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GEO5017
Machine Learning for the Built Environment
https://3d.bk.tudelft.nl/courses/geo5017/

Clustering
&
Nearest Neighbor Classification

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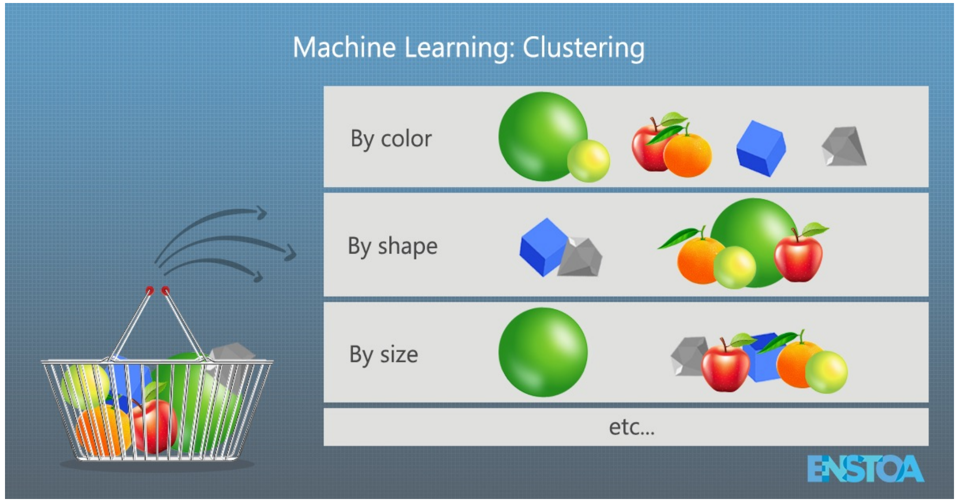
Agenda

- Overview
    - What is clustering?
    - Distance measure (similarity measure)
    - Types of clustering algorithms
- Clustering algorithms
    - K-means clustering
    - Hierarchical clustering
    - Density-based clustering
- Nearest neighbor classification
- Features

What is clustering?

- Clustering
  - A process that **partitions** a given dataset into homogeneous groups based on given features such that **similar** objects are kept in a group whereas **dissimilar** objects are in different groups.



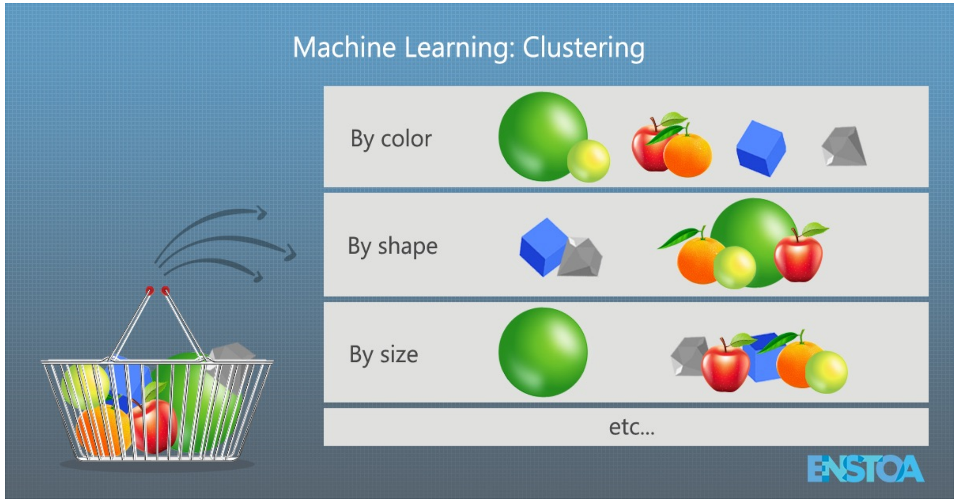
What is a cluster?

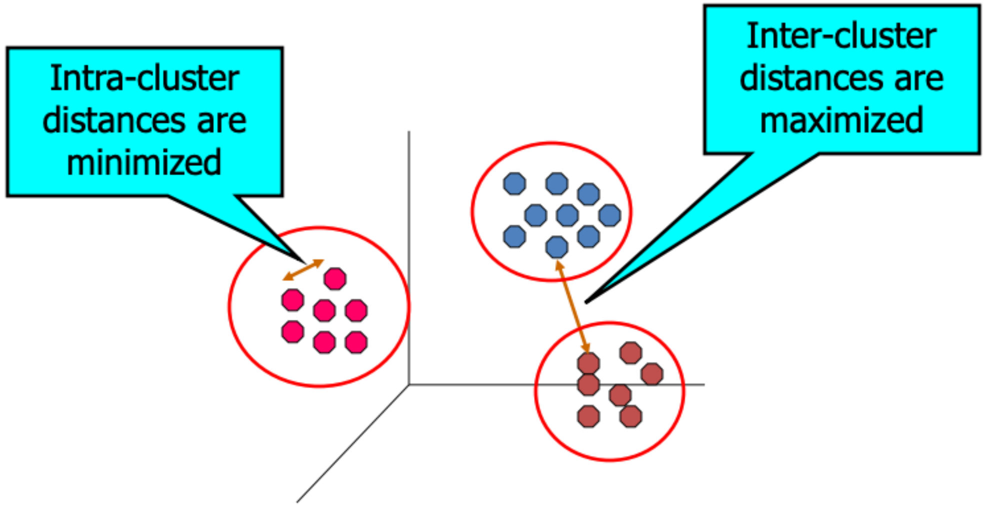
What constitutes a good cluster?

What is the "best" criterion for clustering?

What is clustering?

- Clustering
  - A process that **partitions** a given dataset into homogeneous groups based on given features such that **similar** objects are kept in a group whereas **dissimilar** objects are in different groups.



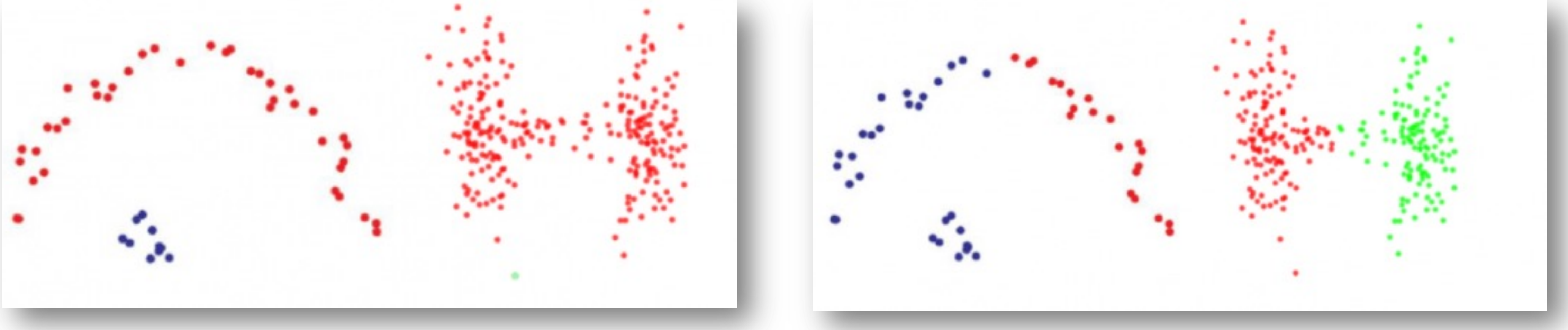


Intra-cluster distances are minimized

Inter-cluster distances are maximized

What is clustering?

- Clustering: two components in an algorithm
  - Distance measure → defines similarities
  - Clustering algorithm → partitions the dataset



Different distance measures lead to different clustering results

Distance measure

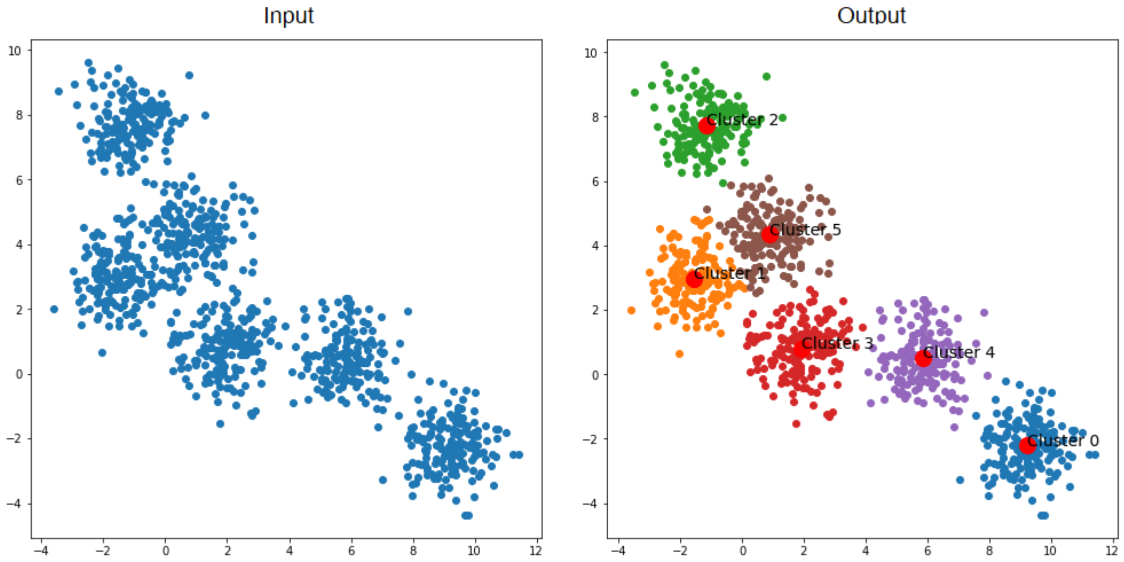
- Problem dependent
  - Minkowski distance/metric is often used
    - Generalization of Euclidean distance (L^2) and Manhattan distance (L^1)

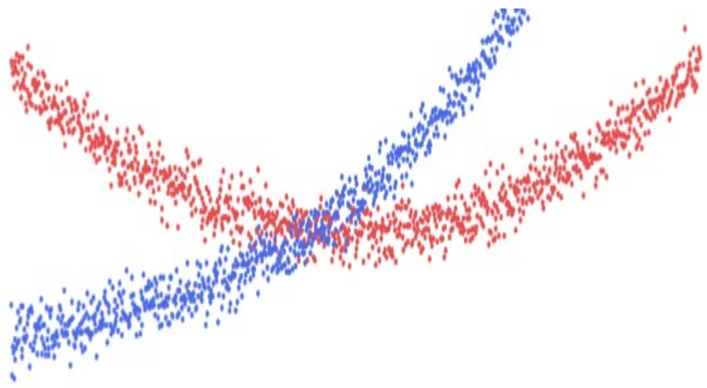
$$D\left(x_i, x_j\right) = \left(\sum_{k=1}^{d} \left|x_{i,k} - x_{j,k}\right|^p\right)^{\frac{1}{p}}$$

  - Domain knowledge is required
    - When components of data feature vectors not immediately comparable, e.g.,
      - color vs size
      - distance to city center vs energy label

Types of clustering algorithms

- Different criteria
  - Exclusive vs overlapping
    - Whether a data point can belong to two or more clusters





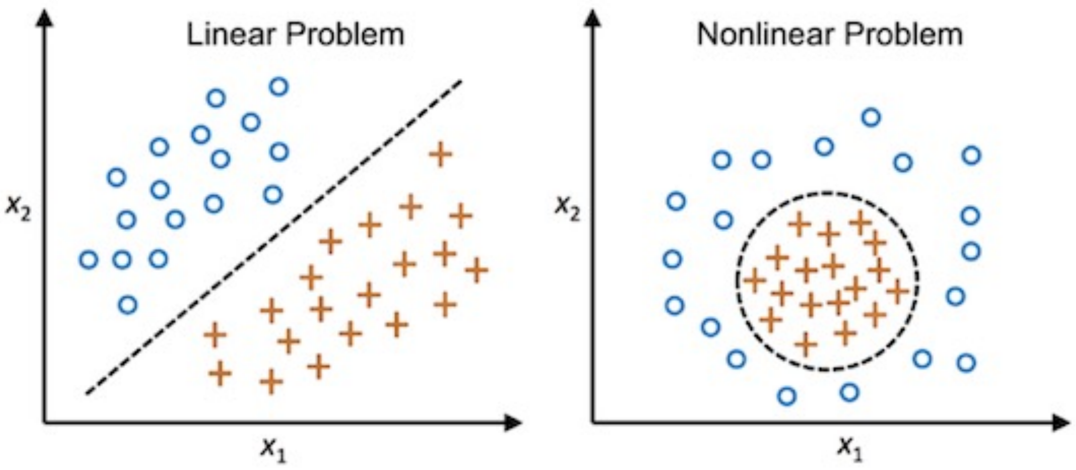
Types of clustering algorithms

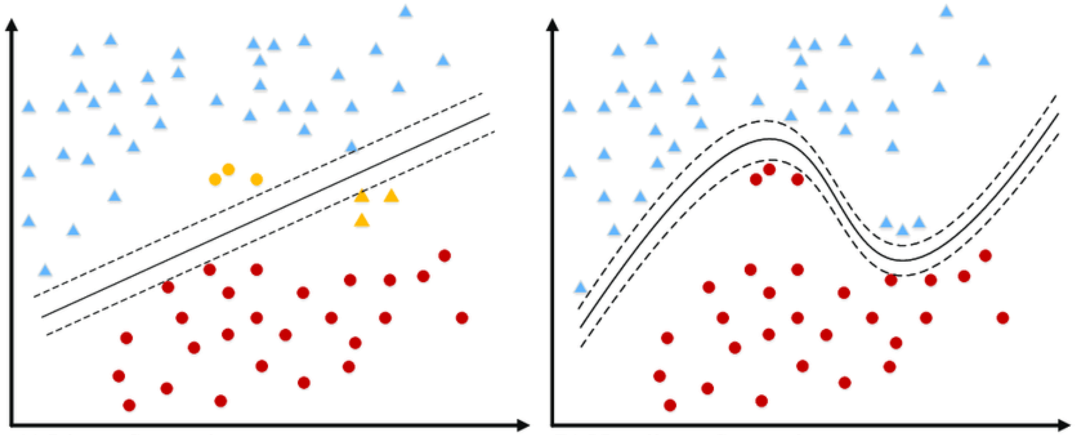
- Different criteria
  - Exclusive vs overlapping
    - Whether a data point can belong to two or more clusters
  - Linear vs non-linear
    - The applicability to different types of data

We will learn:

- Linear: K-means, hierarchical clustering

- Non-linear: density-based clustering




A) Linear Separation

B) Non-linear Separation

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- Clustering algorithms ☜
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k-means

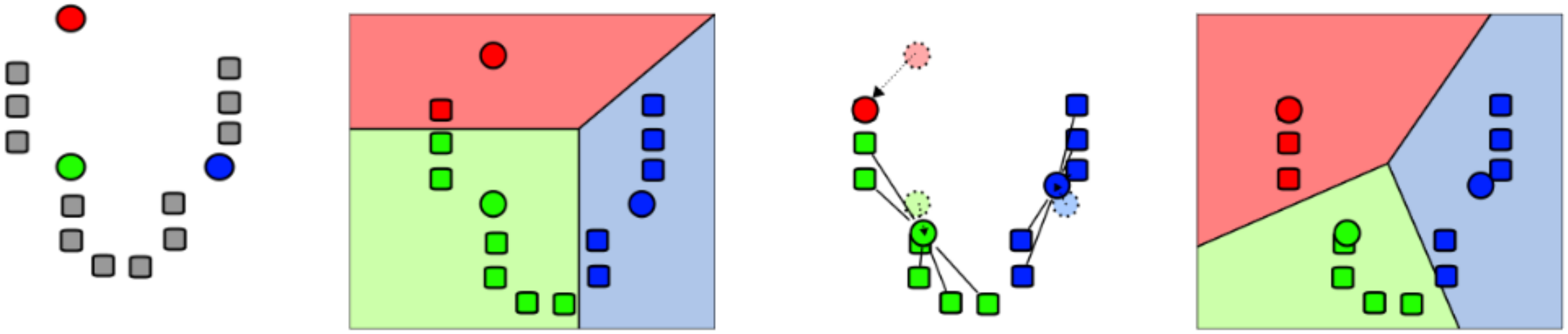
1) Initialize the k clusters $\ell^o = \{c_1^0, c_2^0 \dots c_k^0\}$ in a way such that the initial centroids are placed as far as possible from each other.

2) Calculate the centroids of the clusters: $u_j^i = \frac{1}{|c_j^i|}\sum_{x \in c_j^i} x$, where $j = 1, ..., k$ and i denotes the i-th iteration.

3) Take each point belonging to a given data set and associate it to the nearest centroid:

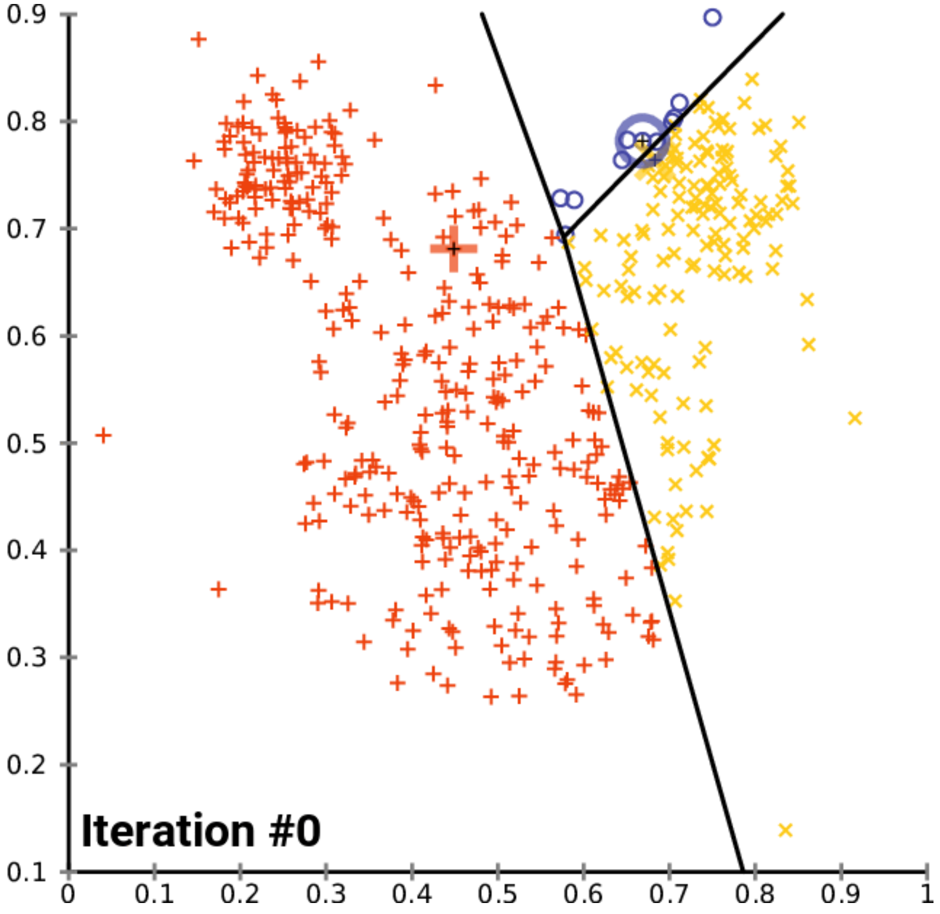
$$\begin{aligned} c_j^{i+1} &= \left\{x \mid d\left(x, u_j^i\right) \leq d\left(x, u_{j'}^i\right), \forall j', 1 \leq j' \leq k\right\} \\ \ell^{i+1} &= \left\{c_j^{i+1} \mid 1 \leq j \leq k\right\} \end{aligned}. \tag{2}$$

4) Repeat steps 2 and 3 until no more changes can be made to the clusters, i.e., $\ell^{i+1} = \ell^i$. In other words, centroids do not move any more.

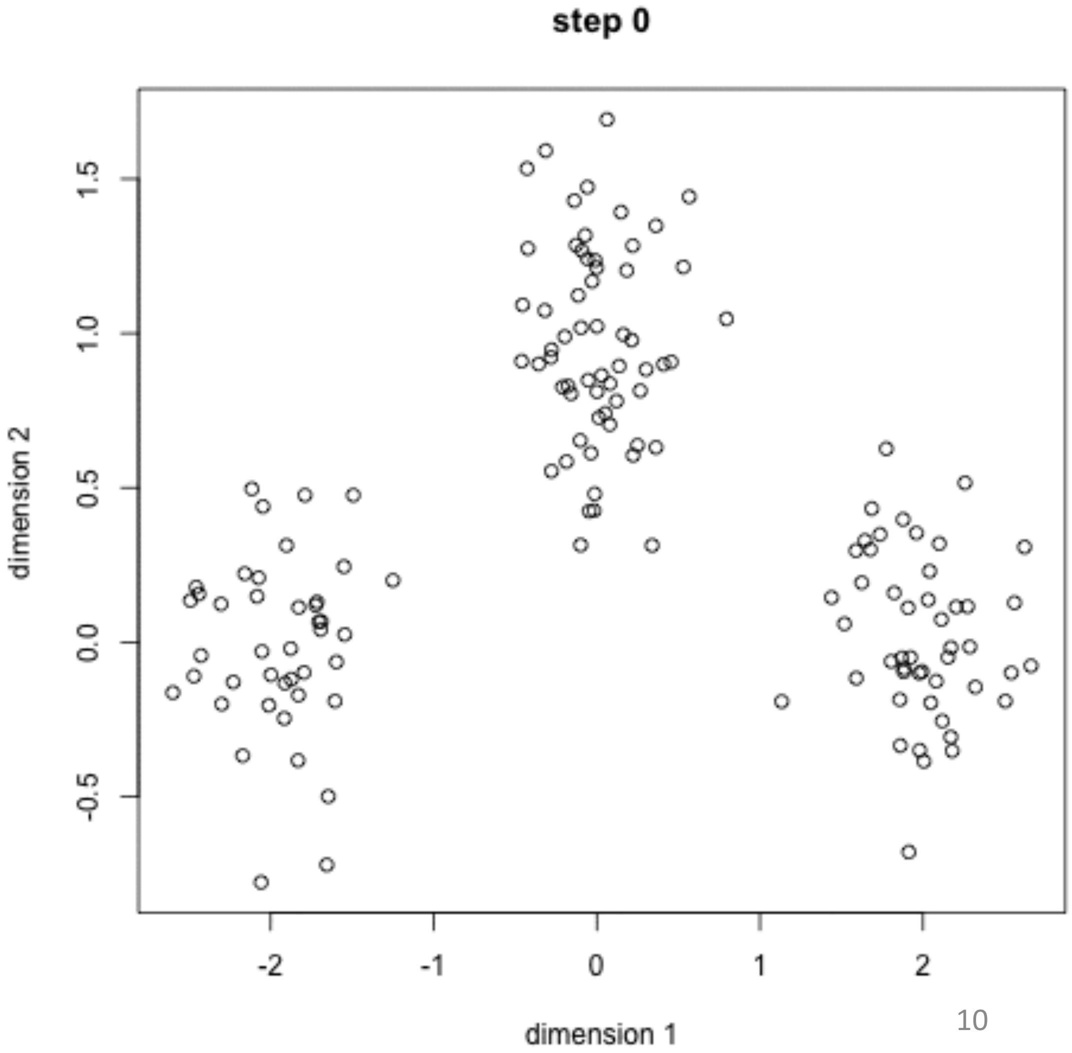


(a) (b) (c) (d)

k-means



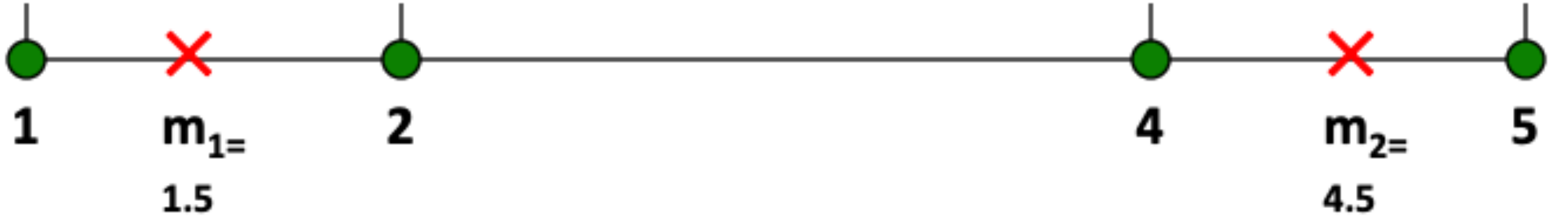
Iteration #0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



step 0
dimension 2
dimension 1
1.5
1.0
0.5
0.0
-0.5
-2
-1
0
1
2

k-means: an optimization perspective

- Objective function
  - SSE (Sum of Squared Error) $J = \sum_{i=1}^{k} \sum_{x \in c_i} \|x - u_i\|^2$



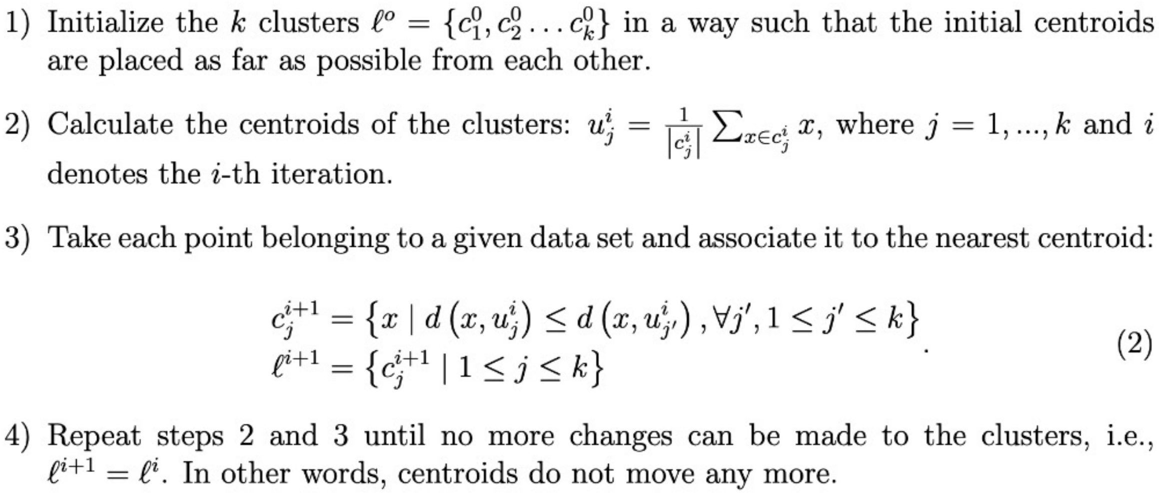
$$SSE = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

k-means: an optimization perspective

- Objective function
  - SSE (Sum of Squared Error)

$$J = \sum_{i=1}^{k} \sum_{x \in c_i} \left\| x - u_i \right\|^2$$

- Convergence
  - K-means is exactly coordinate descent on *J*
    - Step 2: fixed cluster assignment—compute cluster centroids that minimize the current error
    - Step 3: fixed cluster centroids—find cluster assignment that minimizes the current error



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J converges a global minimum?

k-means: an optimization perspective

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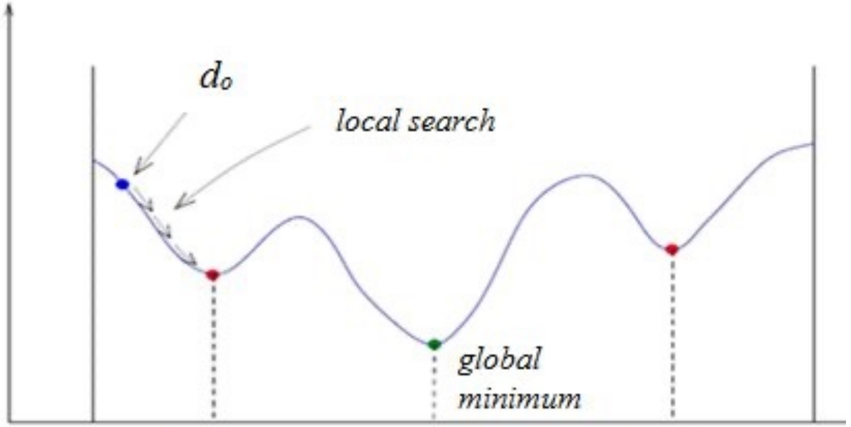
- Not necessarily the optimal configuration
  - i.e., local minimum of the objective function



k-means: an optimization perspective

- Objective function
  - SSE (Sum of Squared Error)

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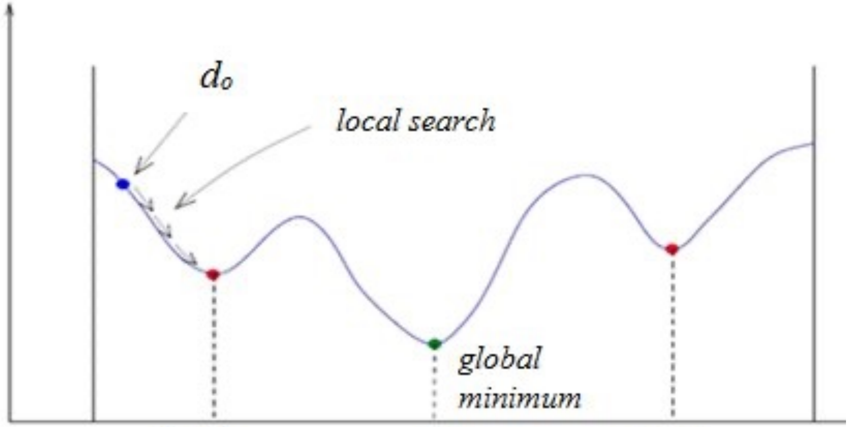
- Not necessarily the optimal configuration
  - i.e., local minimum of the objective function
  - Solution: repeat many times and pick the best
  - Best configuration not guaranteed



k-means

- Advantages
  - Fast and efficient
  - Given good results when groups are distinct or well separated from each other
  - Easy to implement

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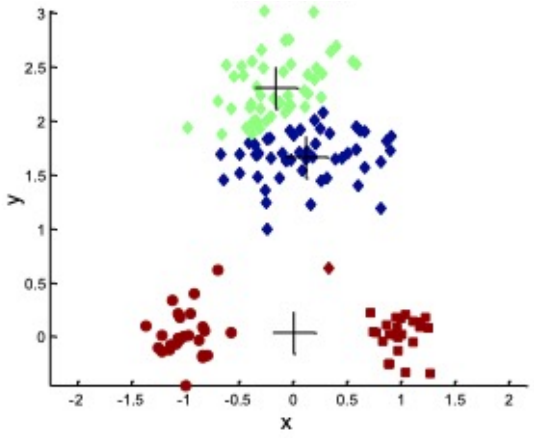
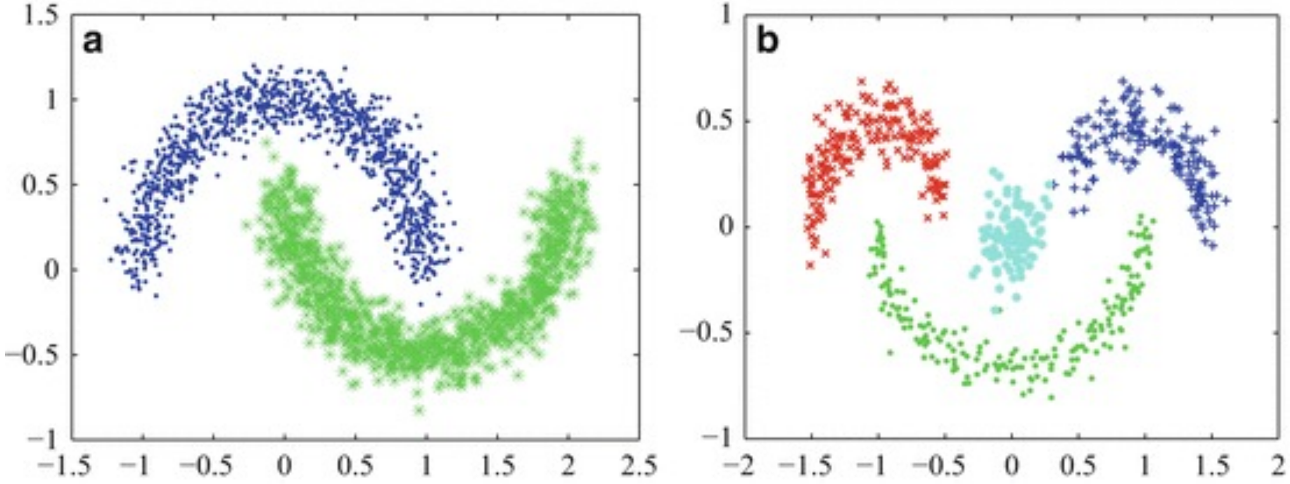
  - Requires a priori specification of the number (i.e., k) of clusters
  - Local minima
    - Sensitive to initialization
    - Cannot guarantee optimal clusters
  - Not invariant to non-linear transformations
    - e.g., cartesian coordinates vs polar coordinates



k-means

- Can k-means handle?



k-means

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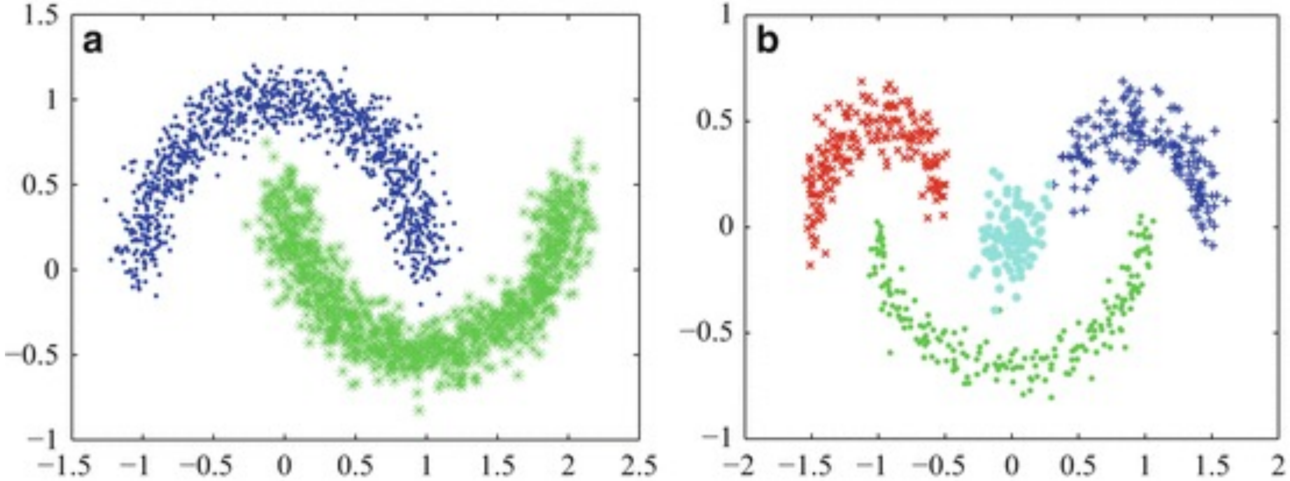

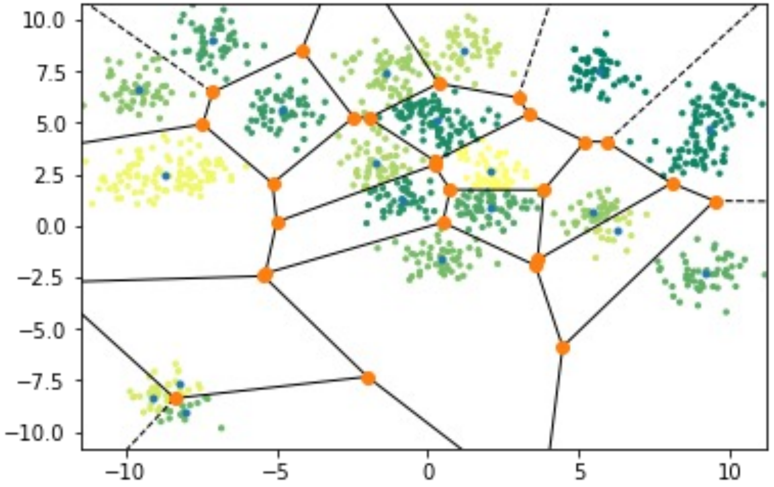

k-means

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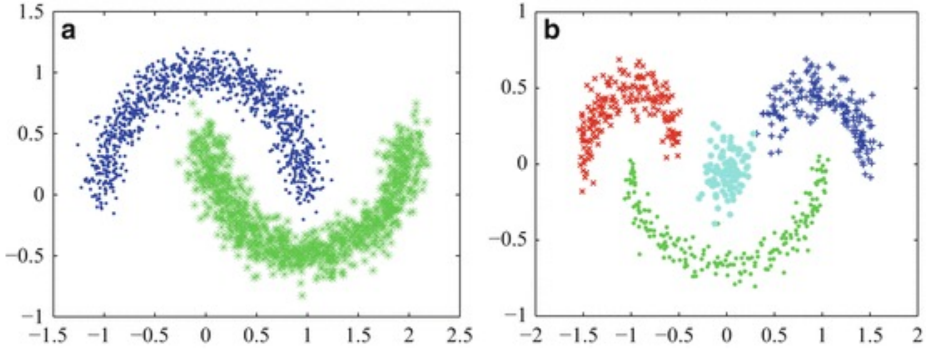
  - Cannot process non-linear datasets



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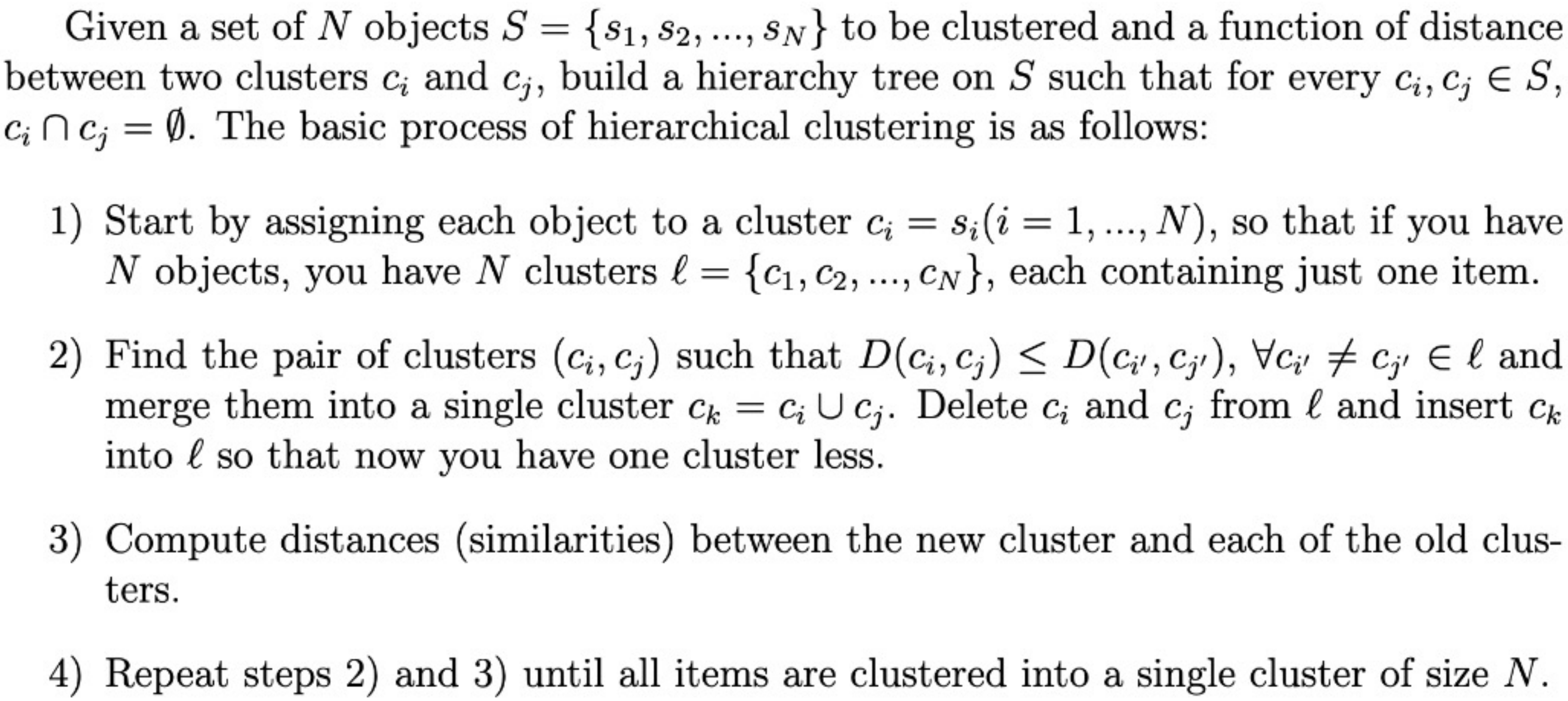
Hierarchical clustering

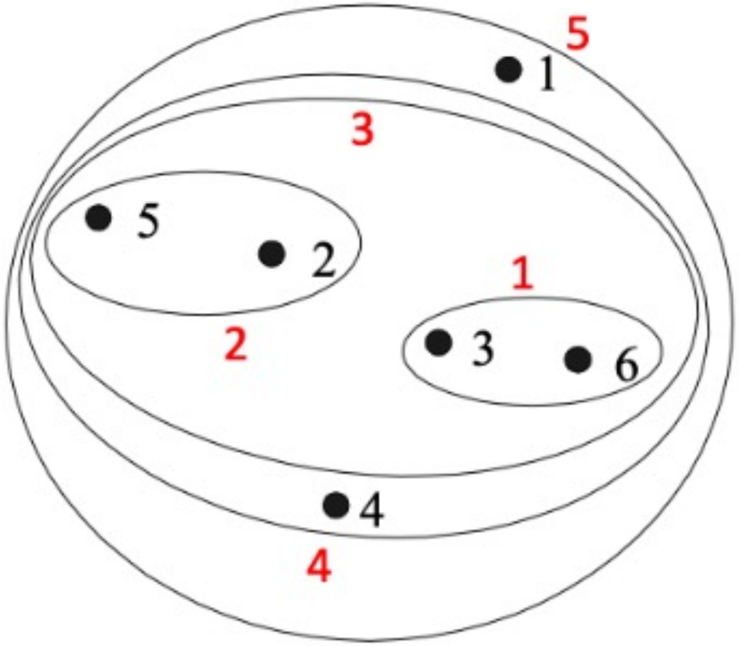


Given a set of N objects $S = \{s_1, s_2, ..., s_N\}$ to be clustered and a function of distance between two clusters c_i and c_j, build a hierarchy tree on S such that for every $c_i, c_j \in S$, $c_i \cap c_j = \emptyset$. The basic process of hierarchical clustering is as follows:

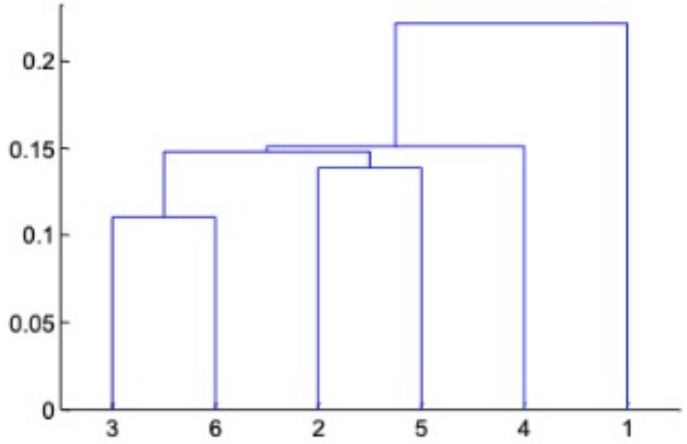
1) Start by assigning each object to a cluster $c_i = s_i (i = 1, ..., N)$, so that if you have N objects, you have N clusters $\ell = \{c_1, c_2, ..., c_N\}$, each containing just one item.
2) Find the pair of clusters (c_i, c_j) such that $D(c_i, c_j) \leq D(c_{i'}, c_{j'}), \forall c_{i'} \neq c_{j'} \in \ell$ and merge them into a single cluster $c_k = c_i \cup c_j$. Delete c_i and c_j from ℓ and insert c_k into ℓ so that now you have one cluster less.
3) Compute distances (similarities) between the new cluster and each of the old clusters.
4) Repeat steps 2) and 3) until all items are clustered into a single cluster of size N.

Hierarchical clustering

- Example



Nested Clusters

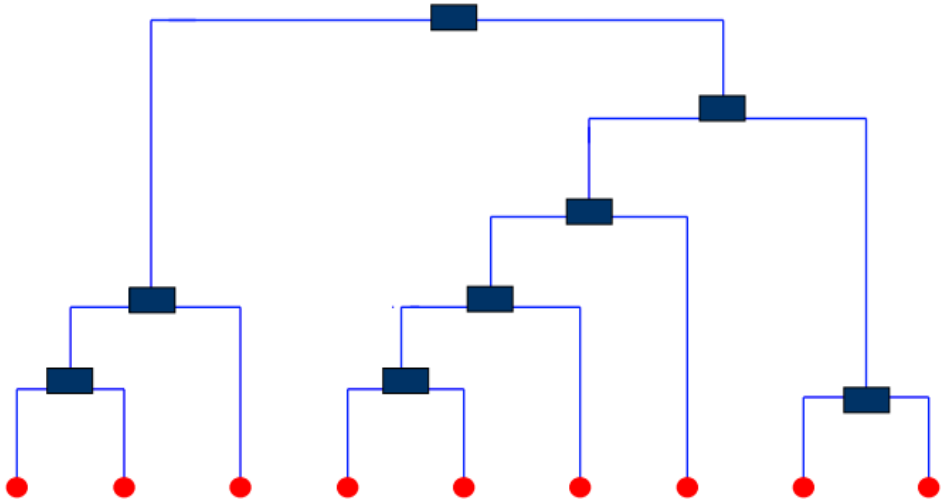


Dendrogram

An example of hierarchical clustering

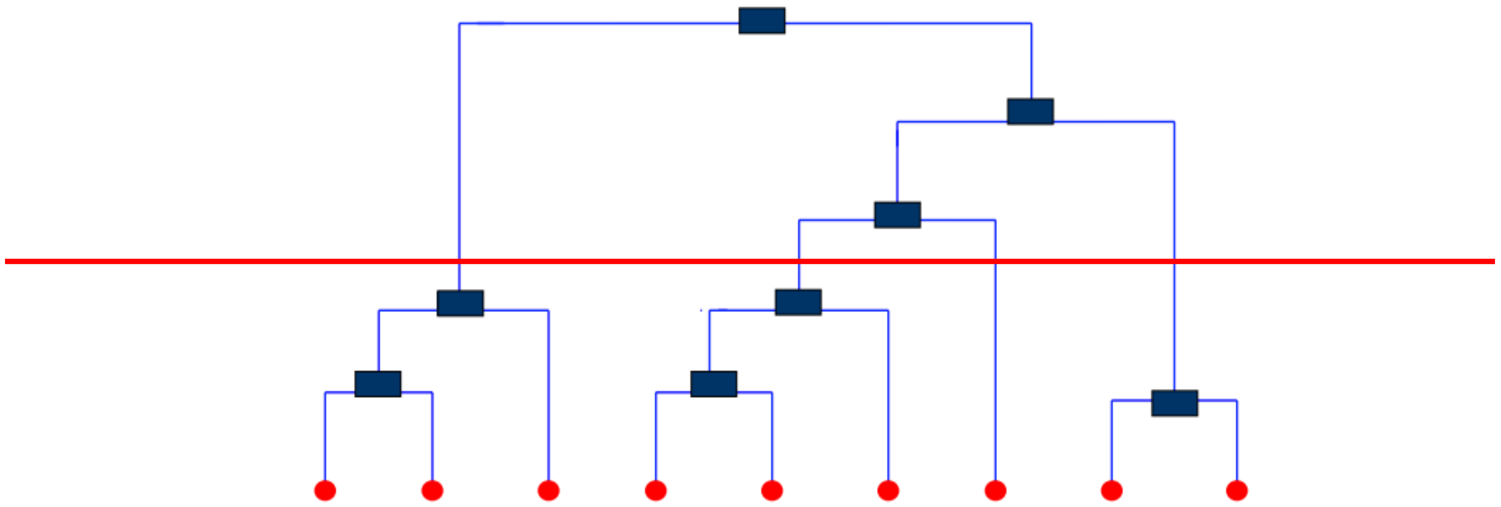
Hierarchical clustering

- Dendrogram
  - A tree that shows how clusters are merged/split hierarchically
  - Each node on the tree is a cluster; each leaf node is a singleton cluster



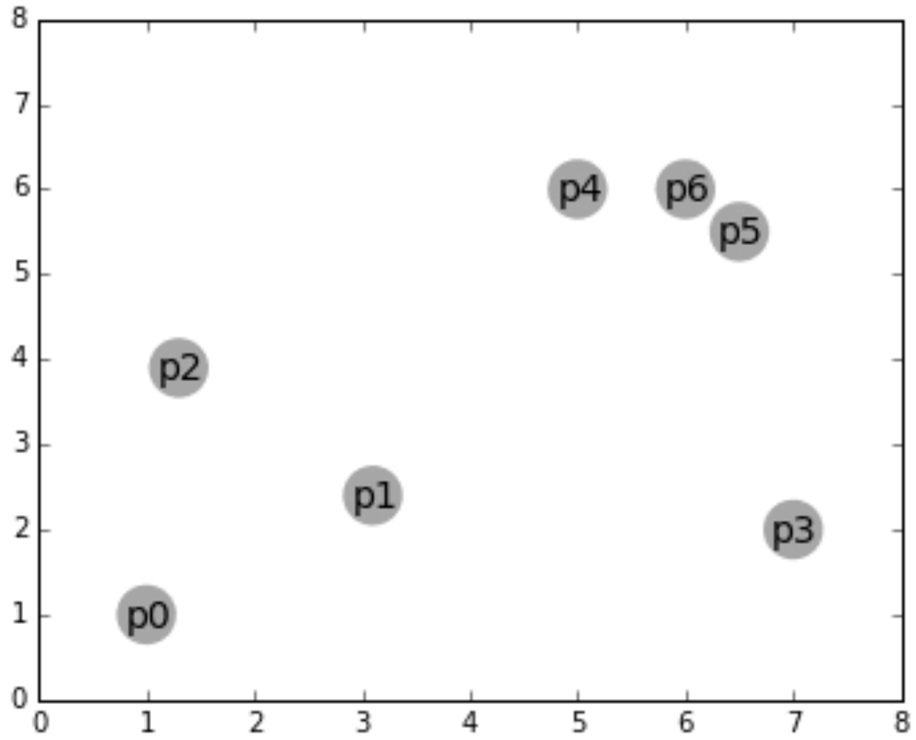
Hierarchical clustering

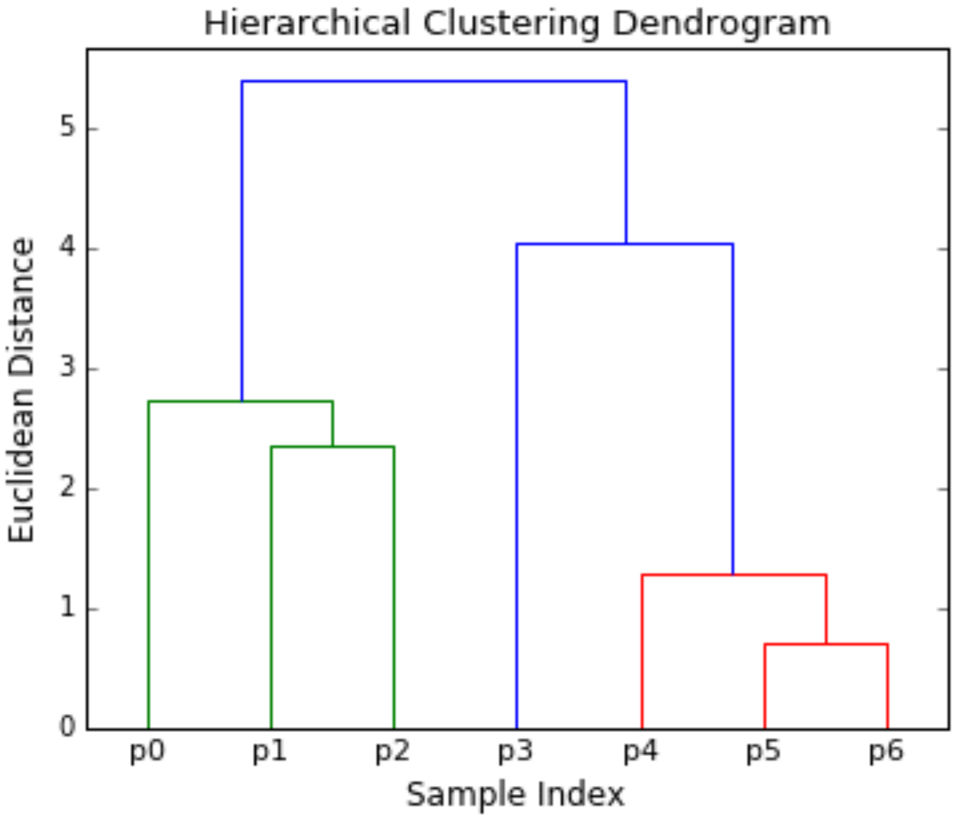
- Dendrogram
  - A tree that shows how clusters are merged/split hierarchically
  - Each node on the tree is a cluster; each leaf node is a singleton cluster
  - A clustering is obtained by cutting the dendrogram at the desired level (then each connected component forms a cluster)



Hierarchical clustering

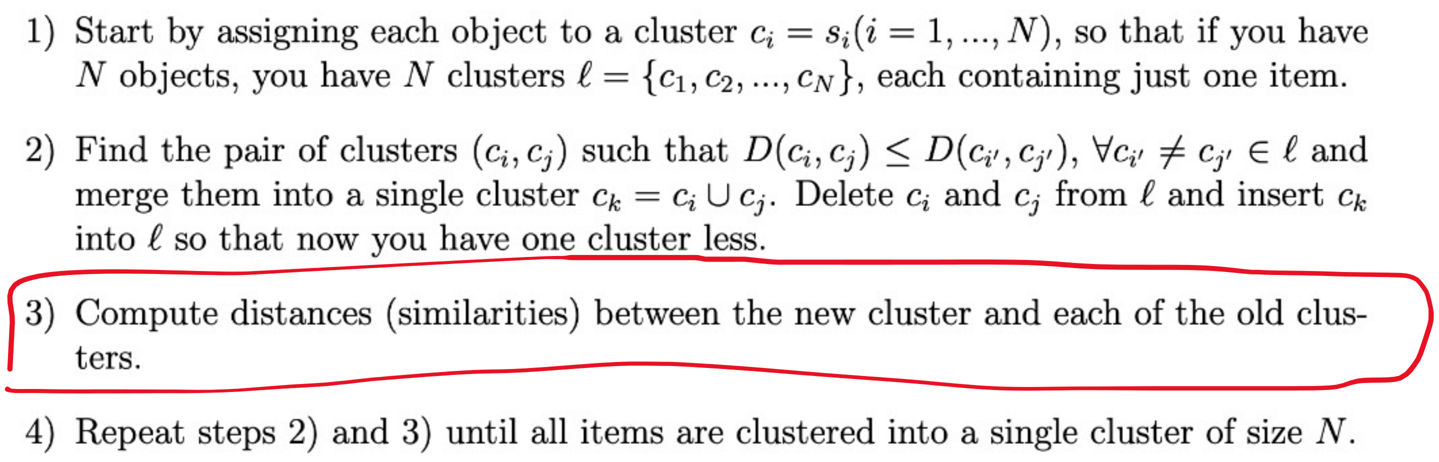
- Example





Hierarchical clustering

- Three different distance measures
  - Single-nearest distance: single linkage
  - Complete-farthest distance: complete linkage
  - Average distance: average linkage



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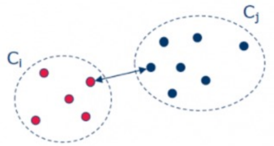
Hierarchical clustering

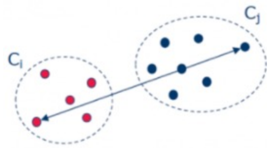
- Three different distance measures
  - Single-nearest distance (single linkage): **shortest** distance between any pair

$$D(c_i, c_j) = \min d(a, b), \forall a \in c_i \text{ and } b \in c_j$$



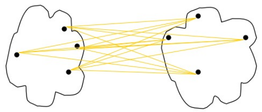
  - Complete-farthest distance (complete linkage): **greatest** distance between any pair

$$D(c_i, c_j) = \max d(a, b), \forall a \in c_i \text{ and } b \in c_j$$



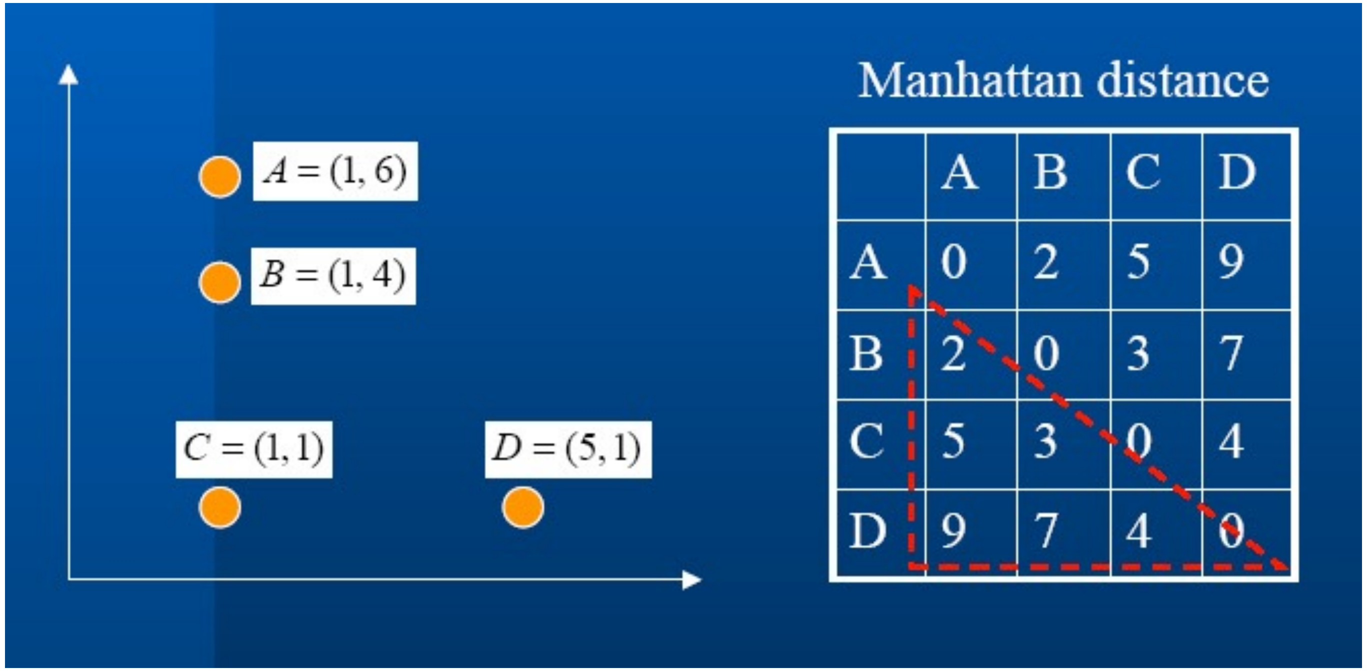
  - Average distance or average linkage: **average** distance between all pairs

$$D\left(c_i, c_j\right) = \frac{1}{|c_i||c_j|} \sum_{a \in c_i, b \in c_j} d(a, b)$$



Hierarchical clustering

- Example: clustering 4 data items in 2D space

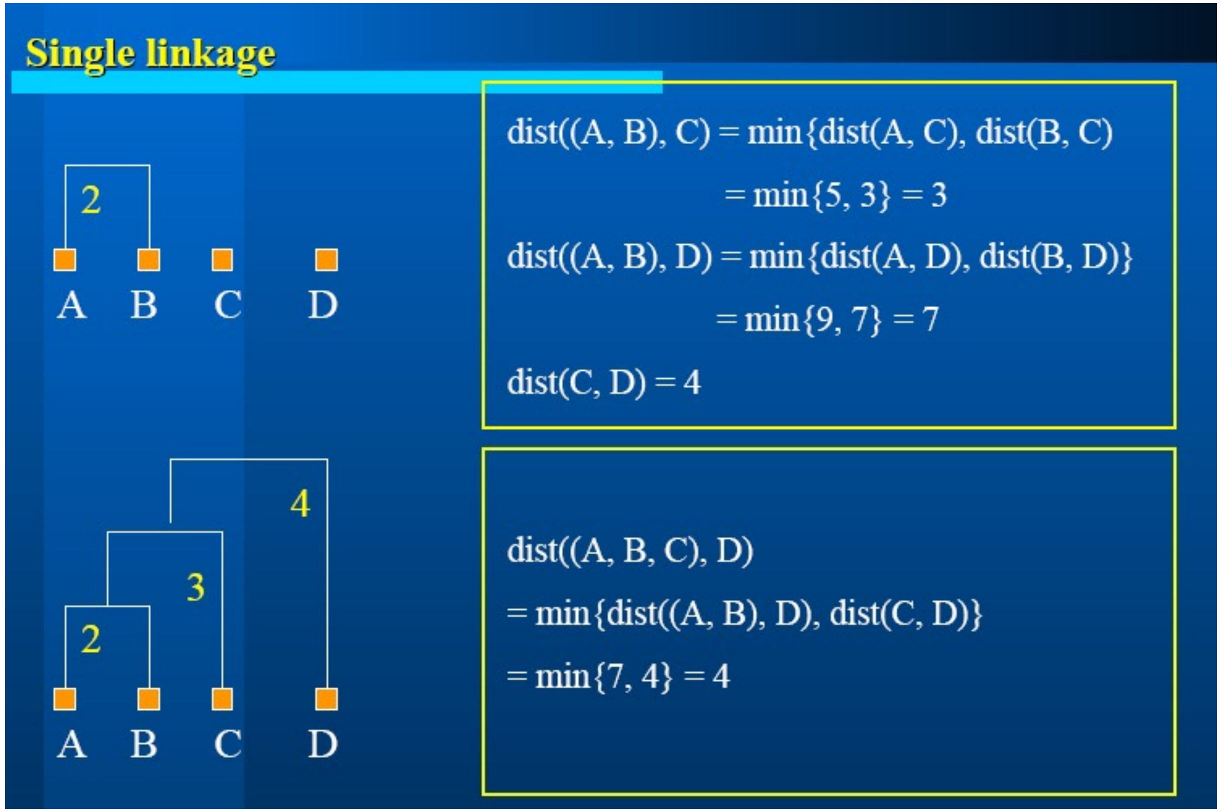


Manhattan distance

	A	B	C	D
A	0	2	5	9
B	2	0	3	7
C	5	3	0	4
D	9	7	4	0

Hierarchical clustering

- Method: *single-linkage* clustering



Single linkage

dist((A, B), C) = min{dist(A, C), dist(B, C)

= min{5, 3} = 3

dist((A, B), D) = min{dist(A, D), dist(B, D)}

= min{9, 7} = 7

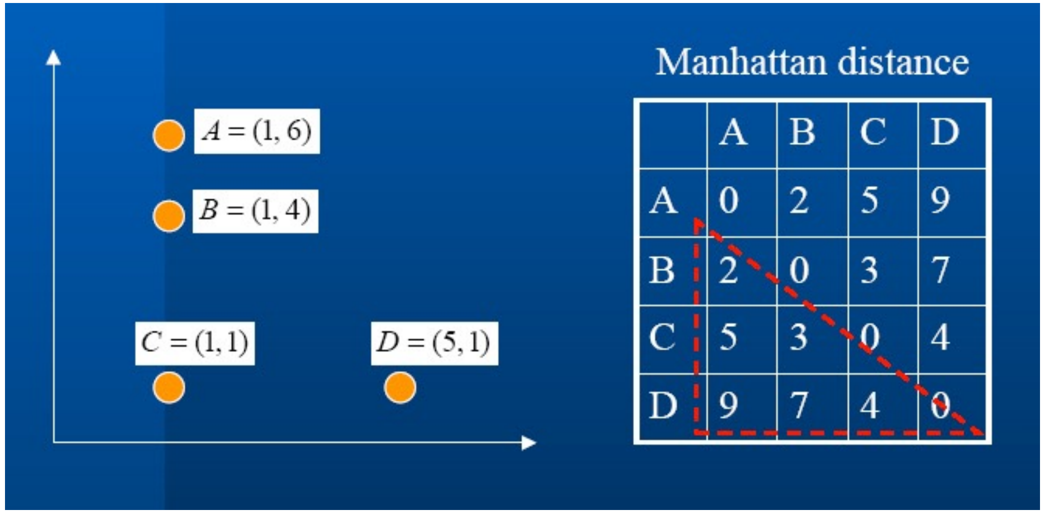
dist(C, D) = 4

dist((A, B, C), D)

= min{dist((A, B), D), dist(C, D)}

= min{7, 4} = 4

$$D(c_i, c_j) = \min d(a,b), \forall a \in c_i \text{ and } b \in c_j$$



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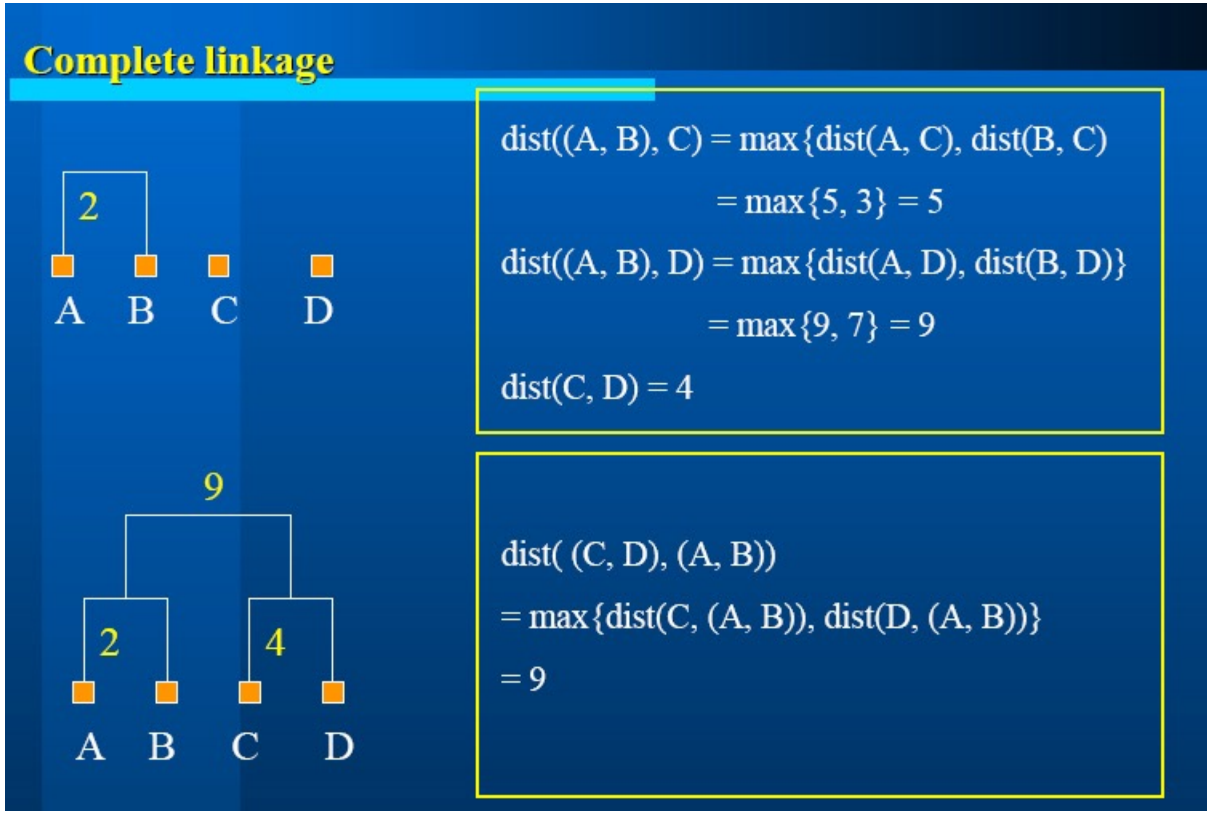
Hierarchical clustering

- Method: *complete-linkage* clustering



Complete linkage

dist((A, B), C) = max{dist(A, C), dist(B, C)

= max{5, 3} = 5

dist((A, B), D) = max{dist(A, D), dist(B, D)}

= max{9, 7} = 9

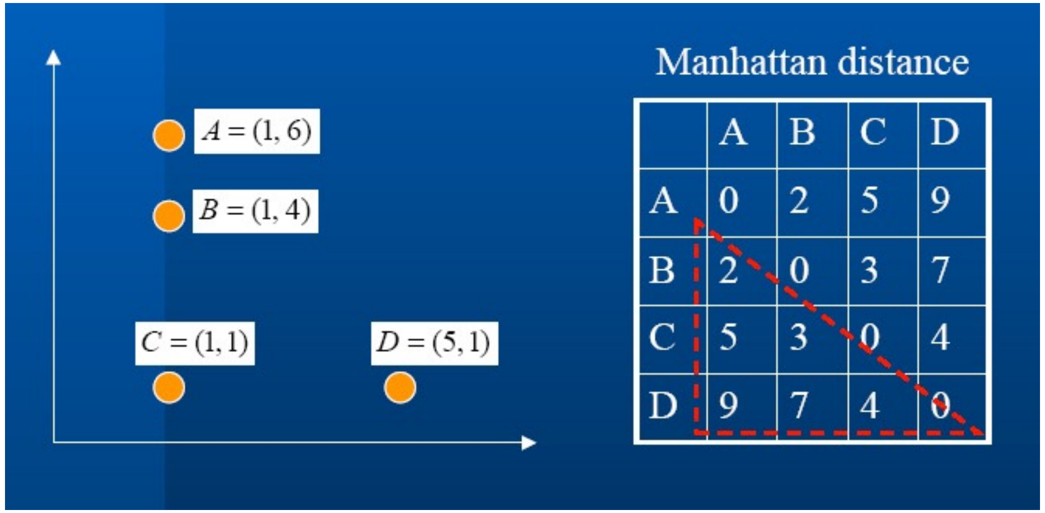
dist(C, D) = 4

dist((C, D), (A, B))

= max{dist(C, (A, B)), dist(D, (A, B))}

= 9

$$D(c_i, c_j) = \max d(a, b), \forall a \in c_i \text{ and } b \in c_j$$



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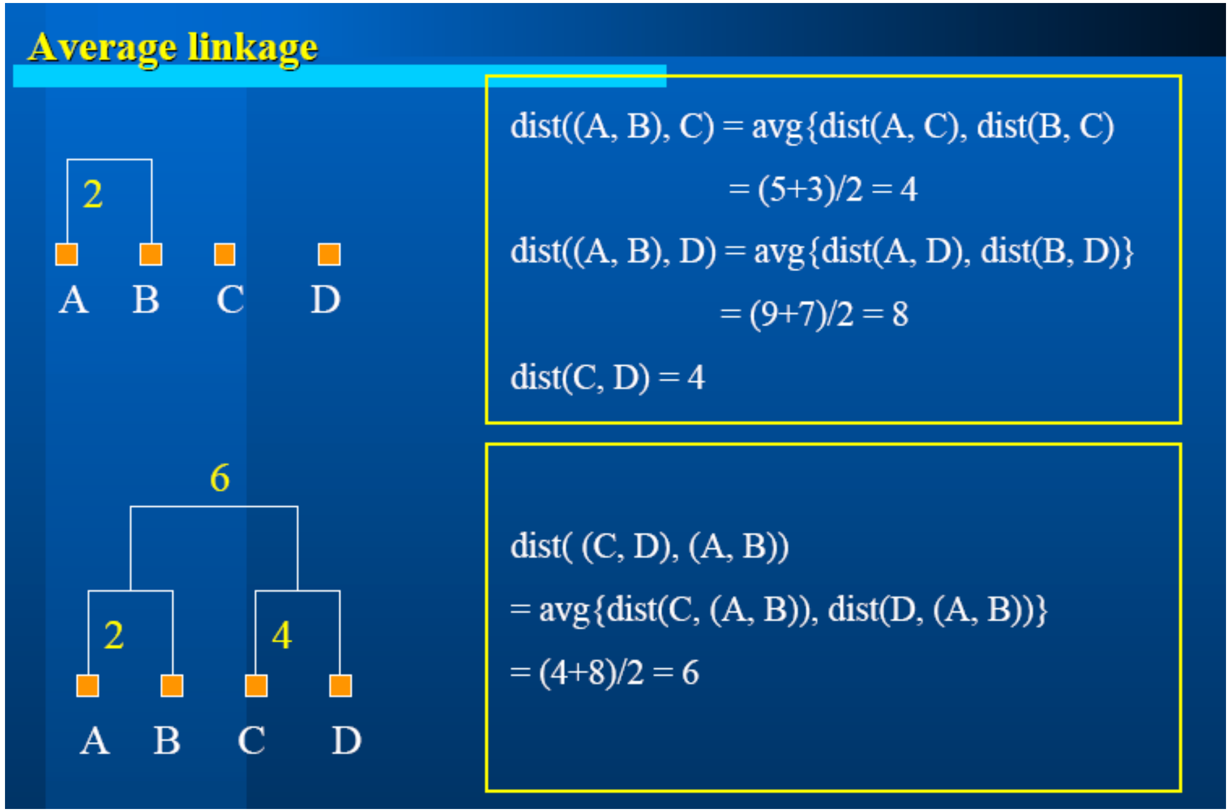
Hierarchical clustering

- Method: *average-linkage* clustering



Average linkage

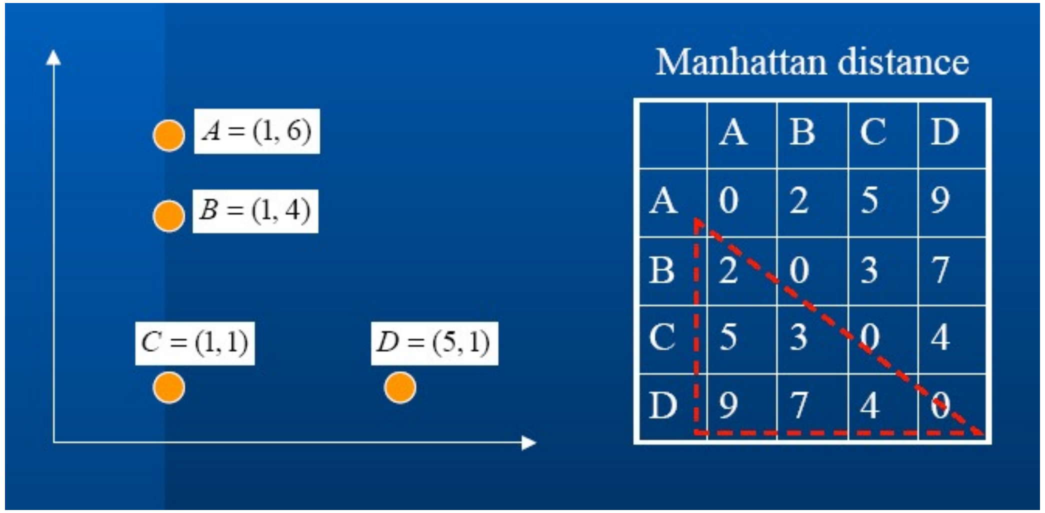
dist((A, B), C) = avg{dist(A, C), dist(B, C)
= (5+3)/2 = 4

dist((A, B), D) = avg{dist(A, D), dist(B, D)}
= (9+7)/2 = 8

dist(C, D) = 4

dist((C, D), (A, B))
= avg{dist(C, (A, B)), dist(D, (A, B))}
= (4+8)/2 = 6

$$D\left(c_i, c_j\right) = \frac{1}{|c_i||c_j|} \sum_{a \in c_i, b \in c_j} d(a, b)$$

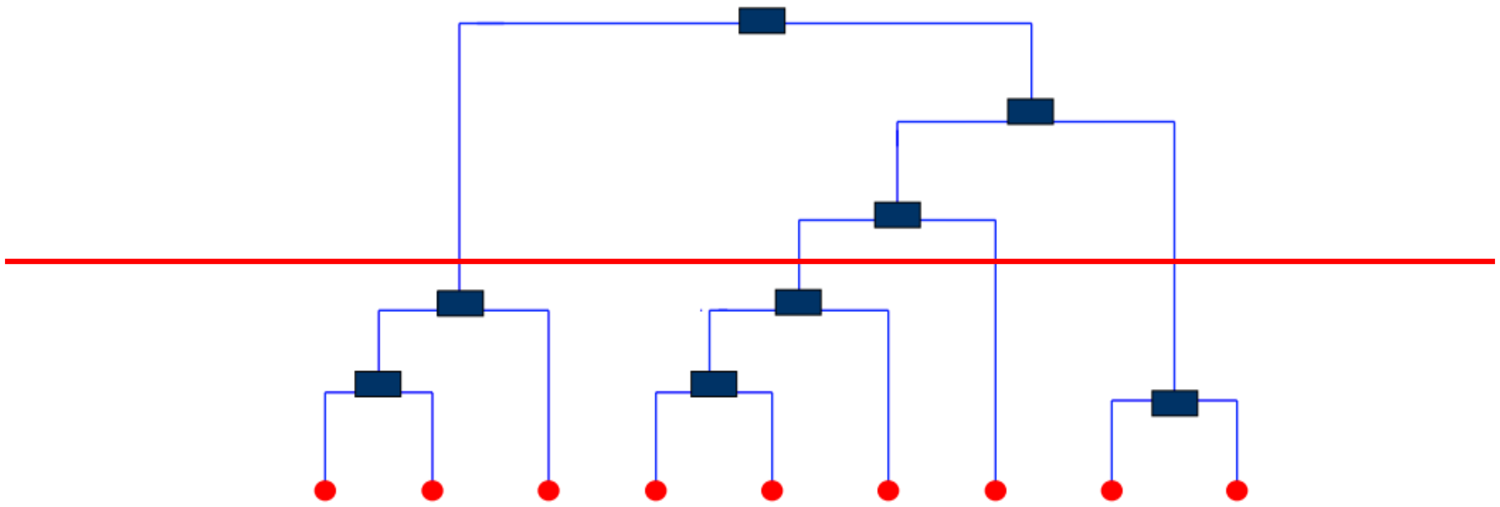


Manhattan distance

	A	B	C	D
A	0	2	5	9
B	2	0	3	7
C	5	3	0	4
D	9	7	4	0

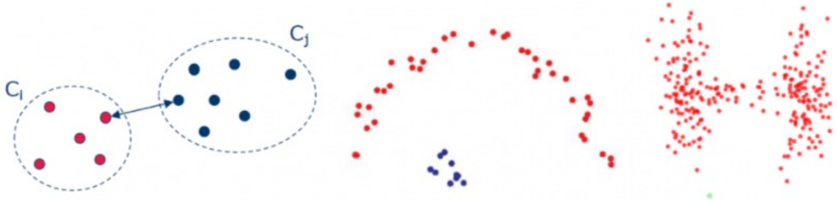
Hierarchical clustering

- Advantages
  - No a priori information about the number of clusters required
    - Any desired number of clusters can be obtained by ‘cutting’ the dendrogram at the proper level
  - Easy to implement and gives best result in some cases

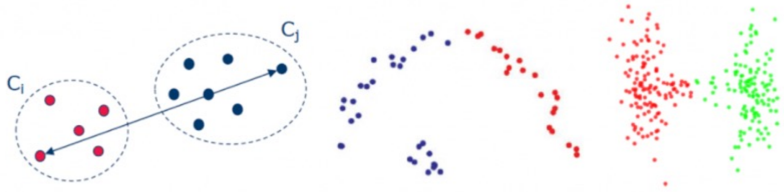


Hierarchical clustering

- Advantages
  - No a priori information about the number of clusters required
  - Easy to implement and gives best result in some cases
- Limitations
  - Can never undo what (i.e., merging two clusters) was done previously
  - Can be slow if a large number data points (due to pairwise distance computation)
  - It may not be easy to choose a proper distance measure



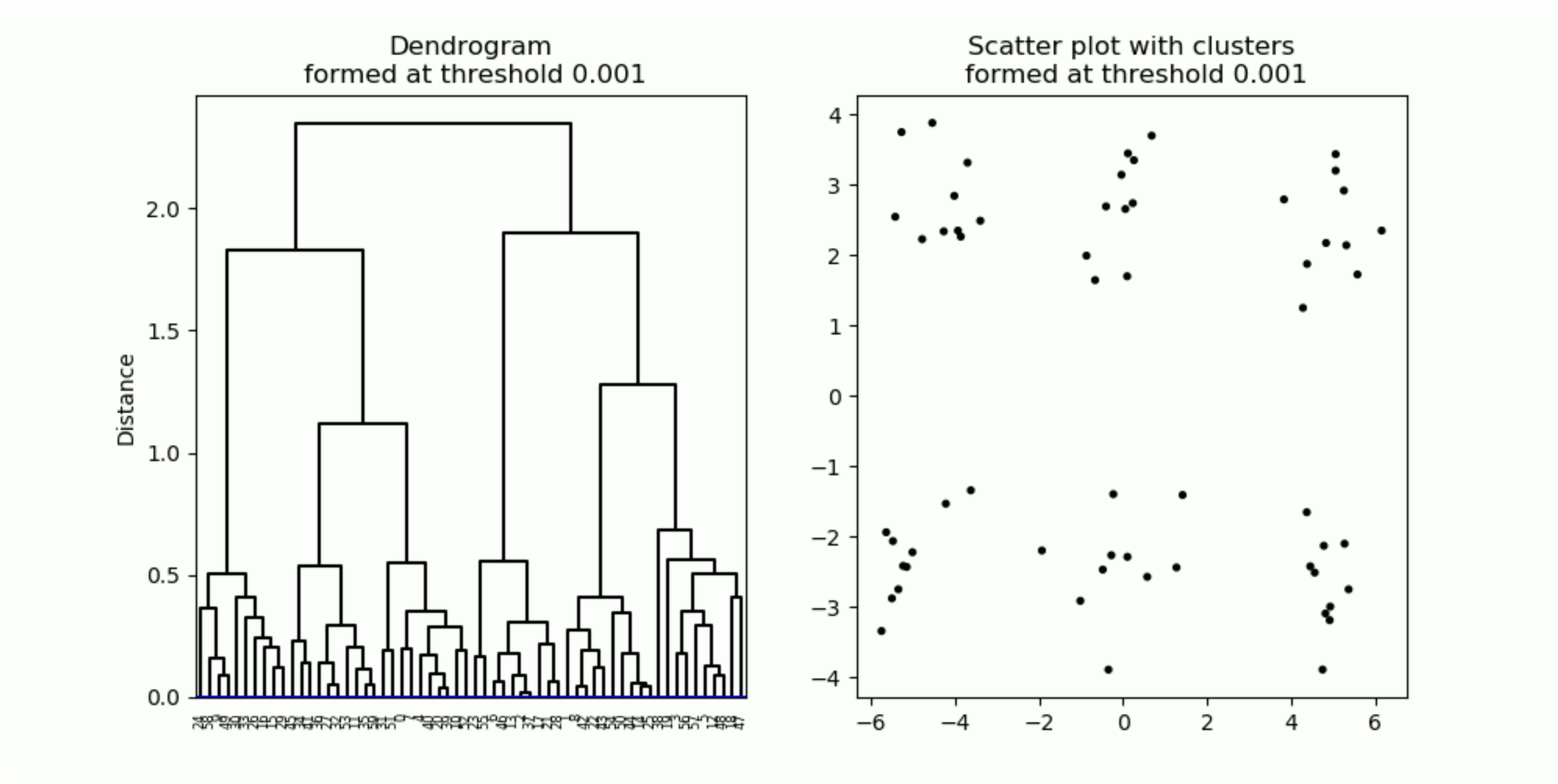
Single linkage: well-separated clusters



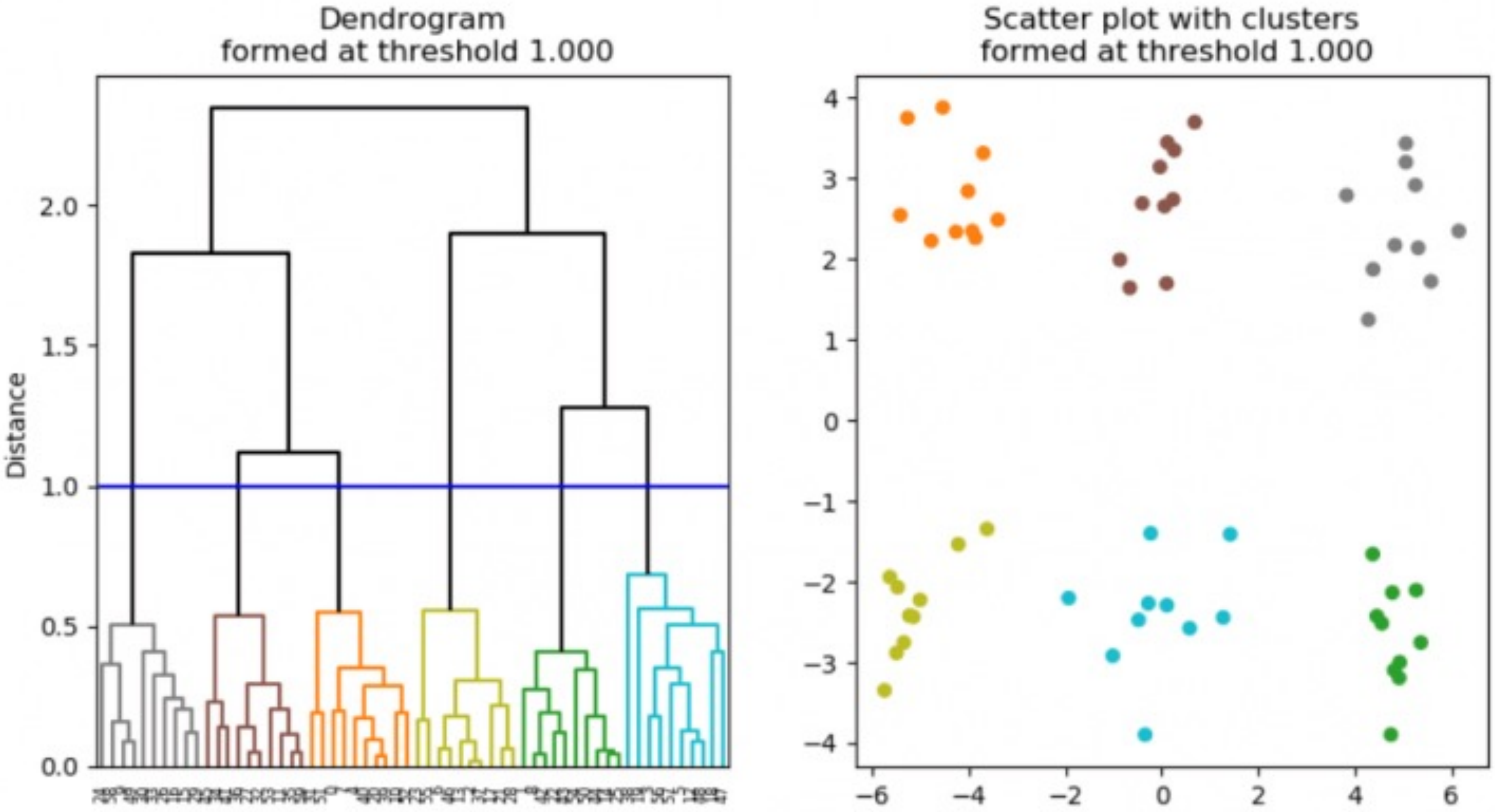
Complete linkage: compact clusters

  - It may not be easy to identify the correct number of clusters by the dendrogram

Hierarchical clustering

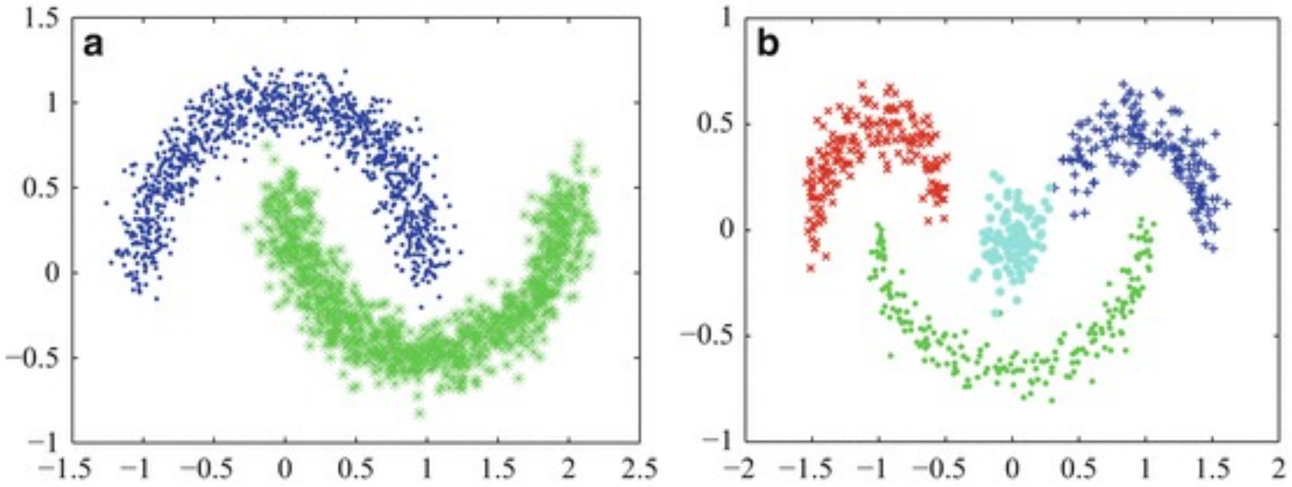


Hierarchical clustering



Hierarchical clustering

- Can hierarchical clustering method handle?

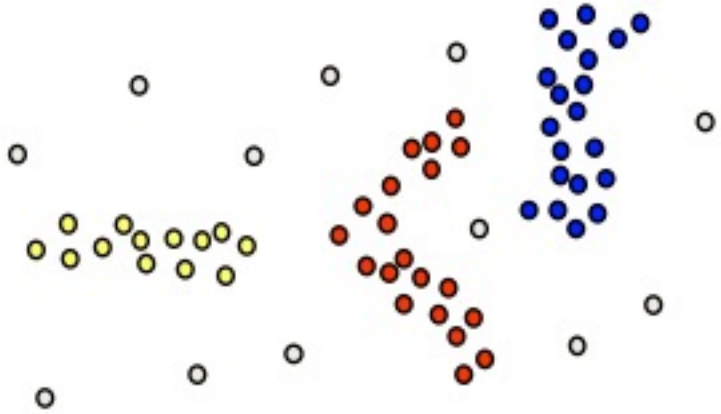


Agenda

- Overview
  - What is clustering?
  - Distance measure (similarity measure)
  - Types of clustering algorithms
- Clustering algorithms
  - K-means clustering
  - Hierarchical clustering
  - Density-based clustering ☜
- Nearest neighbor classification
- Features

Density-based clustering

- Basic ideas
  - Clusters are contiguous regions of high density in the data space, separated by regions of lower data density
  - A cluster is defined as a maximal set of density connected points
- DBSCAN
  - Density-Based Spatial Clustering of Applications with Noise



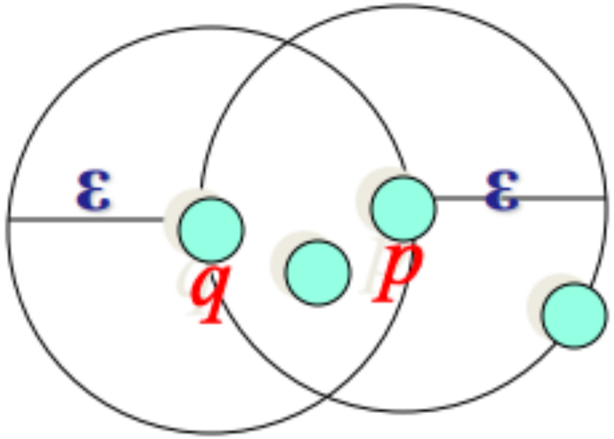
Density definition: two parameters

- ϵ-neighborhood: objects within a radius of ϵ from a cluster

$$N_\varepsilon(p) : \{q \mid d(p,q) \le \varepsilon\}$$

- The minimum number of points required to form a cluster
  - High density: ϵ-neighborhood of an object contains at least *minPts* of objects.

Which point has a higher density?



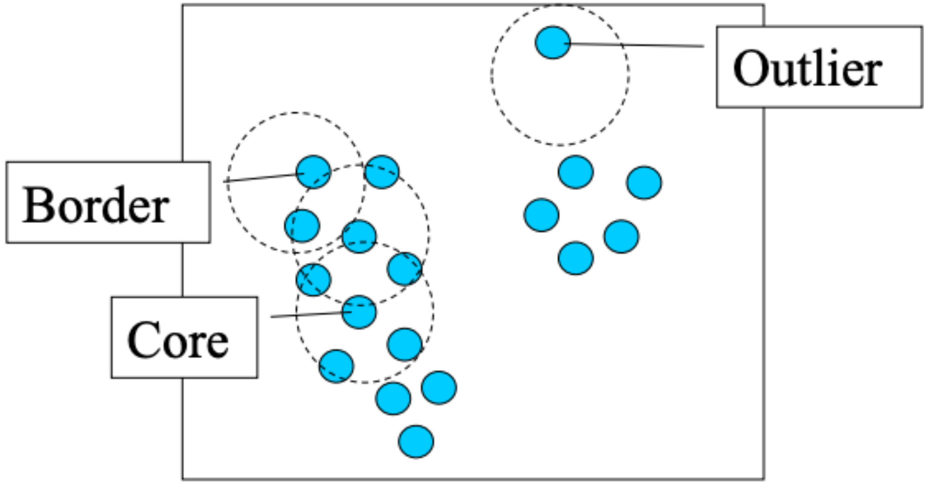
ϵ-neighborhood of *p* and *q*

If *minPts* = 4:

- Density of *p* is "high"
- Density of *q* is "low"

Three types of data points

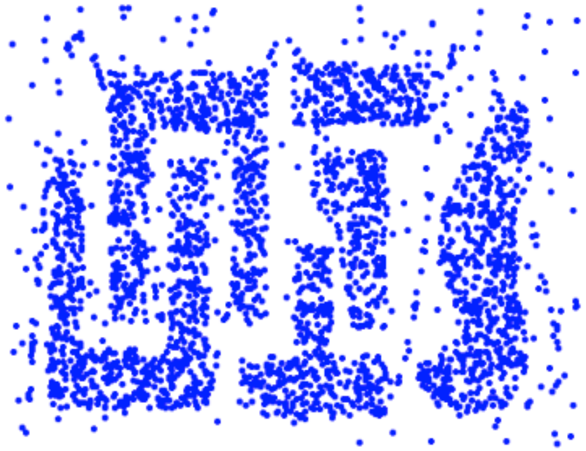
- Given ϵ and *minPts*
  - Core point: has at least *minPts* neighbors within its ϵ-neighborhood
    - At the interior of a cluster
  - Border point
    - has fewer than *minPts* neighbors within its ϵ-neighborhood
    - is within the ϵ-neighborhood of a core point
  - Outlier/Noise
    - Any point that is neither core nor border



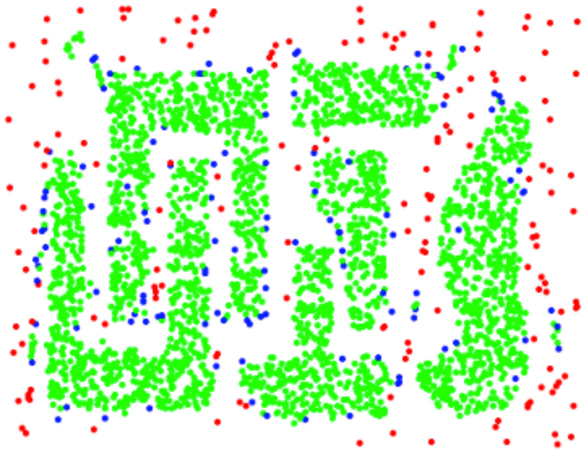
ϵ = circle radius, *minPts* = 5

Three types of data points

- Example



Original Points

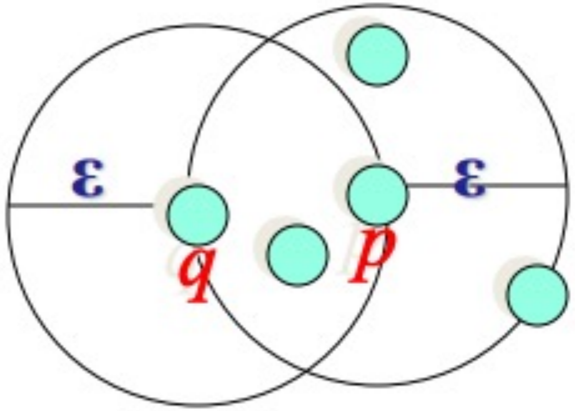


$\epsilon = 10$, $minPts = 4$

Point types: core, border and outliers

Density definition: two concepts

- Density reachability
  - A point *q* is said to be density reachable from a point *p* if
    - *p* is a core point (i.e., has at least *minPts* points within ϵ-neighborhood)
    - point *q* is within the ϵ-neighborhood of *p*

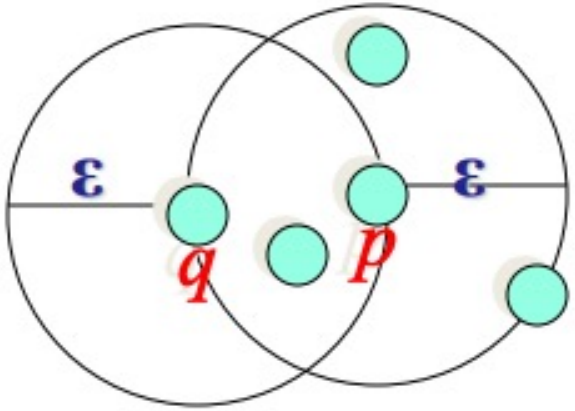


minPts = 4

In this example, *q* is density reachable from *p.*
Is *p* also density reachable from *q*?

Density definition: two concepts

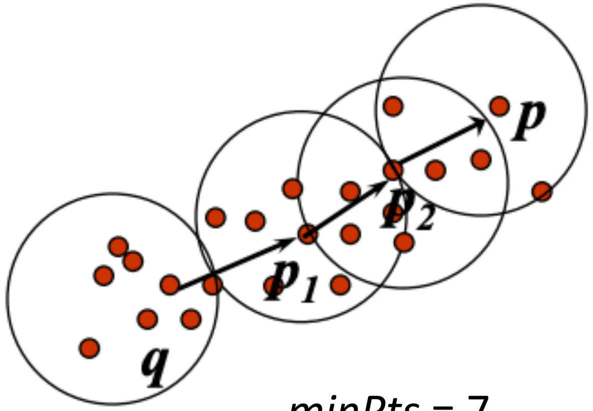
- Density reachability
  - A point q is said to be density reachable from a point p if
    - p is a core point (i.e., has at least *minPts* points within ϵ-neighborhood)
    - point q is within the ϵ-neighborhood of p
  - Density-reachability is asymmetric



minPts = 4

Density definition: two concepts

- Density reachability
- Density connectivity
  - A point *p* and *q* are said to be density connected if
    - There exists another point *r* that has at least *minPts* points within its ϵ-neighborhood
    - *And both p* and *q* are within ϵ-neighborhood of *r*
  - Density connectivity is transitive (i.e., it forms a chain)

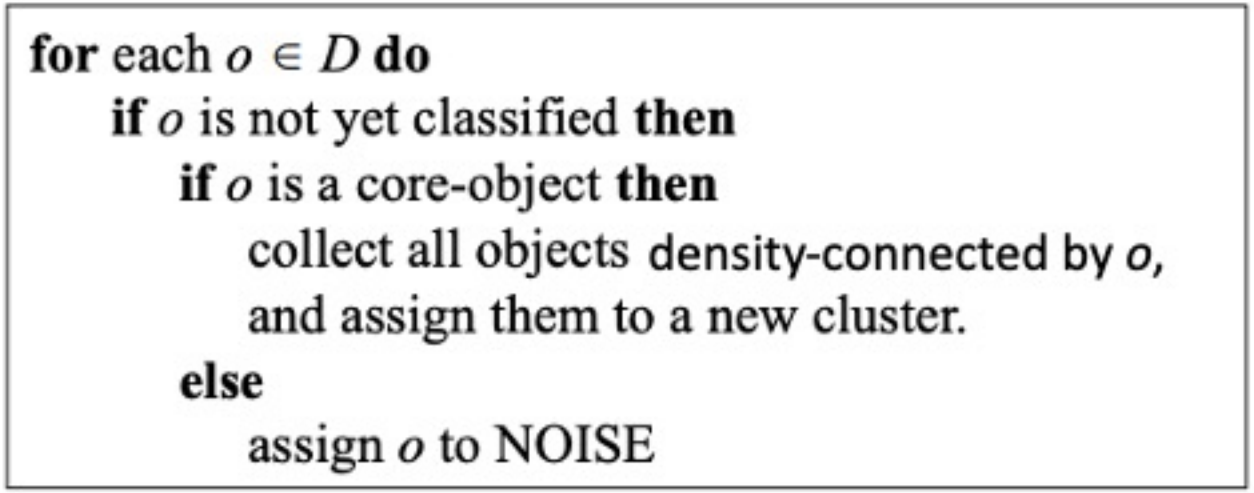


minPts = 7

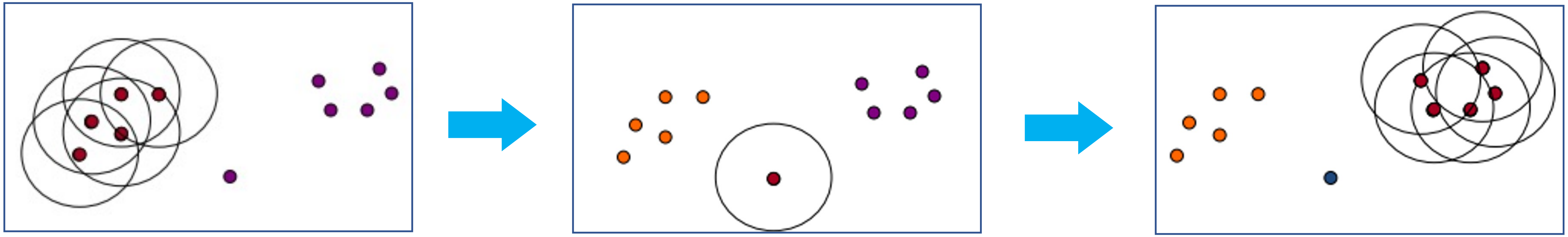
Example:
- *p* is density connected by p_2
- p_2 is density connected by p_1
- p_1 is density connected by *q*

So we say: *p* is density connected by *q*

DBSCAN algorithm



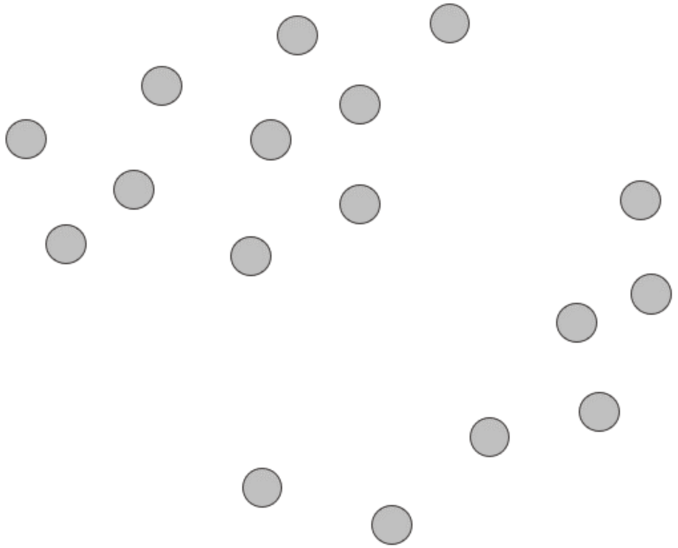
```
for each $o \in D$ do
    if $o$ is not yet classified then
        if $o$ is a core-object then
            collect all objects density-connected by o,
            and assign them to a new cluster.
        else
            assign $o$ to NOISE
```



An example of DBSCAN clustering: ϵ = 1cm, *minPts* = 3

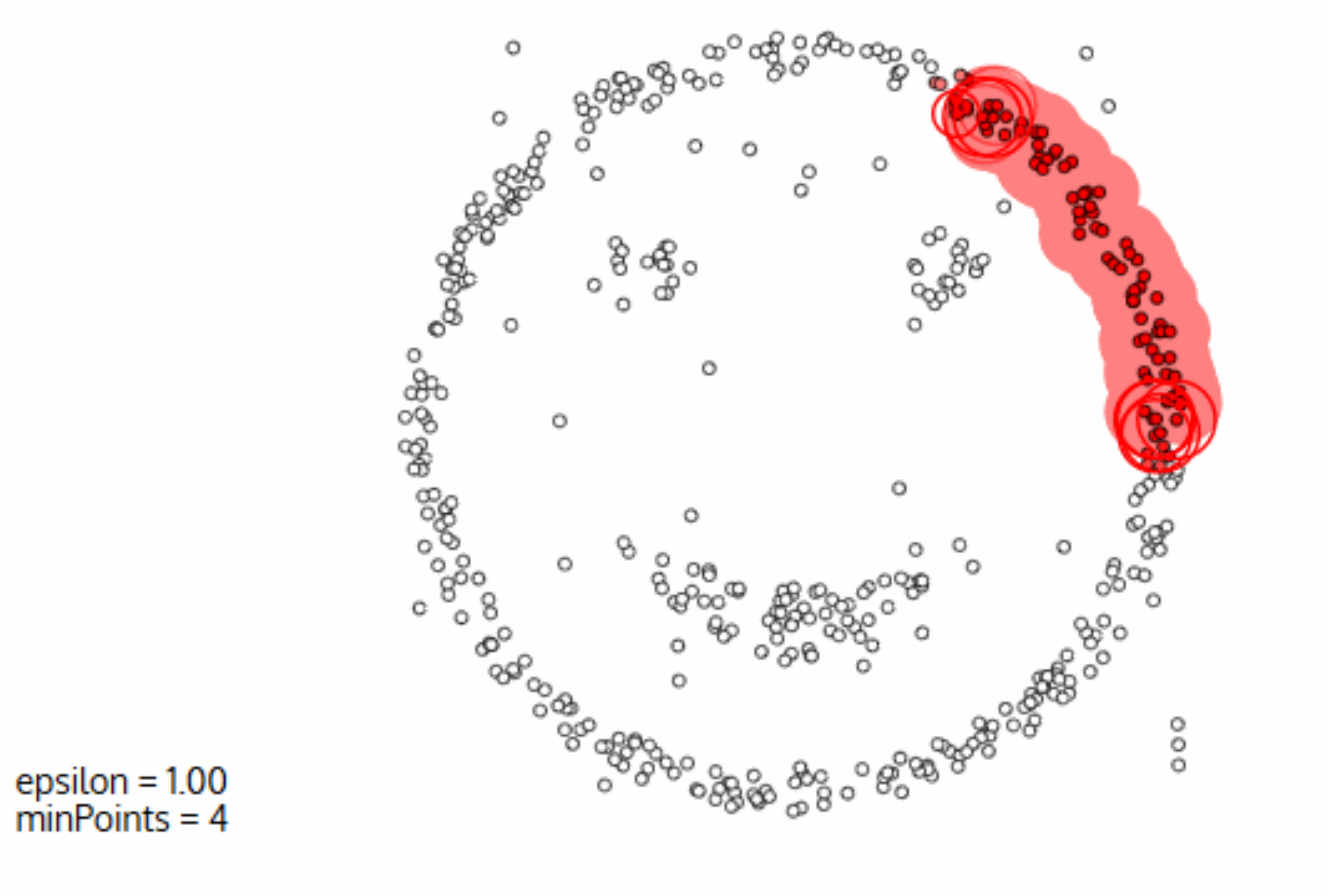
DBSCAN algorithm

- Illustration



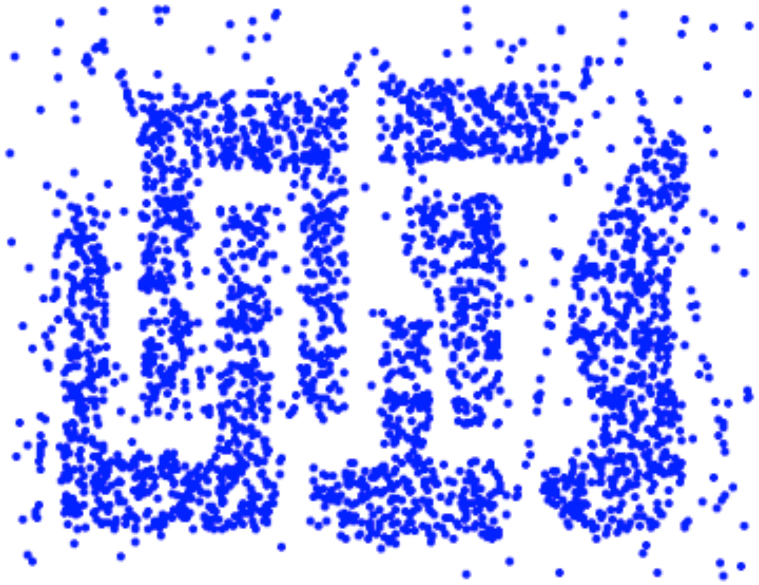
DBSCAN algorithm

- Illustration

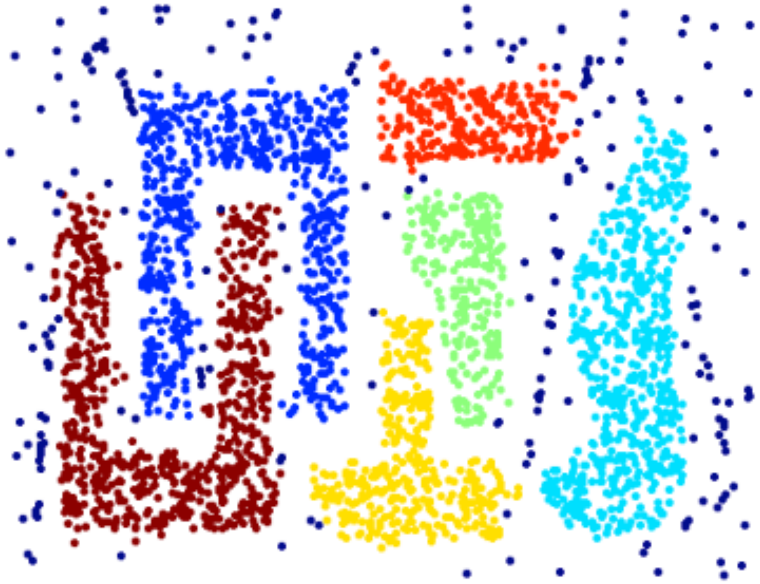


DBSCAN algorithm

- Example



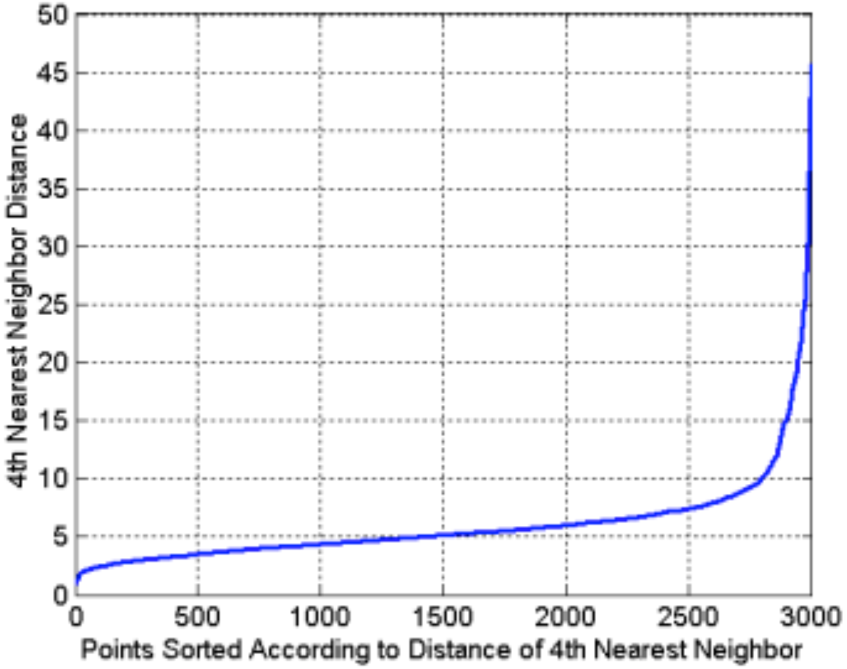
Original Points



Clusters

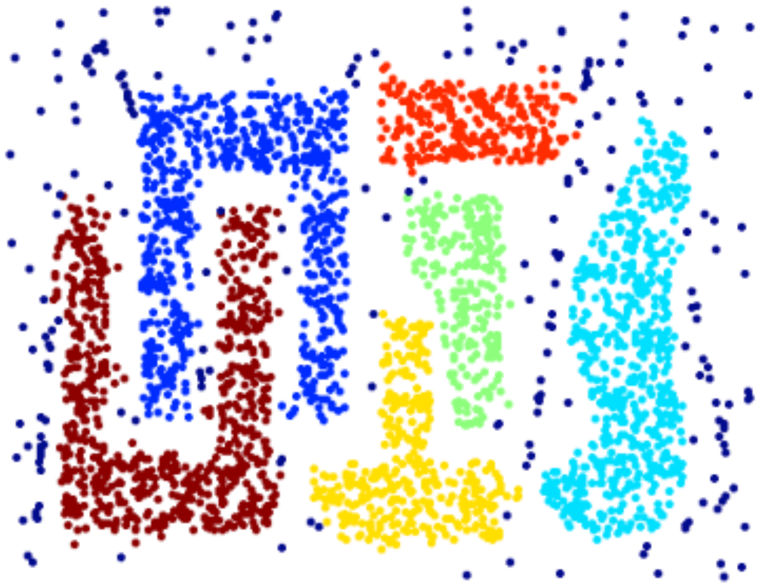
DBSCAN algorithm

- Determining the two parameters
  - *minPts*
    - *minPts* = 1?
    - *minPts* = 2 (same as single linkage hierarchical method)
    - *minPts* = 2 * dimension
  - ϵ (distance threshold)
    - k-distance graph (*k* = *minPts – 1*)
    - Look for the “elbow”



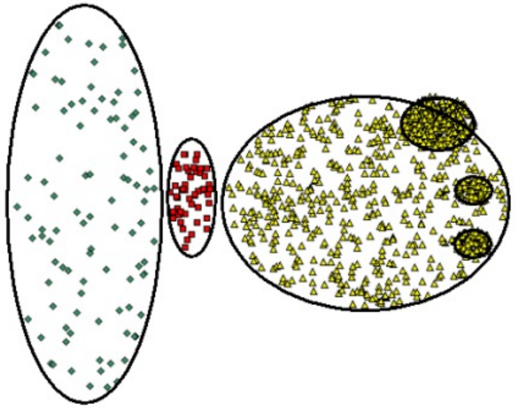
DBSCAN algorithm

- Advantages
  - Resistant to Noise
  - Robust to clusters of different shapes and sizes

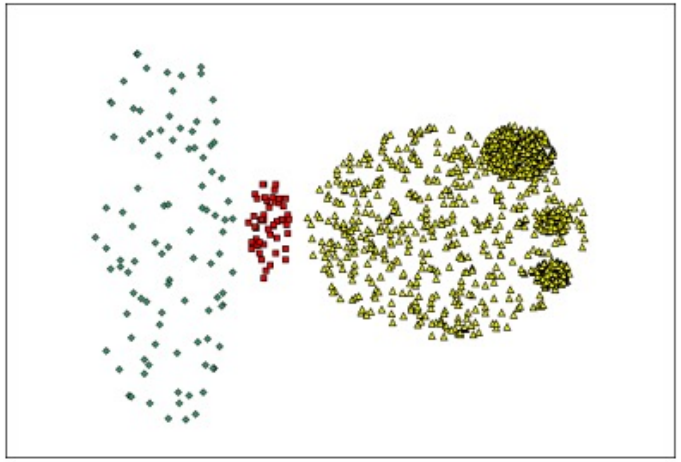


DBSCAN algorithm

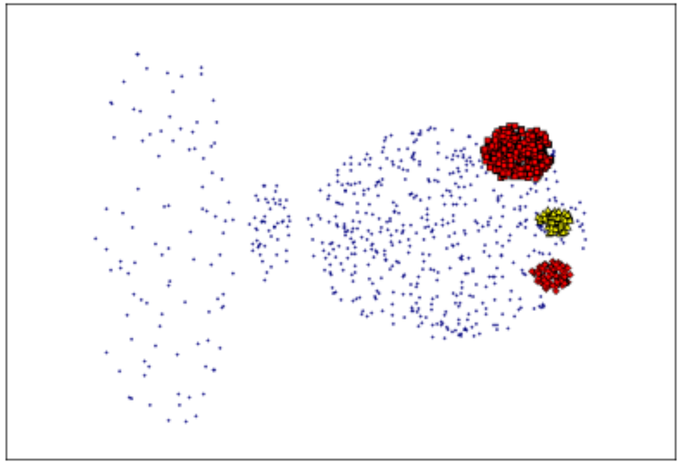
- Limitations
  - Cannot handle varying densities
  - Hard to determine a good set of parameters



Original points



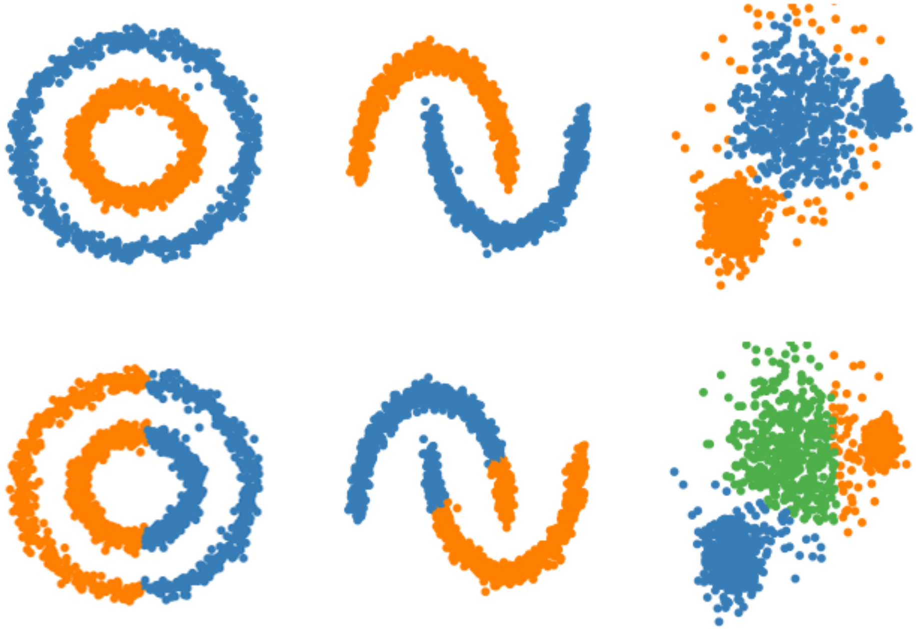
minPts = 4, ϵ = 9.92



minPts = 4, ϵ = 75

Question

- Which method (DBSCAN or k-means) was used to produce each result?



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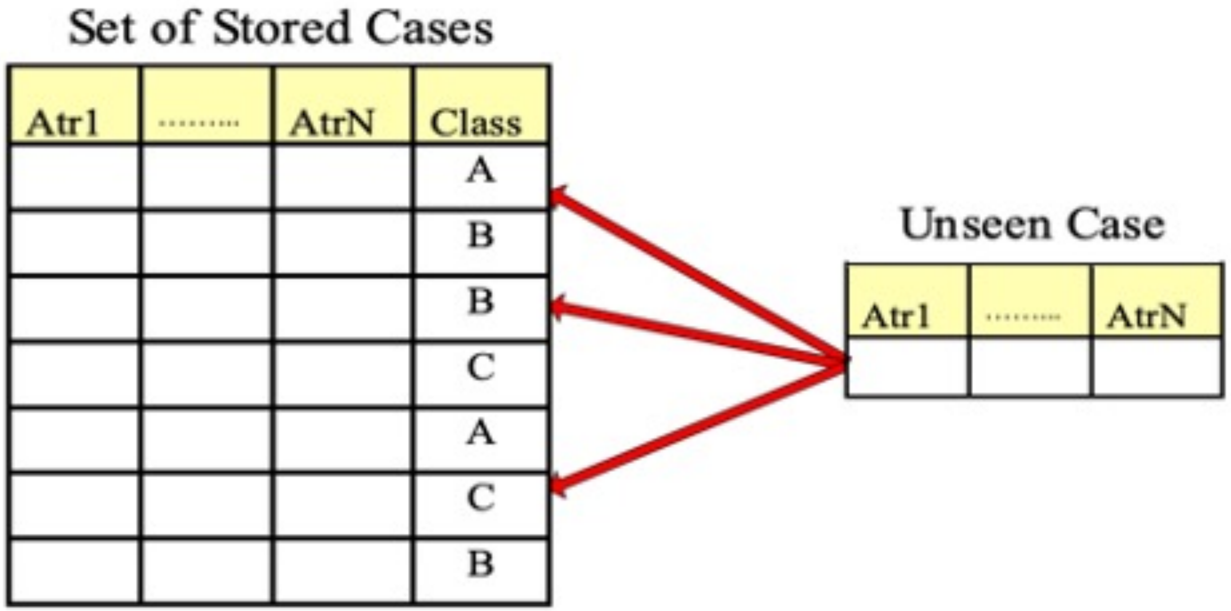
- Nearest neighbor classification ☜
- Features

Nearest neighbor classification

- Basic ideas
  - Store the training records
  - Use training records to predict the class label of unseen cases



Set of Stored Cases

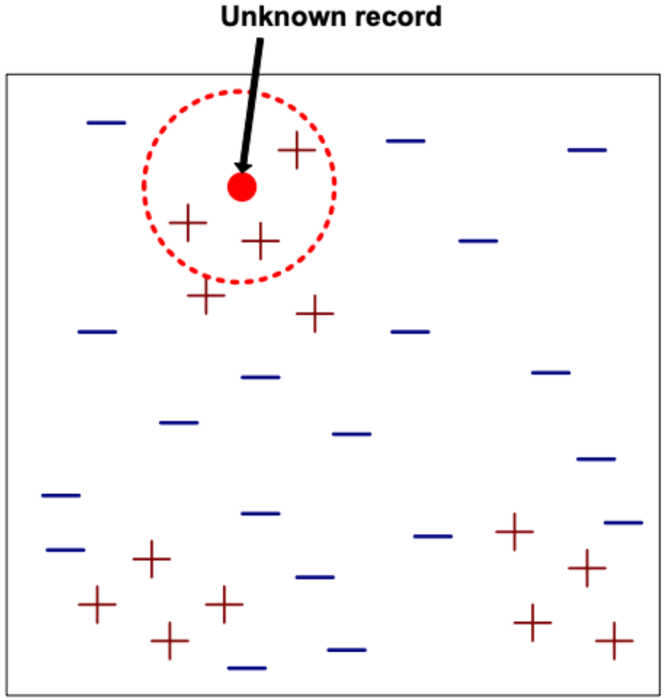
Atr1	………	AtrN	Class
			A
			B
			B
			C
			A
			C
			B

Unseen Case

Atr1	………	AtrN

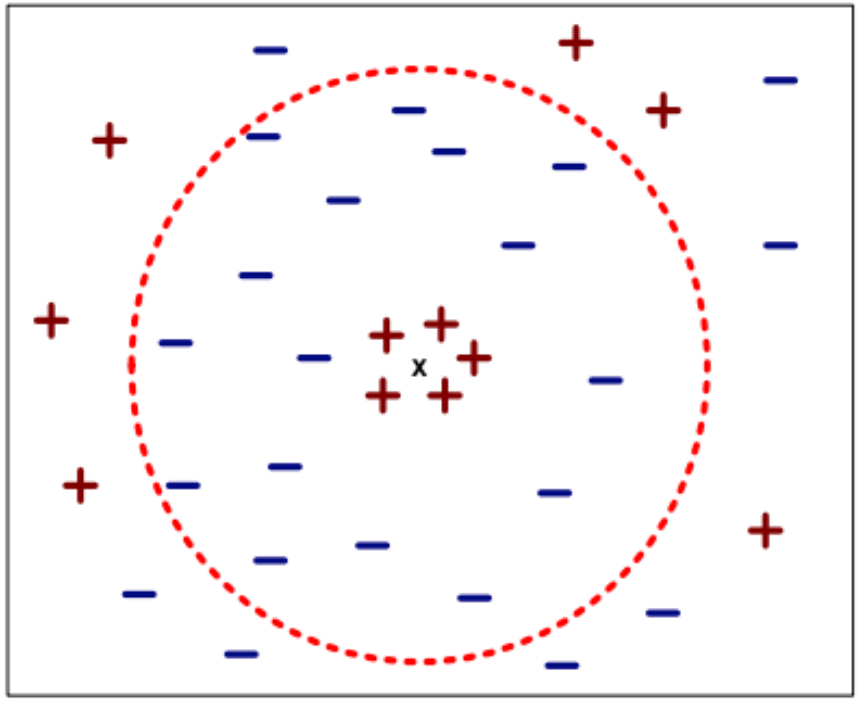
Nearest neighbor classification

- Requires three things
  - The set of stored records
  - Distance metric to compute distance between records
  - The value of k, the number of nearest neighbors to retrieve
- To classify an unknown record
  - Compute distance to other training records
  - Identify k nearest neighbors
  - Use class labels of the k nearest neighbors to determine the class label of the unknown record (e.g., by taking majority vote)



Nearest neighbor classification

- Choosing the value of k
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



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Features

- A set of attributes of an object
- Typically stored as a vector – feature vector
- Scaling issue: distance measure dominated by one of the attributes
  - Example
    - height of a person [1.5m, 1.8m]
    - weight of a person [40kg, 100kg]
    - income of a person [€10K, €1M]
  - Solution
    - Normalization, i.e., $\frac{\text{each attribute value}}{\text{max possible value of this attribute}}$

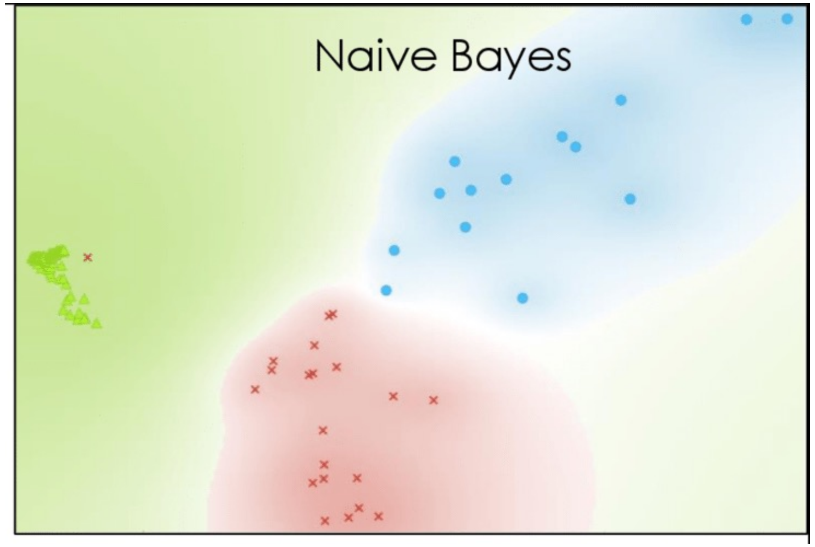
$$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{i=1}^{n}(q_i - p_i)^2}$$

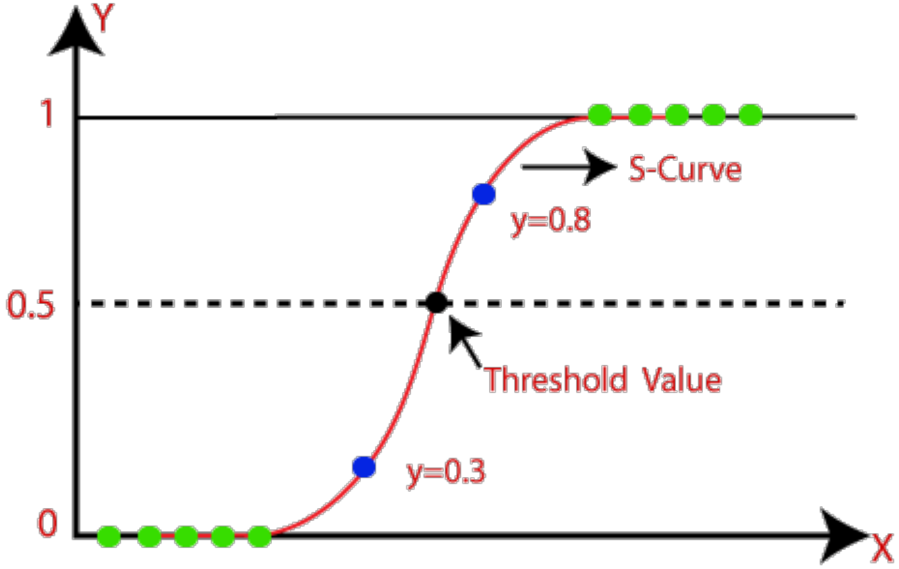
You should have learned

- Clustering
  - The basic ideas, strengths, and weaknesses of the 3 clustering methods
  - K-means
    - How is K-means interpreted as an optimization problem?
  - Hierarchical clustering
    - Several ways of defining inter-cluster distance
  - Density-based clustering
    - The parameters and the definitions of neighborhood and density in DBSCAN
- Classification
  - The basic idea of k-nearest neighbor classifier

Next Lecture

- Bayesian classification & logistic regression


Naive Bayes


Y
X
S-Curve
y=0.8
Threshold Value
y=0.3