Partitions Methods

Partitioning Algorithms: Basic Concepts

- **Partitioning method:** Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions

- ***K*-partitioning method:** Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where c_k is the centroid or medoid of cluster C_k)
  - A typical objective function: **Sum of Squared Errors (SSE)**

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

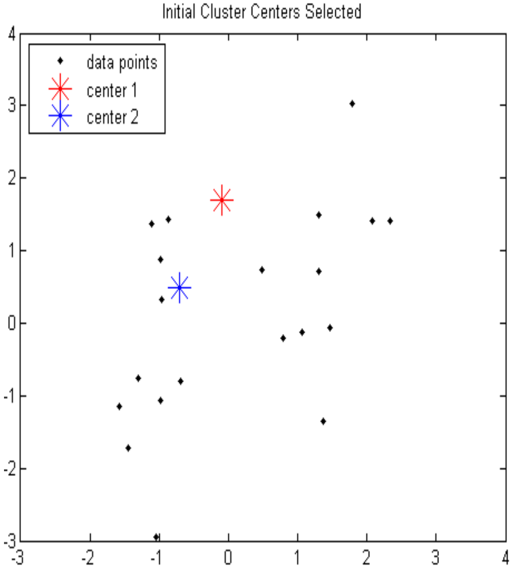
Partitioning Algorithms: Basic Concepts

- Problem definition: Given K, find a partition of K clusters that optimizes the chosen partitioning criterion
  - **Global optimal:** Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): K-Means, K-Medians, K-Medoids, etc.

The *K-Means* Clustering Method

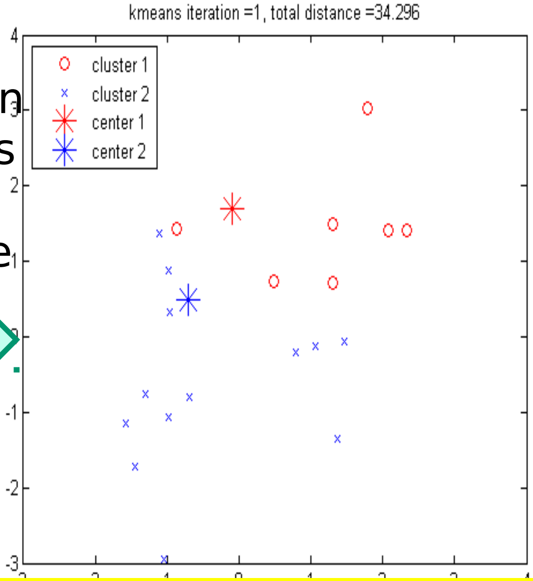
- *K-Means* :Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
    - Select *K* points as initial centroids
    - **Repeat**
        - Form *K* clusters by assigning each point to its closest centroid
        - Re-compute the centroids (i.e., *mean point*) of each cluster
    - **Until** convergence criterion is satisfied
- Different kinds of measures can be used
    - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

Example: *K-Means* Clustering

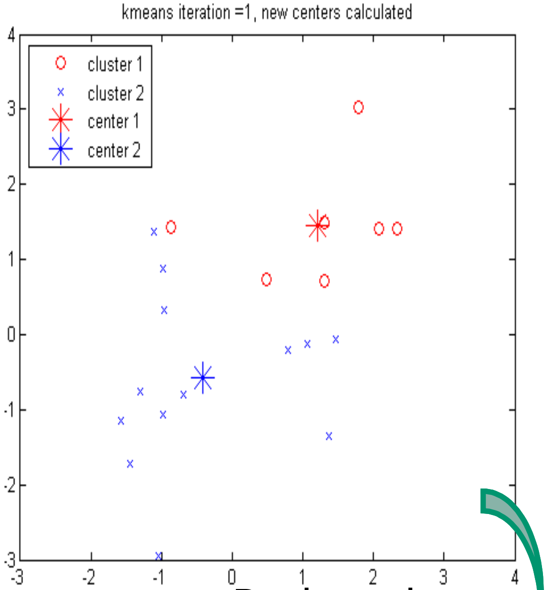


points & randomly select *K* = 2 centroids

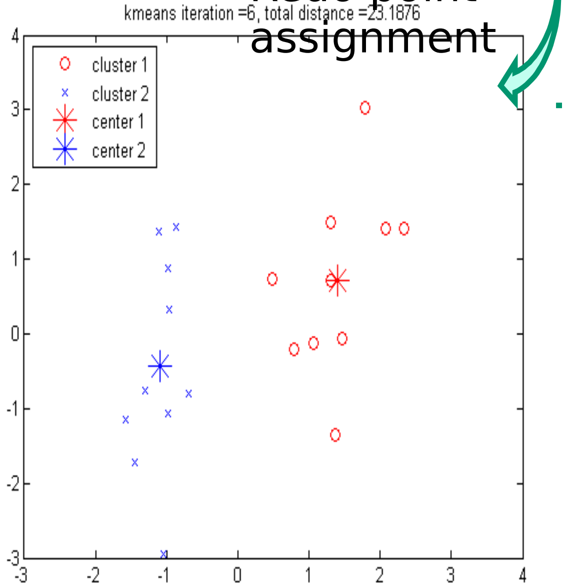
Assign points to clusters.



Recompute cluster centers



Redo point assignment



Execution of the K-Means Clustering Algorithm

Select *K* points as initial centroids

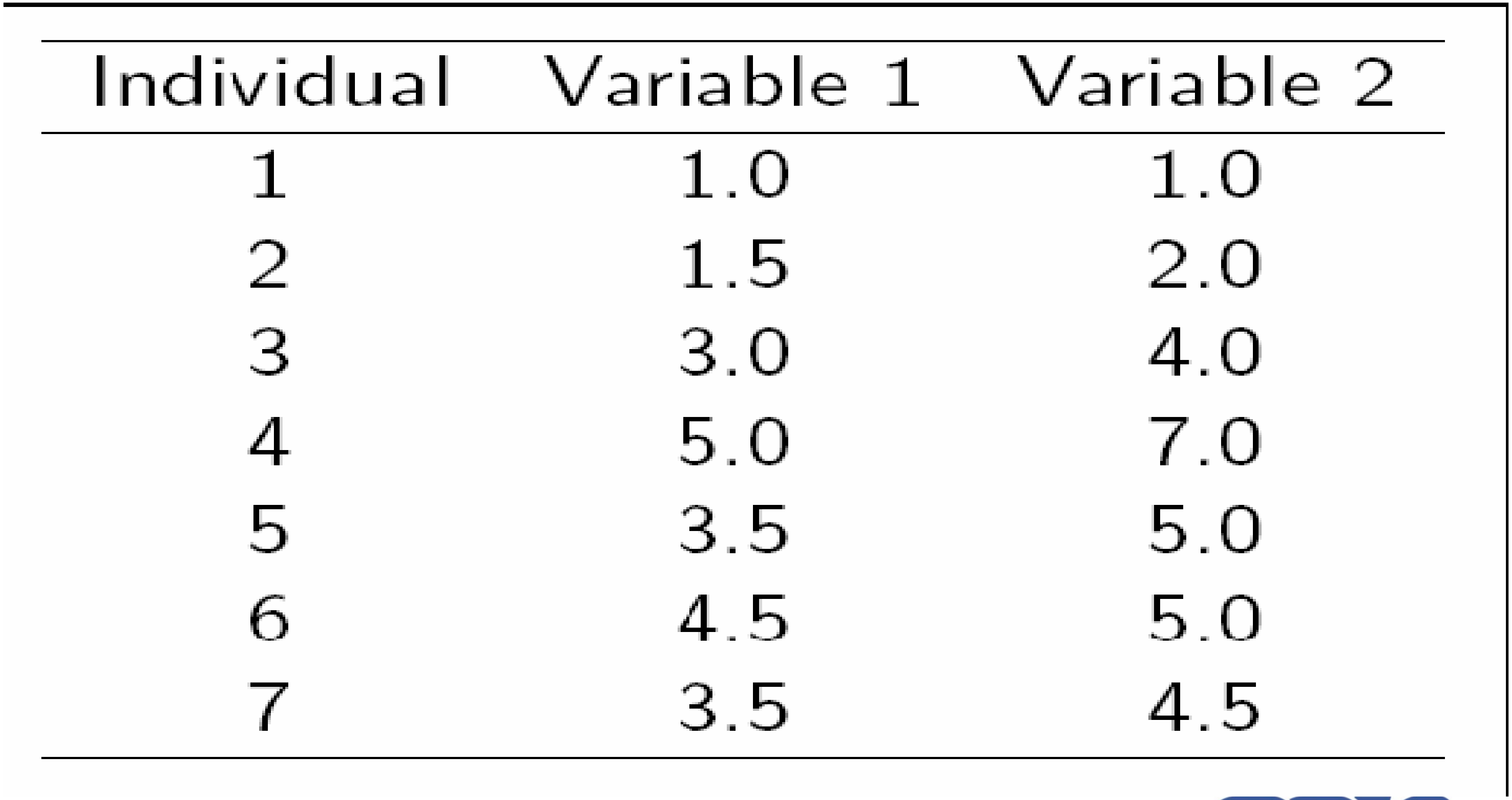
Repeat

•Form *K* clusters by assigning each point to its closest centroid

•Re-compute the centroids (i.e., *mean point*) of each cluster

Until convergence criterion is satisfied

A Simple example showing the implementation of k-means algorithm



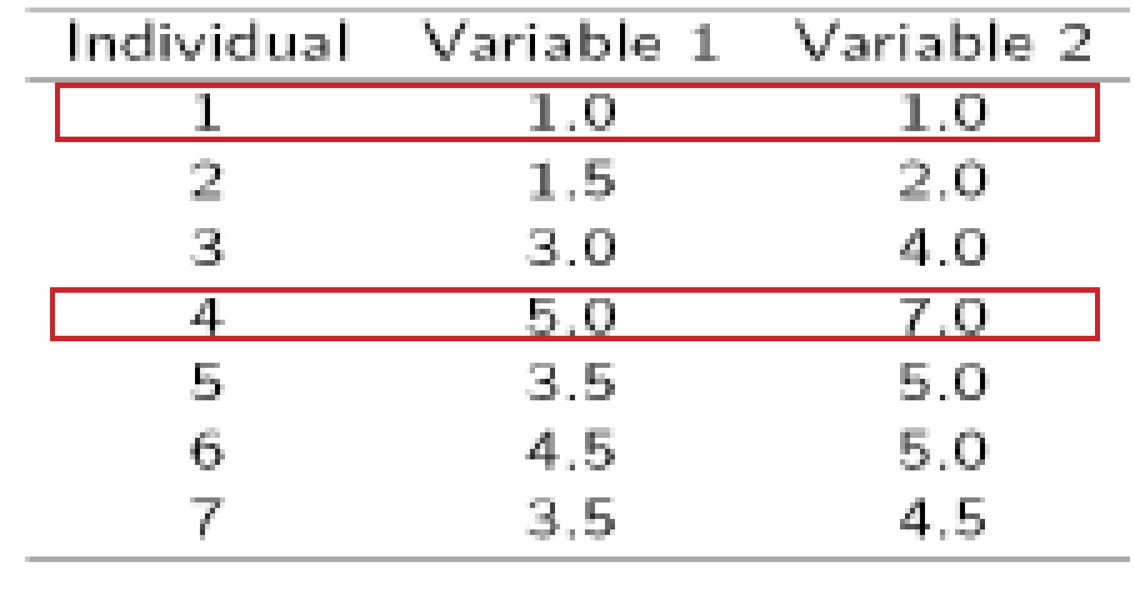
Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

Example: *K-Means* Clustering

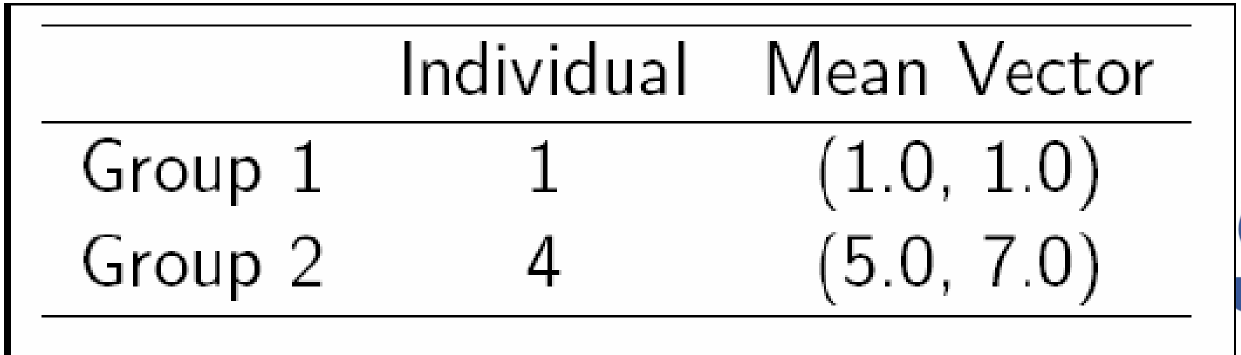
Step 1:

Initialization: Randomly we choose following two centroids (k=2) for two clusters.

In this ca 0,7.0).



Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5



	Individual	Mean Vector
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

Step 2:

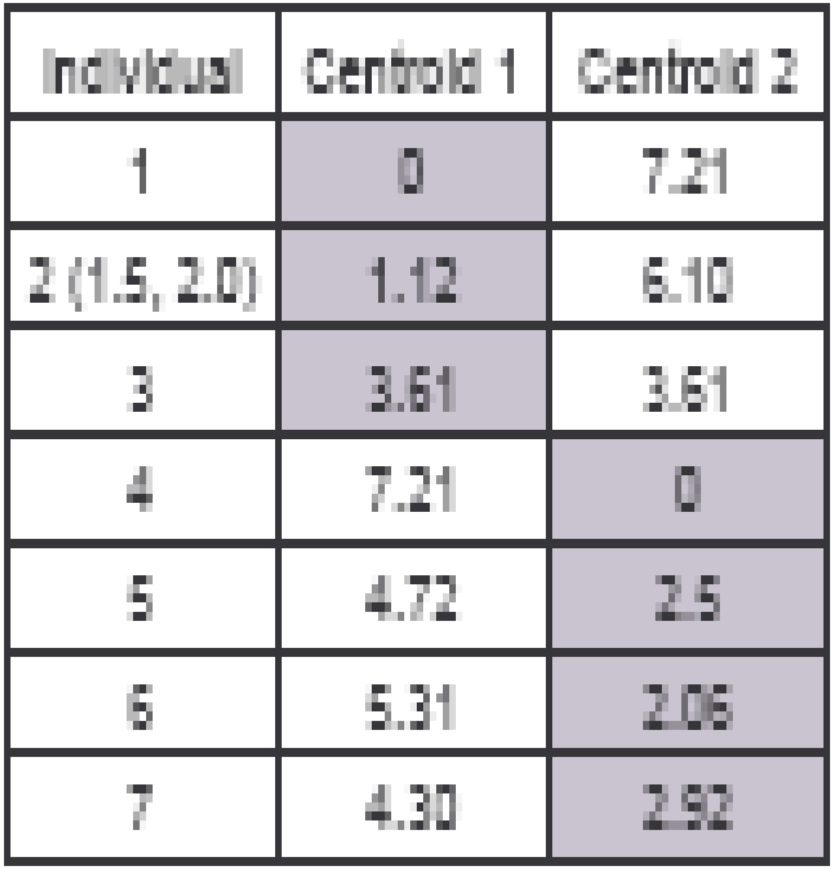
- Thus, we obtain two clusters containing:

$$m_1 = (\frac{1}{3}(1.0+1.5+3.0), \frac{1}{3}(1.0+2.0+4.0)) = (1.83,2.33)$$

$$m_2 = (\frac{1}{4}(5.0+3.5+4.5+3.5), \frac{1}{4}(7.0+5.0+5.0+4.5))$$

- Their new centroids are:

$$= (4.12,5.38)$$



Individual	Centroid 1	Centroid 2
1	0	7.21
2 (1.5, 2.0)	1.12	6.10
3	3.61	3.61
4	7.21	0
5	4.72	2.5
6	5.31	2.06
7	4.30	2.92

$$d(m_1,2) = \sqrt{|1.0-1.5|^2 + |1.0-2.0|^2} = 1.12$$

$$d(m_2,2) = \sqrt{|5.0-1.5|^2 + |7.0-2.0|^2} = 6.10$$

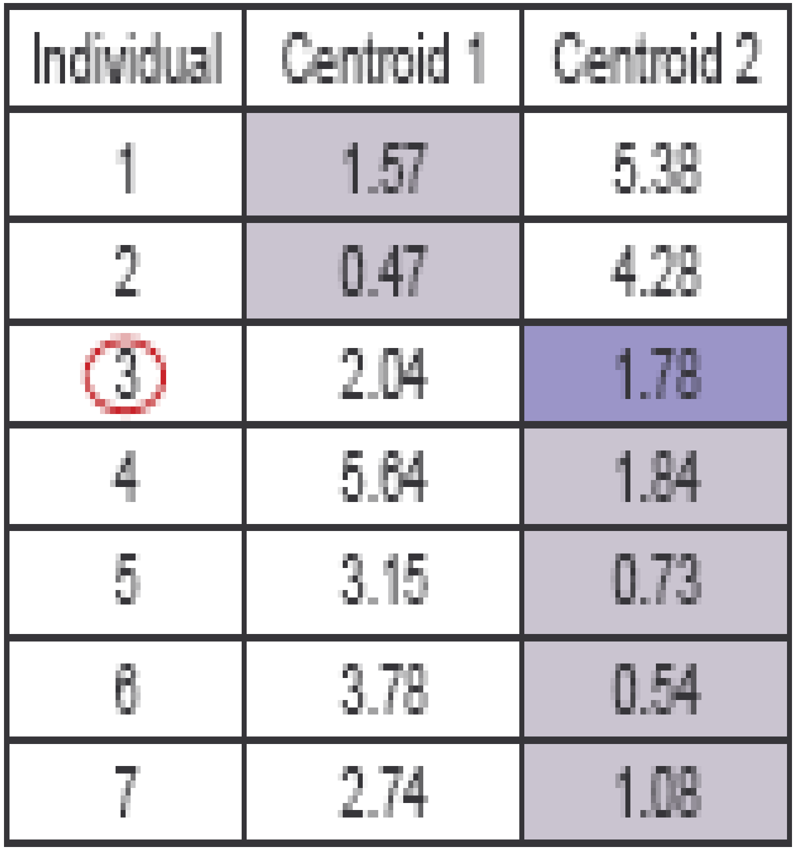
Example: *K-Means* Clustering

Step 3:

- Now using these centroids we compute the Euclidean distance of each object, as shown in table.

- Therefore, the new clusters are:
  {1,2} and {**3**,4,5,6,7}

- Next centroids are: m1=(1.25,1.5) and m2 = (3.9,5.1)



Individual	Centroid 1	Centroid 2
1	1.57	5.38
2	0.47	4.28
3	2.04	1.78
4	5.64	1.84
5	3.15	0.73
6	3.78	0.54
7	2.74	1.08

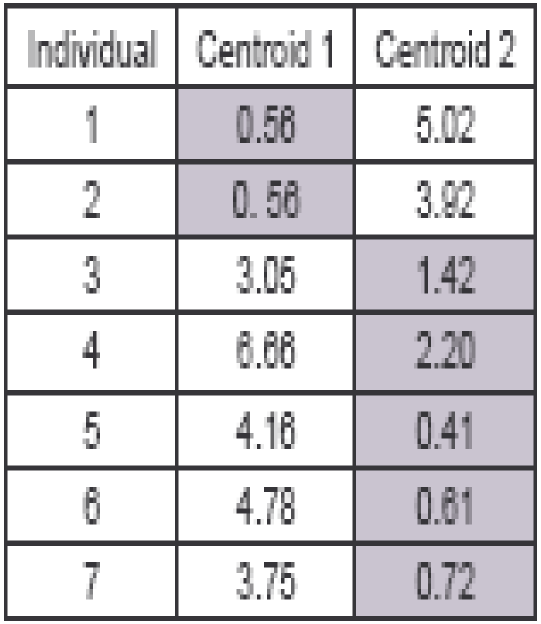
Example: *K-Means* Clustering

- Step 4 :

  The clusters obtained are:

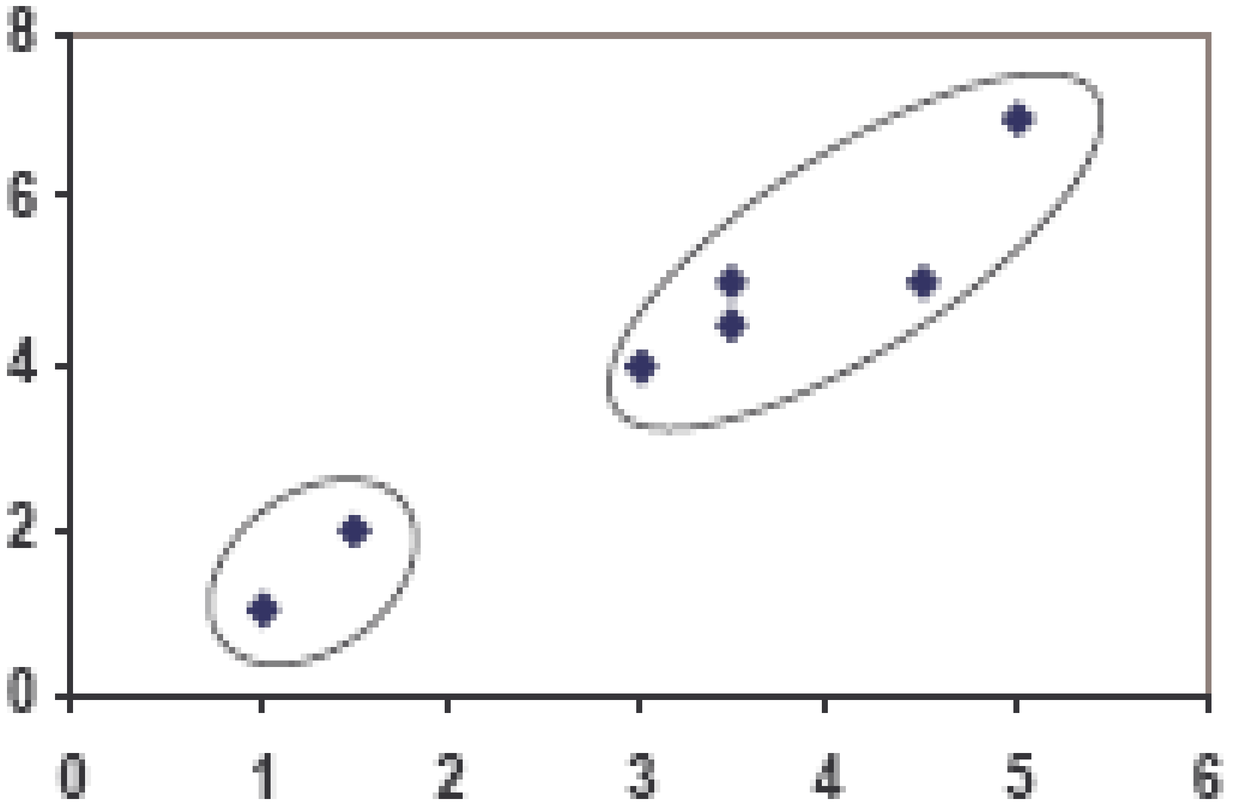
  {1,2} and {3,4,5,6,7}

- Therefore, there is no change in the cluster.
- Thus, the algorithm comes to a halt here and final result consist of 2 clusters {1,2} and {3,4,5,6,7}.

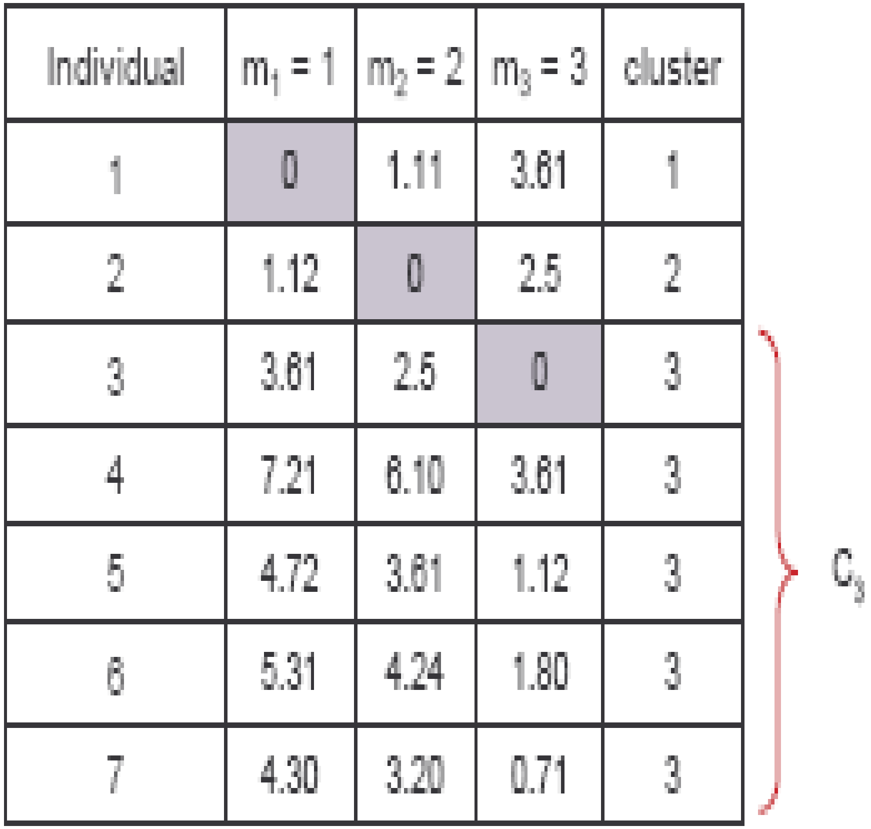


Individual	Centroid 1	Centroid 2
1	0.56	5.02
2	0. 56	3.92
3	3.05	1.42
4	6.66	2.20
5	4.16	0.41
6	4.78	0.61
7	3.75	0.72

PLOT

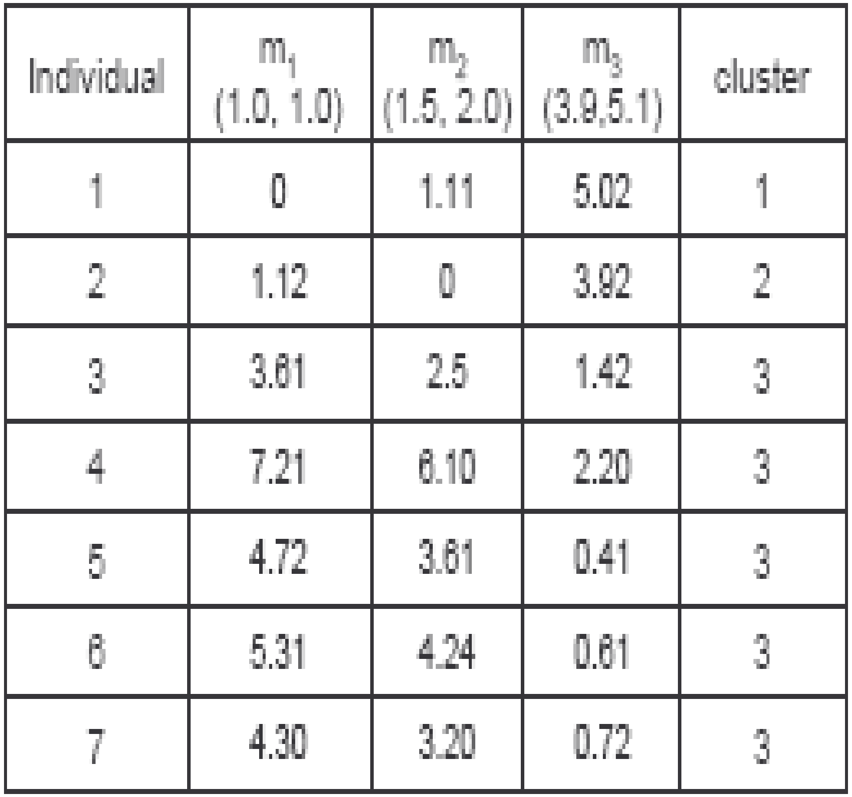


(with K=3)



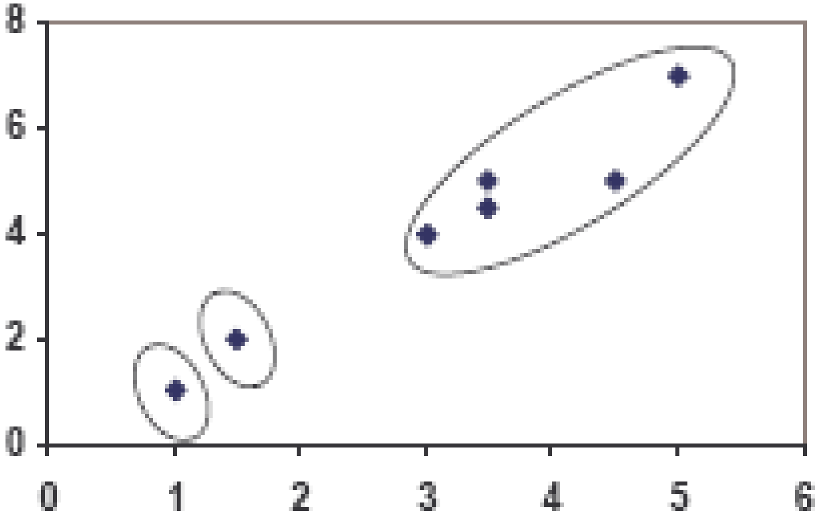
Individual	m_1 = 1	m_2 = 2	m_3 = 3	cluster
1	0	1.11	3.61	1
2	1.12	0	2.5	2
3	3.61	2.5	0	3
4	7.21	6.10	3.61	3
5	4.72	3.61	1.12	3
6	5.31	4.24	1.80	3
7	4.30	3.20	0.71	3

clustering with initial centroids (1, 2, 3)



Individual	m_1 (1.0, 1.0)	m_2 (1.5, 2.0)	m_3 (3.9,5.1)	cluster
1	0	1.11	5.02	1
2	1.12	0	3.92	2
3	3.61	2.5	1.42	3
4	7.21	6.10	2.20	3
5	4.72	3.61	0.41	3
6	5.31	4.24	0.61	3
7	4.30	3.20	0.72	3

PLOT



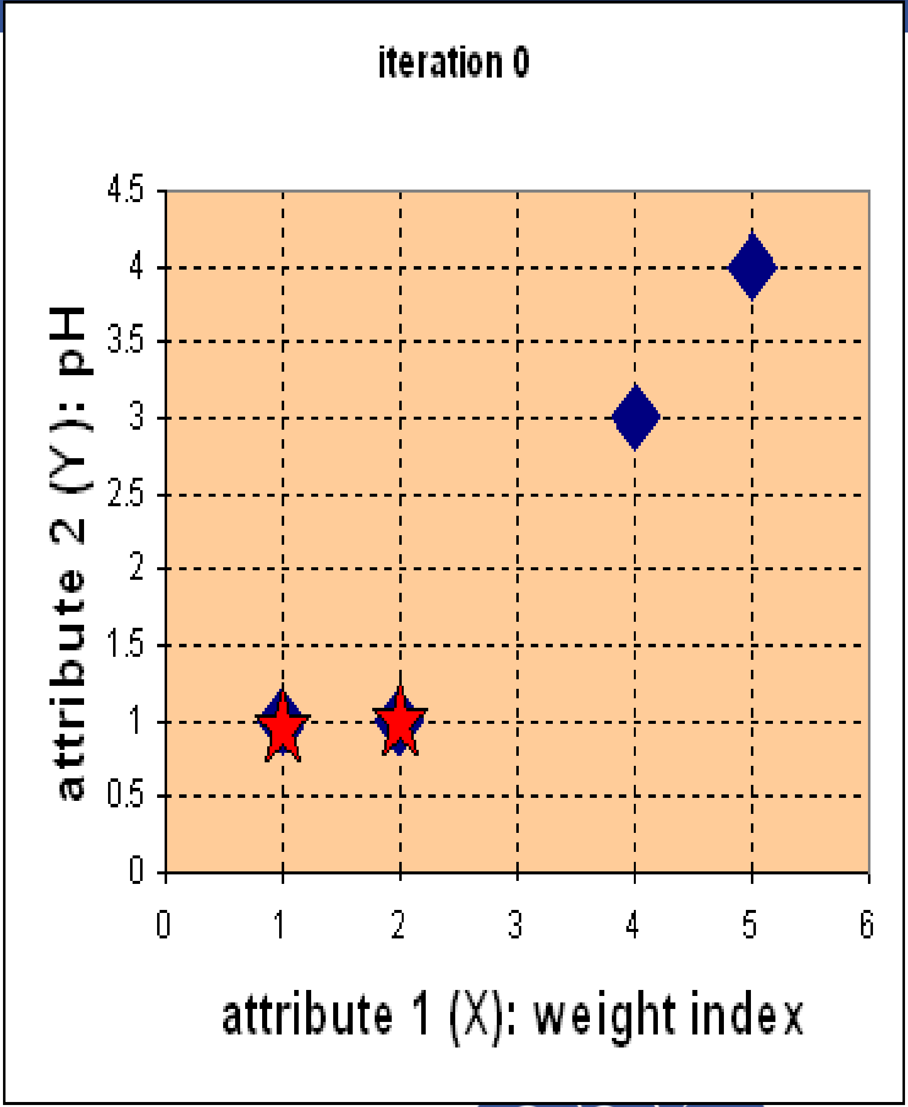
Real-Life Numerical Example of K-Means Clustering

Object	Attribute1 (X): weight index	Attribute 2 (Y): pH
Medicine A	1	1
Medicine B	2	1
Medicine C	4	3
Medicine D	5	4

Real-Life Numerical Example of K-Means Clustering

Step 1:

- **Initial value of centroids** : Suppose we use medicine A and medicine B as the first centroids.
- Let and c_1 and c_2 denote the coordinate of the centroids, then $c_1=(1,1)$ and $c_2=(2,1)$



Real-Life Numerical Example of K-Means Clustering

- **Objects-Centroids distance** : we calculate the distance between cluster centroid to each object using Euclidean distance.

$$\mathbf{D}^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \quad \begin{matrix} \mathbf{c}_1 = (1,1) & group-1 \\ \mathbf{c}_2 = (2,1) & group-2 \end{matrix}$$

$$\begin{array}{cccc|c} A & B & C & D & \\ \hline 1 & 2 & 4 & 5 & X \\ 1 & 1 & 3 & 4 & Y \end{array}$$

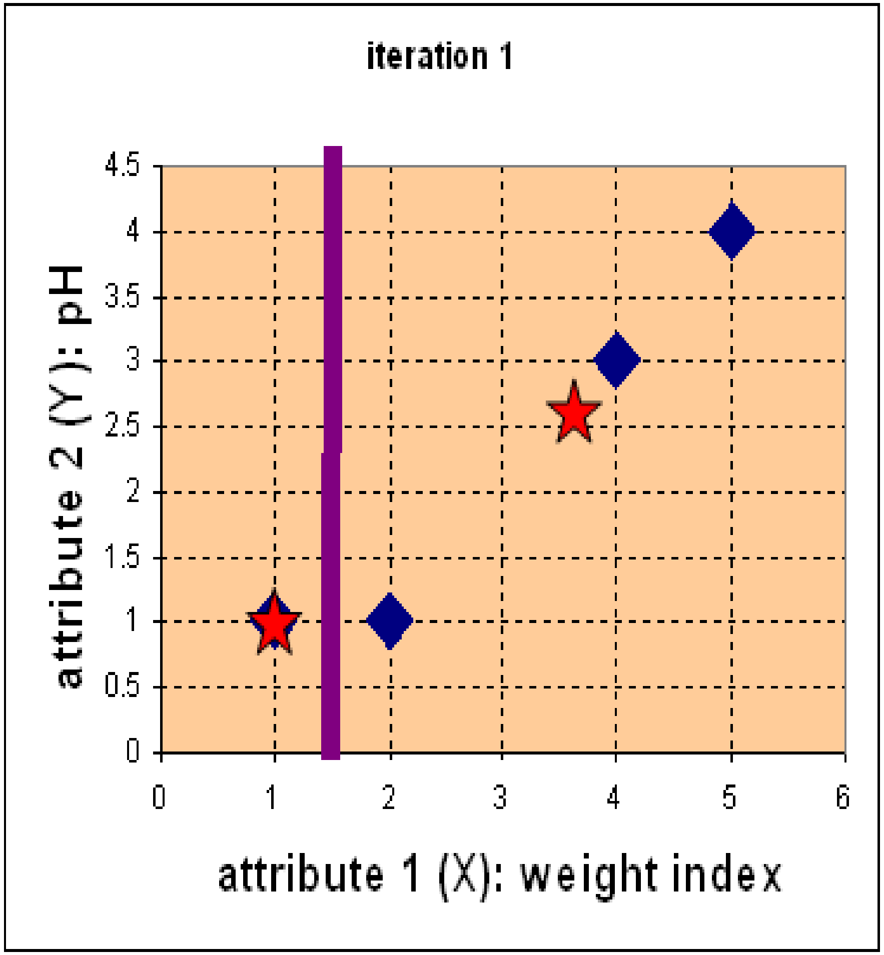
- The first row of the distance matrix corresponds to the distance of each object to the first centroid and the second row is the distance of each object to the second centroid.

$$\mathbf{c}_1 = (1,1)$$

$$\mathbf{c}_2 = (2,1)$$

Step 2:

- **Objects clustering** : We assign each object based on the minimum distance.
- Medicine A is assigned to group 1, medicine B to group 2, medicine C to group 2 and medicine D to group 2.
- The elements of Group matrix below is 1 if and only if the object is assigned to that group.



$$\mathbf{G}^0 = \begin{array}{cc} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{bmatrix} & \begin{array}{l} group-1 \\ group-2 \end{array} \\ \begin{array}{cccc} A & B & C & D \end{array} & \end{array}$$

Real-Life Numerical Example of K-Means Clustering

- **Iteration-1, Objects-Centroids distances** : The next step is to compute the distance of all objects to the new centroids.
- Similar to step 2, we have distance matrix at iteration 1 is

$$\mathbf{D}^1 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 3.14 & 2.36 & 0.47 & 1.89 \end{bmatrix} \quad \begin{matrix} \mathbf{c}_1 = (1,1) & group-1 \\ \mathbf{c}_2 = (\frac{11}{3},\frac{8}{3}) & group-2 \end{matrix}$$

$$\begin{array}{cccc} A & B & C & D \end{array}$$

$$\begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} \quad \begin{matrix} X \\ Y \end{matrix}$$

Real-Life Numerical Example of K-Means Clustering

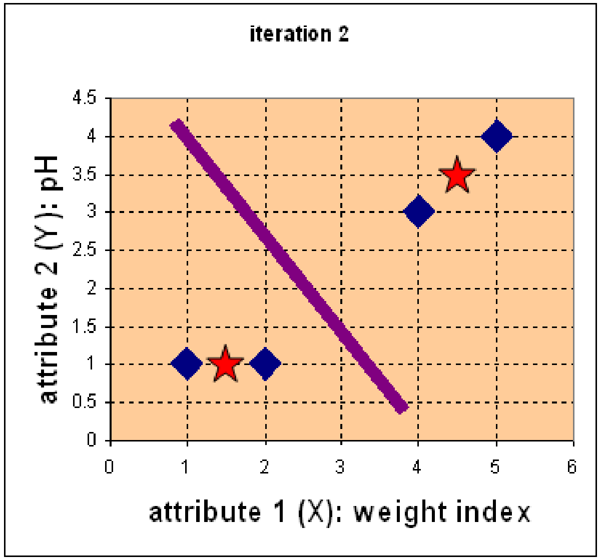
- **Iteration-1, Objects clustering:**Based on the new distance matrix, we move the medicine B to   Group 1 while all the other objects remain. The Group matrix is shown

$$\mathbf{G}^1 = \begin{array}{cc} \left[\begin{array}{cccc} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{array}\right] & \begin{array}{c} group-1 \\ group-2 \end{array} \\ \begin{array}{cccc} A & B & C & D \end{array} & \end{array}$$

- **Iteration 2, determine centroids:** Now we repeat step 4 to calculate the new centroids coordinate based on the clustering of previous iteration. Group1 and group 2 both has two members, thus the new centroids are and

$$\mathbf{c}_1 = \left(\frac{1+2}{2}, \frac{1+1}{2}\right) = (1\tfrac{1}{2}, 1)$$

$$\mathbf{c}_2 = \left(\frac{4+5}{2}, \frac{3+4}{2}\right) = (4\tfrac{1}{2}, 3\tfrac{1}{2})$$



Real-Life Numerical Example of K-Means Clustering

- **Iteration-2, Objects-Centroids distances** : Repeat step 2 again, we have new distance matrix at iteration 2 as

$$\mathbf{D}^2 = \begin{bmatrix} 0.5 & 0.5 & 3.20 & 4.61 \\ 4.30 & 3.54 & 0.71 & 0.71 \end{bmatrix} \quad \begin{array}{ll} \mathbf{c}_1 = (1\tfrac{1}{2}, 1) & group-1 \\ \mathbf{c}_2 = (4\tfrac{1}{2}, 3\tfrac{1}{2}) & group-2 \end{array}$$

$$\begin{array}{cccc|c} A & B & C & D & \\ 1 & 2 & 4 & 5 & X \\ 1 & 1 & 3 & 4 & Y \end{array}$$

Real-Life Numerical Example of K-Means Clustering

- **iteration-2, Objects clustering:** Again, we assign each object based on the minimum distance.

$$\mathbf{G}^{2} = \begin{array}{cc} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} & \begin{array}{l} group-1 \\ group-2 \end{array} \\ \begin{array}{cccc} A & B & C & D \end{array} & \end{array}$$

- We obtain result that $\mathbf{G}^{2} = \mathbf{G}^{1}$. Comparing the grouping of last iteration and this iteration reveals that the objects does not move group anymore.
- Thus, the computation of the k-mean clustering has reached its stability and no more iteration is needed..

Real-Life Numerical Example of K Means Clustering

We get the final grouping as the results as:

Object	Feature1(X): weight index	Feature2 (Y): pH	Group (result)
Medicine A	1	1	1
Medicine B	2	1	1
Medicine C	4	3	2
Medicine D	5	4	2

Discussion on the *K-Means* Method

- **Efficiency**: O(tKn) where n: # of objects, K: # of clusters, and t: # of iterations
  - Normally, K, t << n; thus, an efficient method
- K-means clustering often **terminates at a local optimal**
  - Initialization can be important to find high-quality clusters
- **Need to specify K**, the number of clusters, in advance
  - There are ways to automatically determine the "best" K
  - In practice, one often runs a range of values and selected the "best" K value

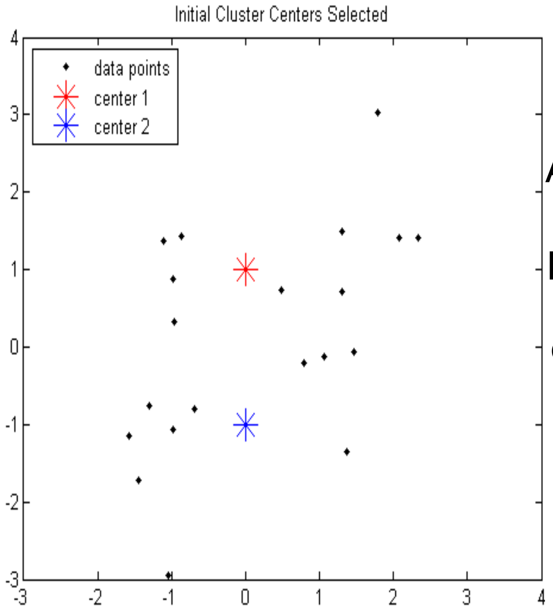
Discussion on the *K-Means* Method

- **Sensitive to noisy data and outliers**
  - Variations: Using K-medians, K-medoids, etc.
- K-means is applicable only to objects in a continuous n-dimensional space
  - Using the K-modes for **categorical data**
- Not suitable to discover clusters with **non-convex shapes**
  - Using density-based clustering, kernel K-means, etc.

Initialization of K-Means

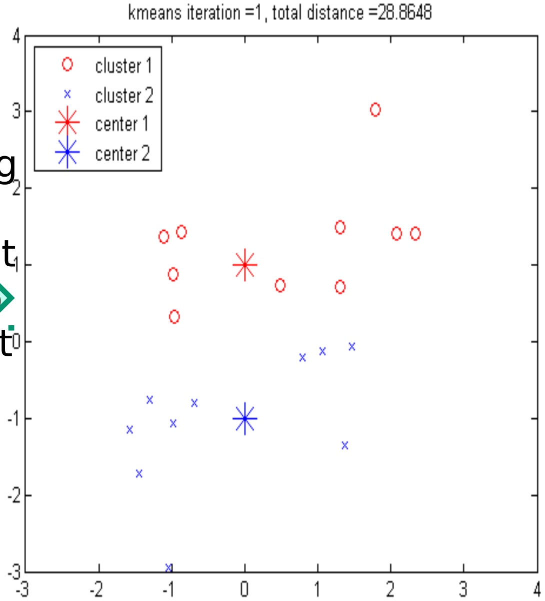
- Different initializations may generate rather different clustering results (some could be far from optimal)
- Original proposal : Select *K* seeds randomly
  - Need to run the algorithm multiple times using different seeds
  - There are many methods proposed for better initialization of *k* seeds (***K-Means++***)
  - The first centroid is selected at random
    - The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score)
    - The selection continues until *K* centroids are obtained

Example: Poor Initialization May Lead to Poor Clustering

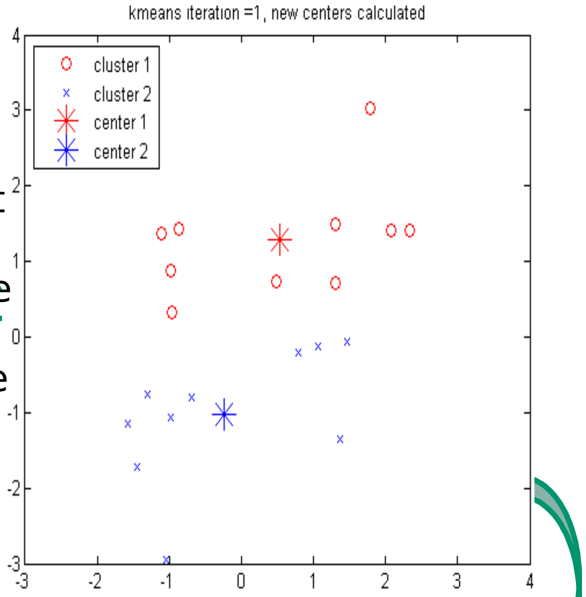

Initial Cluster Centers Selected

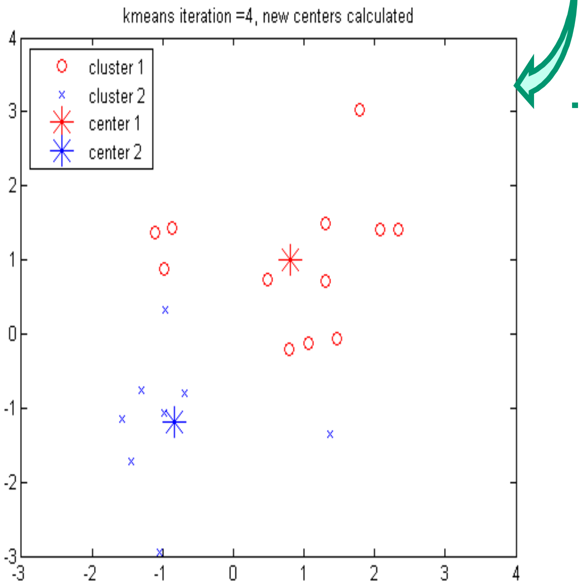
Another random selection of k centroids for the same data points

Assign points to clusters


kmeans iteration =1, total distance =28.8648

Recompute cluster centers


kmeans iteration =1, new centers calculated


kmeans iteration =4, new centers calculated

- Rerun of the *K-Means* using another random *K* seeds
- This run of *K*-Means generates a poor quality clustering

K-Mediods

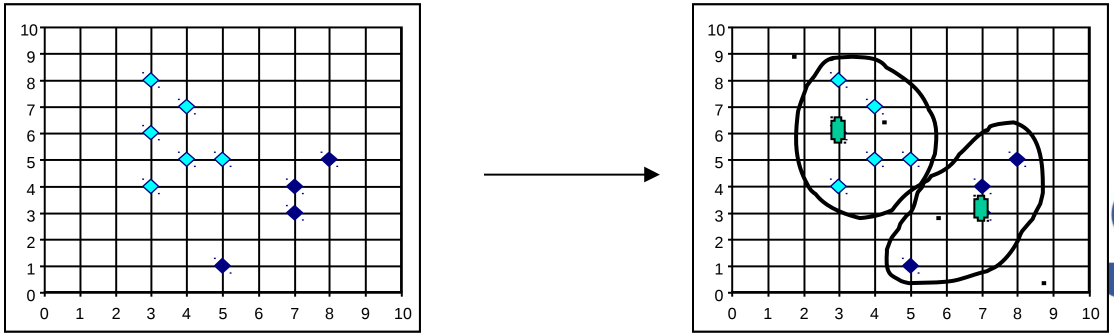
- Consider six points in 1-D space having the values
- 1, 2, 3, 8, 9, 10, and 25, respectively.
- By visual inspection we may partition the points into the clusters {1,2,3} and {8, 9,10} where point 25 is excluded which is an outlier.
- How would k-means partition the values?
- If we apply k-means using mean 2 and 9 and c1{1,2,3} {8,9,10,25} with cluster variation as 196
- With mean as 3.5 and 14.67 for c1{1,2,3,8} and c2{9,10,25} the cluster variation as 189.67
- Assigns 8 to different cluster due to the prsence of outliers

K-Mediods

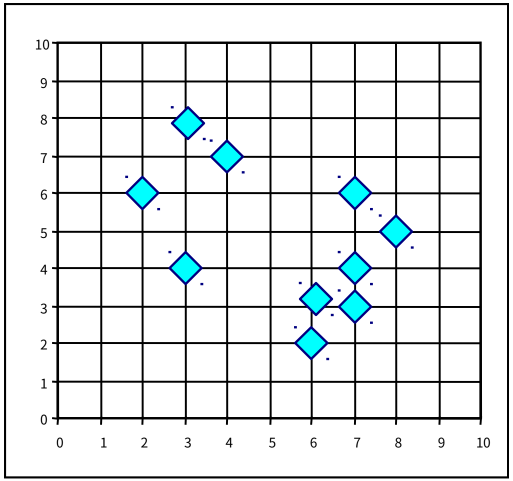
- Avoid taking the mean value of the object as reference point.
- Actual objects to represent the clusters **medoids** can be used, which is the **most centrally located** object in a cluster
- Assign other similar objects as representative object to the cluster.

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} dist(p, o_i),$$

- The absolute-error criterion is defined as O_i representative object and P all objects in the data set

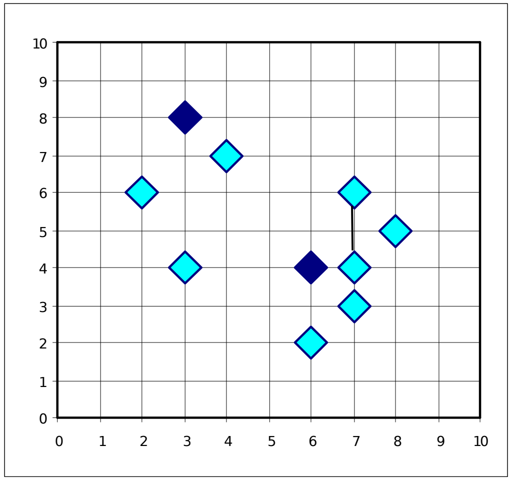


PAM: A Typical K-Medoids Algorithm



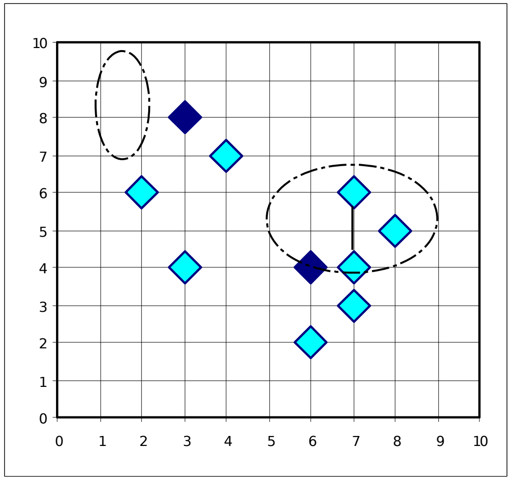
K=2

Arbitrary choose k object as initial medoids

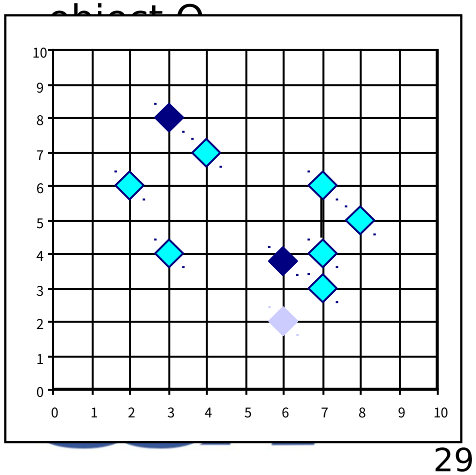


Total Cost = 20

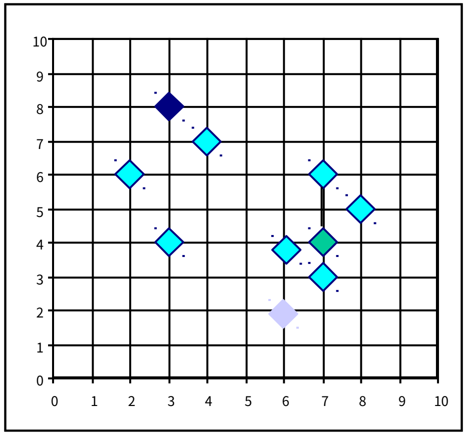
Assign each remaining object to nearest medoids



Randomly select a nonmedoid object O



Compute total cost of swapping



Total Cost = 26

Swapping O and O_{ramdom}

If quality is improved.

Do loop

Until no change

Algorithm for PAM

- The *K-Medoids* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medoids*)
  - **Repeat**
    - – Assigning each point to the cluster with the closest medoid
    - – Randomly select a non-representative object o_i
    - – Compute the total cost *S* of swapping the medoid *m* with o_i
    - – If $S < 0$, then swap *m* with o_i to form the new set of medoids
  - **Until** convergence criterion is satisfied

Discussion on *K-Medoids* Clustering

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
- *PAM* (Partitioning Around Medoids:
  - Starts from an initial set of medoids
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) 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)
  - Computational complexity: PAM: $O(K(n - K)^2)$ (quite expensive!)

Discussion on *K-Medoids* Clustering

- Efficiency improvements on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990):
    - PAM on samples; $O(Ks^2 + K(n - K))$, s is the sample size
    - PAM applied to compute the best medoids from the sample.
    - Representative objects should represent the data set.
    - Build clusterings from multiple random samples and returns the best
    - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

Discussion on *K-Medoids* Clustering

- Efficiency improvements on PAM
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality
  - Randomly select k objects in the data set as current mediods.
  - Conducts randomized search l times
  - After l steps considered as local optimum

K-Medians: Handling Outliers by Computing Medians

- Medians are less sensitive to outliers than means
  - Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- ***K-Medians***: Instead of taking the **mean** value of the object in a cluster as a reference point, **medians** are used (L_1-norm as the distance measure)