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# Clustering

# What is Cluster Analysis?

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- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation*, ...)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- **Unsupervised learning**: no predefined classes
- *learning by observations* vs.  
learning by examples: supervised

# Clustering Applications

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- Information retrieval: document clustering
- Land use: Identification of areas of similar land use in an earth observation database
- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Earth-quake studies: Observed earth quake epi-centers should be clustered along continent faults
- Climate: understanding earth climate, find patterns of atmospheric and ocean
- Economic Science: market resarch

# Clustering as a Preprocessing

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- Summarization:
  - Preprocessing for regression, classification, and association analysis
- Finding K-nearest Neighbors
  - Localizing search to one or a small number of clusters
- Outlier detection
  - Outliers are often viewed as those “far away” from any cluster

# Quality: What Is Good Clustering?

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- A good clustering method will produce high quality clusters
  - high intra-class similarity: **cohesive** within clusters
  - low inter-class similarity: **distinctive** between clusters
- The quality of a clustering method depends on
  - the similarity measure used by the method
  - its implementation, and
  - Its ability to discover some or all of the hidden patterns

# Measure the Quality of Clustering

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- **Dissimilarity/Similarity metric**
  - Similarity is expressed in terms of a distance function, typically metric:  $d(i, j)$
  - The definitions of **distance functions** are usually rather different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables
  - Weights should be associated with different variables based on applications and data semantics
- **Quality of clustering:**
  - There is usually a separate “quality” function that measures the “goodness” of a cluster.
  - It is hard to define “similar enough” or “good enough”

# Considerations for Clustering Analysis

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- Partitioning criteria
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)
- Separation of clusters
  - Exclusive (e.g., one customer belongs to only one region)
  - non-exclusive (e.g., one document may belong to more than one class)
- Similarity measure
  - Distance-based (e.g., Euclidian, vector) vs. connectivity-based (e.g., density or contiguity)
- Clustering space
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

# Major Clustering Approaches

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- Partitioning approach:
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - Typical methods: k-means, k-medoids, CLARANS
- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- Density-based approach:
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue
- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE



# Partitioning Algorithms: Basic Concept

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- Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where  $c_i$  is the centroid or medoid of cluster  $C_i$ )

$$E = \sum_{i=1}^k \sum_{p \in C_i} (p - c_i)^2$$

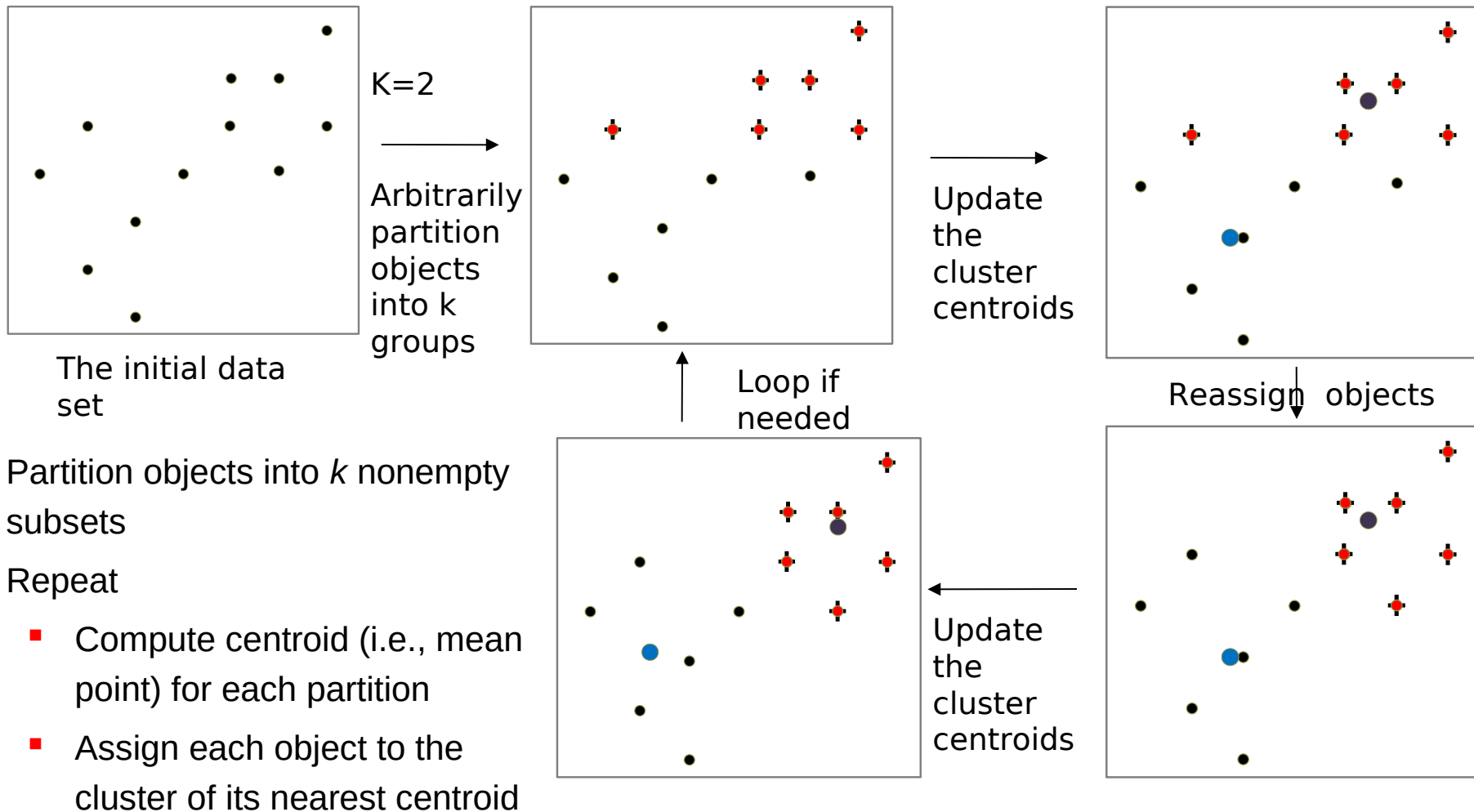
- Given  $k$ , find a partition of  $k$  clusters that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

# The *K-Means* Clustering Method

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- Given  $k$ , the *k-means* algorithm is implemented in four steps:
  - Partition objects into  $k$  nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  - Assign each object to the cluster with the nearest seed point
  - Go back to Step 2, stop when the assignment does not change

# An Example of *K-Means* Clustering



- Partition objects into  $k$  nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

# Comments on the *K-Means* Method

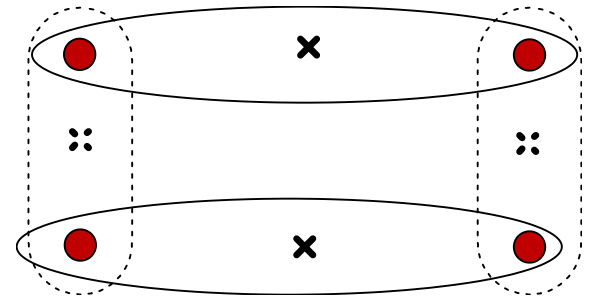
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- Strength: *Efficient*:  $O(tkn)$ , where  $n$  is # objects,  $k$  is # clusters, and  $t$  is # iterations. Normally,  $k, t \ll n$
- Comment: Often terminates at a *local optimal*.
- Weakness
  - Applicable only to objects in a continuous  $n$ -dimensional space
    - In comparison,  $k$ -medoids can be applied to a wide range of data
  - Need to specify  $k$ , the *number* of clusters, in advance (there are ways to automatically determine the best  $k$  (see Hastie et al., 2009))
  - Sensitive to noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*

# Variations of the *K-Means* Method

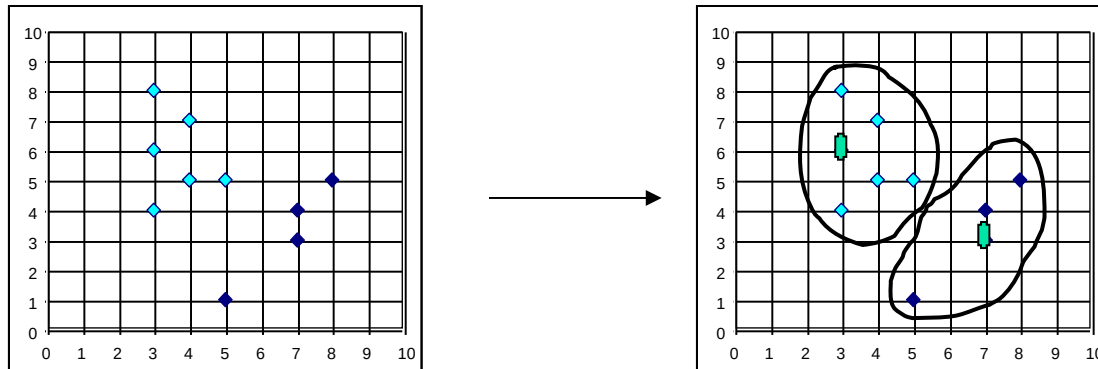
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- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means
- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters

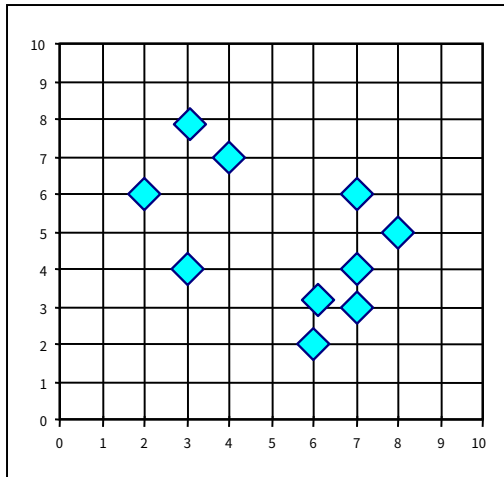


# Problem of the K-Means Method?

- The k-means algorithm is sensitive to outliers !
  - Since an object with an extremely large value may substantially distort the distribution of the data
- K-Medoids: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster



# PAM: A Typical K-Medoids Algorithm



**K=2**

Arbitrary  
choose k  
object as  
initial  
medoids

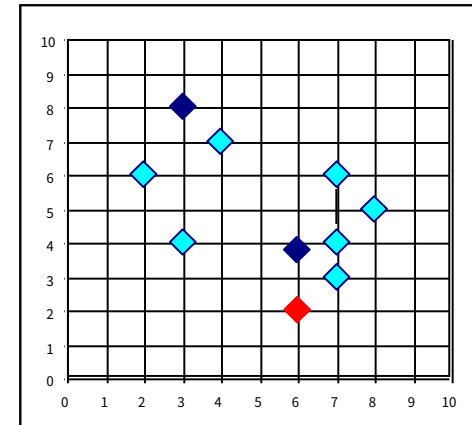
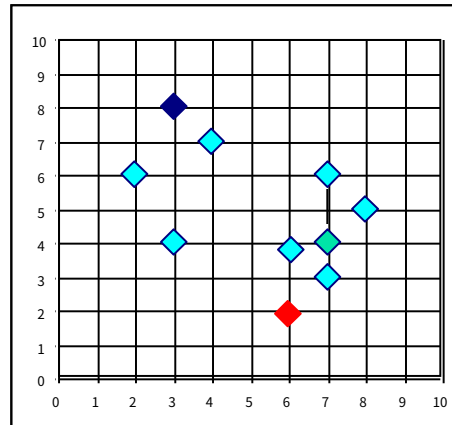
Assign  
each  
remaining  
object to  
nearest  
medoids

Randomly  
select a  
nonmedoid  
object,  $O_{\text{random}}$

**Do loop  
Until no  
change**

Swap Medoid  
If quality is  
improved.

Compute  
total cost  
of  
swapping



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	X	Y
0	8	7
1	3	7
2	4	9
3	9	6
4	8	5
5	5	8
6	7	3
7	8	4
8	7	5
9	4	5

randomly selected 2 medoids,  
so select  $k = 2$  and let  $C1 = (4, 5)$  and  $C2 = (8, 5)$



	X	Y
0	8	7
1	3	7
2	4	9
3	9	6
4	8	5
5	5	8
6	7	3
7	8	4
8	7	5
9	4	5

	X	Y	Dissimilarity from C1	Dissimilarity from C2
0	8	7	6	2
1	3	7	3	7
2	4	9	4	8
3	9	6	6	2
4	8	5	-	-
5	5	8	4	6
6	7	3	5	3
7	8	4	5	1
8	7	5	3	1
9	4	5	-	-

Each point is assigned to the cluster of that medoid whose dissimilarity is less.

The points 1, 2, 5 go to cluster C1 and  
0, 3, 6, 7, 8 go to cluster C2.

$$\text{The Cost} = (3 + 4 + 4) + (3 + 1 + 1 + 2 + 2) = 20$$

randomly selected point be (8, 4).

The dissimilarity of each non-medoid point with the medoids – C1 (4, 5) and C2 (8, 4) is calculated

	X	Y
0	8	7
1	3	7
2	4	9
3	9	6
4	8	5
5	5	8
6	7	3
7	8	4
8	7	5
9	4	5

	X	Y	Dissimilarity from C1	Dissimilarity from C2
0	8	7	6	2
1	3	7	3	7
2	4	9	4	8
3	9	6	6	2
4	8	5	-	-
5	5	8	4	6
6	7	3	5	3
7	8	4	5	1
8	7	5	3	1
9	4	5	-	-

	X	Y	Dissimilarity from C1	Dissimilarity from C2
0	8	7	6	3
1	3	7	3	8
2	4	9	4	9
3	9	6	6	3
4	8	5	4	1
5	5	8	4	7
6	7	3	5	2
7	8	4	-	-
8	7	5	3	2
9	4	5	-	-

The New cost =  $(3 + 4 + 4) + (2 + 2 + 1 + 3 + 3) = 22$   
 Swap Cost = New Cost - Previous Cost =  $22 - 20 = 2 > 0$   
As the swap cost is not less than zero, undo the swap

	X	Y
0	8	7
1	3	7
2	4	9
3	9	6
4	8	5
5	5	8
6	7	3
7	8	4
8	7	5
9	4	5

	X	Y	Dissimilarity from C1	Dissimilarity from C2
0	8	7	6	2
1	3	7	3	7
2	4	9	4	8
3	9	6	6	2
4	8	5	-	-
5	5	8	4	6
6	7	3	5	3
7	8	4	5	1
8	7	5	3	1
9	4	5	-	-

As there is  
no change  
in medoid  
set  
Algorithm  
Terminates

	X	Y	Dissimilarity from C1	Dissimilarity from C2
0	8	7	6	3
1	3	7	3	8
2	4	9	4	9
3	9	6	6	3
4	8	5	4	1
5	5	8	4	7
6	7	3	5	2
7	8	4	-	-
8	7	5	3	2
9	4	5	-	-

# The K-Medoid Clustering Method

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- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
  - *PAM* (Partitioning Around Medoids, Kaufmann & Rousseeuw 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
    - *PAM* works effectively for small data sets, but does not scale well for large data sets (due to the computational complexity)
- Efficiency improvement on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990): PAM on samples