Clustering Analysis

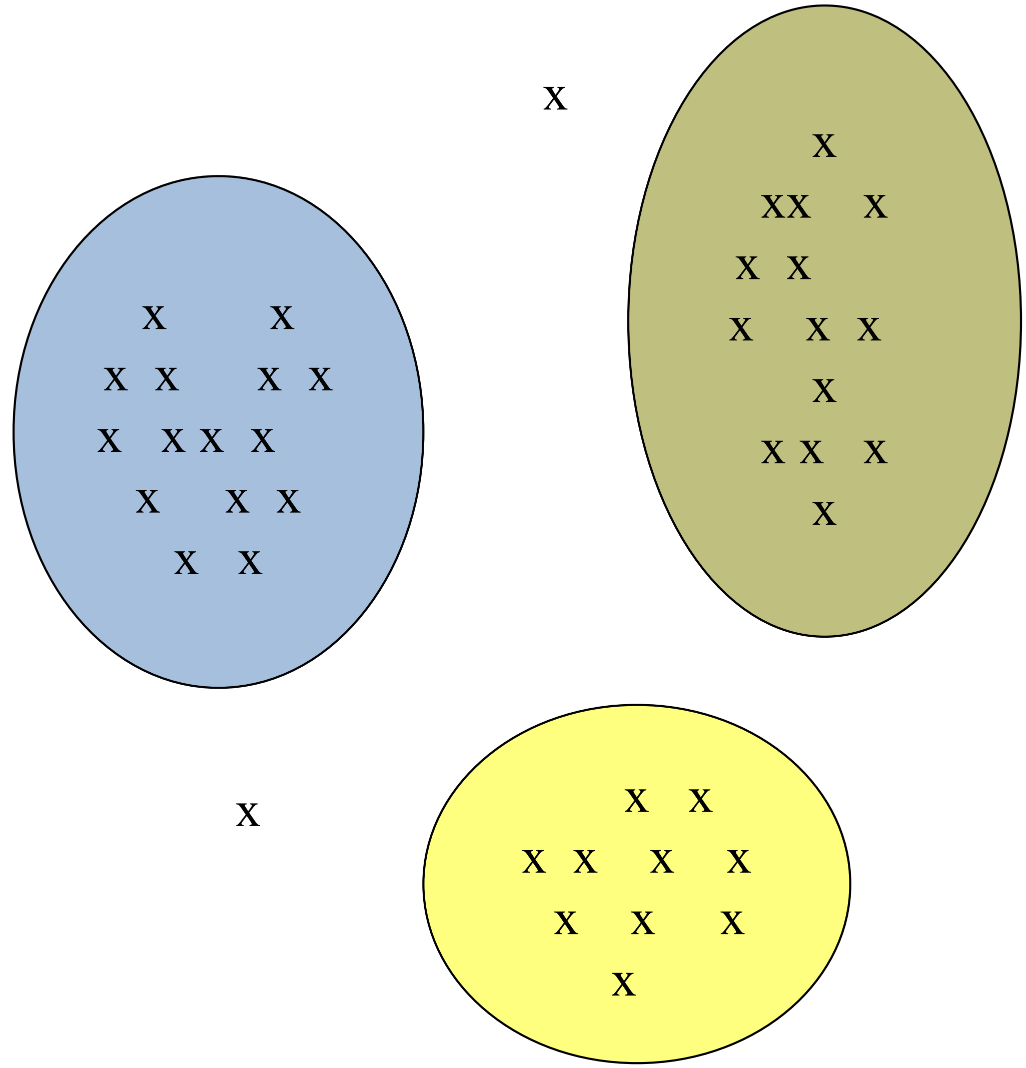
Outline

- What is clustering analysis?
- Types of data in clustering analysis
- A categorization of major clustering methods
  - Partitioning methods
  - Hierarchical methods
  - Model-based clustering methods
- Outlier analysis
- Summary

What Is Clustering Analysis?

- Clustering: a collection of data objects.
  - Similar to one another within the same cluster.
  - Dissimilar to the objects in other clusters.
- Clustering analysis.
  - Grouping a set of data objects into clusters, such that objects within each cluster are similar to each other, objects in different clusters are dissimilar to each other.
- Clustering is unsupervised classification:
  - Objects are not labeled with predefined classes.
  - Different from supervised classification where each training data is labeled with class information

An Example



Problems With Clustering

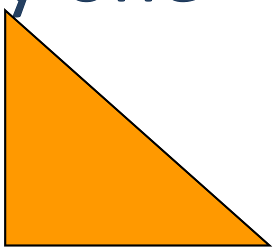
- Clustering in two dimensions looks easy.
- Clustering small amounts of data looks easy.
- And in most cases, looks are *not* deceiving.

The Curse of Dimensionality

- Many applications involve not 2, but 10 or 10,000 dimensions.
- High-dimensional spaces look different: almost all pairs of points are at about the same distance.

Example: Curse of Dimensionality

- Assume random points within a bounding box, e.g., values between 0 and 1 in each dimension.
- In 2 dimensions: a variety of distances between 0 and 1.41.
- In 10,000 dimensions, the difference in any one dimension is distributed as a triangle.



- Actual distance between two random points is the sqrt of the sum of squares of essentially the same set of differences.

General Applications

- Typical applications.
  - As a stand-alone tool to get insight into data distribution.
  - As a preprocessing step for other algorithms.
- (Spatial) data analysis
- Image processing
- Economic science (especially market research)
- WWW
  - Automatic document categorization
  - Web usage mining: cluster web log data to discover groups of similar access patterns
- Business : customer groups
- Biology: animal and plant taxonomy, Categorize genes by functionality

High-Dimension Application: SkyCat

- A catalog of 2 billion “sky objects” represents objects by their radiation in 7 dimensions (frequency bands).
- Problem: cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Sky Survey is a newer, better version.

Clustering CD’s (Collaborative Filtering)

- Intuitively: music divides into categories, and customers prefer a few categories.
  - But what are categories really?
- Represent a CD by the customers who bought it.
- Similar CD’s have similar sets of customers, and vice-versa.

The Space of CD’s

- Think of a space with one dimension for each customer.
  - Values in a dimension may be 0 or 1 only.
- A CD’s point in this space is $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ *iff* the i^{th} customer bought the CD.
  - Compare with boolean matrix: rows = customers; cols. = CD’s.
- For Amazon, the dimension count is tens of millions.

Clustering Documents

- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ *iff* the i^{th} word (in some order) appears in the document.
  – It actually doesn't matter if k is infinite; i.e., we don't limit the set of words.
- Documents with similar sets of words may be about the same topic.

Example: DNA Sequences

- Objects are sequences of {C,A,T,G}.
- Distance between sequences is *edit distance*, the minimum number of inserts and deletes needed to turn one into the other.

What Is Good Clustering?

- A good clustering method will produce high quality clusters with.
  - High intra-class similarity.
  - Low inter-class similarity.
- The quality of a clustering result depends on both the similarity measure used by the method and its clustering approach used.
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

Requirements of Clustering in Data Mining

- Scalability
- Ability to deal with different types of attributes
- Discovery of clusters with arbitrary shape
- Minimal requirements for domain knowledge to determine input parameters
- Able to deal with noise and outliers
- Insensitive to order of input records
- High dimensionality
- Interpretability and usability

Data Structures

- Data matrix

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

Measure the Quality of Clustering

- Dissimilarity/similarity metric: dissimilarity is expressed in terms of a distance function, which is typically metric: d(i, j).
- The definitions of distance functions are usually very different for interval-scaled, boolean, categorical, ordinal variables, and temporal data.
- Weights should be associated with different variables based on applications and data semantics.
- There is a separate "quality" function that measures the "goodness" of a cluster.

Type of Data in Clustering Analysis

- Interval-scaled variables
- Binary variables
- Nominal, and ordinal variables
- Variables of mixed types
- Text
- Temporal

Major Clustering Approaches

- Partitioning algorithms: Construct various partitions and then evaluate them by some criterion
- Hierarchy algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

Partitioning Algorithms: Basic Concept

- Partitioning method: Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters
- Given a *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): 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

- **Objective**: to form a set of clusters that are as compact and separated as possible
- **Distance Measure**: Euclidean distance between data object and cluster center
- **Clustering criterion function**:

  mean squared error (MSE)

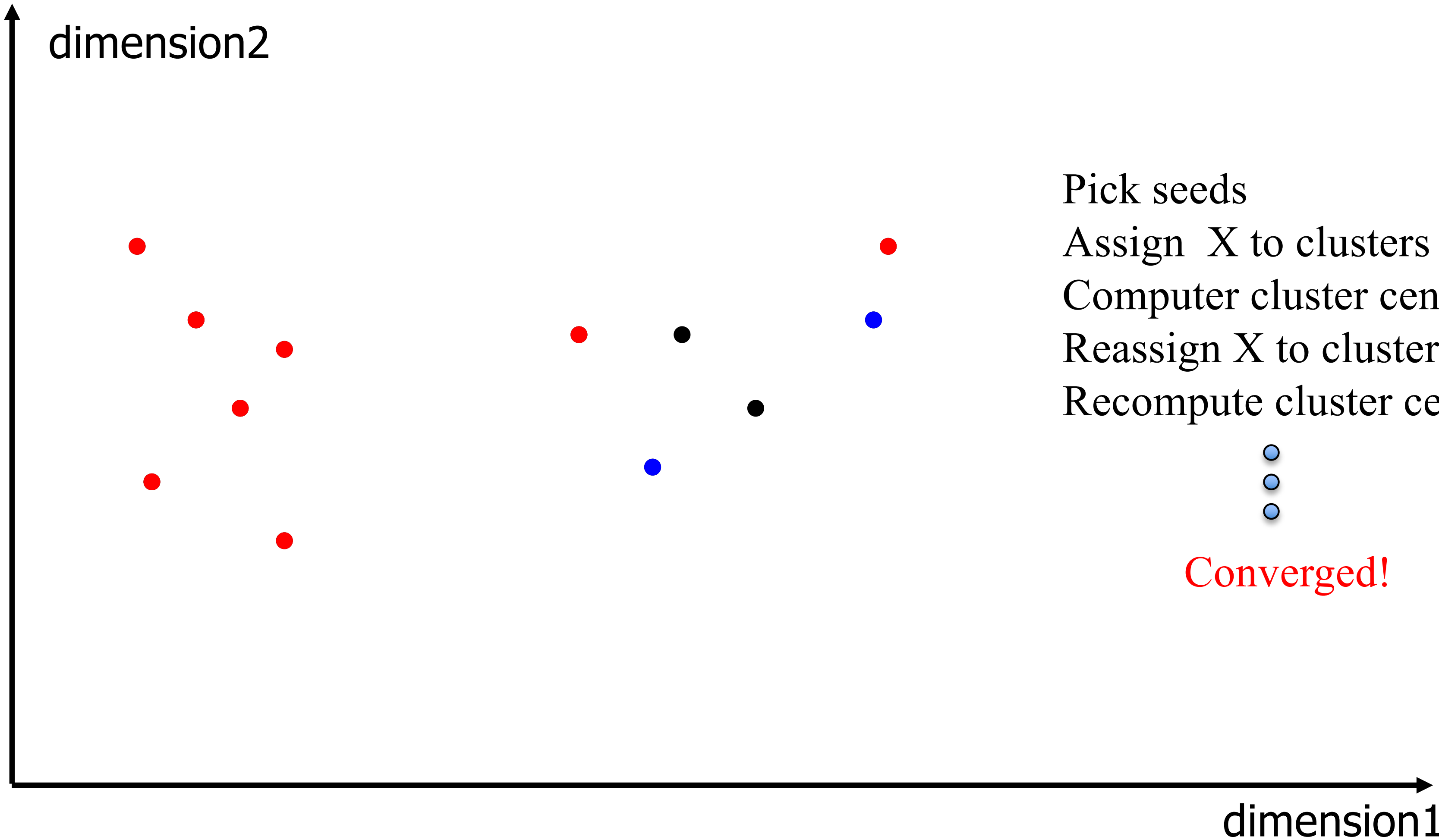
$$MSE = \sum_{i=1}^{k} \sum_{p \subseteq C_i} | x - m_i |^2$$

x: a data object
C_i: cluster i
m_i: center of cluster i
k: number of clusters

The *K-Means* Clustering Method

- **Approach**: Given *k*, the *k-means* algorithm is implemented as the following:
  - arbitrarily choose *K* objects as the initial cluster centers.
  - Repeat:
    - **Compute seed points as the centroids of the clusters of the current partition. The centroid is the center (mean point) of the cluster.**
    - **Assign each object to the cluster with the nearest seed point.**
  - stop when no more new assignment, or when clustering criterion function (mean squared error) converges.

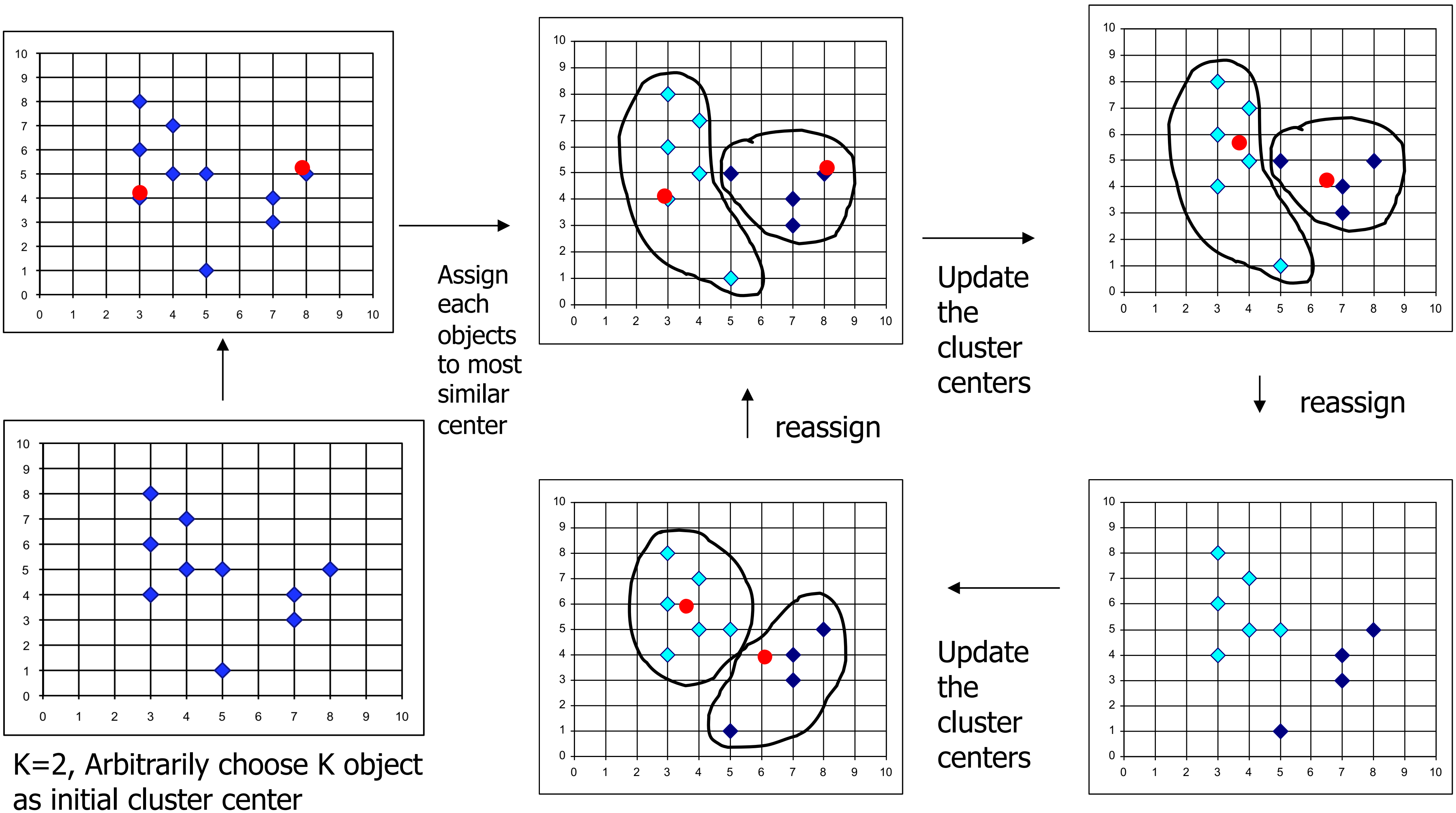
K Means Example (*K*=2)



Pick seeds
Assign X to clusters
Computer cluster centroids
Reassign X to clusters
Recompute cluster centroids

Converged!

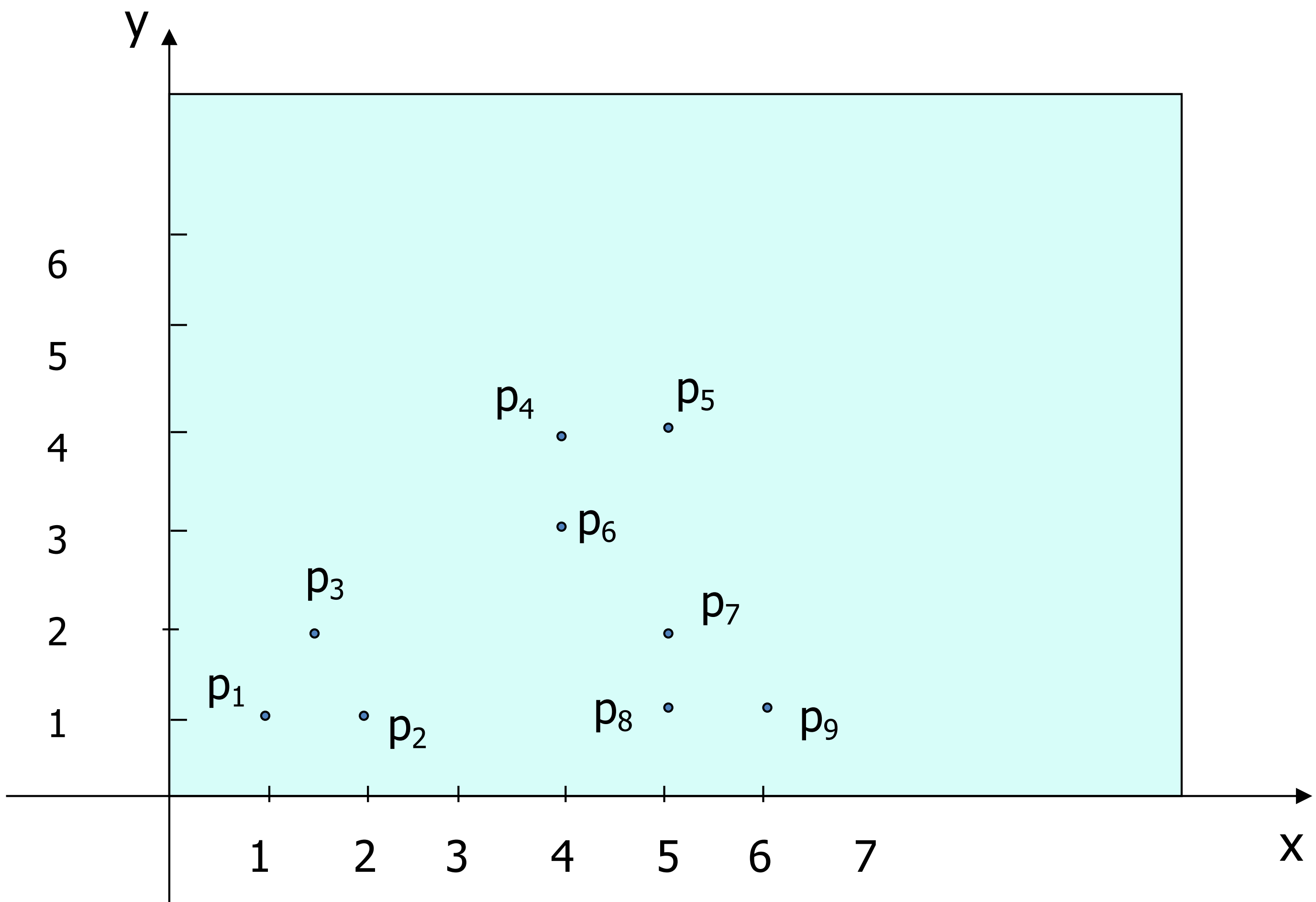
K-Means


Assign each objects to most similar center
Update the cluster centers
reassign
reassign
Update the cluster centers
K=2, Arbitrarily choose K object as initial cluster center

Practice Question

Apply K-means clustering algorithm to partition the following data with 9 data objects:

P1(1, 1)
P2(2,1)
P3(1.5,2)
P4(4, 4)
P5(5,4)
P6(4,3)
P7(5,2)
P8(5,1)
P9(6,1)



Comments on the *K-Means* Method

- <u>Strength</u>
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, $t \ll n$.
  - Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- <u>Weakness</u>
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Sensitive to initial seed selection
  - Unable to handle noisy data and *outliers*

Variations of the *K-Means* Method

- A few 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* (Huang' 98)
  - Replacing means of clusters with modes
    - Using a frequency-based method to update modes of clusters
  - Using new dissimilarity measures to deal with categorical objects
  - A mixture of categorical and numerical data: *k-prototype* method

The *K-Medoids* Clustering Method

- Find *representative* objects, called medoids, in clusters
- *PAM* (Partitioning Around Medoids, 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
- *CLARA* (Kaufmann & Rousseeuw, 1990)
- *CLARANS* (Ng & Han, 1994): Randomized sampling

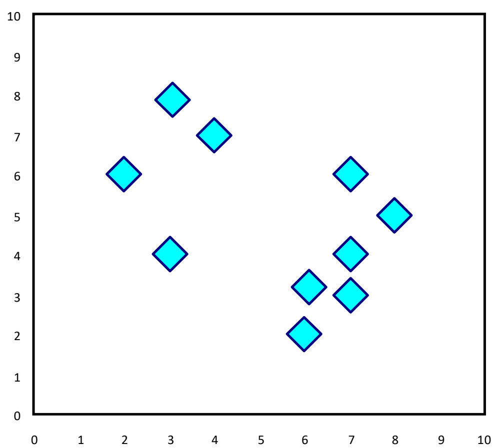
K-Medoids

- Arbitrarily choose K objects as the initial medoids;
- Repeat:
  - Assign each remaining object to the cluster with the nearest medoids;
  - Randomly select a nonmedoid object O_{random};
  - Compute the total cost, S, of swapping O_j with O_{random};
  - If $S<0$, then swap O_j with O_{random} to form the new set of k medoids;
- Until no change

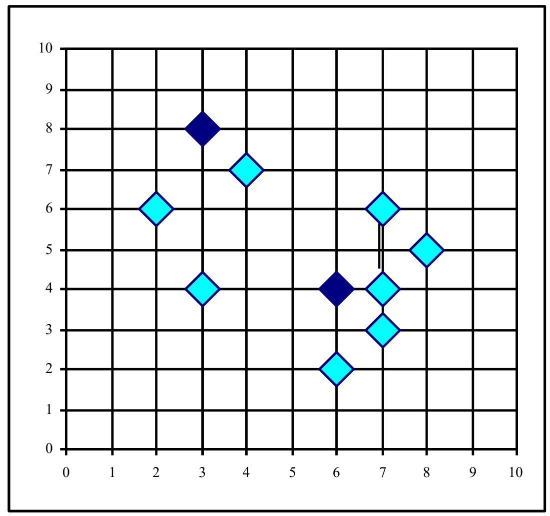
k-Medoids

Total swapping cost $TC_{ih}=\sum_{p}C_{pih}$

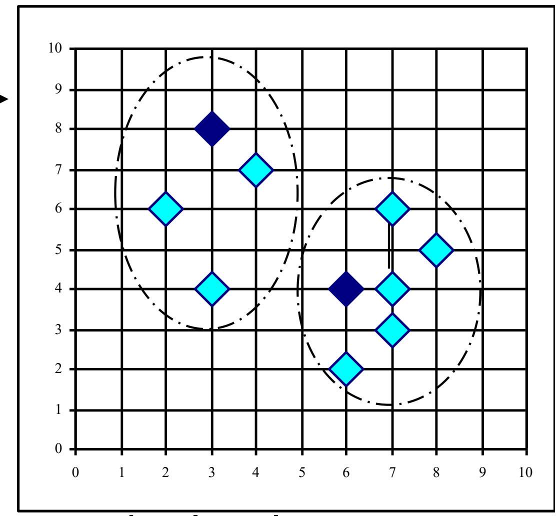
Total Cost = 20



Arbitrary choose k object as initial medoids



Assign each remaining object to nearest medoids



K=2

Total Cost = 18

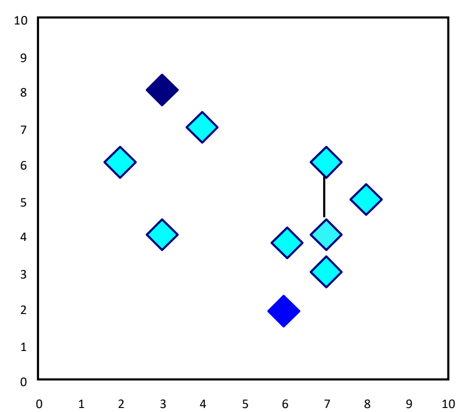
Randomly select a nonmedoid object,O_{ramdom}

Do loop

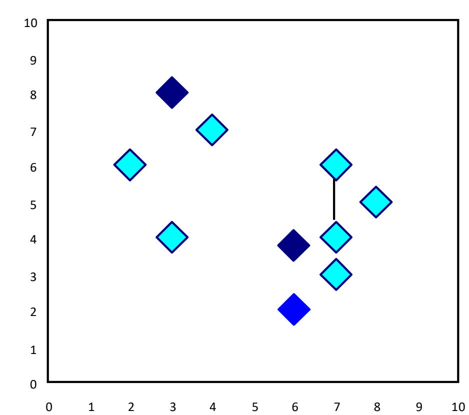
Until no change

Swapping O and O_{ramdom}

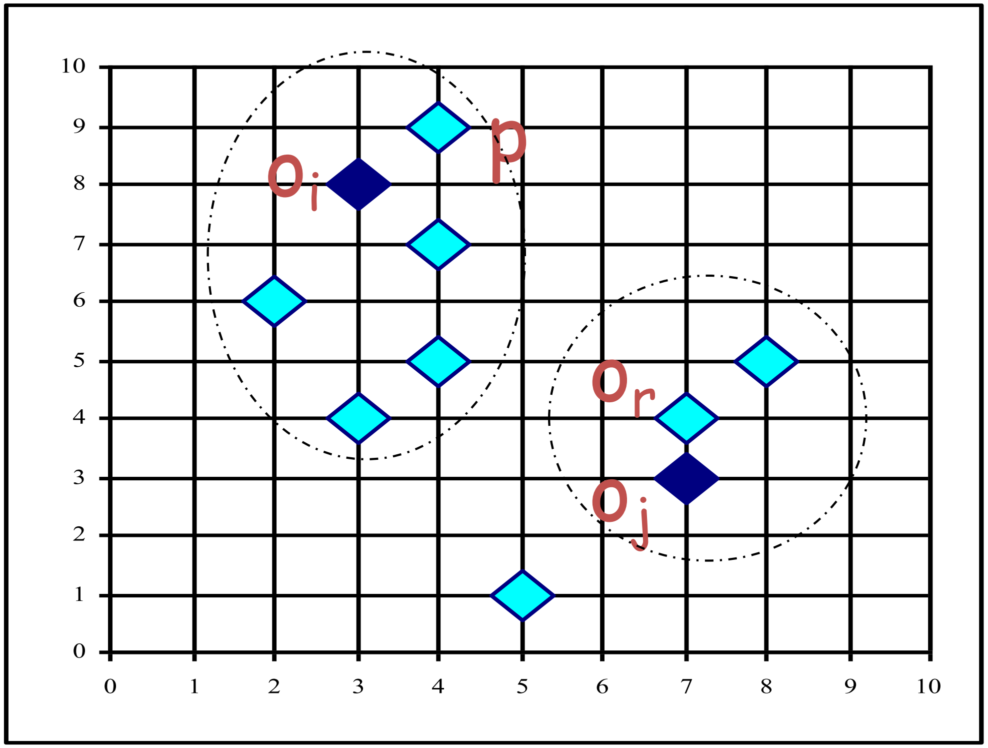
if quality is improved.



Compute total cost of swapping



Four Cases – Case A



Replace o_j with o_r

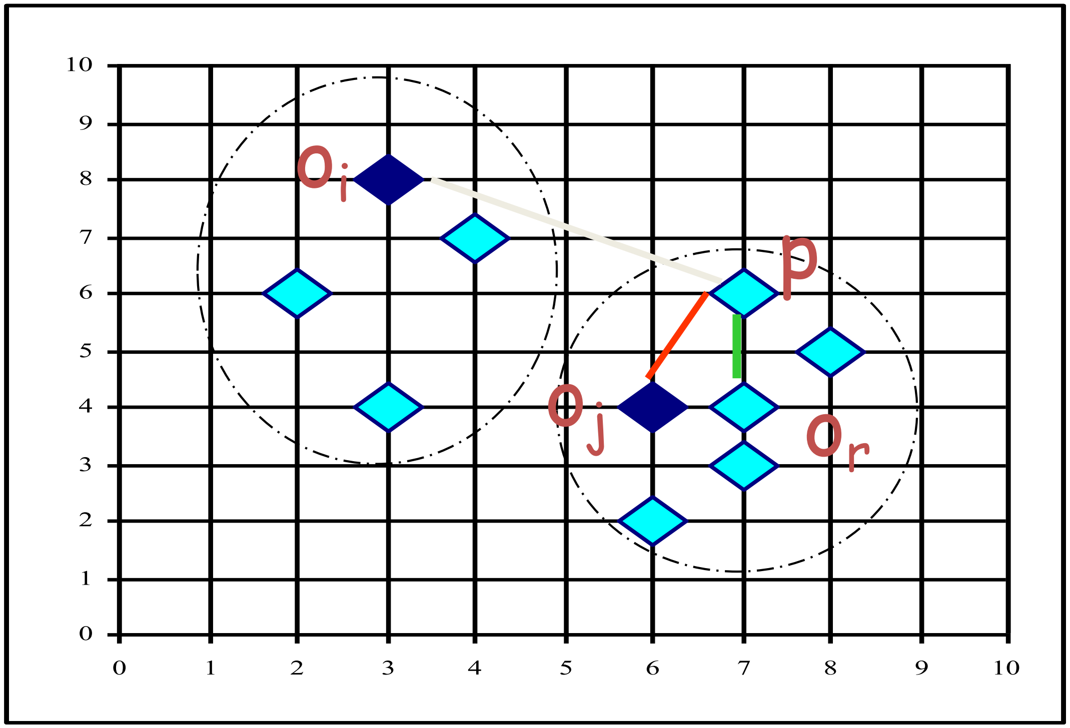
$p \in o_i$; $i \neq j$;

p still closest to o_i

no change

$$C_{p,j,r} = 0$$

Four Cases – Case B



Replace o_j with o_r

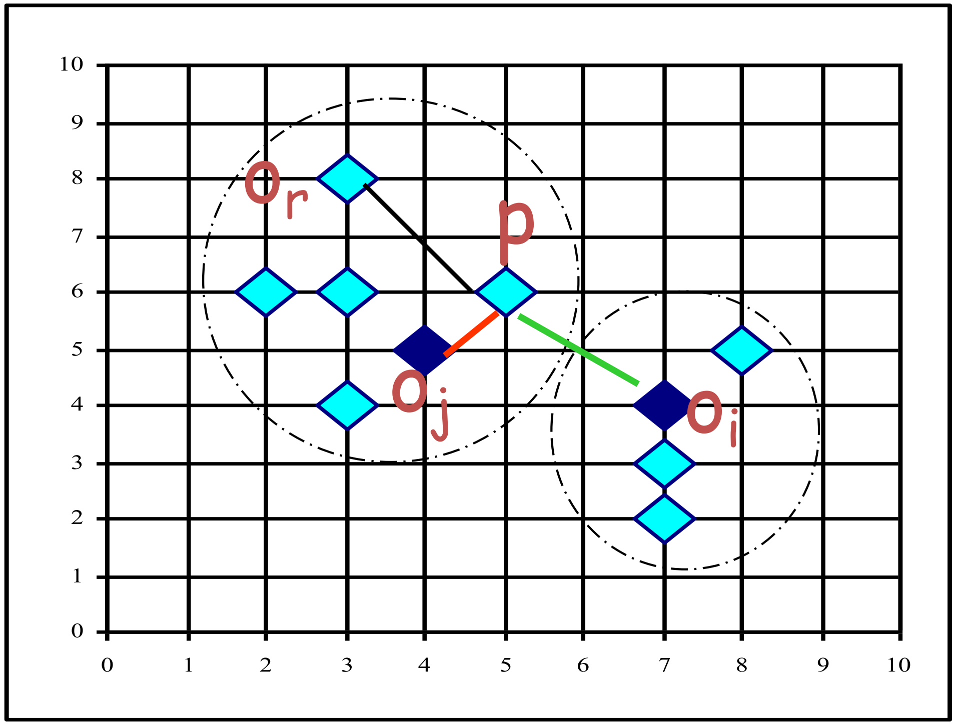
$p \in o_j$

p closest to o_r

Reassign p to O_r

$$C_{p,j,r} = d(p - o_r) - d(p - o_j)$$

Four Cases – Case C



Replace o_j with o_r

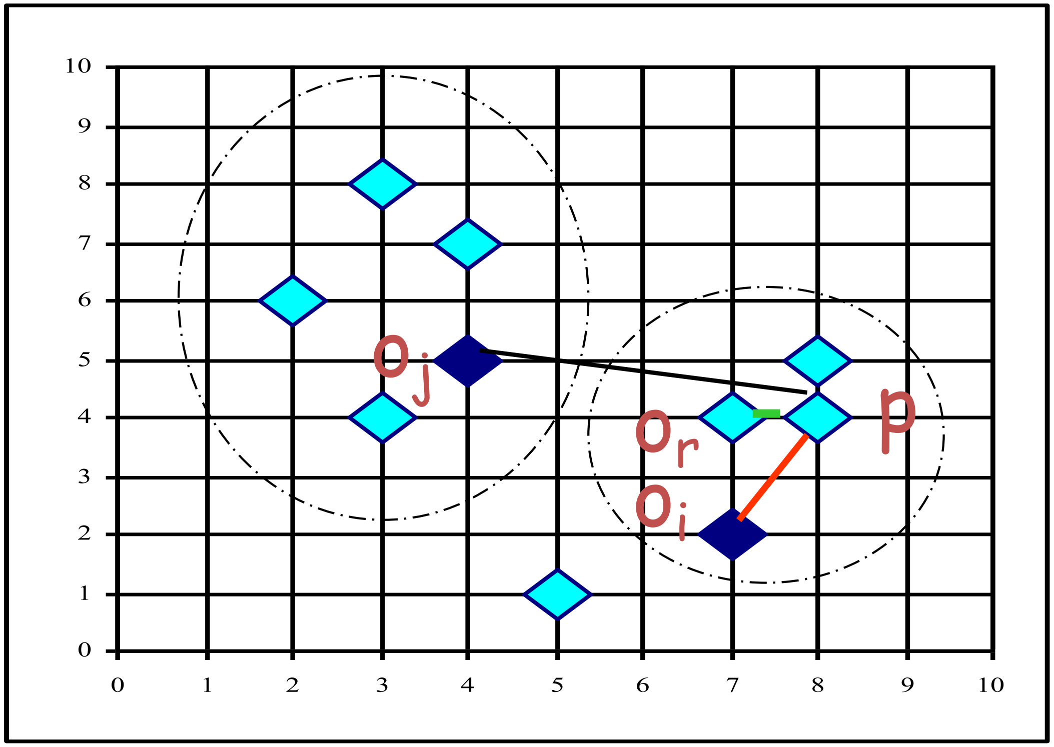
$p \in o_j$

p is now closer to o_i $i \neq j$

Reassign p to O_i

$$C_{p,j,r} = d(p - o_i) - d(p - o_j)$$

Four Cases – Case D



Replace o_j with o_r

$p \in o_i$; $i \neq j$;

p closest to o_r

Reassign p to O_r

$$C_{p,j,r} = d(p - o_r) - d(p - o_i)$$

Practice Question

- Apply PAM on the following data, K=2

	Gender	Age	Time	Fever	Cough
Obj1	F	2	2	Y	N
Obj2	M	2	0.5	N	N
Obj3	F	15	3	Y	Y
Obj4	F	18	0.5	Y	N
Obj5	M	58	4	N	Y
Obj6	F	44	14	N	Y

Assuming O1 and O5 are the medoids of the 2 clusters initially, after objects are distributed to the two clusters, and we randomly selected O2 to replace O1 as the new medoid, should this replacement be carried out?

Practice Question

The distance(dissimilarity) between pairwise objects

	O1	O2	O3	O4	O5	O6
O1	--					
O2	0.94	--				
O3	0.36	0.91	--			
O4	0.19	0.75	0.39	--		
O5	1.15	1.38	0.99	1.3	--	
O6	1.38	2.16	1.22	1.5	1.2	--

Practice Question (2)

Assuming the distance(dissimilarity) between pairwise objects is as the following:

	O1	O2	O3	O4	O5	O6
O1	--					
O2	0.94	--				
O3	0.36	0.91	--			
O4	0.19	0.75	0.39	--		
O5	1.15	1.38	0.99	1.3	--	
O6	1.38	2.16	1.22	1.5	1.2	--

Assuming O1 and O3 are the medoids of the 2 clusters initially, after objects are distributed to the two clusters, and we randomly selected O2 to replace O3 as the new medoid for cluster 2, whats the total cost for this replacement? should this replacement be carried out?

PAM Complexity Analysis

- Total k*(n-k) pairs of (O_i, O_h), k is the number of clusters
- For each pair of (O_i, O_h):
  - compute Tc_{ih} require the examination of (n-k) non-selected objects.
- Total complexity:

  $O(k*(n-k)^2)$

Compare K-means and PAM

- K-means is computationally more efficient
- K-means only handles numeric data
- PAM can handle different types of data
- PAM is better in terms of handling outliers in data

The CLARA algorithm

- Objective: to improve the computational efficiency of PAM, through sampling
- Basic idea:
  - draw a sample (size=40+2k) from the original data set, apply PAM on the sample, and finds the medoids of the sample.
  - Repeat the process a fixed number of times and return the medoids that generate the lowest average dissimilarity from the data objects
- Complexity: $O(k*(40+k)^2 + k*(n-k))$

The CLARA Algorithm

for i=1 to 5, repeat the following steps:

– Draw a sample of 40+2k objects randomly from the entire data set, and call algorithm PAM to find the *k* medoids of the sample

– For each object O_j in the entire data set, determine which of the *k* medoids is the most similar to $O_{j.}$

– Calculate the average dissimilarity of the clustering obtained in the previous step. If this value is < current minimum, set current minimum to this value, and retain the current set of *k* medoids

– Return to step 1 to start the next iteration

CLARANS ("Randomized" CLARA)

- *CLARANS* (A Clustering Algorithm based on Randomized Search)
- CLARANS draws sample of ***neighbors*** dynamically
- The clustering process can be presented as searching a graph where every node is a potential solution, that is, a set of *k* medoids
- If the local optimum is found, *CLARANS* starts with new randomly selected node in search for a new local optimum
- It is more efficient and scalable than both *PAM* and *CLARA*

The CLARANS Algorithm

1. Input *numlocal* and *maxneighbor*
   i=1, mincost=FLT_MAX, bestnode=NULL
2. *current* = an arbitrary *k* modiods
3. j=1
4. Pick random neighbor *S* of *current*, compute the cost difference between *S* and *current*
5. If S has lower cost, set *current* = S, goto 3
   else
      j=j+1;
      if (j <=*maxneighbor*) goto 4
      else
         if (cost(*current*) < *mincost*)
            mincost = cost(*current*)
            bestnode = current
6. i= i+1;
7. If (i <= *numlocal*)
      goto step 2
   else
      output *bestnode* and halt

The CLARANS Algorithm

Outer loop:
i → iterate for numlocal times
    find the local maximum point and update "mincost" and "bestnode"
    inner loop:
    j → iterate for maxneighbor times
        finding the best local maximum k medoids