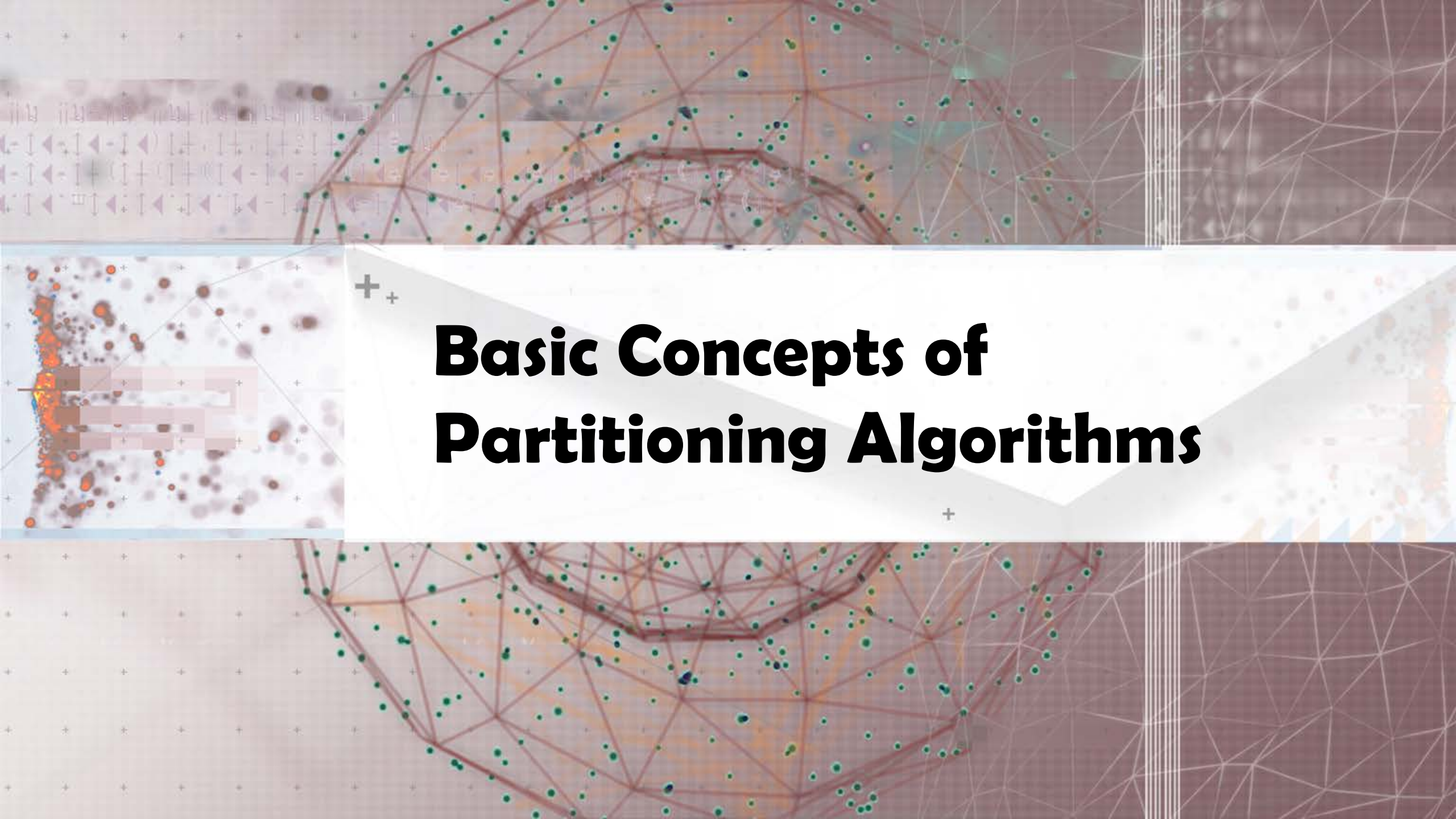


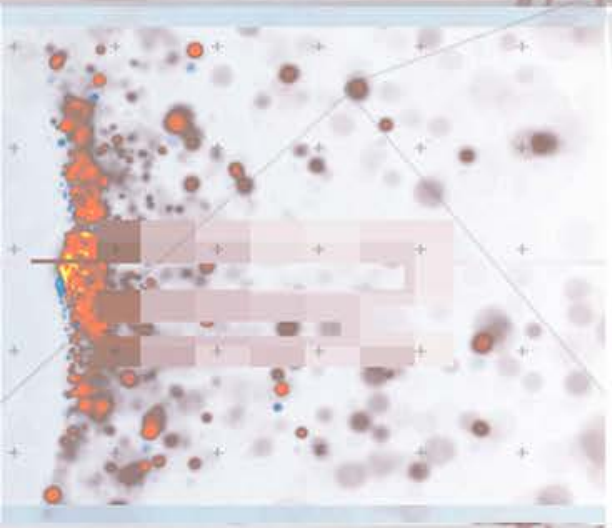
Basic Concepts of Partitioning Algorithms

Partitioning Algorithms: Basic Concepts

- Partitioning method: 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.

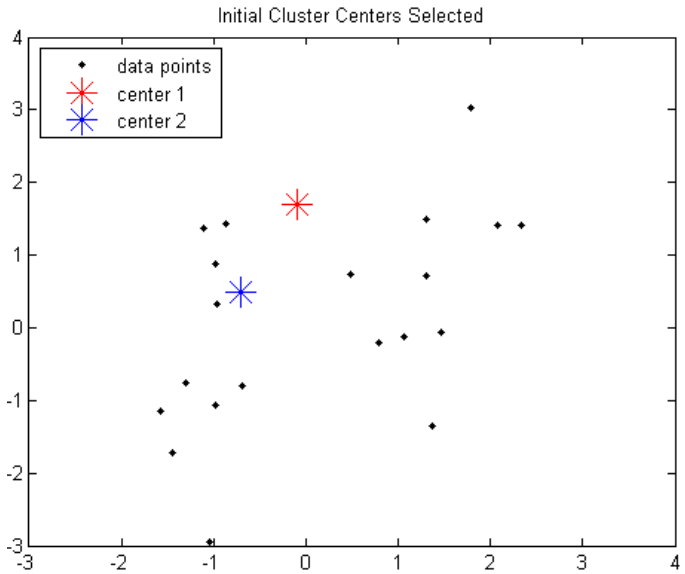


The *K-Means* Clustering Method

The *K-Means* Clustering Method

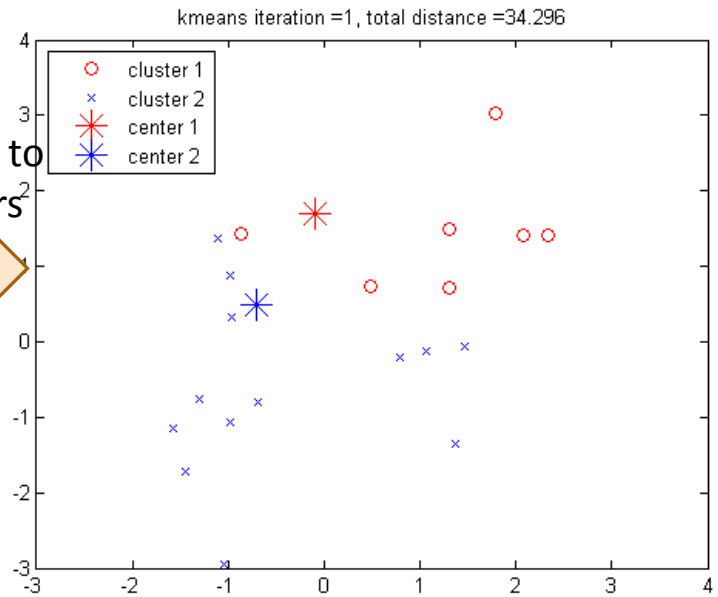
- *K-Means* (MacQueen'67, Lloyd'57/'82)
  - Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
  - Select *K* points as initial centroids
  - **Repeat**
    - Form *K* clusters by assigning each point to 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

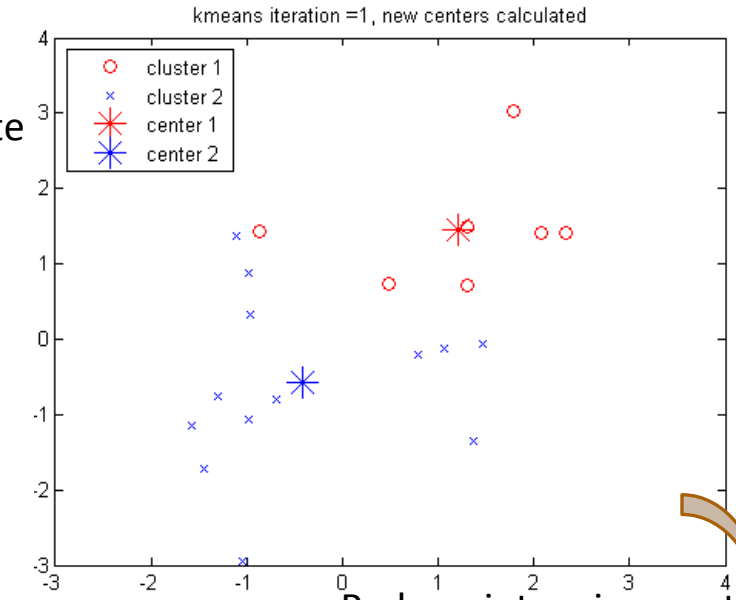


The original data points & randomly select $K = 2$ centroids

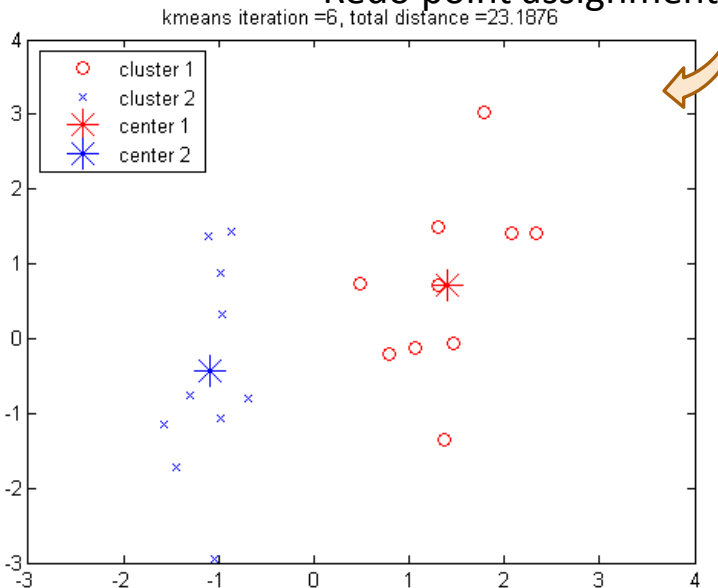
Assign points to clusters



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*

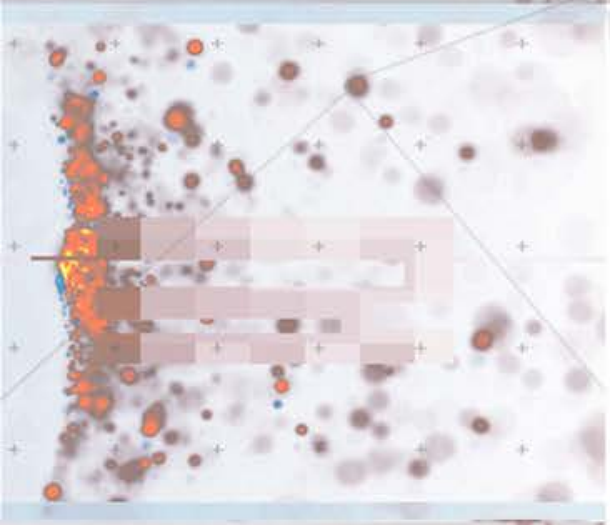
To be discussed in this lecture

  - 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*

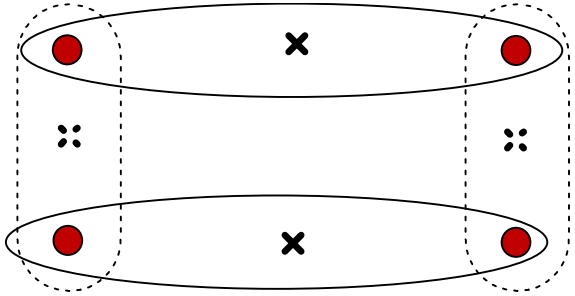
To be discussed in this lecture



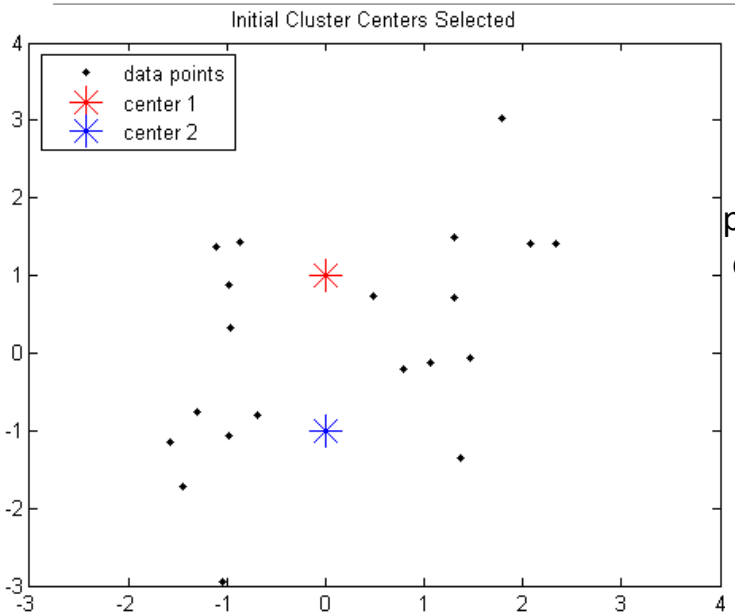
Initialization of K-Means Clustering

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

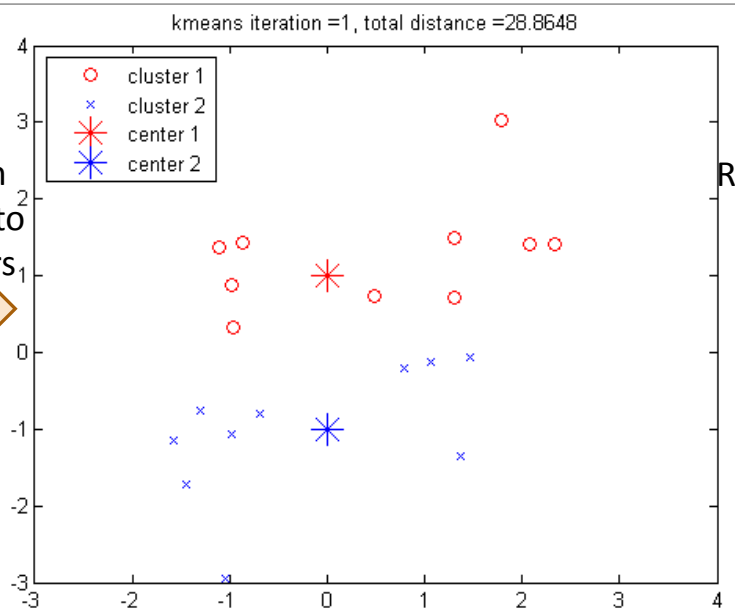


Example: Poor Initialization May Lead to Poor Clustering

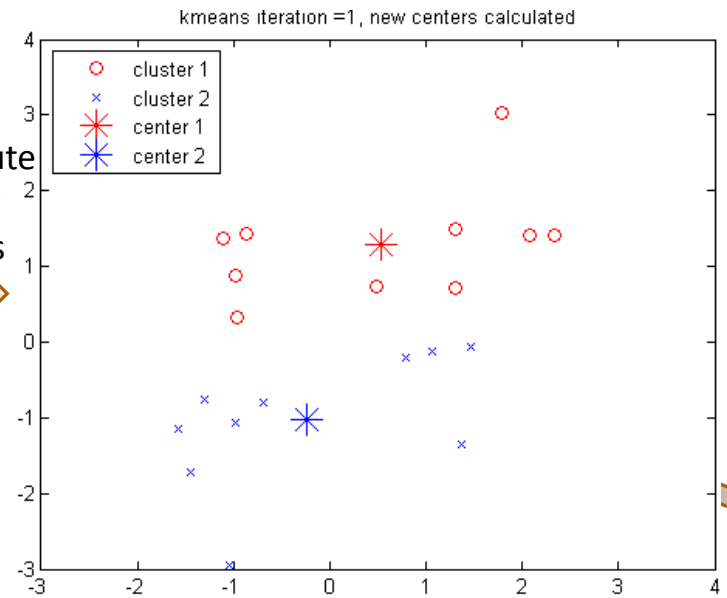


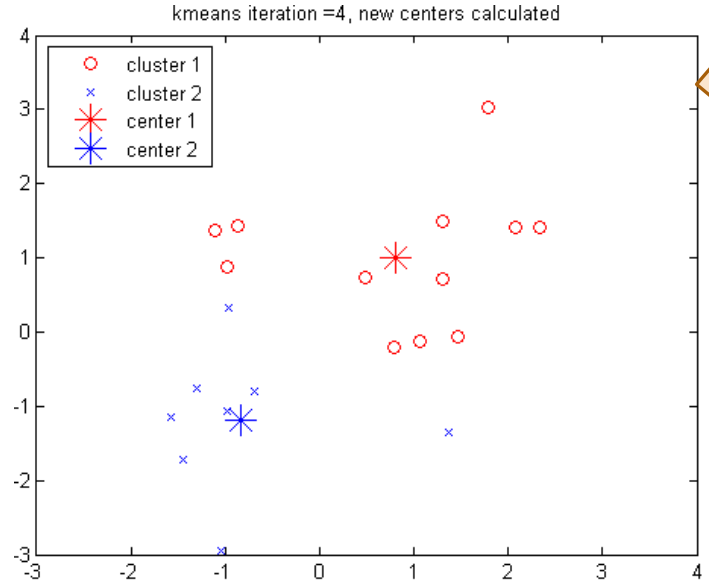
Another random selection of k centroids for the same data points

Assign points to clusters

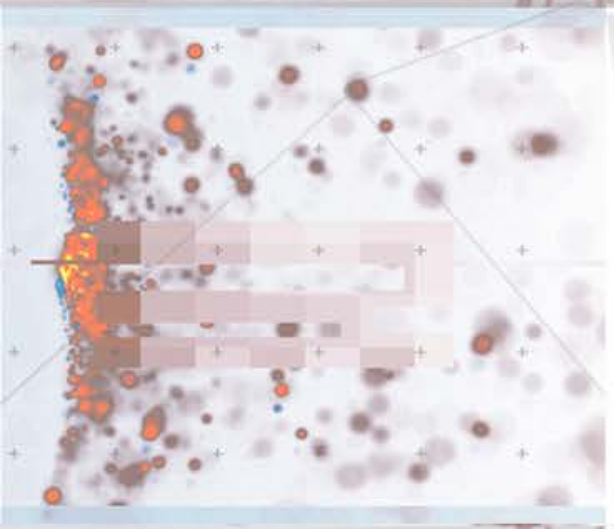


Recompute cluster centers





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

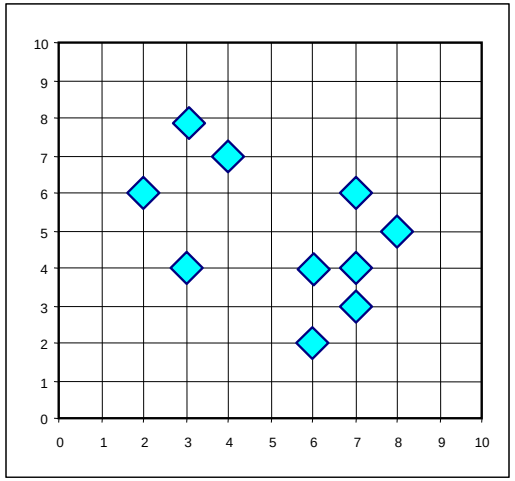


The *K-Medoids* Clustering Method

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

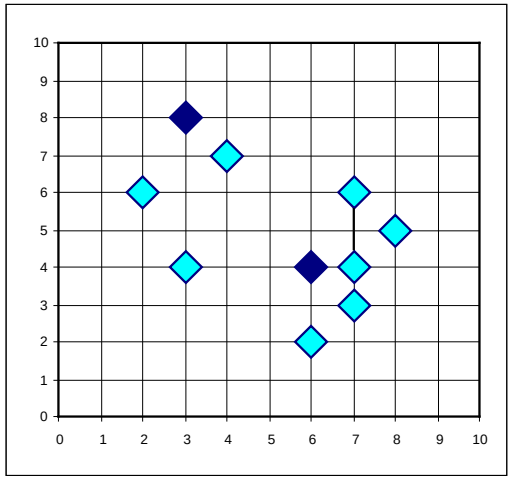
- The *K-Means* algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally 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

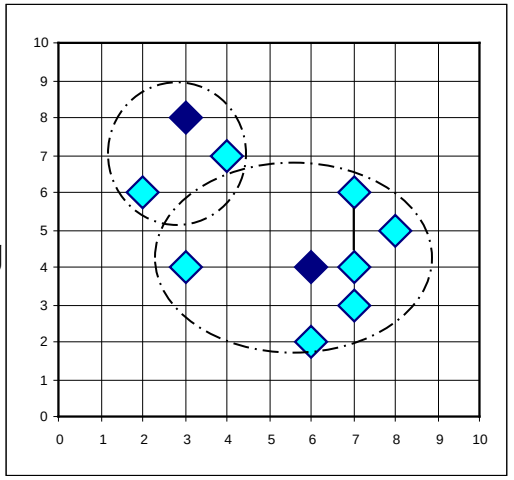


$K = 2$

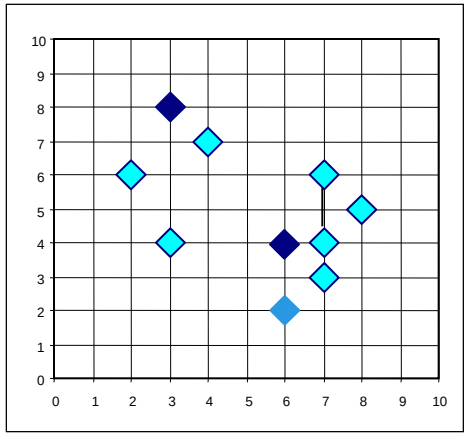
Arbitrary choose *K* object as initial medoids



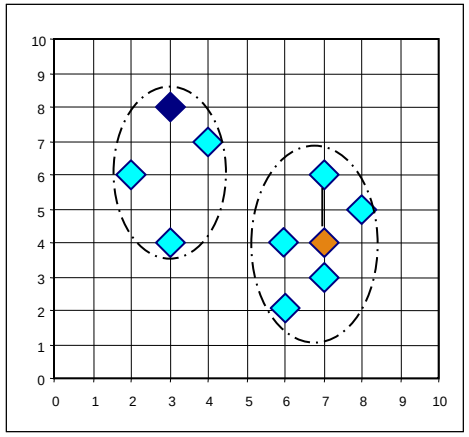
Assign each remaining object to nearest medoids



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

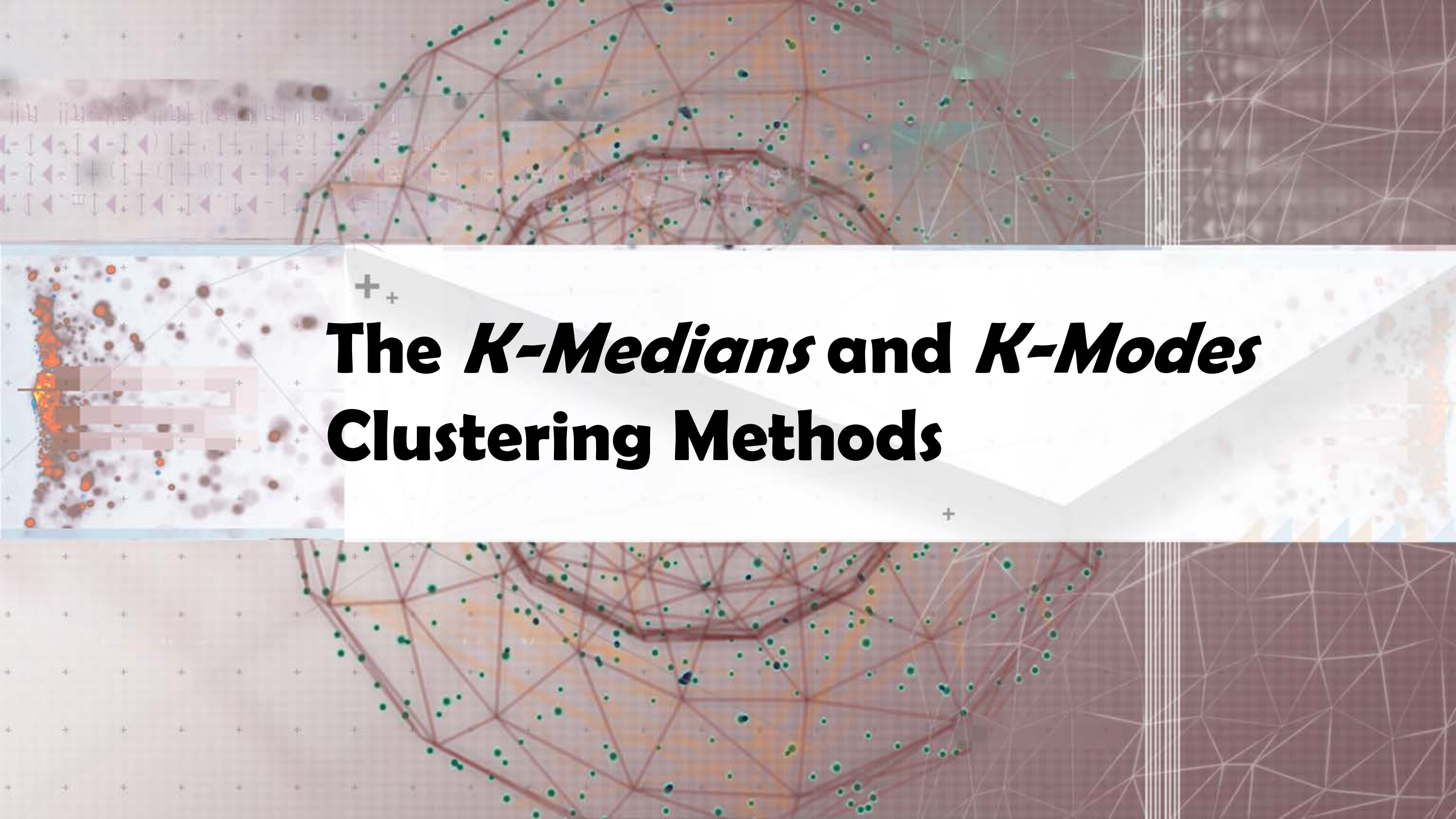
Object re-assignment

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



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:

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

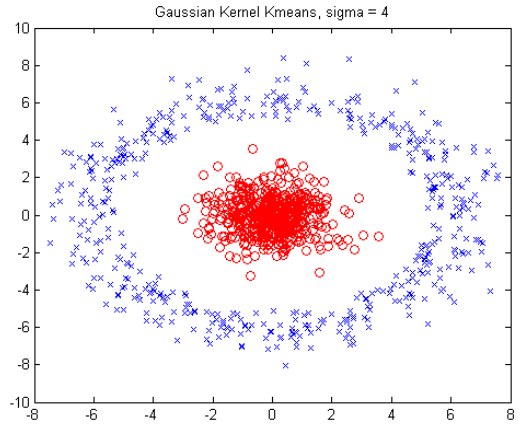
- The *K-Medians* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medians*)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion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

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., $\left|\left|x_1 - x_2\right|\right|^2 = (0-4)^2 + (0-4)^2 = 32$, therefore, $K(x_1, x_2) = e^{-\frac{32}{2 \cdot 4^2}} = e^{-1}$

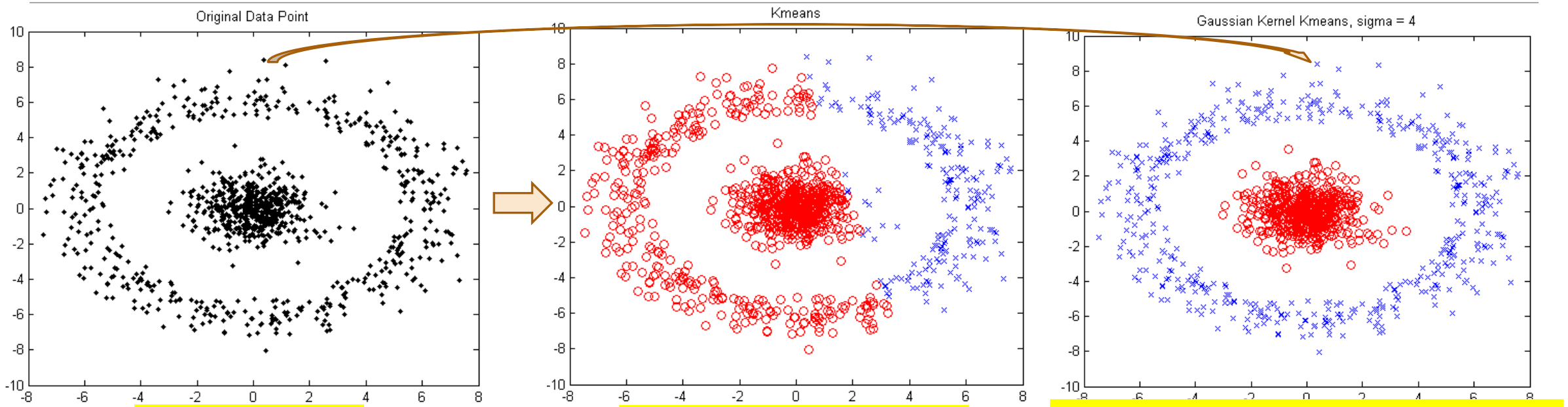
Original Space

	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

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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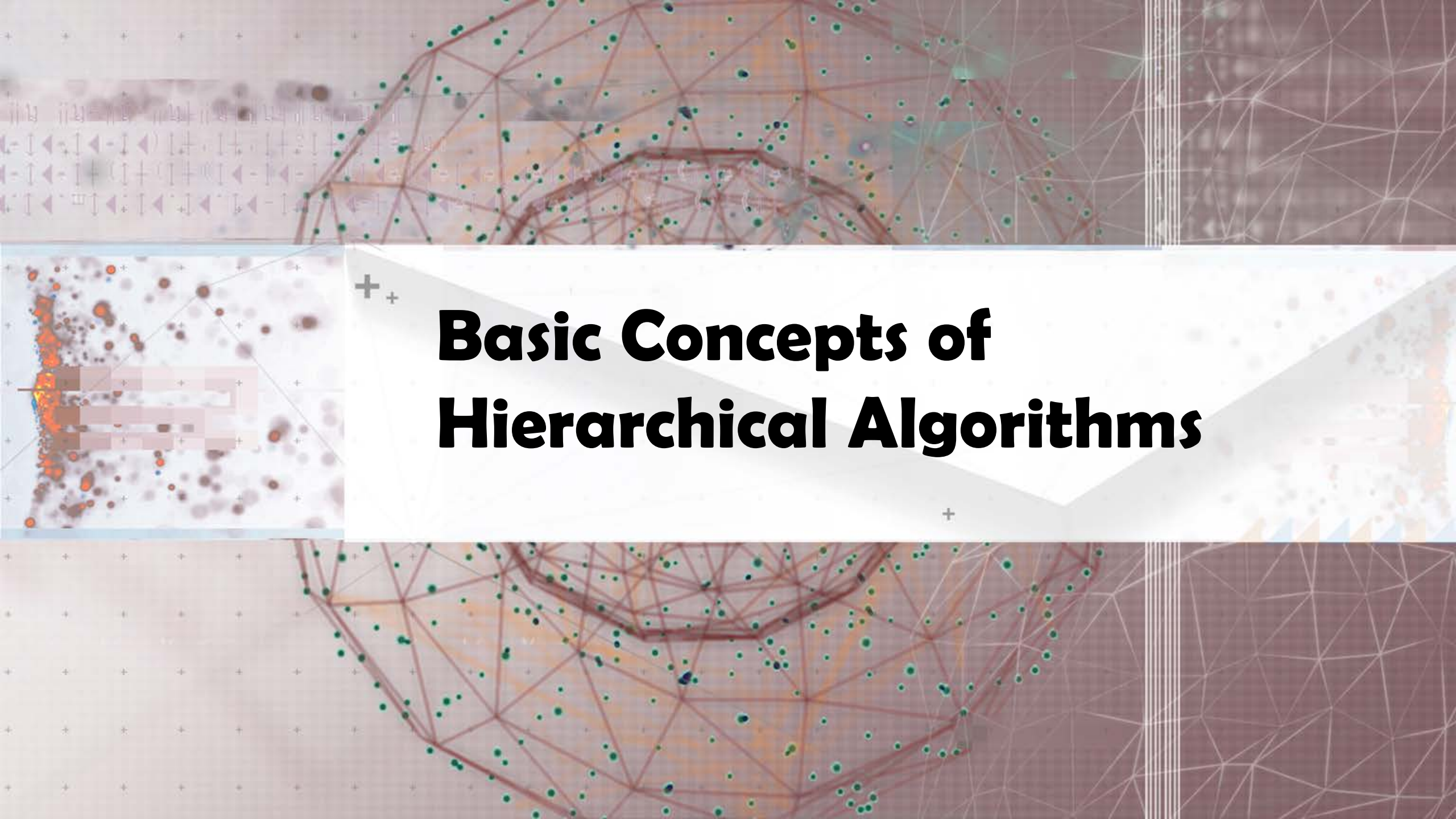
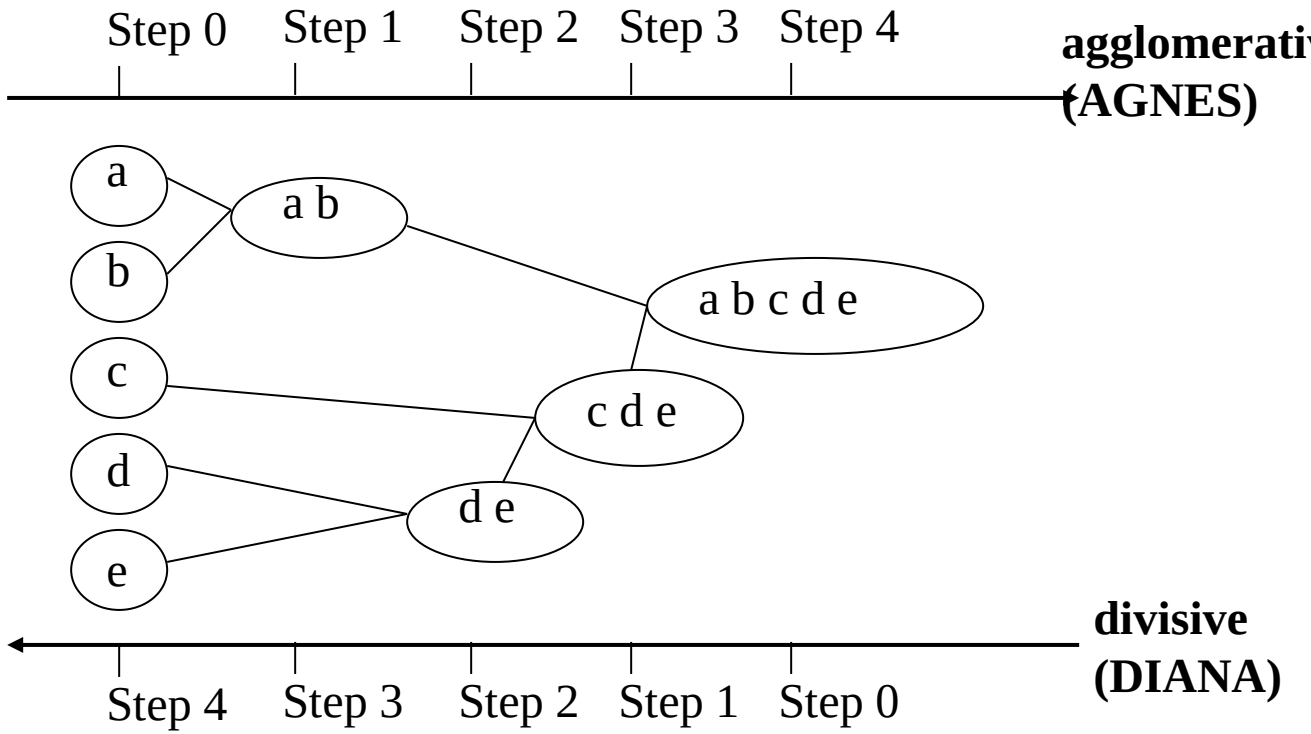


Basic Concepts of Hierarchical Algorithms

Hierarchical Clustering: Basic Concepts

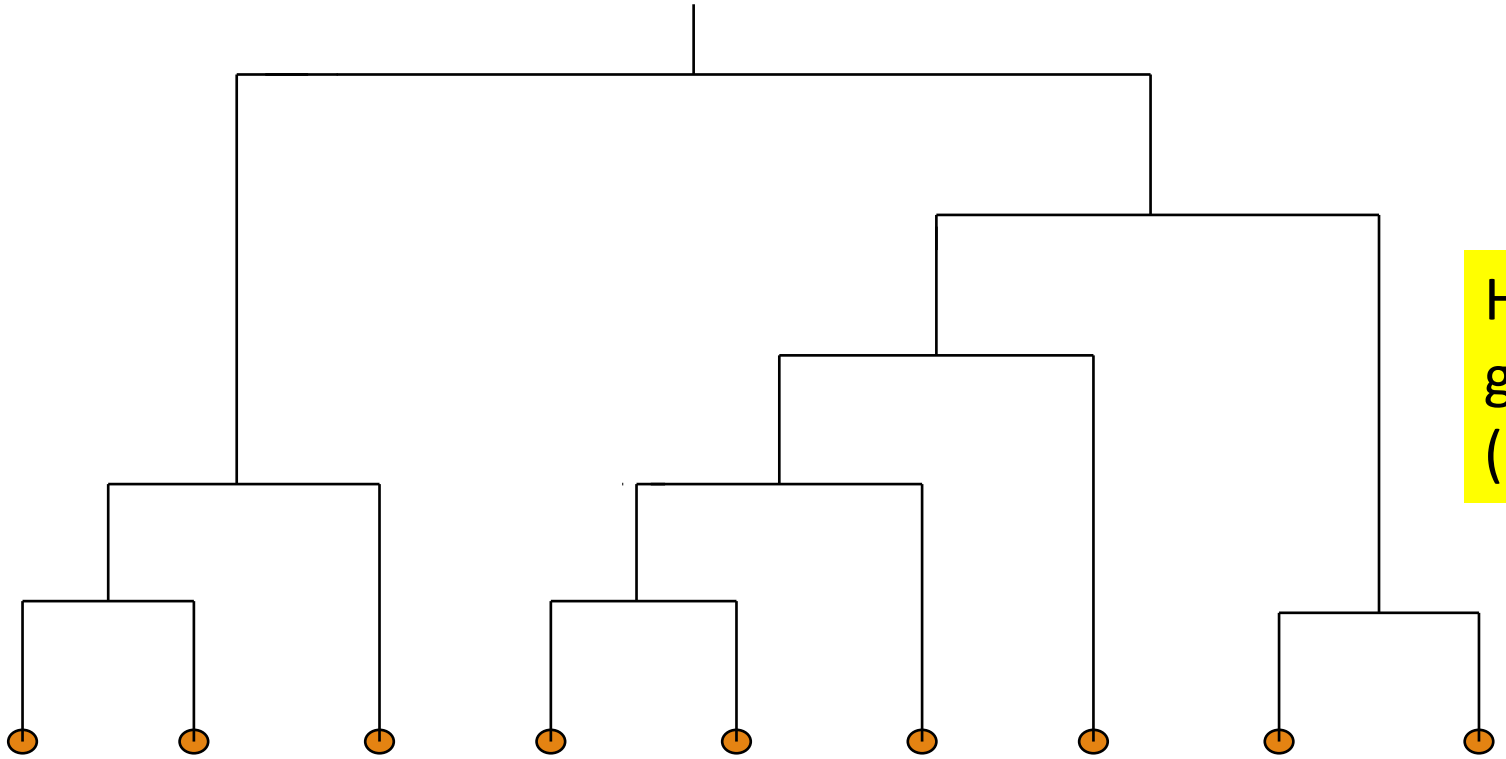
- Hierarchical clustering
  - Generate a clustering hierarchy (drawn as a **dendrogram**)
  - Not required to specify ***K,*** the number of clusters
  - More deterministic
  - No iterative refinement
- Two categories of algorithms:



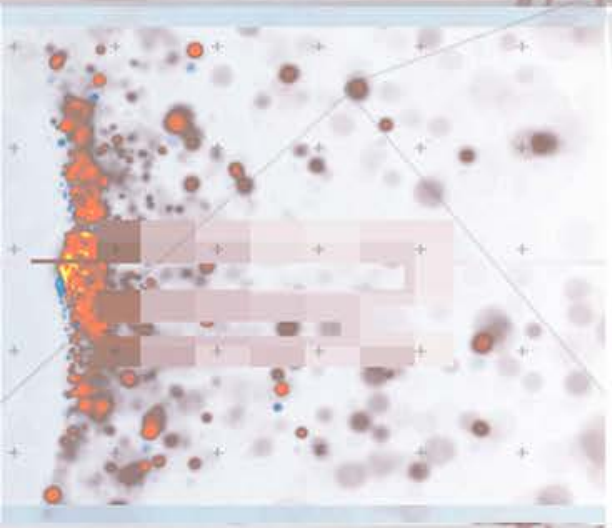
  - **Agglomerative**: Start with singleton clusters, continuously merge two clusters at a time to build a **bottom-up** hierarchy of clusters
  - **Divisive:** Start with a huge macro-cluster, split it continuously into two groups, generating a **top-down** hierarchy of clusters

Dendrogram: Shows How Clusters are Merged

- Dendrogram: Decompose a set of data objects into a tree of clusters by multi-level nested partitioning
- A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



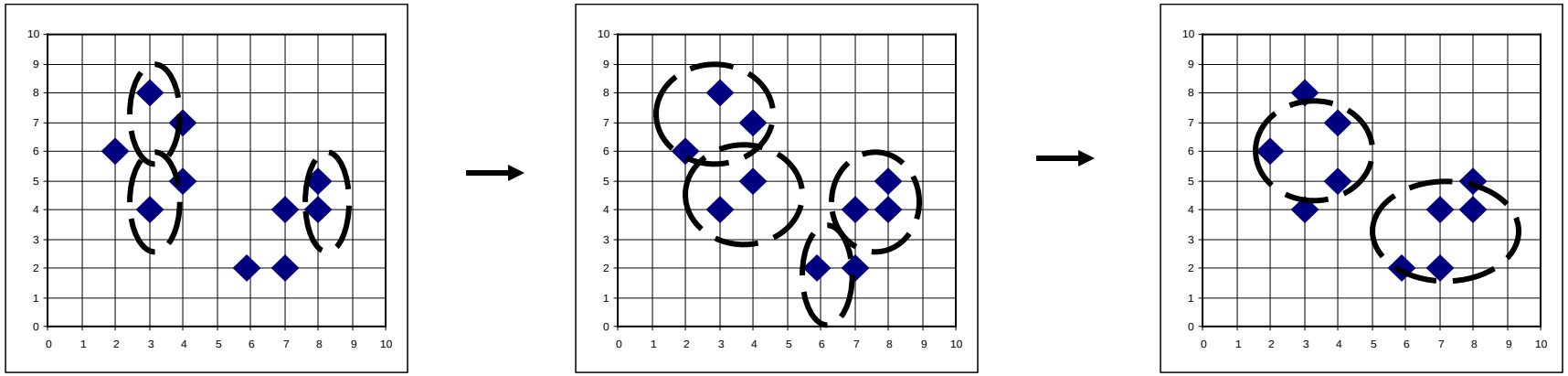
Hierarchical clustering generates a dendrogram (a hierarchy of clusters)



Agglomerative Clustering Algorithms

Agglomerative Clustering Algorithm

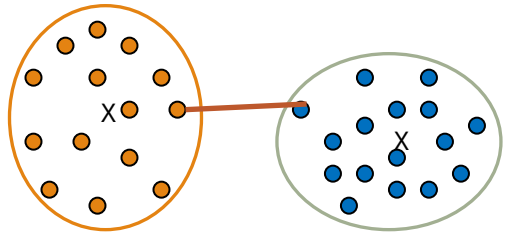
- AGNES (AGglomerative NESting) (Kaufmann and Rousseeuw, 1990)
  - Use the **single-link** method and the dissimilarity matrix
  - Continuously merge nodes that have the least dissimilarity
  - Eventually all nodes belong to the same cluster



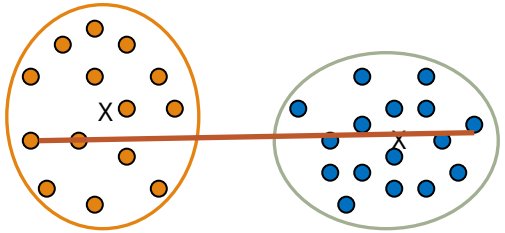
- Agglomerative clustering varies on different similarity measures among clusters
  - Single link (nearest neighbor)
  - Complete link (diameter)
  - Average link (group average)
  - Centroid link (centroid similarity)

Single Link vs. Complete Link in Hierarchical Clustering

- Single link (nearest neighbor)
  - The similarity between two clusters is the similarity between their most similar (nearest neighbor) members
  - Local similarity-based: Emphasizing more on close regions, ignoring the overall structure of the cluster
  - Capable of clustering non-elliptical shaped group of objects
  - Sensitive to noise and outliers

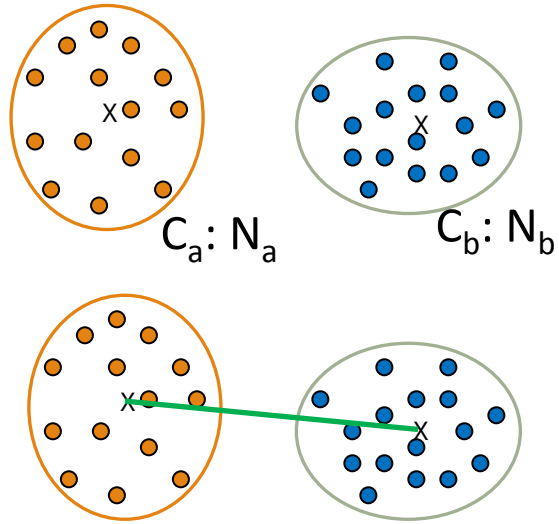


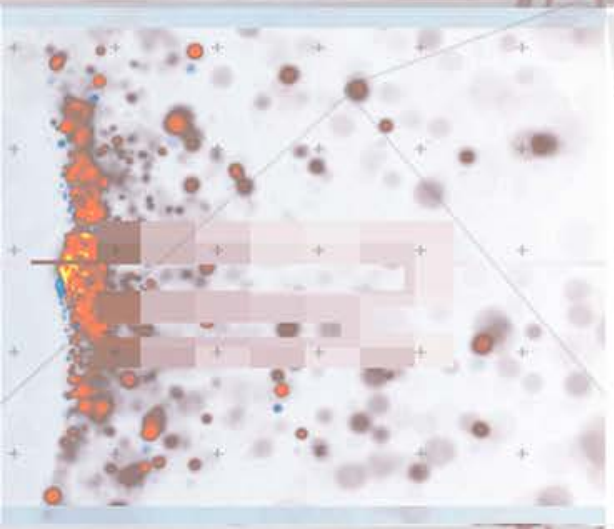
- Complete link (diameter)
  - The similarity between two clusters is the similarity between their most dissimilar members
  - Merge two clusters to form one with the smallest diameter
  - Nonlocal in behavior, obtaining compact shaped clusters
  - Sensitive to outliers



Agglomerative Clustering: Average vs. Centroid Links

- Agglomerative clustering with **average link**
  - **Average link**: The average distance between an element in one cluster and an element in the other (i.e., all pairs in two clusters)
    - Expensive to compute
- Agglomerative clustering with **centroid link**
  - **Centroid link**: The distance between the centroids of two clusters
- **Group Averaged Agglomerative Clustering (GAAC)**
  - Let two clusters C_a and C_b be merged into C_{aUb}. The new centroid is: $c_{a\cup b} = \frac{N_a c_a + N_b c_b}{N_a + N_b}$
    - N_a is the cardinality of cluster C_a, and c_a is the centroid of C_a
  - The similarity measure for GAAC is the average of their distances
- Agglomerative clustering with **Ward's criterion**
  - **Ward's criterion:** The increase in the value of the SSE criterion for the clustering obtained by merging them into C_a U C_b: $W(C_{a\cup b}, c_{a\cup b}) - W(C,c) = \frac{N_a N_b}{N_a + N_b} d(c_a, c_b)$

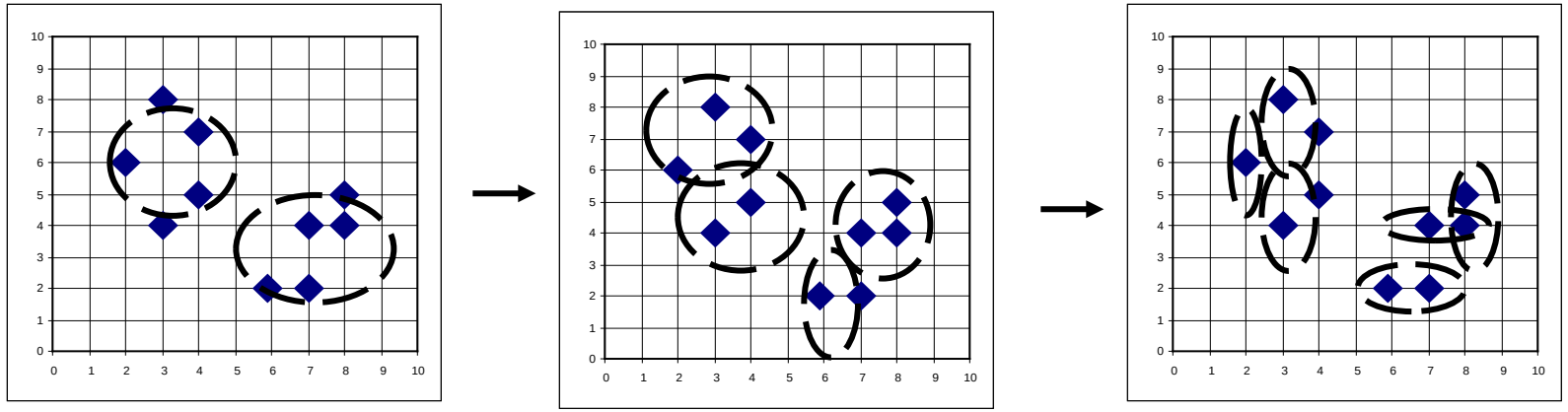




Divisive Clustering Algorithms

Divisive Clustering

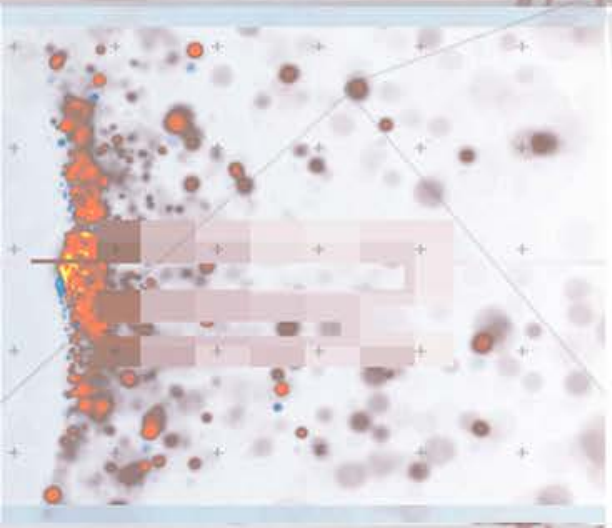
- DIANA (Divisive Analysis) (Kaufmann and Rousseeuw,1990)
  - Implemented in some statistical analysis packages, e.g., Splus
- Inverse order of AGNES: Eventually each node forms a cluster on its own



- Divisive clustering is a top-down approach
  - The process starts at the root with all the points as one cluster
  - It recursively splits the higher level clusters to build the dendrogram
  - Can be considered as a global approach
  - More efficient when compared with agglomerative clustering

More on Algorithm Design for Divisive Clustering

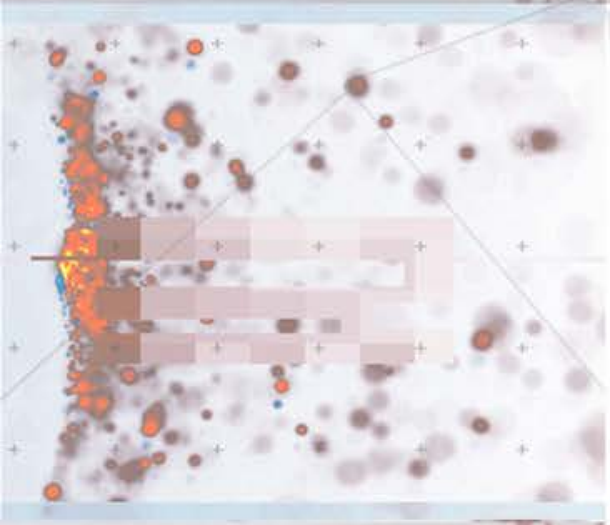
- Choosing which cluster to split
  - Check the sums of squared errors of the clusters and choose the one with the largest value
- Splitting criterion: Determining how to split
  - One may use Ward's criterion to chase for greater reduction in the difference in the SSE criterion as a result of a split
  - For categorical data, Gini-index can be used
- Handling the noise
  - Use a threshold to determine the termination criterion (do not generate clusters that are too small because they contain mainly noises)



Extensions to Hierarchical Clustering

Extensions to Hierarchical Clustering

- Major weaknesses of hierarchical clustering methods
  - Can never undo what was done previously
  - Do not scale well
    - Time complexity of at least $O(n^2)$, where n is the number of total objects
- Other hierarchical clustering algorithms
  - BIRCH (1996): Use CF-tree and incrementally adjust the quality of sub-clusters
  - CURE (1998): Represent a cluster using a set of well-scattered representative points
  - CHAMELEON (1999): Use graph partitioning methods on the K-nearest neighbor graph of the data



BIRCH: A Micro-Clustering-Based Approach

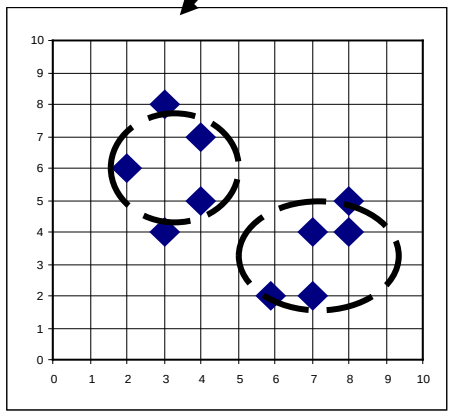
BIRCH (Balanced Iterative Reducing and Clustering Using Hierarchies)

- A multiphase clustering algorithm (Zhang, Ramakrishnan & Livny, SIGMOD'96)
- Incrementally construct a CF (Clustering Feature) tree, a hierarchical data structure for multiphase clustering
  - Phase 1: Scan DB to build an initial in-memory CF tree (a multi-level compression of the data that tries to preserve the inherent clustering structure of the data)
  - Phase 2: Use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree
- Key idea: Multi-level clustering
  - Low-level micro-clustering: Reduce complexity and increase scalability
  - High-level macro-clustering: Leave enough flexibility for high-level clustering
- *Scales linearly*: Find a good clustering with a single scan and improve the quality with a few additional scans

Clustering Feature Vector in BIRCH

- Clustering Feature (CF): *CF = (N, LS, SS)*
  - *N*: Number of data points
  - *LS: linear sum of N points:* $\sum_{i=1}^{N} X_i$
  - *SS: square sum of N points:* $\sum_{i=1}^{N} X_i^2$

CF = (5, (16,30),(54,190))

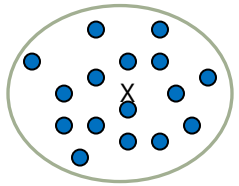


(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

- Clustering feature:
  - Summary of the statistics for a given sub-cluster: the 0-th, 1st, and 2nd moments of the sub-cluster from the statistical point of view
  - Registers crucial measurements for computing cluster and utilizes storage efficiently

Measures of Cluster: Centroid, Radius and Diameter

- Centroid: $\vec{x}_0$
  - the "middle" of a cluster
  - n: number of points in a cluster
  - $\vec{x}_i$ is the *i*-th point in the cluster



$$\vec{x}_0 = \frac{\sum_i^n \vec{x}_i}{n}$$

- Radius: R
  - Average distance from member objects to the centroid
  - The square root of average distance from any point of the cluster to its centroid

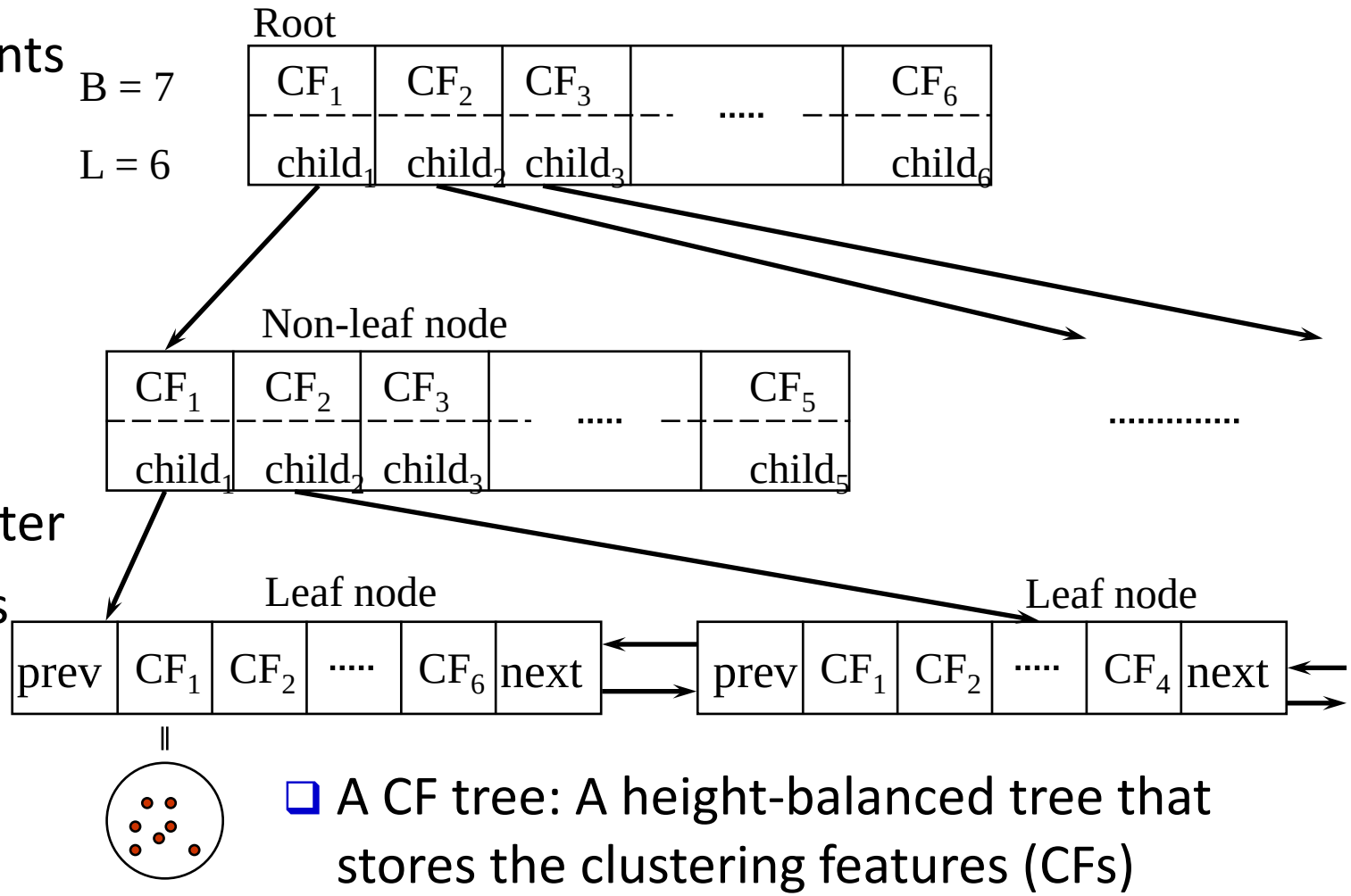
$$R = \sqrt{\frac{\sum_i^n (\vec{x}_i - \vec{x}_0)^2}{n}}$$

- Diameter: D
  - Average pairwise distance within a cluster
  - The square root of average mean squared distance between all pairs of points in the cluster

$$D = \sqrt{\frac{\sum_i^n \sum_j^n (\vec{x}_i - \vec{x}_j)^2}{n(n-1)}}$$

The CF Tree Structure in BIRCH

- Incremental insertion of new points (similar to B+-tree)
- For each point in the input
  - Find closest leaf entry
  - Add point to leaf entry and update CF
  - If entry diameter > max_diameter
    - split leaf, and possibly parents
- A CF tree has two parameters
  - Branching factor: Maximum number of children
  - Maximum diameter of sub-clusters stored at the leaf nodes



- A CF tree: A height-balanced tree that stores the clustering features (CFs)
- The non-leaf nodes store sums of the CFs of their children

BIRCH: A Scalable and Flexible Clustering Method

- An integration of agglomerative clustering with other (flexible) clustering methods
  - Low-level micro-clustering
    - Exploring CP-feature and BIRCH tree structure
    - Preserving the inherent clustering structure of the data
  - Higher-level macro-clustering
    - Provide sufficient flexibility for integration with other clustering methods
- Impact to many other clustering methods and applications
- Concerns
  - Sensitive to insertion order of data points
  - Due to the fixed size of leaf nodes, clusters may not be so natural
  - Clusters tend to be spherical given the radius and diameter measures