Clustering Methods

Clustering Methods

- Clustering is the process of grouping the data into classes or clusters, so that objects within a cluster have high similarity in comparison to one another but are very dissimilar to objects in other clusters.
- Some major clustering approaches are:
  - Partitioning Methods
  - Hierarchical Methods
  - Density based methods

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, 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

Partitioning Methods

- This method generally results in a set of *k* clusters. Each cluster maybe represented by a centroid or a cluster representative

- A partitioning method creates an initial partitioning, given *k*, the number of partitions to construct. It uses an iterative relocation technique that attempts to improve partitioning by moving objects from one group to another

- Partitioning methods can be used for high dimensional data. However, one disadvantage is that a user needs to initialize the number of clusters.

K-Means Clustering Algorithm

Algorithm: ***K-Means***

Input: *k*, *D*

k, is the number of clusters, *D* a data set containing n objects.

Output: A set of *k* clusters

Method:

1: arbitrarily choose k objects from D as the initial cluster centers;

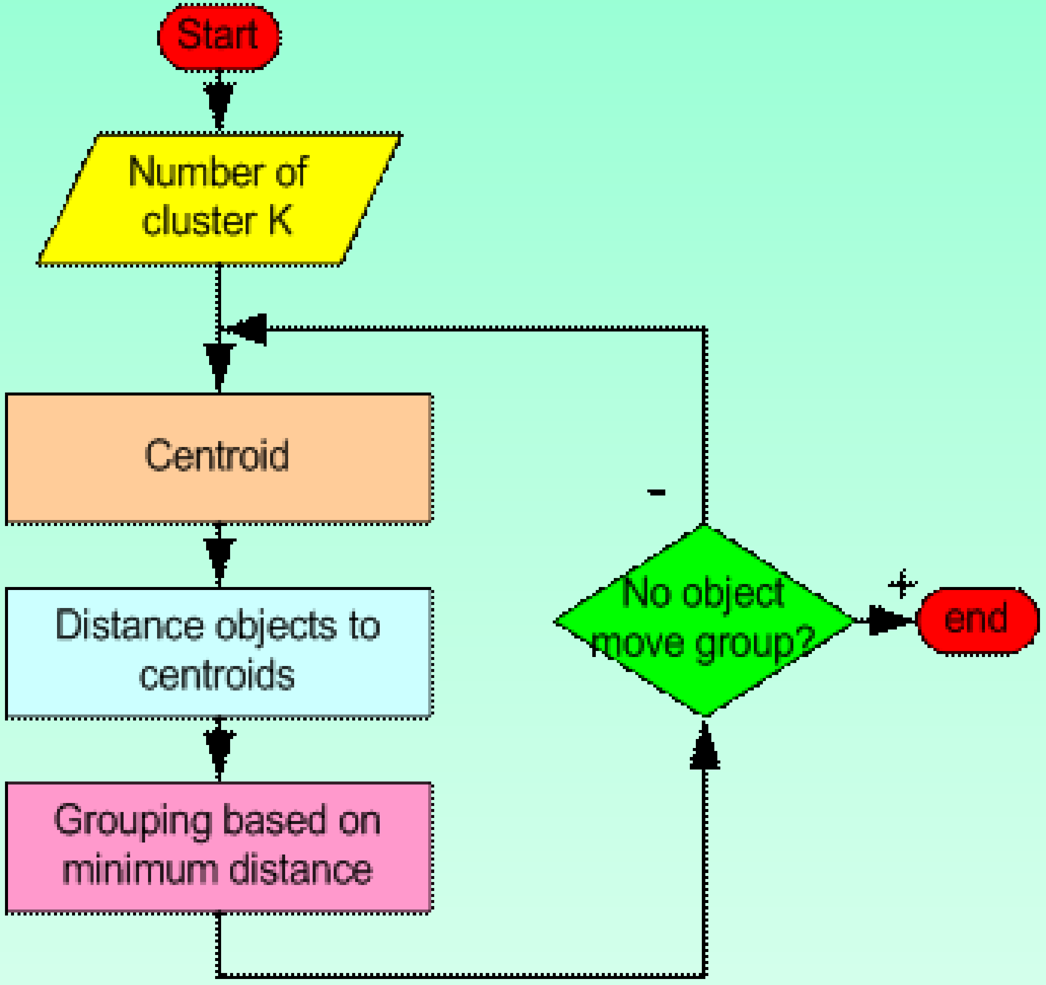
2: **repeat**

3: (re)assign each object to the cluster to which the object is the most similar based on the mean value of the objects in the cluster;

4: update the cluster means, i.e. calculate the mean value of the objects for each cluster;

5: **until** no change;

K-Means Clustering



Example 1: K-Means Clustering

Use k-Means and Euclidean Distance to cluster the following 8 samples into 3 clusters:
A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9)

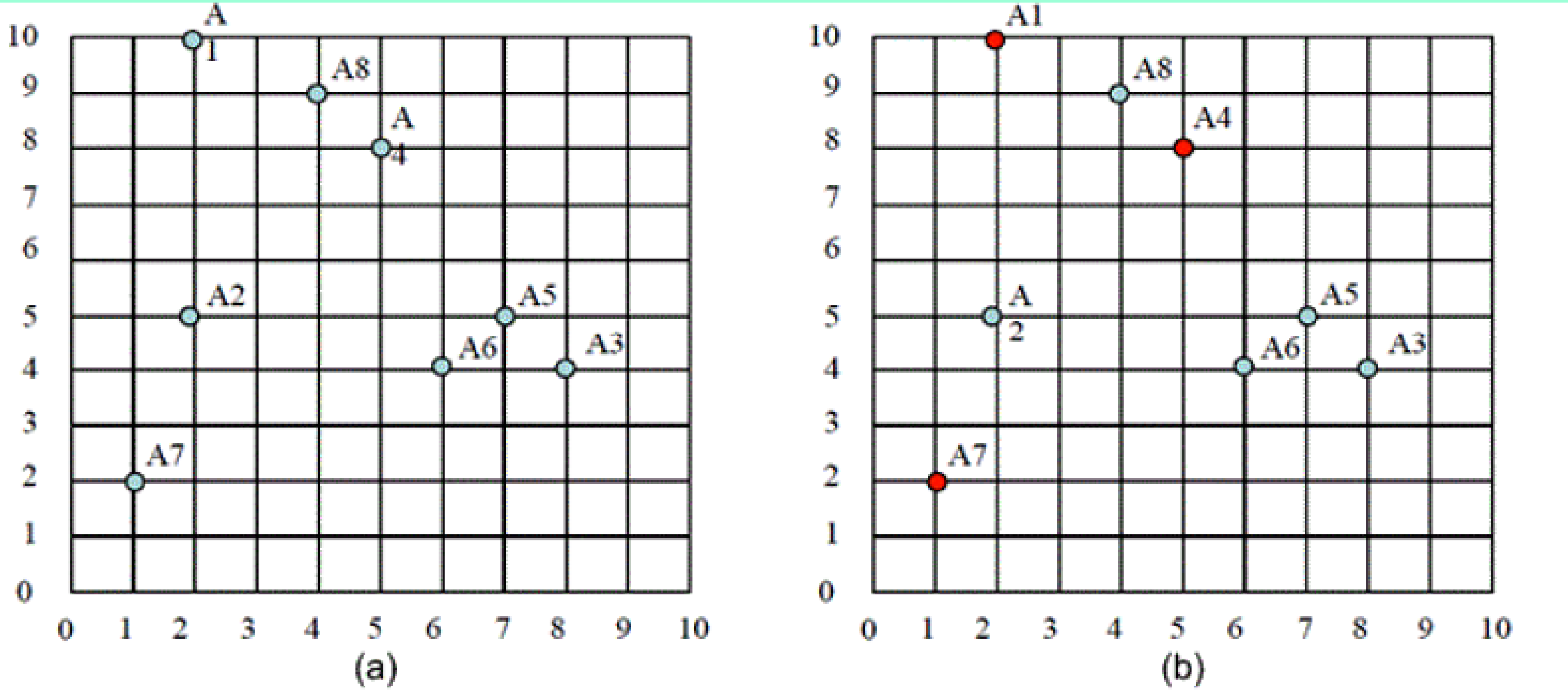


Figure 1: (a) 8 samples (b) 3 clusters (seed1, seed2 and seed3) in red

At the beginning, we initial the centre of the 3 clusters (seed1, seed2 and seed3) to A1, A4 and A7 (Figure 1 (b)).

K-Means Clustering

A1: • d(A1, seed1)=0 as A1 is seed1 (**smallest**) • d(A1, seed2)=$\sqrt{13}$ • d(A1, seed3)=$\sqrt{65}$ → A1 $\in$ cluster1	A2: • d(A2, seed1)= $\sqrt{25}$ • d(A2, seed2)= $\sqrt{18}$ • d(A2, seed3)= $\sqrt{10}$ (**smallest**) → A2 $\in$ cluster3
A3: • d(A3, seed1)= $\sqrt{36}$ • d(A3, seed2)= $\sqrt{25}$ (**smallest**) • d(A3, seed3)= $\sqrt{53}$ → A3 $\in$ cluster2	A4: • d(A4, seed1)= $\sqrt{13}$ • d(A4, seed2)= 0 as A4 is seed2 (**smallest**) • d(A4, seed3)= $\sqrt{52}$ → A4 $\in$ cluster2
A5: • d(A5, seed1)= $\sqrt{50}$ • d(A5, seed2)= $\sqrt{13}$ (**smallest**) • d(A5, seed3)= $\sqrt{45}$ → A5 $\in$ cluster2	A6: • d(A6, seed1)= $\sqrt{52}$ • d(A6, seed2)= $\sqrt{17}$ (**smallest**) • d(A6, seed3)= $\sqrt{29}$ → A6 $\in$ cluster2
A7: • d(A7, seed1)= $\sqrt{65}$ • d(A7, seed2)= $\sqrt{52}$ • d(A7, seed3)= 0 as A7 is seed3 (**smallest**) → A7 $\in$ cluster2	A8: • d(A8, seed1)= $\sqrt{5}$ • d(A8, seed2)= $\sqrt{2}$ (**smallest**) • d(A8, seed3)= $\sqrt{58}$ → A8 $\in$ cluster2

K-Means Clustering

New cluster 1: {A1}, 2: {A3, A4, A5, A6, A8}, 3: {A2, A7}, see Figure 2 (a)

Then, the centres of the new clusters (see Figure 2 (b)):

$$C1=(2,10),\ C2=\left(\frac{8+5+7+6+4}{5}, \frac{4+8+5+4+9}{5}\right)=(6,6),\ C3=\left(\frac{2+1}{2}, \frac{5+2}{2}\right)=(1.5, 3.5)$$

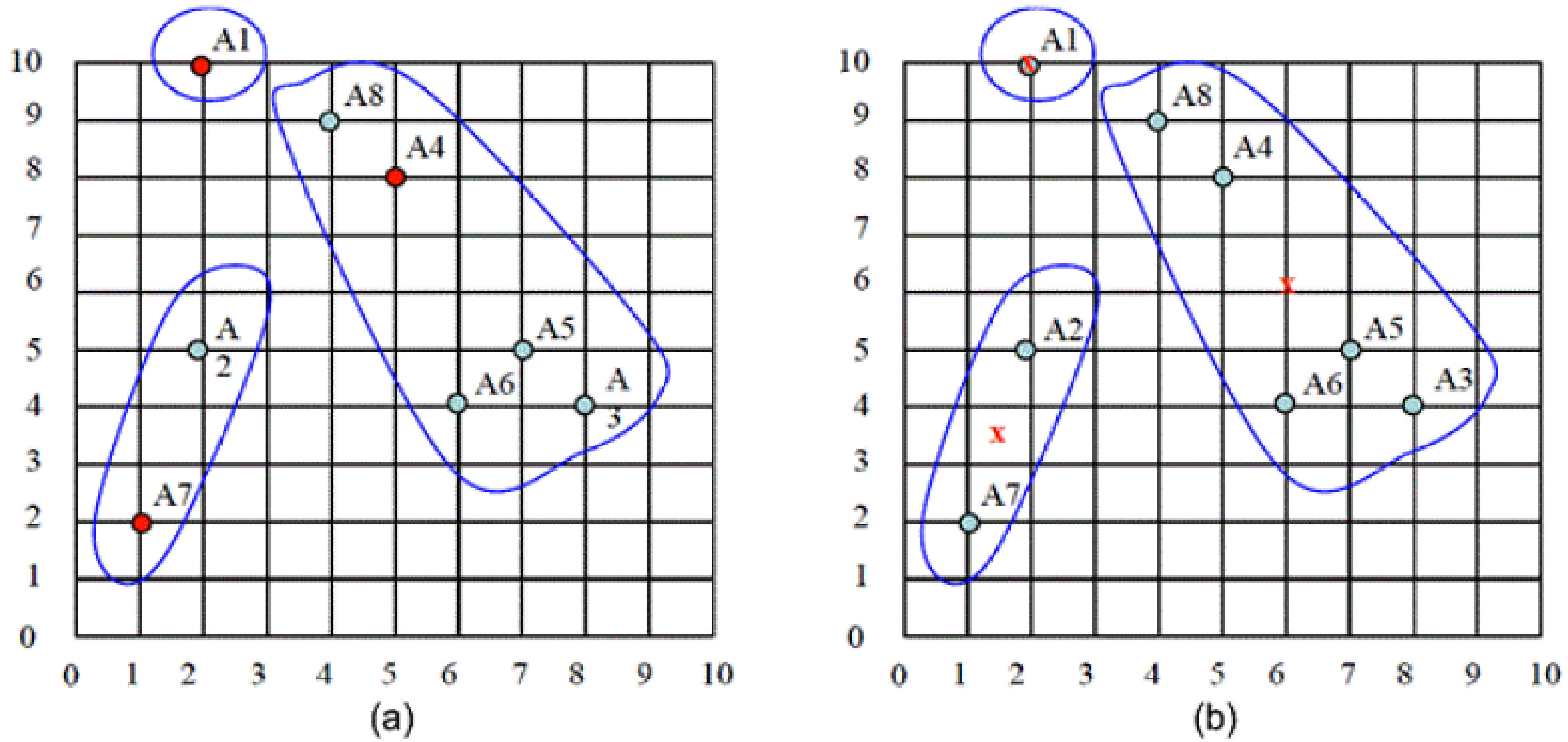


Figure 2: (a) before Epoch 1; (b) centroid has been changed after ***Epoch 1***

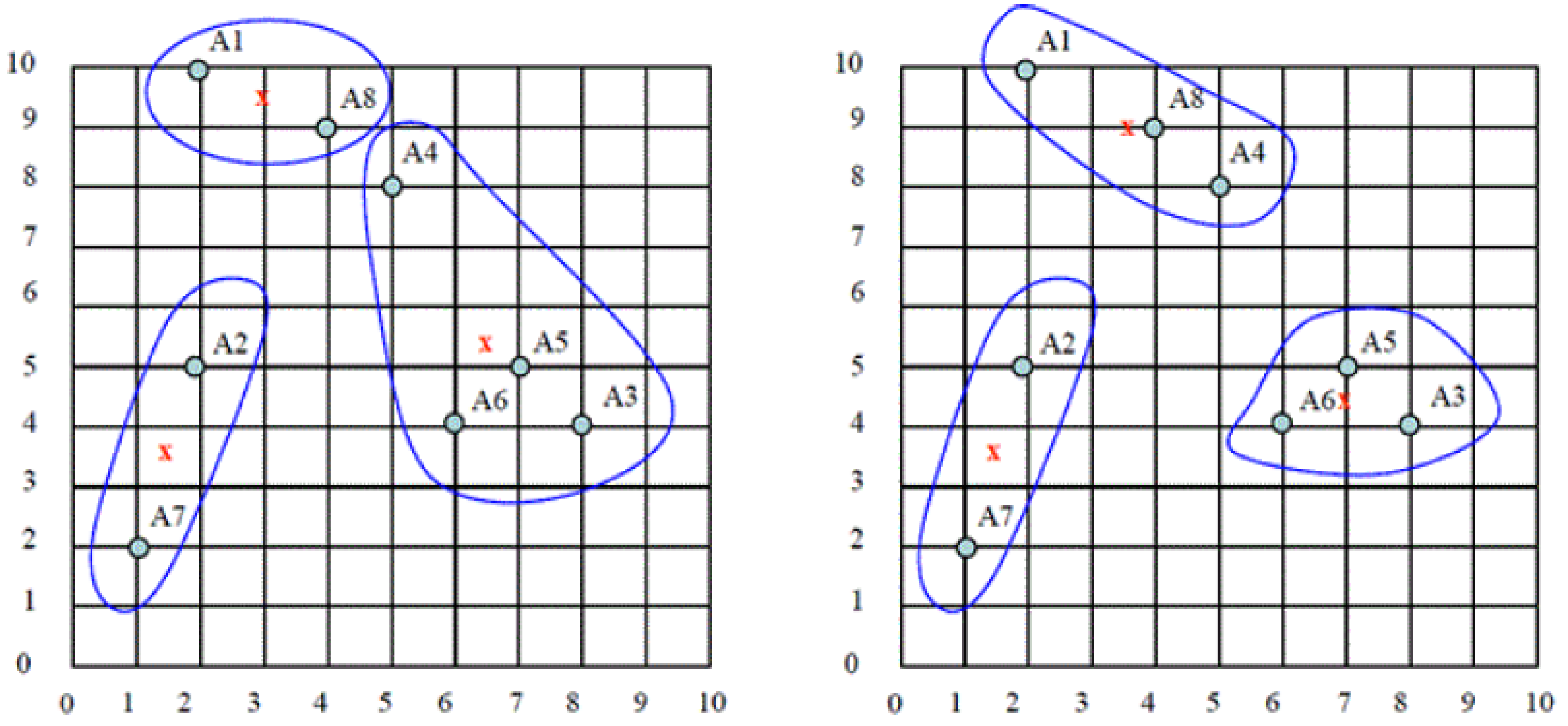
K-Means Clustering

Epoch 2 (Omit), after the 2nd epoch the results would be:

1: {A1, A8}, 2: {A3, A4, A5, A6}, 3: {A2, A7} with centres C1= (3, 9.5), C2= (6.5, 5.25) and C3= (1.5, 3.5)

Epoch 3 (Omit), after the 3rd epoch the results would be:

1: {A1, A4, A8}, 2: {A3, A5, A6}, 3: {A2, A7} with centre C1= (3.66, 9), C2= (7, 4.33) and C3= (1.5, 3.5)



(a) (b)

Strengths and weakness of K-Means Method

- **Strength:** *Efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t \ll n$.
- **Weakness**
  - Need to specify k, the *number* of clusters, in advance (there are ways to automatically determine the best k.
  - Sensitive to noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*