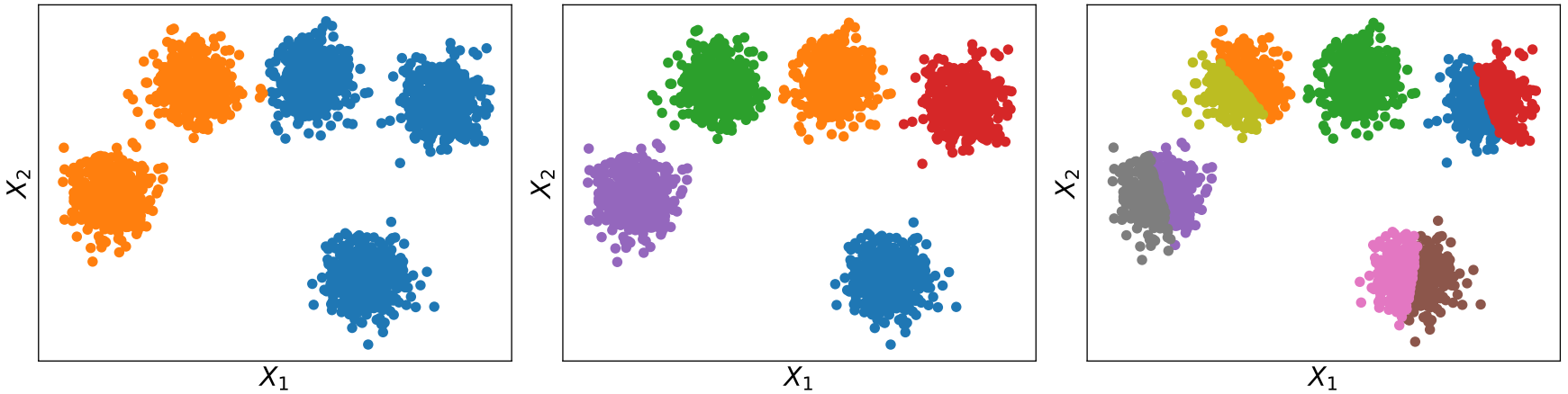
Properties #2

- Solution
  - Depends on starting positions of centers
  - Sensitive to outliers, may create single-object clusters
  - It is recommended to run the algorithm with several different initializations and select solution with the minimal within-cluster distance Q

Elbow method

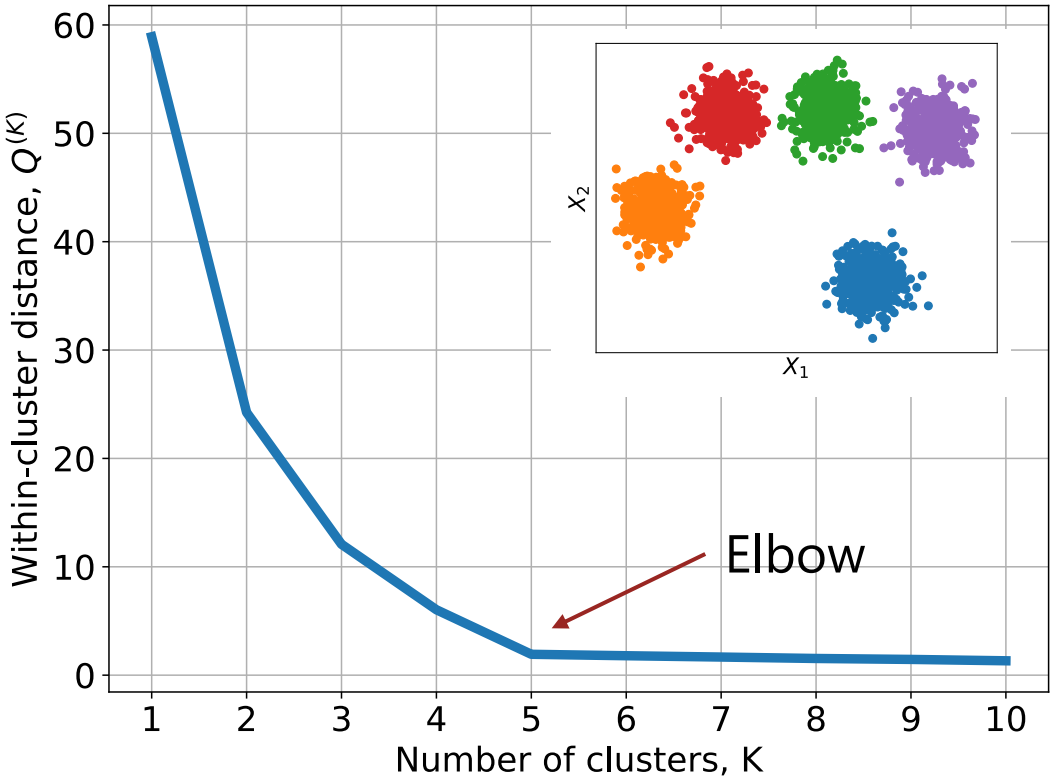
- How to estimate optimal number of clusters K?
- Consider within-cluster distances $Q^{(K)}$ for all possible K:

$$Q^{(K)} = \sum_{n=1}^{N} \left\| x_n - \mu_{z_n} \right\|_2^2 \to \min_{z_1,\ldots,z_N,\mu_1,\ldots,\mu_K}$$



Elbow method

- $Q^{(K)}$ decreases with increasing K
- The dependence has elbow at the optimal number of clusters ($K = 5$)
- Let's try to formalize it

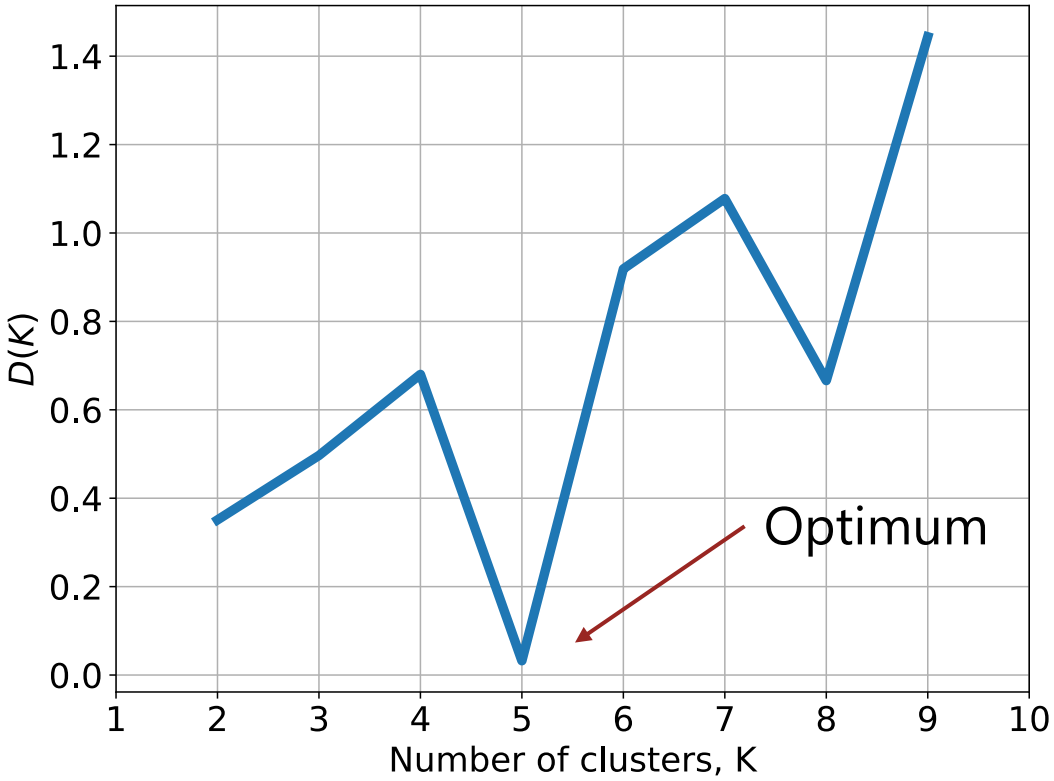


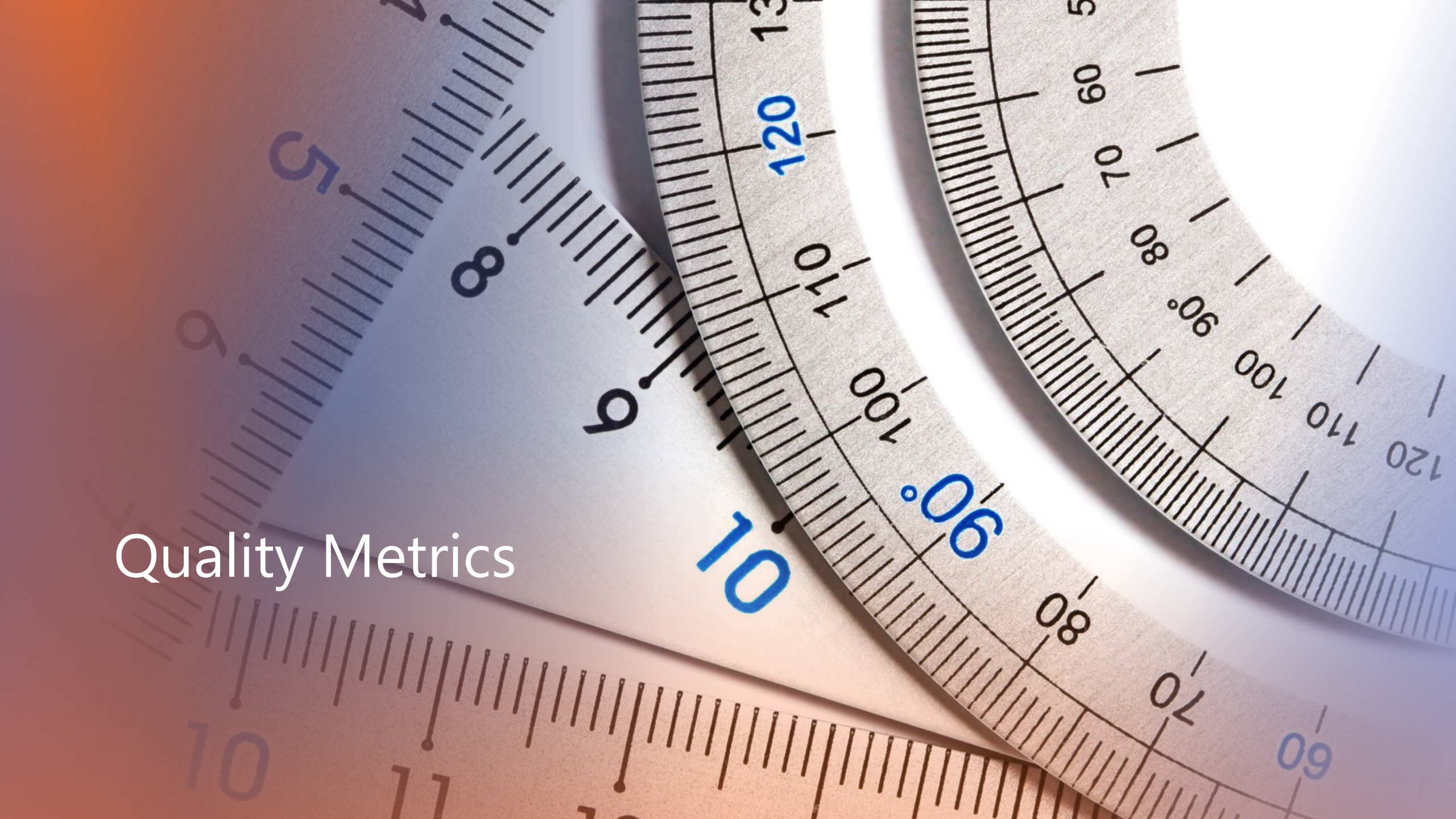
Elbow method

- Let's define $D(K)$:

$$D(K) = \frac{|Q^{(K+1)} - Q^{(K)}|}{|Q^{(K)} - Q^{(K-1)}|}$$

- This function takes small value for the optimal number of clusters





Quality Metrics

Quality metrics

There are two kinds of quality metrics for clustering:

- Supervised
  - Based on ground truth of object labels
  - Invariant to cluster naming
- Unsupervised
  - Based on intuition about “good” clusters:
    - Objects from the same cluster are similar / close to each other
    - Objects from different clusters are dissimilar / distant from each other

Rand Index

Rand Index (RI) is supervised quality metric defined as:

$$\mathrm{RI} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}$$

TP – number of pairs in the same cluster in predictions and the ground truth,

TN – number of pairs from different clusters in predictions and the ground truth,

FP – number of pairs in the same cluster in predictions, but from different clusters in the ground truth,

FN – number of pairs in the same cluster in the ground truth, but from the different clusters in predictions.

Adjusted Rand Index

Adjusted Rand Index (ARI) is modification of RI:

$$\mathrm{ARI} = \frac{\mathrm{RI} - \mathrm{RI}_{\mathrm{Expected}}}{\mathrm{RI}_{\mathrm{Max}} - \mathrm{RI}_{\mathrm{Expected}}}$$

ARI has a value close to 0.0 for random labeling independently of the number of clusters and samples and exactly 1.0 when the clustering is ideal

Metrics for classification

- $\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$
- $\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$
- $\text{F1} - \text{score} = \frac{2 * \text{Precision} * \text{Recall}}{\text{Precision} + \text{Recall}}$
- Fowlkes-Mallows Index (FMI) $= \frac{\text{TP}}{\sqrt{(\text{TP}+\text{FP})(\text{TP}+\text{FN})}}$
- others

Silhouette

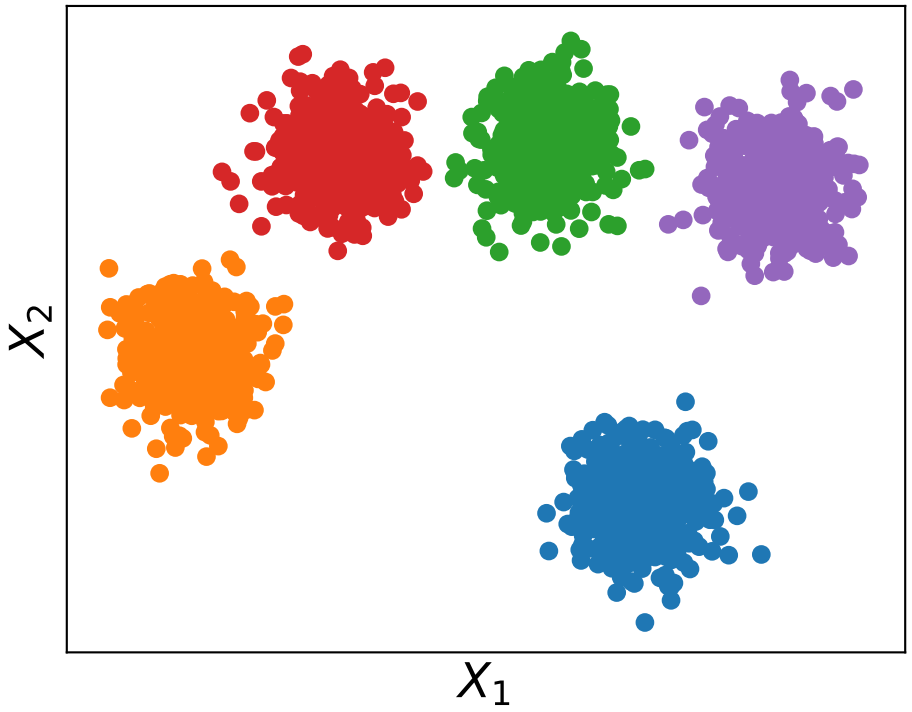
Silhouette is unsupervised quality metric defined as:

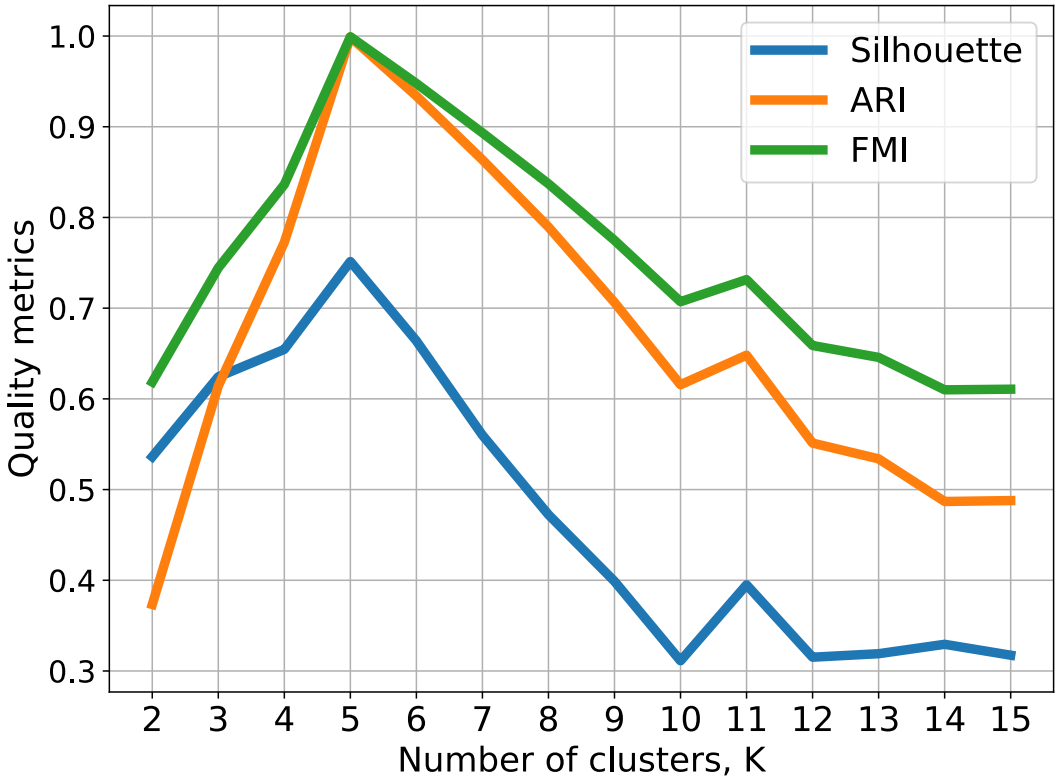
$$\text{Silhouette} = \frac{1}{N}\sum_{i=1}^{N}\frac{d_i - s_i}{\max\{d_i, s_i\}}$$

s_i - mean distance between the i-th object and all objects in the same cluster,

d_i - mean distance between the i-th object and all objects in the nearest cluster.

Example

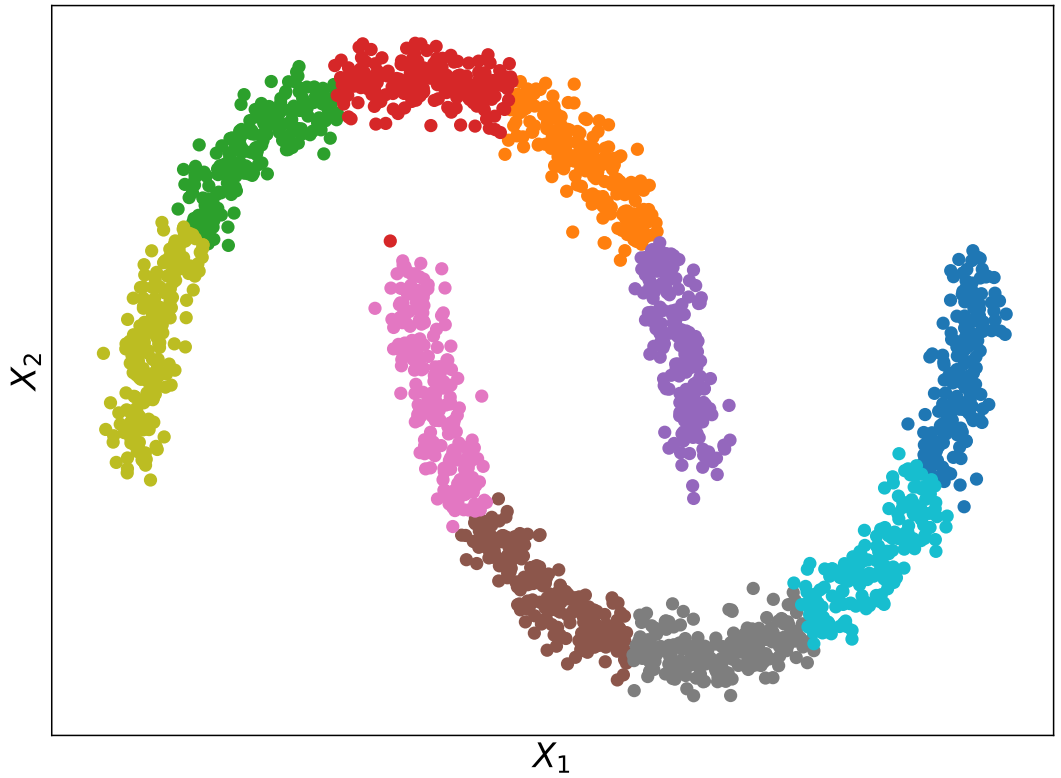

X_2
X_1


Silhouette
ARI
FMI
Quality metrics
Number of clusters, K
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
2 3 4 5 6 7 8 9 10 11 12 13 14 15

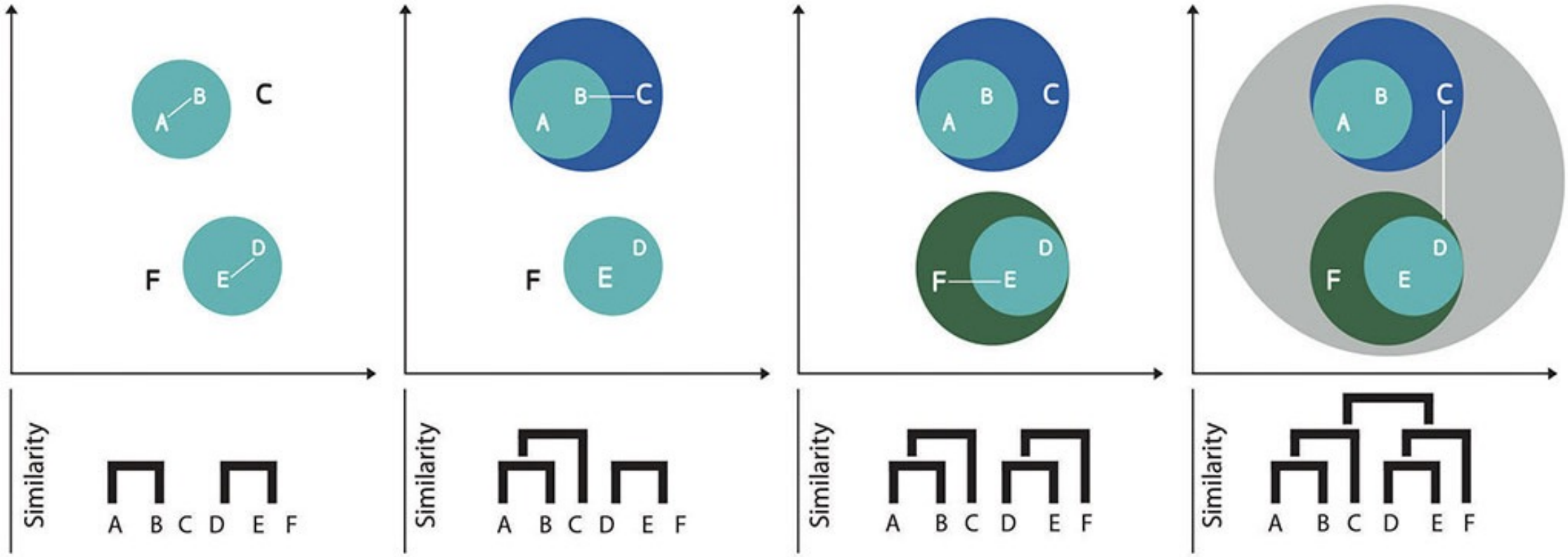
Hierarchical Clustering

Intuition

- Let's ask K-Means to find many clusters
- Each found cluster will be inside a real cluster
- Now, let's unite neighbor found clusters into one
- In result, we will get clusters with more complex shapes



Agglomerative clustering



- Combine A & B based on similarity
- Combine D & E based on similarity

- Combination of A & B is combined with C

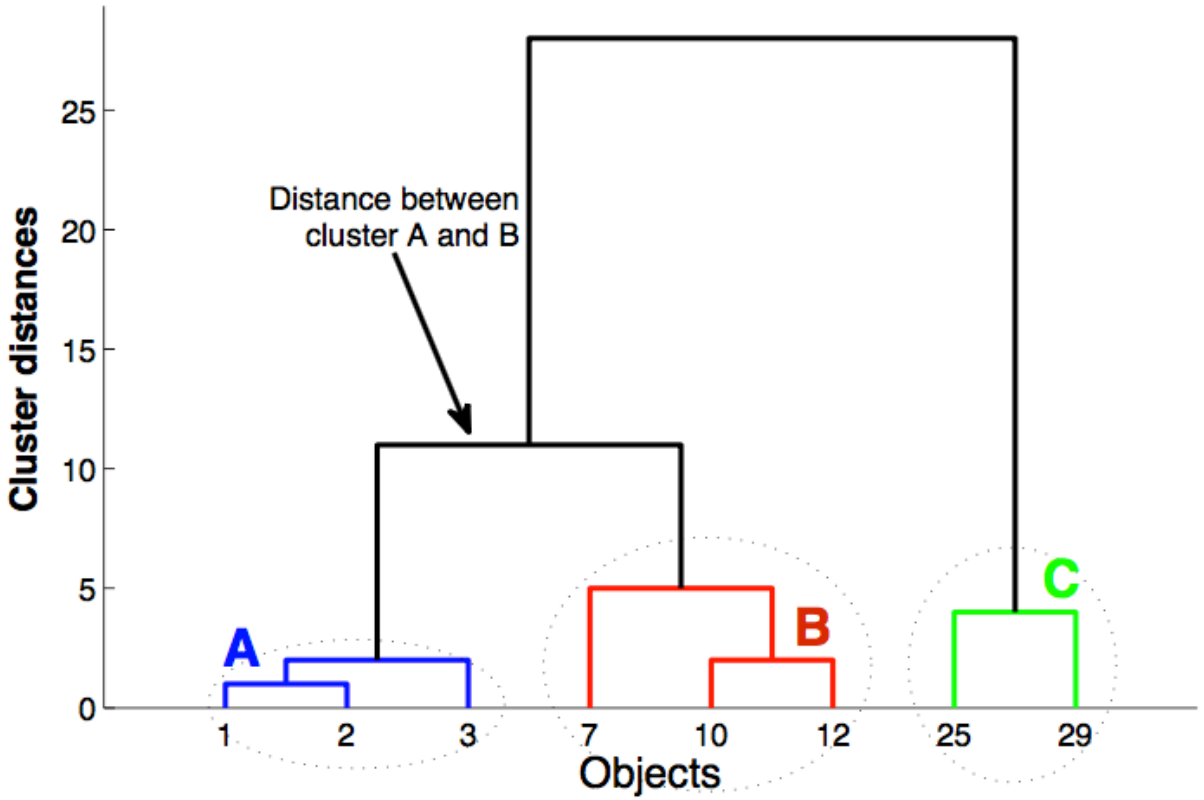
- Combination of D & E is combined with F

- Final tree contains all clusters combined into a single cluster

Link: https://www.brandidea.com/hierarchicalclustering.html

Dendrogram

- Agglomerative clustering algorithms build a dendrogram
- Dendrogram shows hierarchy of clusters in a data sample
- It contains information about objects inside each cluster and distances between these clusters



Algorithm

initialize distance matrix $M \in \mathbb{R}^{N \times N}$ between singleton clusters $\{x_1\}, \ldots \{x_N\}$

REPEAT:

1) pick closest pair of clusters i and j
2) merge clusters i and j
3) delete rows/columns i, j from M and add new row/column for merged cluster
4) recalculate distances between clusters

UNTIL 1 cluster is left

RETURN hiearchical clustering of objects

Distance between clusters #1

- Nearest neighbor (single link):

$$\rho(A, B) = \min_{a \in \mathrm{A},\, b \in B} \rho(a, b)$$

- Furthest neighbor (complete link):

$$\rho(A, B) = \max_{a \in \mathrm{A},\, b \in B} \rho(a, b)$$

where $A = \{x_{i_1}, x_{i_2}, \dots\}$ and $\mathrm{B} = \{x_{j_1}, x_{j_2}, \dots\}$ are two clusters

Distance between clusters #2

- Average (group average link):

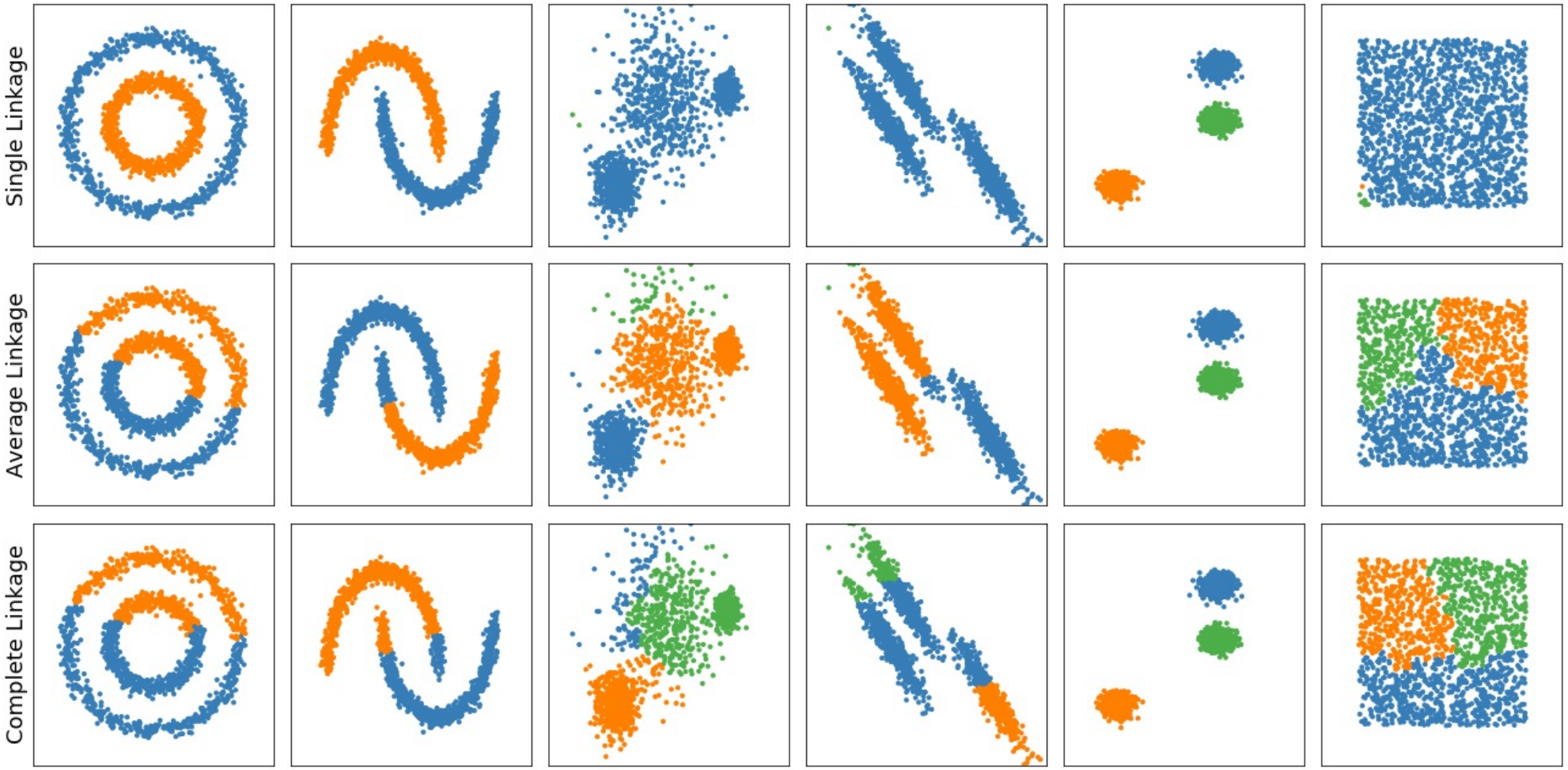
$$\rho(A, B) = \frac{1}{N_A N_B} \sum_{a \in A,\, b \in B} \rho(a, b)$$

- Closest centroid (centroid link):

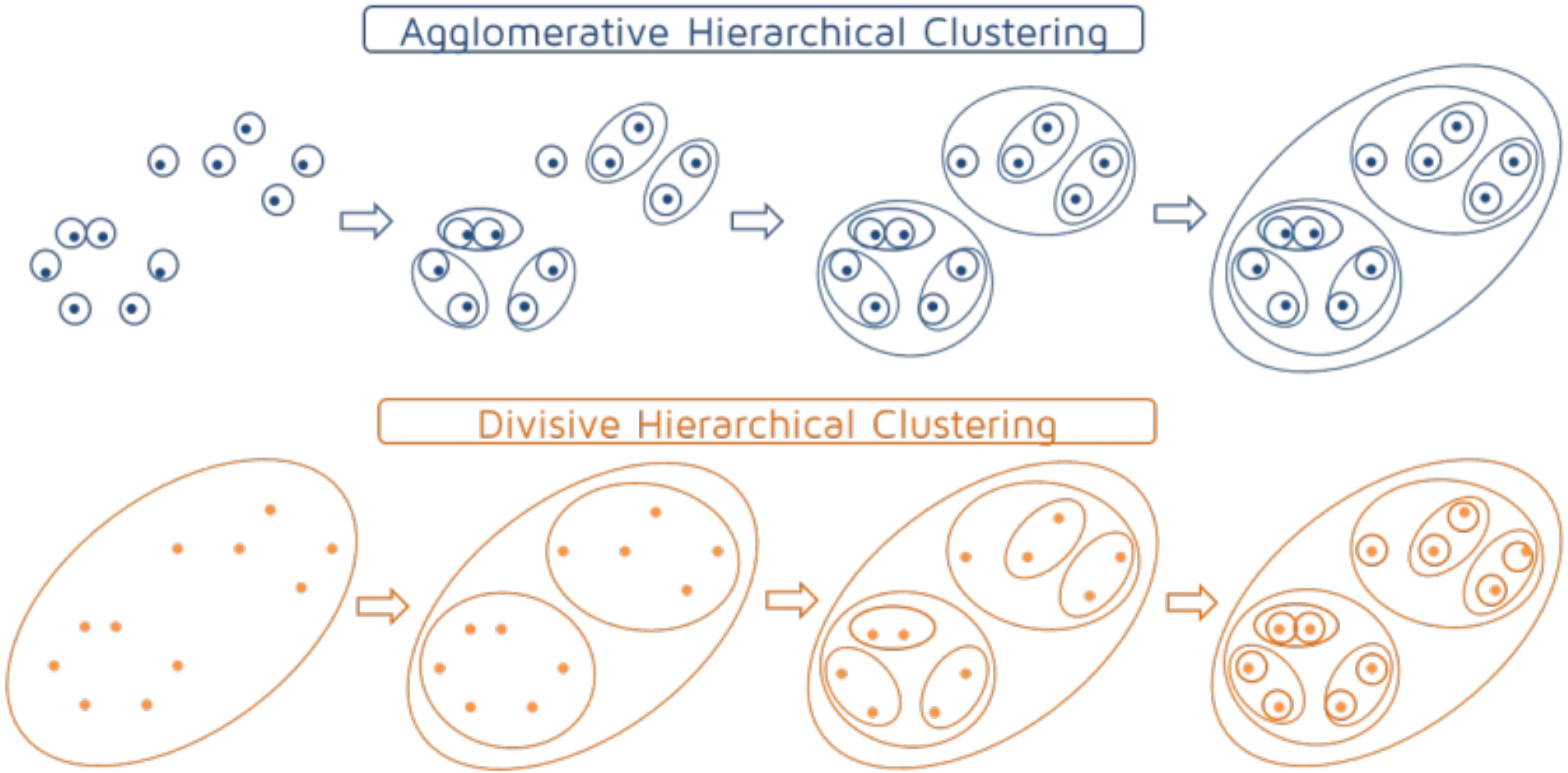
$$\rho(A, B) = \rho(\mu_A, \mu_B)$$

where μ_A and μ_B are cluster centers

Demonstration



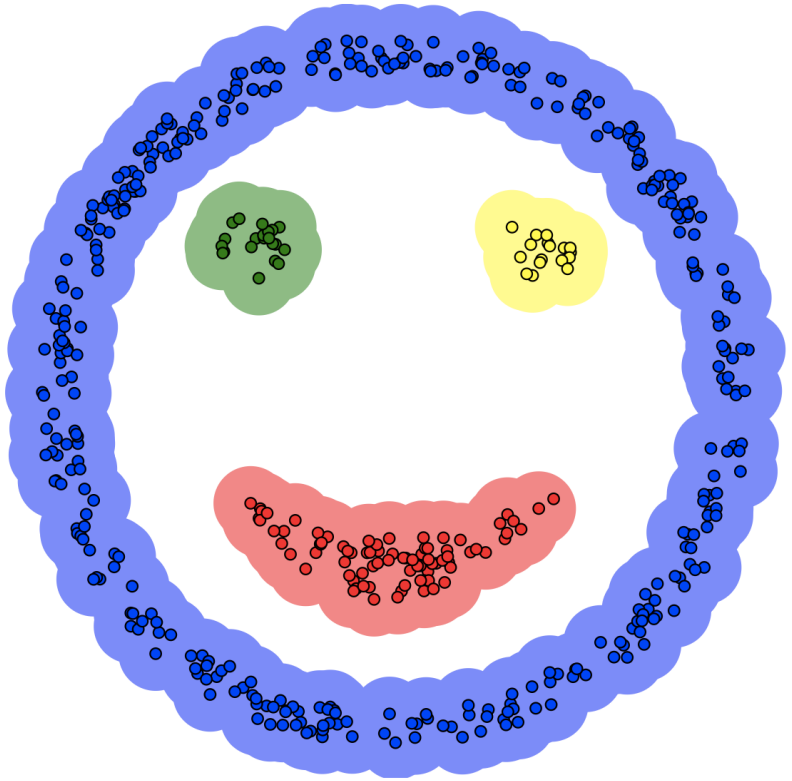
Alternative



DBSCAN

Intuition

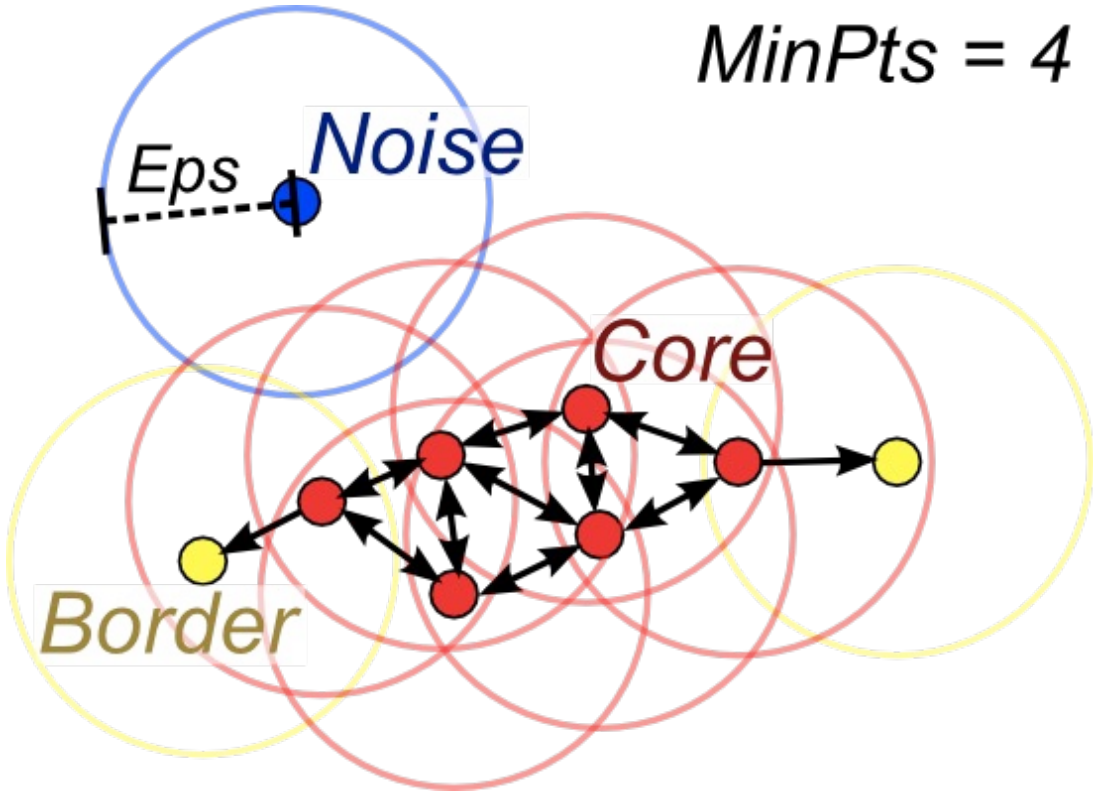
- It supposed that clusters form dense groups of objects
- Areas between the clusters are sparse, with very low densities
- Let’s start from a random object and grow up a cluster by adding neighbor objects within some radius



DBSCAN idea #1

DBSCAN has two parameters:

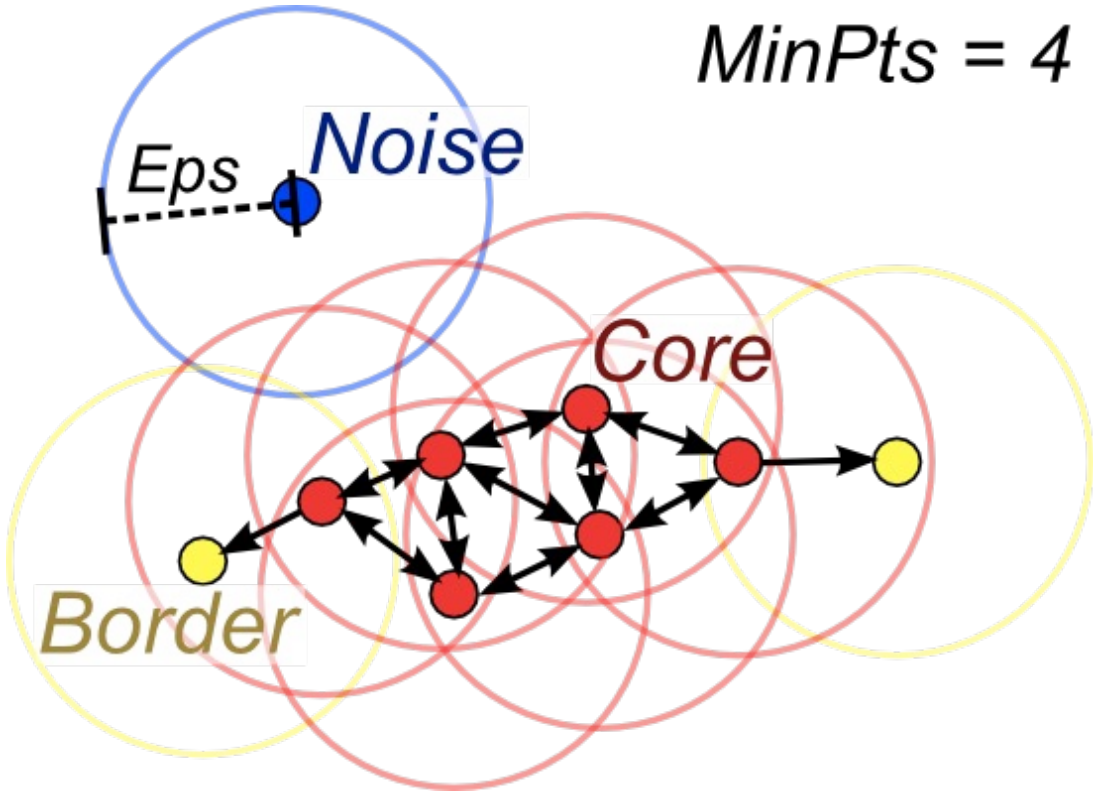
- ϵ – radius of neighborhood of each object
- **MinPts** – minimal number of objects inside the neighborhood



DBSCAN idea #2

Three types of objects:

- **Core:** has ≥ MinPts objects within its ϵ neighborhood
- **Border:** not core object, has at least 1 core object within its ϵ neighborhood
- **Noise:** neither a core nor a border point



Algorithm (short)

Algorithm 1: DBSCAN algorithm.

1: Label all objects as core, border, or noise objects.
2: Eliminate noise objects.
3: Put an edge between all core objects that are within ϵ of each other.
4: Make each group of connected core objects into a separate cluster.
5: Assign each border object to one of the clusters of its associated core objects.

Algorithm (detailed)

```
1.function dbscan(X, eps, min_pts):
2.  initialize NV = X # not visited objects
3.  for x in NV:
4.      remove(NV, x) # mark as visited
5.      nbr = neighbours(x, eps) # set of neighbours
6.      if nbr.size < min_pts:
7.          mark_as_noise(x)
8.      else:
9.          C = new_cluster()
10.         expand_cluster(x, nbr, C, eps, min_pts, NV)
11.         yield C
```

Link: https://shestakoff.github.io/hse_se_ml/2020/l14-cluster/lecture-clust.slides#/4/5

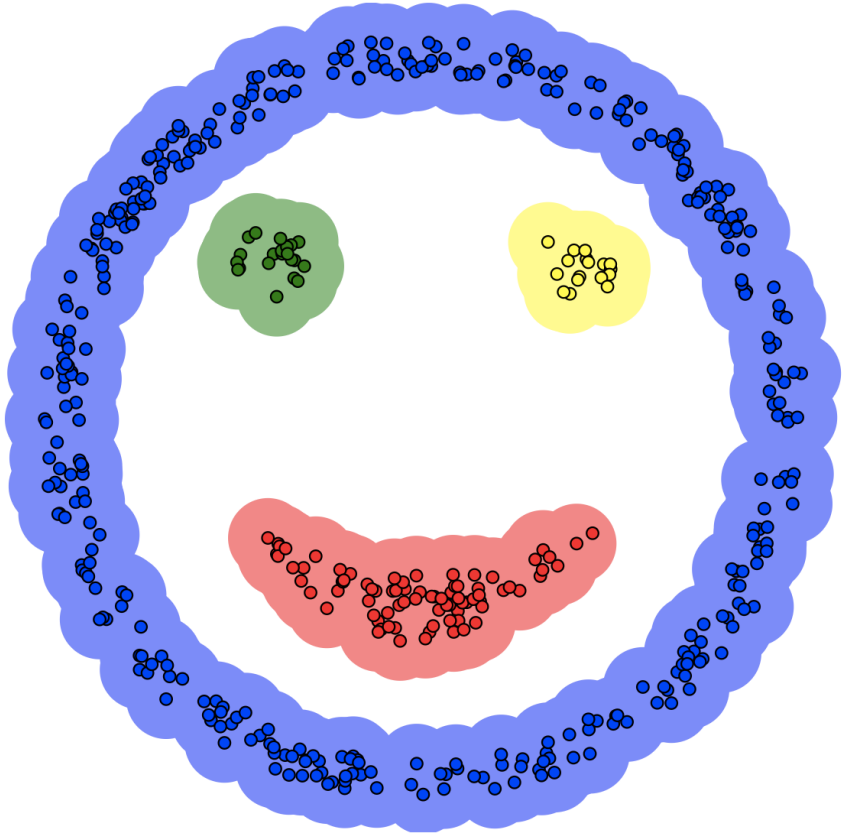
Algorithm (detailed)

```
1. function expand_cluster(x, nbr, C, eps, min_pts, NV):
2.  add(x, C)
3.  for x1 in nbr:
4.      if x1 in NV: # object not visited
5.          remove(NV, x1) # mark as visited
6.          nbr1 = neighbours(x1, eps)
7.          if nbr1.size >= min_pts:
8.              # join sets of neighbours
9.              merge(nbr, nbr_1)
10.     if x1 not in any cluster:
11.         add(x1, C)
```

Link: https://shestakoff.github.io/hse_se_ml/2020/l14-cluster/lecture-clust.slides#/4/5

Demonstration

Demo: https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

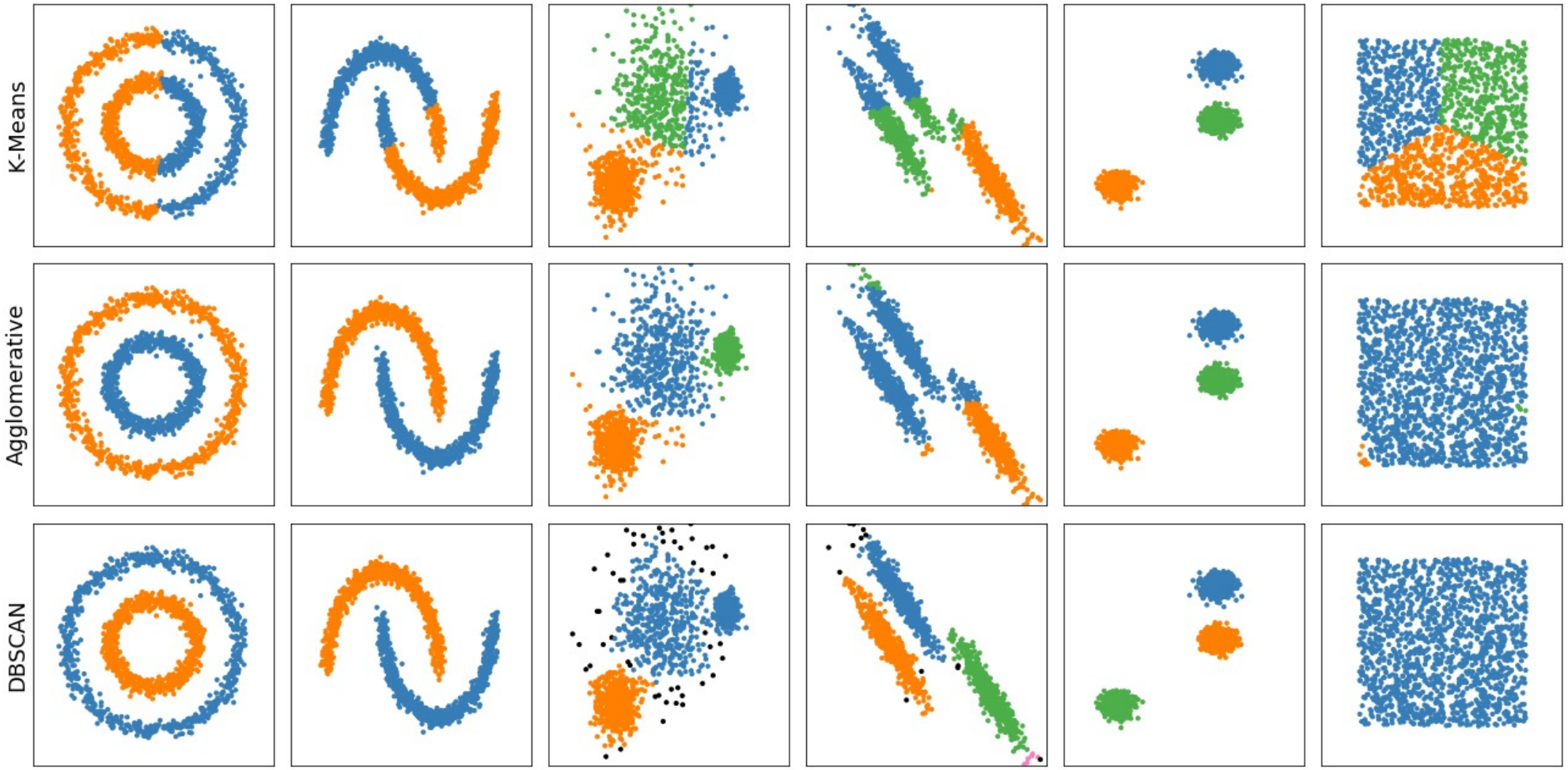


Properties

- Number of clusters is estimated automatically
- Robust to outliers. They are recognized as a noise
- Can find clusters with complex shapes
- Sensitive to objects density variations

Заключение

Резюме



Вопросы

- Что такое задача кластеризации? Как измеряется качество в задаче кластеризации? Запишите формулы для внутрикластерного и межкластерного расстояний.
- Опишите, как работает метод K-Means. Какой критерий он оптимизирует?
- Опишите, как работает метод DBSCAN.
- Как работает подход к кластеризации, основанный на графах? Как работает иерархическая кластеризация?