## CSE 5243 INTRO. TO DATA MINING

Cluster Analysis: Basic Concepts and Methods Huan Sun, CSE@The Ohio State University

Slides adapted from UIUC CS412, Fall 2017, by Prof. Jiawei Han

### Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction
- Partitioning Methods
- Hierarchical Methods
- Density- and Grid-Based Methods
- Evaluation of Clustering
- □ Summary

## **K-means Clustering**

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The basic algorithm is very simple Often chosen
  - 1: Select K points as the initial centroids.

#### 2: repeat

3

- 3: Form K clusters by assigning all points to the <u>closest</u> centroid.
- 4: <u>Recompute the centroid of each cluster</u>.
- 5: **until** The centroids don't change

Typically the mean of the points in the cluster

randomly

Measured by Euclidean distance, cosine similarity, etc.

## K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.
- □ K-means will converge for common similarity measures mentioned above.
- □ Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'

## Example: K-Means Clustering



## **Evaluating K-means Clusters**

□ Most common measure is Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- □ To get SSE, we square these errors and sum them.

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

Using Euclidean Distance

**I**  $X_i$  is a data point in cluster  $C_k$  and  $c_k$  is the representative point for cluster  $C_k$ 

can show that c<sub>k</sub> corresponds to the center (mean) of the cluster

1: Select K points as the initial centroids.

2: repeat

- 3: Form K clusters by assigning all points to the closest centroid.
- 4: Recompute the centroid of each cluster.
- 5: **until** The centroids don't change

=> attempt to minimize SSE

## Derivation of K-means to Minimize SSE

Example: one-dimensional data

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Step 4: how to update centroid

$$\frac{\partial}{\partial c_k} SSE = \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} (c_i - x)^2$$
$$= \sum_{i=1}^K \sum_{x \in C_i} \frac{\partial}{\partial c_k} (c_i - x)^2$$
$$= \sum_{x \in C_k} 2 \times (c_k - x_k) = 0$$

$$\sum_{x \in C_k} 2 \times (c_k - x_k) = 0 \Rightarrow m_k c_k = \sum_{x \in C_k} x_k \Rightarrow c_k = \frac{1}{m_k} \sum_{x \in C_k} x_k$$

## Other distance measures

#### Table 7.2. K-means: Common choices for proximity, centroids, and objective functions.

Proximity Function	Centroid	Objective Function
Manhattan $(L_1)$	median	Minimize sum of the $L_1$ distance of an
		object to its cluster centroid
Squared Euclidean $(L_2^2)$	mean	Minimize sum of the squared $L_2$ distance
		of an object to its cluster centroid
cosine	mean	Maximize sum of the cosine similarity of
		an object to its cluster centroid

## Derivation of K-means to Minimize SSE

Example: What if we choose Manhattan distance?

Step 4: how to update centroid

$$\frac{\partial}{\partial c_k} SAE = \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} |c_i - x|$$
$$= \sum_{i=1}^K \sum_{x \in C_i} \frac{\partial}{\partial c_k} |c_i - x|$$
$$= \sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0$$

$$\sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0 \Rightarrow \sum_{x \in C_k} sign(x - c_k) = 0$$

## Partitioning Algorithms: From Optimization Angle

- 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<sub>k</sub> is the "center" of cluster C<sub>k</sub>)
  - 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.

#### Importance of Choosing Initial Centroids (1)



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#### Importance of Choosing Initial Centroids (2)



# Solutions to Initial Centroids Problem

#### □ Multiple runs

- Helps, but probability is not on your side
- Sample to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated

## Pre-processing and Post-processing

- Pre-processing
  - Normalize the data
  - Eliminate outliers

#### Post-processing

- Eliminate small clusters that may represent outliers
- Split 'loose' clusters, i.e., clusters with relatively high SSE
- Merge clusters that are 'close' and that have relatively low SSE
- Can use these steps during the clustering process
  - ISODATA

### K-Means++

Original proposal (MacQueen'67): Select K seeds randomly

Need to run the algorithm multiple times using different seeds

 $\Box$  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)

 $\Box$  The selection continues until K centroids are obtained



### K-Means++

#### Algorithm 7.2 K-means++ initialization algorithm.

- 1: For the first centroid, pick one of the points at random.
- 2: for i = 1 to number of trials do
- 3: Compute the distance, d(x), of each point to its closest centroid.
- 4: Assign each point a probability proportional to each point's  $d(x)^2$ .
- 5: Pick new centroid from the remaining points using the weighted probabilities.
- 6: end for

# 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<sub>i</sub>
- 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

## Limitations of K-means

□ K-means has problems when clusters are of differing

- Sizes
- Densities
- Non-globular shapes

□ K-means has problems when the data contains outliers.

#### Limitations of K-means: Differing Size





(a) Original points.

(b) Three K-means clusters.

#### Figure 7.9. K-means with clusters of different size.

#### Limitations of K-means: Differing Density



(a) Original points.

(b) Three K-means clusters.

Figure 7.10. K-means with clusters of different density.

#### Limitations of K-means: Non-globular Clusters



(a) Original points.

(b) Two K-means clusters.

Figure 7.11. K-means with non-globular clusters.

#### **Overcoming K-means Limitations:**

#### Breaking Clusters to Subclusters



### 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!

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 $S = \sum_{i=1}^{n} \sum_{i=1}^{n} |x_{ii} - med_{ki}|$ 

 $k=1 x_{i \in C_k}$ 

- K-Medians: Instead of taking the mean value of the object in a cluster as a reference point, medians are used (corresponding to L<sub>1</sub>-norm as the distance measure)
- □ The criterion function for the *K*-Medians algorithm:
  - 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-Medoids: PAM (Partitioning around Medoids)

In general, pick actual data points as "cluster center"

# K-Medoids: PAM (Partitioning around Medoids)



# K-Medoids: PAM (Partitioning around Medoids)

Which one is more robust in the presence of noise and outliers?

A. K-Means

**B. K-Medoids** 

# K-Modes: Clustering Categorical Data

□ *K*-*M*eans 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

$$\Box \Phi(x_i, z_i) = 1 - n_i^r / n_i \text{ when } x_i = z_i \text{ ; } 1 \text{ when } x_i \neq z_i$$

- where z<sub>i</sub> is the categorical value of attribute j in Z<sub>i</sub>, n<sub>i</sub> is the number of objects in cluster l, and n<sub>i</sub><sup>r</sup> 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

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Produces a set of nested clusters organized as a hierarchical tree

Can be visualized as a dendrogram

A tree-like diagram that records the sequences of merges or splits



### Dendrogram: Shows How Clusters are Merged/Splitted

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



# Strengths of Hierarchical Clustering

Do not have to assume any particular number of clusters

Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level

They may correspond to meaningful taxonomies

Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

□ Two main types of hierarchical clustering

Agglomerative:

Divisive:

#### □ Two main types of hierarchical clustering

#### Agglomerative:

- Start with the points as individual clusters
- At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
- Build a bottom-up hierarchy of clusters



#### Divisive:

#### Two main types of hierarchical clustering

#### Agglomerative:

- Start with the points as individual clusters
- At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
- Build a bottom-up hierarchy of clusters



- Start with one, all-inclusive cluster
- At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Generate a top-down hierarchy of clusters



#### Two main types of hierarchical clustering

#### Agglomerative:

- Start with the points as individual clusters
- At each step, merge the closest pair of clusters until only one cluster (or k clusters) left

#### Divisive:

- Start with one, all-inclusive cluster
- At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
   Merge or split one cluster at a time

## Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  - 1. Compute the proximity matrix
  - 2. Let each data point be a cluster
  - 3. Repeat
  - 4. Merge the two closest clusters
  - 5. Update the proximity matrix
  - 6. **Until** only a single cluster remains



## Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  - 1. Compute the proximity matrix
  - 2. Let each data point be a cluster
  - 3. Repeat
  - 4. Merge the two closest clusters
  - 5. Update the proximity matrix
  - 6. **Until** only a single cluster remains
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance/similarity between clusters distinguish the different algorithms

# **Starting Situation**

Start with clusters of individual points and a proximity matrix

p1



12 data points



## Intermediate Situation

□ After some merging steps, we have some clusters



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

**Proximity Matrix** 



## Intermediate Situation

□ We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.





#### **Proximity Matrix**



# After Merging

□ How do we update the proximity matrix?





#### **Proximity Matrix**





- Image: MIN
- MAX
- Group Average
- Distance Between Centroids

	р1	p2	р3	р4	р5	<u> </u>
р1						
p2						
р3						
p4						
р5						
_						

**Proximity Matrix** 

•



- □ MIN
- MAX
- □ Group Average
- Distance Between Centroids

	р1	p2	р3	р4	р5	<u> </u>
р1						
p2						
р3						
p4						
р5						
_						

• Proximity Matrix

•



- MIN
- □ MAX
- □ Group Average
- Distance Between Centroids

	р1	p2	р3	p4	р5	<u> </u>
р1						
p2						
р3						
p4						
р5						
_						

• Proximity Matrix

•



- MIN
- MAX
- Group Average
- Distance Between Centroids

	р1	p2	р3	p4	р5	<u> </u>
р1						
p2						
р3						
р4						
р5						
_						

• Proximity Matrix

.



- □ MIN
- MAX
- □ Group Average
- Distance Between Centroids

	р1	p2	р3	р4	р5	<u> </u>
р1						
p2						
р3						
p4						
р5						

• Proximity Matrix

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Similarity of two clusters is based on the two most similar (closest) points in the different clusters

Similarity of two clusters is based on the two most similar (closest) points in the different clusters

Determined by one pair of points, i.e., by one link in the proximity graph.

 |
 |
 |
 |

 1
 2
 3
 4
 5

	1	2	13	4	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00

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Similarity of two clusters is based on the two most similar (closest) points in the different clusters

	1	12	13	4	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00

Similarity of two clusters is based on the two most similar (closest) points in the different clusters

	1	12	13	4	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00



Similarity of two clusters is based on the two most similar (closest) points in the different clusters

	1	12	13	4	15
11	1.00	0.90	0.10	0.65	0.20
2	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00



Similarity of two clusters is based on the two most similar (closest) points in the different clusters

Determined by one pair of points, i.e., by one link in the proximity graph.

	{ <b>I</b> 1, <b>I</b> 2}	3	<b>I</b> 4	15
{ <b>I</b> 1, <b>I</b> 2}	1.00	0.70	0.65	0.50
<b>I</b> 3	0.70	1.00	0.40	0.30
<b>I</b> 4	0.65	0.40	1.00	0.80
<b>I</b> 5	0.50	0.30	0.80	1.00

Update proximity matrix with new cluster {11, 12}

Similarity of two clusters is based on the two most similar (closest) points in the different clusters

Determined by one pair of points, i.e., by one link in the proximity graph.



Update proximity matrix with new cluster {11, 12}



Similarity of two clusters is based on the two most similar (closest) points in the different clusters

Determined by one pair of points, i.e., by one link in the proximity graph.



Update proximity matrix with new cluster {11, 12} and {14, 15}



Similarity of two clusters is based on the two most similar (closest) points in the different clusters



Only two clusters are left.







**Nested Clusters** 

Dendrogram

## Strength of MIN





**Original Points** 

**Two Clusters** 

Can handle non-elliptical shapes

### Limitations of MIN





**Original Points** 

**Two Clusters** 

Sensitive to noise and outliers

Similarity of two clusters is based on the two least similar (most distant) points in the different clusters

Determined by all pairs of points in the two clusters

	11	12	13	4	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00



Similarity of two clusters is based on the two least similar (most distant) points in the different clusters

Determined by all pairs of points in the two clusters



Similarity of two clusters is based on the two least similar (most distant) points in the different clusters

Determined by all pairs of points in the two clusters

	{ <b>I</b> 1, <b>I</b> 2}	13	<b>I</b> 4	15	
11	1.00	0.10	0.60	0.20	
13	0.10	1.00	0.40	0.30	
<b> </b> 4	0.60	0.40	1.00	0.80	
15	0.20	0.30	0.80	1.00	



Which two clusters should be merged next?

Similarity of two clusters is based on the two least similar (most distant) points in the different clusters

Determined by all pairs of points in the two clusters

	{ <b>I</b> 1, <b>I</b> 2}	13	<b>I</b> 4	15	
11	1.00	0.10	0.60	0.20	
13	0.10	1.00	0.40	0.30	
<b> </b> 4	0.60	0.40	1.00	0.80	
15	0.20	0.30	0.80	1.00	







**Nested Clusters** 

Dendrogram

## Strength of MAX





**Original Points** 

**Two Clusters** 

• Less susceptible to noise and outliers

### Limitations of MAX



**Original Points** 

**Two Clusters** 

•Tends to break large clusters

•Biased towards globular clusters

## **Cluster Similarity: Group Average**

Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

$$proximity(Cluster_{i}, Cluster_{j}) = \frac{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{j}}}{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{j}}} |Cluster_{i}| * |Cluster_{i}|$$

□ Need to use average connectivity for scalability since total proximity favors large clusters

-	11	12	13	<b> </b> 4	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
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### Hierarchical Clustering: Group Average





**Nested Clusters** 

Dendrogram

## Hierarchical Clustering: Group Average

Compromise between Single and Complete Link

- Strengths
  - Less susceptible to noise and outliers

- Limitations
  - Biased towards globular clusters

#### Hierarchical Clustering: Time and Space requirements

 $\Box$  O(N<sup>2</sup>) space since it uses the proximity matrix.

N is the number of points.

 $\Box$  O(N<sup>3</sup>) time in many cases

There are N steps and at each step the size, N<sup>2</sup>, proximity matrix must be updated and searched

• Complexity can be reduced to  $O(N^2 \log(N))$  time for some approaches

#### Hierarchical Clustering: Problems and Limitations

□ Once a decision is made to combine two clusters, it cannot be undone

□ No objective function is directly minimized

Different schemes have problems with one or more of the following:

- Sensitivity to noise and outliers
- Difficulty handling different sized clusters and convex shapes
- Breaking large clusters