LECTURE 31

Unit IV – FP Growth Algorithm & Evaluation of Association Patterns from Textbook

LECTURE 32

Cluster Analysis

Source: Chapter 10, Data Mining: Concepts and Techniques(3rd ed.)

Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: Basic Concepts
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- ~~Grid-Based Methods~~
- Evaluation of Clustering
- Summary

What is Cluster Analysis?

- 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 (i.e., *learning by observations* vs. learning by examples: supervised)
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Applications of Cluster Analysis

- Data reduction
  - Summarization: Preprocessing for regression, PCA, classification, and association analysis
  - Compression: Image processing: vector quantization
- Hypothesis generation and testing
- Prediction based on groups
  - Cluster & find characteristics/patterns for each group
- 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

Clustering: Application Examples

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- 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
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earthquake epicenters should be clustered along continent faults
- Climate: understanding earth climate, find patterns of atmospheric and ocean
- Economic Science: market resarch

Basic Steps to Develop a Clustering Task

- Feature selection
  - Select info concerning the task of interest
  - Minimal information redundancy
- Proximity measure
  - Similarity of two feature vectors
- Clustering criterion
  - Expressed via a cost function or some rules
- Clustering algorithms
  - Choice of algorithms
- Validation of the results
  - Validation test (also, *clustering tendency* test)
- Interpretation of the results
  - Integration with applications

Quality: What Is Good Clustering?

- 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 the hidden patterns

Measure the Quality of Clustering

- 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"
    - The answer is typically highly subjective

Considerations for Cluster Analysis

- 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) vs. non-exclusive (e.g., one document may belong to more than one class)
- Similarity measure
  - Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- Clustering space
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

Requirements and Challenges

- Scalability
  - Clustering all the data instead of only on samples
- Ability to deal with different types of attributes
  - Numerical, binary, categorical, ordinal, linked, and mixture of these
- Constraint-based clustering
  - User may give inputs on constraints
  - Use domain knowledge to determine input parameters
- Interpretability and usability
- Others
  - Discovery of clusters with arbitrary shape
  - Ability to deal with noisy data
  - Incremental clustering and insensitivity to input order
  - High dimensionality

Major Clustering Approaches (I)

- 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 (Partitioning Around Medoids PAM) , CLARA (Clustering LARge Applications) CLARANS(Clustering Large Applications based upon RANdomized Search)

Major Clustering Approaches (II)

- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Typical methods: DIANA (DIvisive ANAlysis), AGNES (AGglomerative NESting), BIRCH(Balanced Iterative Reducing and Clustering using Hierarchies), CAMELEON(Multiphase Hierarchical Clustering Using Dynamic Modeling)
- Density-based approach:
  - Based on connectivity and density functions
- Typical methods: DBSCAN(Density-Based Spatial Clustering of Applications with Noise) , OPTICS(Ordering Points to Identify the Clustering Structure), DenClue(Clustering Based on Density Distribution Functions

Major Clustering Approaches (III)

- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE

Major Clustering Approaches (IV)

- Model-based:
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: EM, SOM, COBWEB
- Frequent pattern-based:
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- User-guided or constraint-based:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), constrained clustering
- Link-based clustering:
  - Objects are often linked together in various ways
  - Massive links can be used to cluster objects: SimRank, LinkClus

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Partitioning Algorithms: Basic Concept

- 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)

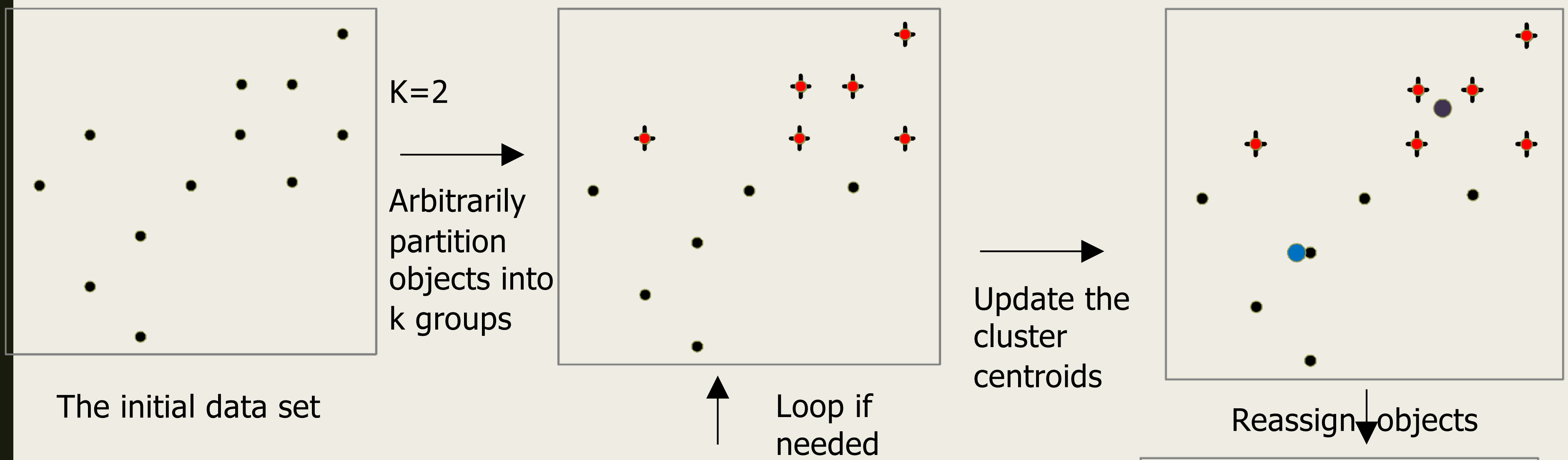
$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (d(p, c_i))^2$$

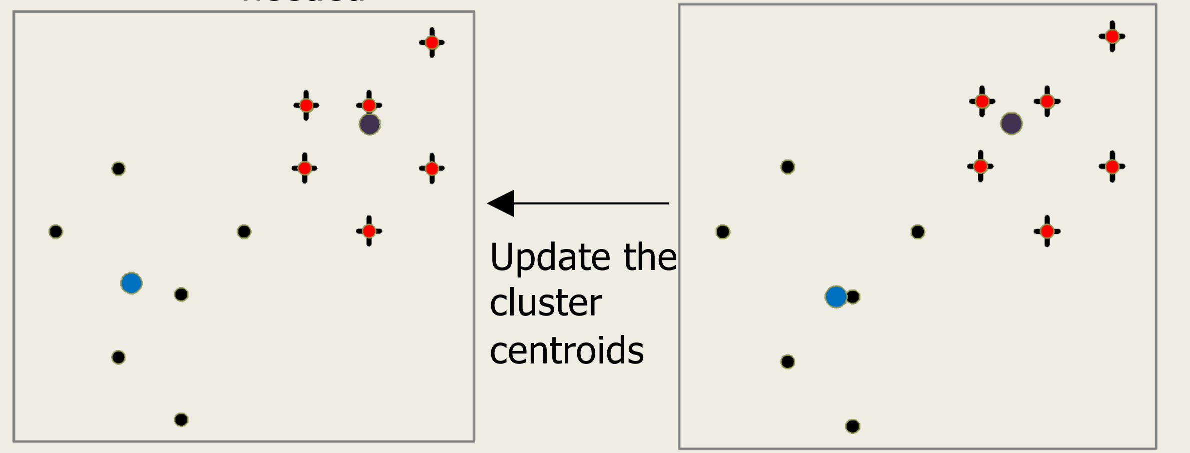
- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of 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

- 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

- <u>Strength:</u> *Efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, $t << n$.
    - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- <u>Comment:</u> Often terminates at a *local optimal*
- <u>Weakness</u>
  - Applicable only to objects in a continuous n-dimensional space
    - Using the k-modes method for categorical data
    - 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*

Validity of clusters

- Why validity of clusters?
  - *Given some data, any clustering algorithm generates clusters*
  - *So, we need to make sure the clustering results are valid and meaningful.*
- Measuring the validity of clustering results usually involve
  - *Optimality of clusters*
  - *Verification of meaning of clusters*

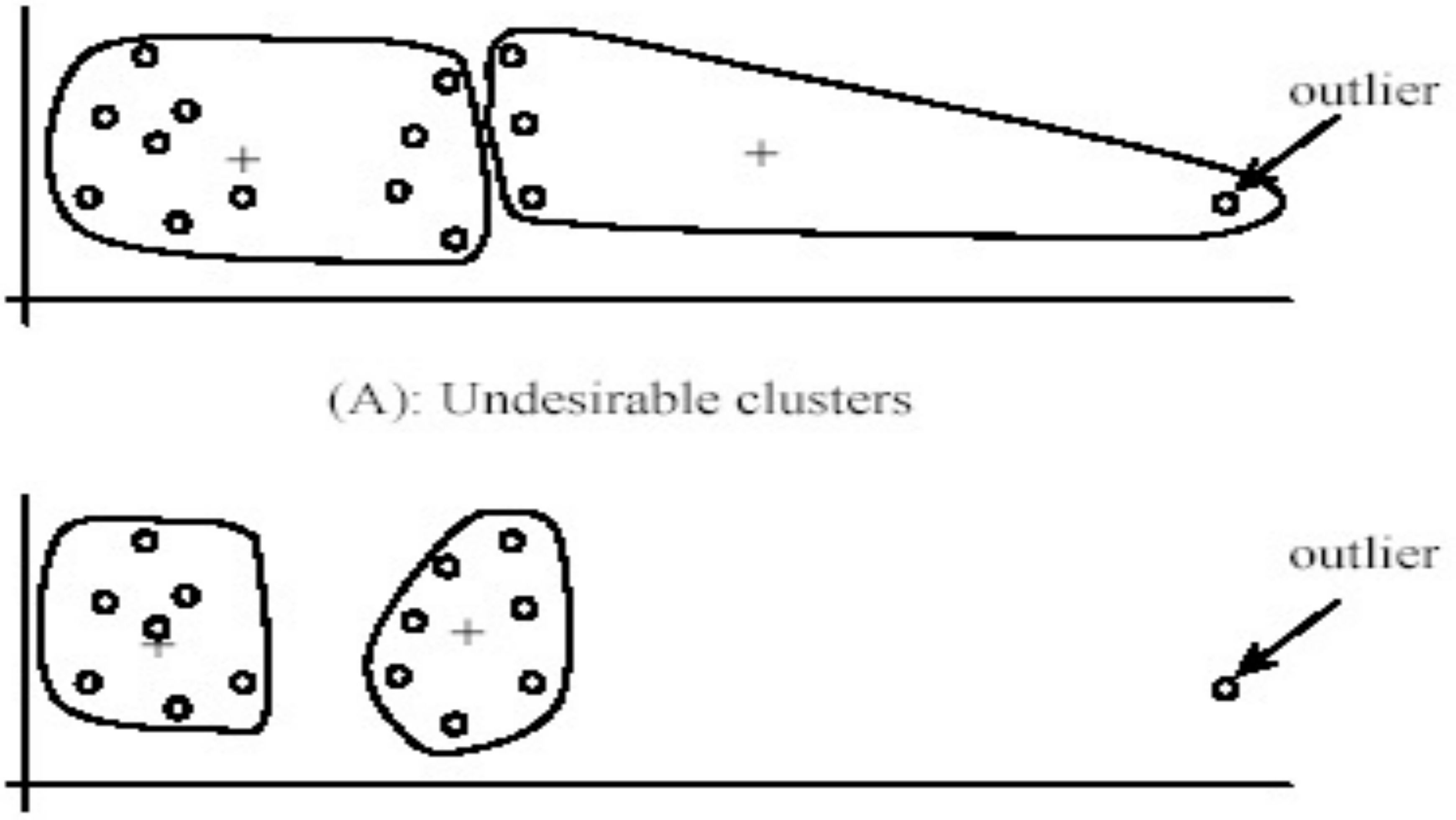
Optimality of clusters

- Optimal clusters should
  - *minimize distance **within** clusters (intracluster)*
  - *maximize distance **between** clusters (intercluster)*
- Example of intracluster measure
  - Squared error *se*

    where m_i is the mean of all instances in cluster c_i

$$\boxed{se = \sum_{i=1}^{k} \sum_{p \in c_i} \| p - m_i \|^2}$$

Weaknesses of k-means: Problems with outliers

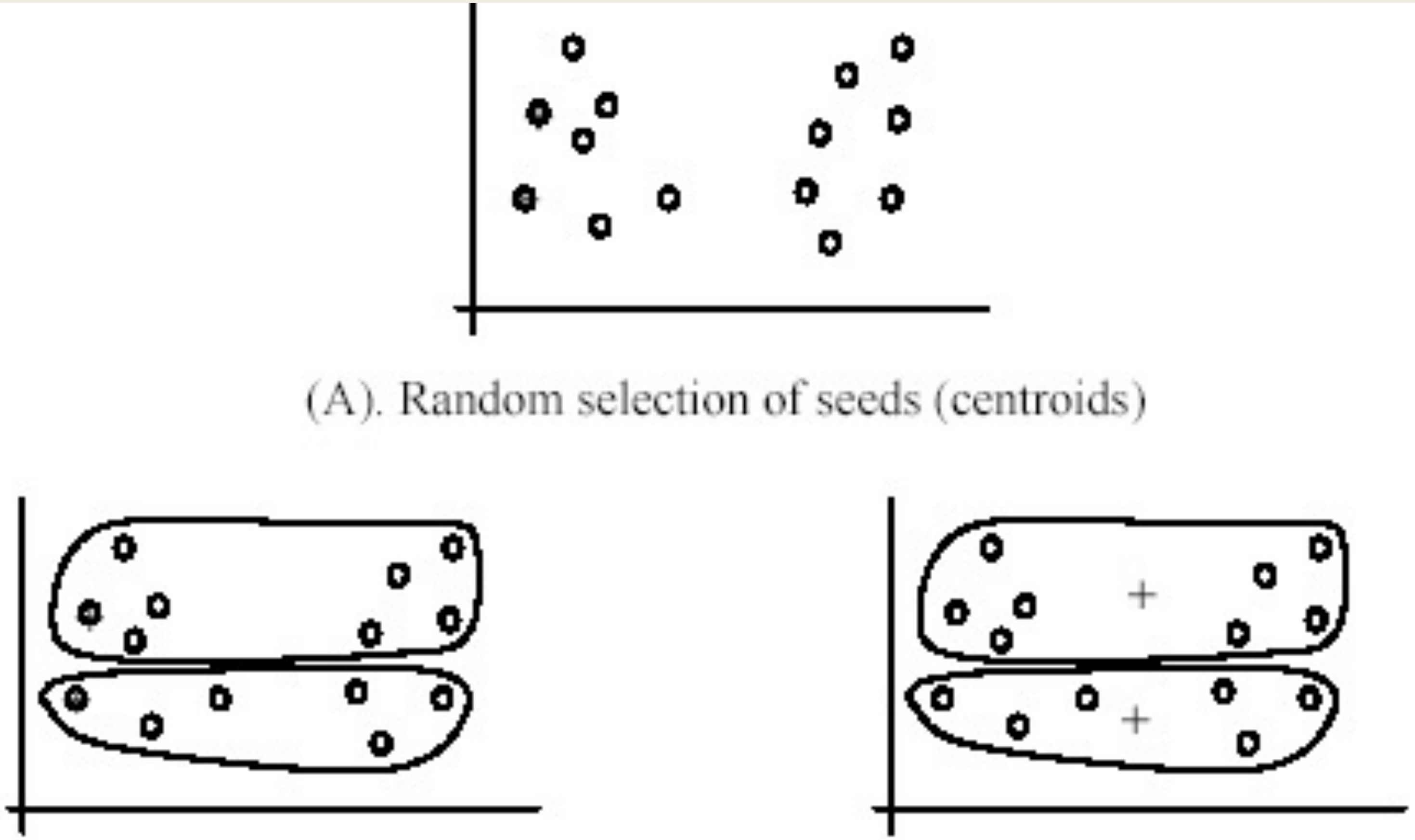


(A): Undesirable clusters

(B): Ideal clusters

Weaknesses of k-means (cont …)

- The algorithm is sensitive to initial seeds.



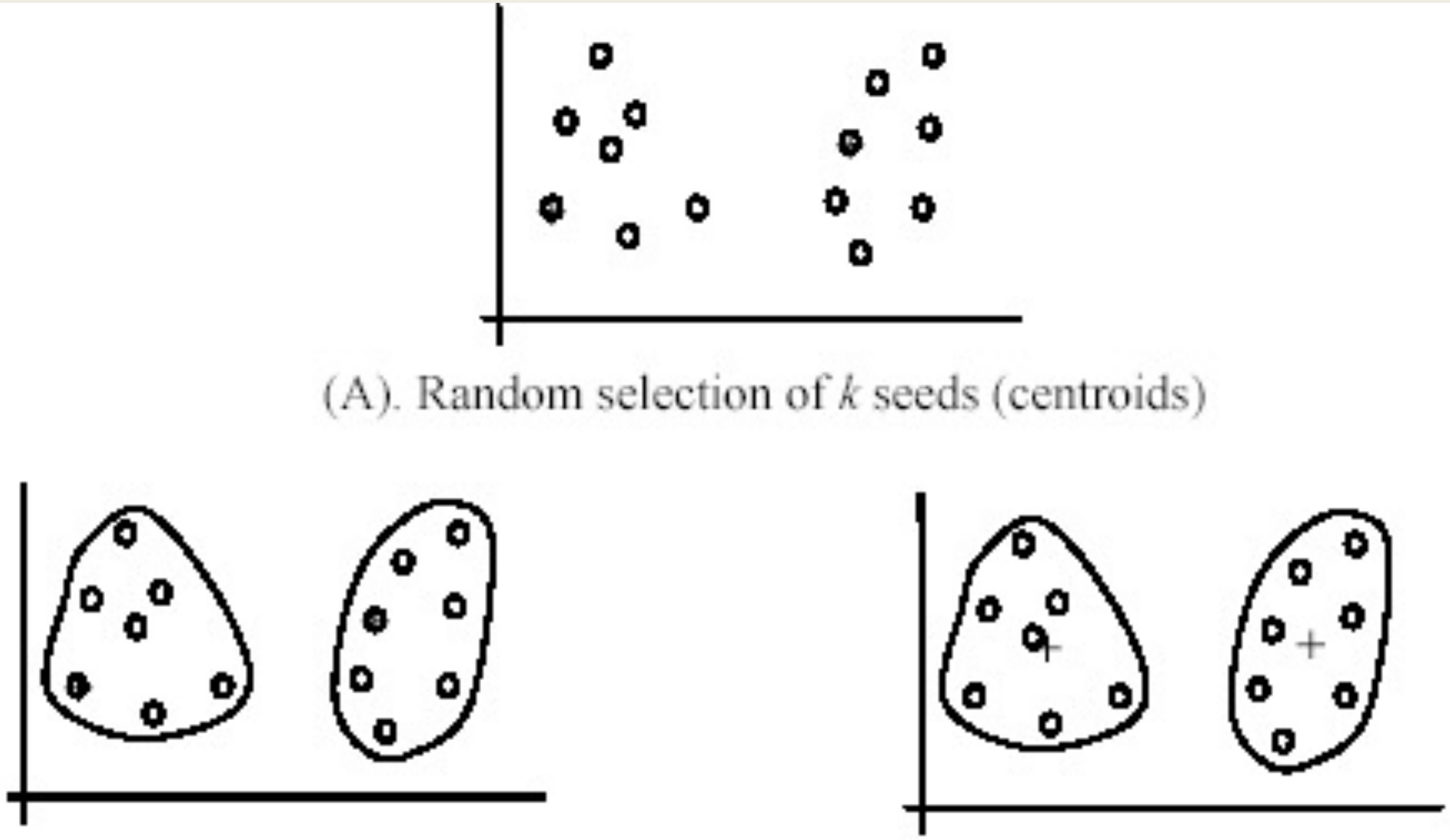
(A). Random selection of seeds (centroids)

(B). Iteration 1

(C). Iteration 2

Weaknesses of k-means (cont ...)

- If we use different seeds: good results



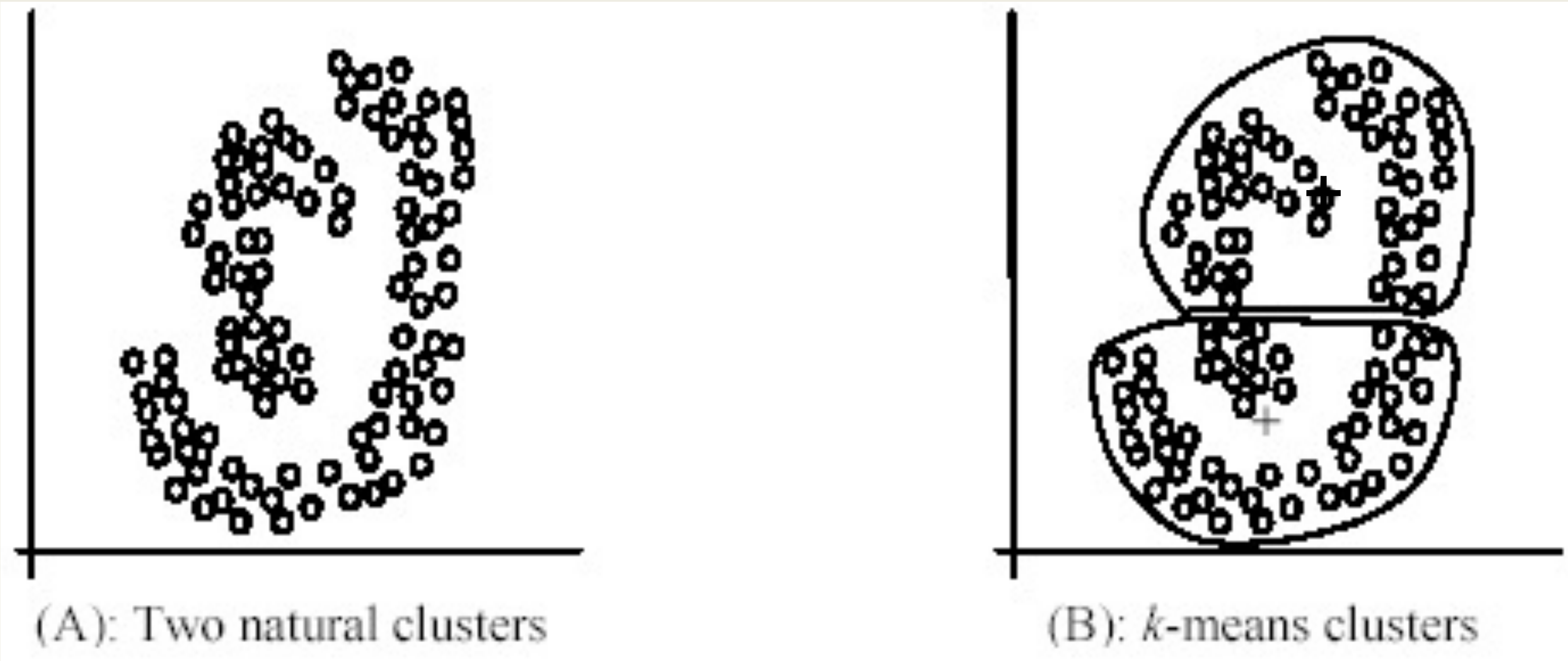
(A). Random selection of *k* seeds (centroids)

(B). Iteration 1

(C). Iteration 2

Weaknesses of k-means (cont …)

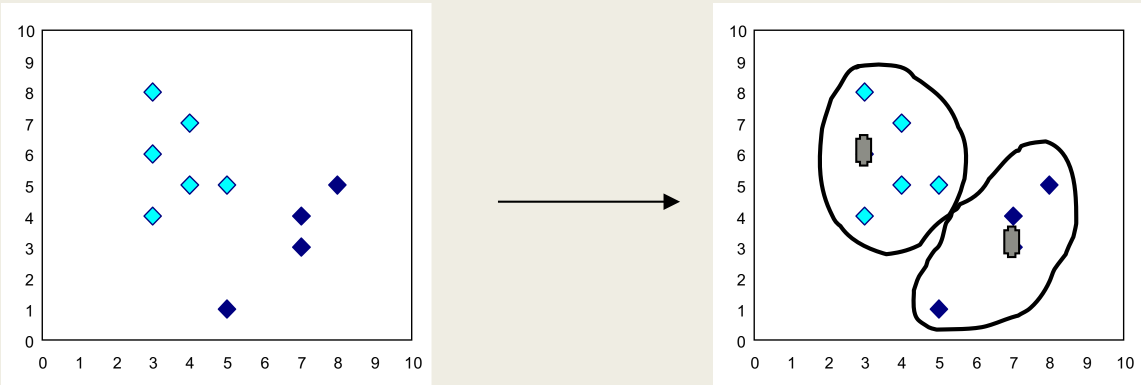
- The *k*-means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).



What is the problem of 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.



Termination conditions

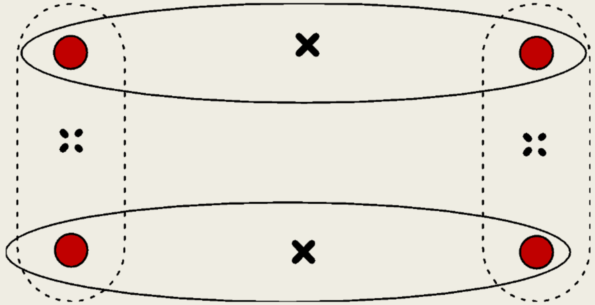
- Several possibilities, e.g.,
  - *A fixed number of iterations.*
  - *Cluster partition unchanged.*
  - *Centroid positions don't change.*

K-means: summary

- Algorithmically, very simple to implement
- *K*-means converges, but it finds a local minimum of the cost function
- Works only for numerical observations
- *K* is a user input;
- Outliers can be considerable trouble to *K*-means

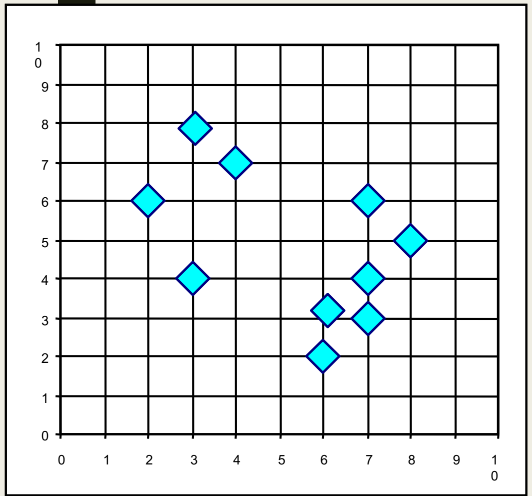
Variations of the *K-Means* Method

- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means



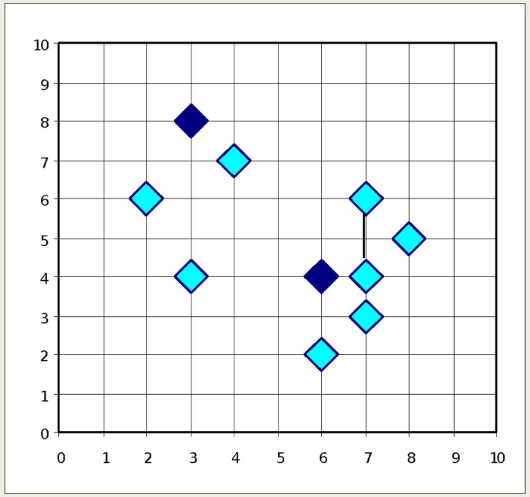
- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

PAM: A Typical K-Medoids Algorithm



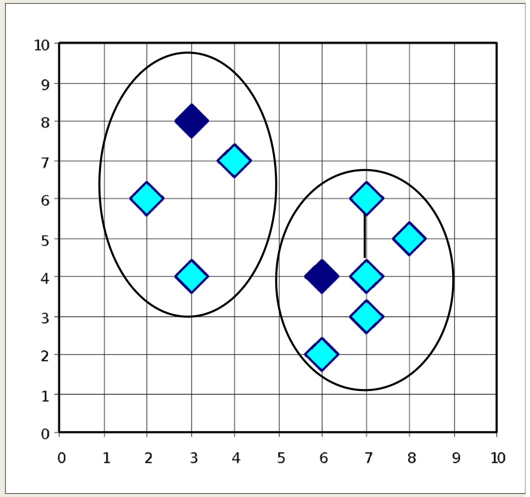
K=2

Arbitrary choose k object as initial medoids

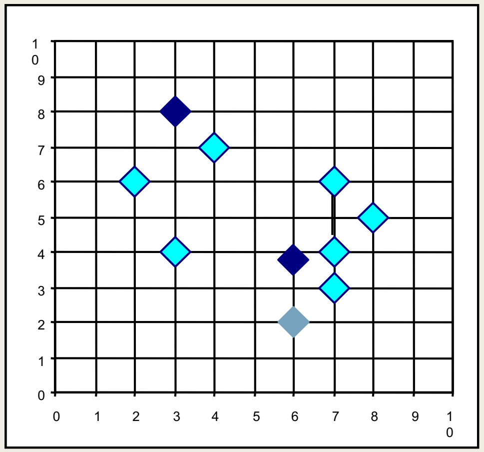


Assign each remaining object to nearest medoids

Total Cost = 20

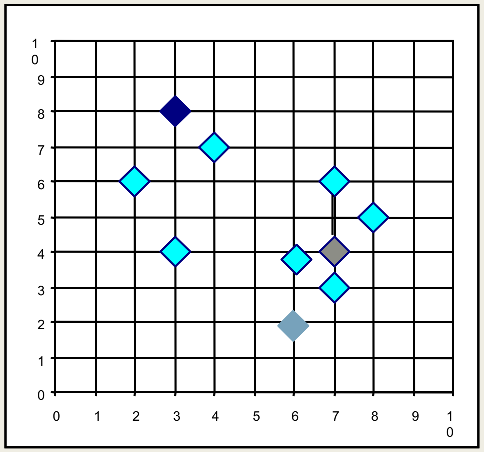


Randomly select a nonmedoid object, O_{ramdom}



Compute total cost of swapping

Total Cost = 26



Swapping O and O_{ramdom}

If quality is improved.

Do loop

Until no change