Lecture 3. Partitioning-Based Clustering Methods

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- Basic Concepts of Partitioning Algorithms
- The K-Means Clustering Method
- Initialization of K-Means Clustering
- The K-Medoids Clustering Method
- The K-Medians and K-Modes Clustering Methods
- The Kernel K-Means Clustering Method
- Summary

Session 1: Basic Concepts of Partitioning Algorithms

Partitioning Algorithms: Basic Concepts

- <u>Partitioning method:</u> Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
- *K*-partitioning method: Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where c_k is the centroid or medoid of cluster C_k)
  - A typical objective function: **Sum of Squared Errors** (**SSE**)

$$SSE(C) = \sum_{k=1}^{K} \sum_{x_i \in C_k} || x_i - c_k ||^2$$

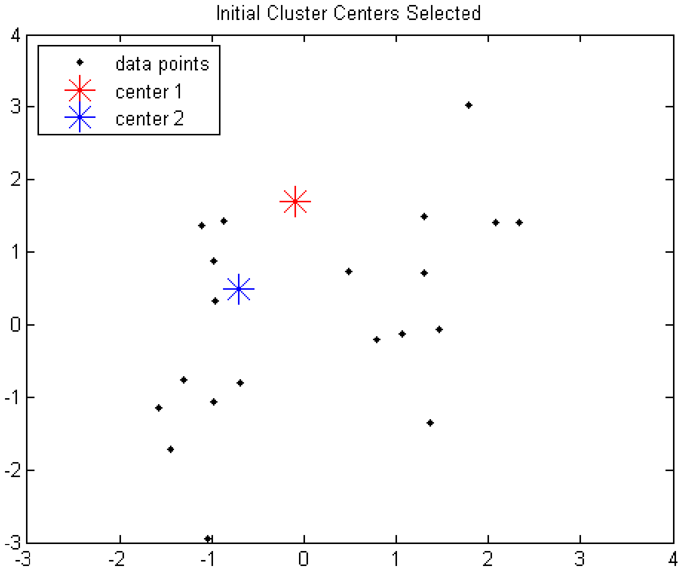
- Problem definition: Given *K*, find a partition of *K clusters* that optimizes the chosen partitioning criterion
  - Global optimal: Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): *K-Means*, *K-Medians*, *K-Medoids*, etc.

Session 2: The *K-Means* Clustering Method

The *K-Means* Clustering Method

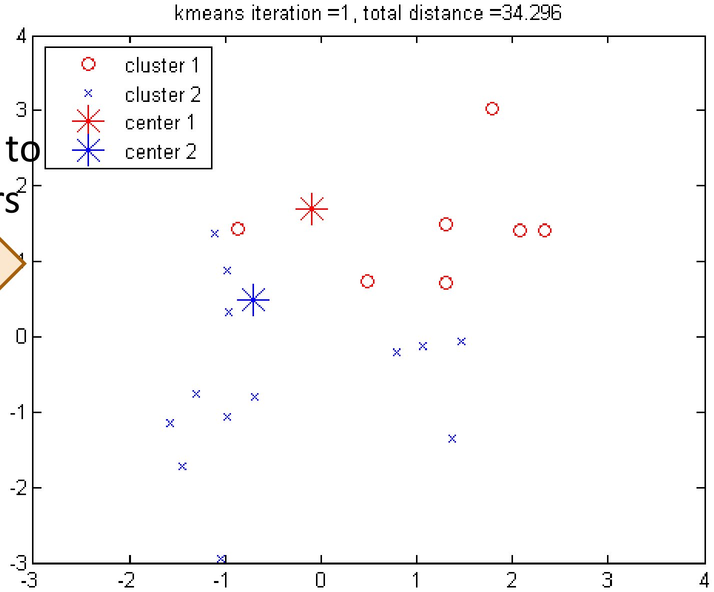
- *K-Means* (MacQueen’67, Lloyd’57/’82)
  - Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
  - Select *K* points as initial centroids
  - **Repeat**
    - Form *K* clusters by assigning each point to its closest centroid
    - Re-compute the centroids (i.e., *mean point*) of each cluster
  - **Until** convergence criterion is satisfied
- Different kinds of measures can be used
  - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

Example: *K-Means* Clustering

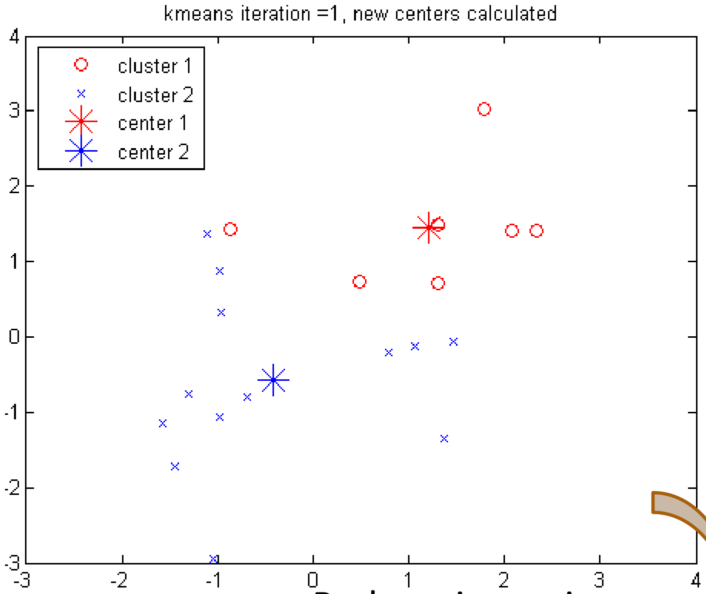


The original data points & randomly select *K* = 2 centroids

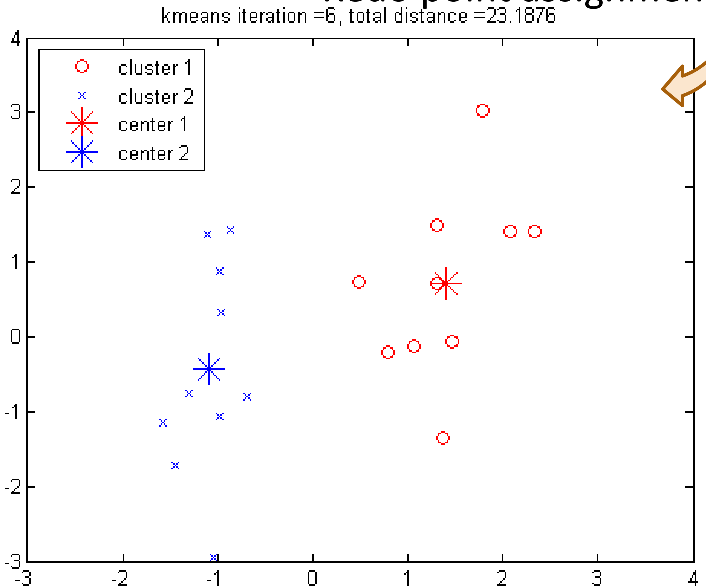
Assign points to clusters



Recompute cluster centers



Redo point assignment



Execution of the K-Means Clustering Algorithm

Select *K* points as initial centroids

Repeat

- Form *K* clusters by assigning each point to its closest centroid
- Re-compute the centroids (i.e., *mean point*) of each cluster

Until convergence criterion is satisfied

Discussion on the *K-Means* Method

- **Efficiency**: $O(tKn)$ where n: # of objects, K: # of clusters, and t: # of iterations
  - Normally, K, $t << n$; thus, an efficient method
- K-means clustering often ***terminates at a local optimal***
  - Initialization can be important to find high-quality clusters
- **Need to specify *K*,** the *number* of clusters, in advance
  - There are ways to automatically determine the "*best*" *K*
  - In practice, one often runs a range of values and selected the "*best*" *K* value
- **Sensitive to noisy data and *outliers***
  - Variations: Using K-medians, K-medoids, etc.
- K-means is applicable only to objects in a continuous n-dimensional space
  - Using the K-modes for ***categorical data***
- Not suitable to discover clusters with ***non-convex shapes***
  - Using density-based clustering, kernel *K*-means, etc.

Variations of *K-Means*

- There are many variants of the *K-Means* method, varying in different aspects
  - Choosing better initial centroid estimates
    - *K-means++, Intelligent K-Means, Genetic K-Means*

      To be discussed in this lecture
  - Choosing different representative prototypes for the clusters
    - *K-Medoids, K-Medians, K-Modes*

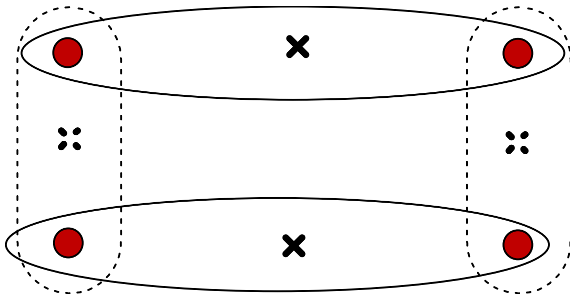
      To be discussed in this lecture
  - Applying feature transformation techniques
    - *Weighted K-Means, Kernel K-Means*

      To be discussed in this lecture

Session 3: Initialization of K-Means Clustering

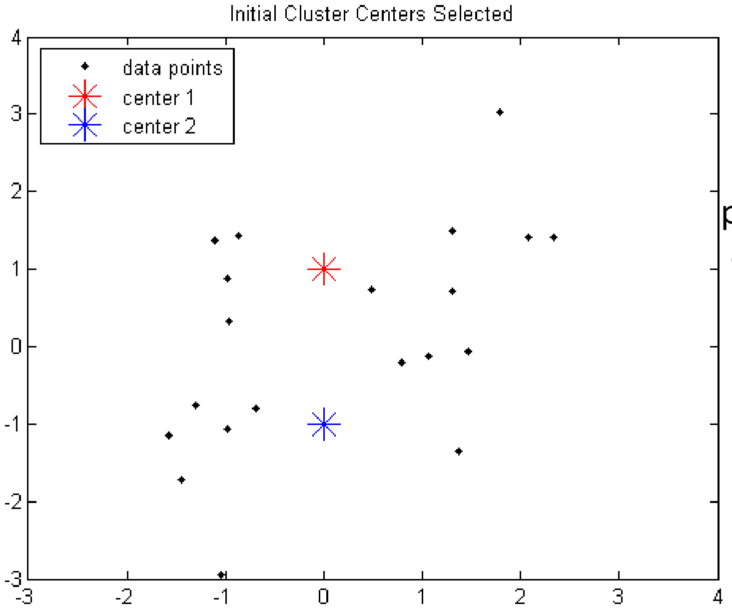
Initialization of K-Means

- Different initializations may generate rather different clustering results (some could be far from optimal)



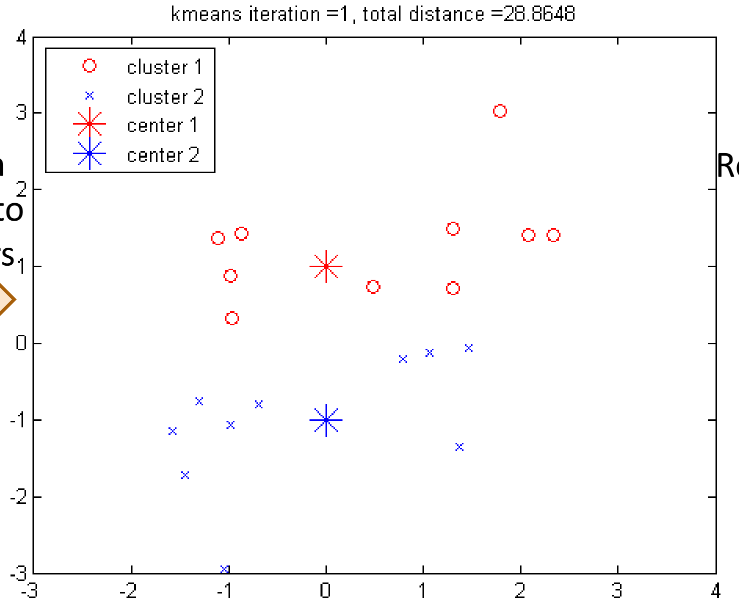
- Original proposal (MacQueen'67): Select *K* seeds randomly
  - Need to run the algorithm multiple times using different seeds
- There are many methods proposed for better initialization of *k* seeds
  - ***K-Means++*** (Arthur & Vassilvitskii'07):
    - The first centroid is selected at random
    - The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score)
    - The selection continues until *K* centroids are obtained

Example: Poor Initialization May Lead to Poor Clustering

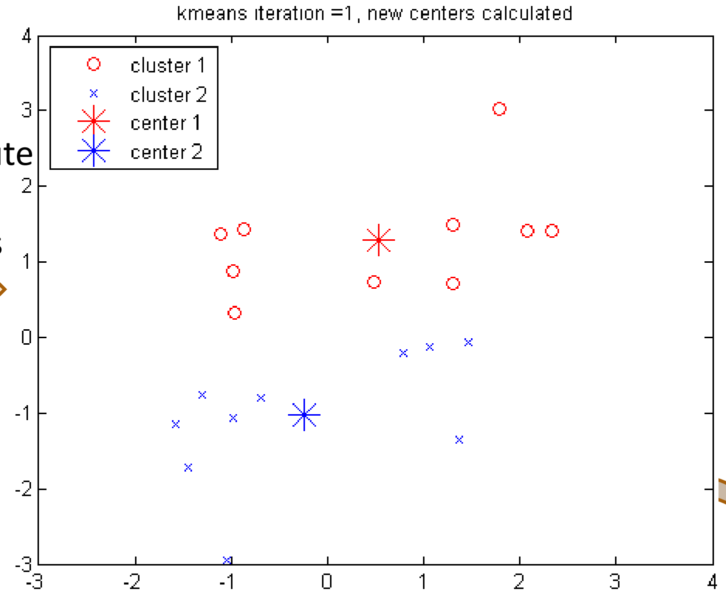


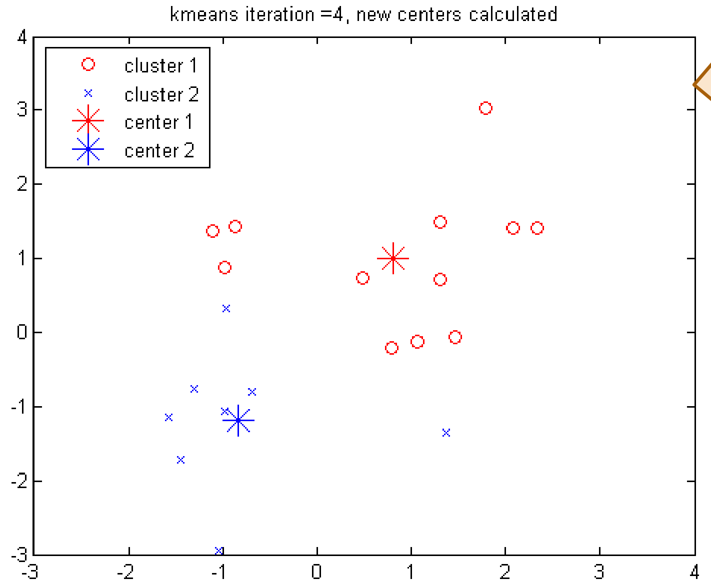
Another random selection of k centroids for the same data points

Assign points to clusters



Recompute cluster centers





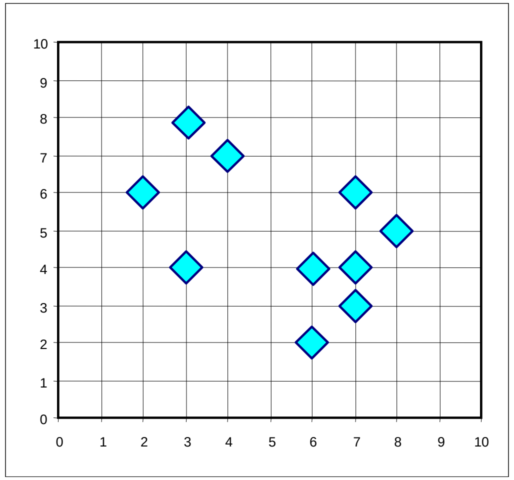
- Rerun of the *K-Means* using another random *K* seeds
- This run of *K*-Means generates a poor quality clustering

Session 4: The *K-Medoids* Clustering Method

Handling Outliers: From *K-Means* to *K-Medoids*

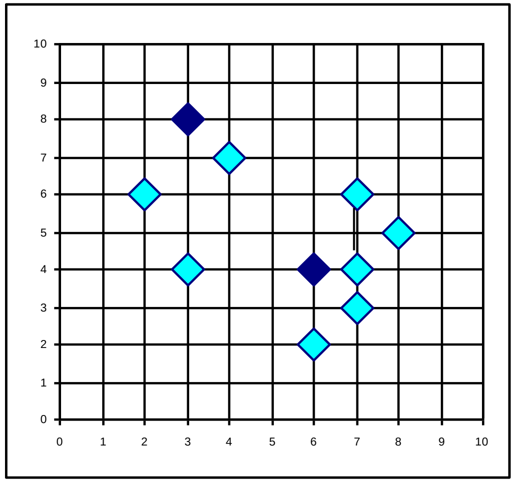
- The *K-Means* algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medoids*)
  - **Repeat**
    - Assigning each point to the cluster with the closest medoid
    - Randomly select a non-representative object o_i
    - Compute the total cost *S* of swapping the medoid *m* with o_i
    - If $S < 0$, then swap *m* with o_i to form the new set of medoids
  - **Until** convergence criterion is satisfied

PAM: A Typical *K-Medoids* Algorithm

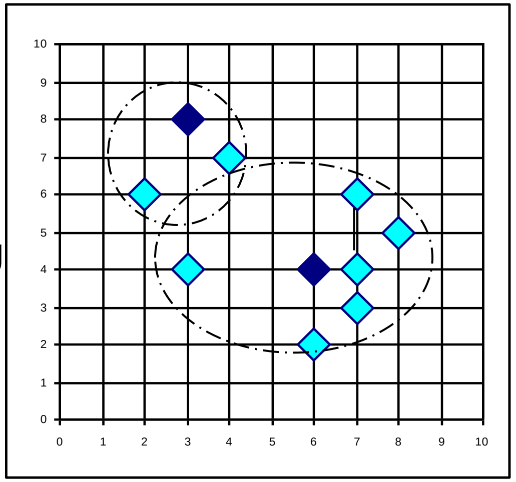


K = 2

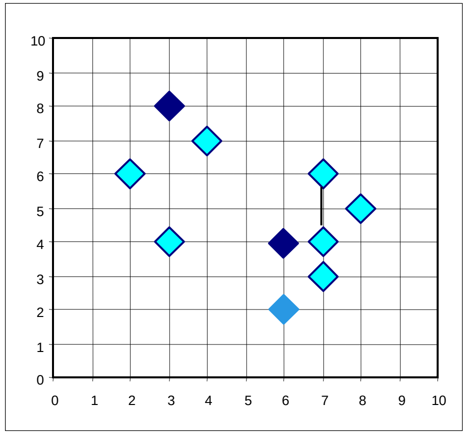
Arbitrary choose *K* object as initial medoids



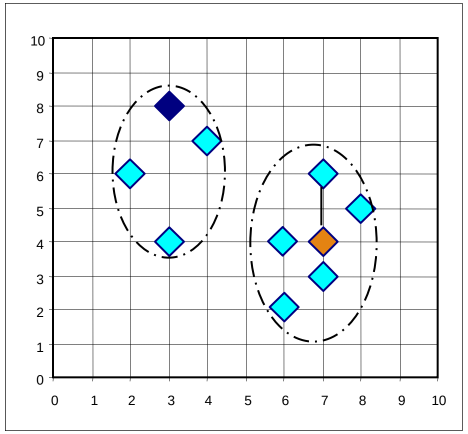
Assign each remaining object to nearest medoids



Randomly select a non-medoid object,O_{ramdom}



Compute total cost of swapping



Swapping O and O_{ramdom}

If quality is improved

Select initial *K medoids* randomly

Repeat

Object re-assignment

Swap medoid *m* with o_i if it improves the clustering quality

Until convergence criterion is satisfied

Discussion on *K-Medoids* Clustering

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
- *PAM* (Partitioning Around Medoids: Kaufmann & Rousseeuw 1987)
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - *PAM* works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational complexity: PAM: $O(K(n - K)^2)$ (quite expensive!)
- Efficiency improvements on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990):
    - PAM on samples; $O(Ks^2 + K(n - K))$, s is the sample size
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

Session 5: The *K-Medians* and *K-Modes* Clustering Methods

K-Medians: Handling Outliers by Computing Medians

- Medians are less sensitive to outliers than means
  - Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- ***K-Medians***: Instead of taking the **mean** value of the object in a cluster as a reference point, **medians** are used (L_1-norm as the distance measure)
- The criterion function for the *K-Medians* algorithm:

$$S = \sum_{k=1}^{K} \sum_{x_{i \in C_k}} | x_{ij} - med_{kj} |$$

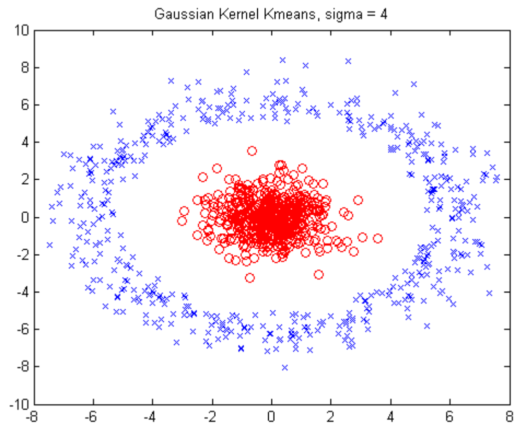
- The *K-Medians* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medians*)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion is satisfied

K-Modes: Clustering Categorical Data

- *K-Means* cannot handle non-numerical (categorical) data
  - Mapping categorical value to 1/0 cannot generate quality clusters for high-dimensional data
- ***K-Modes***: An extension to *K-Means* by replacing means of clusters with ***modes***
- Dissimilarity measure between object X and the center of a cluster Z
  - $\Phi(x_j, z_j) = 1 - n_j^r/n_l$ when $x_j = z_j$; 1 when $x_j \neq z_j$
    - where z_j is the categorical value of attribute j in Z_l, n_l is the number of objects in cluster *l*, and n_j^r is the number of objects whose attribute value is r
- This dissimilarity measure (distance function) is **frequency-based**
- Algorithm is still based on iterative *object cluster assignment* and *centroid update*
- A ***fuzzy K-Modes*** method is proposed to calculate a ***fuzzy cluster membership value*** for each object to each cluster
- A mixture of categorical and numerical data: Using a ***K-Prototype*** method

Session 6: Kernel K-Means Clustering

Kernel K-Means Clustering



- ❑ *Kernel K-Means* can be used to detect non-convex clusters
  - ❑ *K-Means* can only detect clusters that are linearly separable
- ❑ Idea: Project data onto the high-dimensional kernel space, and then perform *K-Means* clustering
  - ❑ Map data points in the input space onto a high-dimensional feature space using the kernel function
  - ❑ Perform *K-Means* on the mapped feature space
- ❑ Computational complexity is higher than K-Means
  - ❑ Need to compute and store n x n kernel matrix generated from the kernel function on the original data
- ❑ The widely studied spectral clustering can be considered as a variant of Kernel K-Means clustering

Kernel Functions and Kernel K-Means Clustering

- Typical kernel functions:
  - Polynomial kernel of degree h: $K(\boldsymbol{X_i}, \boldsymbol{X_j}) = (\boldsymbol{X_i} \cdot \boldsymbol{X_j} + 1)^h$
  - Gaussian radial basis function (RBF) kernel: $K(\boldsymbol{X_i}, \boldsymbol{X_j}) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$
  - Sigmoid kernel: $K(\boldsymbol{X_i}, \boldsymbol{X_j}) = \tanh(\kappa \boldsymbol{X_i} \cdot \boldsymbol{X_j} - \delta)$
- The formula for kernel matrix K for any two points $x_i, x_j \in C_k$ is $K_{x_i x_j} = \phi(x_i) \bullet \phi(x_j)$
- The SSE criterion of *kernel K-means*: $SSE(C) = \sum_{k=1}^{K} \sum_{x_{i \in C_k}} \| \phi(x_i) - c_k \|^2$
  - The formula for the cluster centroid:

$$c_k = \frac{\sum_{x_{i \in C_k}} \phi(x_i)}{|C_k|}$$

- Clustering can be performed without the actual individual projections $\phi(x_i)$ and $\phi(x_j)$ for the data points $x_i, x_j \in C_k$

Example: Kernel Functions and Kernel K-Means Clustering

- Gaussian radial basis function (RBF) kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|X_i - X_j\|^2/2\sigma^2}$
- Suppose there are 5 original 2-dimensional points:
  - $x_1(0, 0)$, $x_2(4, 4)$, $x_3(-4, 4)$, $x_4(-4, -4)$, $x_5(4, -4)$
- If we set σ to 4, we will have the following points in the kernel space
  - E.g., $||x_1 - x_2||^2 = (0-4)^2 + (0-4)^2 = 32$, therefore, $K(x_1, x_2) = e^{-\frac{32}{2\cdot 4^2}} = e^{-1}$

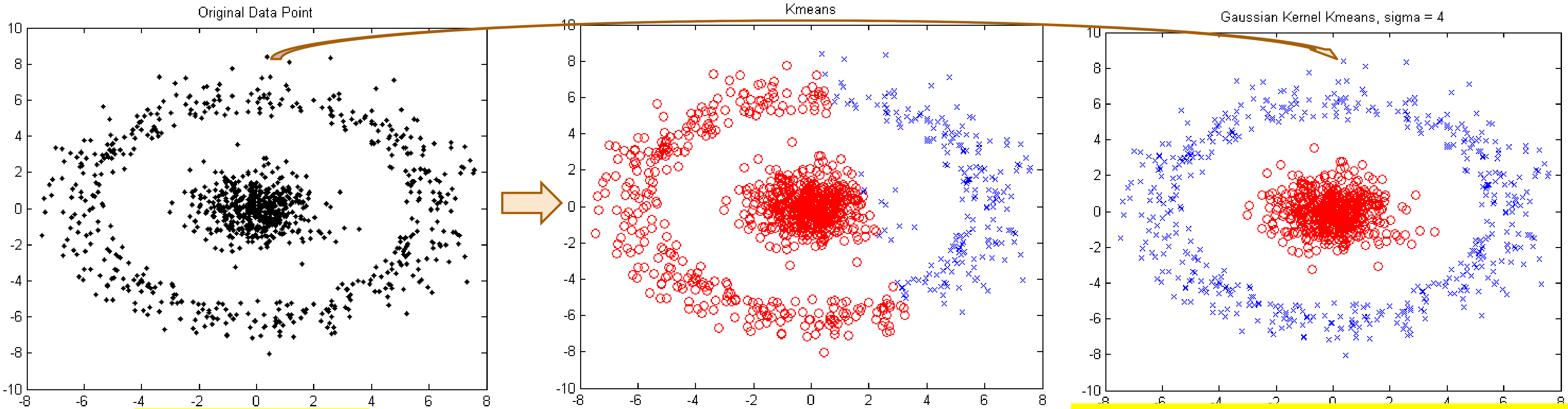
Original Space

	x	y
x_1	0	0
x_2	4	4
x_3	-4	4
x_4	-4	-4
x_5	4	-4

RBF Kernel Space ($\sigma = 4$)

$K(x_i, x_1)$	$K(x_i, x_2)$	$K(x_i, x_3)$	$K(x_i, x_4)$	$K(x_i, x_5)$
0	$e^{-\frac{4^2+4^2}{2\cdot 4^2}} = e^{-1}$	e^{-1}	e^{-1}	e^{-1}
e^{-1}	0	e^{-2}	e^{-4}	e^{-2}
e^{-1}	e^{-2}	0	e^{-2}	e^{-4}
e^{-1}	e^{-4}	e^{-2}	0	e^{-2}
e^{-1}	e^{-2}	e^{-4}	e^{-2}	0

Example: Kernel K-Means Clustering



The original data set | The result of K-Means clustering | The result of Gaussian Kernel K-Means clustering

- The above data set cannot generate quality clusters by K-Means since it contains non-covex clusters
- Gaussian RBF Kernel transformation maps data to a kernel matrix K for any two points x_i, x_j: $K_{x_i x_j} = \phi(x_i) \bullet \phi(x_j)$ and Gaussian kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$
- K-Means clustering is conducted on the mapped data, generating quality clusters

Session 7: Summary

Summary: Partitioning-Based Clustering Methods

- Basic Concepts of Partitioning Algorithms
- The K-Means Clustering Method
- Initialization of K-Means Clustering
- The K-Medoids Clustering Method
- The K-Medians and K-Modes Clustering Methods
- The Kernel K-Means Clustering Method
- Summary

Recommended Readings

- J. MacQueen. Some Methods for Classification and Analysis of Multivariate Observations. In *Proc. of the 5th Berkeley Symp. on Mathematical Statistics and Probability*, 1967
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- M. J. Zaki and W. Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge Univ. Press, 2014