K-MEANS CLUSTERING

INTRODUCTION-
What is clustering?

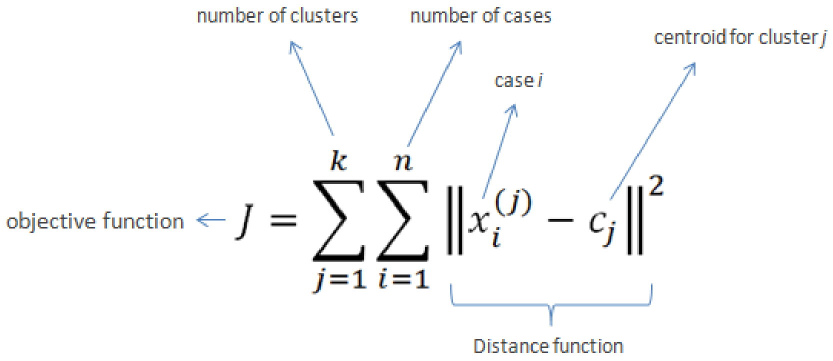
- **Clustering** is the classification of objects into different groups, or more precisely, the partitioning of a data set into subsets (clusters), so that the data in each subset (ideally) share some common trait - often according to some defined distance measure.

K-MEANS CLUSTERING

- The **k-means algorithm** is an algorithm to cluster *n* objects based on attributes into *k* partitions, where $k < n$.

K-MEANS CLUSTERING

- An algorithm for partitioning (or clustering) N data points into K disjoint subsets S_j (k clusters) containing data points so as to minimize the sum-of-squares criterion



number of clusters

number of cases

case *i*

centroid for cluster *j*

objective function ←

$$J = \sum_{j=1}^{k} \sum_{i=1}^{n} \underbrace{\left\| x_i^{(j)} - c_j \right\|^2}_{\text{Distance function}}$$

where x_i is a vector representing the the n^{th} data point and c_j is the geometric centroid of the data points in S_j (k^{th} cluster)

K-MEANS CLUSTERING

- Simply speaking k-means clustering is an algorithm to classify or to group the objects based on attributes/features into K number of group.
- K is positive integer number.
- The grouping is done by minimizing the sum of squares of distances between data and the corresponding cluster centroid.

How the K-Mean Clustering algorithm works?

- **Initialization:** once the number of groups, *k* has been chosen, *k* centroids are established in the data space, for instance, choosing them randomly.
- **Assignment of objects to the centroids:** each object of the data is assigned to its nearest centroid.
- **Centroids update:** The position of the centroid of each group is updated taking as the new centroid the average position of the objects belonging to said group.

K-MEANS CLUSTERING

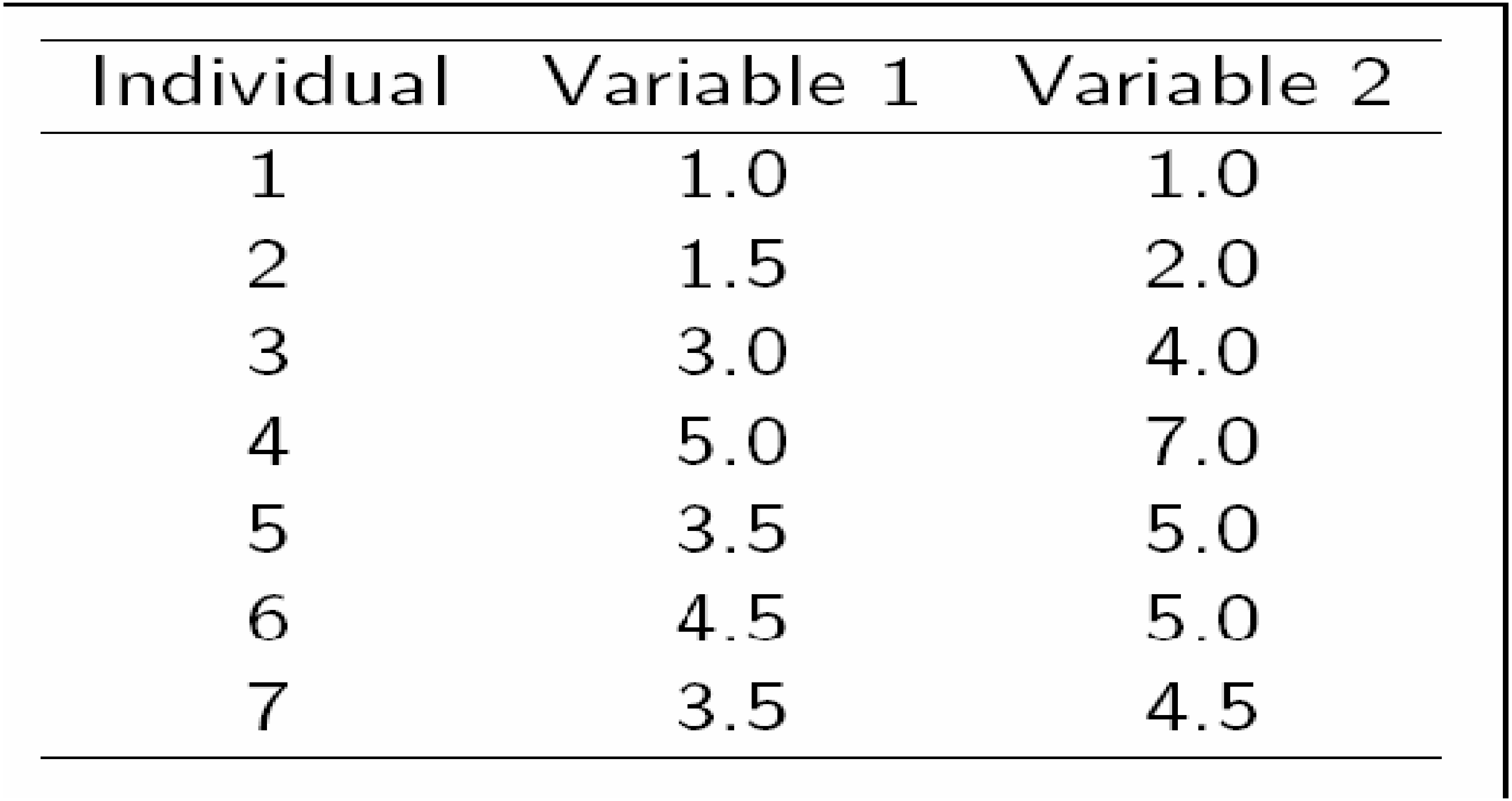
- **Step 1:** Begin with a decision on the value of k = number of clusters.
- **Step 2**: Put any initial partition that classifies the data into k clusters. You may assign the training samples randomly, or systematically as the following:

1. Take the first k training sample as single-element clusters
2. Assign each of the remaining (N-k) training sample to the cluster with the nearest centroid. After each assignment, recompute the centroid of the clusters.

K-MEANS CLUSTERING

- **Step 3:** Take each sample in sequence and compute its distance from the centroid of each of the clusters. If a sample is not currently in the cluster with the closest centroid, switch this sample to that cluster and update the centroid of the cluster gaining the new sample and the cluster losing the sample.
- **Step 4 .** Repeat step 3 until convergence is achieved, that is until a pass through the training sample causes no new assignments.

A Simple example showing the implementation of k-means algorithm (using K=2)

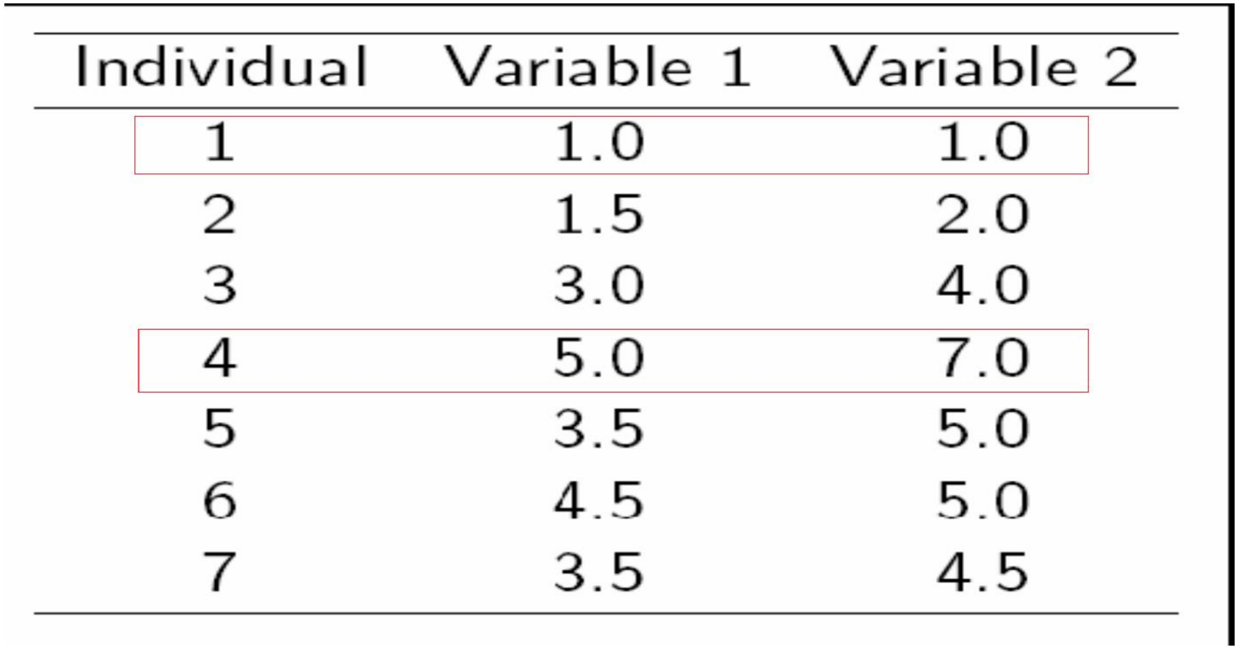


Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

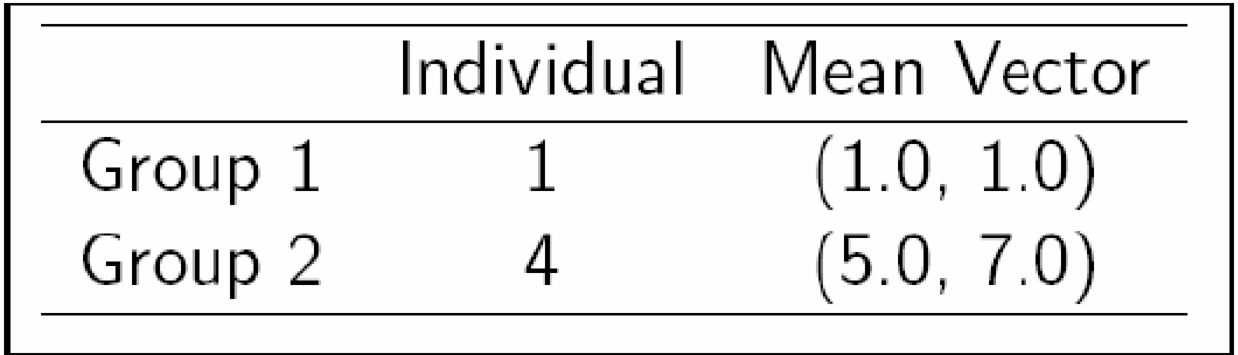
Step 1:

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)

Step 2:

- Thus, we obtain two clusters containing:

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

$$d(m_1,2)=\sqrt{|1.0-1.5|^2+|1.0-2.0|^2}=1.12$$
$$d(m_2,2)=\sqrt{|5.0-1.5|^2+|7.0-2.0|^2}=6.10$$

- Their new centroids are:

$$m_1=(\frac{1}{3}(1.0+1.5+3.0),\frac{1}{3}(1.0+2.0+4.0))=(1.83,2.33)$$
$$m_2=(\frac{1}{4}(5.0+3.5+4.5+3.5),\frac{1}{4}(7.0+5.0+5.0+4.5))=(4.12,5.38)$$

Individual	Centroid 1	Centroid 2
1	0	7.21
2	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

Distance from individual points to the two centroids

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

Distance from individual points to the two centroids

Step 4 :

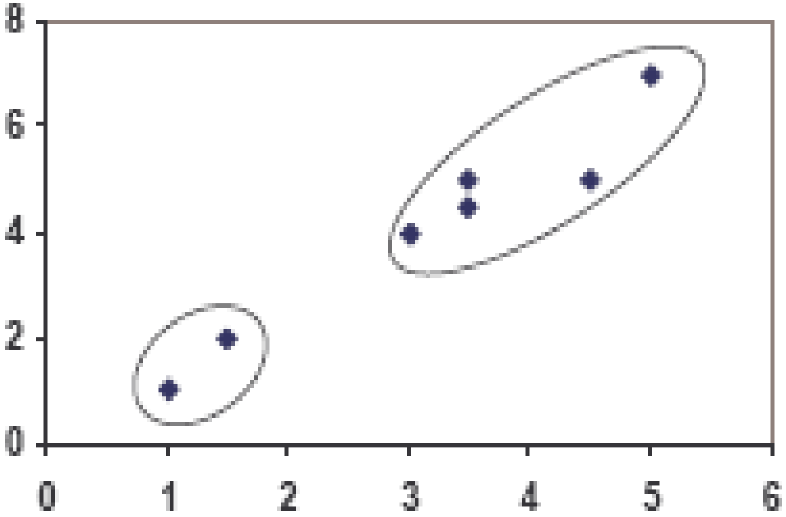
The clusters obtained are:

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

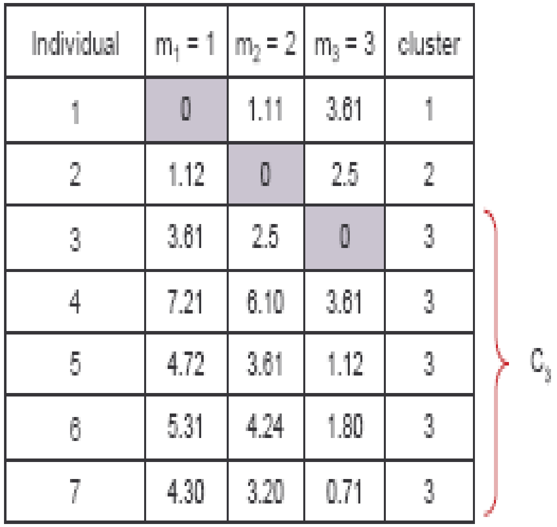
- Therefore, there is no change in the cluster.
- Thus, the algorithm comes to a halt here and final result consist of 2 clusters {1,2} and {3,4,5,6,7}.

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

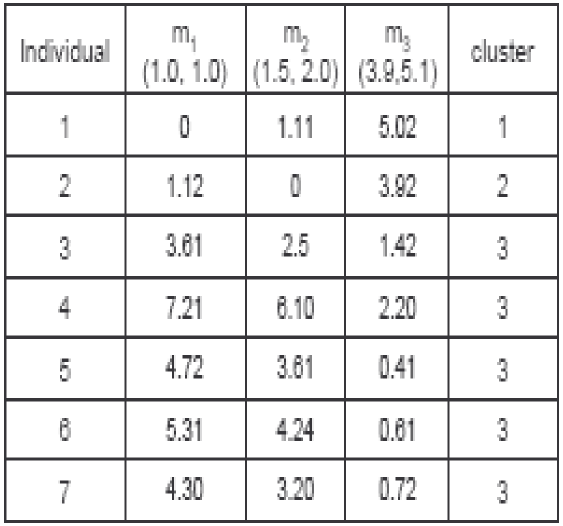


(with K=3)



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)

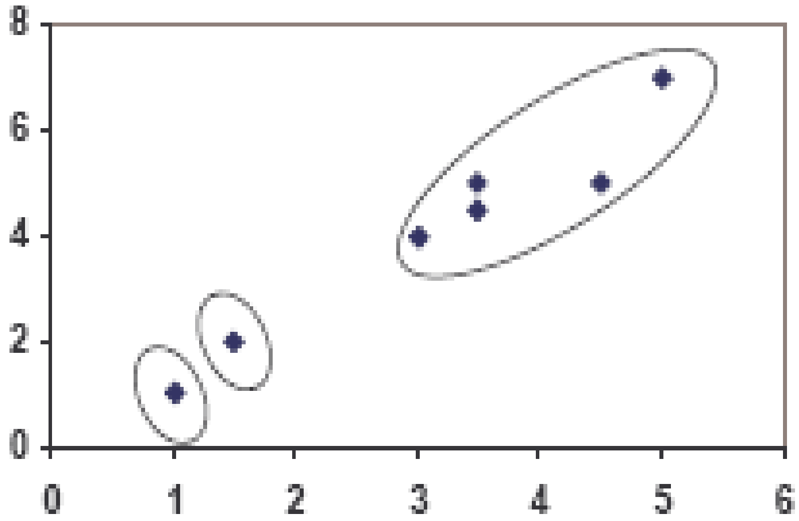


Individual	m_1 (1.0, 1.0)	m_2 (1.5, 2.0)	m_3 (3.9,5.1)	cluster
1	0	1.11	5.02	1
2	1.12	0	3.92	2
3	3.61	2.5	1.42	3
4	7.21	6.10	2.20	3
5	4.72	3.61	0.41	3
6	5.31	4.24	0.61	3
7	4.30	3.20	0.72	3

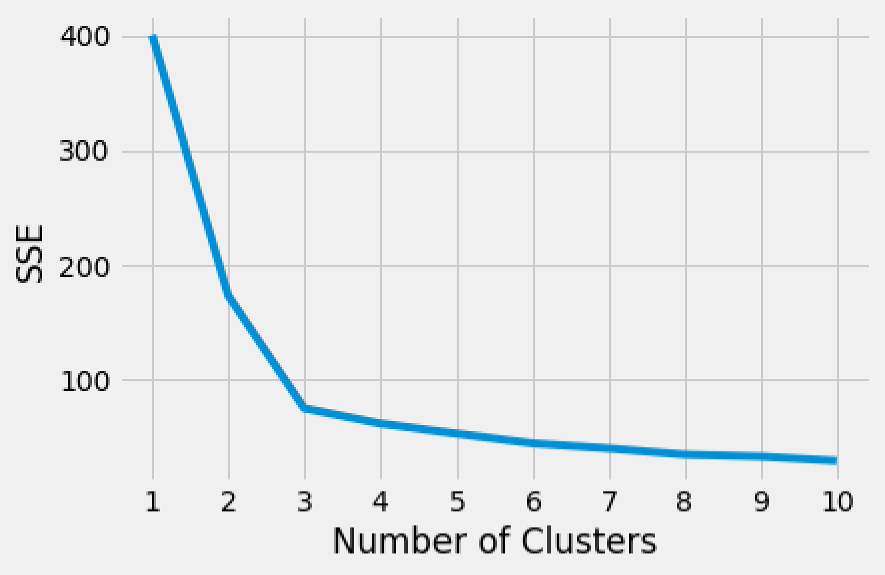
Step 1

Step 2

PLOT



Elbow Method (choosing the number of clusters)



Elbow Method

Another Method - silhouette coefficient (self study)

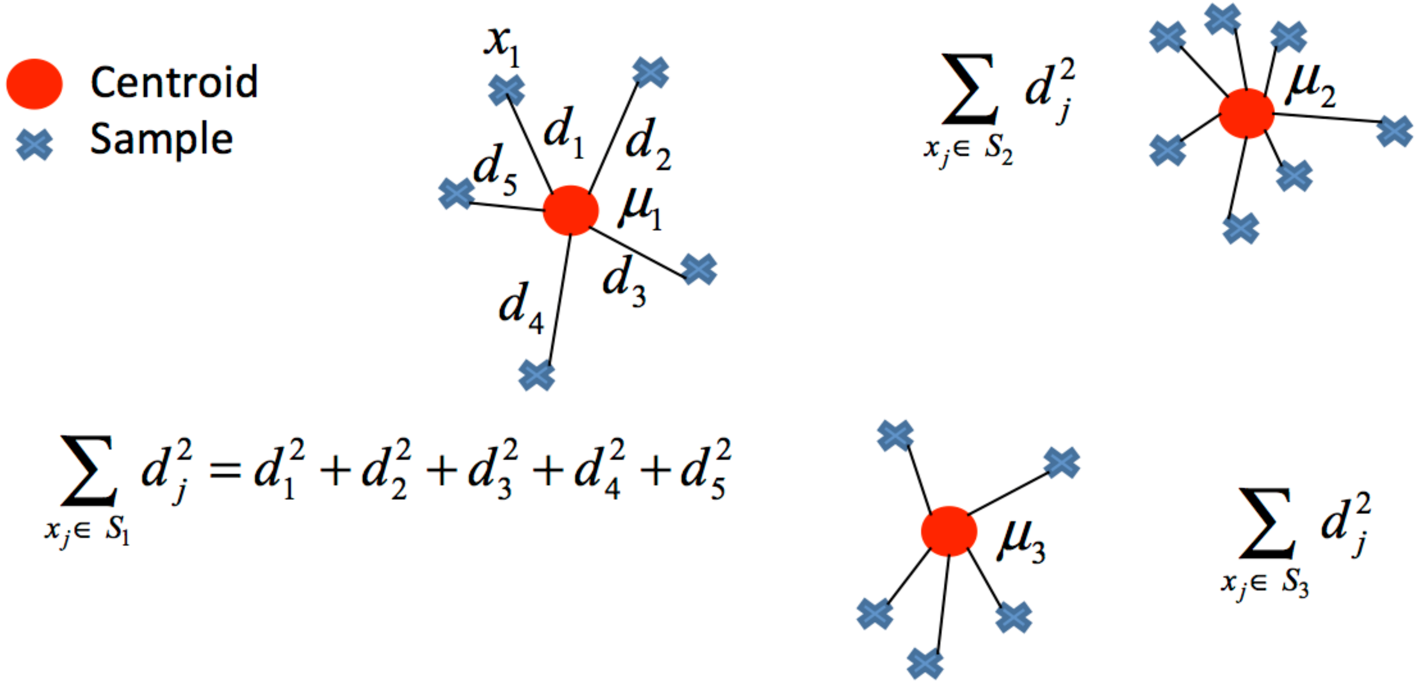
Weaknesses of K-Mean Clustering

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*.

Applications of K-Mean Clustering

- It is relatively *efficient and fast.*
- k-means clustering can be applied to *machine learning or data mining*
- *Used on acoustic data in speech understanding to convert waveforms into one of k categories or Image Segmentation.*

Visualization: Example



● Centroid

✖ Sample

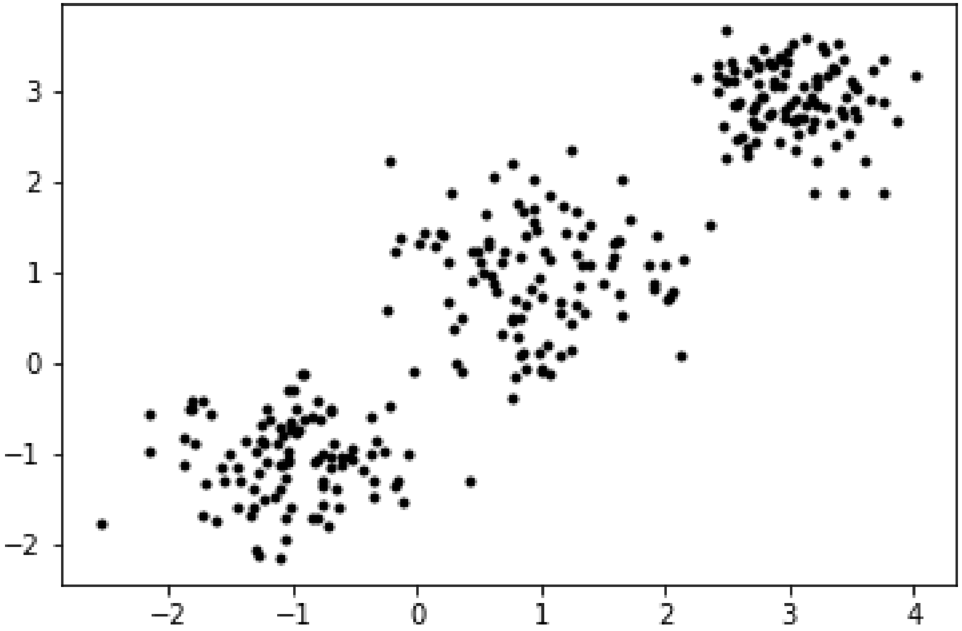
$$\sum_{x_j \in S_1} d_j^2 = d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2$$

$$\sum_{x_j \in S_2} d_j^2$$

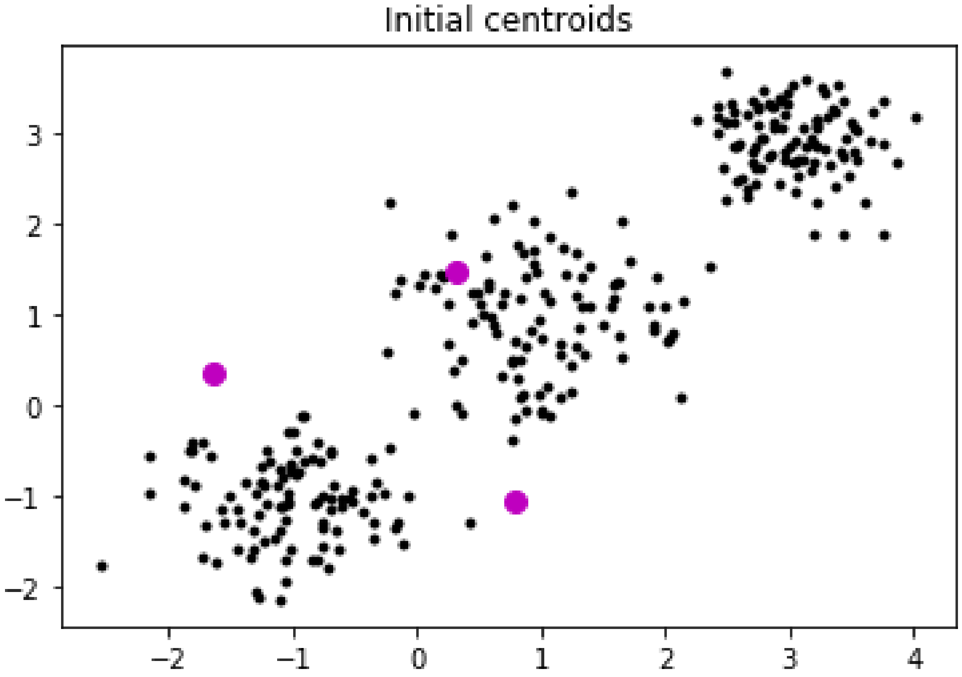
$$\sum_{x_j \in S_3} d_j^2$$

$$\min_S E(\mu_i) = \sum_{x_j \in S_1} d_j^2 + \sum_{x_j \in S_2} d_j^2 + \sum_{x_j \in S_3} d_j^2$$

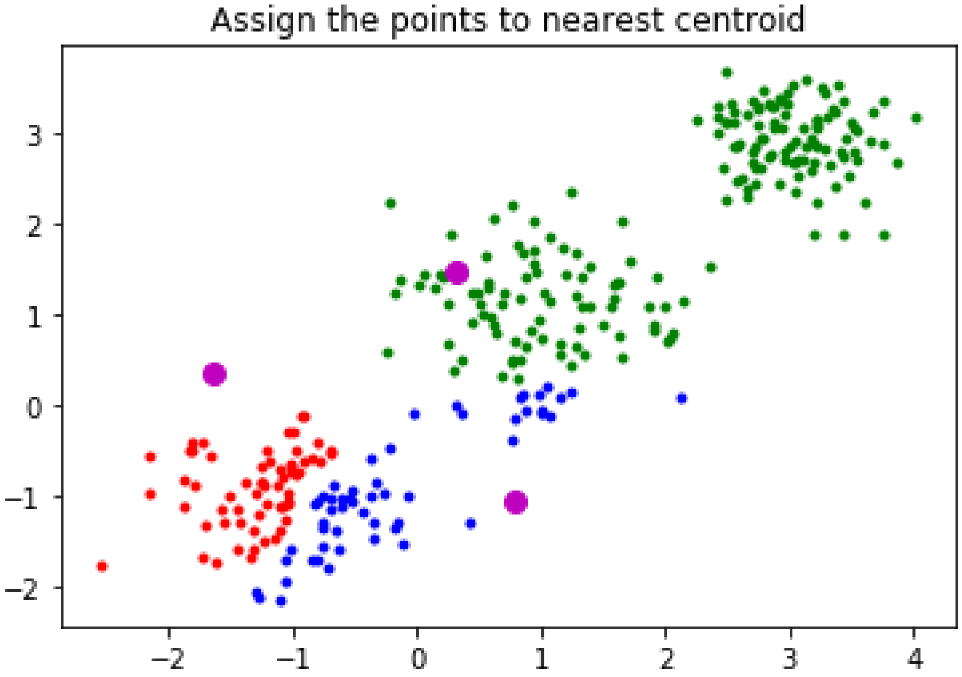
Visualization: Example



Visualization: Example



Visualization: Example



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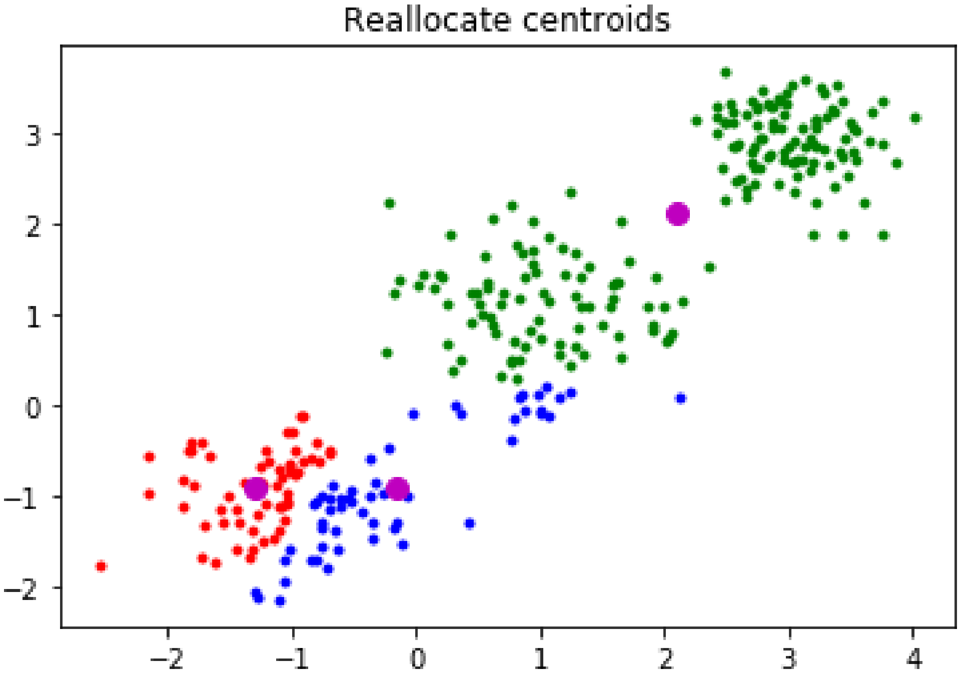

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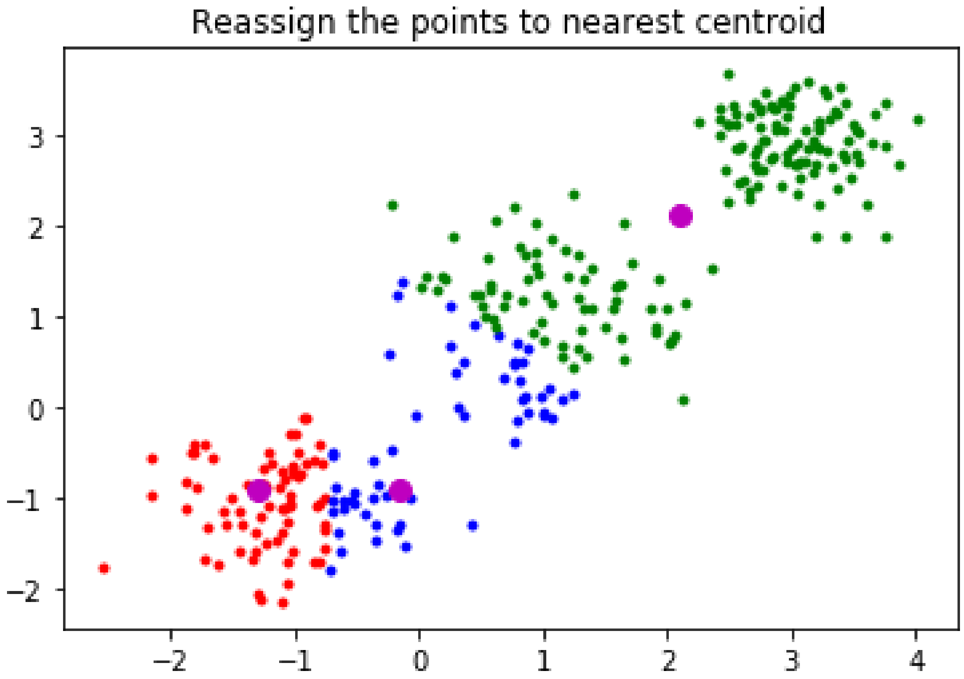

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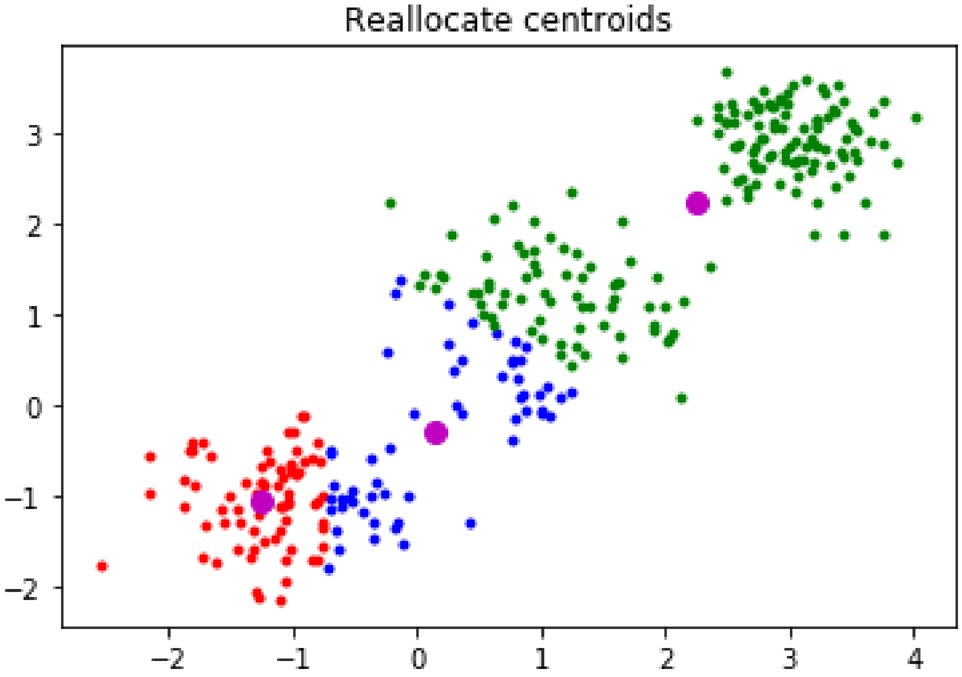

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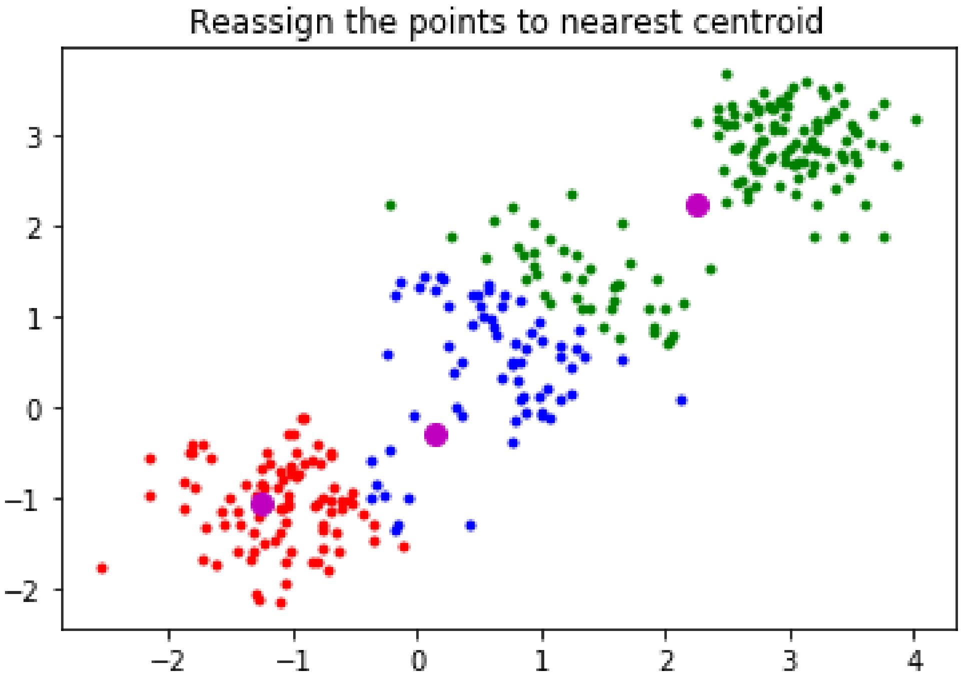

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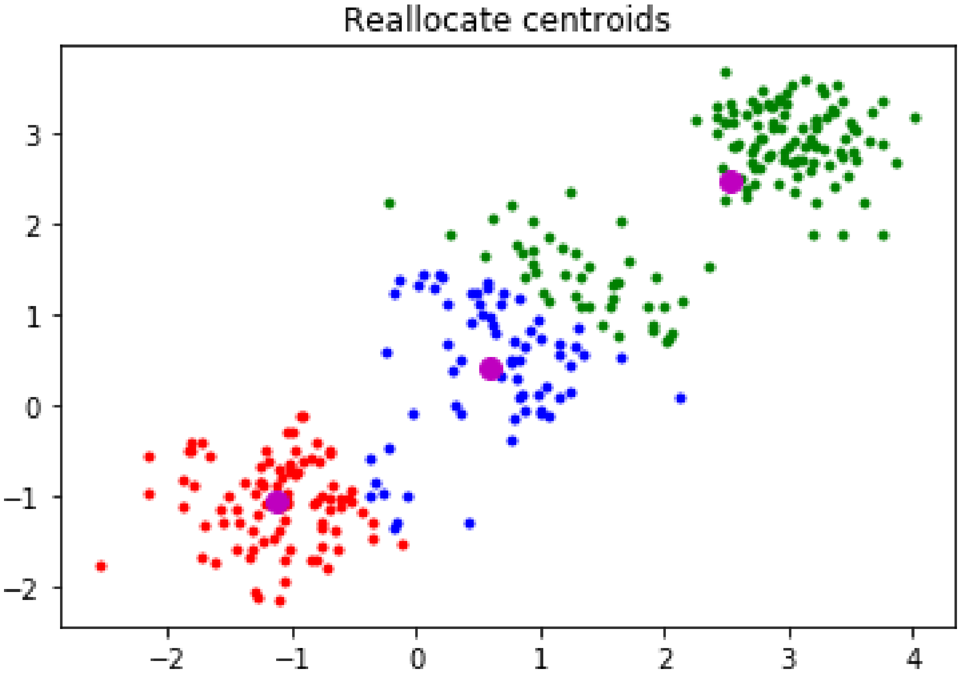

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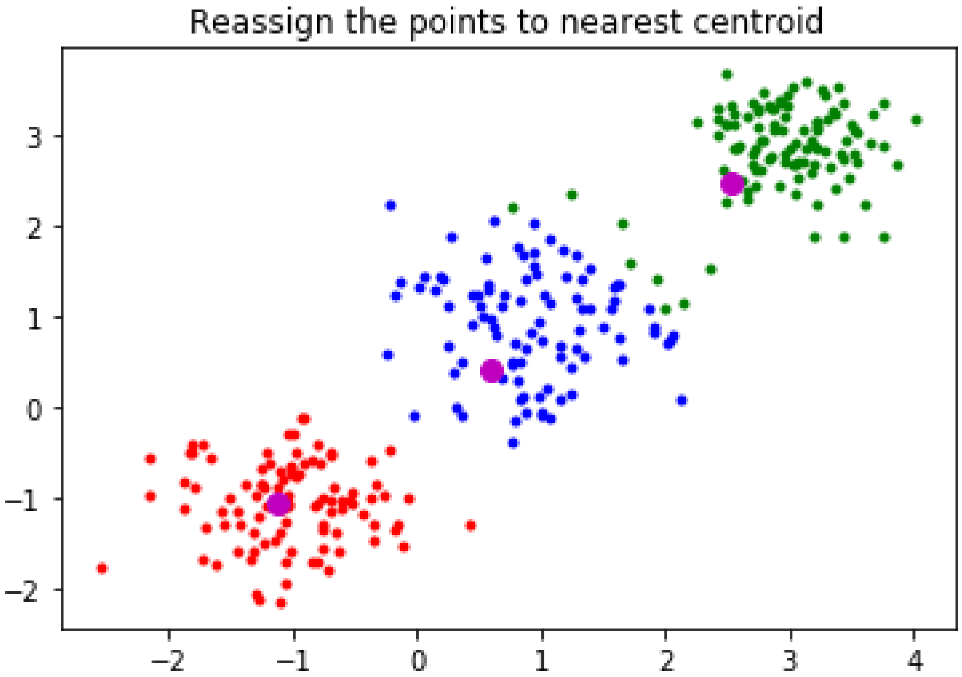

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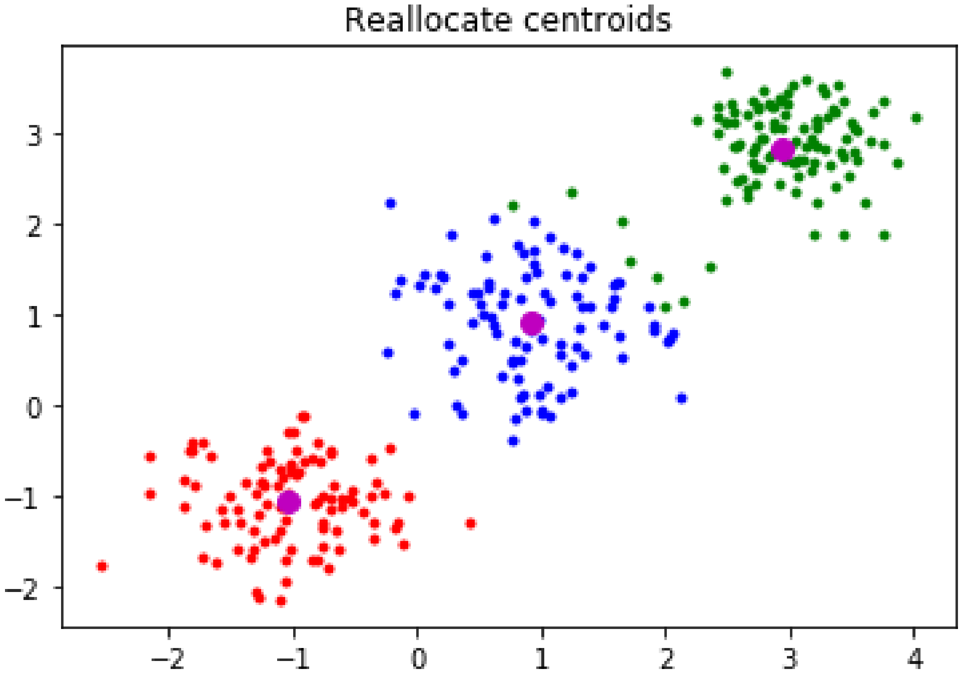

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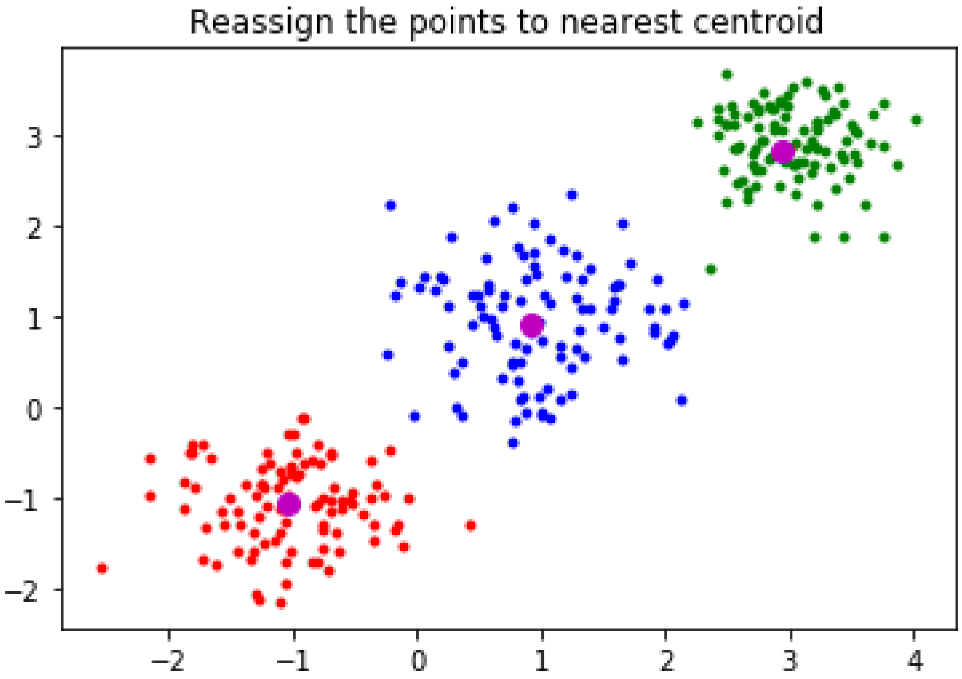

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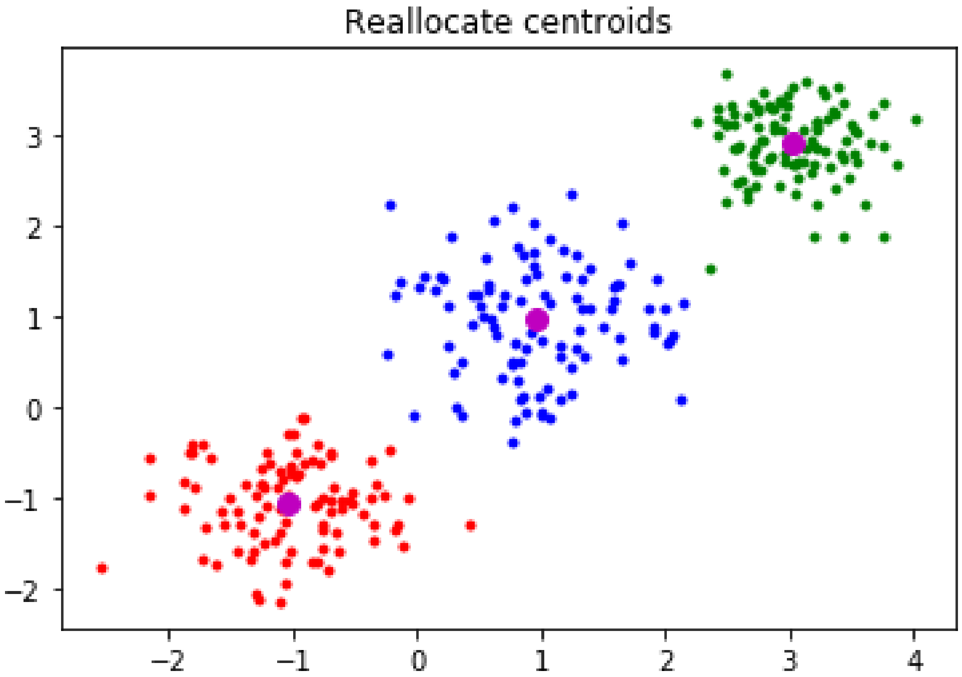

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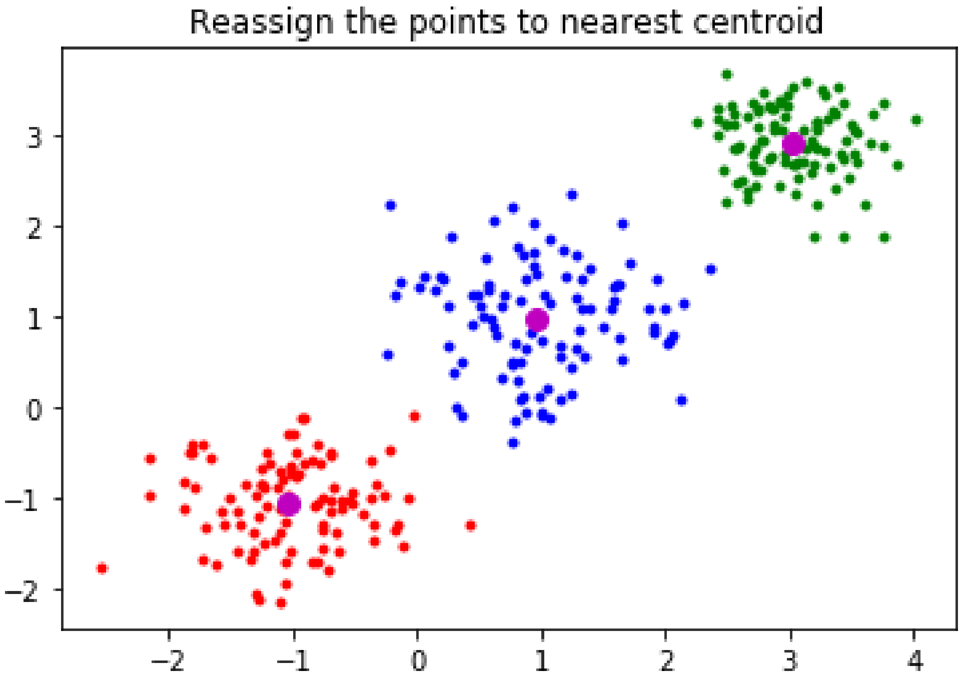

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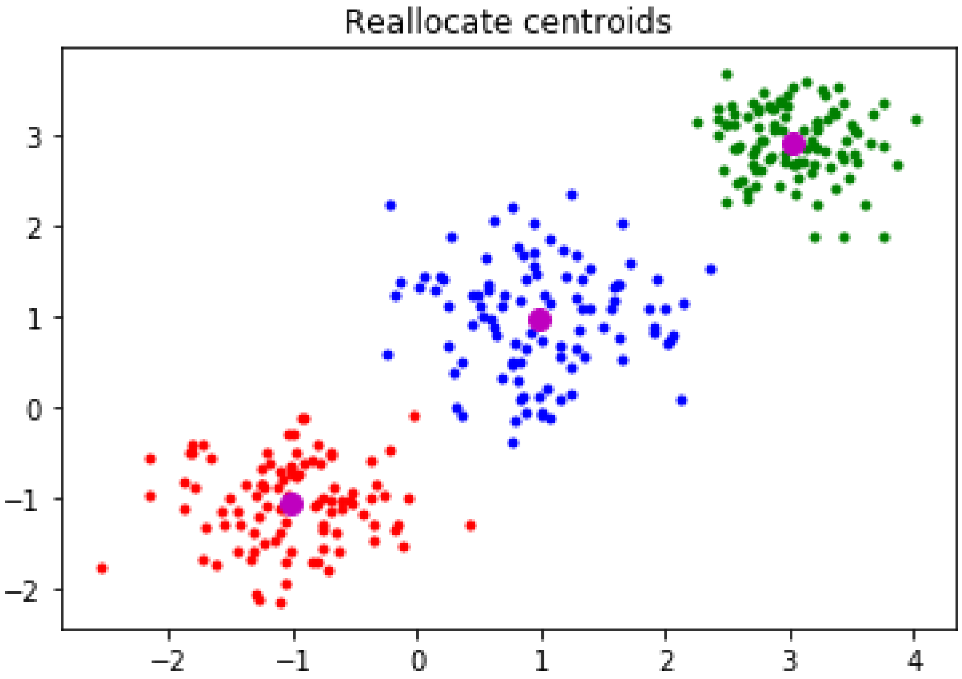
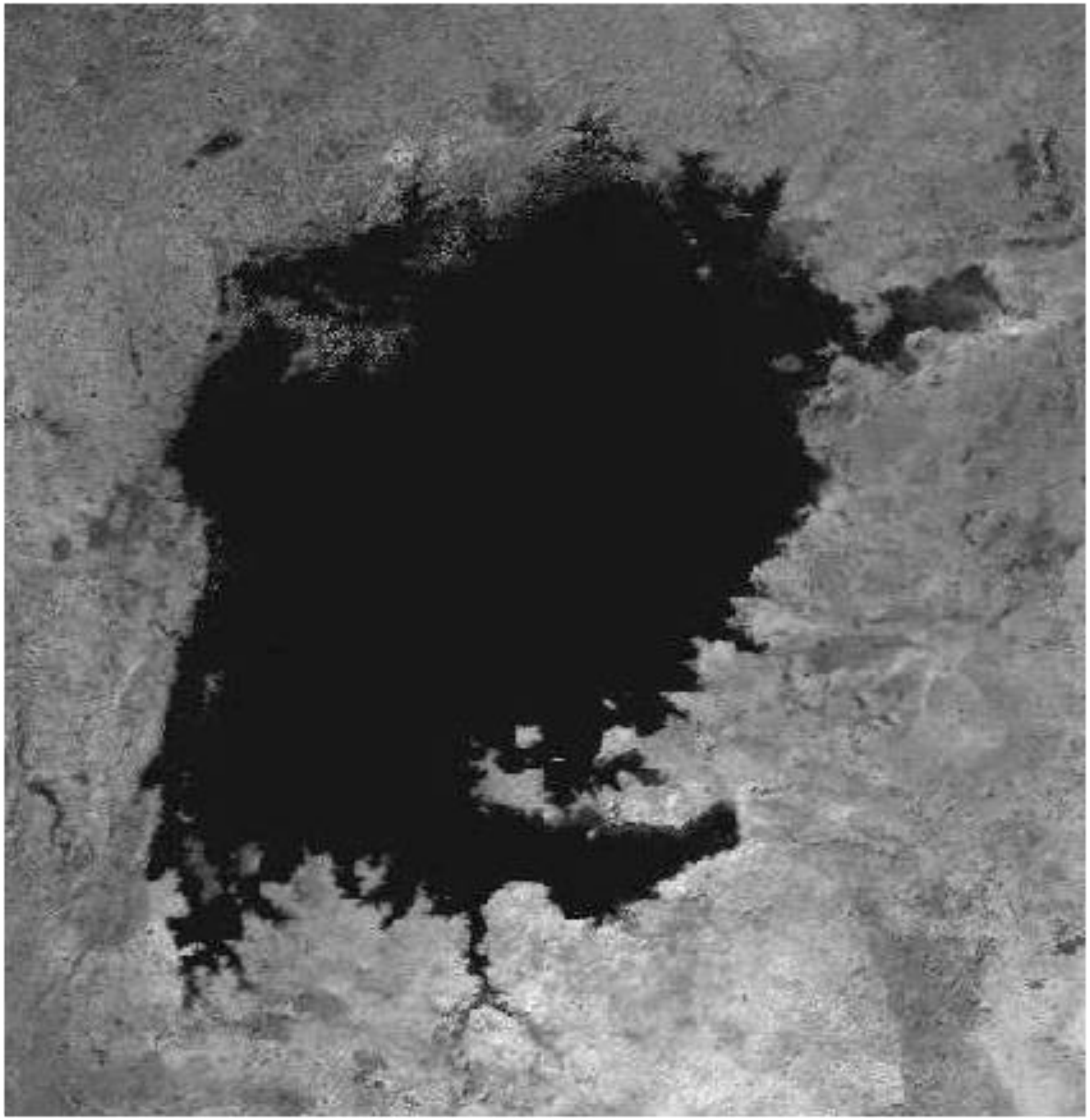
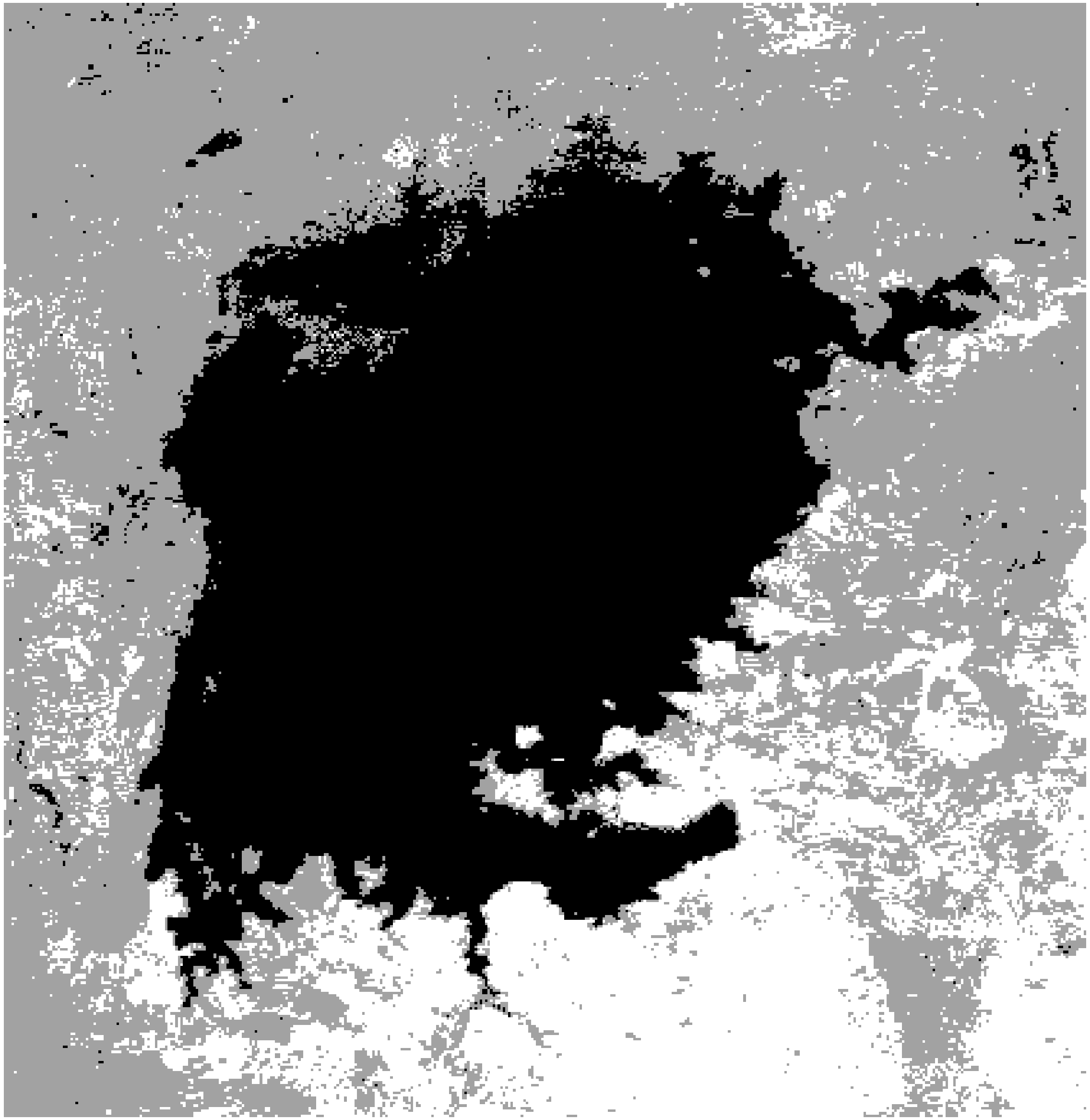


Application: Segmentation





Segmentation