Chapter 10. Cluster Analysis: Basic Concepts and Methods

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

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_k is the centroid or medoid of cluster C_k)

$$SSE = \sum_k \sum_{x_i \in C_k} ||x_i - C_k||^2$$

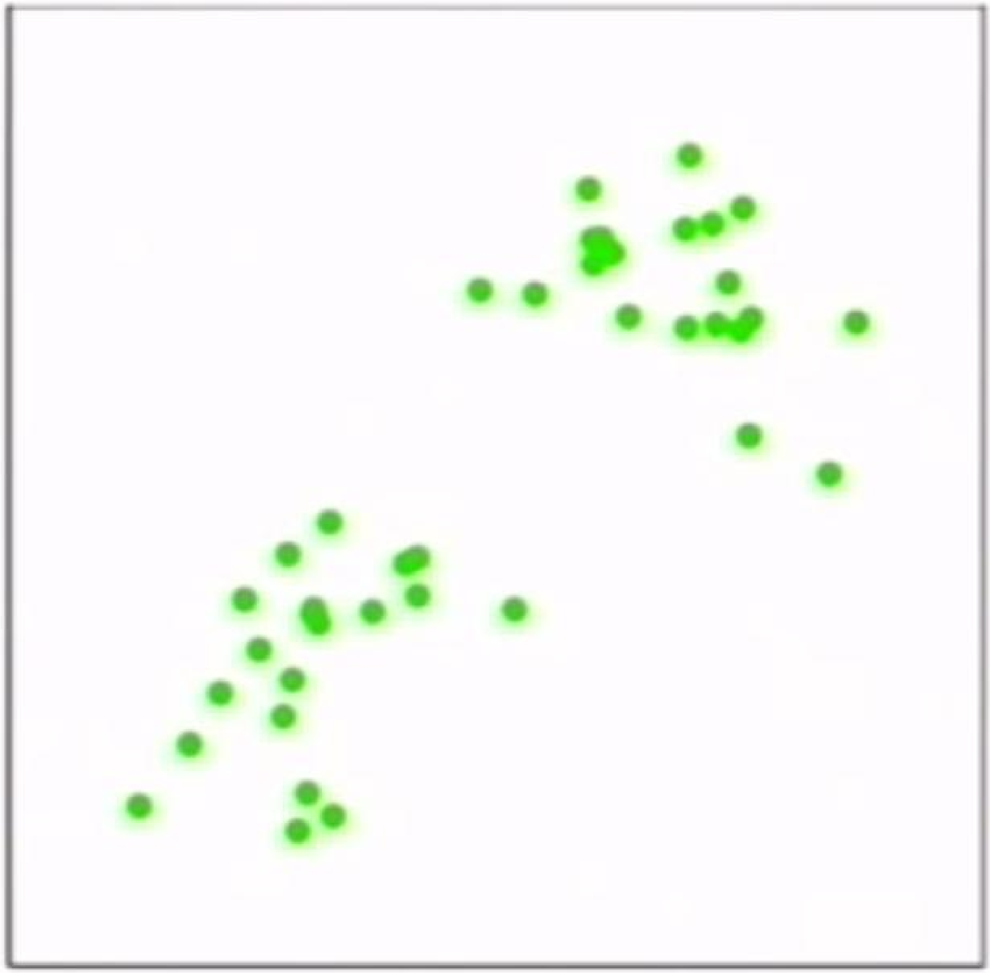
- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids)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

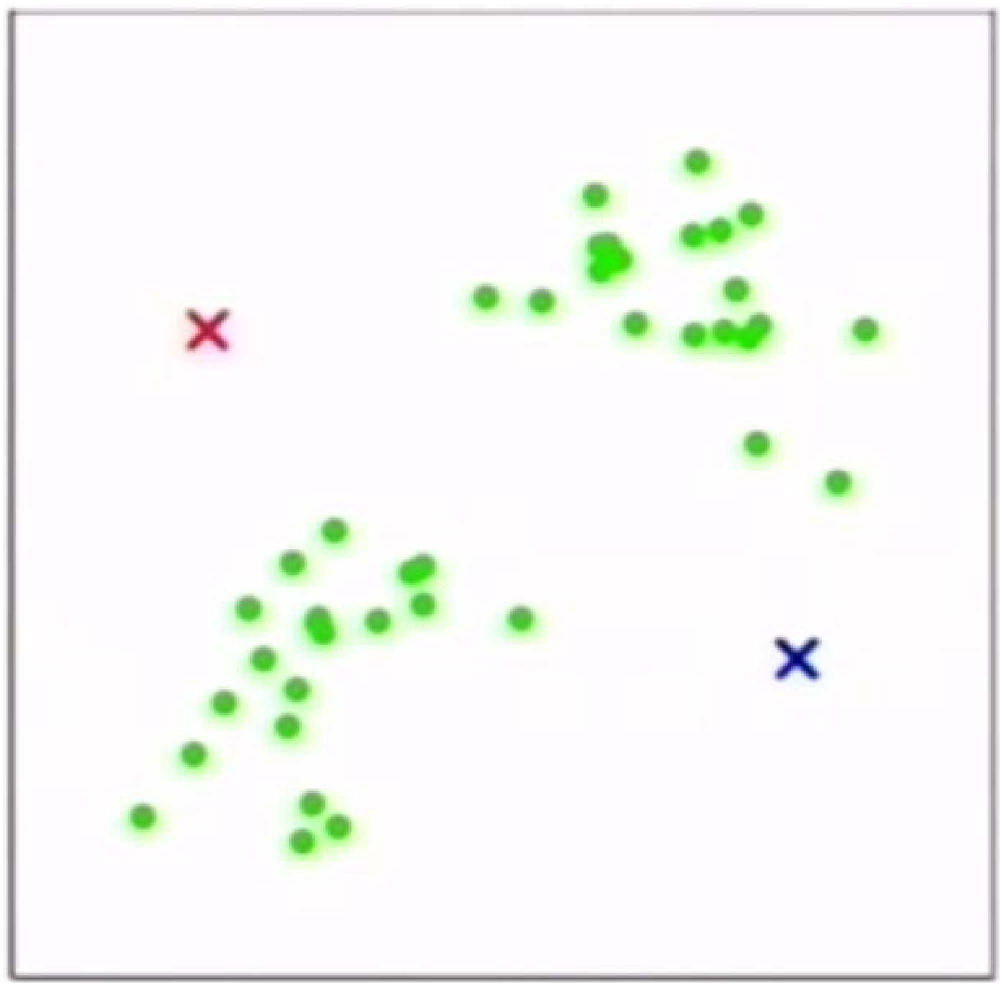
The *K-Means* Clustering Method

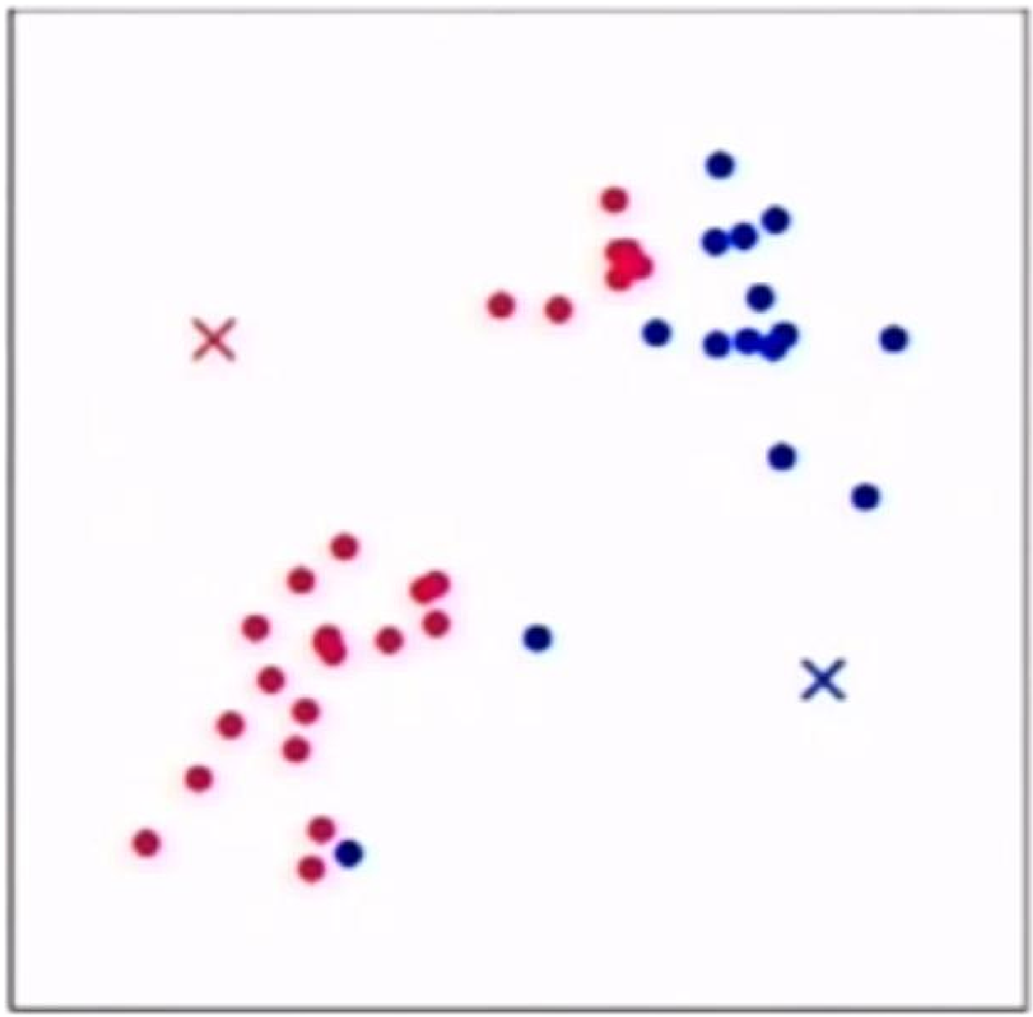
Inputs: The initial data set & *k* : number of clusters

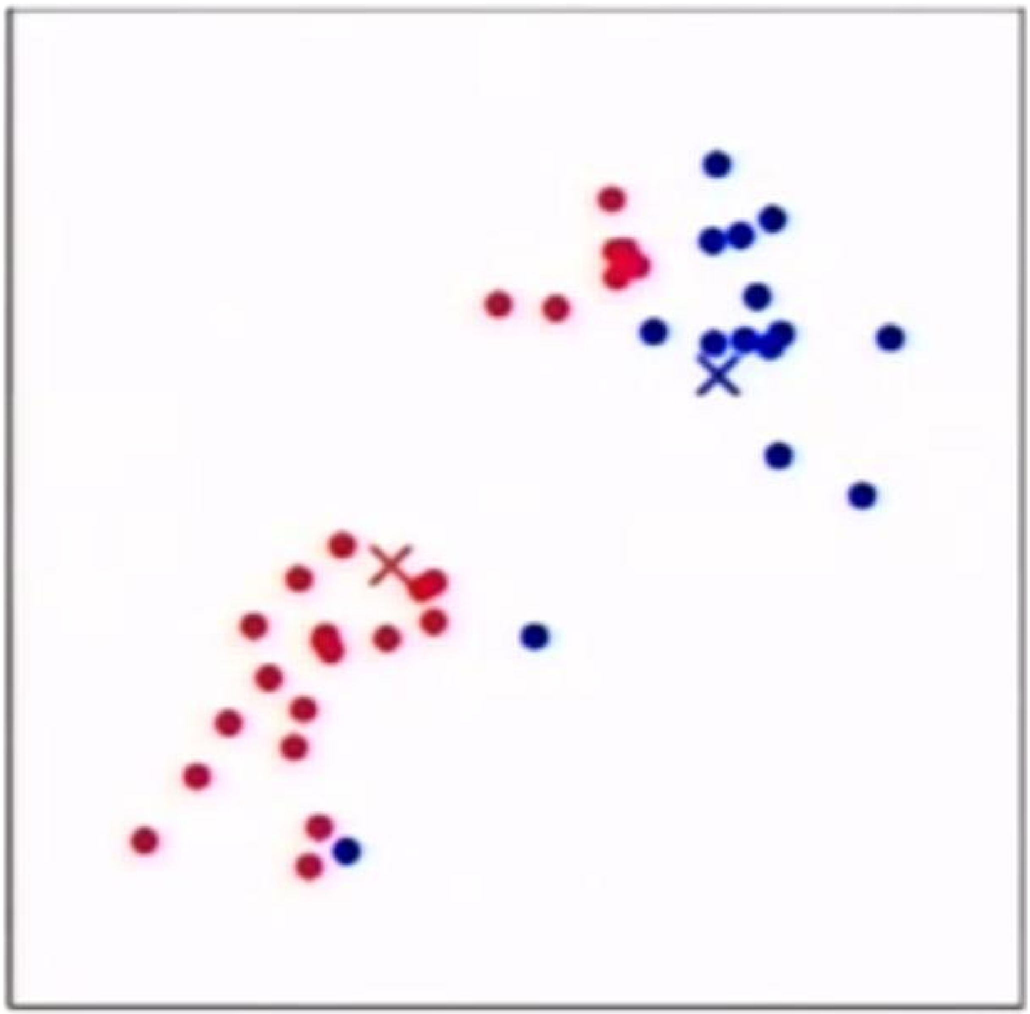
- Initialize *k* random centroids
- Repeat
  - Assign each object to the cluster of its nearest centroid
  - Compute centroid (i.e., mean point) for each partition
- Until no change

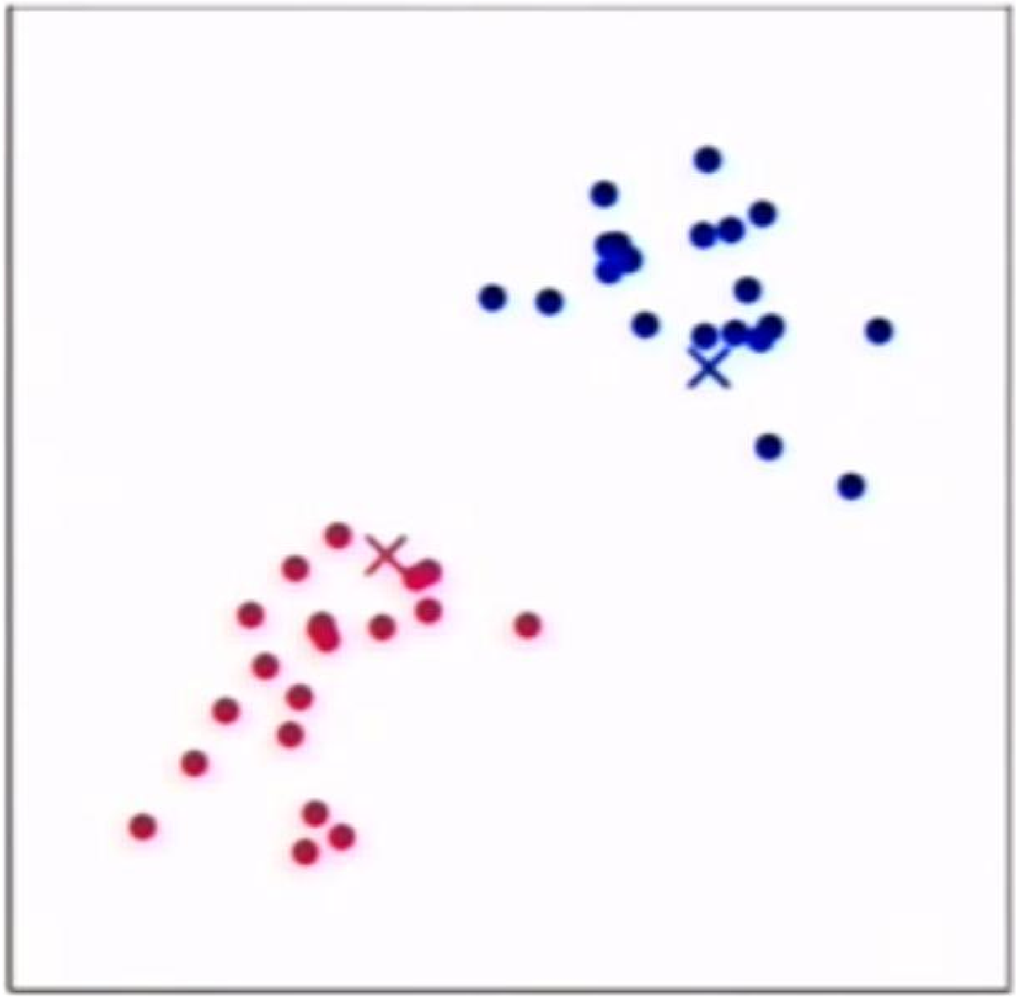
K-Means Clustering Example

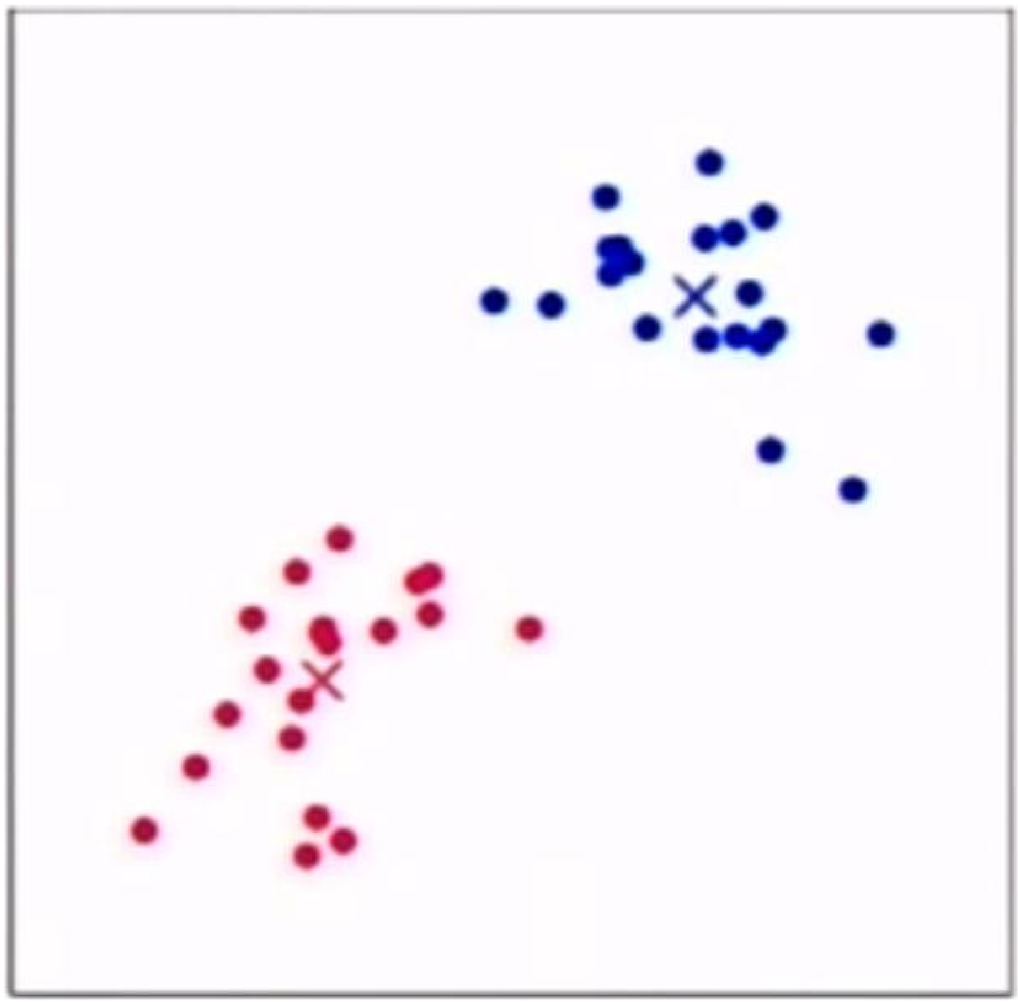






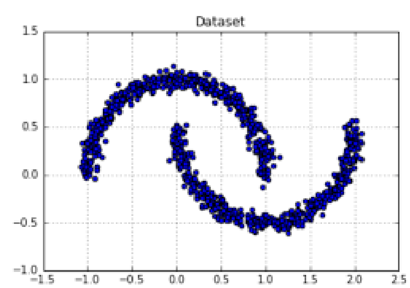






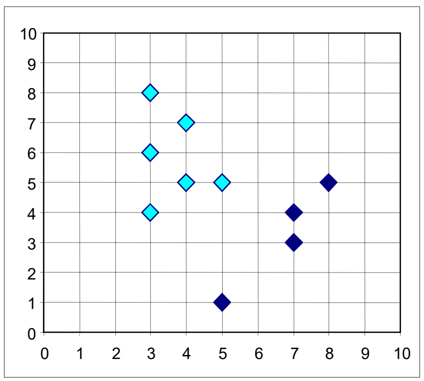
Comments on the *K-Means* Method

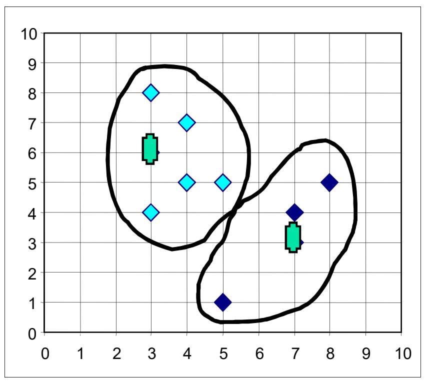
- <u>Strength:</u> *Efficient*: *O*(*tkn*), where *n* is # objects, *k* is # clusters, and *t* is # iterations. Normally, *k*, *t* << *n*.
- <u>Comment:</u> Often terminates at a *local optimal*.
- <u>Weakness</u>
  - Applicable only to objects in a continuous n-dimensional space
    - Using the k-modes 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*



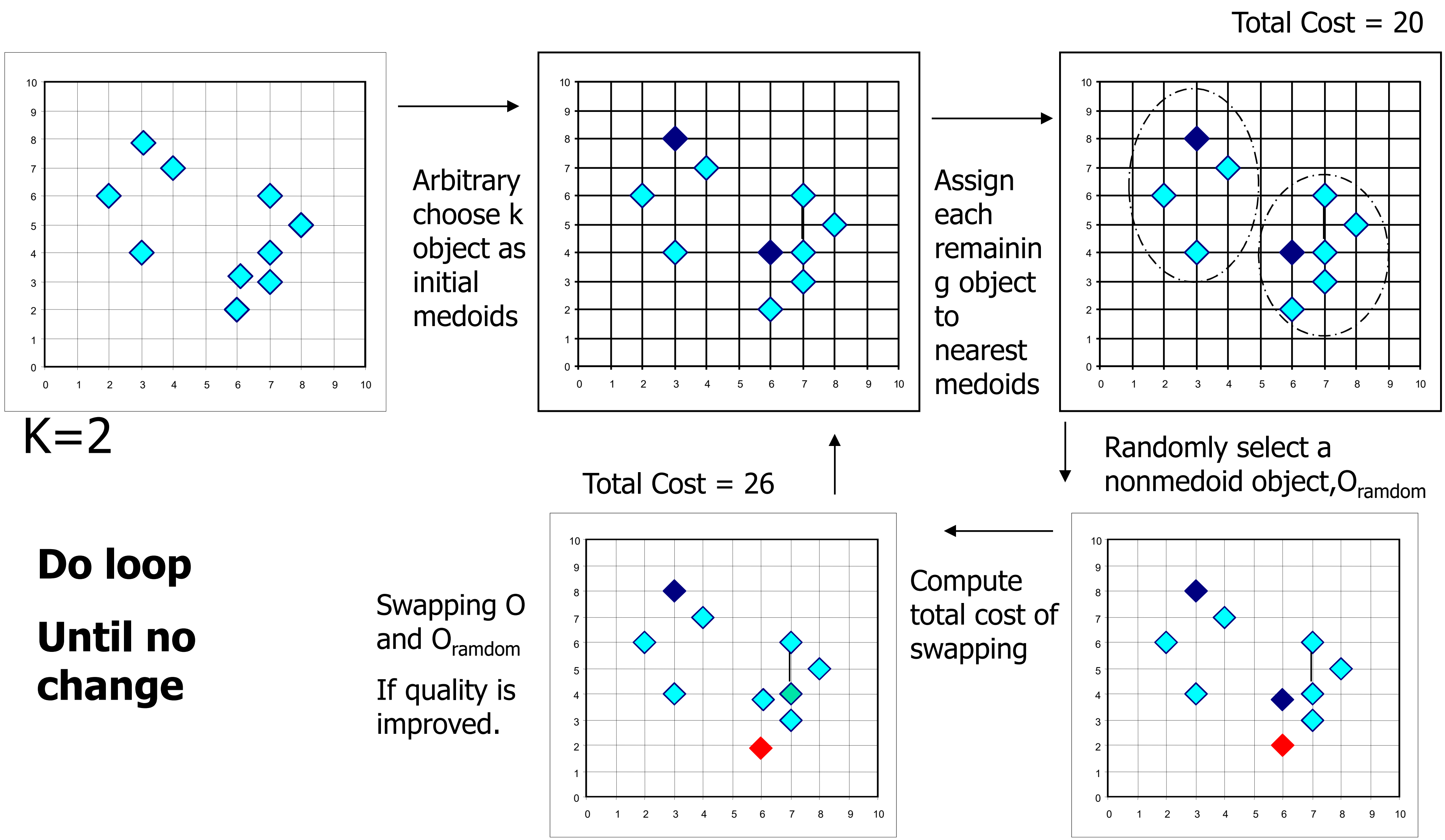
What Is the Problem of the K-Means Method?

- 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



The K-Medoid Clustering Method

- *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
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling

Number of Clusters

- The Elbow method