COMP 7990
Principles and Practices of Data Analytics

Lecture 6: Unsupervised Learning

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Outline for Data Preprocessing and Data Mining

- **Data Preprocessing**
- **Supervised learning**
- Regression
  1. Linear regression with one variable
  2. Linear Regression with multiple variables
  3. The relationship between Correlation and Regression
- Classification
  1. Perceptron
  2. Artificial Neural Network
  3. Support Vector Machine
  4. K Nearest Neighbor
- **Unsupervised learning**
  1. K-means Clustering
  2. Hierarchical Clustering

Classification

Classification

$$\mathbf{X} \longrightarrow y$$

- Input X
  - an $m*n$ matrix
  - Each row represents one data sample

- Output y
  - an $m*1$ vector
  - Each element in y represents the output (i.e., label) of one data sample
  - y_i is a **discrete value** for classification problem
    - $y_i \in \{0, 1\}$ for binary classification
    - $y_i \in \{1, \ldots, k\}$ for multi-class classification

Regression

Regression

$$\mathbf{X} \longrightarrow y$$

- Input X
  - an $m*n$ matrix
  - Each row represents one data sample
- Output y
  - an $m*1$ vector
  - Each element in y represents the output (i.e., label) of one data sample
  - y_i **is a continuous value** for regression problem

Clustering

Clustering

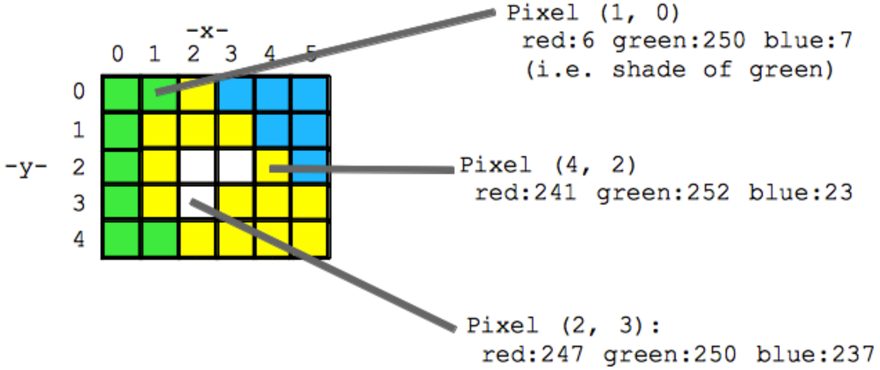
X

- The given data does not contain any output y
- Clustering tries to group input samples into different groups based on data similarities.

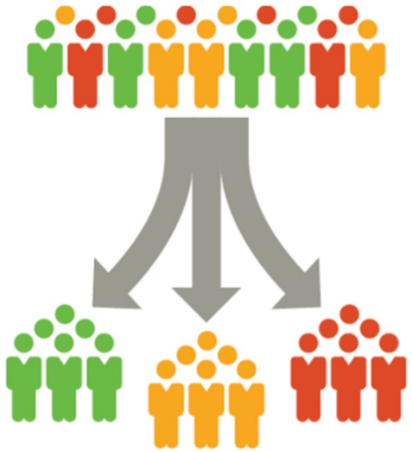
- Input X
  - an $m*n$ matrix
  - Each row represents one data sample

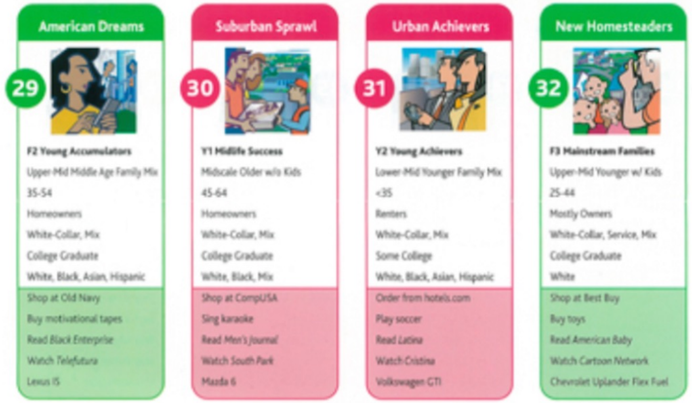
Clustering: Some Real-World Examples

- Clustering pixel values in an image to do image segmentation

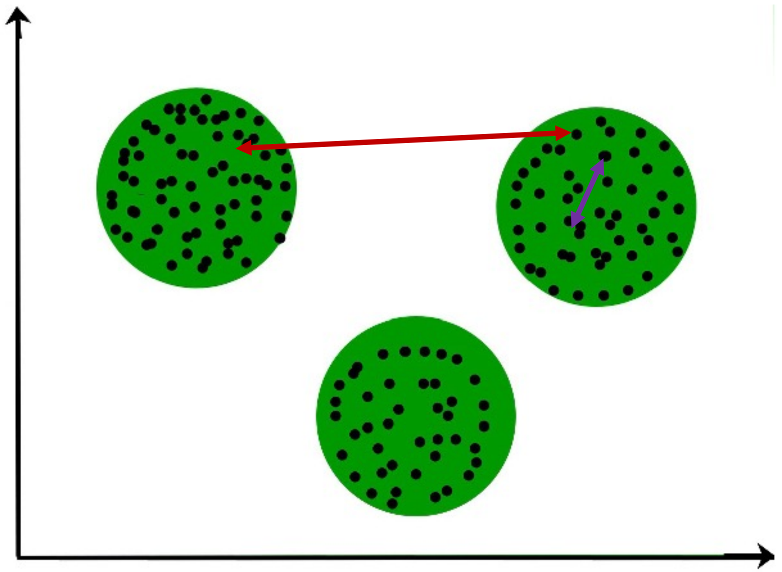


- Clustering customers based on their profile or purchase history





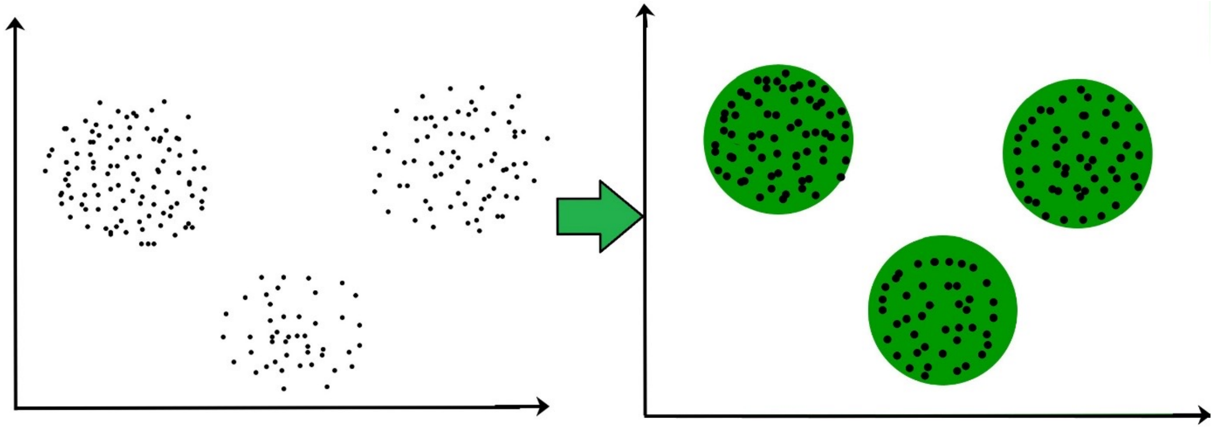
What is Clustering?



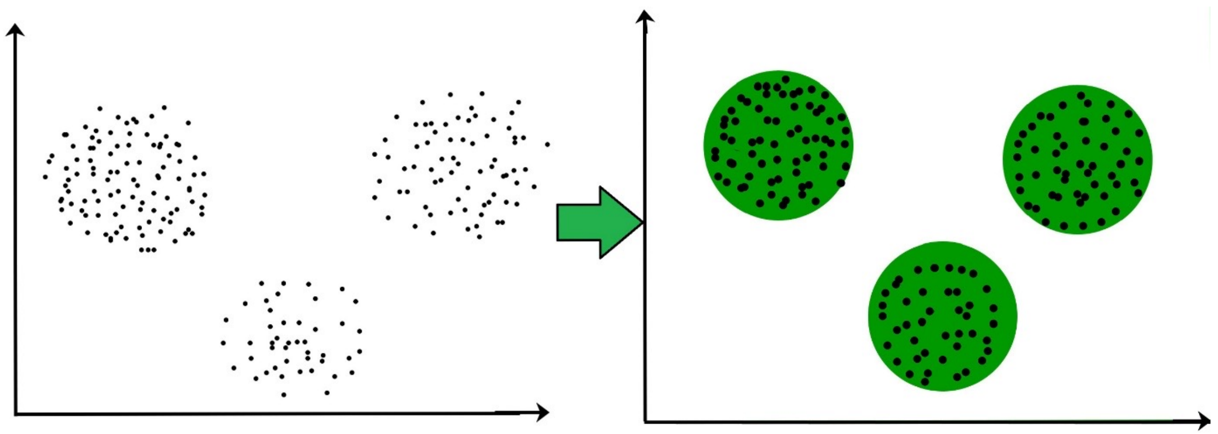
- Cluster: A collection of data points
  - With a cluster, the data points are close to each other.
  - For the data points in different clusters, they are far from each other.
- Clustering
  - Compute similarities (distance) between data points
  - Group similar (close) data points into clusters
  - Clusters/Groups/Partitions are used interchangeably in the literature but are essentially the same concept.
- Unsupervised learning: no predefined class labels

What is Clustering?

- Data Clustering is an unsupervised learning problem.
- Given *m* unlabeled samples $\{\mathbf{x}_i\}_{i=1}^{m}$, where $\mathbf{x}_i$ is a *n* dimensional input feature vector; the number of clusters *K*
- Goal: Group *m* samples into *K* clusters



What is Clustering?



- The only information clustering uses is the similarity between samples
- A good clustering is the one that can achieve:
  - High intra-cluster similarity: cohesive within cluster
  - Low inter-cluster similarity: distinctive between clusters

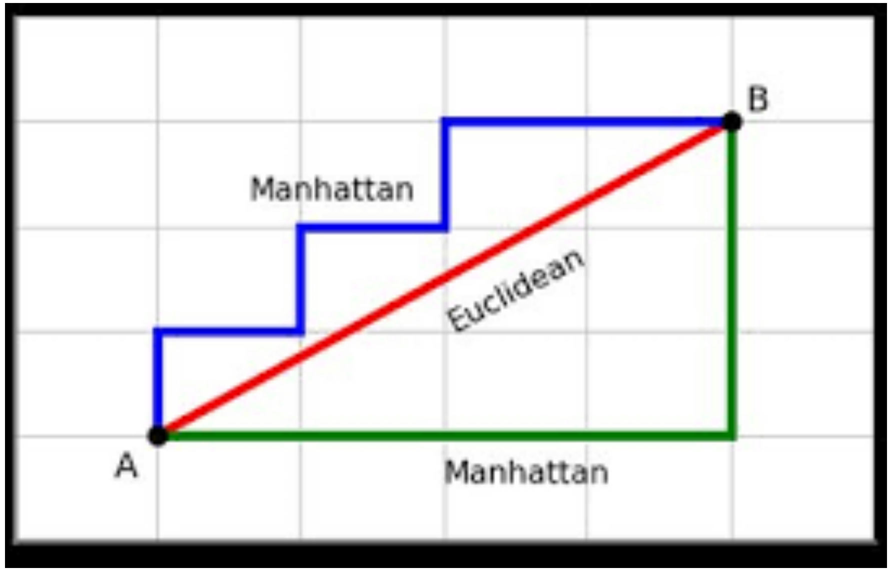
Notions of Similarity/Distance

- The choice of the similarity measure is very important for clustering.
- Similarity is inversely related to distance.
- There are different ways to measure the distances between two data points.
  - L_2 (Euclidean) distance: $d(\mathbf{x}, \mathbf{z}) = \|\mathbf{x} - \mathbf{z}\| = \sqrt{\sum_{j=1}^{n} (x_j - z_j)^2}$
  - L_1 (Manhattan) distance: $d(\mathbf{x}, \mathbf{z}) = \sum_{j=1}^{n} |x_j - z_j|$
  - L_p distance: $d(\mathbf{x}, \mathbf{z}) = \left(\sum_{j=1}^{n} |x_j - z_j|^p\right)^{1/p}$
  - L_∞ distance: $\max\{x_j - z_j\}$, j=1…n

  - Kernelized (non-linear) distance: $d(\mathbf{x}, \mathbf{z}) = \|\phi(\mathbf{x}) - \phi(\mathbf{z})\|$

Euclidean and Manhattan Distance: Difference?

E.g. 1



L_2 (Euclidean) distance $= \sqrt{3^2 + 4^2} = 5$

L_1 (Manhattan) distance $= 3 + 4 = 7$

L_∞ distance$= \max(\{3, 4\}) = 4$

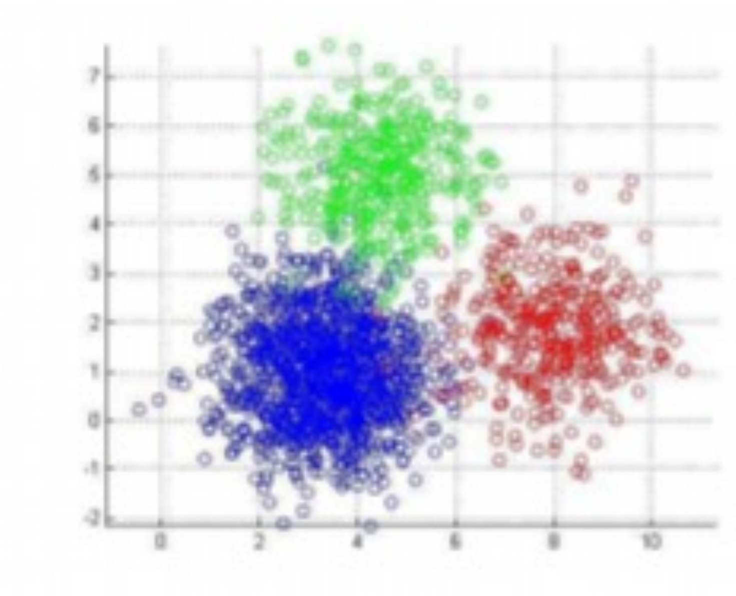
E.g. 2 Distance along different dimensions $= (2, 3, 2, 3, 100, 2)$

L_2 distance $= \sqrt{4 + 9 + 4 + 9 + 10000 + 4}$

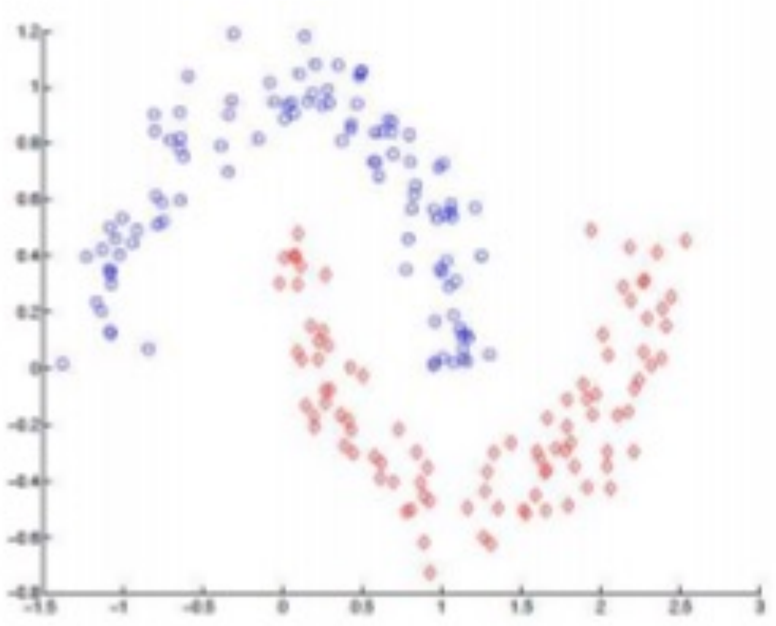
L_1 distance $= 2 + 3 + 2 + 3 + 100 + 2$

L_∞ distance $= 100$

Kernelized (non-linear) Distance



Use of Euclidean distance is reasonable.

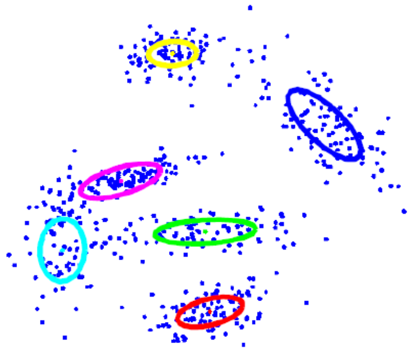


Kernelized distance is needed.

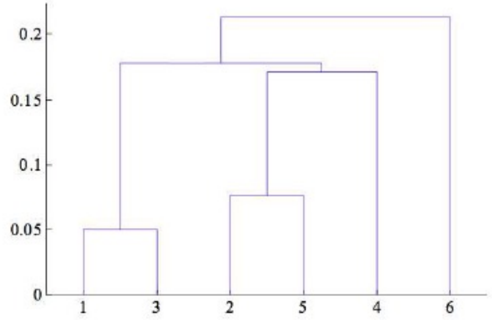
$$d(\mathbf{x}, \mathbf{z}) = \|\phi(\mathbf{x}) - \phi(\mathbf{z})\|$$

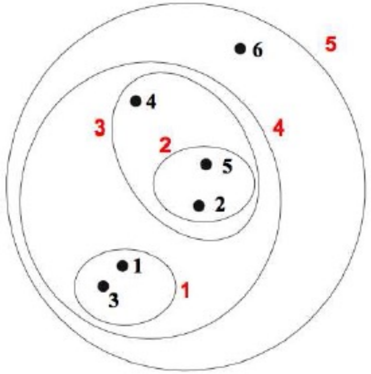
Types of Clustering

- Partitional Clustering (e.g., *K*-means)
  - Partitions are independent of each other.
  - Hierarchical relationship not considered.



- Hierarchical Clustering (e.g., agglomerative clustering, divisive clustering)
  - Partitions can be visualized using a tree structure (a dendrogram)
  - Does not need the number of clusters as input
  - Allows partitions at different levels of granularities (i.e., can refine/coarsen clusters)





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- **Data Preprocessing**
- **Supervised learning**

❖ Regression

1. Linear regression with one variable
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3. The relationship between Correlation and Regression

❖ Classification

1. Perceptron
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3. Support Vector Machine
4. K Nearest Neighbor

- **Unsupervised learning**

1. K-means Clustering
2. Hierarchical Clustering

K-means Algorithm

- **Input:** Samples $\{\mathbf{x}_i\}_{i=1}^{m}$, parameter K (i.e., number of clusters)
- **Initialize:** K cluster centers (means) $\mathbf{c}_1, \ldots, \mathbf{c}_k$. Several initialization options:
  - Randomly initialized anywhere in the input space
  - Randomly choose K samples from the data as the cluster centers
- **Iterate:**
  - Assign each sample $\mathbf{x}_i$ to its closest cluster center

$$k = \arg\min_k \|\mathbf{x}_i - \mathbf{c}_k\|$$

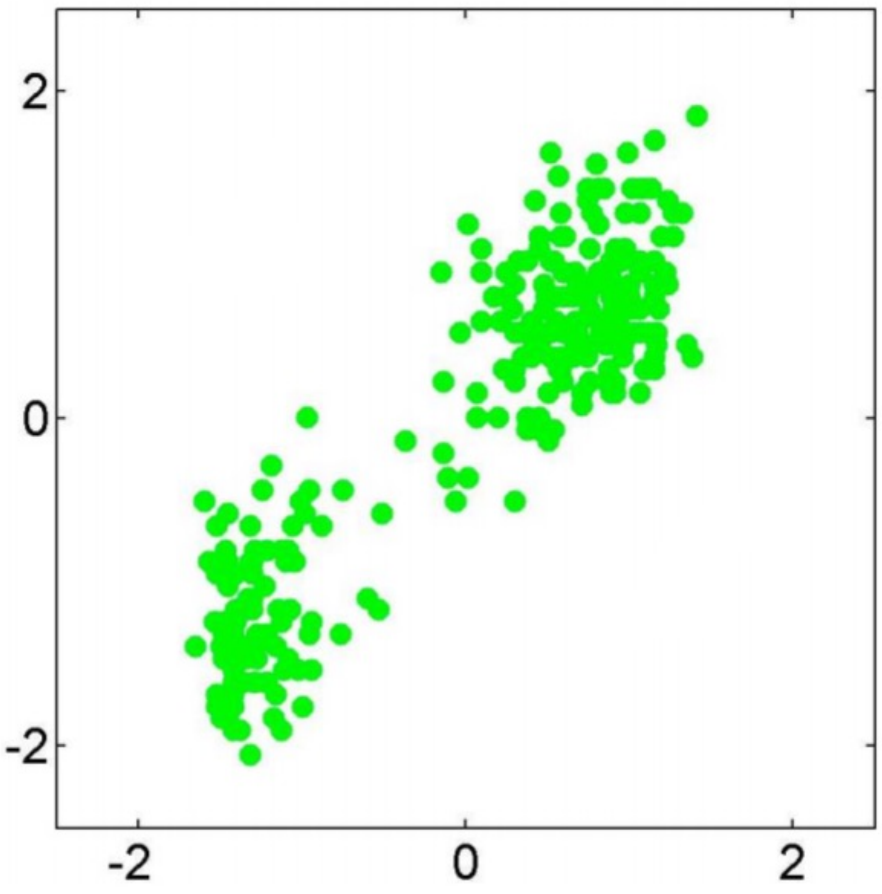
  - Re-compute the cluster center $\mathbf{c}_k$ for every new cluster

$$\mathbf{c}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$$

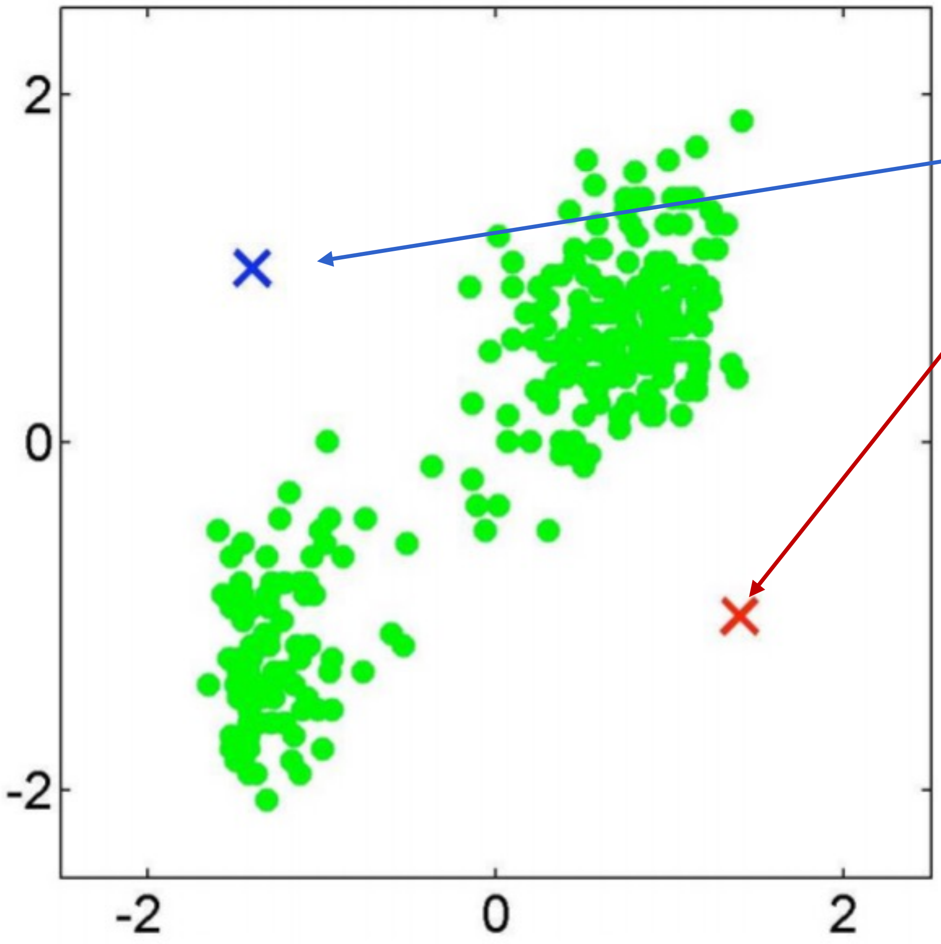
C_k is the set of samples in cluster k
$|C_k|$ denotes the number of samples in C_k

  - Repeat while not converged
- Converge criteria: Cluster centers do not change anymore

K-means Example (Assume K = 2)

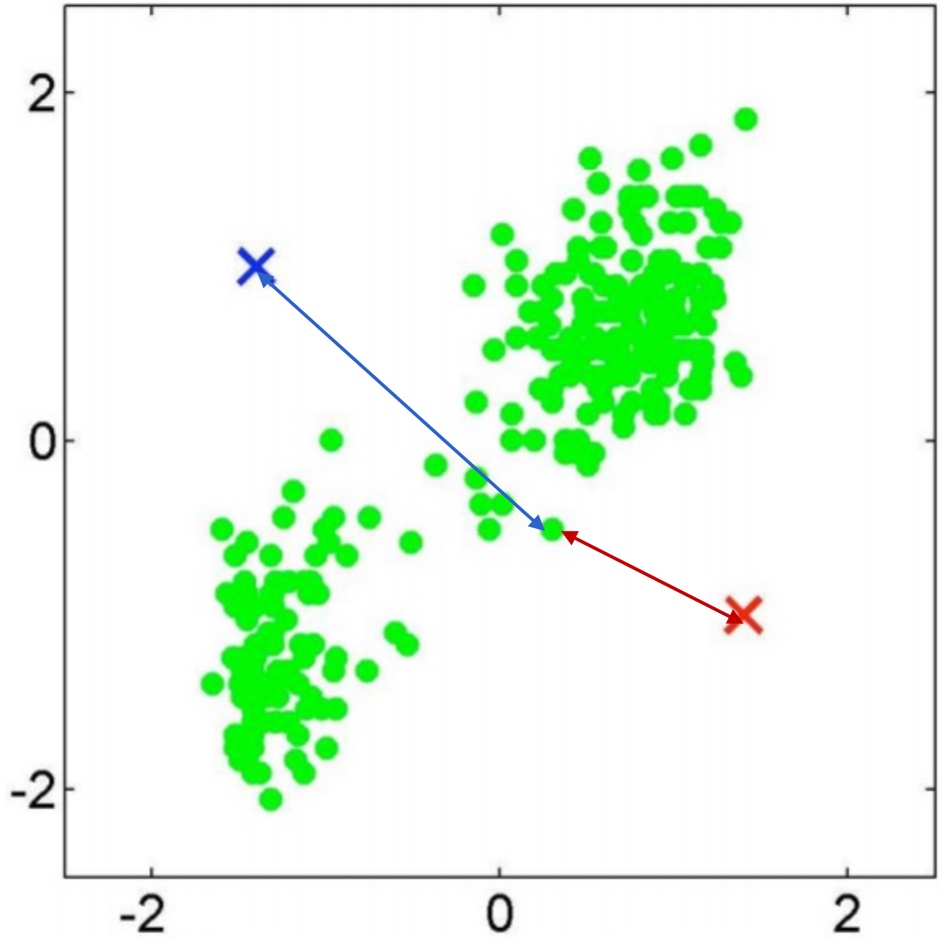


K-means Example: Initialization



- Randomly initialize two data points in the input space as the cluster centers.

K-means Iteration 1: Assign Data Points to Cluster

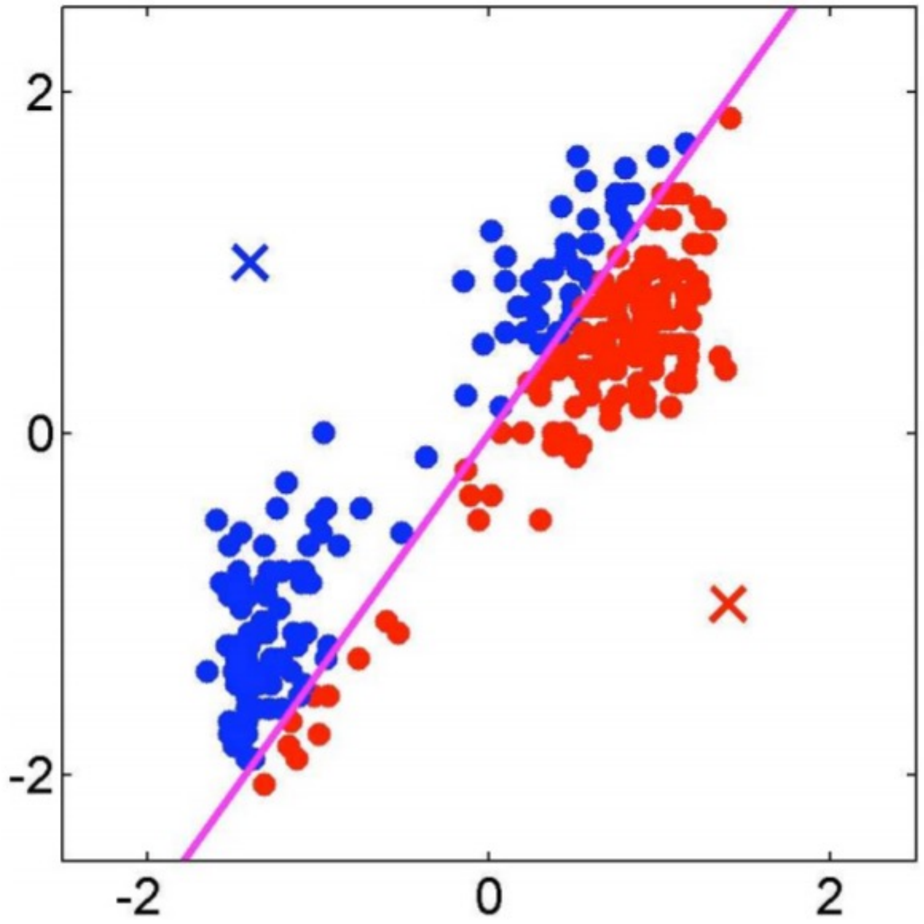


- For each sample, compute its distance from the cluster centers.

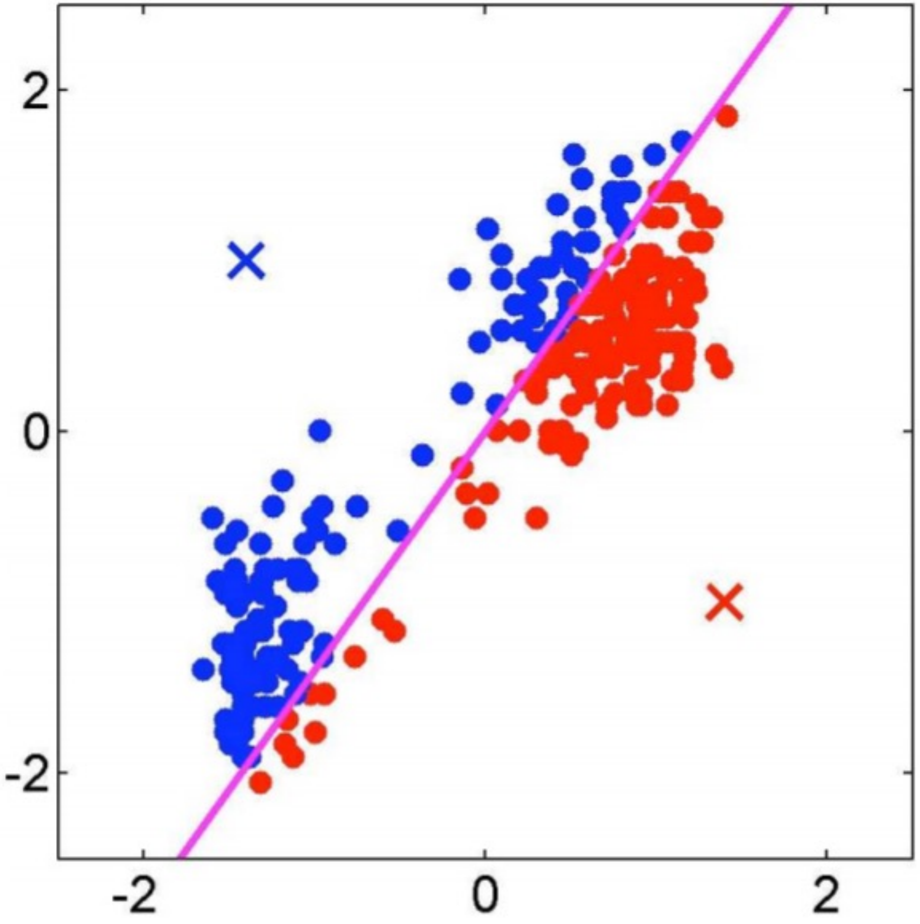
- Assign each sample $\mathbf{x}_i$ to its closest cluster center.

$$k = \arg\min_k \|\mathbf{x}_i - \mathbf{c}_k\|$$

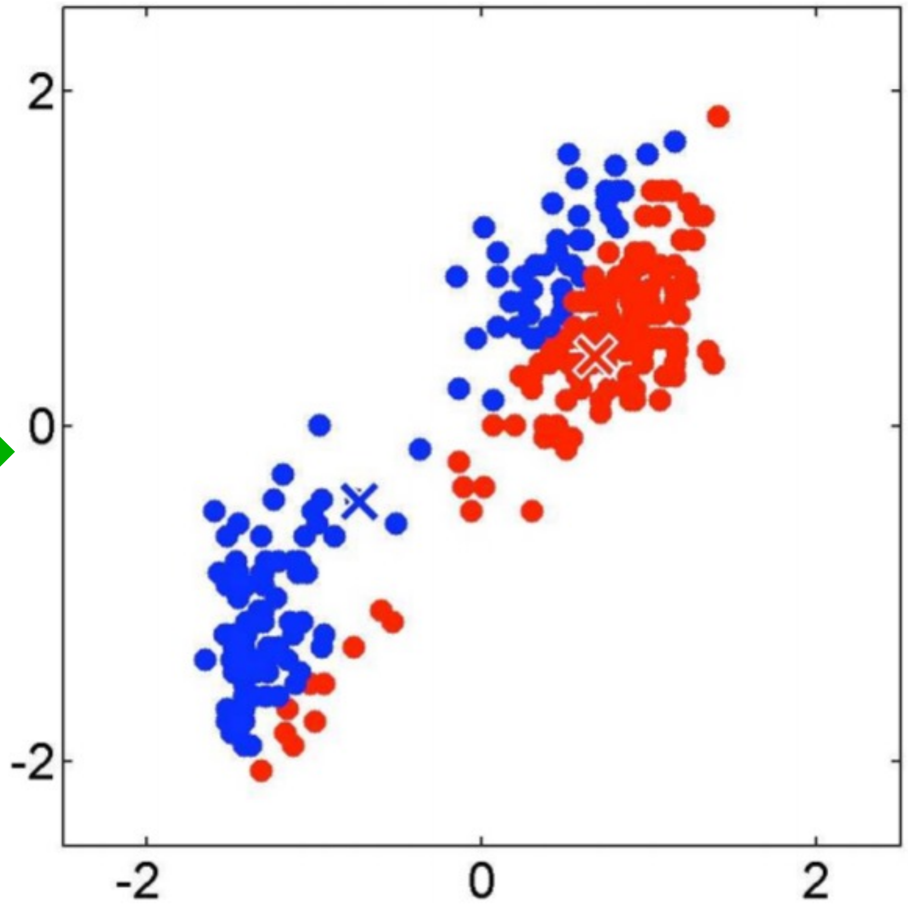
K-means Iteration 1: Assign Data Points to Cluster



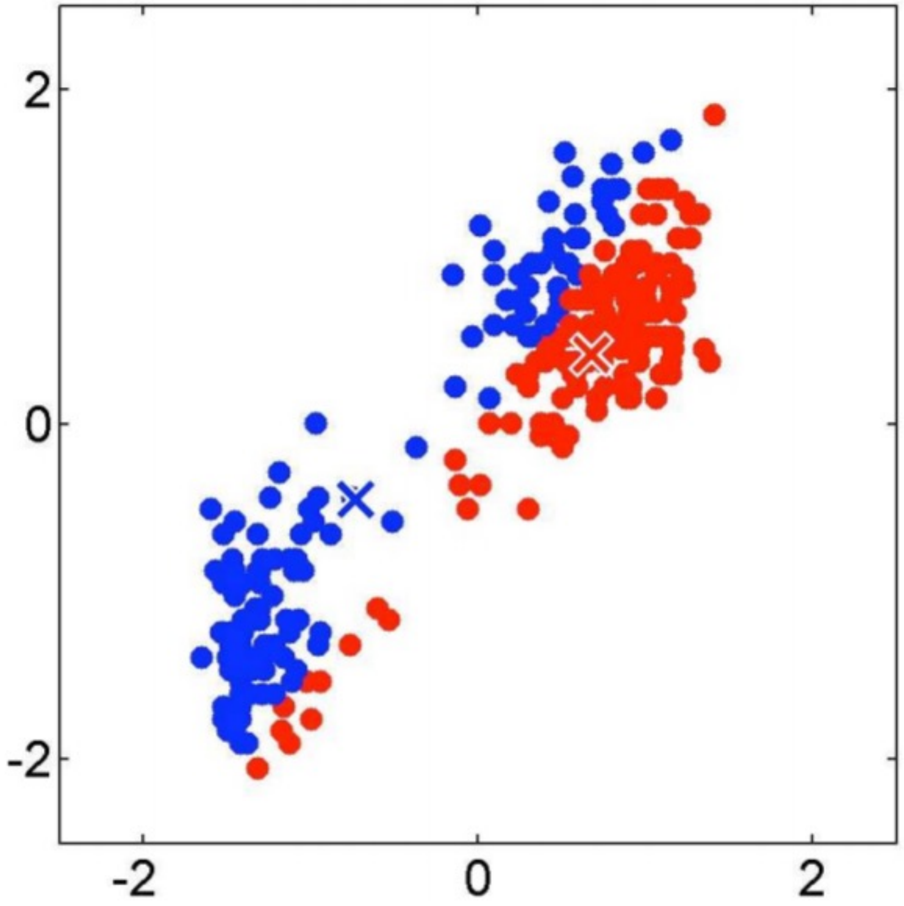
K-means Iteration 1: Recompute the Cluster Centers



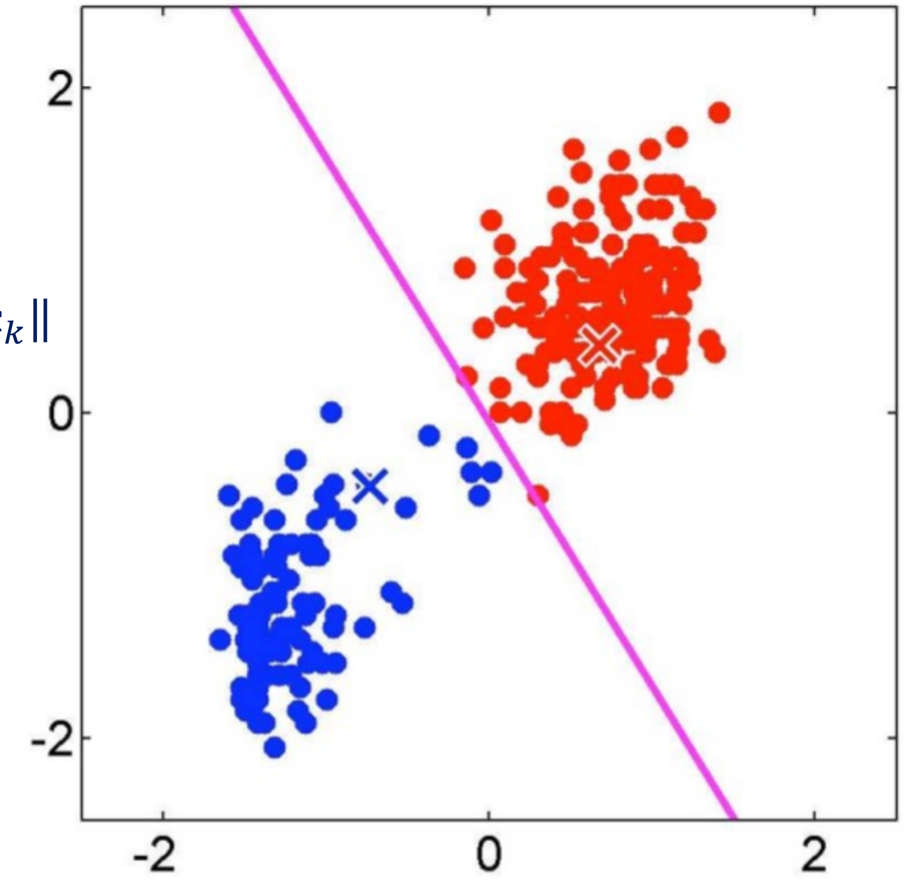
$$\mathbf{c}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$$



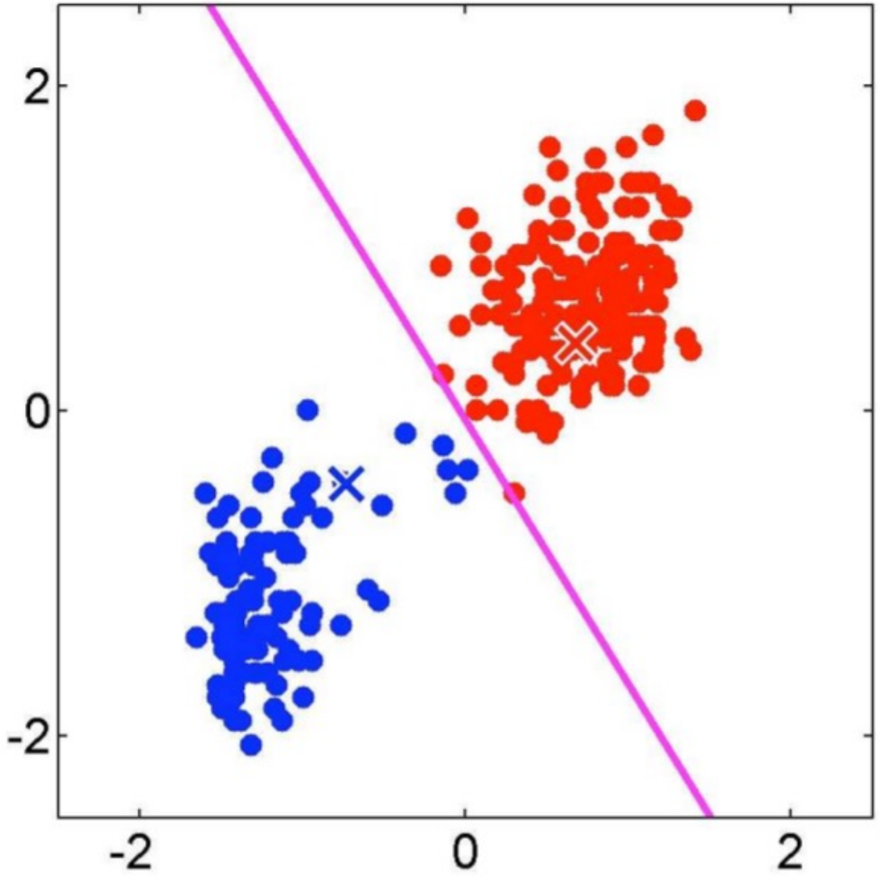
K-means iteration 2: Assign Data Points to Cluster



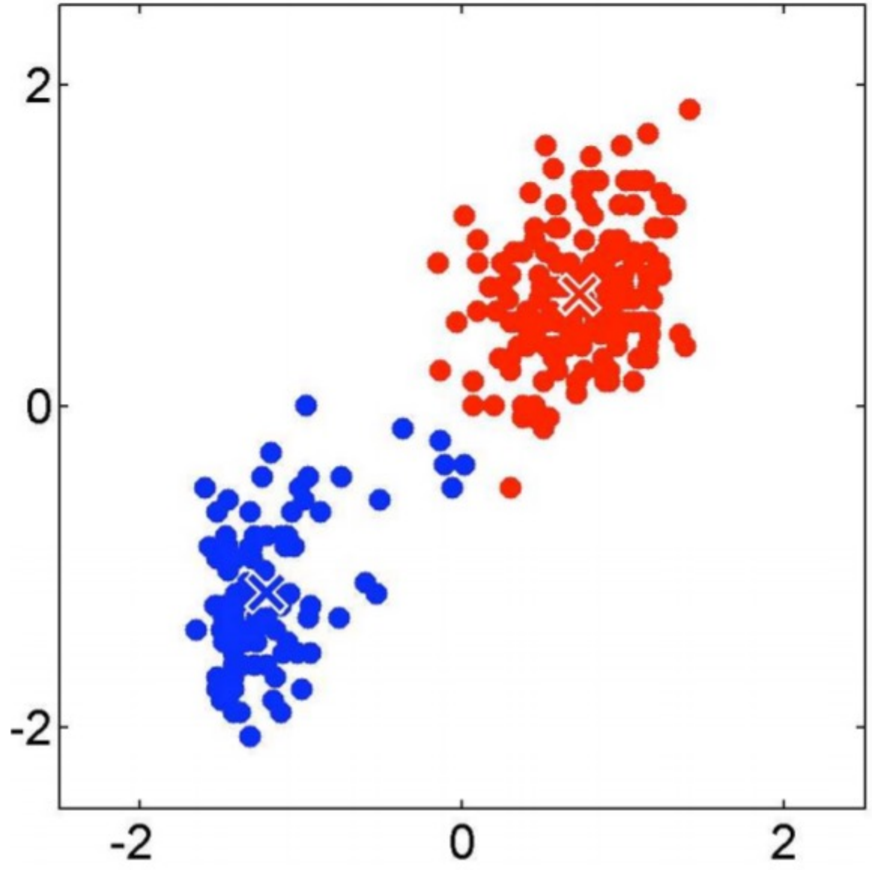
$$k = \arg\min_{k} \|\mathbf{x}_i - \mathbf{c}_k\|$$



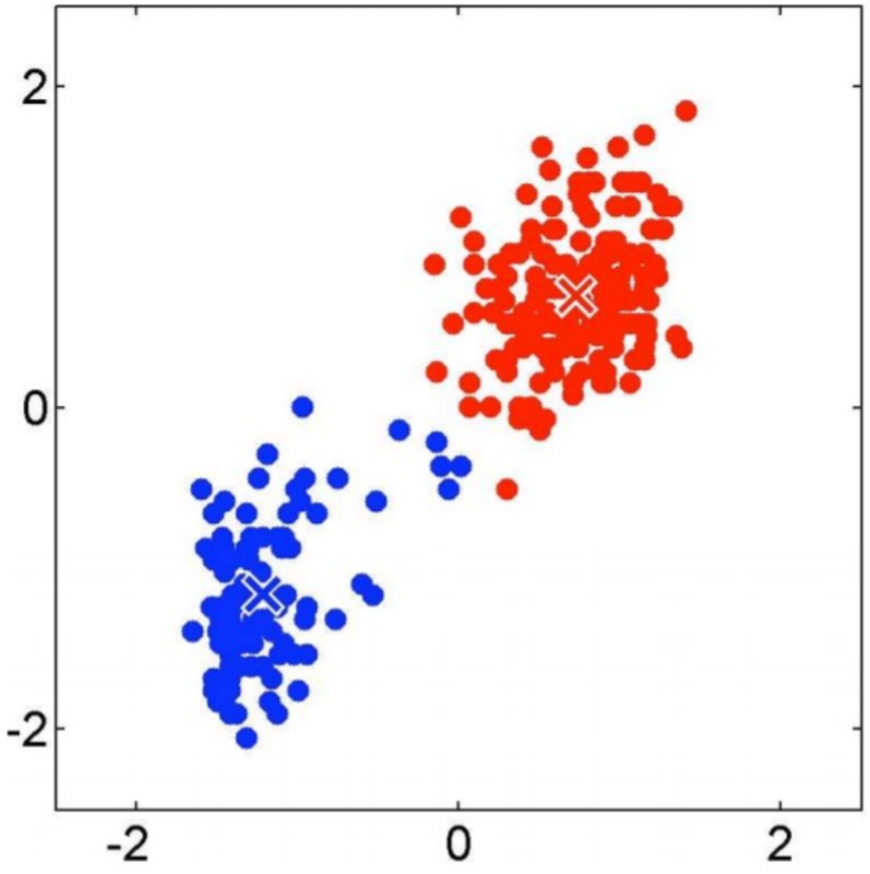
K-means Iteration 2: Recompute the Cluster Centers



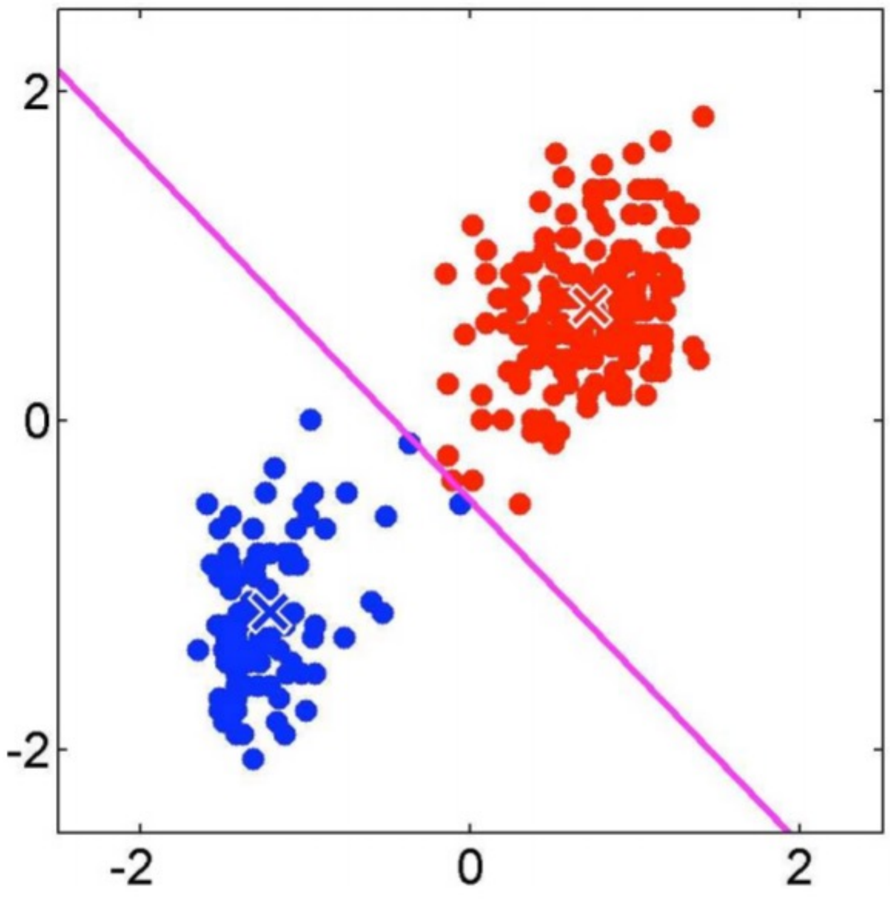
$$\mathbf{c}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$$



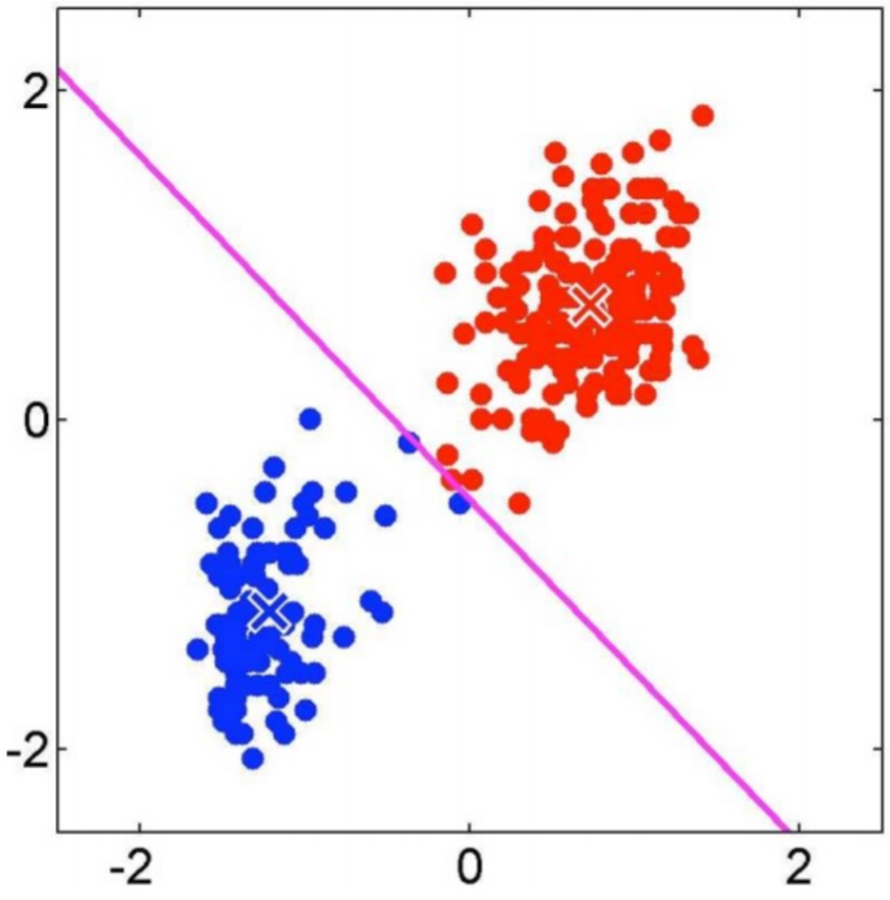
K-means Iteration 3: Assign Data Points to Cluster



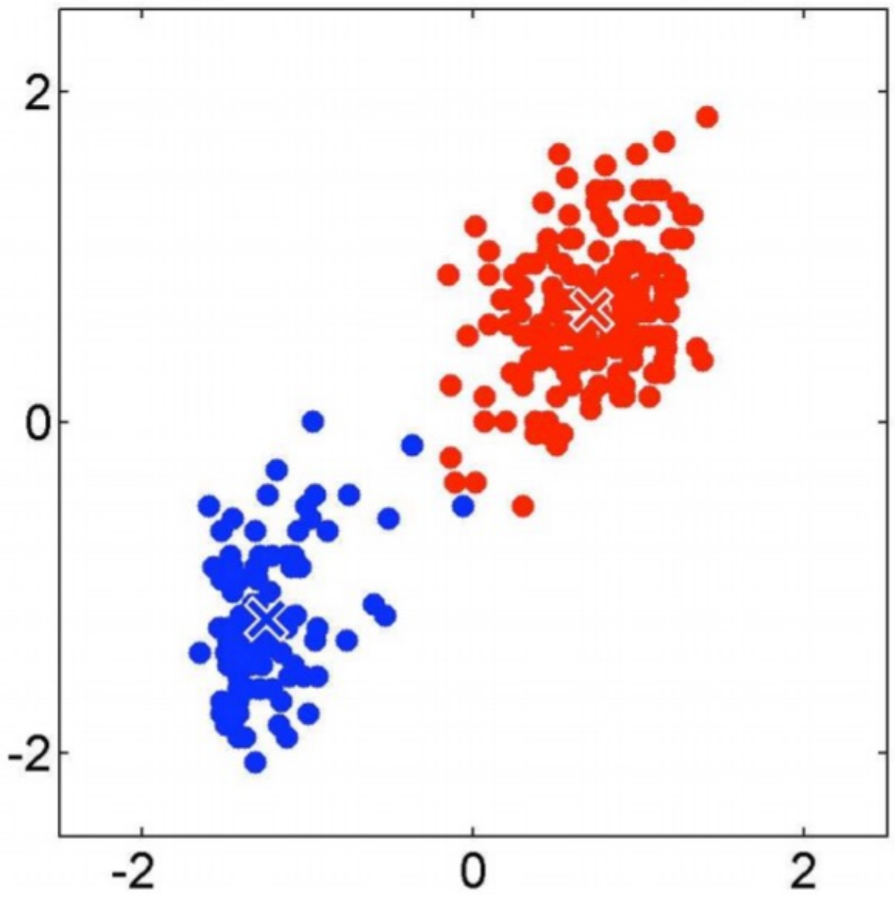
$$k = \arg\min_k \|\mathbf{x}_i - \mathbf{c}_k\|$$



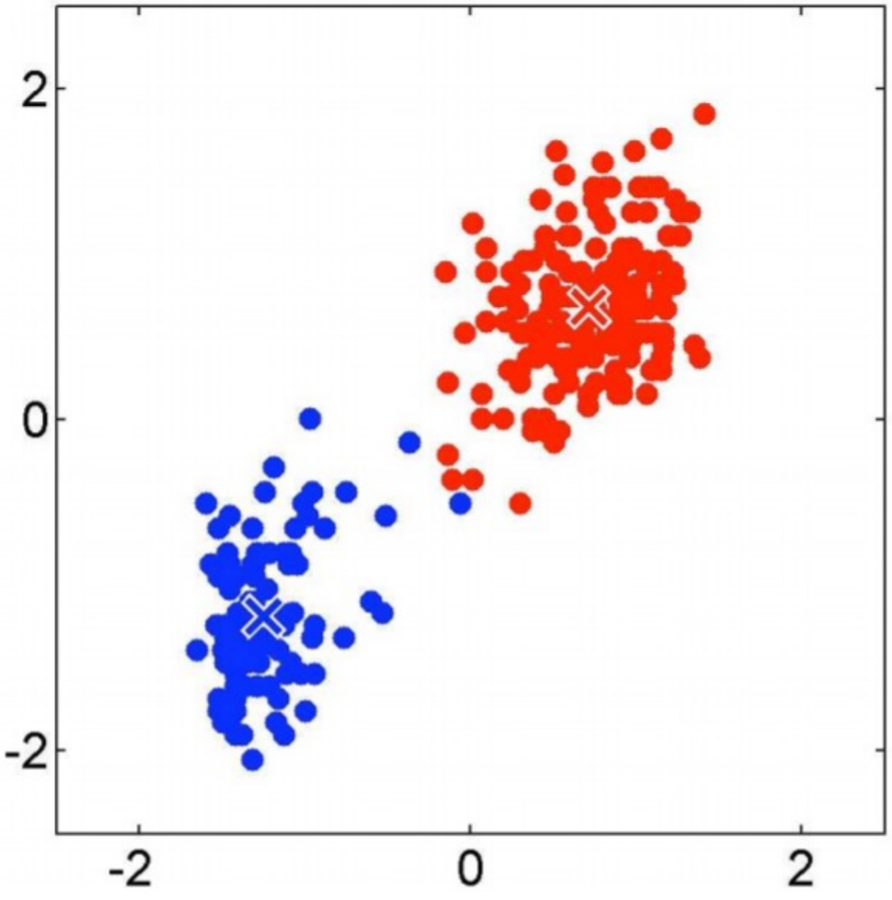
K-means Iteration 3: Recompute the Cluster Centers



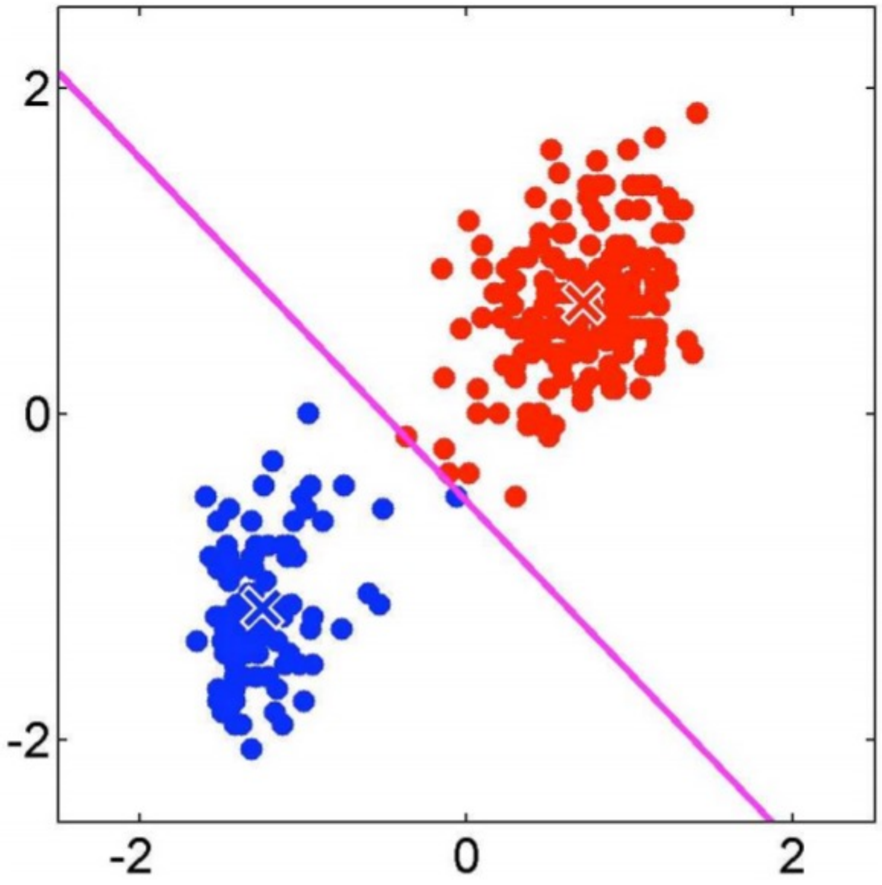
$$\mathbf{c}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$$



K-means Iteration 4: Assign Data Points to Cluster

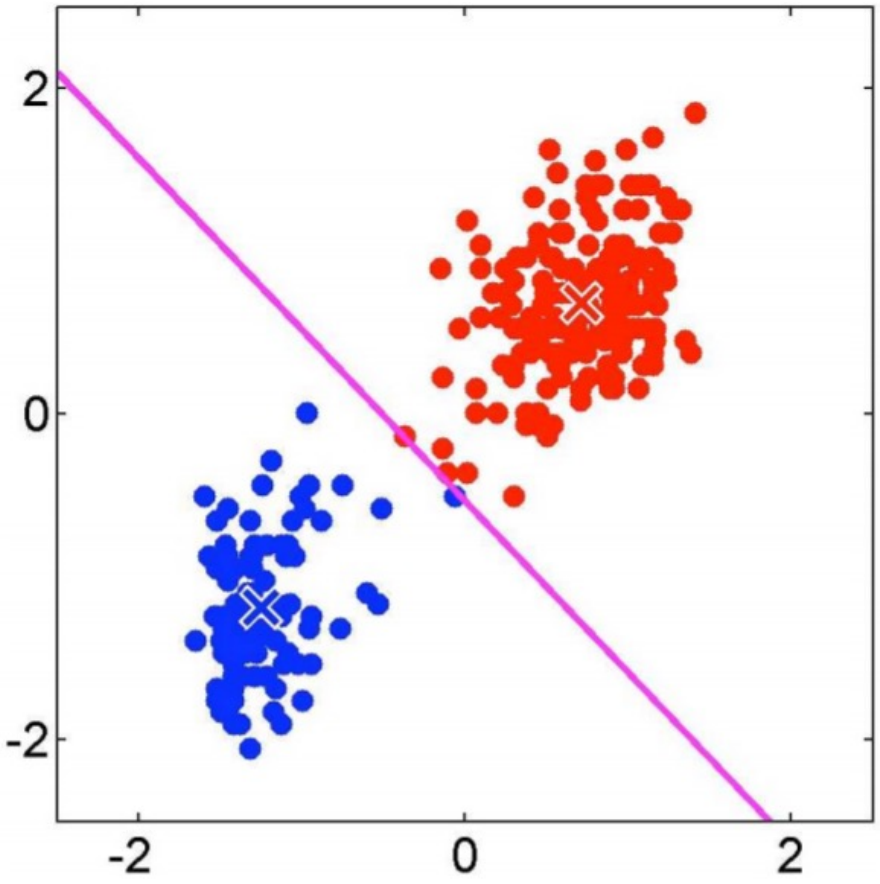


$$k = \arg\min_k \|\mathbf{x}_i - \mathbf{c}_k\|$$

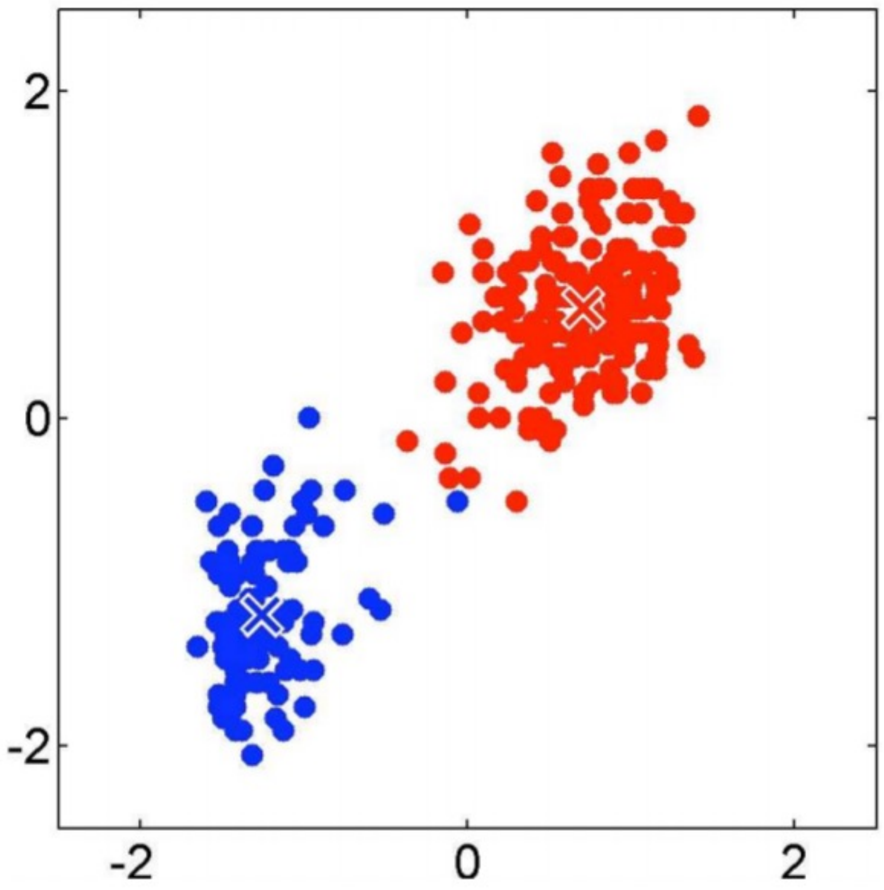


The cluster information does not change. The algorithm converged.

K-means iteration 4: Recompute the Cluster Centers



$$\mathbf{c}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$$



The cluster centers do not change. The algorithm converged.

K-means: The Objective Function for Optimization

- The *K*-means objective function
  - Let $\mathbf{c}_1, \ldots, \mathbf{c}_K$ be the K cluster centers (means)
  - Let $\gamma_{ik} \in \{0,1\}$ be indicator variable denoting whether data point $\mathbf{x}_i$ belongs to cluster k

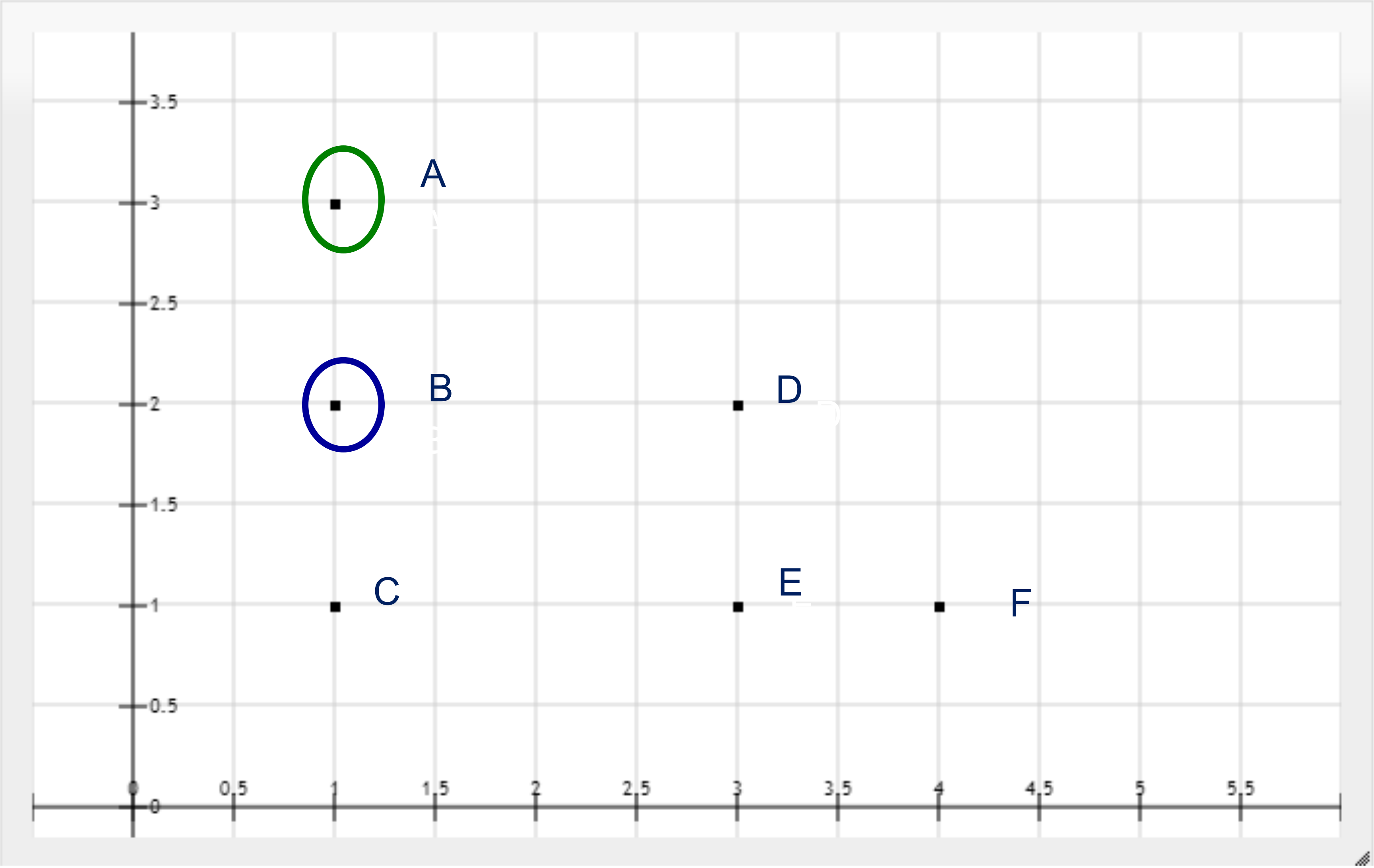
$$\gamma_{ik} = \begin{cases} 1 \text{ if } \mathbf{x}_i \text{ belongs to cluster } k \\ 0 \text{ if } \mathbf{x}_i \text{ not belongs to cluster } k \end{cases}$$

  - *K-means algorithm aims to minimize the total sum of distances of points from their cluster centers.*

$$J = \sum_{i=1}^{m} \sum_{k=1}^{K} \gamma_{ik} \|\mathbf{x}_i - \mathbf{c}_k\|^2$$

  - **Note:** Exact optimization of the *K*-means objective function needs exhaustively enumerate all partitions. It is a NP-hard problem (to compute global optimal solution).
  - The *K*-means algorithm is a **heuristic way** to obtain a local optimal solution.

Another K-means Example



Iteration #1

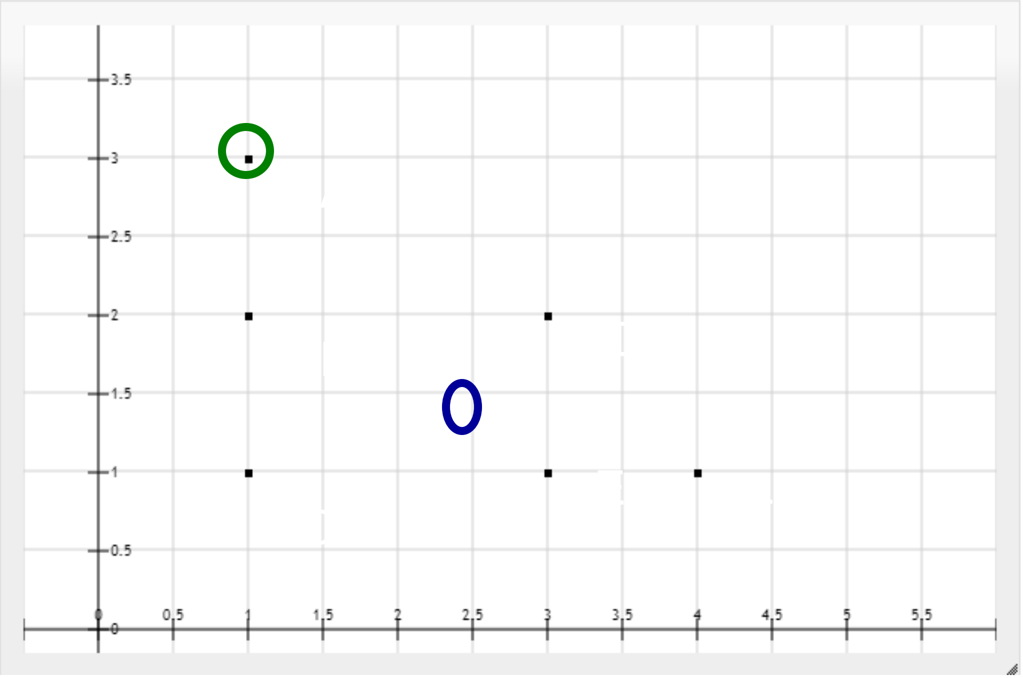
- Assume A and B were randomly picked as initial centroids.
- Computes the distance for each points

Points	Centroids 1 (A)	Centroids 2(B)
A (1,3)	***0***	1
B (1,2)	1	***0***
C (1,1)	2	***1***
D (3,2)	sqrt(5)	***2***
E (3,1)	sqrt(8)	***sqrt(5)***
F (4,1)	sqrt(13)	***sqrt(10)***

Compute New Centroids #2

- New centroids:
- Centroids 1: A
- Centroids 2: Mean of (B,C,D,E,F)

$$(x, y) = (\frac{1+1+3+3+4}{5}, \frac{2+1+2+1+1}{5}) = (2.4, 1.4)$$



Iteration #2

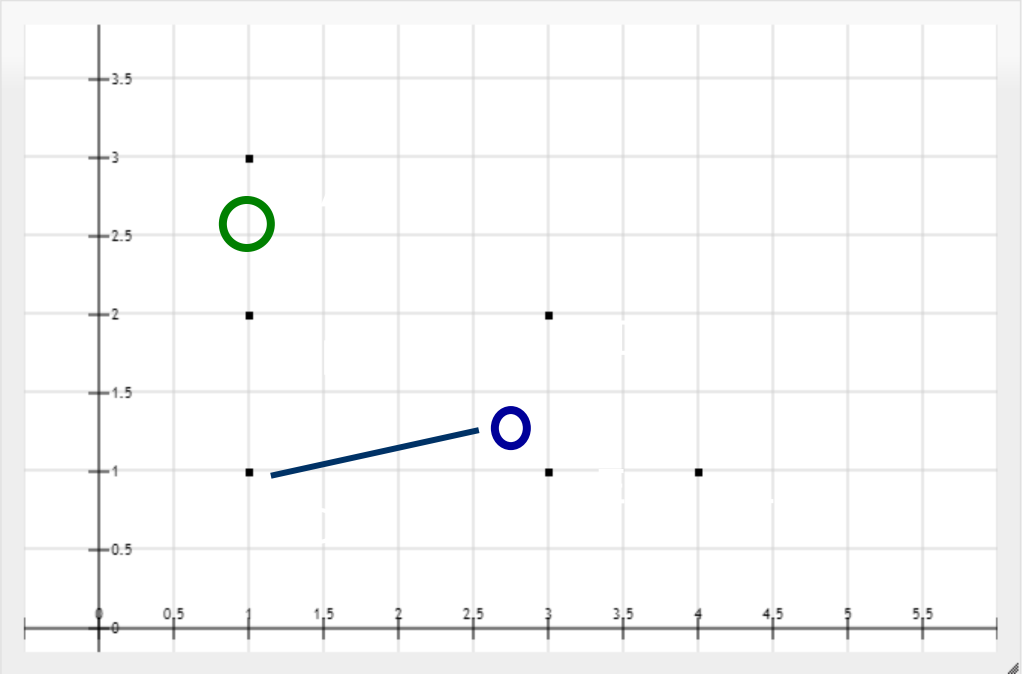
- Computes the distance for each points

Points	Centroids 1 (A)	Centroids 2(2.4,1.4)
A (1,3)	***0***	2.13
B (1,2)	***1***	1.523
C (1,1)	2	***1.46***
D (3,2)	2.24	***0.85***
E (3,1)	2.83	***0.72***
F (4,1)	3.61	***1.65***

Compute New Centroids #3

- New centroids:
- Centroids 1: Mean of (A, B) = (1, 2.5)
- Centroids 2: Mean of (C,D,E,F)

$$(x, y) = \left(\frac{1+3+3+4}{4}, \frac{1+2+1+1}{4}\right) = (2.75, 1.25)$$



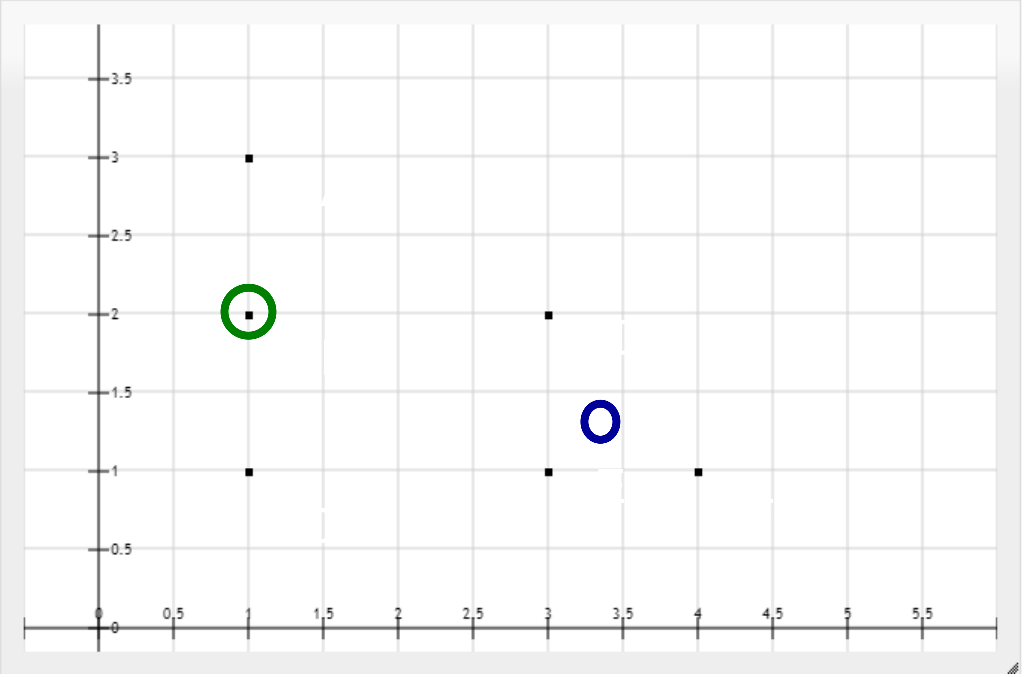
Distance between c and new centroids 2 is1.77

Thus, new group is (A,B,C), (D,E,F)

Compute New Centroids #4

- New centroids:
- Centroids 1: Mean of (A, B, C) = B
- Centroids 2: Mean of (D,E,F)

$$(x, y) = \left(\frac{3+3+4}{3}, \frac{2+1+1}{3}\right) = (3.33, 1.33)$$



Obviously the new group is (A,B,C), (D,E,F).

Stop here.

K-means: The Objective Function for Optimization

- The *K*-means objective function

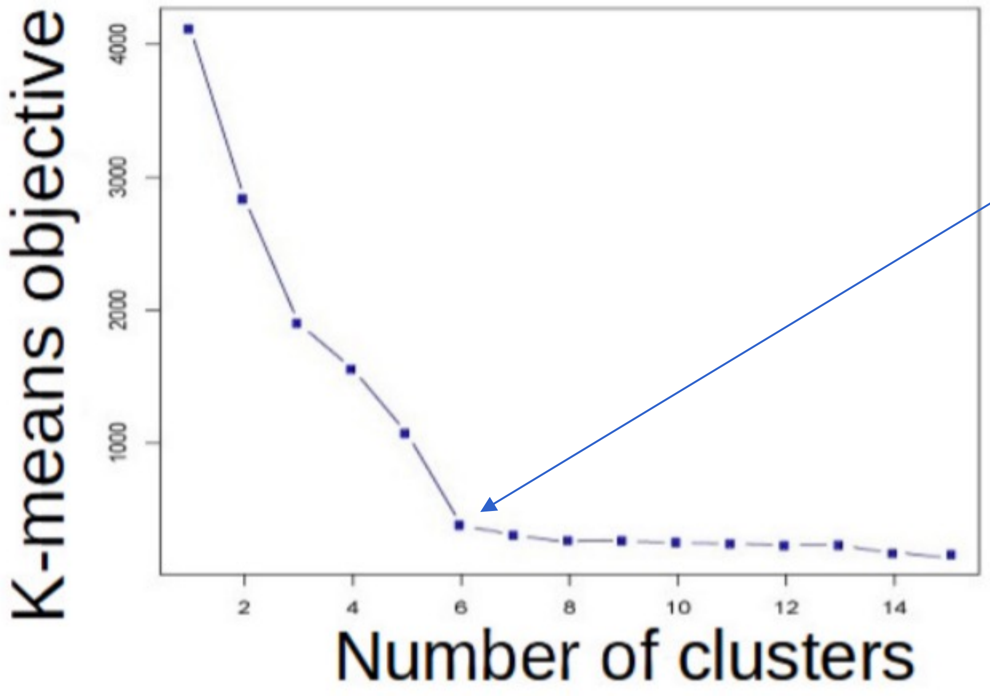
$$J = \sum_{i=1}^{m} \sum_{k=1}^{K} \gamma_{ik} \|\mathbf{x}_i - \mathbf{c}_k\|^2$$

- *K*-means algorithm is a heuristic to optimize this function. It works iteratively between two steps
  - Fix cluster centers $\mathbf{c}_k$, find best γ_{ik} (assign data points to cluster)
  - Fix γ_{ik}, find the best $\mathbf{c}_k$ (re-compute the cluster center)

- Convergence of *K*-means algorithm
  - Each step can never increase the objective

How to choose *K* (number of clusters)

- One way to select *K* for the *K*-means algorithm is to try different values of *K*, plot the *K*-means objective versus *K*, and look at the “elbow-point” in the plot.



K = 6 is the elbow point.

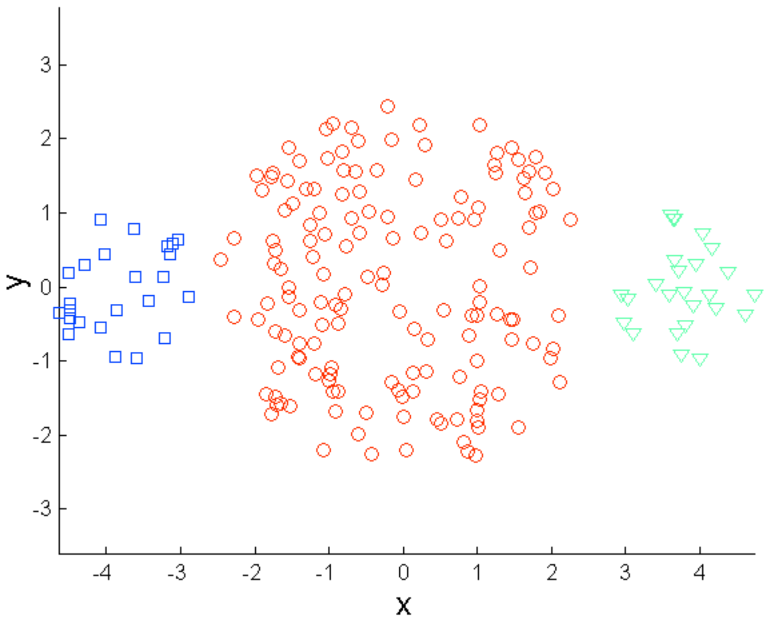
K-means: Initialization Issues

- *K*-means is extremely sensitive to cluster center initialization
- Bad initialization can lead to
  - Poor convergence speed
  - Bad overall clustering
- Possibly solutions
  - Choose the first center as one of the samples, the second which is the farthest from the first, the third which is the farthest from both, and so on.
  - Try multiple initializations and choose the best result.

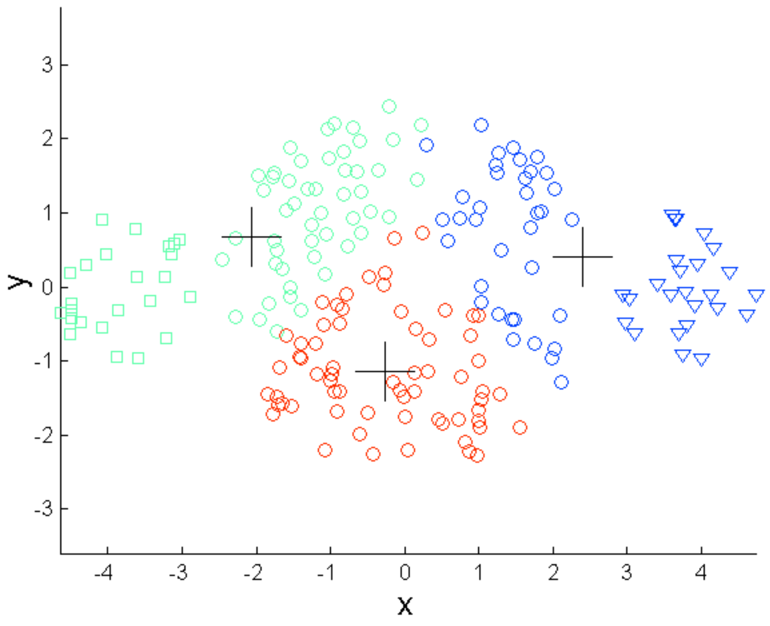
K-means: Limitations

- 1. K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- 2. Makes hard assignments of points to clusters
  - A point either completely belongs to a cluster or does not belong
  - Soft assignment ignored (i.e., probability of being assigned to each cluster: say $K = 3$ for some points $\mathbf{x}_i$, $p_1 = 0.7$, $p_2 = 0.2$, $p_3 = 0.1$)

Limitations of K-means: Differing Sizes

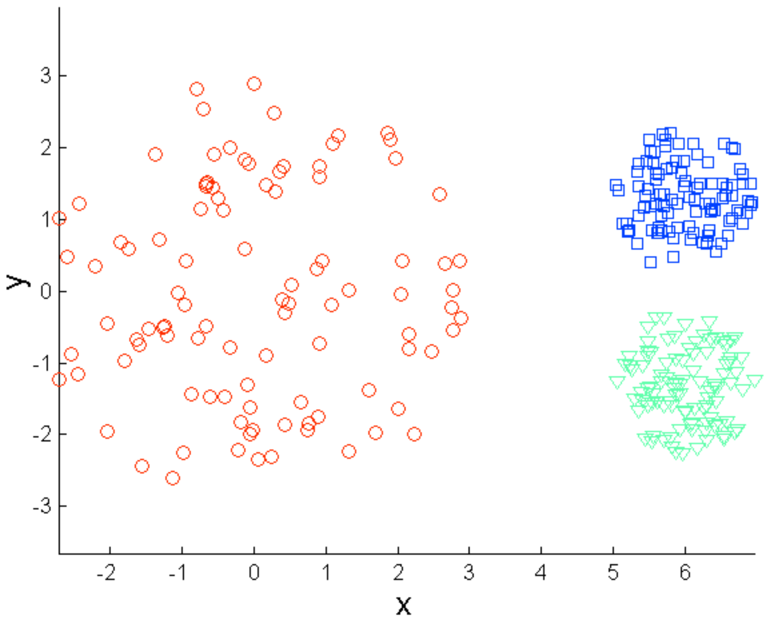


Original Points

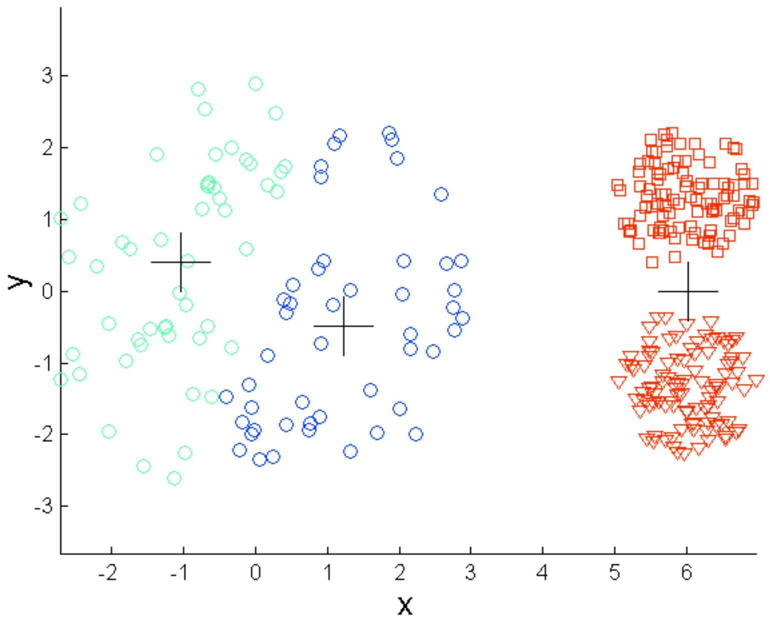


K-means (3 Clusters)

Limitations of K-means: Differing Density

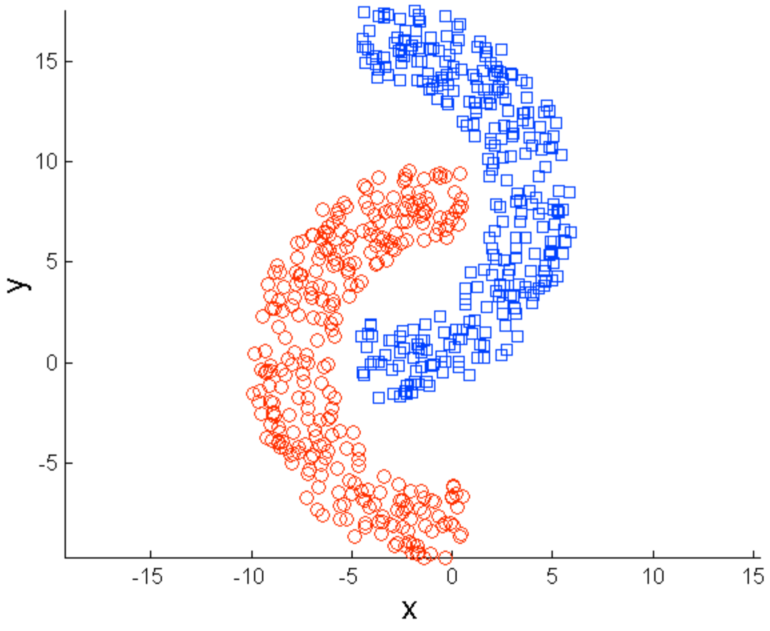


Original Points

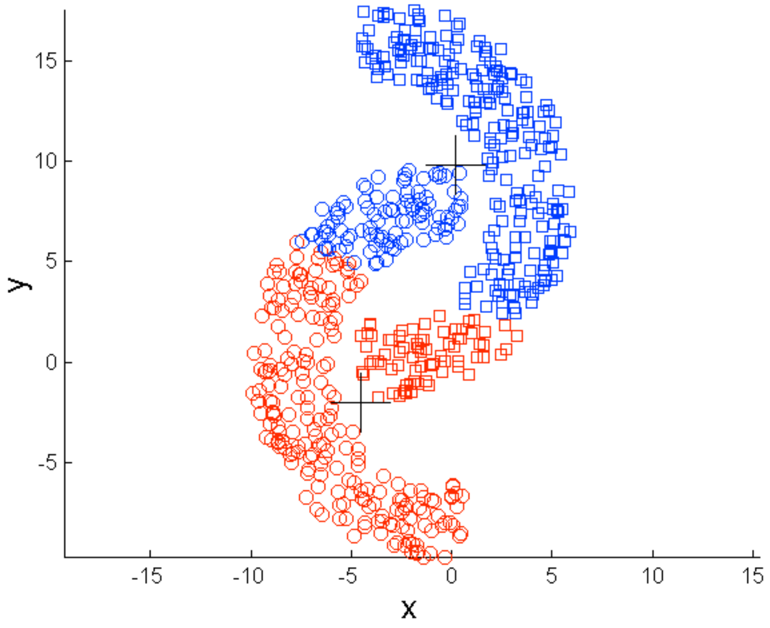


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



Original Points

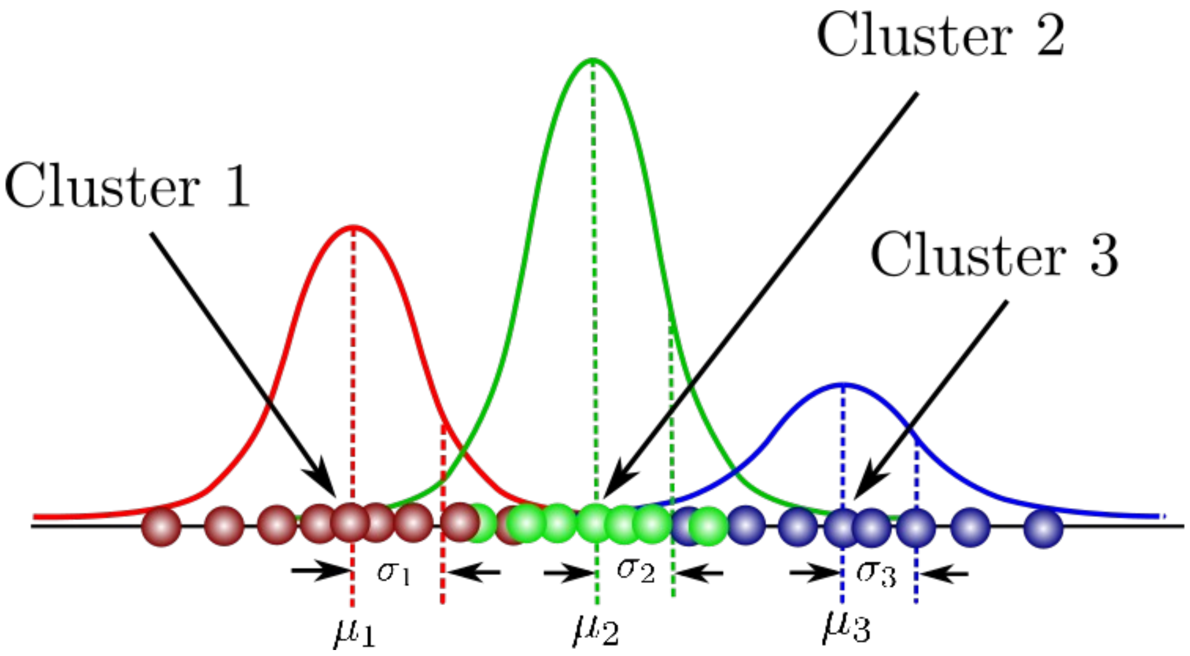


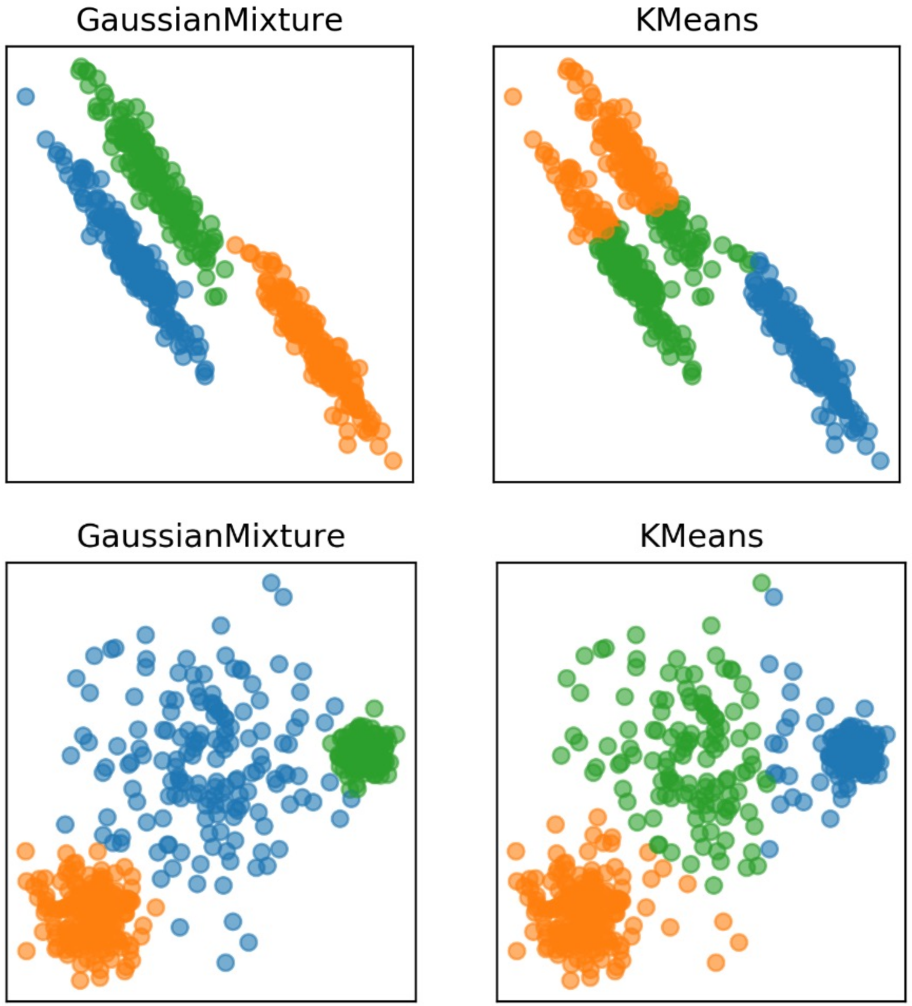
K-means (2 Clusters)

K-means: Limitations

- 1. K-means has problems when clusters are of differing
  - Sizes (*Gaussian Mixture Models*)
  - Densities (*Gaussian Mixture Models*)
  - Non-globular shapes (Kernel *K*-means)
- 2. Makes hard assignments of points to clusters (*Gaussian Mixture Models*)
  - A point either completely belongs to a cluster or does not belong
  - Soft assignment ignored (i.e., probability of being assigned to each cluster: say $K = 3$ for some points $\mathbf{x}_i$, $p_1 = 0.7$, $p_2 = 0.2$, $p_3 = 0.1$)
- *Solution: Gaussian Mixture Models and* Kernel *K*-means

Gaussian Mixture Models





Kernel *K*-means

- The idea: Replace the Euclidean distance/similarity computations in *K*-means by the kernelized version $d(\mathbf{x}_i, \mathbf{c}_k) = \|\phi(\mathbf{x}_i) - \phi(\mathbf{c}_k)\|$

$$\begin{aligned}\|\phi(\mathbf{x}_i) - \phi(\mathbf{c}_k)\|^2 &= \|\phi(\mathbf{x}_i)\|^2 + \|\phi(\mathbf{c}_k)\|^2 - 2\phi(\mathbf{x}_i)^T\phi(\mathbf{c}_k) \\ &= k(\mathbf{x}_i, \mathbf{x}_i) + k(\mathbf{c}_k, \mathbf{c}_k) - 2k(\mathbf{x}_i, \mathbf{c}_k)\end{aligned}$$

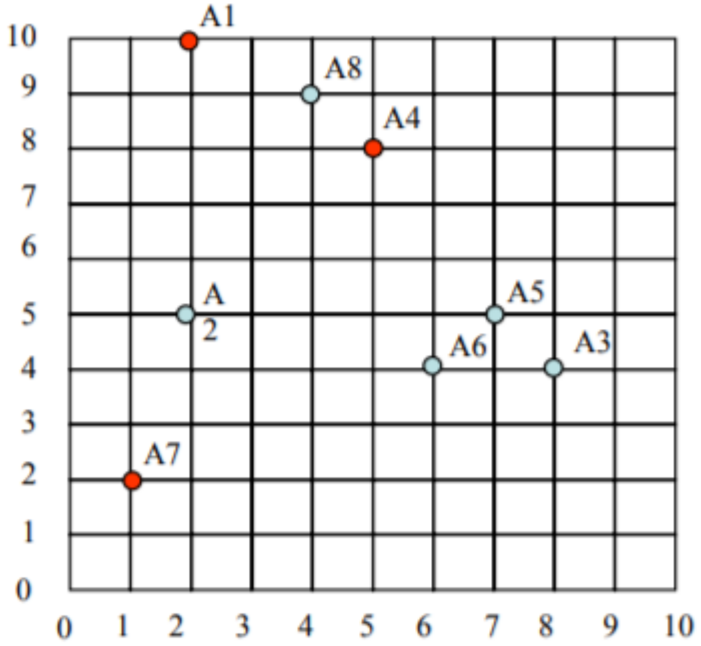
- Here *k*(.,.) denotes the kernel function and ϕ is its (implicit) feature map

- Note: ϕ does not have to be computed/stored because computation only depends on kernel evaluations

An Exercise on *K*-means Algorithm

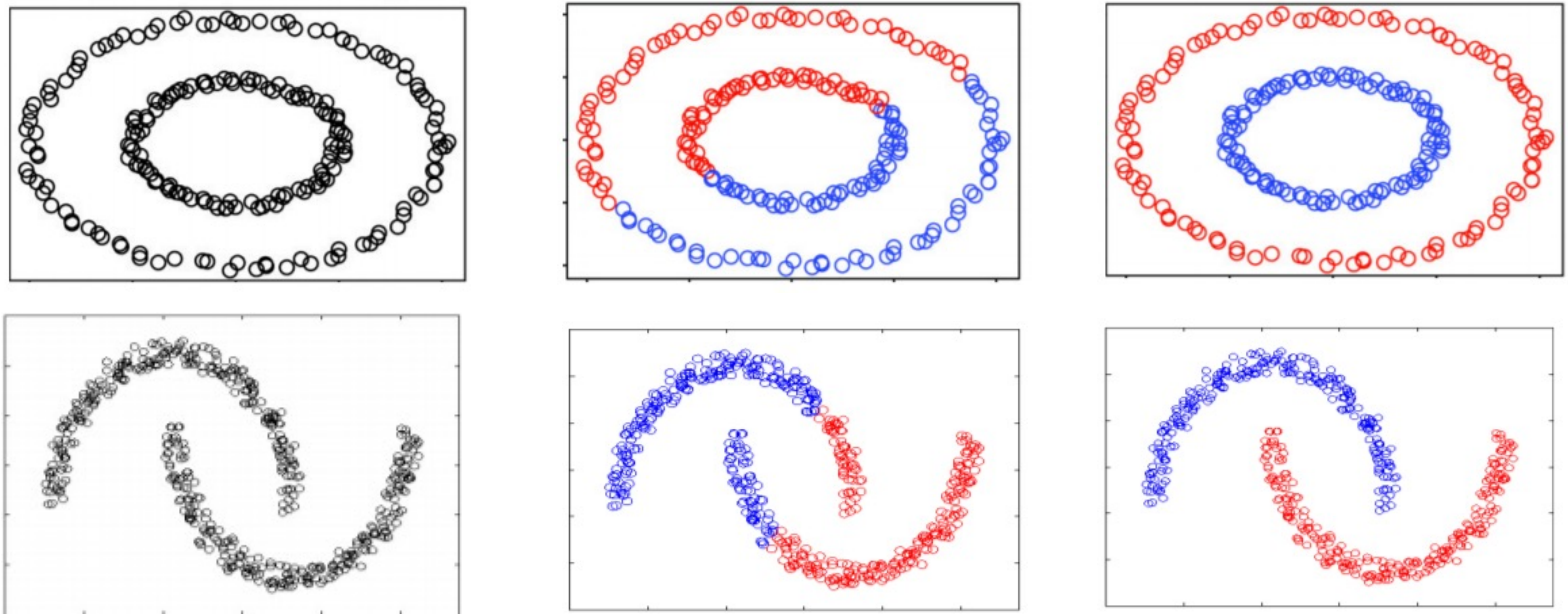
Use the *K*-means algorithm and Euclidean distance to cluster the following eight samples into three clusters. Suppose that the initial centers of the clusters are A1, A4 and A7 (as shown in red in the figure). Run the *K*-means algorithm on this data and show the results of each iteration.

ID	x_1	x_2
A1	2	10
A2	2	5
A3	8	4
A4	5	8
A5	7	5
A6	6	4
A7	1	2
A8	4	9



K-means vs Kernel *K*-means

Input Data | *K*-means | Kernel *K*-means



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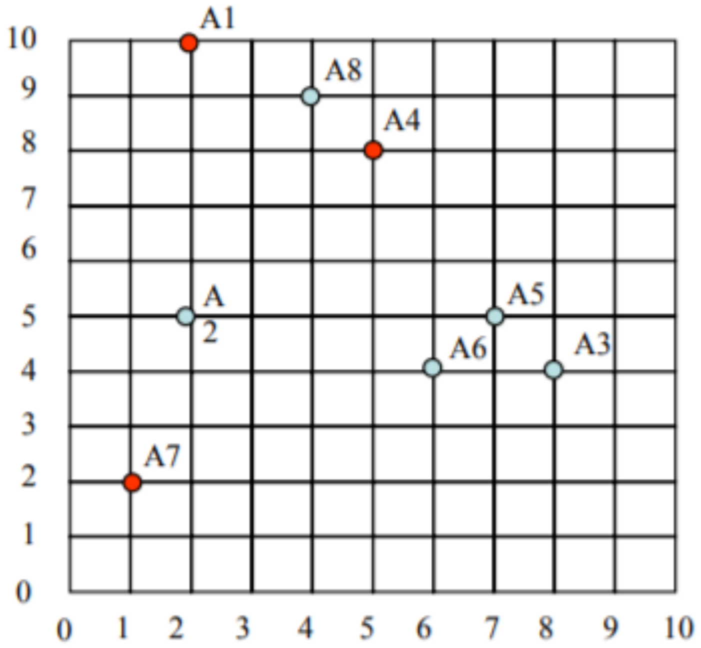


Outline for Data Preprocessing and Data Mining

- **Data Preprocessing**
- **Supervised learning**

❖ Regression

1. Linear regression with one variable
2. Linear Regression with multiple variables
3. The relationship between Correlation and Regression

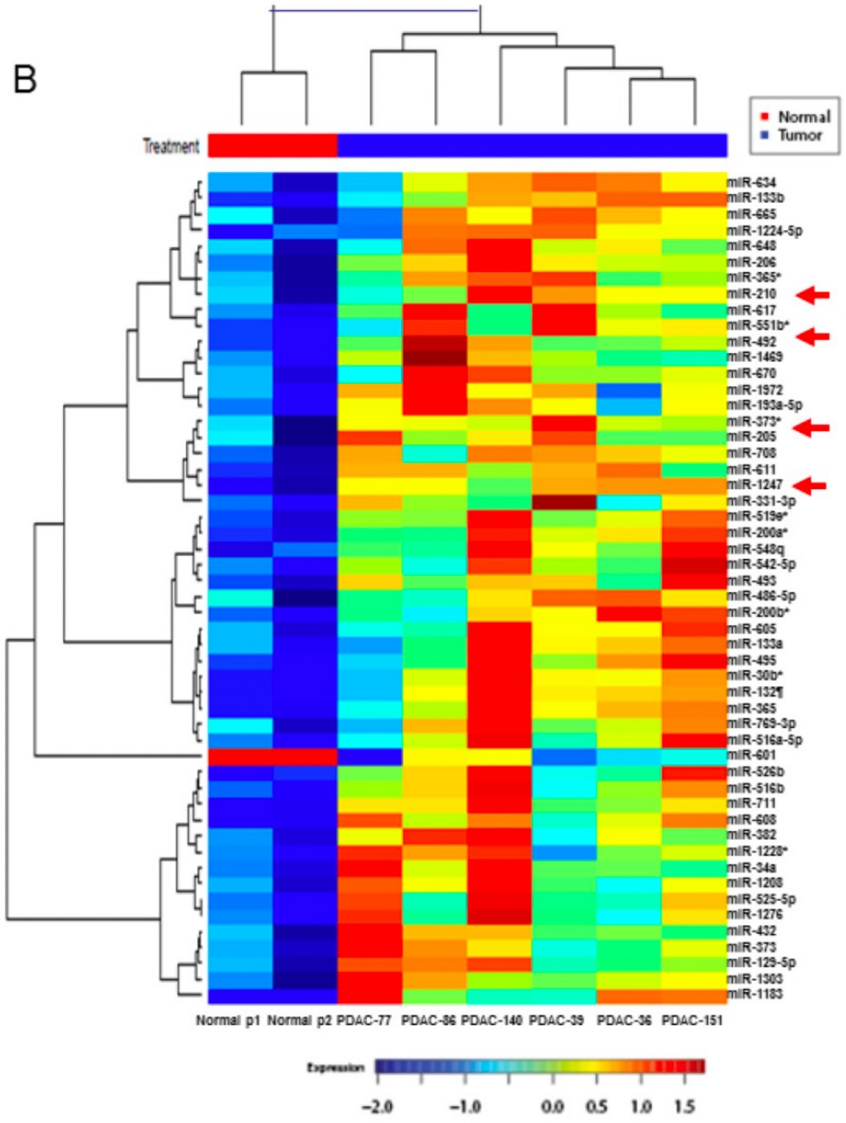
❖ Classification

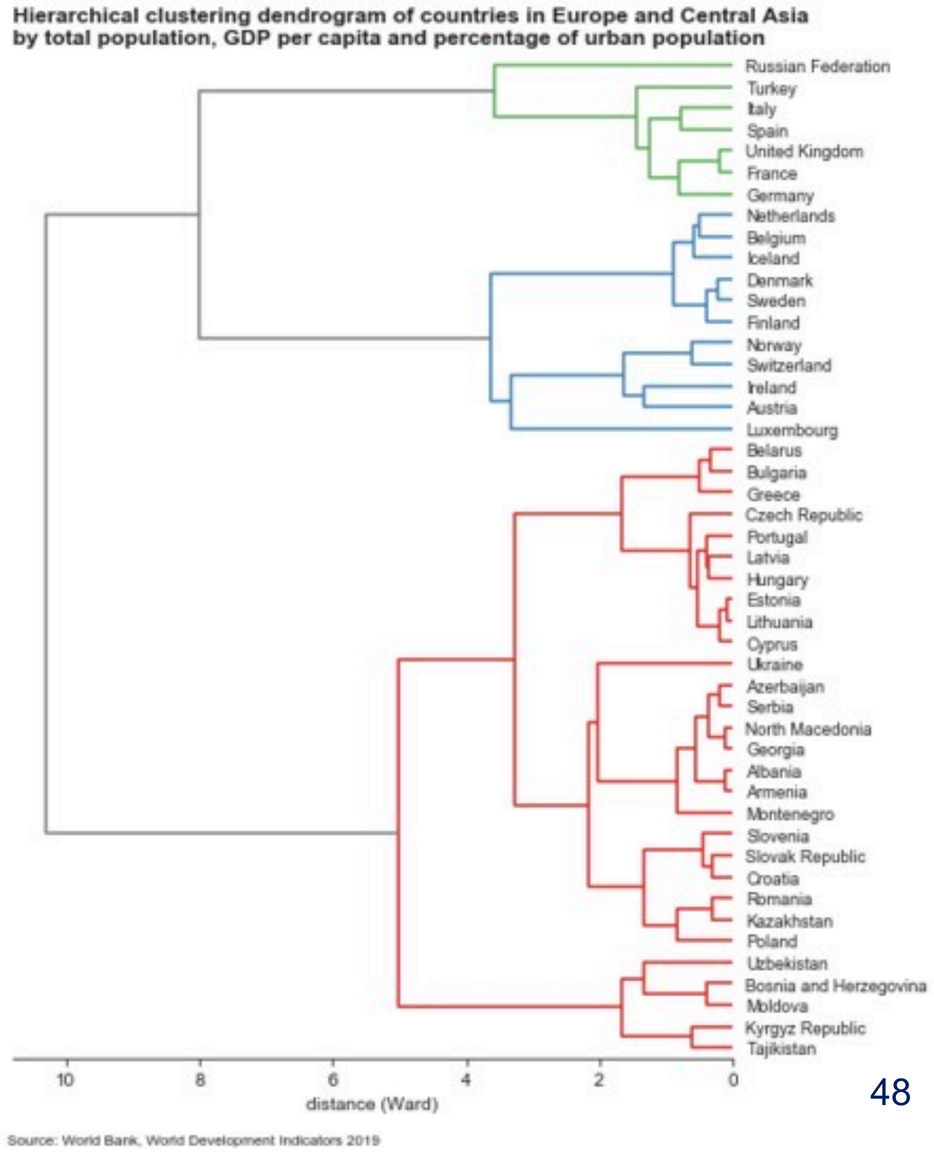
1. Perceptron
2. Artificial Neural Network
3. Support Vector Machine
4. K Nearest Neighbor

- **Unsupervised learning**

1. K-means Clustering
2. Hierarchical Clustering

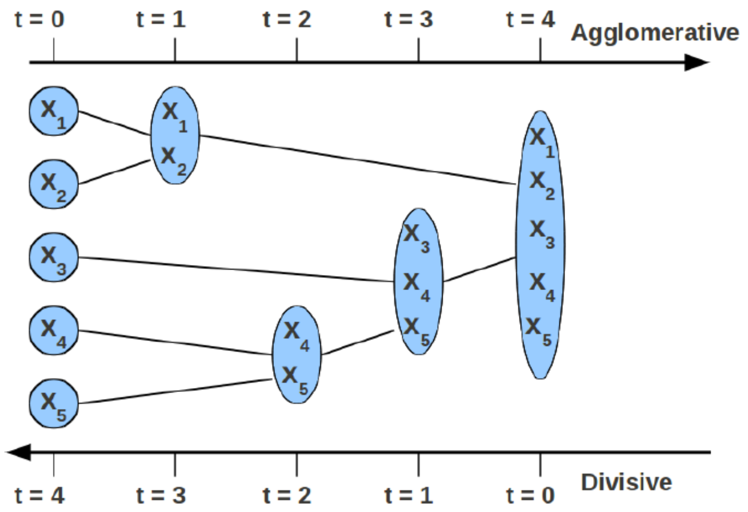
Why Hierarchical Clustering? Some Real-World Examples





Hierarchical Clustering

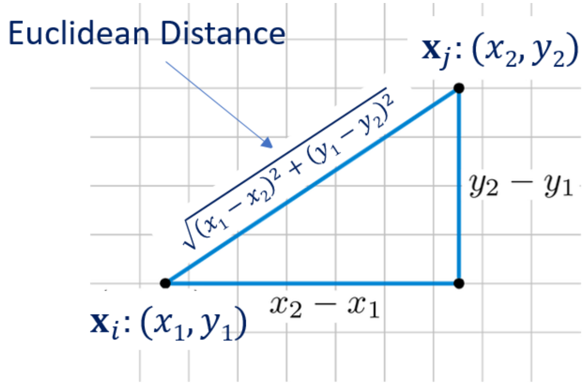
- Agglomerative (bottom-up) clustering
  - Start with each sample in its own singleton cluster.
  - At each iteration, greedily merge two most similar clusters.
  - Stop when there is a single cluster of all samples.
- Divisive (top-down) clustering
  - Start with all samples in a single cluster (i.e, the same cluster)
  - At each iteration, partition cluster(s) into smaller subclusters.
  - Stop when each sample is in its own singleton cluster.
- Agglomerative clustering is more popular and simpler than divisive clustering.



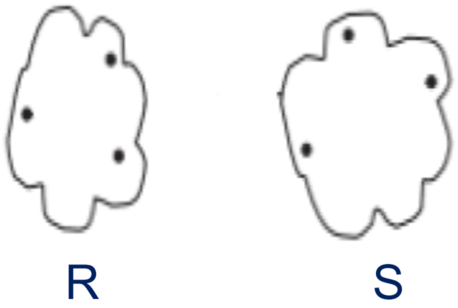
Hierarchical Clustering: (Dis)similarity Between Clusters

- We know how to compute the dissimilarity $d(\mathbf{x}_i,\mathbf{x}_j)$ between two samples (e.g., Euclidean distance)

$$\|\mathbf{x}_i - \mathbf{x}_j\|_2 = \sqrt{\sum_{k=1}^{n}(x_{ik} - x_{jk})^2}$$

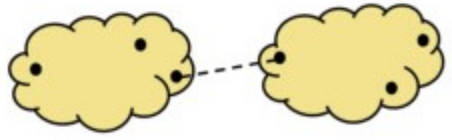


- How to compute the dissimilarity between two clusters R and S?

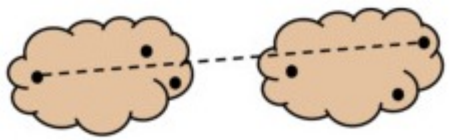


Hierarchical Clustering: (Dis)similarity Between Clusters

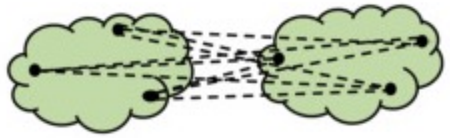
- **Single Linkage**
  - **Smallest** distances between samples, where each one is taken from one of the two groups
- **Complete Linkage**
  - **Largest** distances between samples, where each one is taken from one of the two groups
- **Average Linkage**
  - **Average** distance between all samples in one cluster to all points in another cluster
- **Centroid Linkage**
  - Distance between their **centroids**.



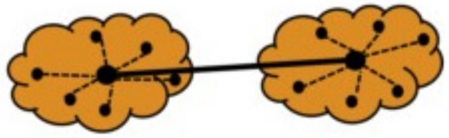
Single Linkage



Complete Linkage

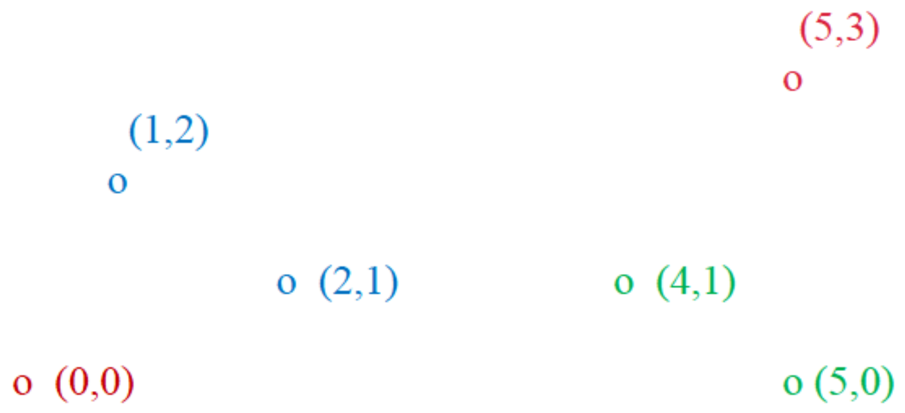


Average Linkage



Centroid Linkage

Example: Hierarchical Clustering (with Centroid Linkage)

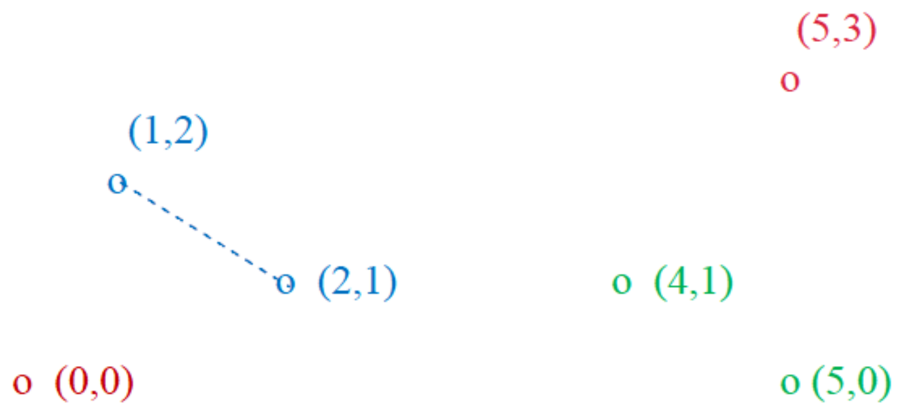


x_1	x_2
0	0
1	2
2	1
4	1
5	0
5	3

Data:
o … data point

Dendrogram

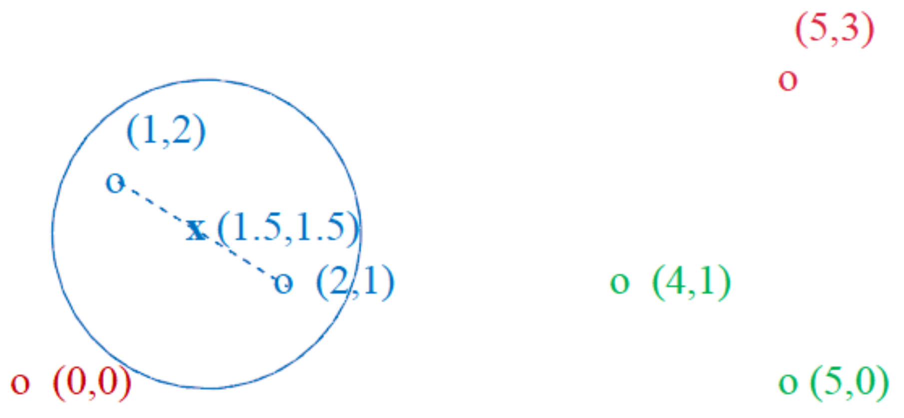
Example: Hierarchical Clustering (with Centroid Linkage) Step 1



Data:
o … data point

Dendrogram

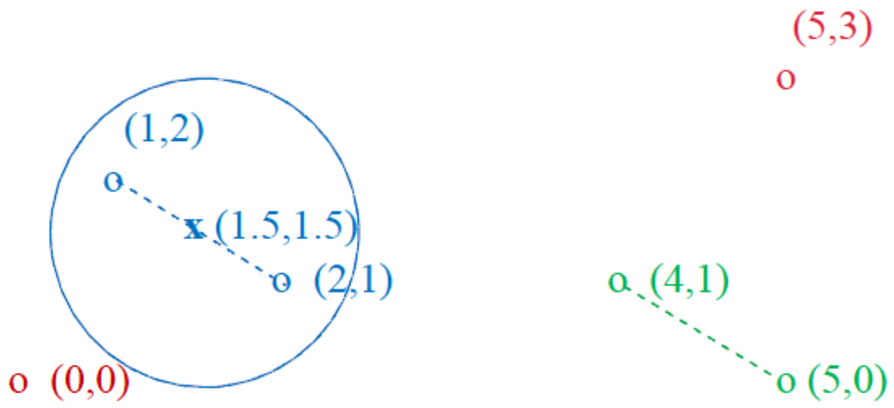
Example: Hierarchical Clustering (with Centroid Linkage) Step 2



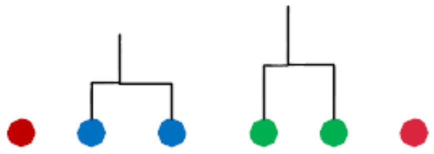
Data:
o … data point
x … centroid

Dendrogram

Example: Hierarchical Clustering (with Centroid Linkage) Step 3

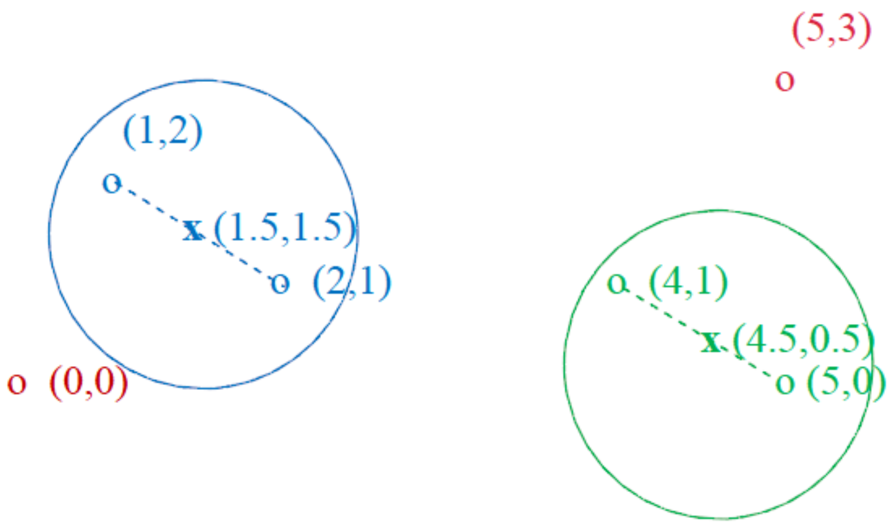


Data:
o … data point
x … centroid

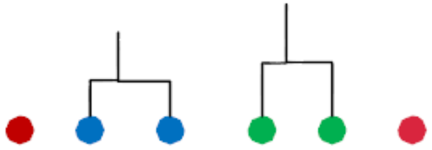


Dendrogram

Example: Hierarchical Clustering (with Centroid Linkage) Step 4

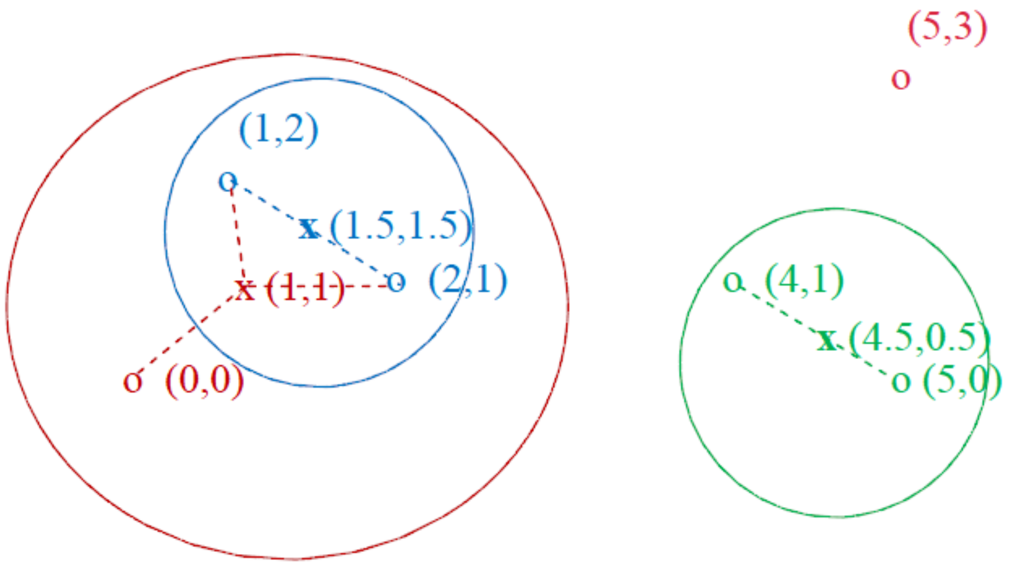


Data:
o … data point
x … centroid

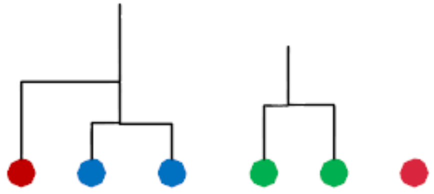


Dendrogram

Example: Hierarchical Clustering (with Centroid Linkage) Step 5

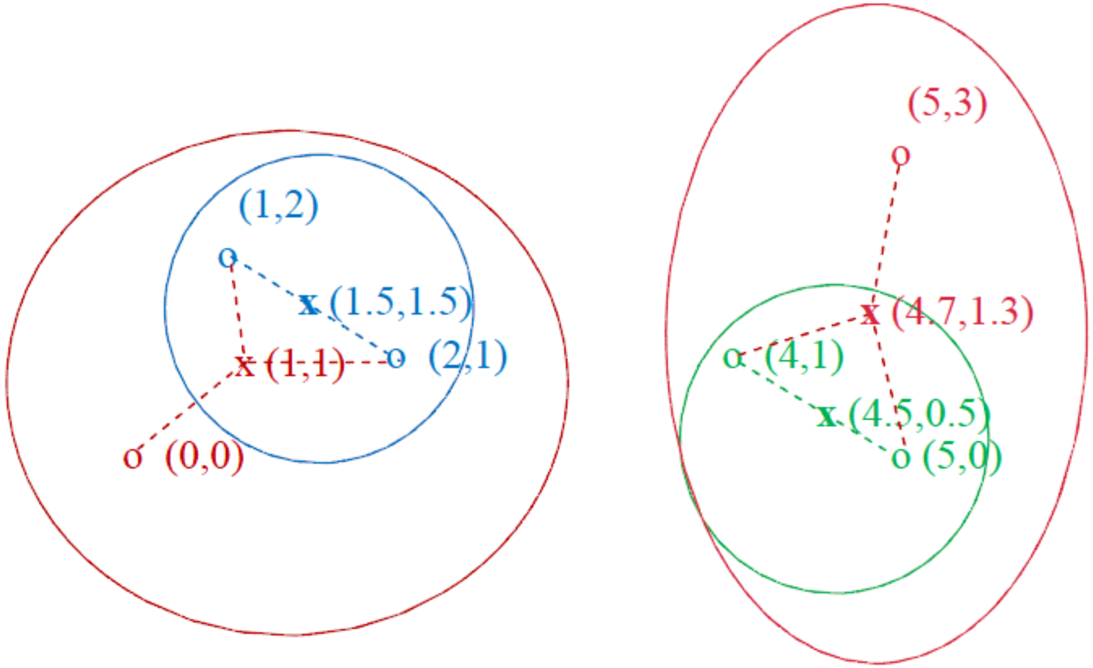


Data:
o … data point
x … centroid

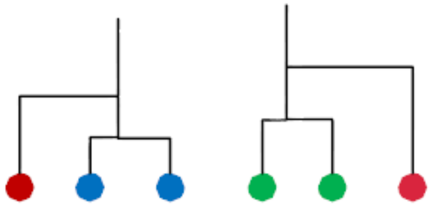


Dendrogram

Example: Hierarchical Clustering (with Centroid Linkage) Step 6

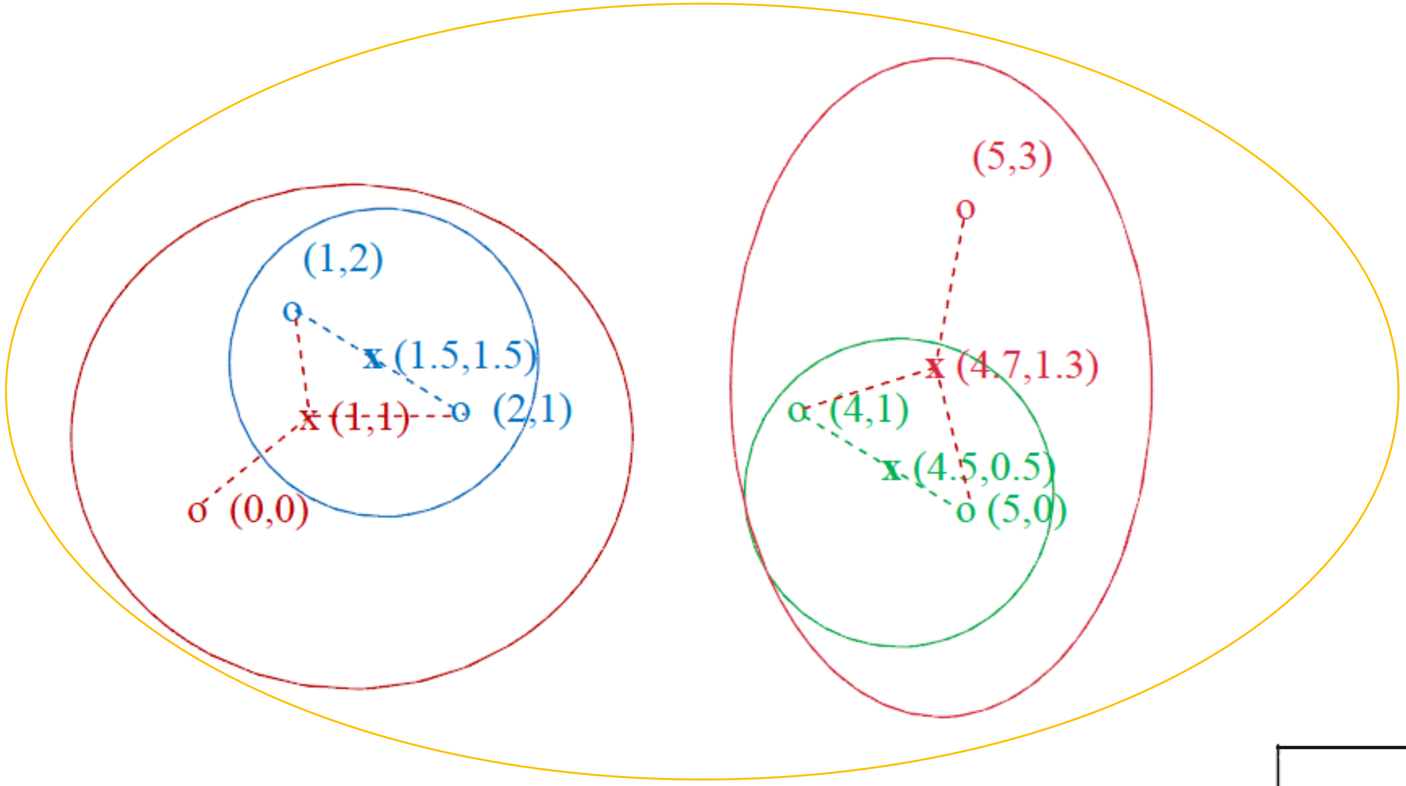


Data:
o … data point
x … centroid

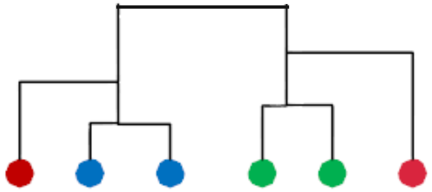


Dendrogram

Example: Hierarchical Clustering (with Centroid Linkage) Step 7



Data:
o … data point
x … centroid

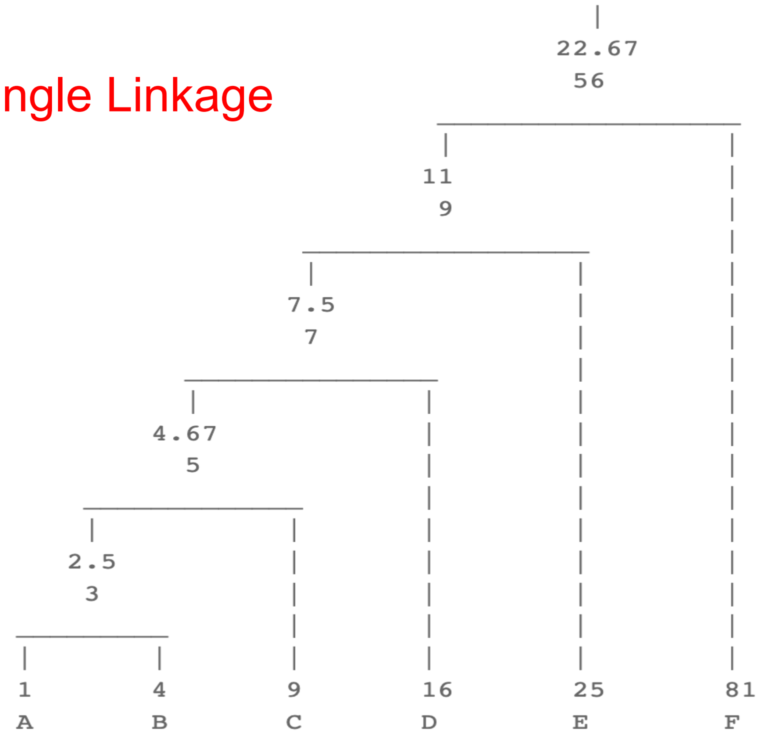


Dendrogram

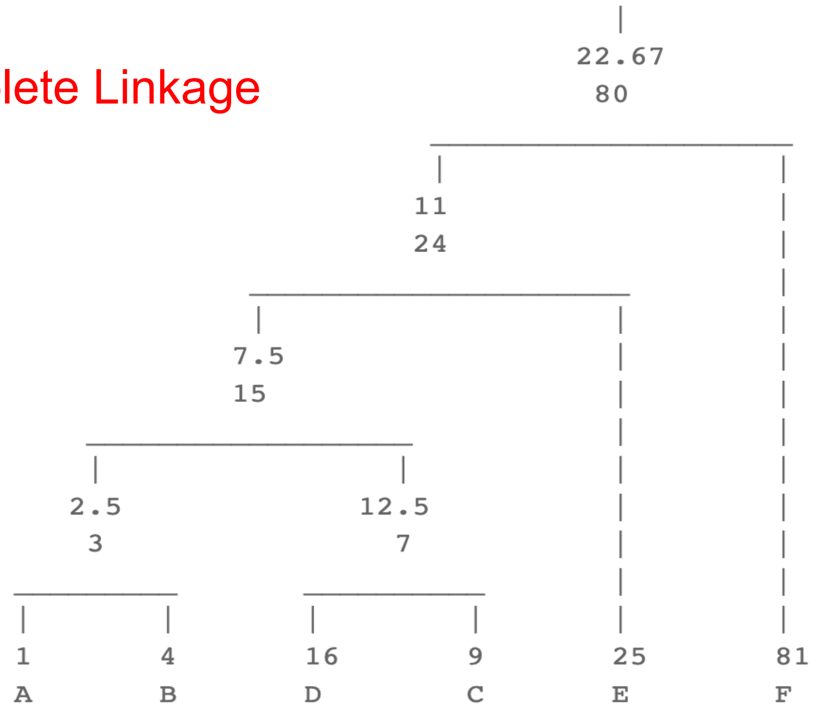
An Exercise on Bottom-up Hierarchical Clustering

- Perform a bottom-up hierarchical clustering on a one-dimensional data set {1, 4, 9, 16, 25, 81} and draw the dendrogram. Assume that the distance between clusters is computed using single linkage or complete linkage

Single Linkage



Complete Linkage



Partitional clustering vs Hierarchical Clustering

- Partitional clustering (e.g., *k*-means) produces a single partitioning.
- Hierarchical Clustering can give different partitionings depending on the level-of-granularity we are looking at.
- Partitional clustering needs the number of clusters to be specified.
- Hierarchical clustering doesn't need the number of clusters to be specified.
- Partitional clustering is usually more efficient.
- Hierarchical clustering can be slow (due to the merge/split decisions)
- No clear consensus on which of the two produces better clustering.