# CSE 5243 INTRO. TO DATA MINING 

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

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

|  | Cluster Analysis: An Introduction |
| :--- | :--- |
| Partitioning Methods |  |

- Hierarchical Methods
$\square \quad$ Density- and Grid-Based Methods
- Evaluation of Clustering
$\square$ Summary


## K-means Clustering

$\square$ Partitional clustering approach
$\square$ Each cluster is associated with a centroid (center point)
$\square$ Each point is assigned to the cluster with the closest centroid
$\square$ Number of clusters, K, must be specified
$\square$ The basic algorithm is very simple

## Often chosen randomly

Measured by Euclidean distance, cosine similarity, etc.

1: Select $K$ points as the initial centroids.
2: repeat
3: Form $K$ clusters by assigning all points to the closest centroid.
4: $\quad$ Recompute the centroid of each cluster.
Typically the mean of
5: until The centroids don't change

## K-means Clustering - Details

$\square \quad$ Initial centroids are often chosen randomly.

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


## Example: K-Means Clustering



## Evaluating K-means Clusters

$\square$ Most common measure is Sum of Squared Error (SSE)
$\square$ For each point, the error is the distance to the nearest cluster

- To get SSE, we square these errors and sum them.

$$
S S E(C)=\sum_{k=1}^{K} \sum_{x_{i \in C_{k}}}\left\|x_{i}-c_{k}\right\|^{2}
$$

Using Euclidean Distance
$\square X_{i}$ is a data point in cluster $C_{k}$ and $c_{k}$ is the representative point for cluster $C_{k}$ - can show that $c_{k}$ 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.
=> attempt to minimize SSE
5: until The centroids don't change

## Derivation of K-means to Minimize SSE

$\square$ Example: one-dimensional data
Step 4: how to update centroid

$$
\begin{aligned}
\frac{\partial}{\partial c_{k}} \mathrm{SSE} & =\frac{\partial}{\partial c_{k}} \sum_{i=1}^{K} \sum_{x \in C_{i}}\left(c_{i}-x\right)^{2} \\
& =\sum_{i=1}^{K} \sum_{x \in C_{i}} \frac{\partial}{\partial c_{k}}\left(c_{i}-x\right)^{2} \\
& =\sum_{x \in C_{k}} 2 \times\left(c_{k}-x_{k}\right)=0 \\
\sum_{x \in C_{k}} 2 \times\left(c_{k}-x_{k}\right)=0 & \Rightarrow m_{k} c_{k}=\sum_{x \in C_{k}} x_{k} \Rightarrow c_{k}=\frac{1}{m_{k}} \sum_{x \in C_{k}} x_{k}
\end{aligned}
$$

## Other distance measures

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

| Proximity Function | Centroid | Objective Function |
| :---: | :---: | :--- |
| Manhattan $\left(\mathrm{L}_{1}\right)$ | median | Minimize sum of the $\mathrm{L}_{1}$ distance of an <br> object to its cluster centroid |
| Squared Euclidean $\left(\mathrm{L}_{2}^{2}\right)$ | mean | Minimize sum of the squared $\mathrm{L}_{2}$ distance <br> of an object to its cluster centroid |
| cosine | mean | $\frac{\text { Maximize sum of the cosine similarity of }}{\text { an object to its cluster centroid }}$ |

## Derivation of K-means to Minimize SSE

$\square$ Example: What if we choose Manhattan distance?

$$
\begin{aligned}
\frac{\partial}{\partial c_{k}} \mathrm{SAE} & =\frac{\partial}{\partial c_{k}} \sum_{i=1}^{K} \sum_{x \in C_{i}}\left|c_{i}-x\right| \\
& =\sum_{i=1}^{K} \sum_{x \in C_{i}} \frac{\partial}{\partial c_{k}}\left|c_{i}-x\right| \\
& =\sum_{x \in C_{k}} \frac{\partial}{\partial c_{k}}\left|c_{k}-x\right|=0 \\
\sum_{x \in C_{k}} \frac{\partial}{\partial c_{k}}\left|c_{k}-x\right| & =0 \Rightarrow \sum_{x \in C_{k}} \operatorname{sign}\left(x-c_{k}\right)=0
\end{aligned}
$$

Step 4: how to update centroid

## Partitioning Algorithms: From Optimization Angle

$\square$ Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
$\square K$-partitioning method: Partitioning a dataset $\boldsymbol{D}$ of $\boldsymbol{n}$ objects into a set of $\boldsymbol{K}$ clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where $c_{k}$ is the "center" of cluster $C_{k}$ )

- A typical objective function: Sum of Squared Errors (SSE)

$$
S S E(C)=\sum_{k=1}^{K} \sum_{x_{i \in c_{k}}}\left\|x_{i}-c_{k}\right\|^{2}
$$

$\square$ 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)


## Importance of Choosing Initial Centroids (2)



## Solutions to Initial Centroids Problem

$\square$ Multiple runs

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


## Pre-processing and Post-processing

$\square$ Pre-processing
$\square$ Normalize the data
$\square$ Eliminate outliers
$\square$ Post-processing
$\square$ Eliminate small clusters that may represent outliers
$\square$ Split 'loose' clusters, i.e., clusters with relatively high SSE
$\square$ Merge clusters that are 'close' and that have relatively low SSE
$\square$ Can use these steps during the clustering process

- ISODATA


## K-Means++

$\square$ Original proposal (MacQueen'67): Select $K$ seeds randomly
$\square$ Need to run the algorithm multiple times using different seeds

$\square$ There are many methods proposed for better initialization of $k$ seeds
$\square$ 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)
$\square$ 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

$\square$ The K-Means algorithm is sensitive to outliers!-since an object with an extremely large value may substantially distort the distribution of the data
$\square$ 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
$\square$ 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
$\square$ 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


## Limitations of K-means

$\square$ K-means has problems when clusters are of differing
$\square$ Sizes

- Densities
$\square$ Non-globular shapes
$\square$ 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.


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


Original Points


K-means Clusters

## K-Medians: Handling Outliers by Computing Medians

$\square$ Medians are less sensitive to outliers than means
$\square$ Think of the median salary vs. mean salary of a large firm when adding a few top executives!

## K-Medians: Handling Outliers by Computing Medians

- Medians are less sensitive to outliers than means
$\square$ Think of the median salary vs. mean salary of a large firm when adding a few top executives!
$\square$ K-Medians: Instead of taking the mean value of the object in a cluster as a reference point, medians are used (corresponding to $\mathrm{L}_{1}$-norm as the distance measure)
$\square$ The criterion function for the K-Medians algorithm: $\quad S=\sum_{k=1}^{K} \sum_{x_{i \in C_{k}}} \mid x_{i j}-$ med $_{k j} \mid$
$\square$ 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


## K-Medoids: PAM (Partitioning around Medoids)

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

## K-Medoids: PAM (Partitioning around Medoids)



$$
K=2
$$

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

$\uparrow$
Arbitrary choose $K$ medoids
$\qquad$ object as initial



Randomly select a nonmedoid object, $\mathrm{O}_{\text {ramdom }}$


## 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

$\square$ K-Means cannot handle non-numerical (categorical) data

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


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## Hierarchical Clustering

$\square$ Produces a set of nested clusters organized as a hierarchical tree
$\square$ Can be visualized as a dendrogram
$\square$ A tree-like diagram that records the sequences of merges or splits



## Dendrogram: Shows How Clusters are Merged/Splitted

$\square$ Dendrogram: Decompose a set of data objects into a tree of clusters by multi-level nested partitioning
$\square$ 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)

## Strengths of Hierarchical Clustering

$\square$ Do not have to assume any particular number of clusters
$\square$ Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level
$\square$ They may correspond to meaningful taxonomies
$\square$ Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

## Hierarchical Clustering

$\square$ Two main types of hierarchical clustering
$\square$ Agglomerative:
$\square$ Divisive:

## Hierarchical Clustering

$\square$ 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
$\square$ Divisive:



## Hierarchical Clustering

## $\square$ Two main types of hierarchical clustering

$\square$ 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:
- 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



## Hierarchical Clustering

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


## Agglomerative Clustering Algorithm

$\square \quad$ More popular hierarchical clustering technique
$\square \quad$ Basic algorithm is straightforward

1. Compute the proximity matrix
2. Let each data point be a cluster
3. Repeat

Merge the two closest clusters
Update the proximity matrix
6. Until only a single cluster remains


## Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
$\square \quad$ 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
$\square$ 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

$\square$ Start with clusters of individual points and a proximity matrix


## Intermediate Situation

$\square$ After some merging steps, we have some clusters


|  | C1 | C2 | C3 | C4 | C5 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| C 1 |  |  |  |  |  |
| C |  |  |  |  |  |
| C |  |  |  |  |  |
| C |  |  |  |  |  |
| C |  |  |  |  |  |
|  |  |  |  |  |  |

Proximity Matrix


## Intermediate Situation

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


## After Merging

$\square$ How do we update the proximity matrix?

| C 2 |  |  |  |  |
| ---: | :---: | :---: | :---: | :---: |
|  | C 1 | C 5 | C 3 | C 4 |
| C 1 |  | $?$ |  |  |
| C 2 U 5 | $?$ | $?$ | $?$ | $?$ |
| C 3 |  | $?$ |  |  |
| C |  | $?$ |  |  |

Proximity Matrix


## How to Define Inter-Cluster Similarity


$\square \mathrm{MIN}$

- MAX
- Group Average
- Distance Between Centroids

- MIN
- MAX
- Group Average
- Distance Between Centroids

|  | p1 | p2 | p3 | p4 | p5 | $\ldots$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| p1 |  |  |  |  |  |  |
| p2 |  |  |  |  |  |  |
| p3 |  |  |  |  |  |  |
| p4 |  |  |  |  |  |  |
| p5 |  |  |  |  |  |  |
| . |  |  |  |  |  |  |

- Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

|  | p1 | p2 | p3 | p4 | p5 | $\ldots$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| p1 |  |  |  |  |  |  |
| p2 |  |  |  |  |  |  |
| p3 |  |  |  |  |  |  |
| p4 |  |  |  |  |  |  |
| p5 |  |  |  |  |  |  |
| . |  |  |  |  |  |  |

- Proximity Matrix

How to Define Inter-Cluster Similarity

$\square \mathrm{MIN}$

- MAX
- Group Average
- Distance Between Centroids

|  | p1 | p2 | p3 | p4 | p5 | $\ldots$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| p1 |  |  |  |  |  |  |
| p2 |  |  |  |  |  |  |
| p3 |  |  |  |  |  |  |
| p4 |  |  |  |  |  |  |
| p5 |  |  |  |  |  |  |
| . |  |  |  |  |  |  |

Proximity Matrix

How to Define Inter-Cluster Similarity


- MIN
- MAX
- Group Average
- Distance Between Centroids

|  | p1 | p2 | p3 | p4 | p5 | $\ldots$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| p1 |  |  |  |  |  |  |
| p2 |  |  |  |  |  |  |
| p3 |  |  |  |  |  |  |
| p4 |  |  |  |  |  |  |
| p5 |  |  |  |  |  |  |
| . |  |  |  |  |  |  |

Proximity Matrix

## Cluster Similarity: MIN or Single Link

$\square$ Similarity of two clusters is based on the two most similar (closest) points in the different clusters
$\square$ Determined by one pair of points, i.e., by one link in the proximity graph.

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|  | 11 | 12 | 13 | 14 | 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 |


| $\mid$ | $\mid$ | $\mid$ | $\mid$ | $\mid$ |
| :--- | :--- | :--- | :--- | :--- |
| 1 | 2 | 3 | 4 | 5 |

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| :---: | :---: | :---: | :---: | :---: | :---: |
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| 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 |
| 5 | 0.20 | 0.50 | 0.30 | 0.80 | 1.00 |

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| 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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$\square$ Similarity of two clusters is based on the two most similar (closest) points in the different clusters
$\square$ Determined by one pair of points, i.e., by one link in the proximity graph.

|  | $\{\|1\| 2\}$, | 13 | 14 | 15 |
| ---: | :--- | :--- | :--- | :--- |
| $\{11, \mid 2\}$ | 1.00 | 0.70 | 0.65 | 0.50 |
| 13 | 0.70 | 1.00 | 0.40 | 0.30 |
| 14 | 0.65 | 0.40 | 1.00 | 0.80 |
| 15 | 0.50 | 0.30 | 0.80 | 1.00 |
|  |  |  |  |  |

Update proximity matrix with new
cluster $\{11, \mid 2\}$

## Cluster Similarity: MIN or Single Link

$\square$ Similarity of two clusters is based on the two most similar (closest) points in the different clusters
$\square$ Determined by one pair of points, i.e., by one link in the proximity graph.

|  | \{11,12\} | 13 | 14 | 15 |
| :---: | :---: | :---: | :---: | :---: |
| \{11, 21$\}$ | 1.00 | 0.70 | 0.65 | 0.50 |
| 13 | 0.70 | 1.00 | 0.40 | 0.30 |
| 14 | 0.65 | 0.40 | 1.00 | 0.80 |
| 15 | 0.50 | 0.30 | 0.80 | 1.00 |

Update proximity matrix with new cluster $\{11,12\}$

## Cluster Similarity: MIN or Single Link

$\square$ Similarity of two clusters is based on the two most similar (closest) points in the different clusters
$\square$ Determined by one pair of points, i.e., by one link in the proximity graph.

|  | $\{11,12\}$ | 13 | $\{4,15\}$ |
| ---: | ---: | ---: | ---: |
| $\{11,12\}$ | 1.00 | 0.70 | 0.65 |
| 13 | 0.70 | 1.00 | 0.40 |
| $\{14,15\}$ | 0.65 | 0.40 | 1.00 |

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


## Cluster Similarity: MIN or Single Link

$\square$ Similarity of two clusters is based on the two most similar (closest) points in the different clusters
$\square$ Determined by one pair of points, i.e., by one link in the proximity graph.

|  | $\{\|1,\|2\| 3\}$, | $\{\|4\| 5\}$, |
| ---: | ---: | ---: |
| $\{\|1,\|2\| 3\}$, | 1.00 | 0.65 |
| $\{\|4\| 5\}$, | 0.65 | 1.00 |

Only two clusters are left.


## Hierarchical Clustering: MIN



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


## Cluster Similarity: MAX or Complete Linkage

$\square$ Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
$\square$ Determined by all pairs of points in the two clusters

|  |  | 12 | 13 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1.00 | 0. | 0.10 | 0.65 |  |
| 2 | 0.90 | 1.00 | 0.70 | 0.60 |  |
| 3 | 0.10 | 0.70 | 1. | 0.40 |  |
|  | 0.65 | 0.60 | 0.40 | 1.00 | 0.80 |
|  | 0.2 | 0.5 | 0.30 | 0.80 |  |


| 1 |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |  |
| 1 | 2 | 3 | 4 | 5 |  |

## Cluster Similarity: MAX or Complete Linkage

$\square$ Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
$\square$ Determined by all pairs of points in the two clusters

|  | $\multicolumn{1}{c}{11, \mid 2} \mid 3$ | 14 | 15 |  |
| :--- | :--- | :--- | :--- | :--- |
| 11 | 1.00 | 0.10 | 0.60 | 0.20 |
| 13 | 0.10 | 1.00 | 0.40 | 0.30 |
| 14 | 0.60 | 0.40 | 1.00 | 0.80 |
| 15 | 0.20 | 0.30 | 0.80 | 1.00 |
|  |  |  |  |  |



## Cluster Similarity: MAX or Complete Linkage

$\square$ Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
$\square$ Determined by all pairs of points in the two clusters



Which two clusters should be merged next?

## Cluster Similarity: MAX or Complete Linkage

$\square$ Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
$\square$ Determined by all pairs of points in the two clusters



## Hierarchical Clustering: MAX



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

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

$$
\begin{aligned}
& \sum \text { proximity }\left(\mathbf{p}_{\mathrm{i}}, \mathbf{p}_{\mathrm{j}}\right) \\
& \text { proximity } \left.\text { Cluster }_{i}, \text { Cluster }_{j}\right)=\frac{\substack{p_{i} \in \text { Clister } \\
p_{j} \\
\mathcal{C C l u s t e r}_{j}}}{\mid \text { Cluster }_{i}|*| \text { Cluster }_{j} \mid}
\end{aligned}
$$

$\square$ Need to use average connectivity for scalability since total proximity favors large clusters

|  | 11 | 12 | 13 | 14 | 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 |
| 1 |  |  |  |  |  |



## Hierarchical Clustering: Group Average



Nested Clusters


Dendrogram

## Hierarchical Clustering: Group Average

$\square$ Compromise between Single and Complete Link
$\square$ Strengths

- Less susceptible to noise and outliers
$\square$ Limitations
$\square$ Biased towards globular clusters


## Hierarchical Clustering: Time and Space requirements

$\square \mathrm{O}\left(\mathrm{N}^{2}\right)$ space since it uses the proximity matrix.
$\square \mathrm{N}$ is the number of points.
$\square \mathrm{O}\left(\mathrm{N}^{3}\right)$ time in many cases

- There are $N$ steps and at each step the size, $N^{2}$, proximity matrix must be updated and searched
$\square$ Complexity can be reduced to $\mathrm{O}\left(\mathrm{N}^{2} \log (\mathrm{~N})\right)$ time for some approaches


## Hierarchical Clustering: Problems and Limitations

$\square$ Once a decision is made to combine two clusters, it cannot be undone
$\square$ No objective function is directly minimized
$\square$ Different schemes have problems with one or more of the following:
$\square$ Sensitivity to noise and outliers
$\square$ Difficulty handling different sized clusters and convex shapes
$\square$ Breaking large clusters

