KMeans Clustering Overview

Abdullah Al Safi Chowdhury Porosh

Msc. in Data and knowledge Engineering

Otto-von-Guericke University of Magdeburg

- Algorithm

K-means algorithm

The Lloyd's algorithm, mostly known as k-means algorithm, is used to solve the k-means clustering problem and works as follows. First, decide the number of clusters k. Then:

1. Initialize the center of the clusters	$\mu_i =$ some value $, i = 1, \ldots, k$
2. Attribute the closest cluster to each data point	$\mathbf{c}_i = \{j : d(\mathbf{x}_j, \mu_i) \leq d(\mathbf{x}_j, \mu_l), l \neq i, j = 1, \ldots, n\}$
3. Set the position of each cluster to the mean of all data points belonging to that cluster	$\mu_i = \frac{1}{\lvert c_i \rvert} \sum_{j \in c_i} \mathbf{x}_j, \forall i$
4. Repeat steps 2-3 until convergence	
Notation	$\lvert \mathbf{c} \rvert =$ number of elements in $\mathbf{c}$

The algorithm eventually converges to a point, although it is not necessarily the minimum of the sum of squares. That is because the problem is non-convex and the algorithm is just a heuristic, converging to a local minimum. The algorithm stops when the assignments do not change from one iteration to the next.

- Objective function(Euclidean distance)

$$\mathrm{d}(\mathbf{p}, \mathbf{q}) = \mathrm{d}(\mathbf{q}, \mathbf{p}) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2 + \cdots + (q_n - p_n)^2}$$

$$= \sqrt{\sum_{i=1}^{n} (q_i - p_i)^2}.$$

Fig: Euclidean distance between p and q vectors of n feature space

- Kmeans Example

Step 1:

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

In this case the 2 centroid are: m1=(1.0,1.0) and m2=(5.0,7.0).

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)

- KMeans Example

Step 2:

- Thus, we obtain two clusters containing:

  {1,2,3} and {4,5,6,7}.
- Their new centroids are:

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

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

$$= (4.12, 5.38)$$

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

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

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

We start calculating distances for the next step ->

- KMeans Example

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

- KMeans Example

  - Step 4 :

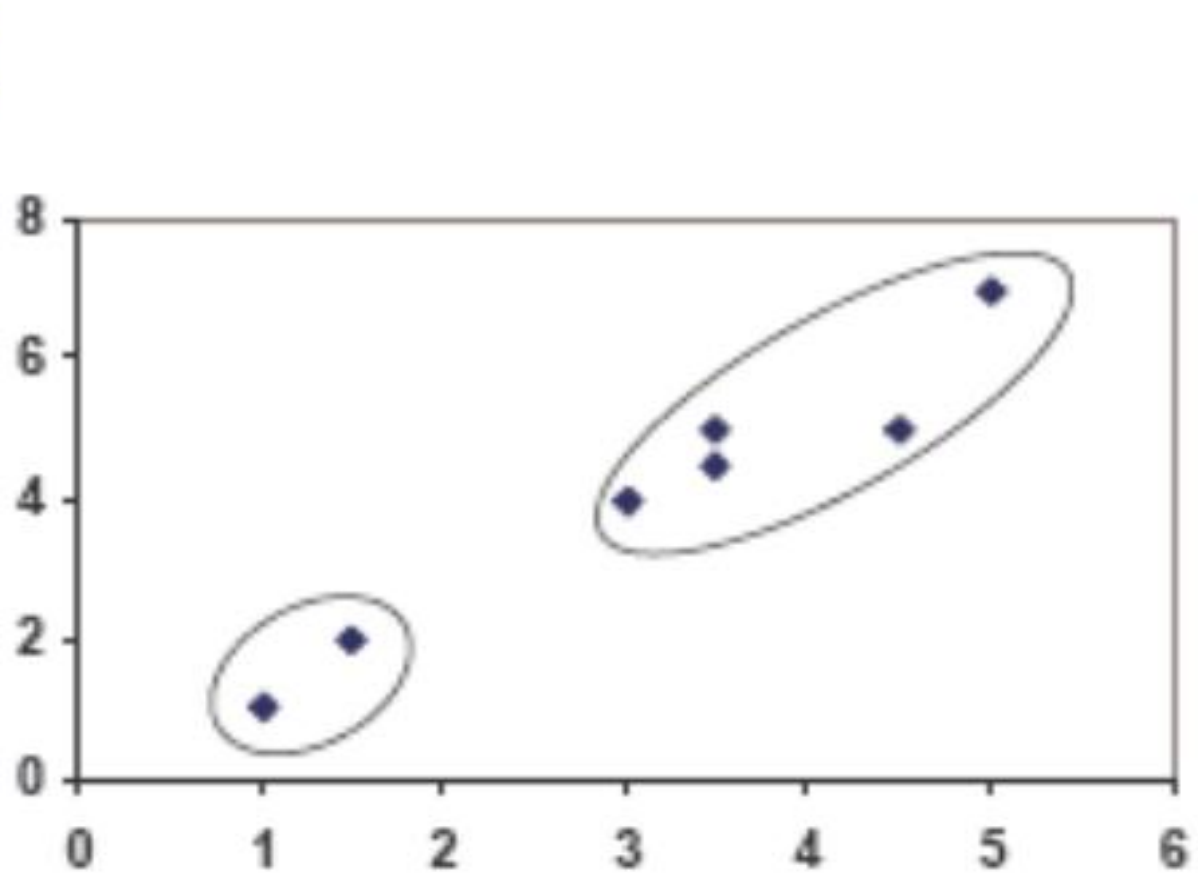
    The clusters obtained are:

    {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}.

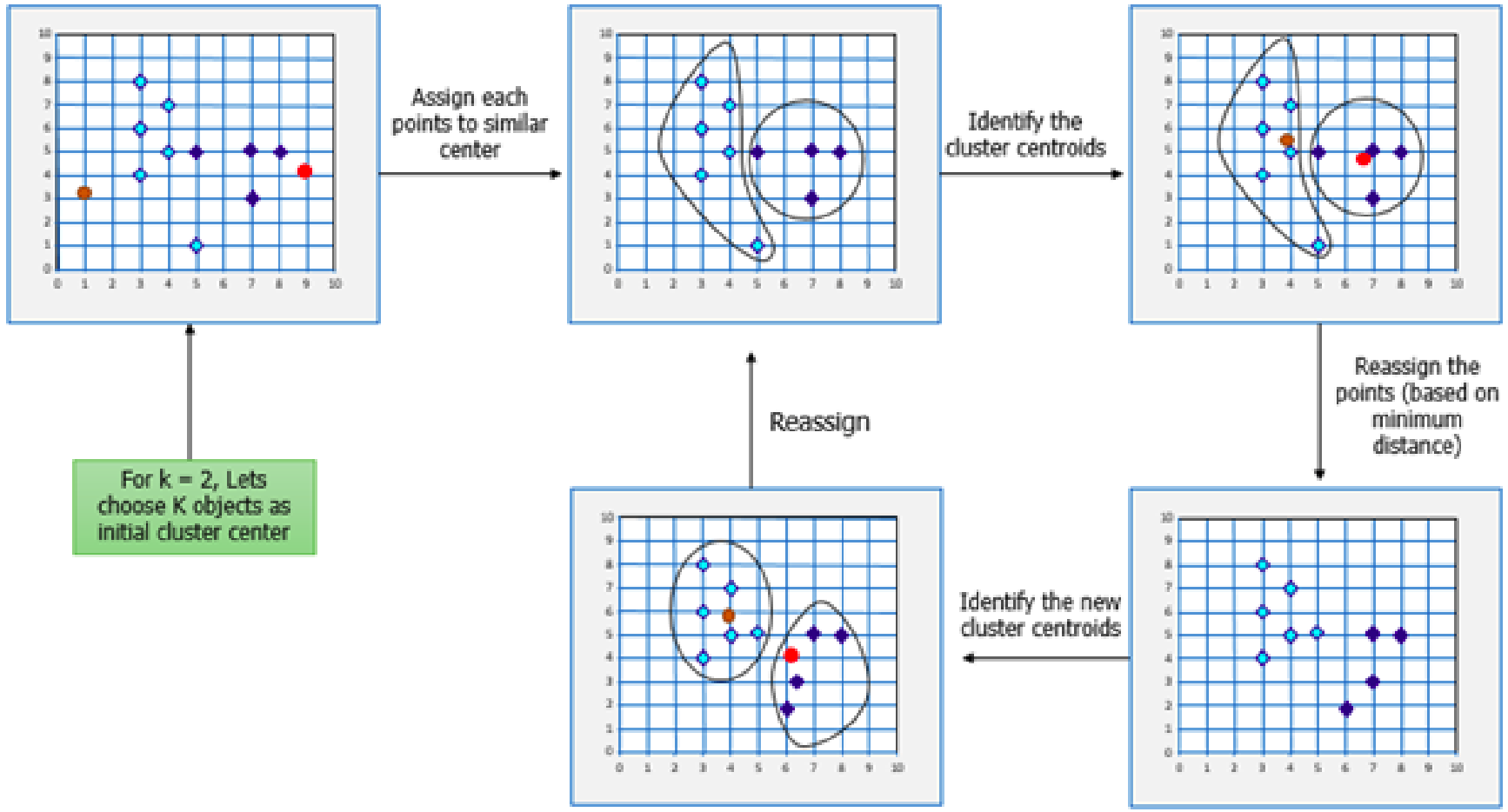
Individual	Centroid 1	Centroid 2
1	0.56	5.02
2	0. 56	3.92
3	3.05	1.42
4	6.66	2.20
5	4.16	0.41
6	4.78	0.61
7	3.75	0.72

- KMeans Example



- KMeans clustering step by step

The step by step process:



- KMeans Clustering in 2D & 3D

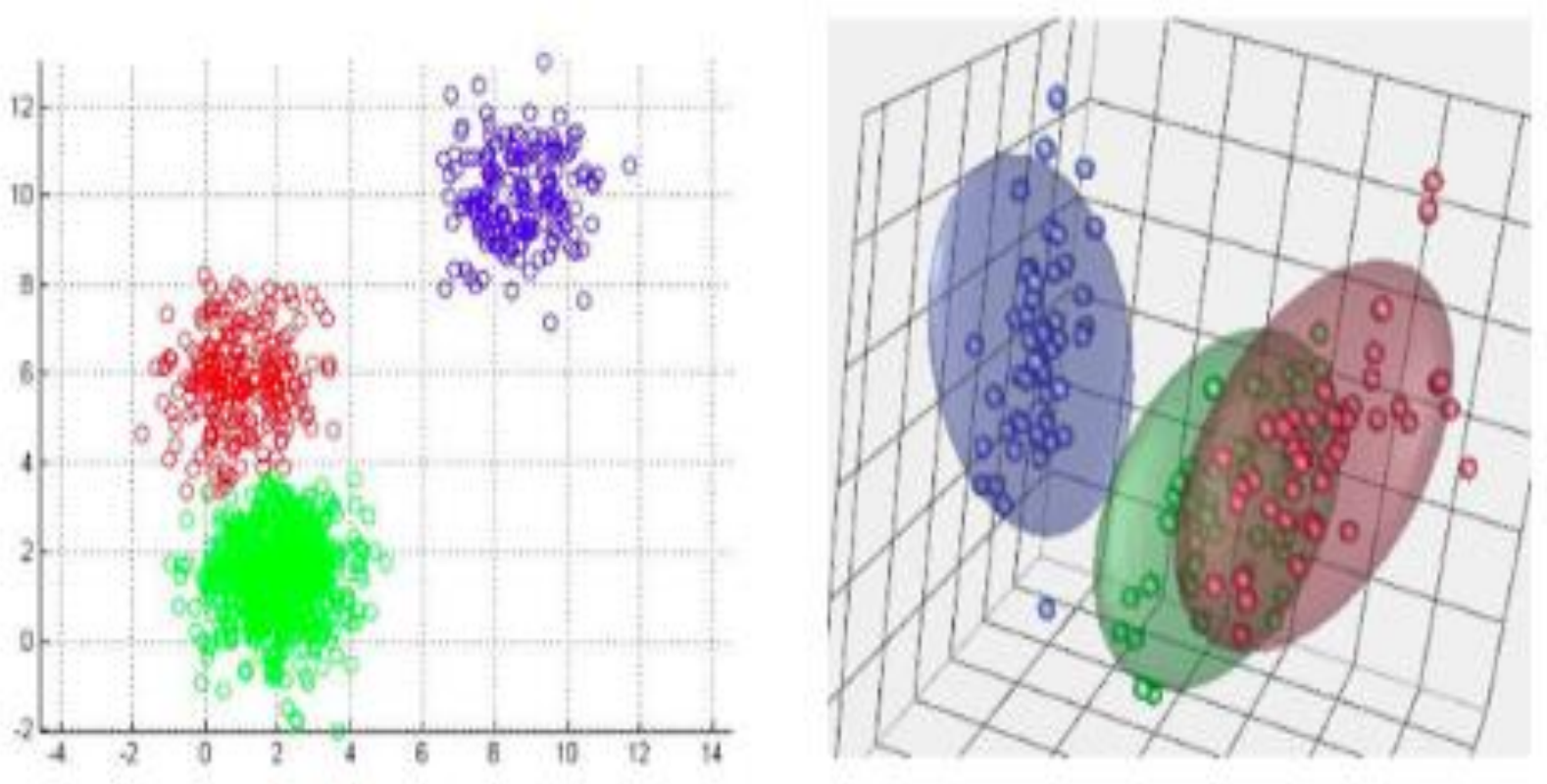


Fig: KMeans in 2D and 3D.

- Weakness of KMeans

1. When the numbers of data are not so many, initial grouping will determine the cluster significantly.
2. The number of cluster, K, must be determined before hand. Its disadvantage is that it does not yield the same result with each run, since the resulting clusters depend on the initial random assignments.
3. We never know the real cluster, using the same data, because if it is inputted in a different order it may produce different cluster if the number of data is few.
4. It is sensitive to initial condition. Different initial condition may produce different result of cluster. The algorithm may be trapped in the *local optimum*.

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