Lesson 11. Cluster Analysis

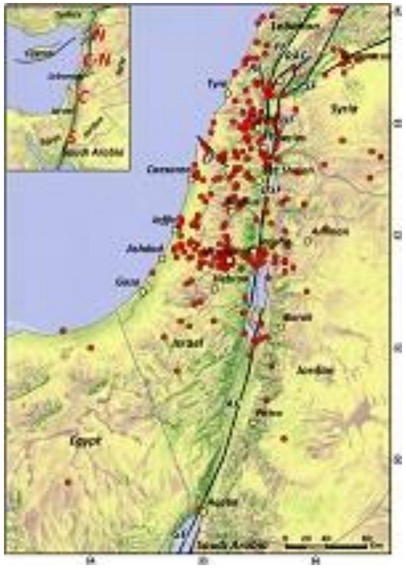
- What is Cluster Analysis?
- Types of Data in Cluster Analysis
- A Categorization of Major Clustering Methods
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- Grid-Based Methods
- Model-Based Clustering Methods
- Outlier Analysis
- Summary

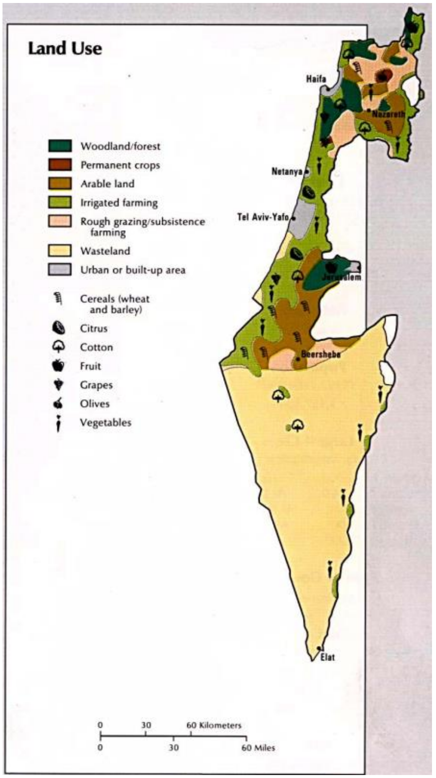
What is Cluster Analysis?

- Cluster: a collection of data objects
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters
- Cluster analysis
  - Grouping a set of data objects into clusters
- Clustering is unsupervised classification: no predefined classes
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Examples of Clustering Applications

- **Information retrieval**: document clustering
- **Land use**: Identification of areas of similar land use in an earth observation database
- **Marketing**: Develop targeted marketing programs
- **City planning**: Identifying groups of houses according to their house type, value, and geographical location
- **Earthquake studies**: Observe earthquake epicenters
- **Climate**: understanding earth climate, find patterns of atmospheric and ocean





What Is Good Clustering?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation.
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns.

Requirements of Clustering in Data Mining

- Scalability (Big Data)
- Ability to deal with different types of attributes
- Discovery of clusters with arbitrary shape
- Minimal requirements for domain knowledge to determine input parameters
- Able to deal with noise and outliers
- Incremental clustering and insensitivity to input order
- High dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability

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Data Structures

- Data matrix
  - p – number of variables
  - n – number of objects
  - x_{if} - value of variable i in record f

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix
  - $d\ (i,j)$ – distance between objects i and j

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ : & : & : & & \\ d(n,1) & d(n,2) & \ldots & \ldots & 0 \end{bmatrix}$$

Attribute Types in Clustering Analysis

- **Nominal:** categories, states, or "names of things"
  - *Hair_color = {auburn, black, blond, brown, grey, red, white}*
  - marital status, occupation, ID numbers, zip codes

- **Binary**
  - Nominal attribute with only 2 states (0 and 1)
  - <u>Symmetric binary</u>: both outcomes equally important
    - e.g., gender
  - <u>Asymmetric binary</u>: outcomes not equally important.
    - e.g., medical test (positive vs. negative), TF
    - Convention: assign 1 to most important outcome (e.g., HIV positive)

- **Ordinal**
  - Values have a meaningful order (ranking) but magnitude between successive values is not known.
  - *Size = {small, medium, large}*, grades, army rankings

Numeric Attribute Types

- Quantity (integer or real-valued)
- **Interval**
  - Measured on a scale of **equal-sized units**
  - Values have order
    - E.g., *temperature in C˚or F˚, calendar dates*
  - No true zero-point
- **Ratio**
  - Inherent **zero-point**
  - We can speak of values as being an order of magnitude larger than the unit of measurement (10 K˚ is twice as high as 5 K˚).
    - e.g., *temperature in Kelvin, length, counts, monetary quantities*

Interval-scaled variables

- Goal: give all variables (age (years), height (cm), etc.) an <u>equal weight</u>
- Standardize data (*n* – number of objects)
  - Calculate the mean absolute deviation for variable *f*:
    $$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + ... + |x_{nf} - m_f|)$$
  - Where the mean value of *f* is $m_f = \frac{1}{n}(x_{1f} + x_{2f} + ... + x_{nf})$.
  - Calculate the standardized measurement (z-score)
    $$z_{if} = \frac{x_{if} - m_f}{s_f}$$
- Using mean absolute deviation is more robust than using standard deviation, since deviations are not squared

Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
  - Requirements
    - *Non-negativity:* $d(i,j) \geq 0$
    - *Distance to itself:* $d(i,i) = 0$
    - *Symmetry:* $d(i,j) = d(j,i)$
    - *Triangular inequality:* $d(i,j) \leq d(i,k) + d(k,j)$
- Some popular ones include: Minkowski distance:

$$d(i,j) = \sqrt[q]{(|x_{i_1} - x_{j_1}|^q + |x_{i_2} - x_{j_2}|^q + \ldots + |x_{i_p} - x_{j_p}|^q)}$$

  - where $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ are two p-dimensional data objects, and q is a positive integer

Similarity and Dissimilarity Between Objects (Cont.)

- If q = 1, d is Manhattan distance

$$d(i,j) = |x_{i_1} - x_{j_1}| + |x_{i_2} - x_{j_2}| + \ldots + |x_{i_p} - x_{j_p}|$$

- *If q = 2, d* is Euclidean distance:

$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \ldots + |x_{i_p} - x_{j_p}|^2)}$$

- Other dissimilarity measures are available

Binary Variables

- A contingency table for binary data
  - *p* – number of variables

		Object *j*		
		1	0	*sum*
Object *i*	1	a	b	$a+b$
	0	c	d	$c+d$
	sum	$a+c$	$b+d$	p

- Distance measure for <u>symmetric</u> binary variables:

$$d(i,j) = \frac{b+c}{a+b+c+d}$$

- Distance measure for <u>asymmetric</u> binary variables:

$$d(i,j) = \frac{b+c}{a+b+c}$$

- Jaccard coefficient (*similarity* measure for <u>*asymmetric*</u> binary variables):

$$sim_{Jaccard}(i,j) = \frac{a}{a+b+c}$$

Dissimilarity between Binary Variables

Example

Name	~~Gender~~	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	~~M~~	Y	N	P	N	N	N
Mary	~~F~~	Y	N	P	N	P	N
Jim	~~M~~	Y	P	N	N	N	N

- gender is a symmetric attribute
- the remaining attributes are asymmetric binary
- let the values *Y* and *P* be set to 1, and the value *N* be set to 0

$$d(i,j) = \frac{b+c}{a+b+c}$$

$$d(jack, mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(jack, jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(jim, mary) = \frac{1+2}{1+1+2} = 0.75$$

Mary \ Jack	1	0	*sum*
1	2	1	3
0	0	3	3
sum	2	4	6

Nominal Variables

- A generalization of the binary variable in that it can take more than 2 states, e.g., red, yellow, blue, green
- Method 1: Simple matching
  - *m*: # of matches, *p*: total # of variables

$$d(i,j) = \frac{p-m}{p}$$

- Method 2: use a large number of binary variables
  - creating a new binary variable for each of the *M* nominal states

Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank
- Can be treated like interval-scaled
  - replace x_{if} by their rank $r_{if} \in \{1, \ldots, M_f\}$
  - map the range of each variable onto [0, 1] by replacing *i*-th object in the *f*-th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

    - Example: academic ranks in Israel
  - compute the dissimilarity using methods for interval-scaled variables

Ratio-Scaled Variables

- Ratio-scaled variable: a positive measurement on a nonlinear scale, approximately at exponential scale, such as Ae^{Bt} or Ae^{-Bt}
  - Examples: salaries, web links
- Methods:
  - treat them like interval-scaled variables—*not a good choice!* (why?—the scale can be distorted)
  - apply logarithmic transformation

$$y_{if} = log(x_{if})$$

  - treat them as continuous ordinal data treat their rank as interval-scaled

Variables of Mixed Types

- A database may contain all the six types of variables
  - symmetric binary, asymmetric binary, nominal, ordinal, interval and ratio
- One may use a weighted formula to combine their effects

$$d(i,j) = \frac{\sum_{f=1}^{p} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} \delta_{ij}^{(f)}}$$

  - $\delta_{ij}(f)$ – binary indicator ($\delta_{ij}(f)$ = 0 if a variable f should be skipped)
  - $d_{ij}^{(f)}$ – contribution of variable f to dissimilarity between i and j
  - *Variable f* is binary or nominal:

    $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, or $d_{ij}^{(f)} = 1$ otherwise
  - *Variable f* is interval-based: use the normalized distance
  - *Variable f* is ordinal or ratio-scaled
    - compute ranks r_{if} and
    - and treat z_{if} as interval-scaled

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

Vector Objects

- Vector objects: keywords in documents, gene features in micro-arrays, etc.
- Broad applications: information retrieval, biologic taxonomy, etc.
- Cosine measure

$$s(\vec{X}, \vec{Y}) = \frac{\vec{X}^t \cdot \vec{Y}}{|\vec{X}||\vec{Y}|},$$

$\vec{X}^t$ is a transposition of vector $\vec{X}$, $|\vec{X}|$ is the Euclidean normal of vector $\vec{X}$,

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Major Clustering Approaches (I)

- Partitioning approach:
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - Typical methods: k-means, k-medoids, CLARANS
- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- Density-based approach:
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue
- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE

Major Clustering Approaches (II)

- Model-based:
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: EM, SOM, COBWEB
- Frequent pattern-based:
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- User-guided or constraint-based:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), constrained clustering
- Link-based clustering:
  - Objects are often linked together in various ways
  - Massive links can be used to cluster objects: SimRank, LinkClus

Typical Alternatives to Calculate the Distance between Clusters

- Single link: smallest distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_j) = min(t_{ip}, t_{jq})$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_j) = max(t_{ip}, t_{jq})$
- Average: avg distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_j) = avg(t_{ip}, t_{jq})$
- Centroid: distance between the centroids of two clusters, i.e., $dis(K_i, K_j) = dis(C_i, C_j)$
- Medoid: distance between the medoids of two clusters, i.e., $dis(K_i, K_j) = dis(M_i, M_j)$
  - Medoid: one chosen, centrally located object in the cluster

Centroid, Radius and Diameter of a Cluster (for numerical data sets)

- Centroid: the "middle" of a cluster

$$C_m = \frac{\sum_{i=1}^{N}(t_{ip})}{N}$$

- Radius: square root of average distance from any point of the cluster to its centroid

$$R_m = \sqrt{\frac{\sum_{i=1}^{N}(t_{ip} - c_m)^2}{N}}$$

- Diameter: square root of average mean squared distance between all pairs of points in the cluster

$$D_m = \sqrt{\frac{\sum_{i=1}^{N}\sum_{i=1}^{N}(t_{ip} - t_{iq})^2}{N(N-1)}}$$

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Partitioning Algorithms: Basic Concept

- Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

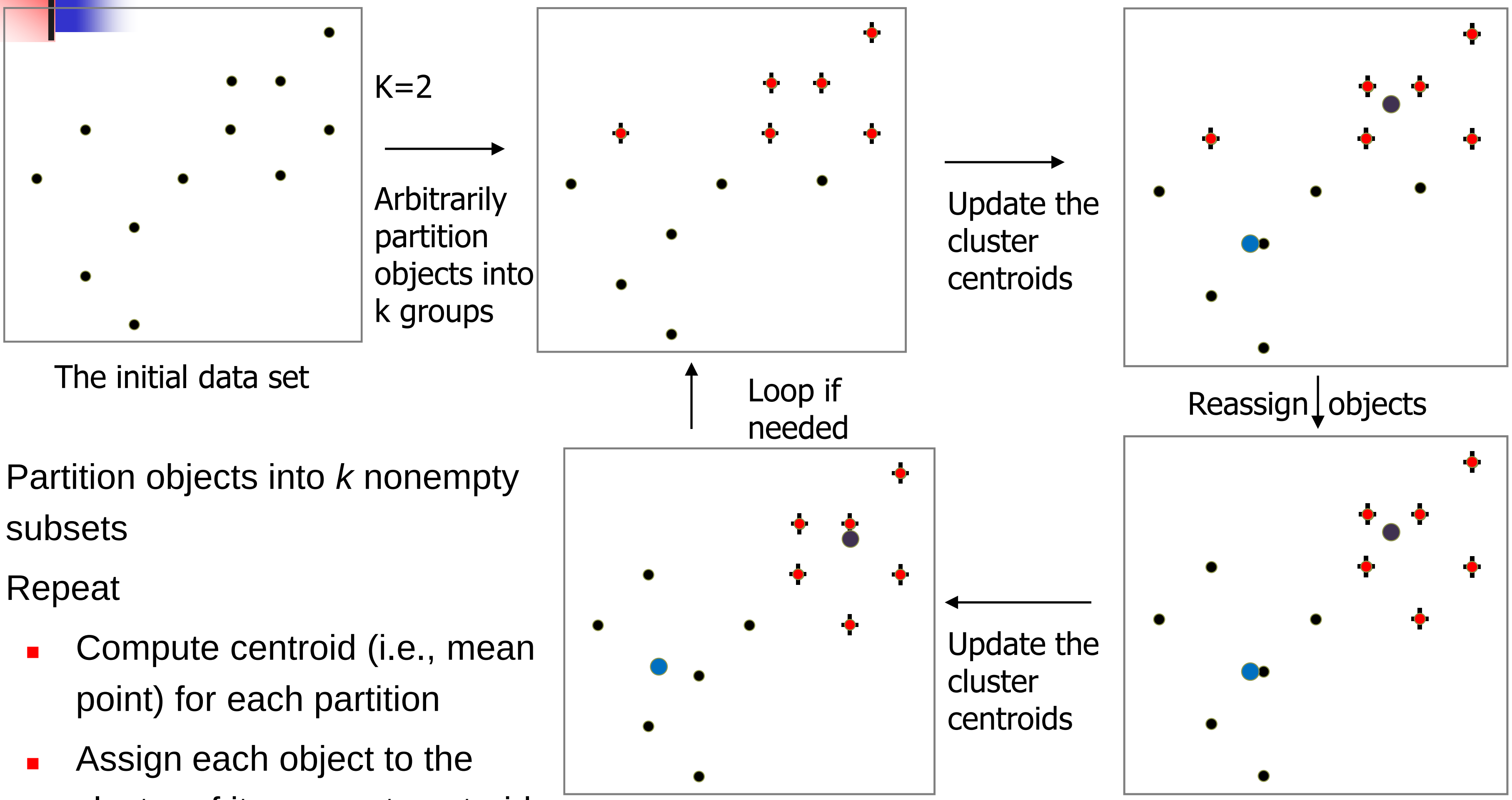
$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (p - c_i)^2$$

- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in four steps:
  - Partition objects into *k* nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  - Assign each object to the cluster with the nearest seed point
  - Go back to Step 2, stop when the assignment does not change

An Example of *K-Means* Clustering



- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

K-Means Example (k = 2)

Iteration 1

Cluster 1

Rec No	X1	X2	X3	X4	X5
1	0	0	0	0	0
2	0	0	0	0	0
3	1	1	1	1	1
Mean	**0.33**	**0.33**	**0.33**	**0.33**	**0.33**

Cluster 2

Rec No	X1	X2	X3	X4	X5
4	1	0	1	0	1
5	0	1	0	1	0
6	1	0	1	1	1
7	1	1	1	1	1
Mean	**0.75**	**0.5**	**0.75**	**0.75**	**0.75**

Objects Re-assignment

Rec No	Old	to Cluster 1	to Cluster 2	Min	New
1	1	0.745	1.581	0.745	1
2	1	0.745	1.581	0.745	1
3	1	1.491	0.707	0.707	2
4	2	1.247	1.000	1.000	2
5	2	1.106	1.414	1.106	1
6	2	1.374	0.707	0.707	2
7	2	1.491	0.707	0.707	2

K-Means Example (k = 2)

Iteration 2

Cluster 1

Rec No	X1	X2	X3	X4	X5
1	0	0	0	0	0
2	0	0	0	0	0
5	0	1	0	1	0
Mean	**0.00**	**0.33**	**0.00**	**0.33**	**0.00**

Cluster 2

Rec No	X1	X2	X3	X4	X5
3	1	1	1	1	1
4	1	0	1	0	1
6	1	0	1	1	1
7	1	1	1	1	1
Mean	**1**	**0.5**	**1**	**0.75**	**1**

Objects Re-assignment

Rec No	Old	to Cluster 1	to Cluster 2	Min	New
1	1	0.471	1.953	0.471	1
2	1	0.471	1.953	0.471	1
3	2	1.972	0.559	0.559	2
4	2	1.795	0.901	0.901	2
5	1	0.943	1.820	0.943	1
6	2	1.886	0.559	0.559	2
7	2	1.972	0.559	0.559	2

Comments on the *K-Means* Method

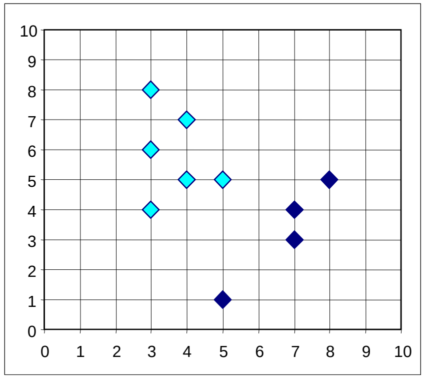
- Strength: *Efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, $t << n$.
    - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- Comment: Often terminates at a *local optimal*.
- Weakness
    - Applicable only to objects in a continuous n-dimensional space
        - Using the k-modes method for categorical data
        - In comparison, k-medoids can be applied to a wide range of data
    - Need to specify *k,* the *number* of clusters, in advance (there are ways to automatically determine the best k (see Hastie et al., 2009)
    - Sensitive to noisy data and *outliers*
    - Not suitable to discover clusters with *non-convex shapes*

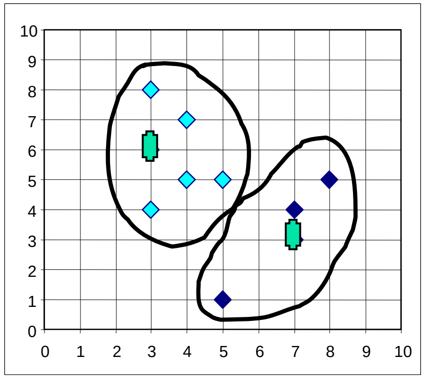
Variations of the *K-Means* Method

- A few variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means
- Handling categorical data: *k-modes* (Huang'98)
  - Replacing means of clusters with <u>modes</u>
  - Using new dissimilarity measures to deal with categorical objects
  - Using a <u>frequency</u>-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

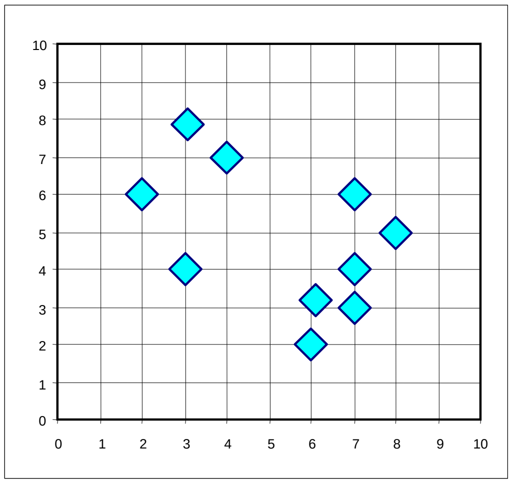
What is the problem of k-Means Method?

- 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.



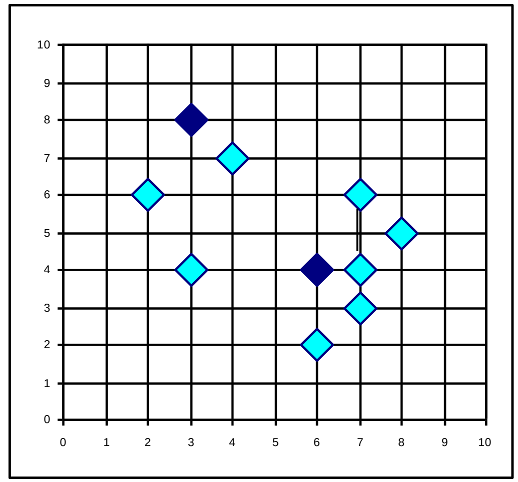


PAM: A Typical K-Medoids Algorithm



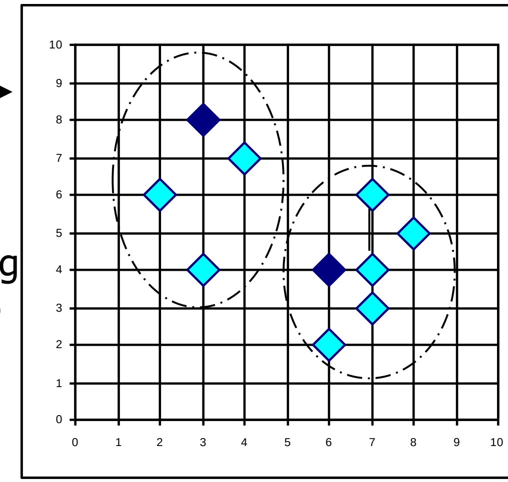
K=2

Arbitrary choose *k* objects as initial medoids

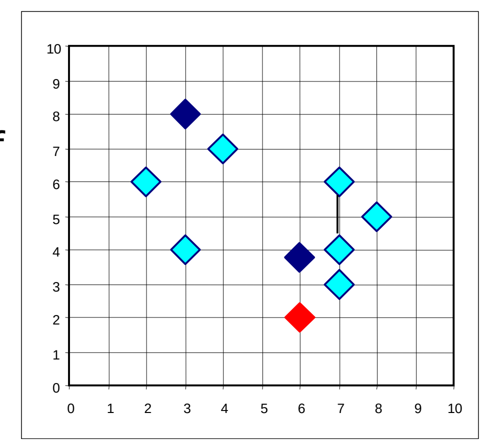


Assign each remaining object to nearest medoids

Total Cost = 20

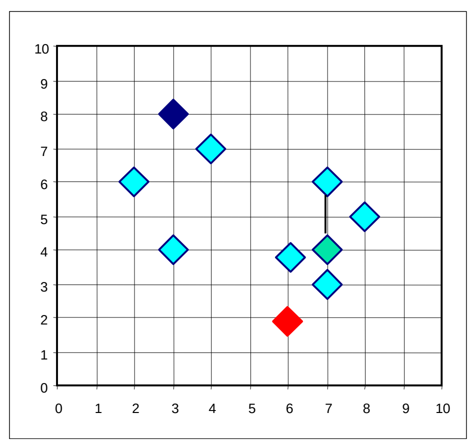


Randomly select a nonmedoid object, O_{random}



Compute total cost of swapping

Total Cost = 26



Swapping O and O_{random}

If quality is improved.

Do loop

Until no change

The K-Medoid Clustering Method

- *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 randomly selected non-medoids if it decreases the total distance of the resulting clustering
      - Each object is assigned to a cluster represented by the nearest medoid
    - *PAM* works effectively for small data sets, but does not scale well for large data sets (due to the computational complexity)
- Efficiency improvement on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990): PAM on samples
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling

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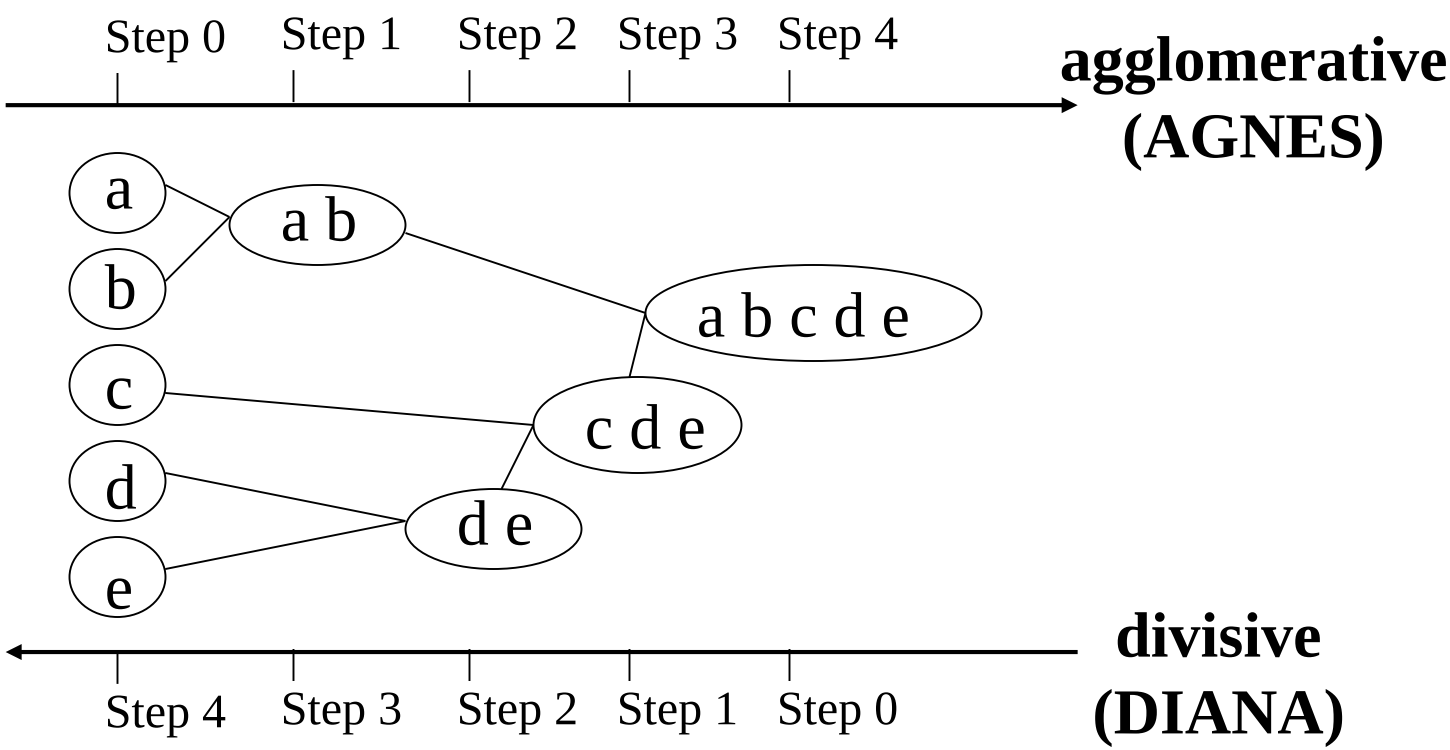
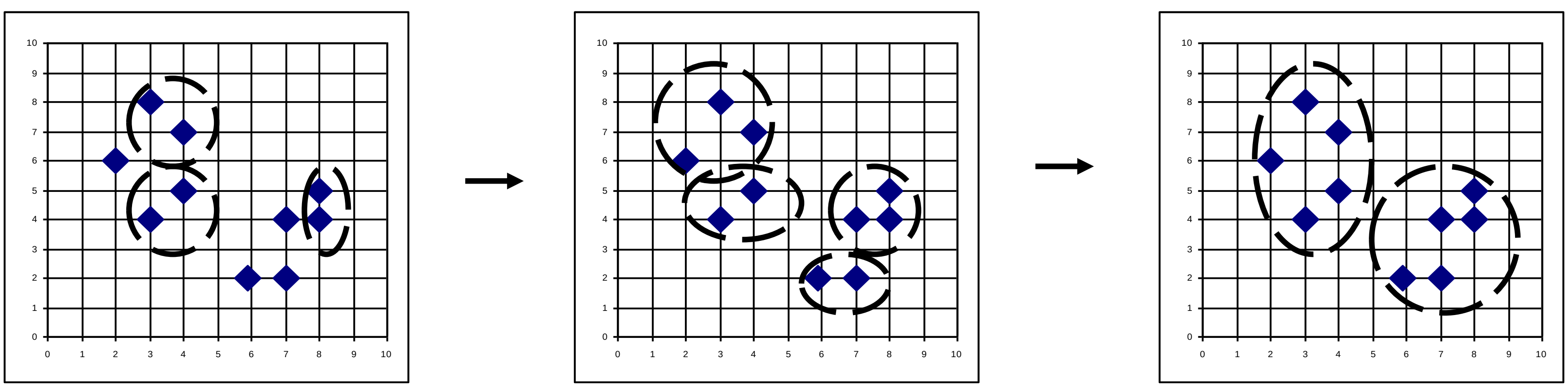
Hierarchical Clustering

- Use distance matrix as clustering criteria. This method does not require the number of clusters ***k*** as an input, but needs a termination condition



AGNES (Agglomerative Nesting)

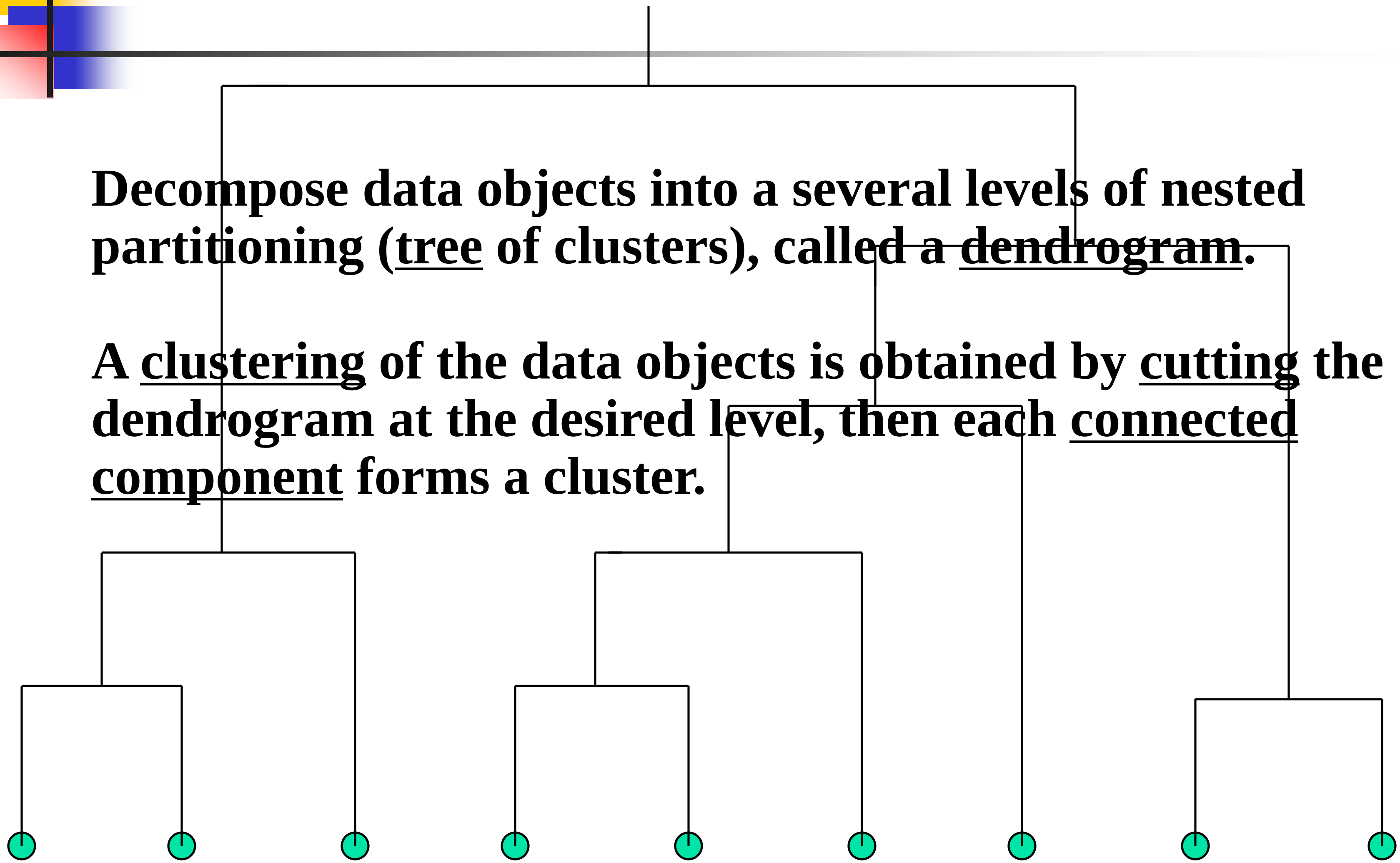
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Use the Single-Link method and the dissimilarity matrix.
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



Dendrogram: Shows How the Clusters are Merged

Decompose data objects into a several levels of nested partitioning (<u>tree</u> of clusters), called a <u>dendrogram</u>.

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.



Agglomerative Clustering Example

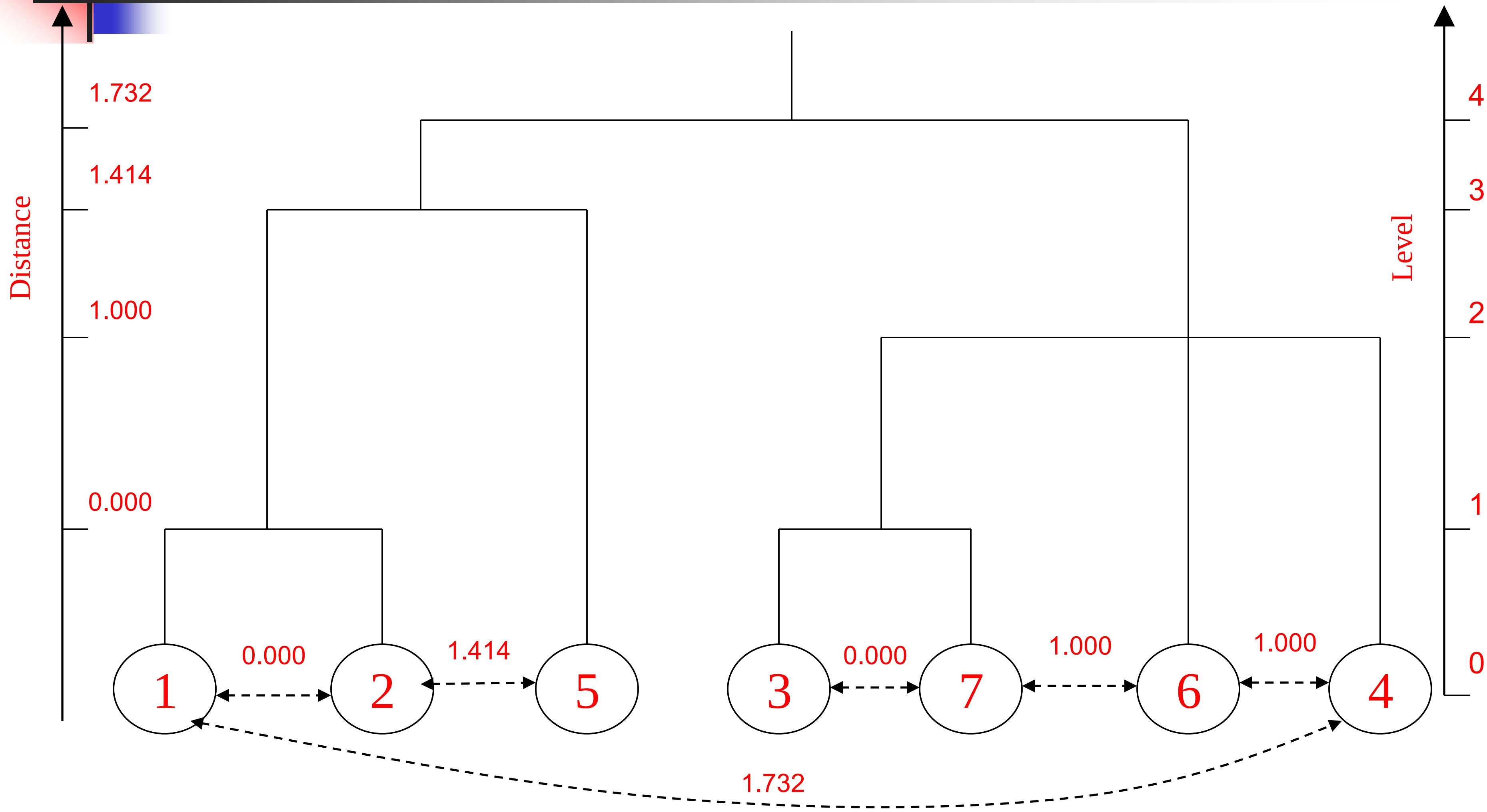
Data Objects:

Rec No	X1	X2	X3	X4	X5
1	0	0	0	0	0
2	0	0	0	0	0
3	1	1	1	1	1
4	1	0	1	0	1
5	0	1	0	1	0
6	1	0	1	1	1
7	1	1	1	1	1

Dissimilarity Matrix (Euclidean Distances):

Rec No	Dist1	Dist2	Dist3	Dist4	Dist5	Dist6	Dist7
1							
2	0.000						
3	2.236	2.236					
4	1.732	1.732	1.414				
5	1.414	1.414	1.732	2.236			
6	2.000	2.000	1.000	1.000	2.000		
7	2.236	2.236	0.000	1.414	1.732	1.000	

Agglomerative Clustering Example (cont.)



More on Hierarchical Clustering Methods

- Major weakness of agglomerative clustering methods
  - do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects
  - can never undo what was done previously
- Integration of hierarchical with distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
  - CURE (1998): selects well-scattered points from the cluster and then shrinks them towards the center of the cluster by a specified fraction
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Measure of similarity can be computed for various types of data
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- Outlier detection and analysis are very useful for fraud detection, etc. and can be performed by statistical, distance-based or deviation-based approaches
- There are still lots of research issues on cluster analysis, such as efficient clustering in big data environment

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