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WYDZIAŁ MATEMATYKI, INFORMATYKI I MECHANIKI

Unsupervised learning - algorithms for data partitioning (part 2)

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THE PLAN

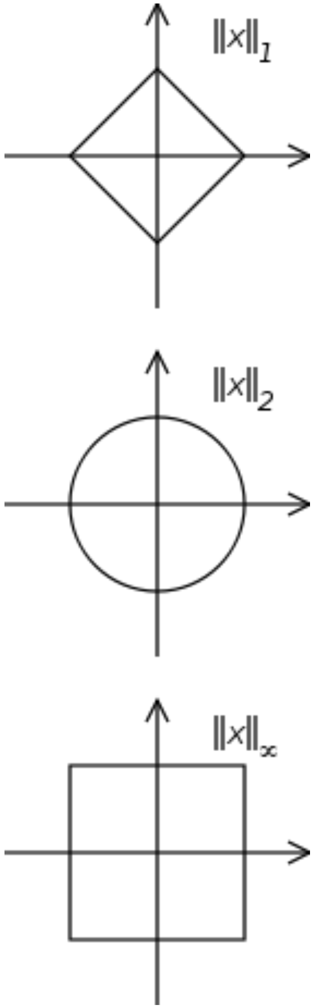
- A recap of the previous lectures.
- Hierarchical clustering.
- Density-based algorithms.
- Deep neural networks for clustering.
- Semi-(un)supervised learning.
- Examples of commonly used algorithms.
- Summary.

Unsupervised learning

- Given a cloud of data points, we want to understand its structure.
    - A common step in the exploratory data analysis.
    - Provides insights about the data.
    - Helps at identifying outliers.
    - <u>Can help in finding a reliable initial data batch for active learning!</u>
- Desirable properties of clustering:
    - Members of a cluster should be similar to each other.
    - Dissimilar samples should be placed in different clusters.
    - Clustering can be efficiently re-computed to allow interactive data analysis.

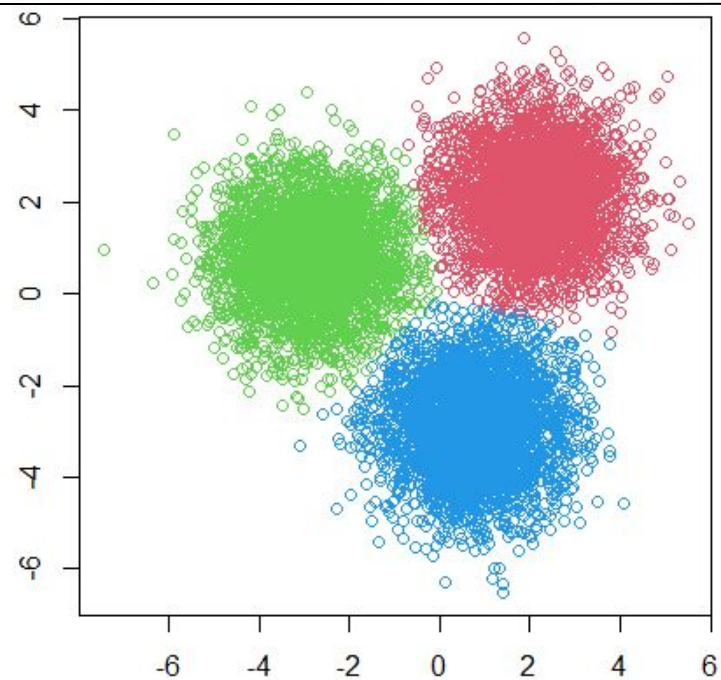
Distance and similarity metrics

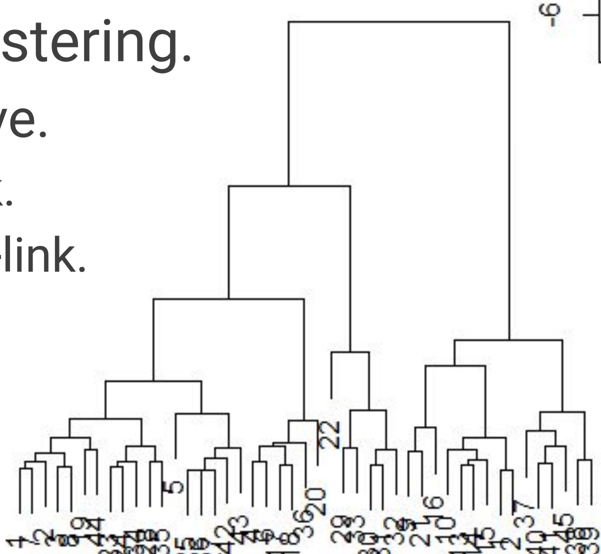
- Most of the clustering algorithms make use of some similarity or distance measure.
- Examples of popular distance measures:
  - Minkowski distances: $d(p,q) = \sqrt[m]{\sum_i^n (p_i - q_i)^m}$
    - Manhattan distance (p = 1)
    - Euclidean distance (p = 2)
  - The Canberra distance: $d(p,q) = \sum_i^n \frac{|p_i - q_i|}{|p_i| + |q_i|}$
  - We don't always need all properties of a distance metric.
- Examples of popular similarity measures:
  - Cosine similarity (of vectors): $sim(p,q) = \frac{p \cdot q}{\|p\| \, \|q\|}$
  - Jaccard similarity (of sets): $sim(A,B) = \frac{|A \cap B|}{|A \cup B|}$



Taxonomy of clustering algorithms

- Flat-partition clustering:
  - Hard partitioning:
    - k-means, BFR.
    - EM, DBscan.
  - Soft partitioning:
    - fuzzy c-means.
    - rough c-means.
- Hierarchical clustering.
  - Agglomerative.
    - single-link.
    - complete-link.
  - Divisive.
    - Daina.
- Hybrids.





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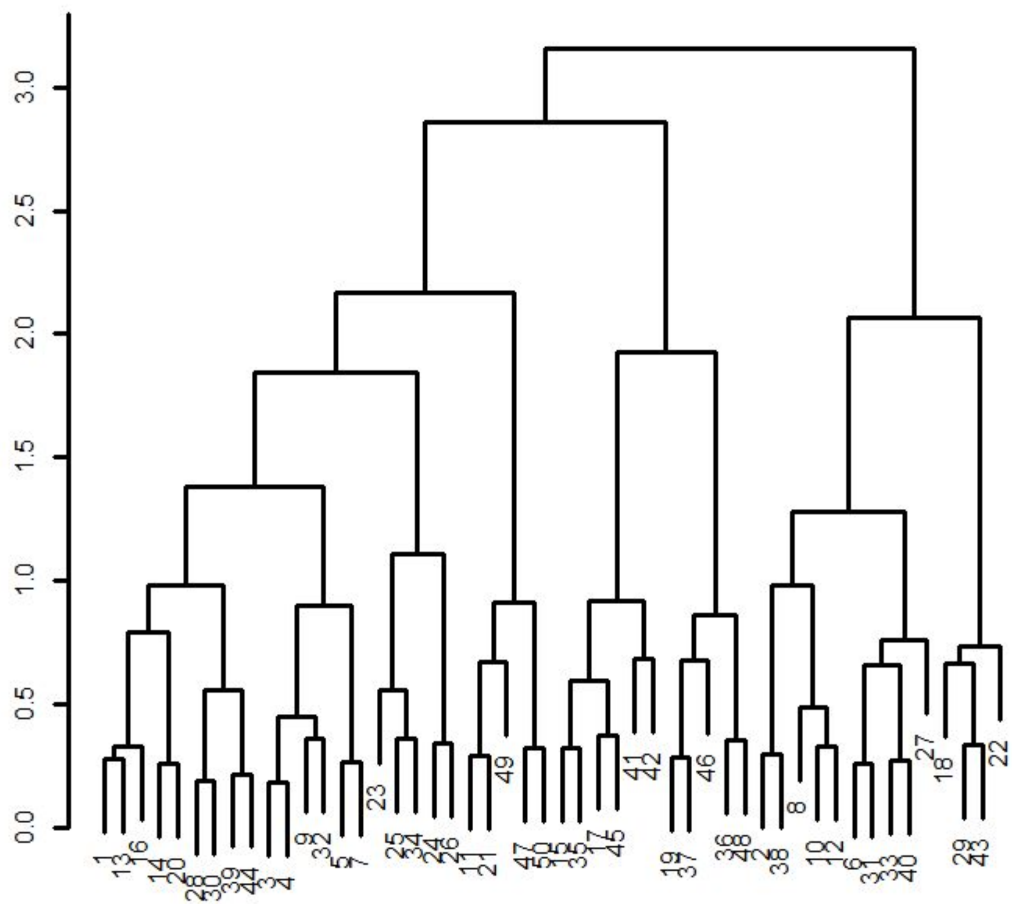
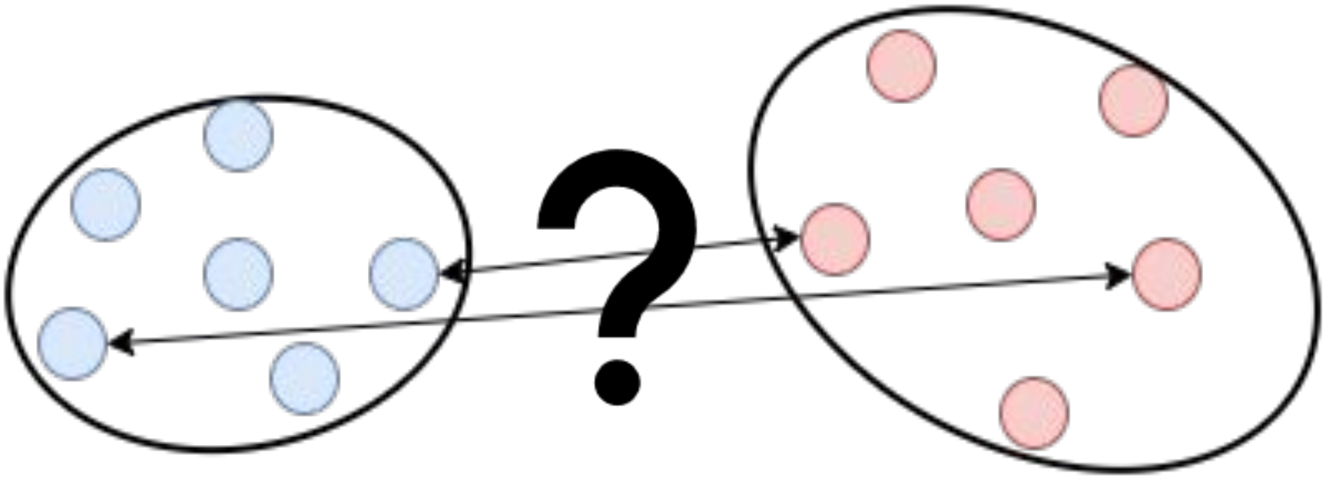
Agglomerative clustering

- The most common approach to the hierarchical clustering.
- Starts with as many clusters as there are data samples.
- In each iteration, join two most “closest” clusters until all samples are in a single group.
- How to define the cluster proximity?



Linkage functions

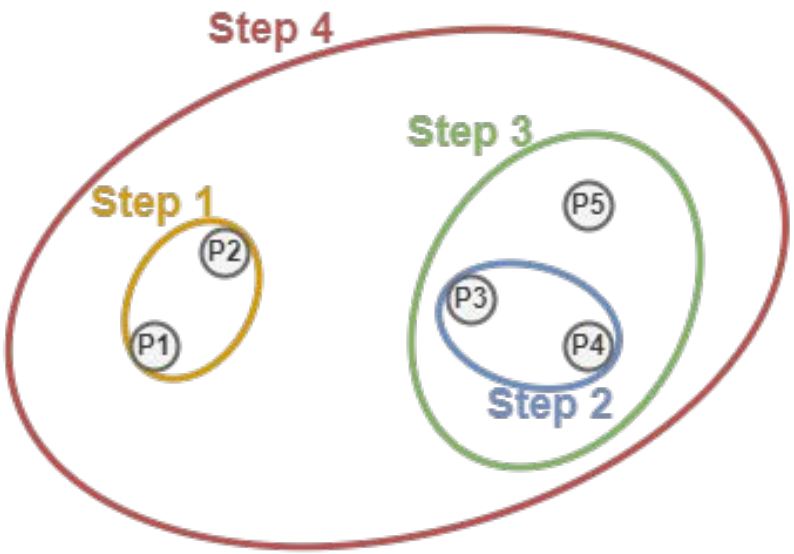
- Linkage functions are used to measure cluster proximity.
- The choice of a linkage function determines the shape of the resulting clustering tree.
- Typical implementations of hierarchical clustering use distance matrices to efficiently compute the linkage values.

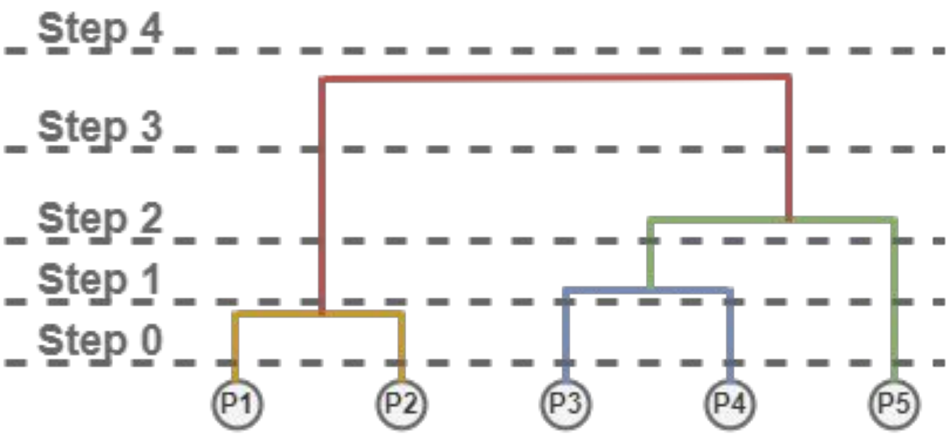


Exemplary linkage functions

- Single linkage: $$D(C_1, C_2) = \min_{c_1 \in C_1, c_2 \in C_2} d(c_1, c_2)$$
- Complete linkage: $$D(C_1, C_2) = \max_{c_1 \in C_1, c_2 \in C_2} d(c_1, c_2)$$
- Average linkage: $$D(C_1, C_2) = \frac{1}{|C_1| \times |C_2|} \sum_{c_1 \in C_1} \sum_{c_2 \in C_2} d(c_1, c_2)$$
- Centroid linkage: $$D(C_1, C_2) = d\left(\frac{1}{|C_1|} \sum_{c_1 \in C_1} c_1, \frac{1}{|C_2|} \sum_{c_2 \in C_2} c_2 \right)$$
- Ward's linkage: $$D(C_1, C_2) = \sum_{c \in C_1 \cup C_2} d\left(c, \frac{1}{|C_1| + |C_2|} \sum_{c' \in C_1 \cup C_2} c' \right)^2$$

An example

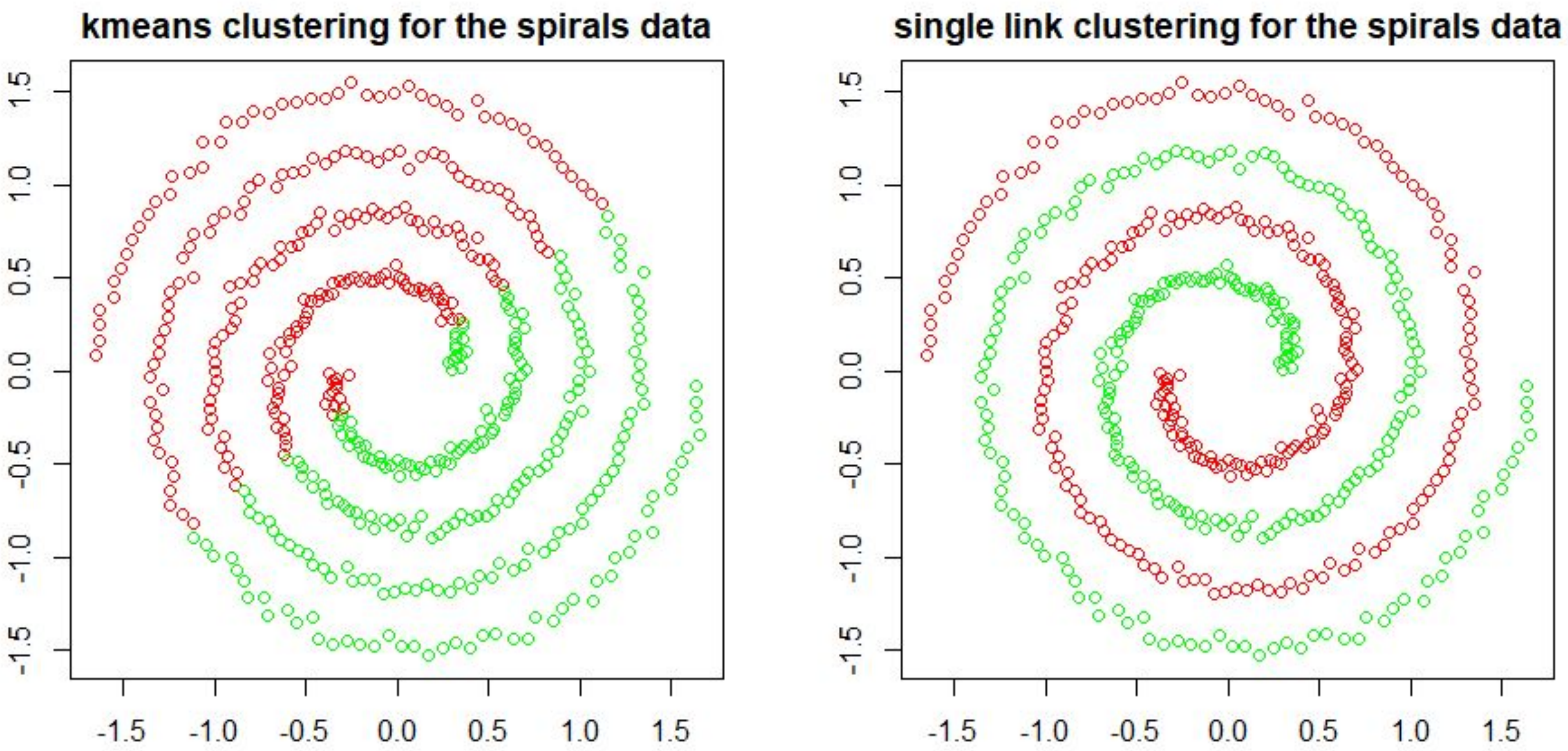

Step 4
Step 3
Step 1
P2
P5
P3
P1
P4
Step 2


Step 4
Step 3
Step 2
Step 1
Step 0
P1
P2
P3
P4
P5

Divisive clustering

- Unlike in the agglomerative approach, we start from a single cluster containing all data.
- We recursively divide "*the largest*" cluster into two smaller ones, in a way that maximizes a predefined gain function.
  - We measure the cluster "*size*" in terms of its *compactness*, not the actual cardinality.
  - Gain functions measure the difference between the cluster "*size*" and the sum of resulting cluster "*sizes*".
- An exemplary algorithm: DIANA.
  - The "*size*" is expressed as the cluster variance.

Discovering complex cluster shapes



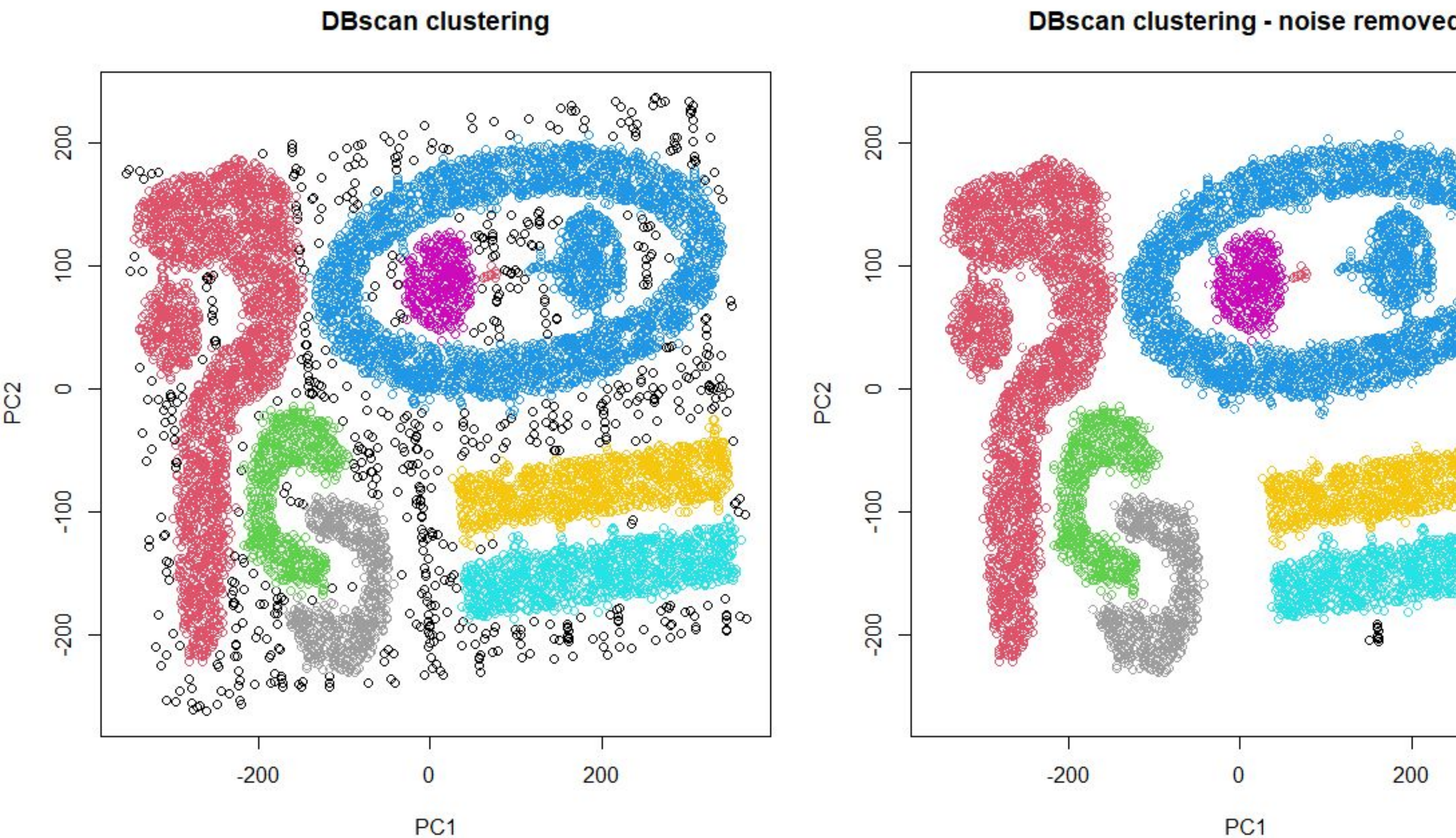
Problems with hierarchical clustering

- **<u>Computational complexity!</u>**
  - For most of the linkage functions, the agglomerative approach has at least $O(n^2 \log(n))$ time complexity.
  - Hierarchical clustering usually requires the computation of a distance matrix (at least $O(n^2)$ memory requirements).
- Quality of hierarchical clustering depends on the selection of a distance metric and the linkage function.

Density-based clustering

- Density-based clustering algorithms identify regions of high data density that are separated by regions of low data density.
  - Density is typically understood as a number of data samples inside a sphere of a fixed radius.
- Major features of the density-based clustering:
  - Can discover clusters of arbitrary shape.
  - Can handle noise and detect outliers.
  - Need density parameters as a clustering condition.
    - Often doesn’t need explicit number of clusters.

Example

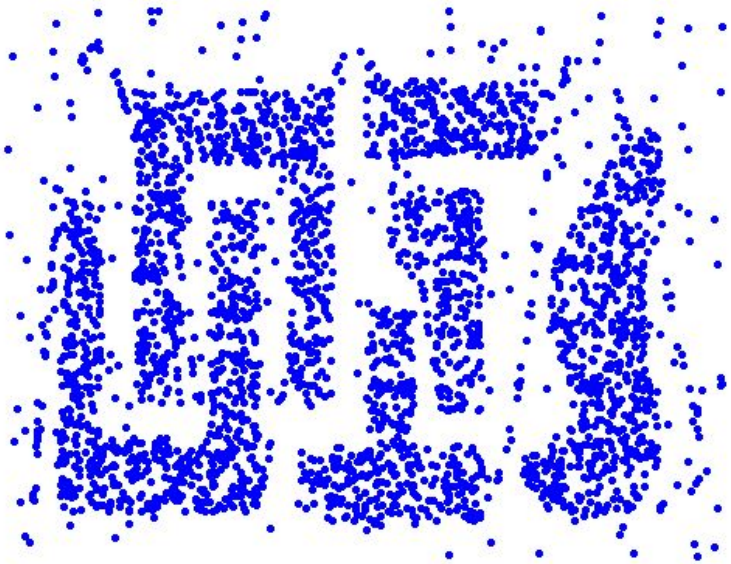

DBscan clustering
DBscan clustering - noise removed
PC1
PC2
-200
0
200
100
-100

The DBSCAN algorithm

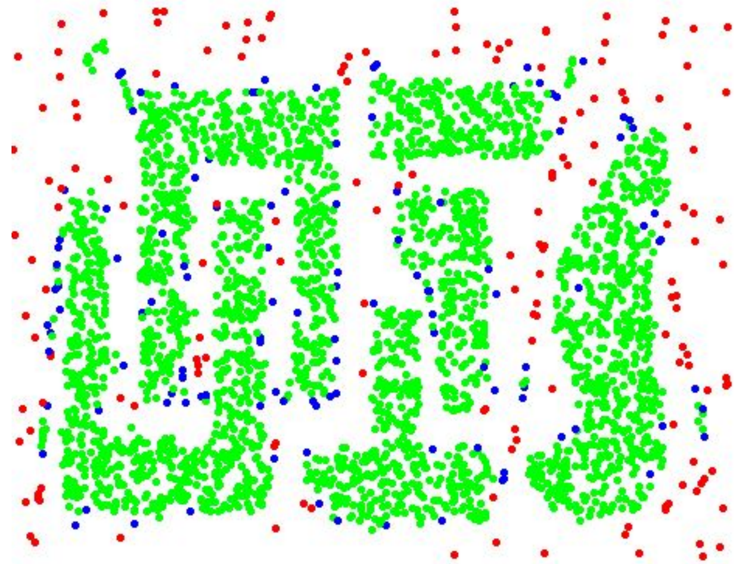
- **D**ensity-**B**ased **S**patial **C**lustering of **A**pplications with **N**oise:
  - One of the most widely used clustering algorithms.
- Main input parameters:
  - ***Eps*** - the radius of local neighborhoods.
  - ***MinPts*** - the minimal number of points in a neighborhood.
- The algorithm divides data into three categories:
  - Core points (CP) - dense cluster interiors.
  - Border points (BP) - have fewer than *MinPts* neighbors within *Eps*, but are in the neighborhood of some core point.
  - Noise points (NP) - all remaining data points.

Core points, border points, and noise points

Original data:

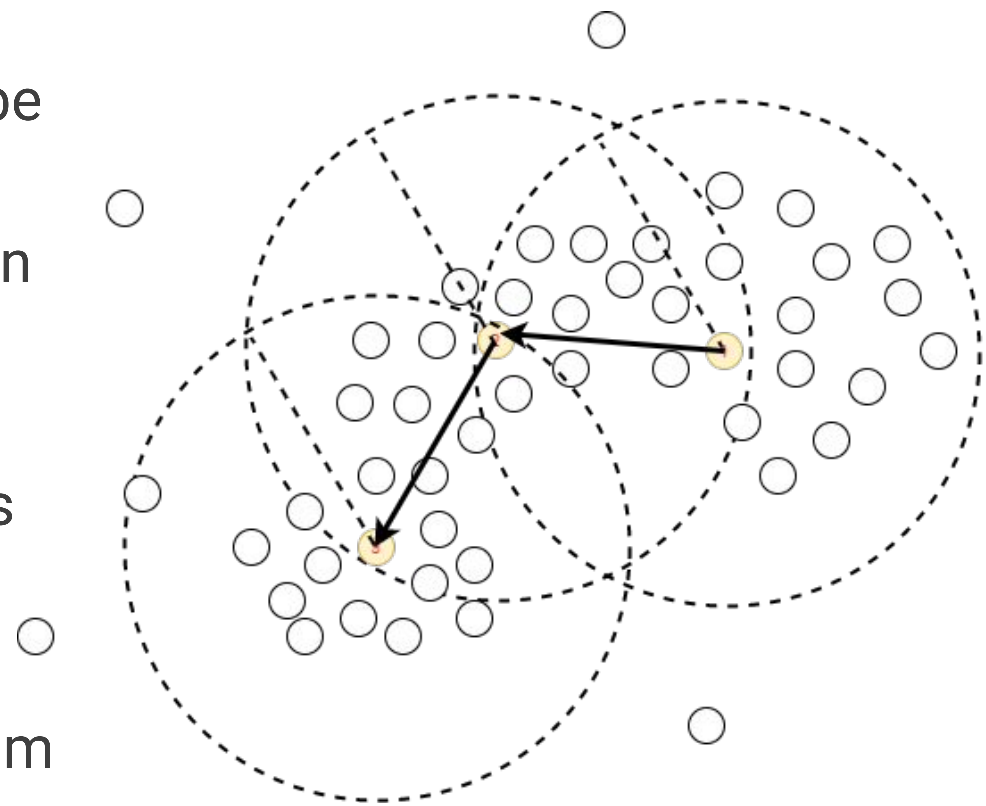


Core points, **border points**, and **noise points**:



How does it work?

- Two points are density-reachable is they can be connected by dense neighborhoods (there is a chain of core points with distances < Eps between them).
- Any two density-reachable CPs will be placed in the same cluster.
- If a BP is density-reachable from a CP, it will be placed in the same cluster.
- All NPs will be discarded.



MinPts = 20

The algorithm

Set clusterID := 0; Draw a single sample u from U:

1. If u <u>is not a CP</u>, assign a null label to u (e.g., zero label).
2. If u <u>is a CP</u>, create a new cluster with clusterID := clusterID+1;

   Assign the label clusterID to u;

   Find all points density-reachable from u and assign them to clusterID (you may re-assign cases with the null label);

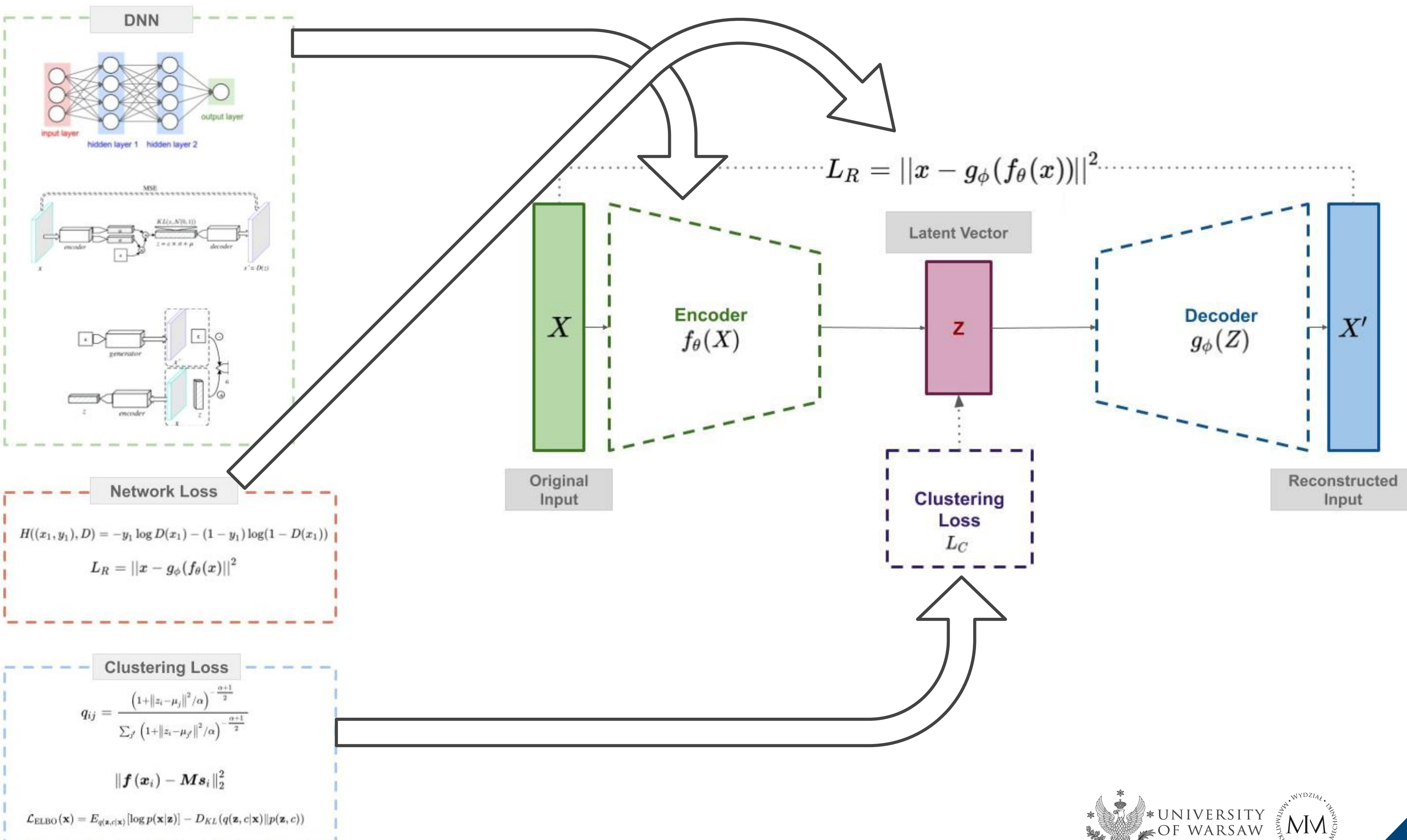
Repeat the above procedure until you visit all cases from U.

DBSCAN implemented using, e.g., KD-trees, has O(nlog(n)) time complexity.

Deep learning vs. the clustering task

- Typically, we have a lot of unlabeled data.
  - It seems to be a perfect circumstance for deep learning.
- Deep clustering models have two essential components:
  - **Deep neural network architecture** for the representation learning.
    - Auto-encoders - a very common choice.
    - Generative model-based architectures.
    - Direct cluster optimization approaches.
  - **Loss functions.**
    - Cluster assignment losses, e.g., *k-means loss*.
    - Cluster regularization losses, e.g., *locality preserving loss*, *group sparsity loss*.

Building blocks of deep clustering methods



Exemplary DNN clustering algorithm

- Deep Clustering Network (DCN).
  - Simple and intuitive model.
  - Uses an autoencoder to learn a data representation suitable for k-means clustering.
  - Uses the k-means loss function:

$$L_{k-means} = \sum_{u \in U} \left(\ell\left(g(f(u)), u\right) + \frac{\lambda}{2} ||f(u) - M s_u||_2^2 \right)$$

    where *f*, *g* are encoder and decoder functions, respectively.
  - Optimizes the representation and the centroids matrix *M*.

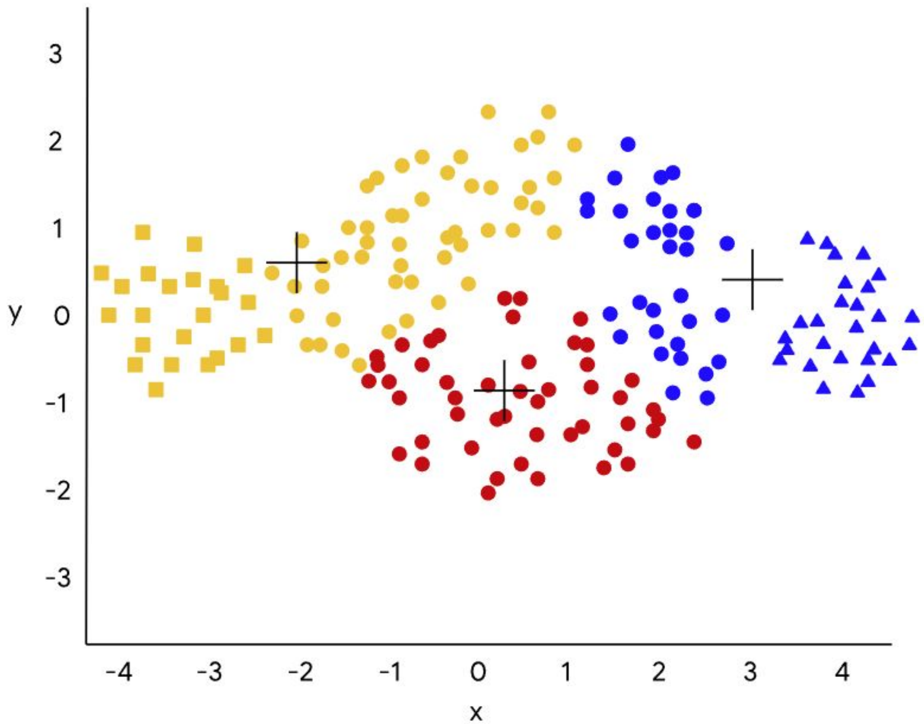
- Obtains good results on popular benchmarks:
  - MNIST: NMI = 0.63
  - 20Newsgroup: NMI = 0.48
  - RCV1(20): NMI ranging from 0.88 to 0.63 (depending on the number of considered clusters).

Semi-(un)supervised learning

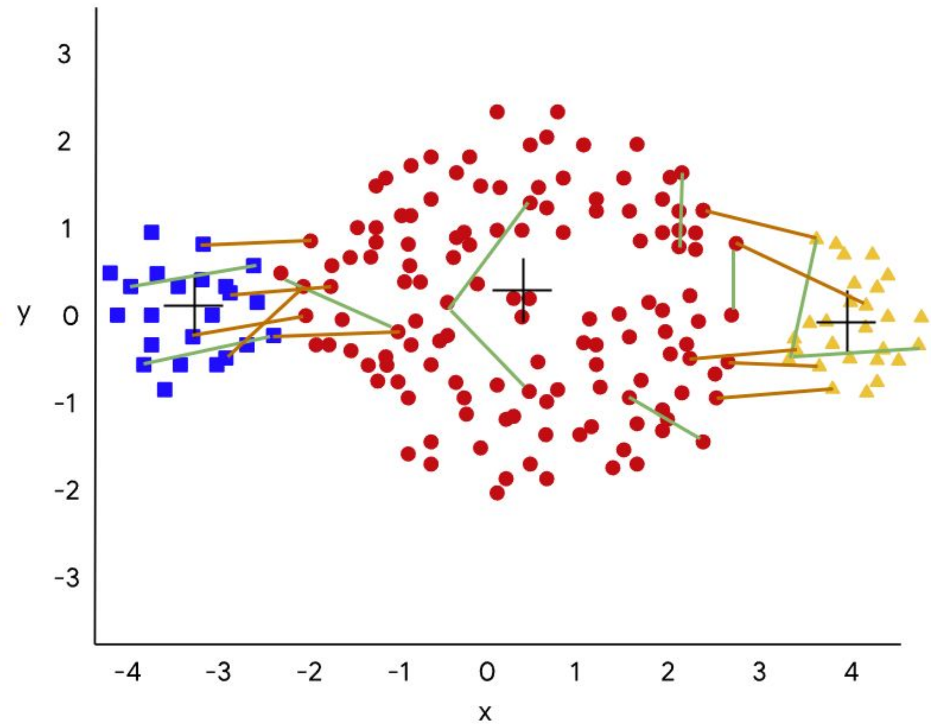
- Sometimes, we may not have class labels but we can get some similarity constraints:
  - Must-links - two cases have to be placed in the same cluster.
  - Cannot-links - two cases must not be in the same cluster.
- Exemplary algorithm: COP k-means.
  - Check constraint consistency. Extend and fix the constraint set if possible.
  - Initialize k cluster centers.
  - Repeat until convergence:
    - **Assign phase**: objects are assigned to the closest cluster center without violating constraints.
    - **Update phase**: cluster centers are updated to the mean of constituent objects.

Semi-(un)supervised clustering example

standard k-means



constrained k-means



Active learning can be used to acquire constraints!

Summary

- We continued the discussion on the unsupervised learning task.
- We discussed agglomerative and divisive approaches to hierarchical clustering.
- We talked about density-based clustering methods using as an example the DBSCAN algorithm.
- We considered deep learning point of view on the clustering task and discussed the Deep Clustering Network model.
- We talked about clustering with constraints with an example of COP k-means.

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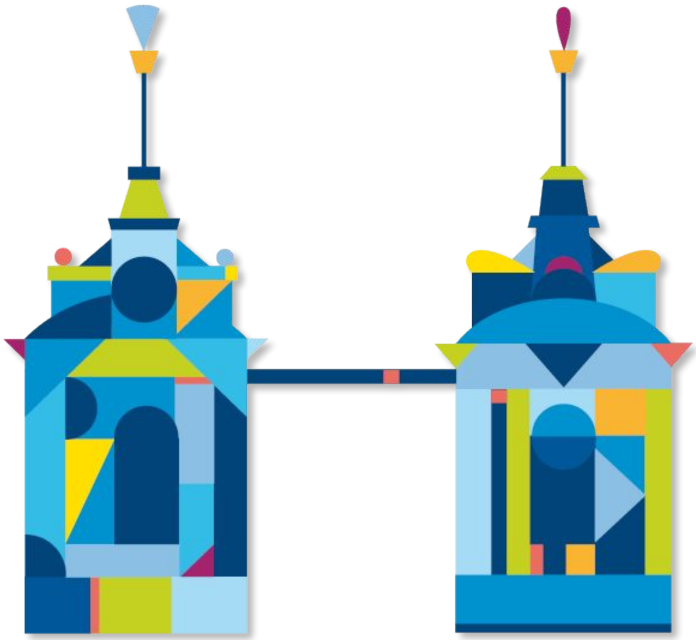

QUESTIONS OR COMMENTS?

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