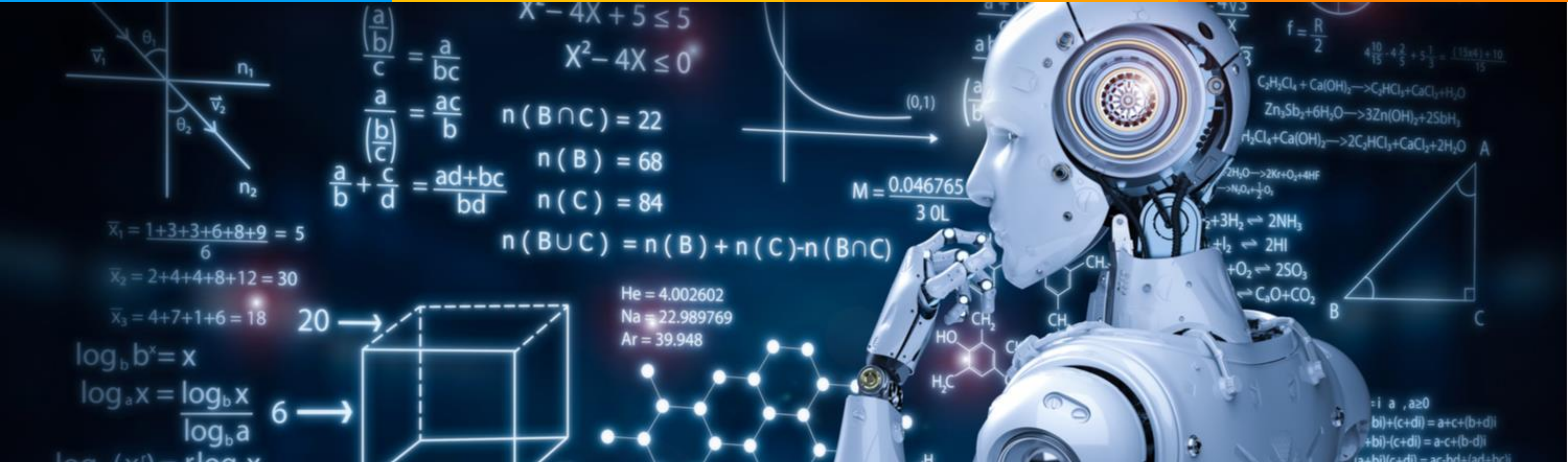
Duration: 60 min | Srikanth Shenoy | AML 5102 | M.E. AI & ML



Lecture 13: K Means Clustering

Recap

- Clustering properties & metrics
  - Inertia (WCSS), Silhouette score, Dunn Index
- Elbow plot, Silhouette plot

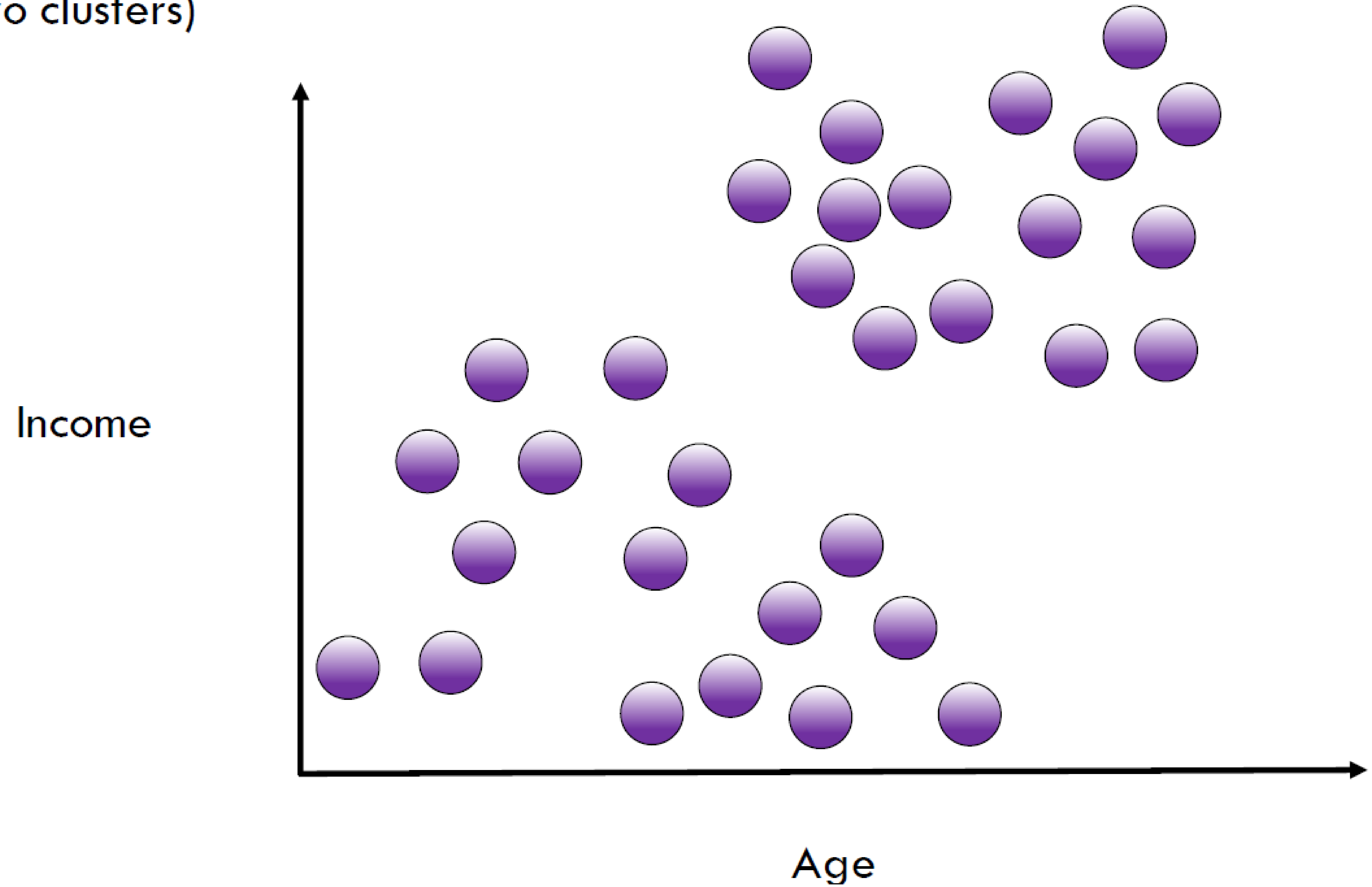
K-means clustering algorithm

K-Means Algorithm – Input and outputs

- Input:
  - Set of data points xi
  - K
  - No labels
- Output:
  - Grouping of data points into K clusters
  - A centroid for each group - prototypical representation of the group

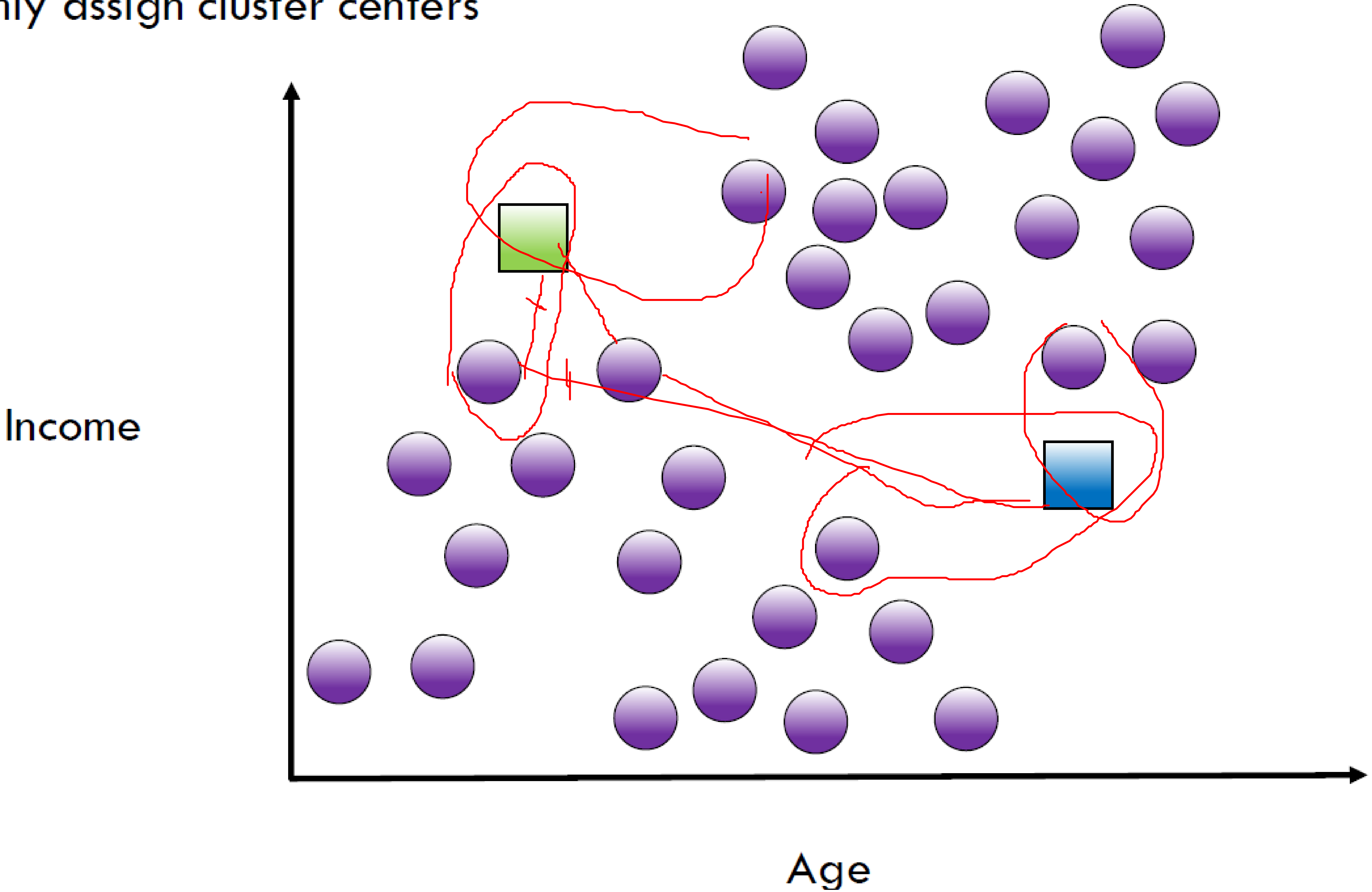
K-Means Algorithm

K = 2 (find two clusters)



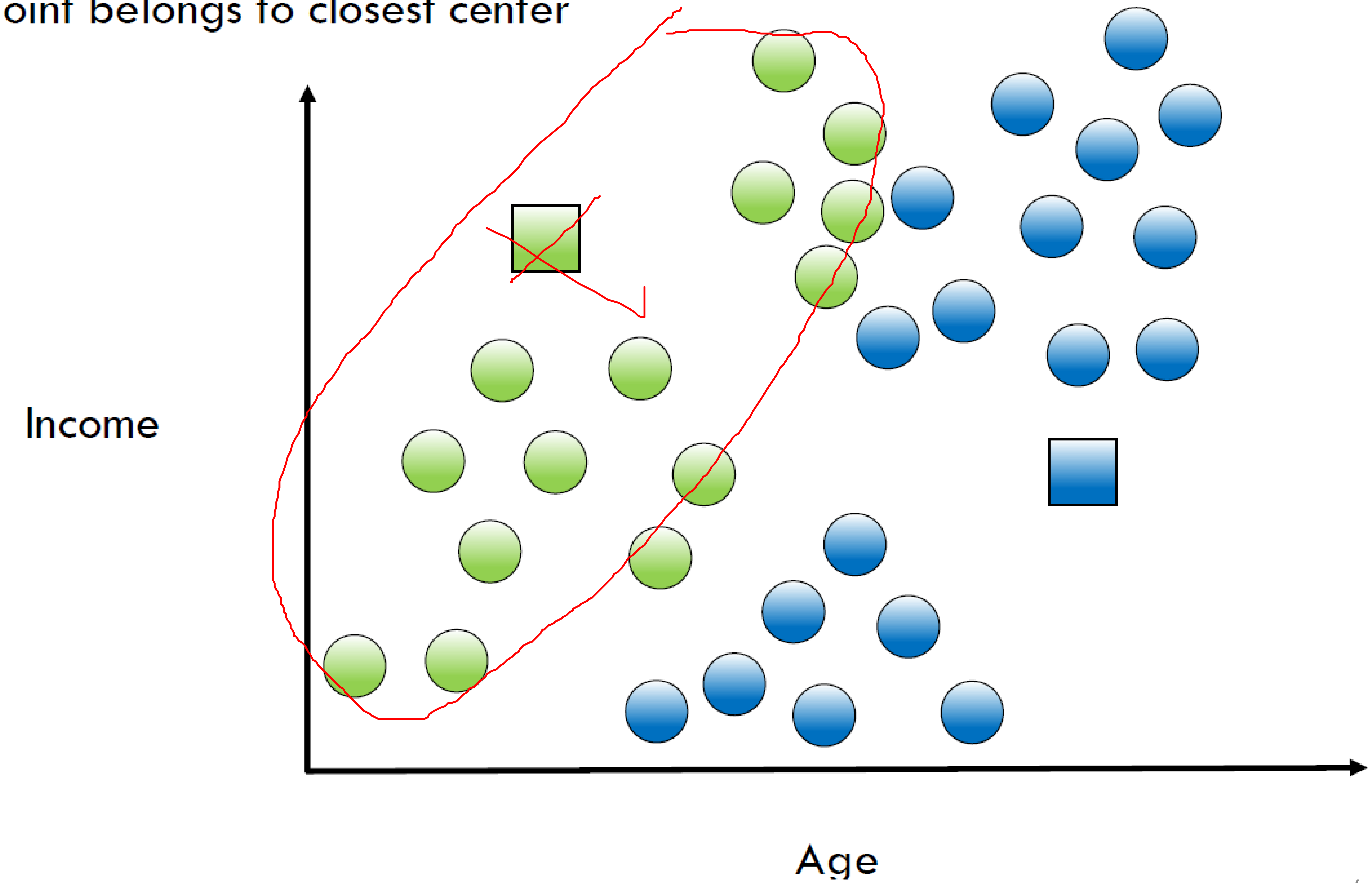
K-Means Algorithm

K = 2, Randomly assign cluster centers



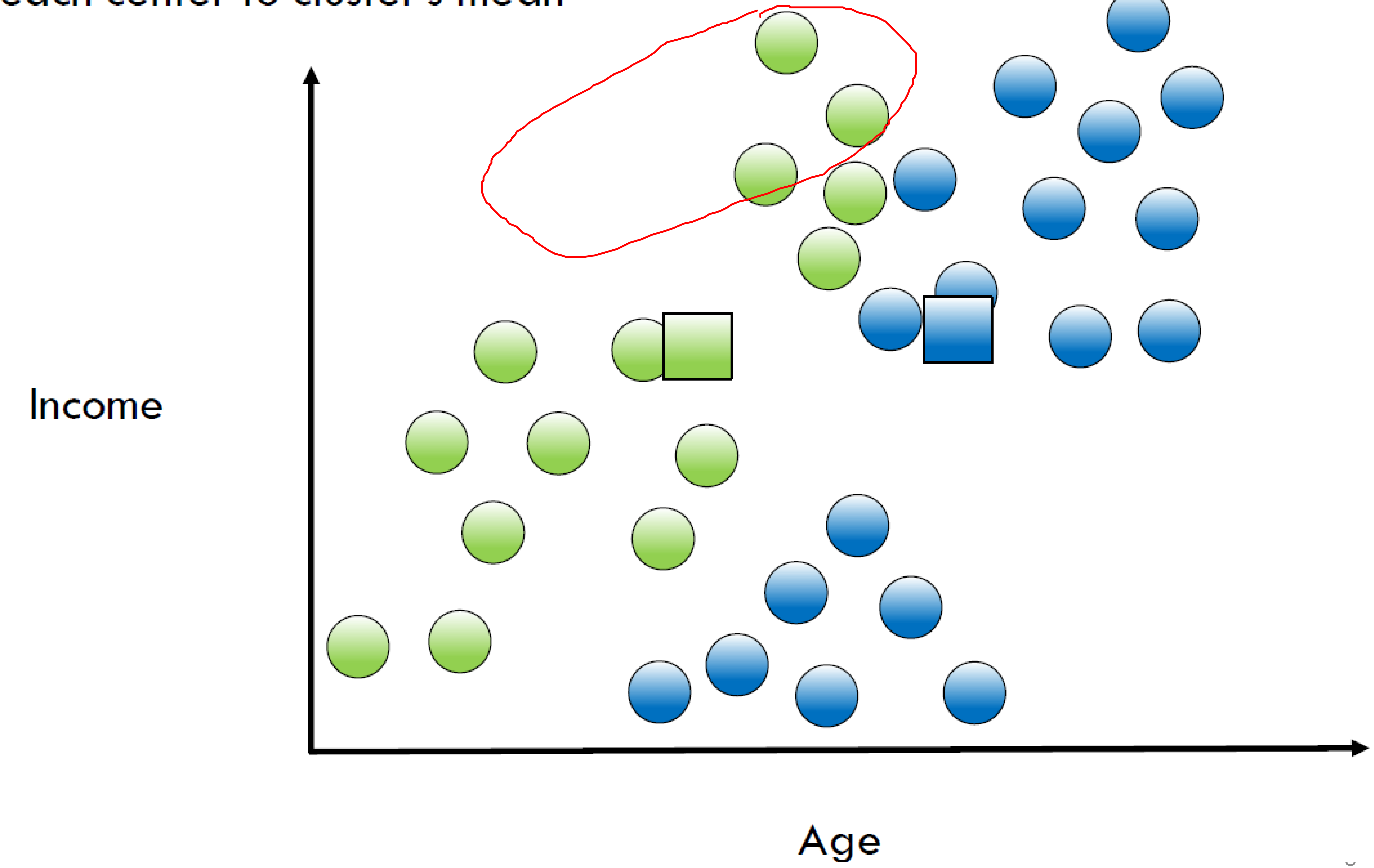
K-Means Algorithm

K = 2, Each point belongs to closest center



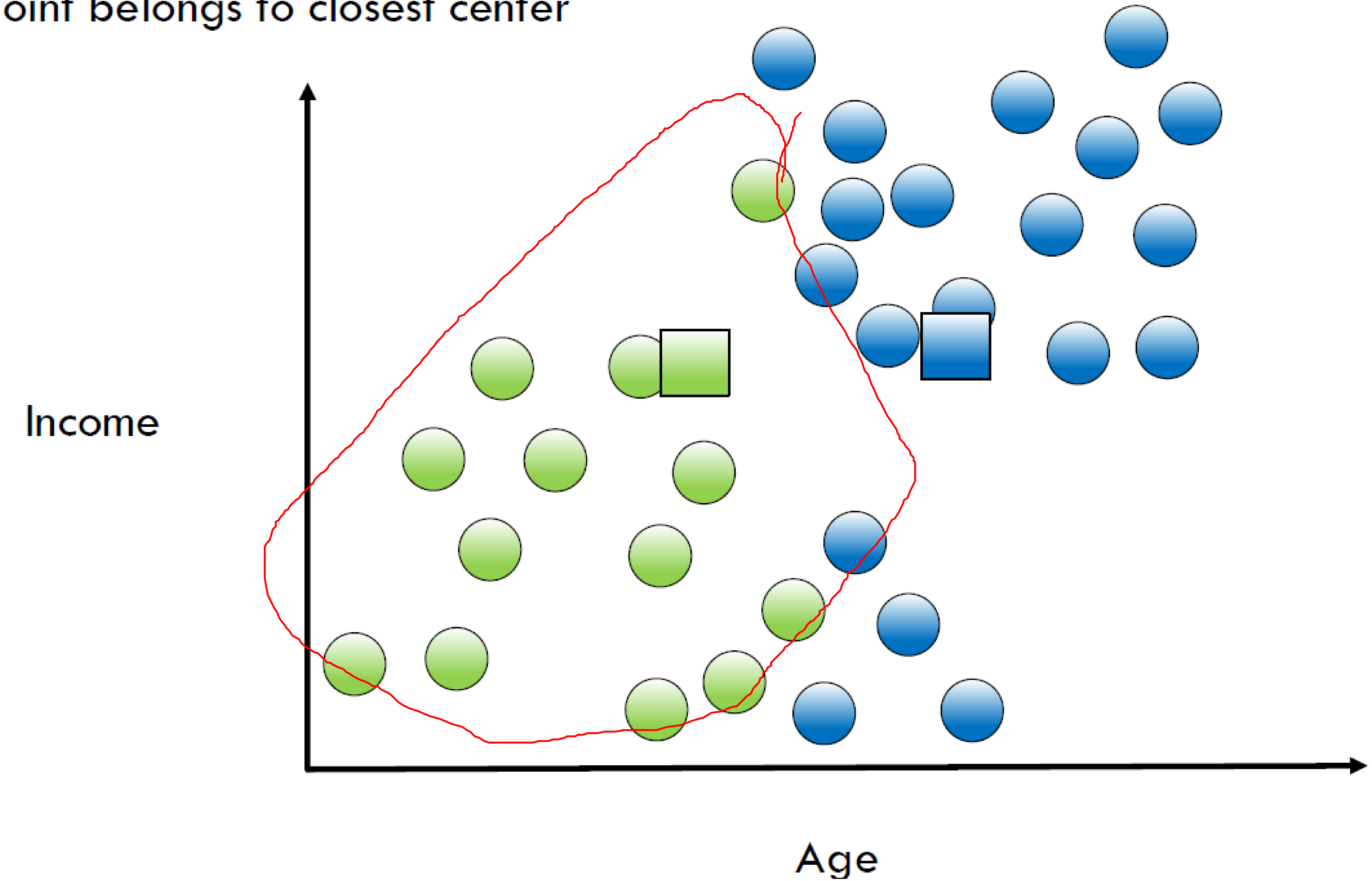
K-Means Algorithm

K = 2, Move each center to cluster's mean



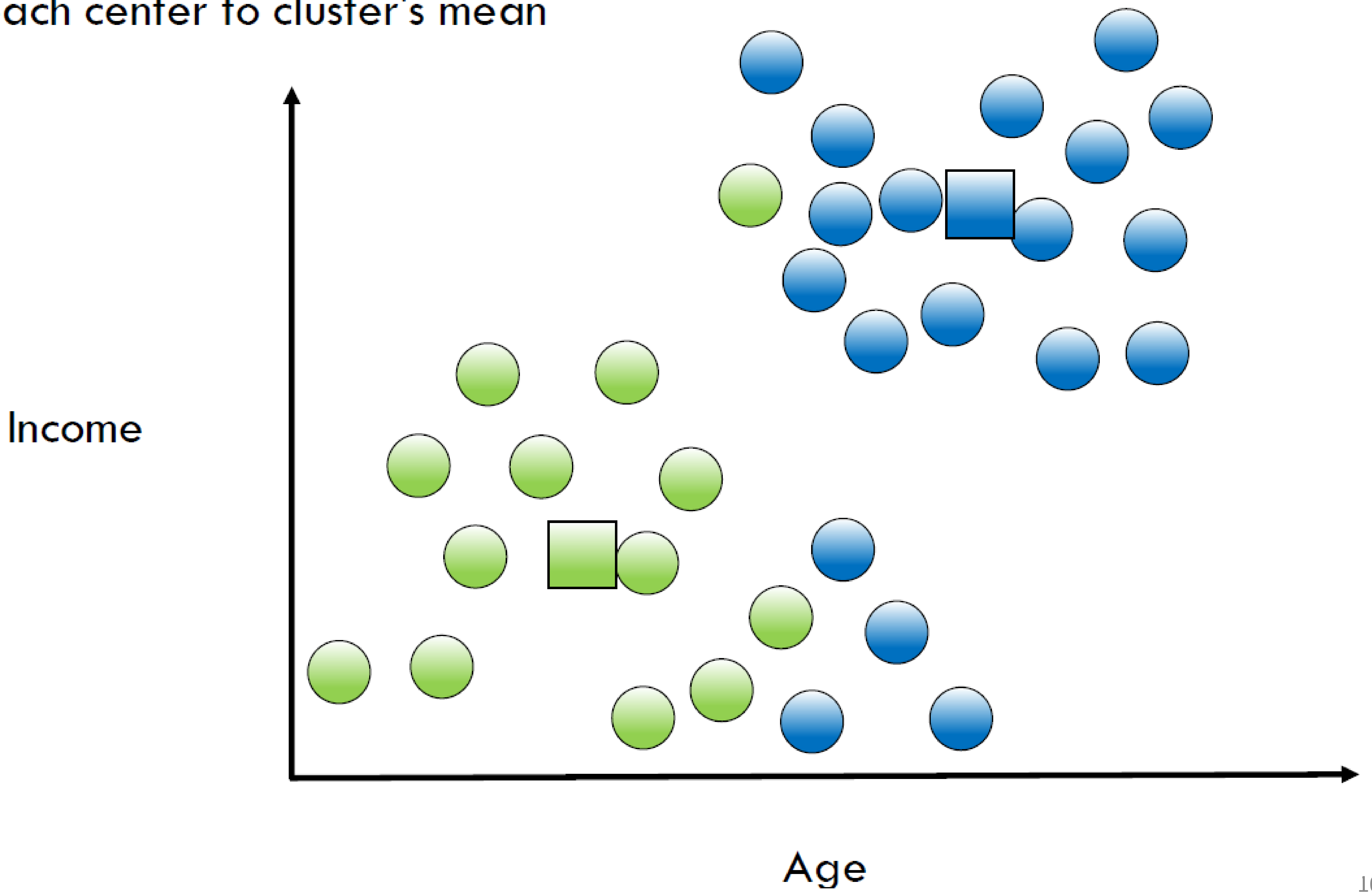
K-Means Algorithm

K = 2, Each point belongs to closest center



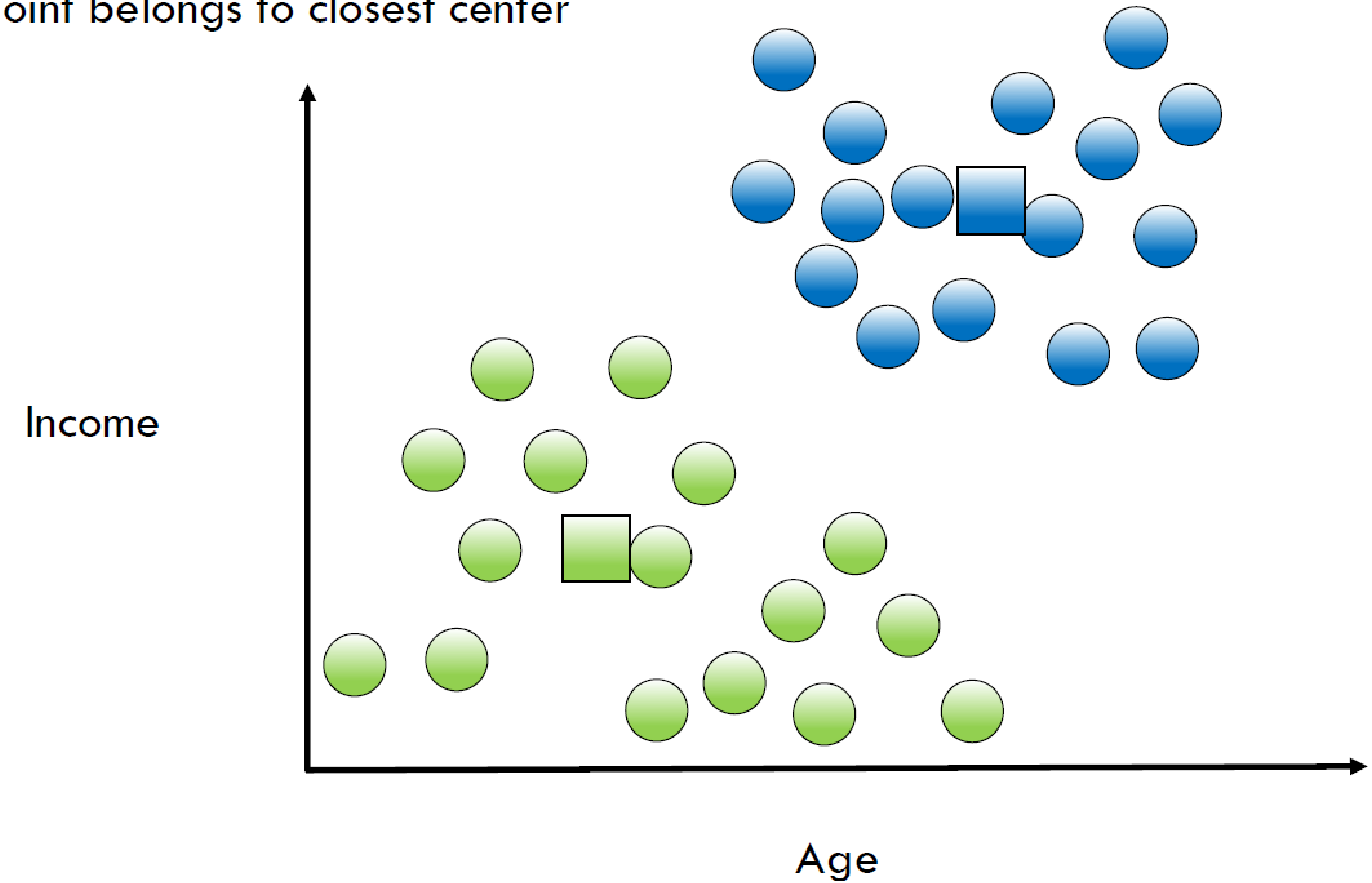
K-Means Algorithm

K = 2, Move each center to cluster's mean



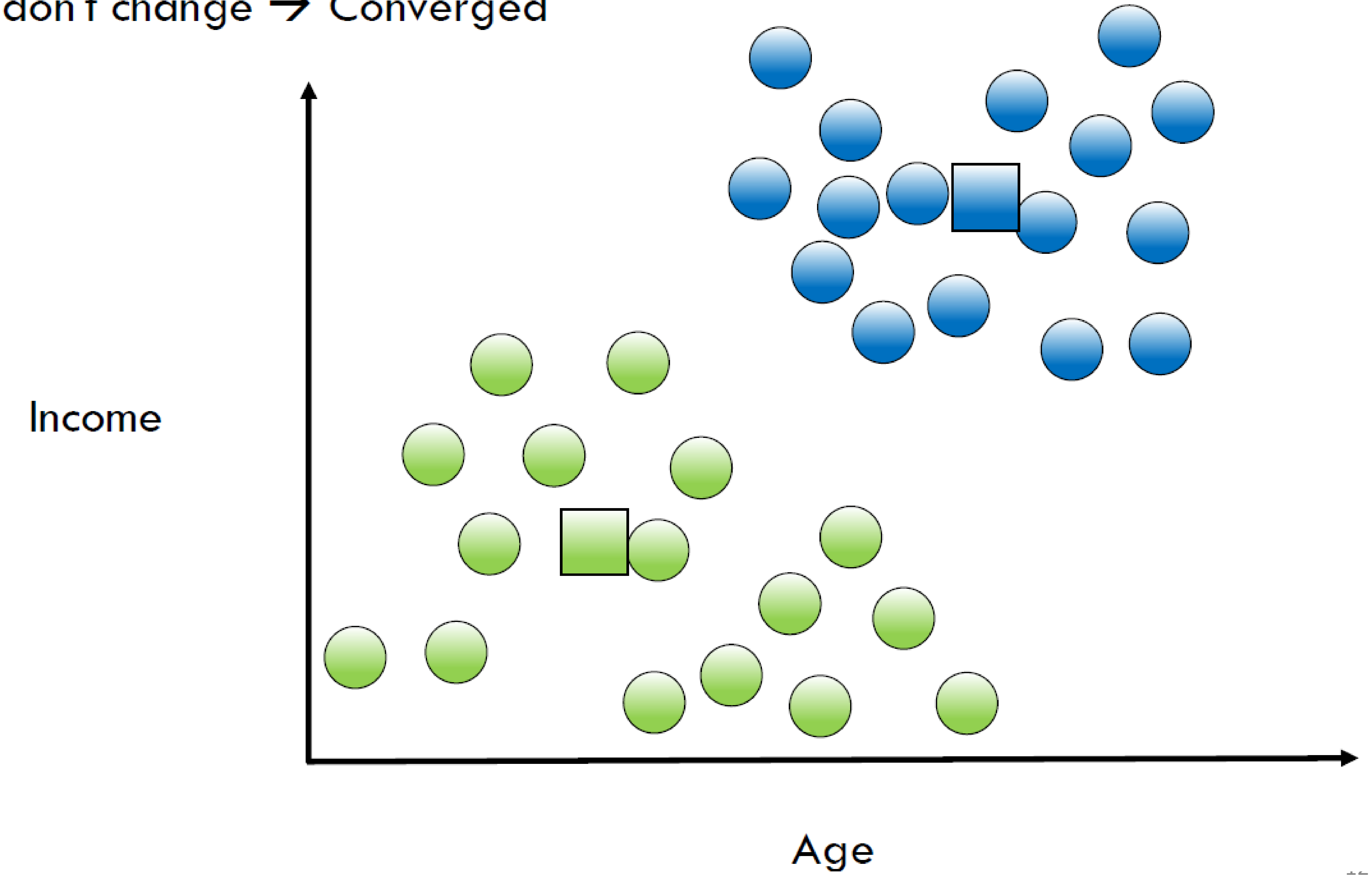
K-Means Algorithm

K = 2, Each point belongs to closest center



K-Means Algorithm

K = 2, Points don't change → Converged



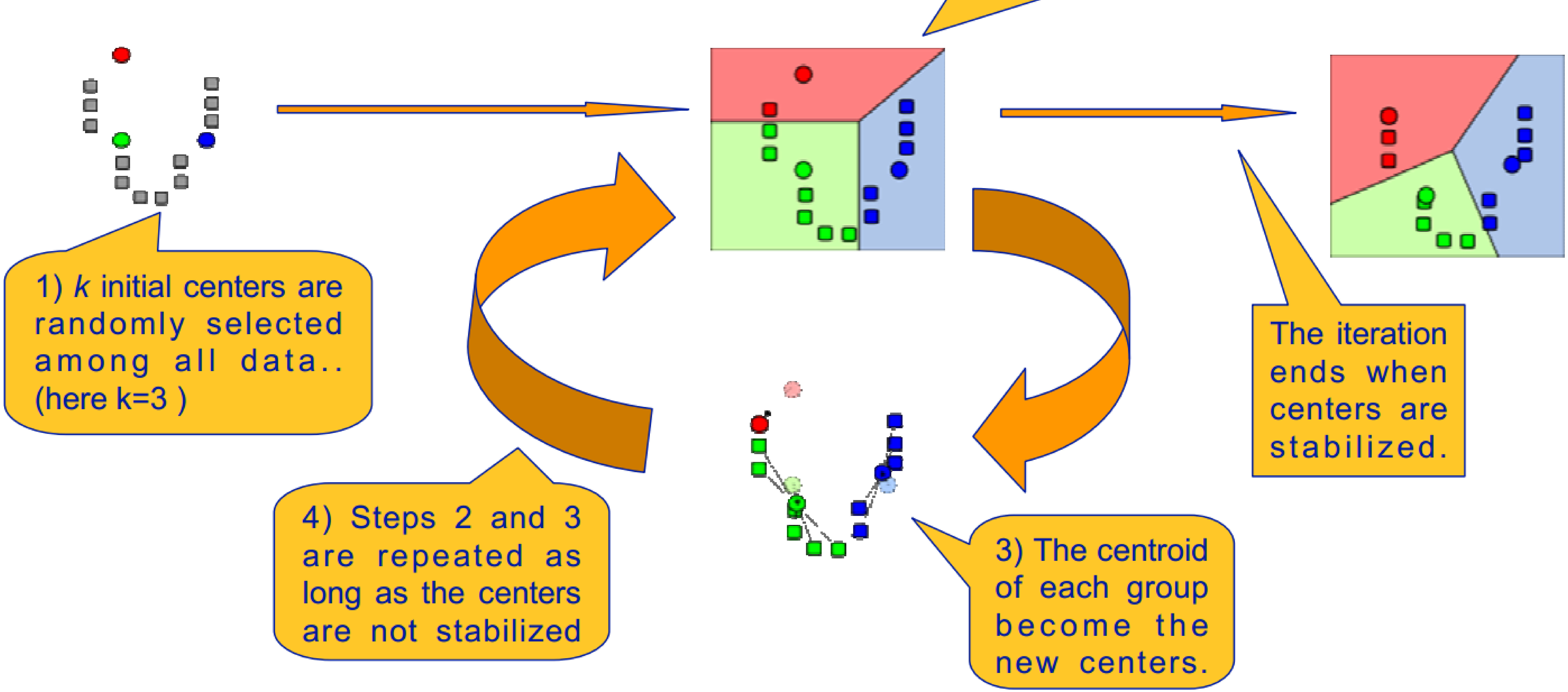
K-Means Algorithm

- Randomly select k points as centroids for k clusters
  - J = 1 to k Centroids are Mu1 to muk
- while (true):
  - for each point xi $\forall j \in [1, k]$
    - find nearest centroid muj $\arg\min_j D(x^{(i)}, \mu_j)$
    - assign the point xi to cluster j
  - for each cluster j = 1 to k
    - Update the centroid muj of each cluster (using points assigned to cluster j in previous step)
  - Stop when cluster assignments don't change (i.e. centroids don't change)

K-means

An unsupervised method.

MacQueen, 1967



Interpreting K-means as Expectation Maximization

K-Means as EM: Steps 1& 2 Guess, Expect

- **Guessing step**: Randomly guess k centroids

$$\mu_1, \ldots \mu_j, \ldots, \mu_k$$

- **Expectation Step**: Cluster assignment
  - Assign datapoints to clusters whose centroids they are closest (closest = minimum distance)

$$\forall j \in [1, k] \quad \arg\min_j D(x^{(i)}, \mu_j)$$

For every data point

  - Called expectation because we update our expectation on which cluster does the point belong

K-Means as EM: Step 3 Maximize

- **<u>Maximization Step</u>**: Set the mean of cluster data points as the new centroid

$$\mu_j = \frac{1}{|C_j|} \sum_{x \in C_j} x$$

  - Called maximization because we maximize the fitness function defining cluster centers
- Repeat E & M till convergence $new \ \ \mu_j = old \ \ \mu_j$

K-Means as EM algorithm steps rigorously

- **<u>Guessing step</u>**: Randomly guess k centroids

$$\mu_1, \ldots \mu_j, \ldots, \mu_k$$

O(iterations * data points * clusters * features)

- **<u>Expectation Prep</u>**

$$\forall j \in [1, k] \qquad C_j = \{\} \quad \mu_{j_{new}} = \mu_{j_{old}}$$

- **<u>Expectation Step</u>**: Cluster assignment for each x(i)

$$C_j \leftarrow C_j + \{\ \forall j \in [1, k] \quad \arg\min_j D(x^{(i)}, \mu_j)\ \}$$

- **<u>Maximization Step</u>**: Set the new clusters

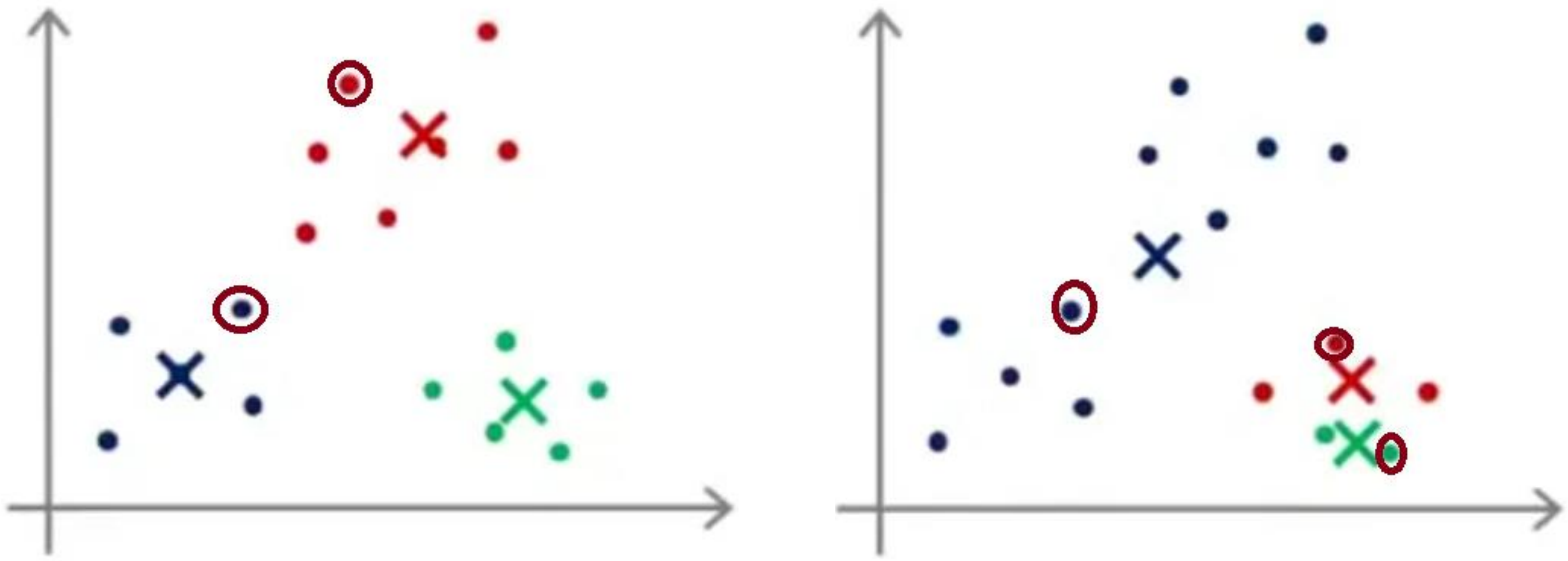
$$\mu_{j_{new}} = \frac{1}{|C_j|} \sum_{x \in C_j} x$$

- Go to Expectation Prep & loop if $\mu_{j_{new}} \neq \mu_{j_{old}}$

K-Means initialization

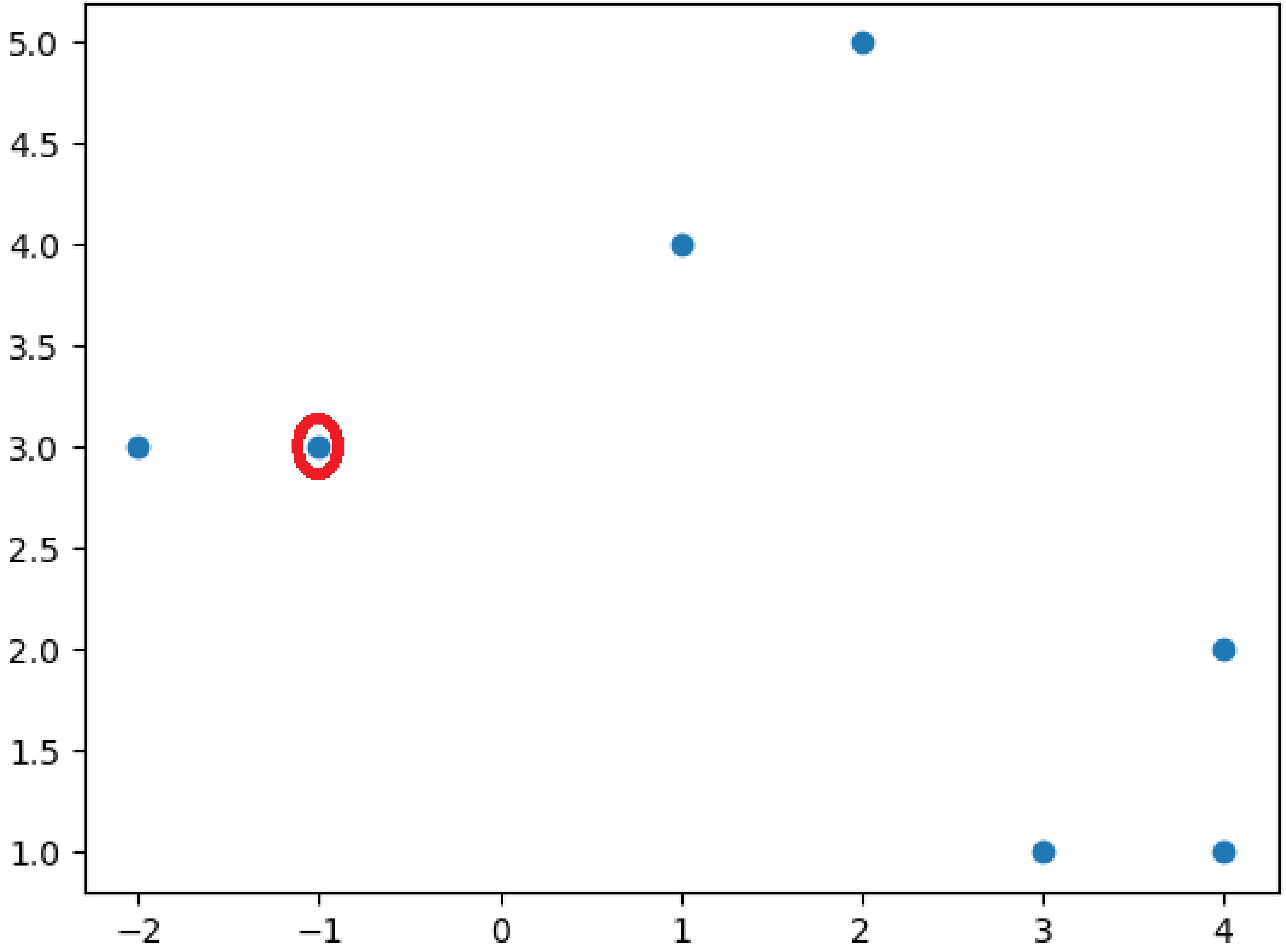
Impact of non-deterministic K-Means algorithm

- Might get wrong centroids & wrong clusters in every run
- K = 3 and random initialization



How to initialize initial centroids

- First centroid chosen randomly
- Centroids should be as far as possible from each other



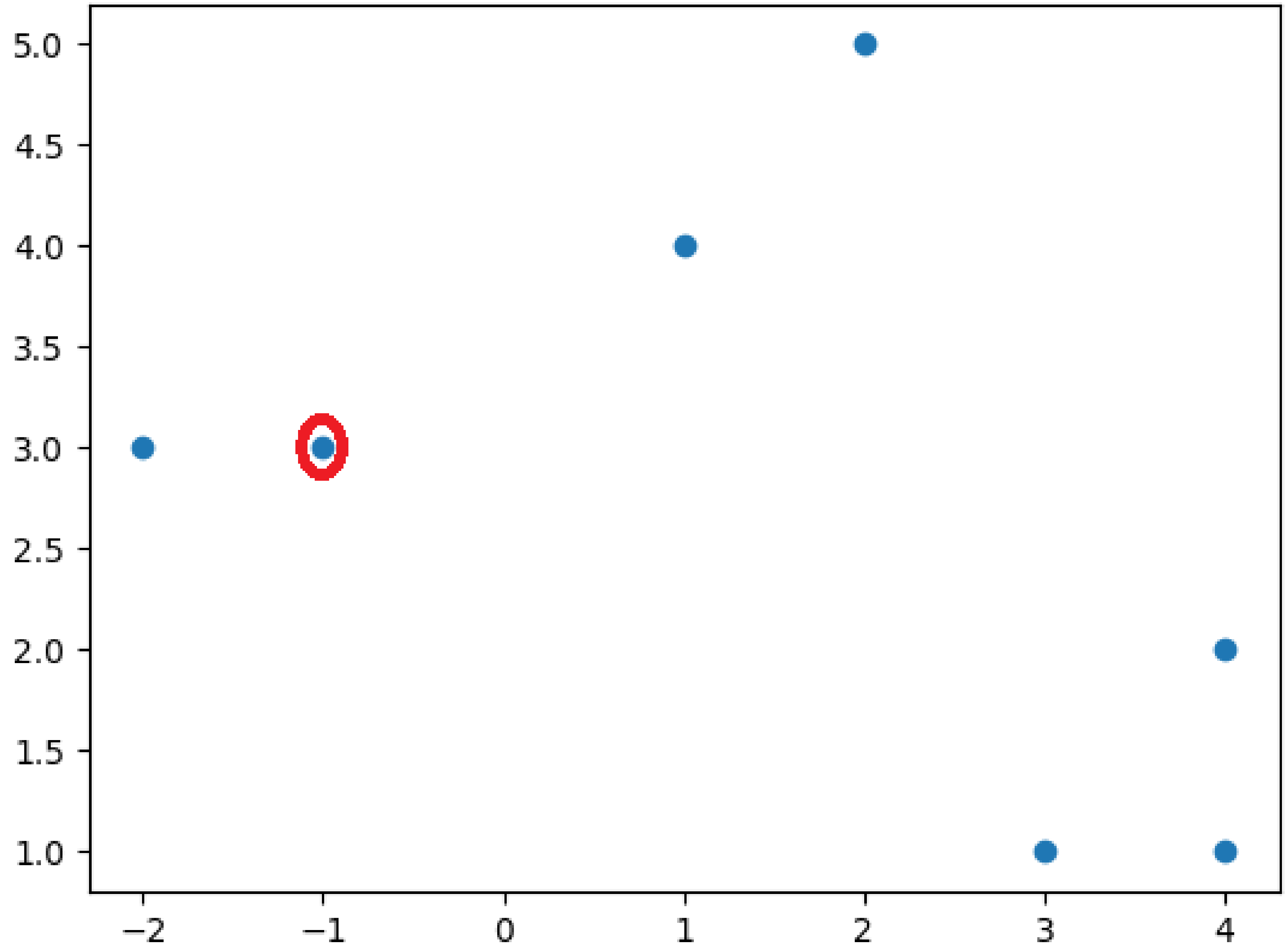
Different initialization different results

- Random
  - We have been doing this
- Kmeans++
  - Will cover next
- Naïve sharding
  - not covered

Kmeans++

- First centroid chosen randomly
- Probability of next centroid selection proportional to distance

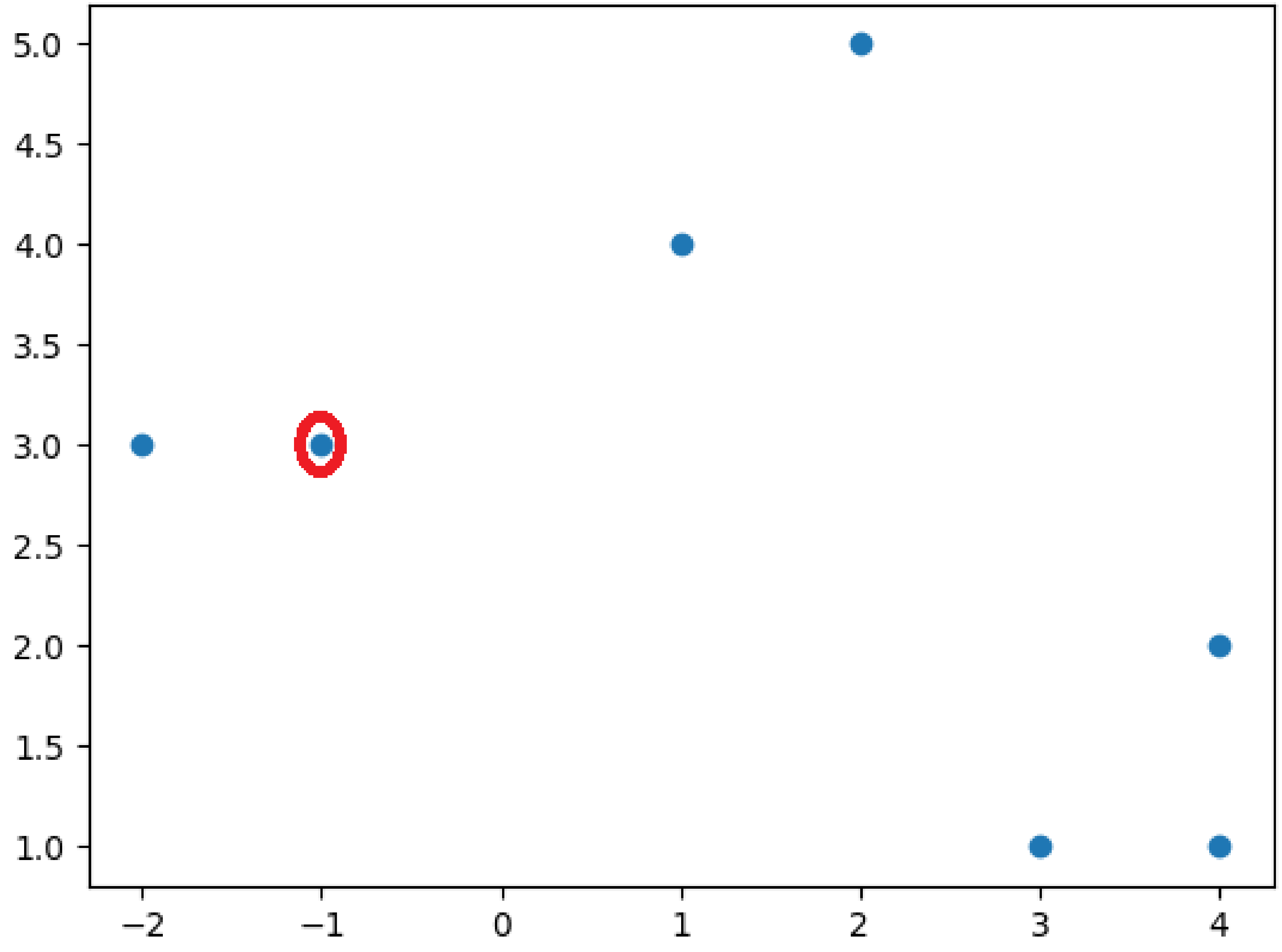
X	Dist (x, c1)^2
(2,5)	
(-1,3)	Centroid
(-2,3)	
(3,1)	
(1,4)	
(4,1)	
(4,2)	
Total	



Kmeans++

- Calculate all distances square from centroid

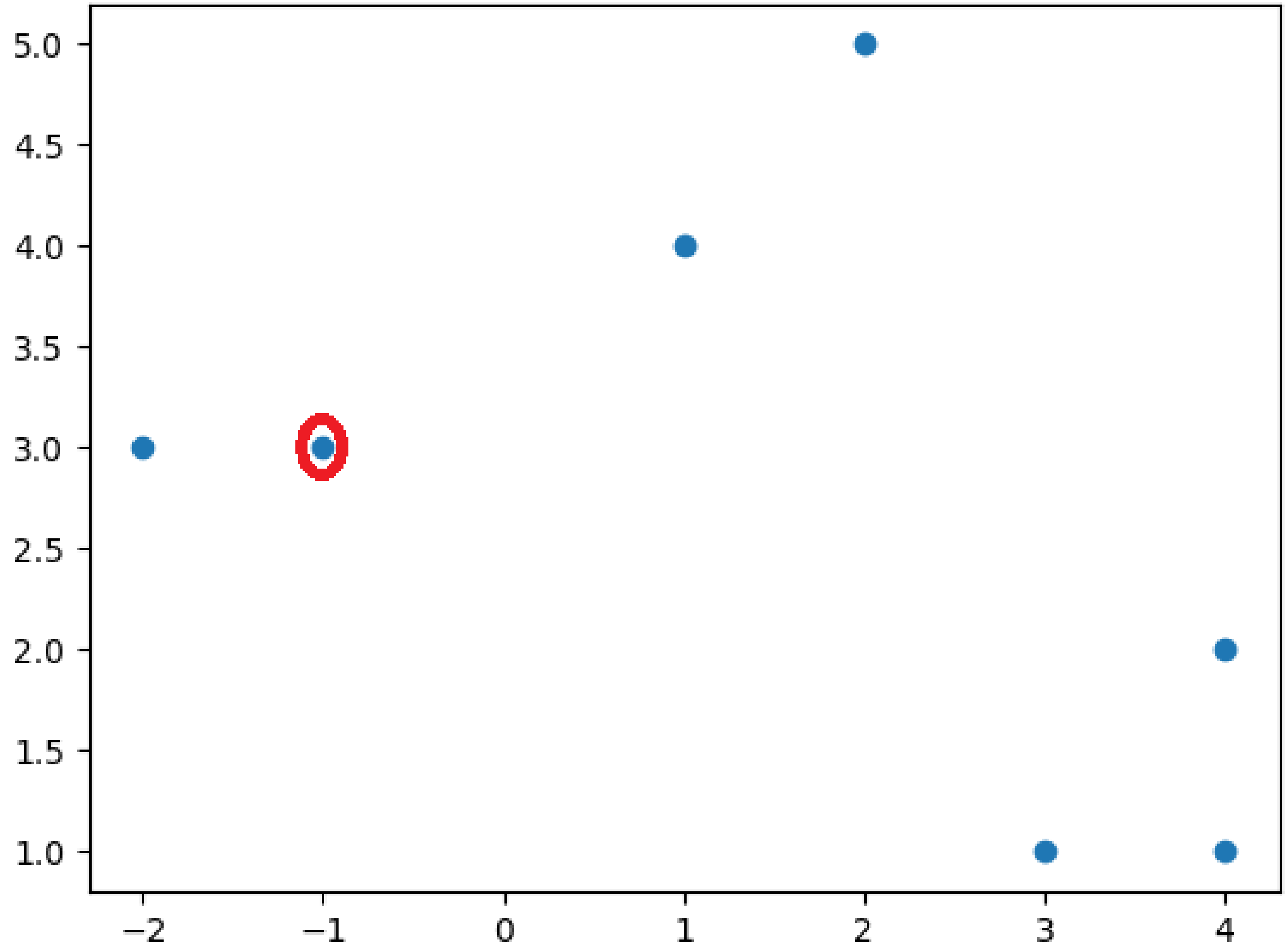
X	Dist (x, c1)^2
(2,5)	13
(-1,3)	Centroid
(-2,3)	1
(3,1)	20
(1,4)	5
(4,1)	29
(4,2)	26
Total	94



Kmeans++

- Calculate all distances square from centroid
- Convert to probability

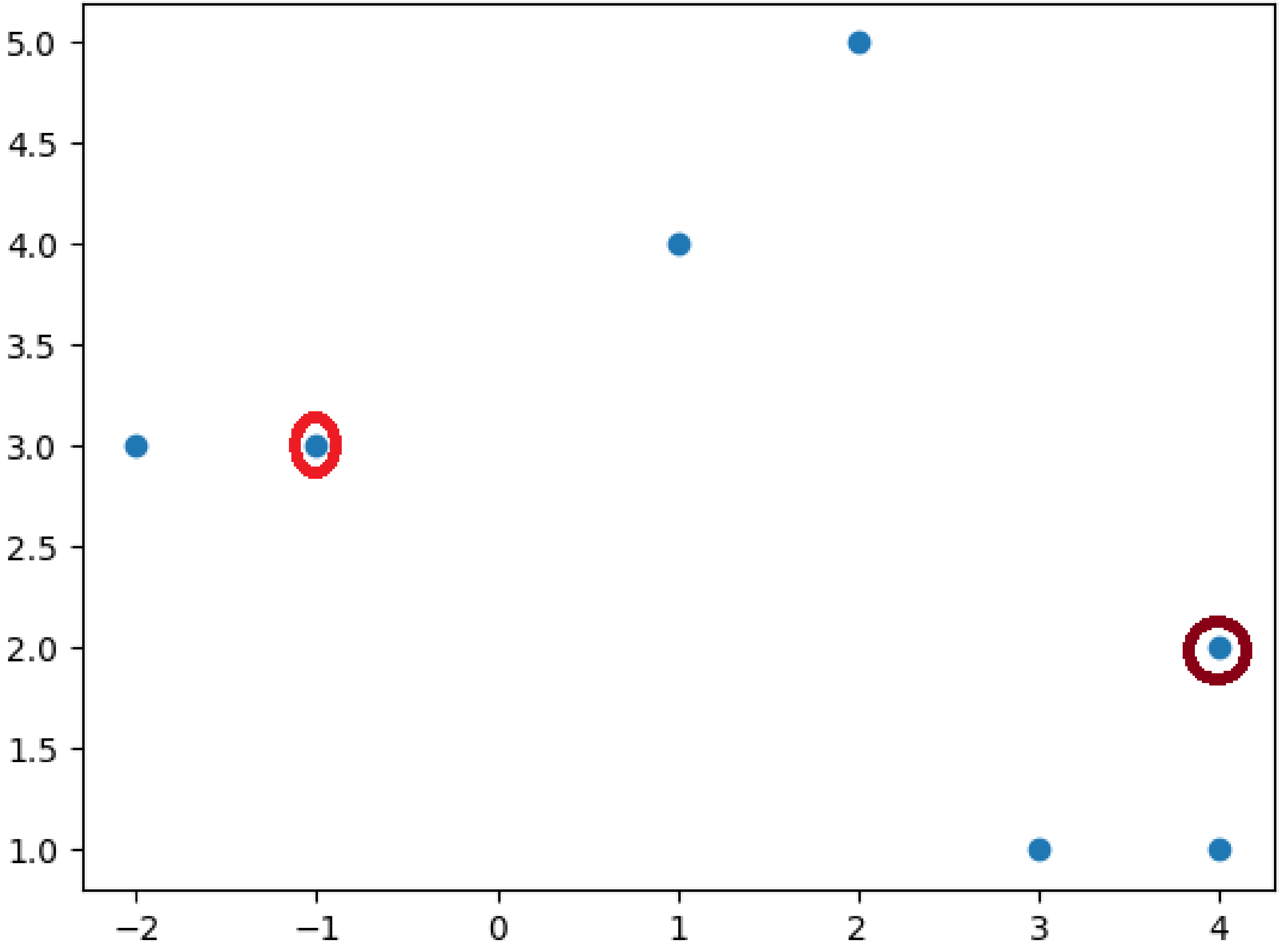
X	Dist (x, c1)^2	Prob
(2,5)	13	13/94
(-1,3)	Centroid	–
(-2,3)	1	1/94
(3,1)	20	20/94
(1,4)	5	5/94
(4,1)	29	29/94
(4,2)	26	26/94
Total	94	



Kmeans++

- Sample from remaining points weighted by probabilities
- Find the minimum of distance from both centroids

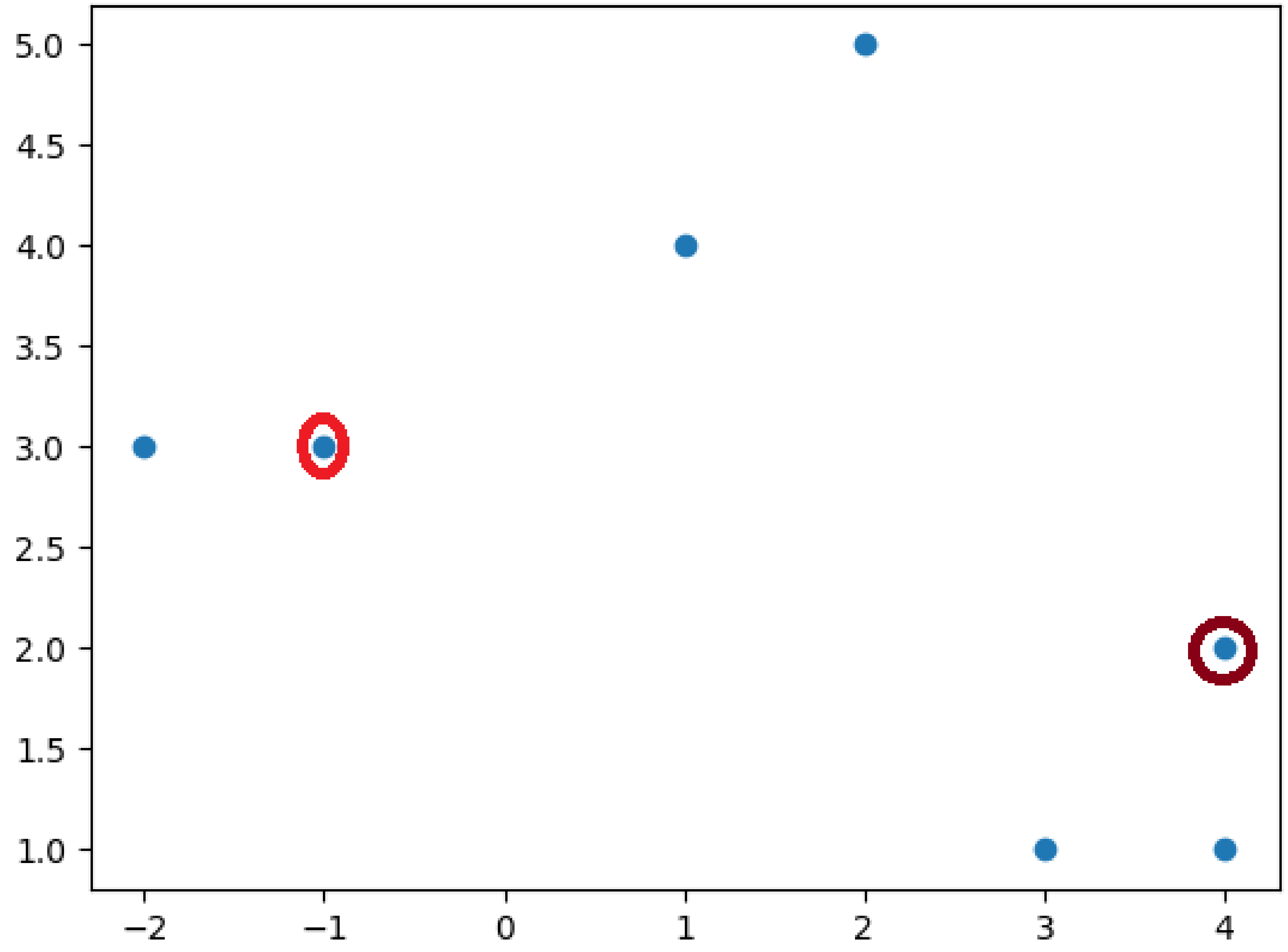
X	Dist (x, c1)^2	Prob	Dist(x, c1, c2)^2
(2,5)	13	13/94	min(13,13)
(-1,3)	Centroid	–	–
(-2,3)	1	1/94	min(1,37)
(3,1)	20	20/94	min(20, 2)
(1,4)	5	5/94	min(5,13)
(4,1)	29	29/94	min(29,1)
(4,2)	26	26/94	Centroid
Total	94		Not min(94, 92), But 22



Kmeans++

- Normalize the probabilities again and do weighted sampling

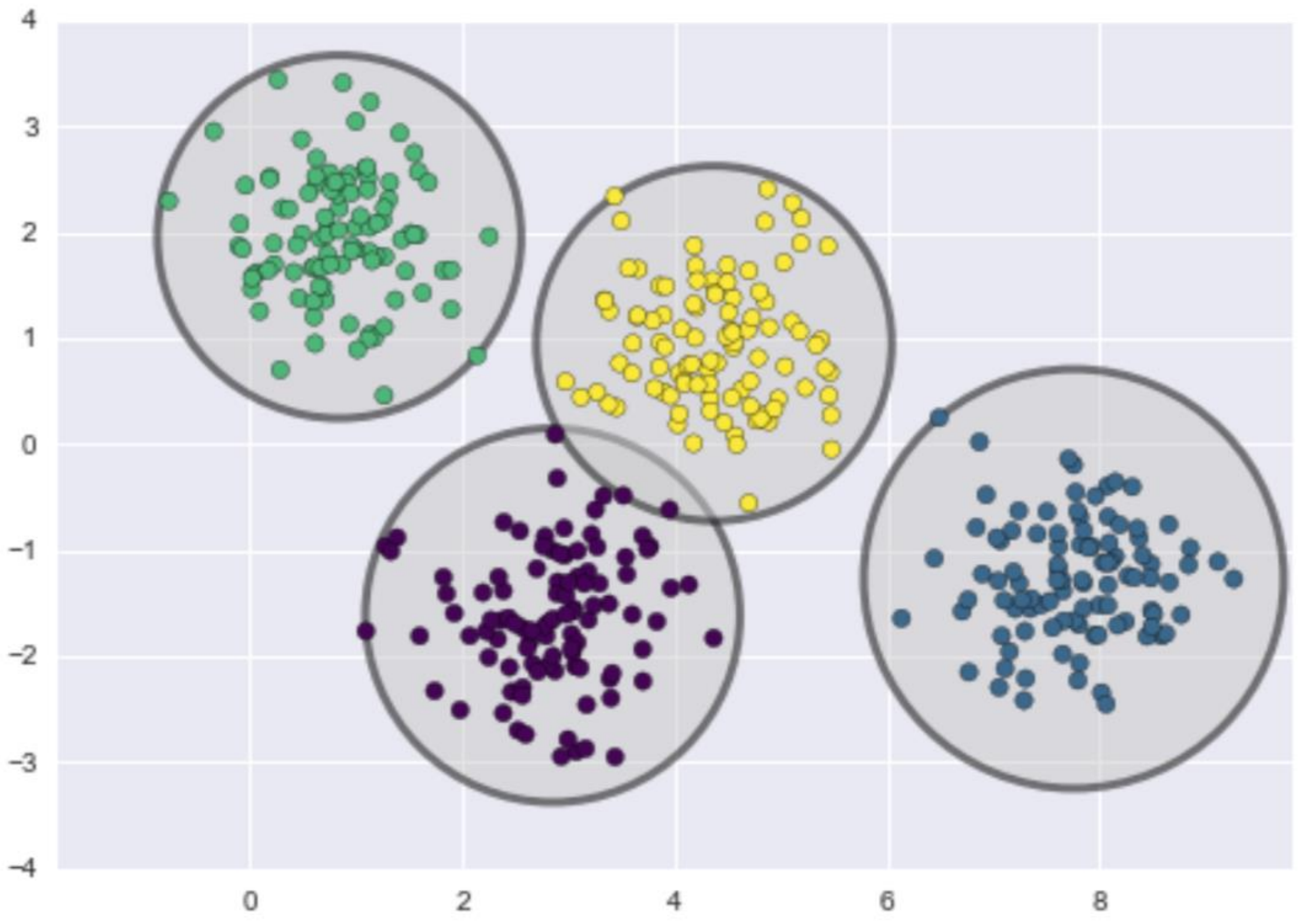
X	Dist (x, c1)^2	Prob	Dist(x, c1, c2)^2	Prob
(2,5)	13	13/94	min(13,13)	13/22
(-1,3)	Centroid	–	–	–
(-2,3)	1	1/94	min(1,37)	1/22
(3,1)	20	20/94	min(20, 2)	2/22
(1,4)	5	5/94	min(5,13)	5/22
(4,1)	29	29/94	min(29,1)	1/22
(4,2)	26	26/94	Centroid	–
Total	94		Not min(94, 92), But 22	

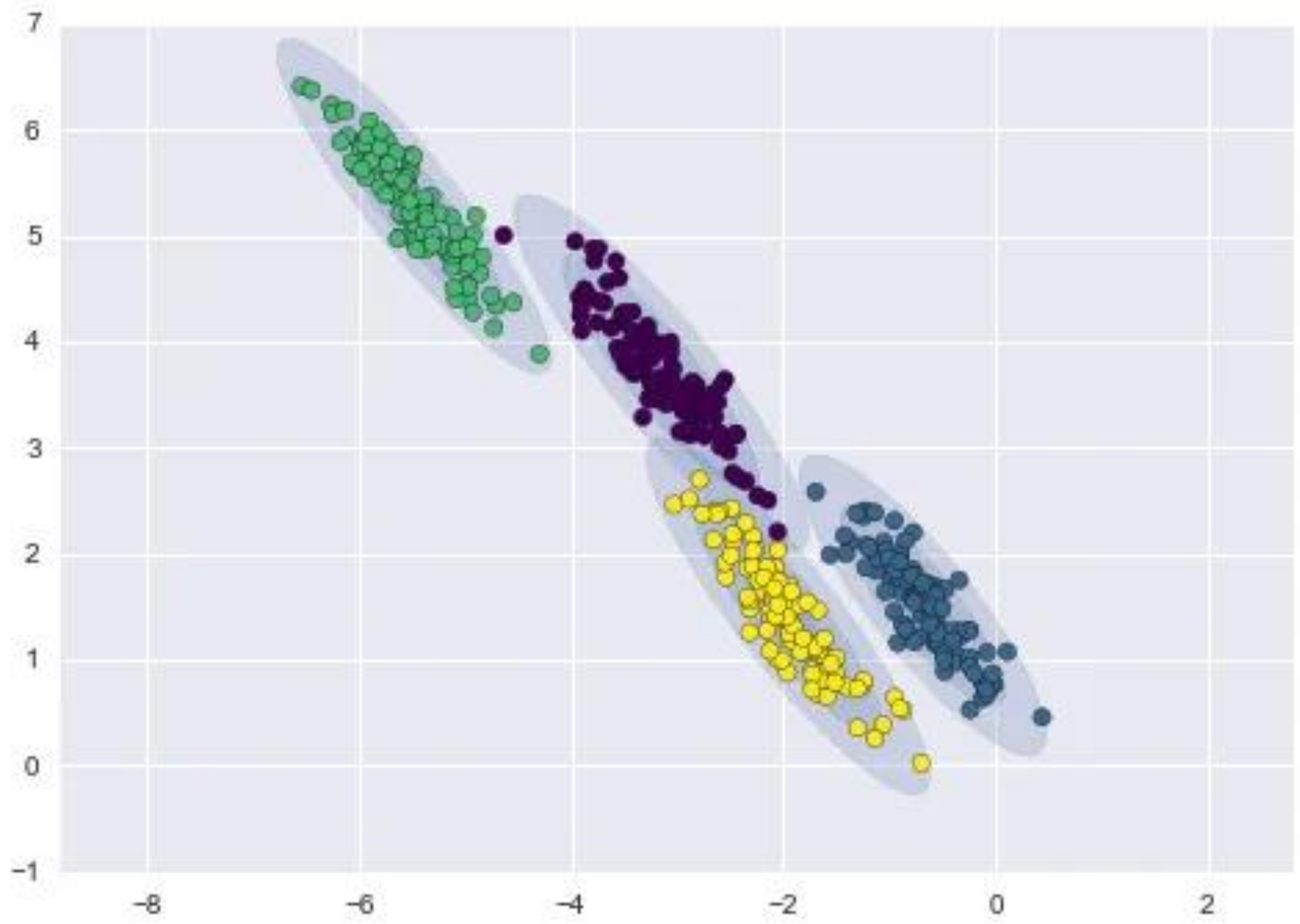


K-Means limitations

K means limitations

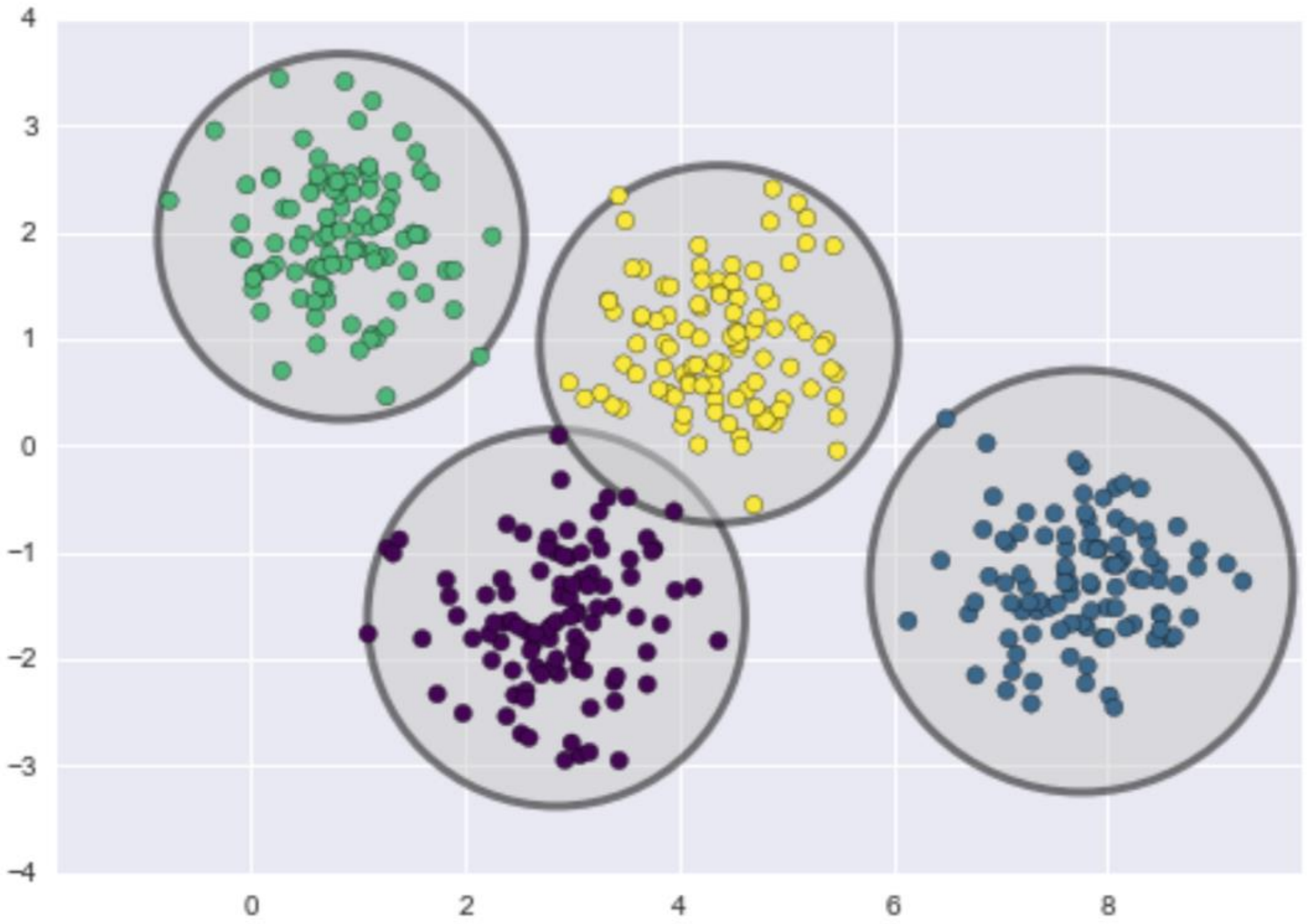
- Oblong data cannot be clustered well
  - Recall nearest centroid classification

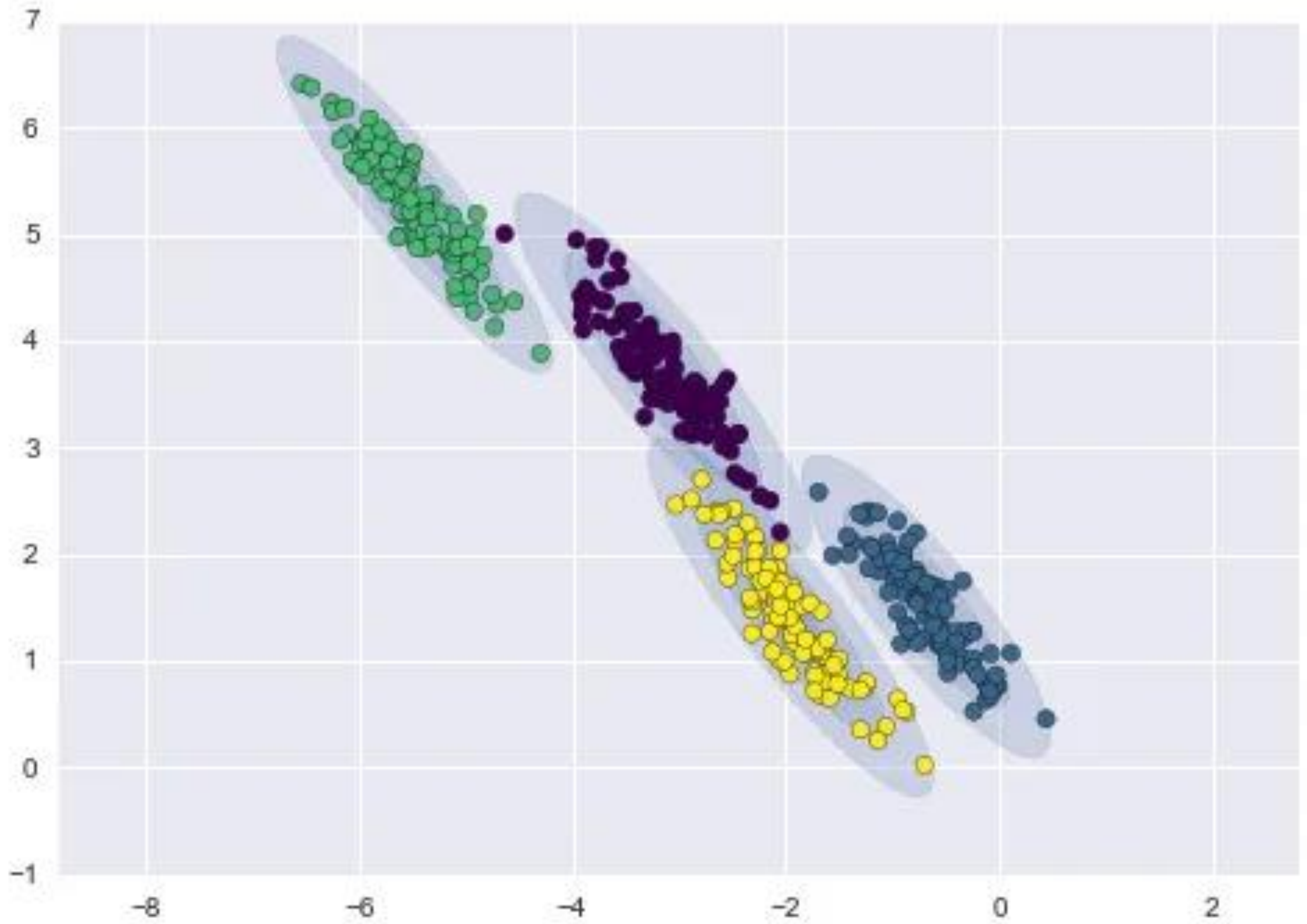




K means limitations

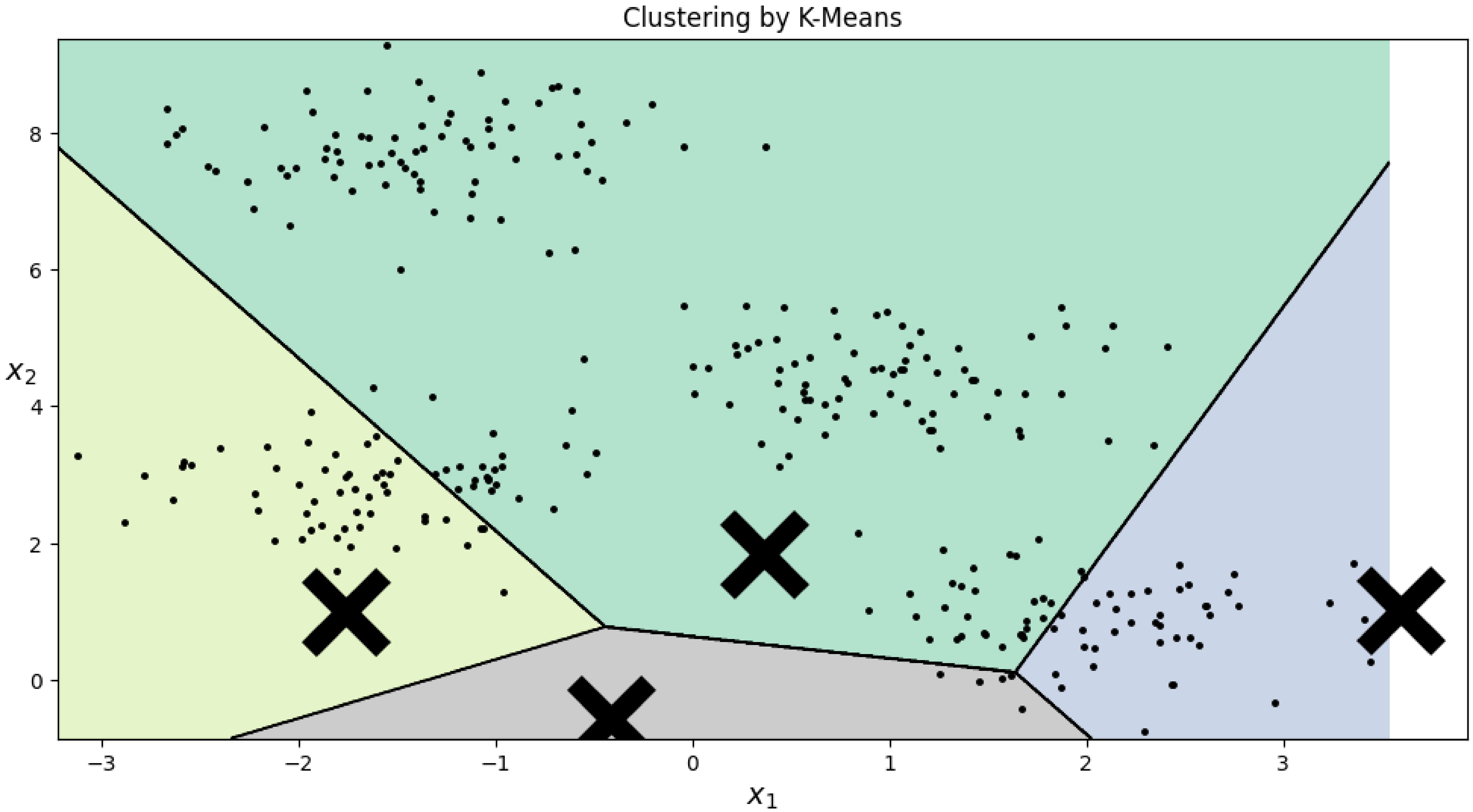
- Clustering every time when new data comes is hard
- Could use extracted centroids as model
  - Nearest Centroid from scratch without labels!!





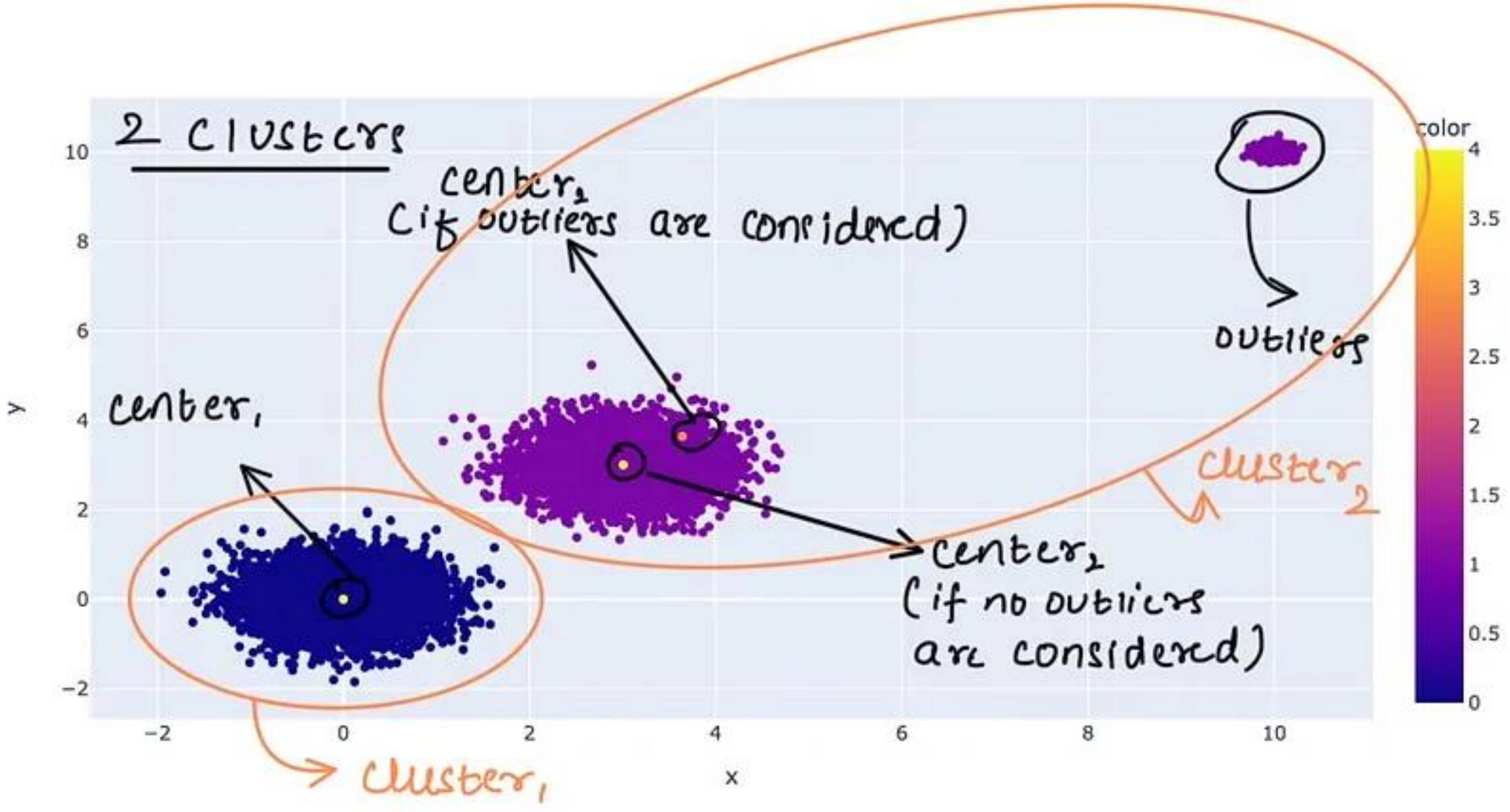
K means decision boundary

- Linear decision boundary

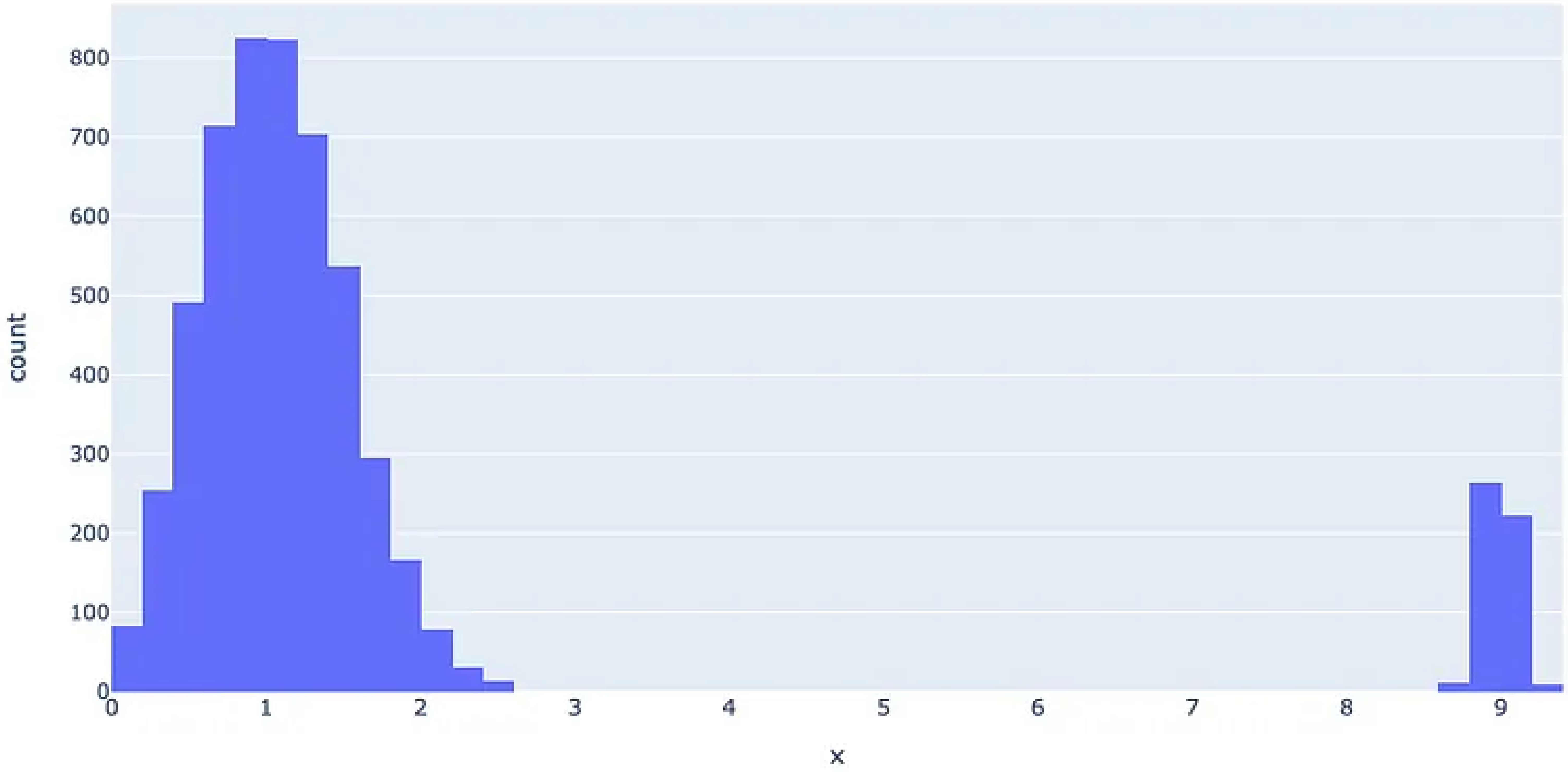


Handling outliers with K-Means

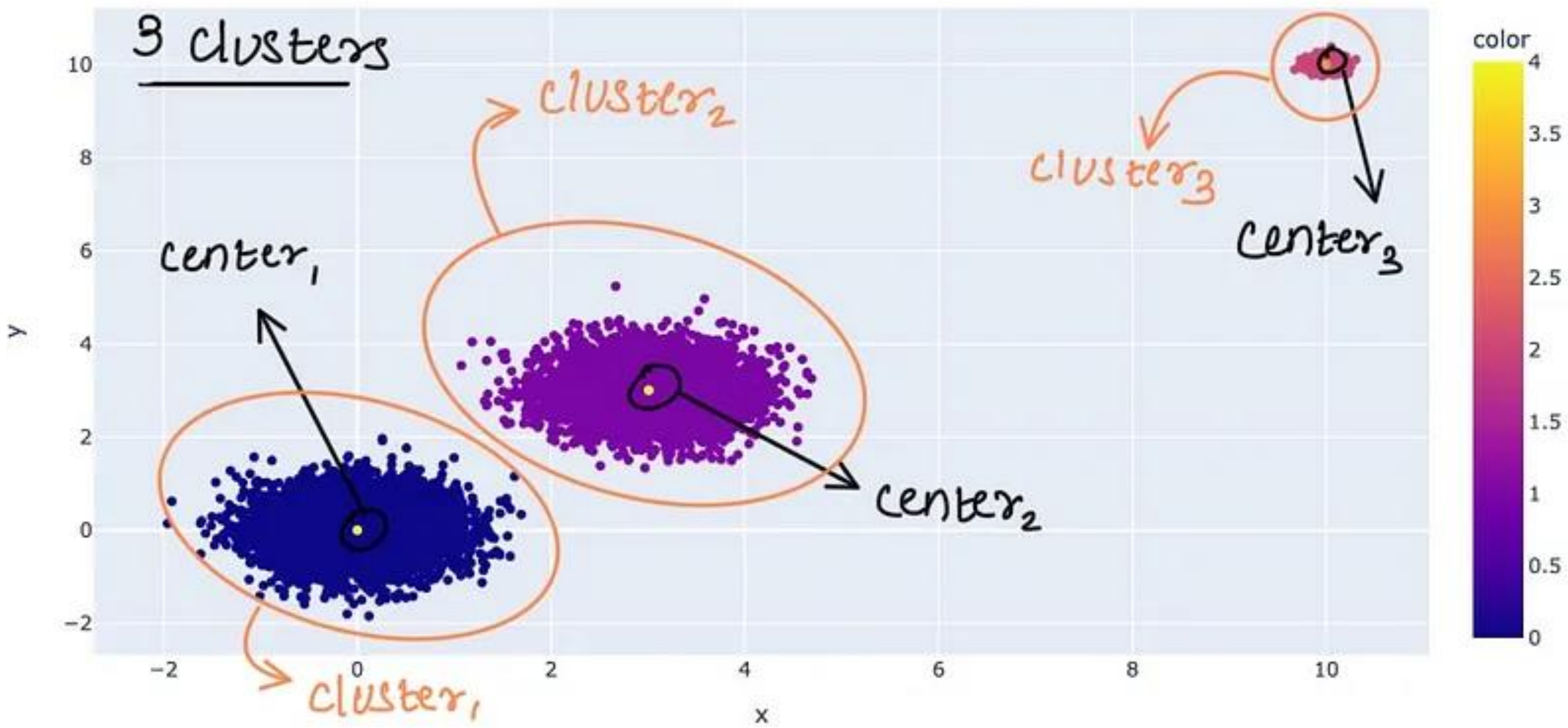
K-Means is sensitive to outliers



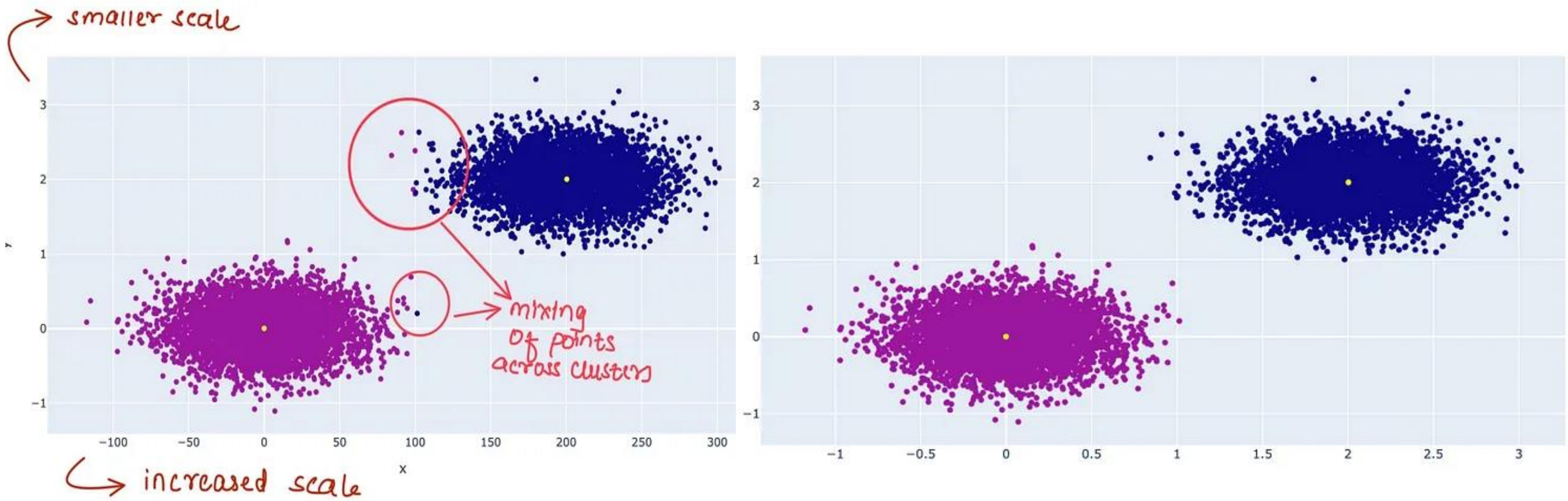
K-Means is sensitive to outliers



K-Means is sensitive to outliers

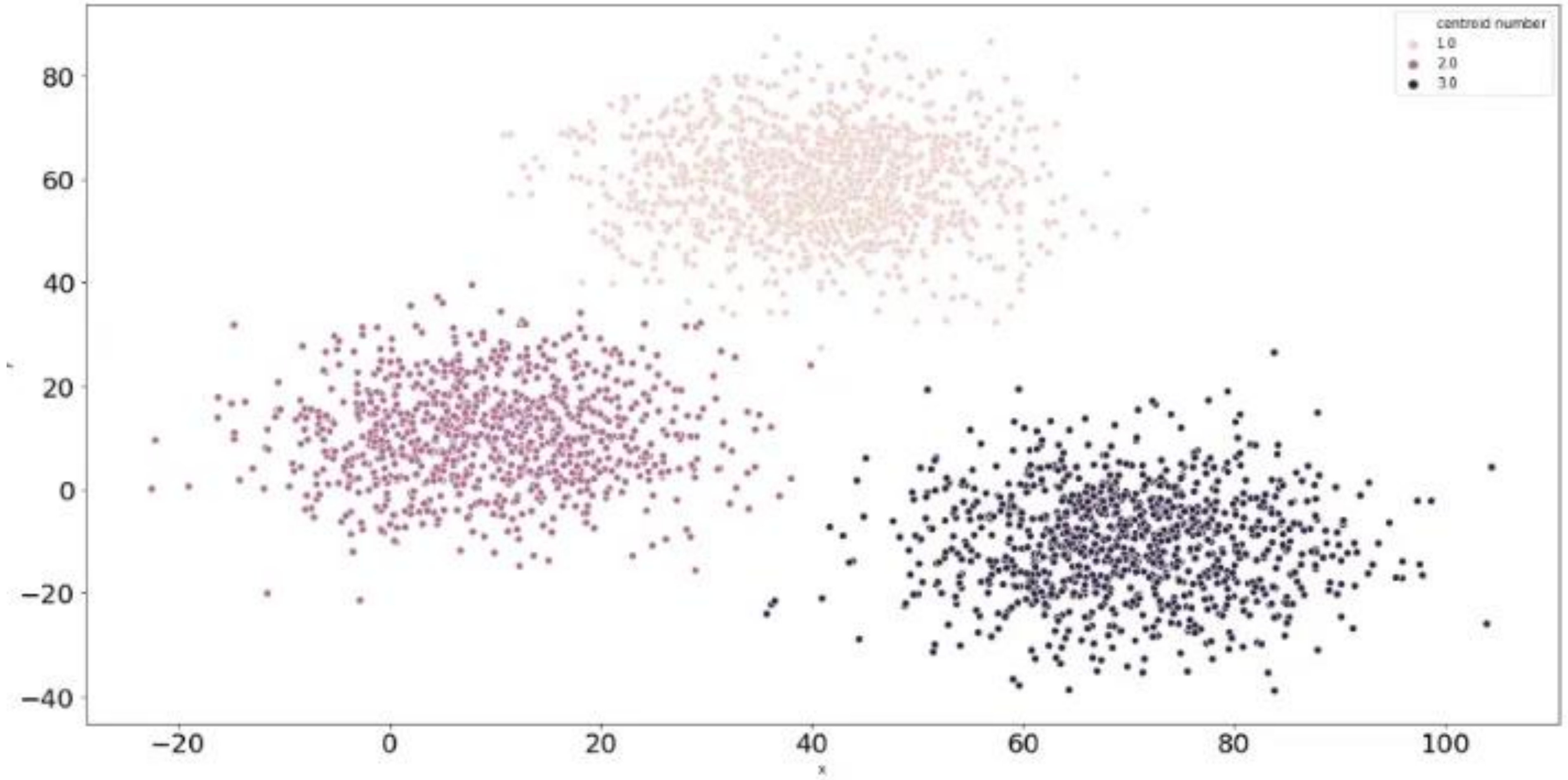


K-Means and scaling



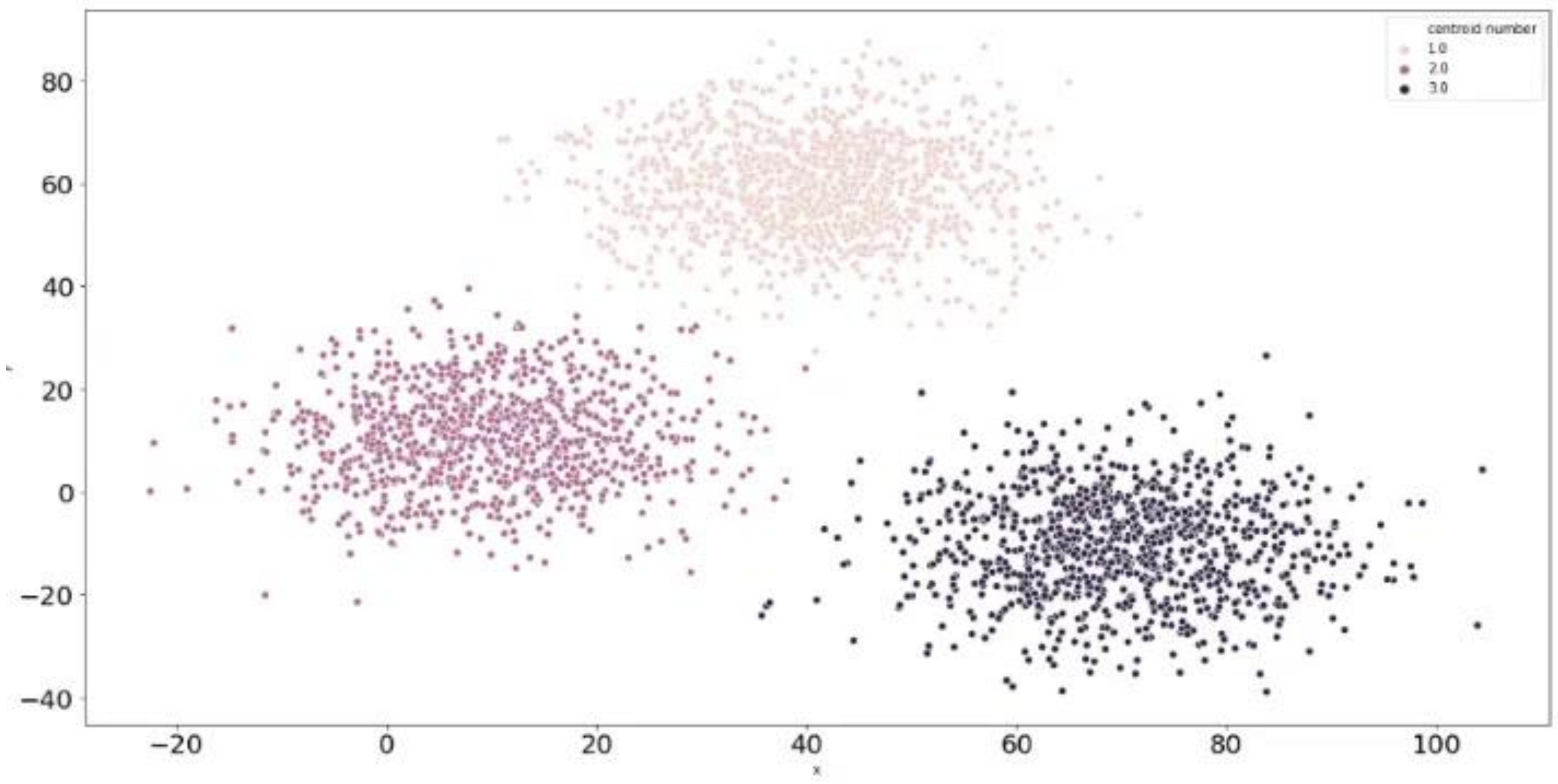
K means limitations

- K-Means is sensitive to outliers
  - Clusters become bigger to accommodate outliers
- Can use statistical techniques or silhouette analysis

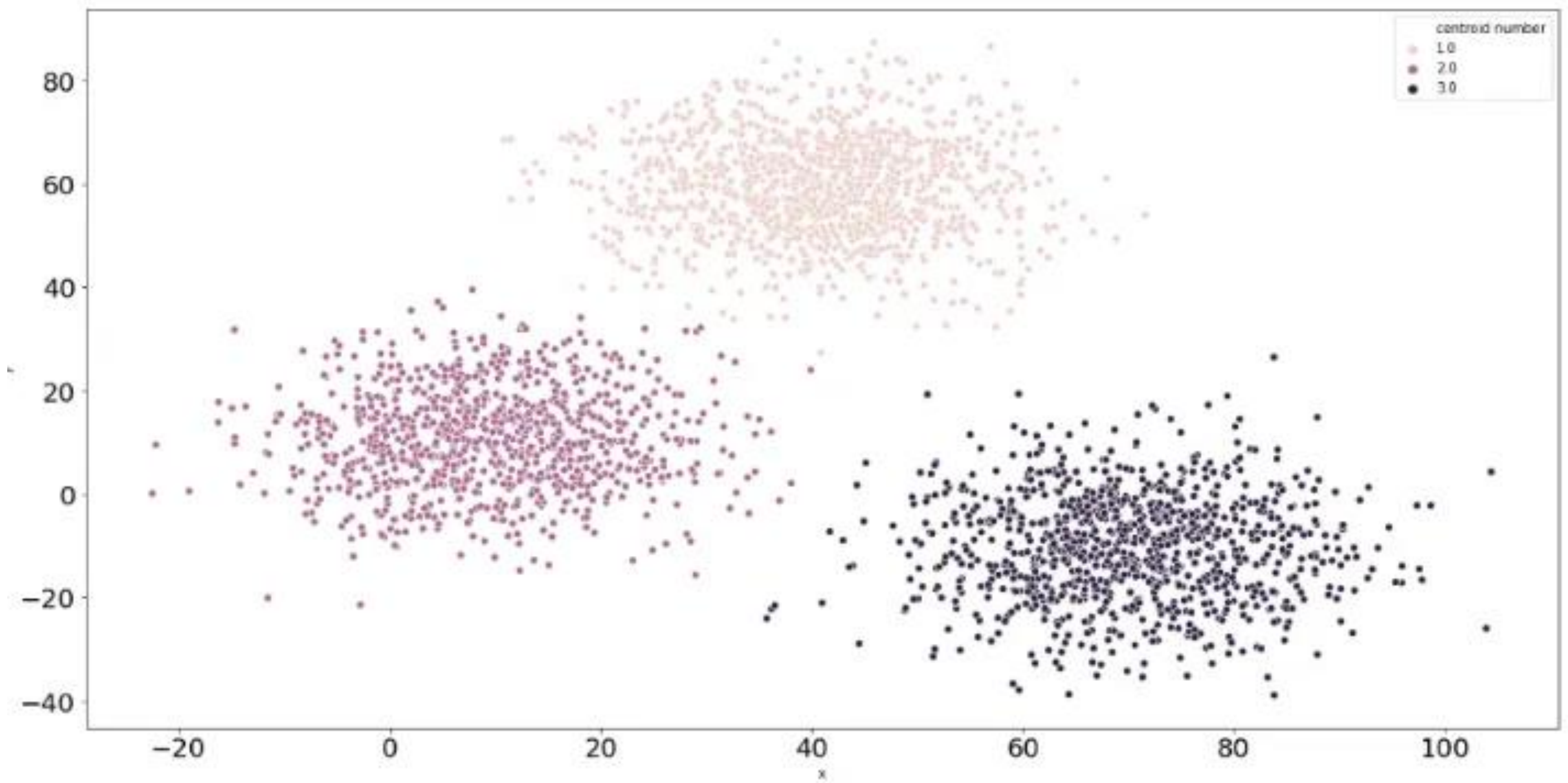


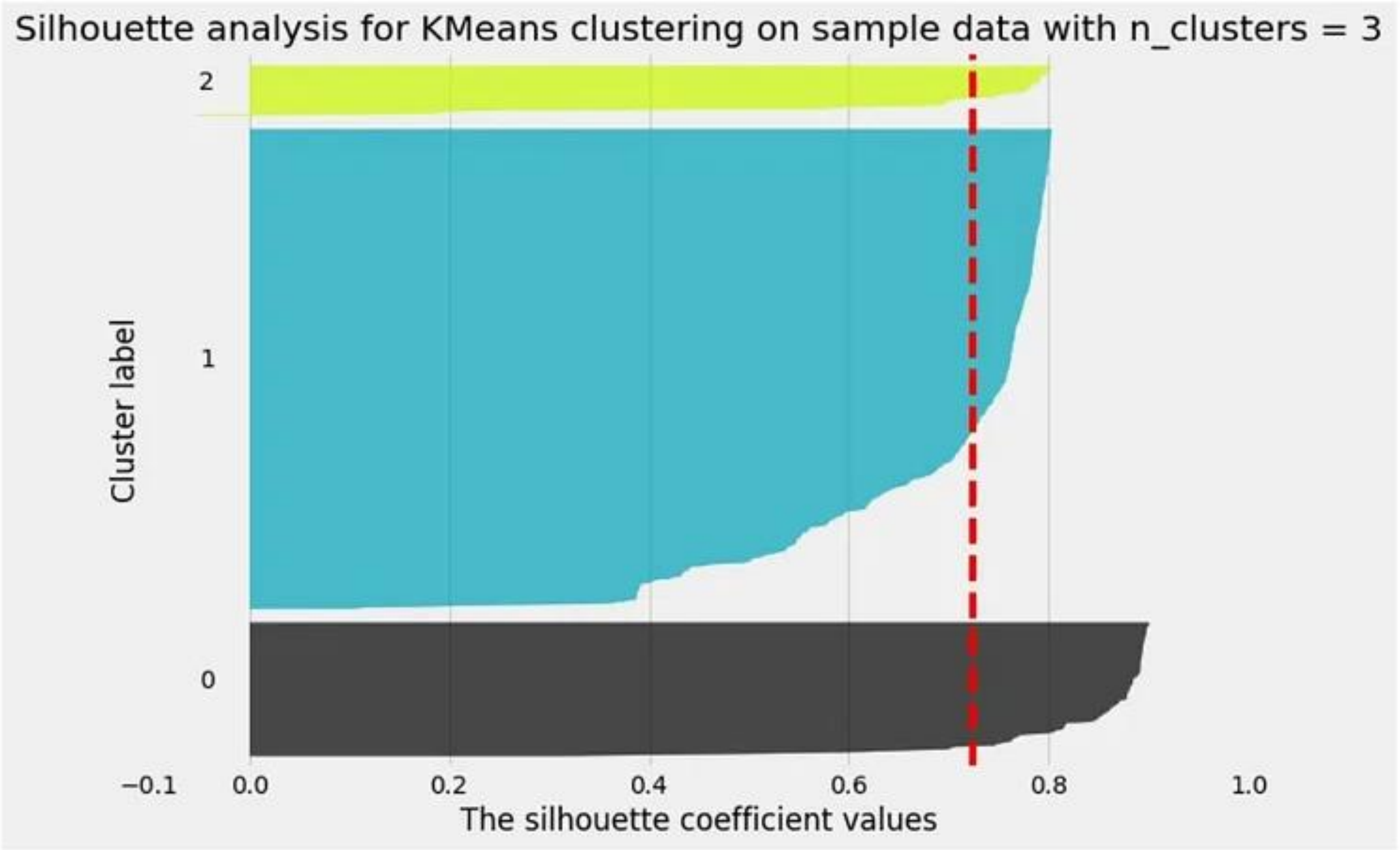
Handling outliers with K means & statistical analysis

- Statistical techniques to analyze each cluster
  - IQR
  - 3 standard deviations



Handling outliers with K means & silhouette analysis





- Analyze Silhouette plots for outlier detection
  - Variation of score gives clues of outlier presence
  - Negative values are sure outliers
  - Values with score less than 0.4 are potential outliers