Unit V - Cluster Analysis

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
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Clustering: Rich Applications and Multidisciplinary Efforts

- Pattern Recognition
- Spatial Data Analysis
  - Create thematic maps in GIS by clustering feature spaces
  - Detect spatial clusters or for other spatial mining tasks
- Image Processing
- Economic Science (especially market research)
- WWW
  - Document classification
  - Cluster Weblog data to discover groups of similar access patterns

Examples of Clustering Applications

- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Land use: Identification of areas of similar land use in an earth observation database
- Insurance: Identifying groups of motor insurance policy holders with a high average claim cost
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults

Quality: 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

Measure the Quality of Clustering

- Dissimilarity/Similarity metric: Similarity is expressed in terms of a distance function, typically metric: $d(i, j)$
- There is a separate "quality" function that measures the "goodness" of a cluster.
- The definitions of distance functions are usually very different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables.
- Weights should be associated with different variables based on applications and data semantics.
- It is hard to define "similar enough" or "good enough"
  - the answer is typically highly subjective.

Requirements of Clustering in Data Mining

- Scalability
- Ability to deal with different types of attributes
- Ability to handle dynamic data
- Discovery of clusters with arbitrary shape
- Minimal requirements for domain knowledge to determine input parameters
- Able to deal with noise and outliers
- Insensitive to order of input records
- High dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability

Data Structures

- Data matrix
  - (two modes)

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

- Dissimilarity matrix
  - (one mode)

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

Type of data in clustering analysis

- Interval-scaled variables
- Binary variables
- Nominal, ordinal, and ratio variables
- Variables of mixed types

Interval-valued variables

- Standardize data
  - Calculate the mean absolute deviation:

$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + ... + |x_{nf} - m_f|)$$

where $m_f = \frac{1}{n}(x_{1f} + x_{2f} + ... + x_{nf})$.

  - 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

Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

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

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

- If $q = 1$, d is Manhattan distance

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

Similarity and Dissimilarity Between Objects (Cont.)

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

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

  - Properties
    - $d(i,j) \geq 0$
    - $d(i,i) = 0$
    - $d(i,j) = d(j,i)$
    - $d(i,j) \leq d(i,k) + d(k,j)$
- Also, one can use weighted distance, parametric Pearson product moment correlation, or other disimilarity measures

Binary Variables

- A contingency table for binary data

		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 symmetric binary variables:

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

- Distance measure for asymmetric binary variables:

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

- Jaccard coefficient (*similarity* measure for *asymmetric* 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

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

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

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

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

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

  - 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}
- 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

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

  - *f* is binary or nominal:

    $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, or $d_{ij}^{(f)} = 1$ otherwise
  - *f* is interval-based: use the normalized distance
  - *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 $\vec{X}$,

- A variant: Tanimoto coefficient $$s(\vec{X}, \vec{Y}) = \frac{\vec{X}^t \cdot \vec{Y}}{\vec{X}^t \cdot \vec{X} + \vec{Y}^t \cdot \vec{Y} - \vec{X}^t \cdot \vec{Y}},$$

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, ROCK, CAMELEON
- Density-based approach:
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue

Major Clustering Approaches (II)

- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE
- 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: pCluster
- User-guided or constraint-based:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), constrained clustering

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

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

Partitioning Algorithms: Basic Concept

- Partitioning method: Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters, s.t., min sum of squared distance

$$\sum_{m=1}^{k}\sum_{t_{mi}\in Km}(C_m - t_{mi})^2$$

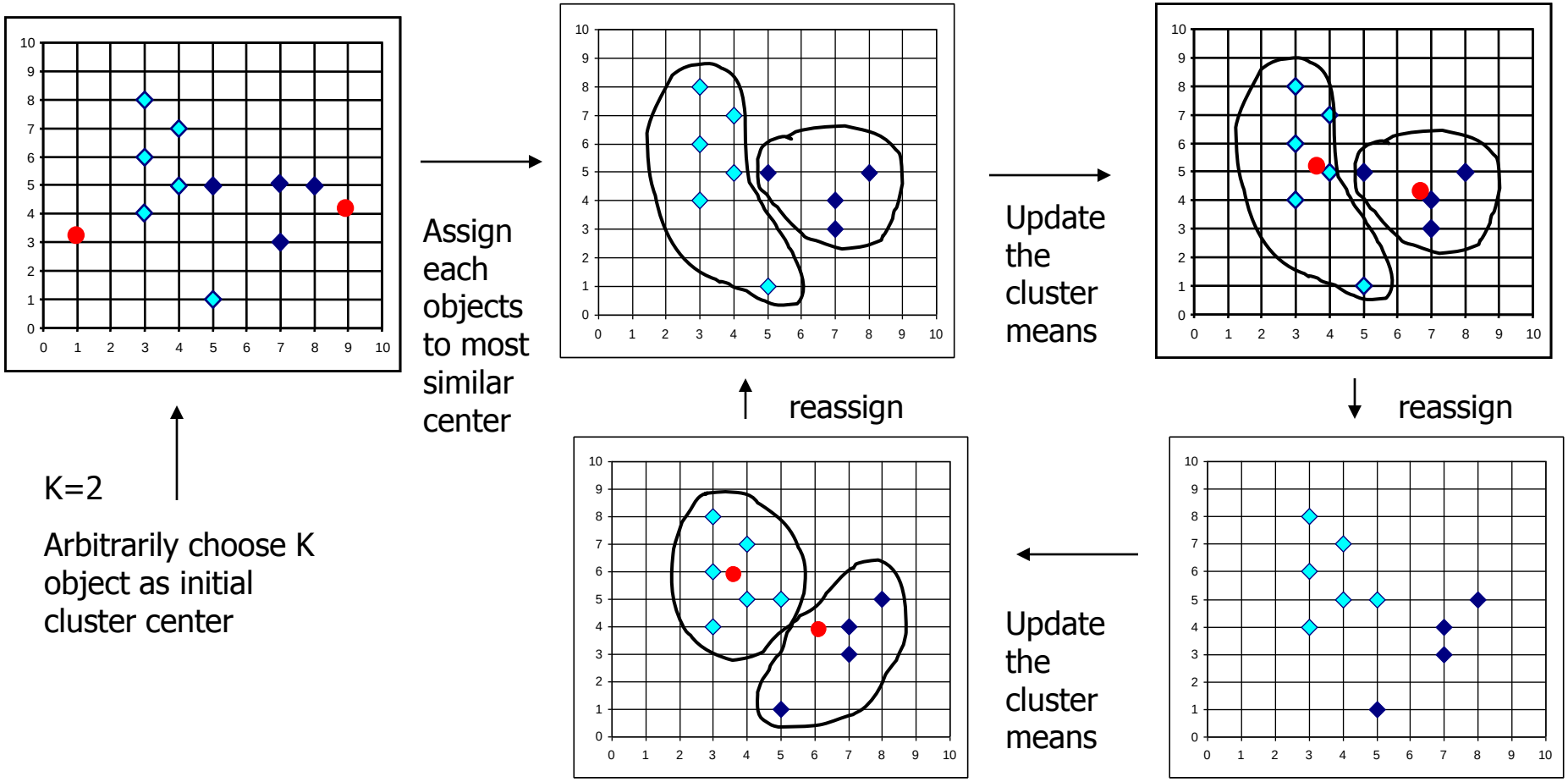
- Given a *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67): Each cluster is represented by the center of the cluster
  - *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 partition (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 no more new assignment

The *K-Means* Clustering Method

- Example



Comments on the *K-Means* Method

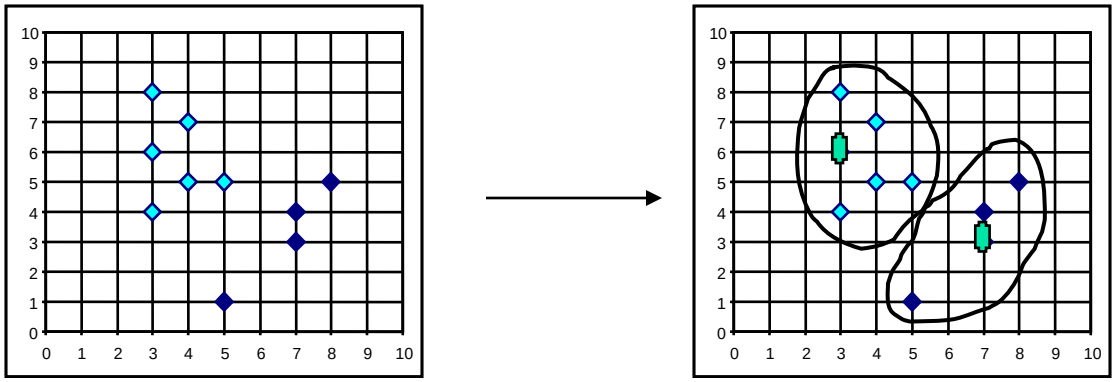
- Strength: *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t << n$.
  - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- Comment: Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Weakness
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Unable to handle 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 modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

What Is the Problem of the K-Means Method?

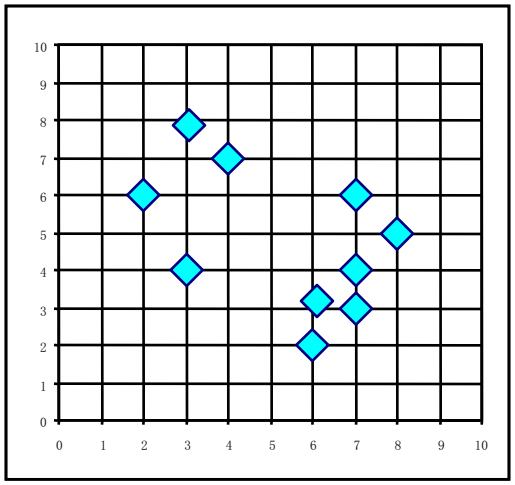
- The k-means algorithm is sensitive to outliers !
  - Since an object with an extremely large value may substantially distort the distribution of the data.
- K-Medoids: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most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



The *K-Medoids* Clustering Method

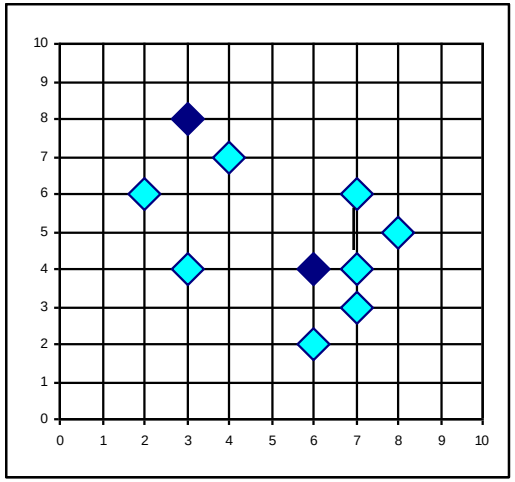
- Find *representative* objects, called medoids, in clusters
- *PAM* (Partitioning Around Medoids, 1987)
  - starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering
  - *PAM* works effectively for small data sets, but does not scale well for large data sets
- *CLARA* (Kaufmann & Rousseeuw, 1990)
- *CLARANS* (Ng & Han, 1994): Randomized sampling
- Focusing + spatial data structure (Ester et al., 1995)

A Typical K-Medoids Algorithm (PAM)



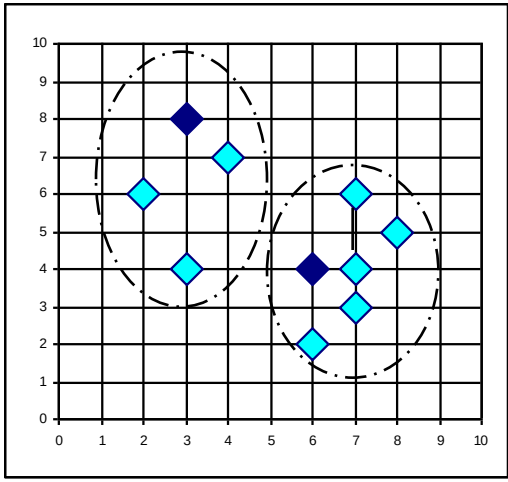
K=2

Arbitrary choose k object as initial medoids

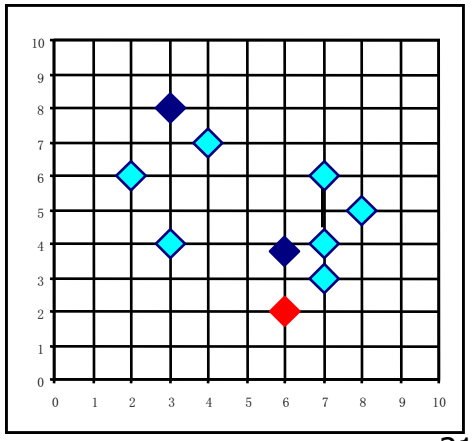


Assign each remaining object to nearest medoids

Total Cost = 20

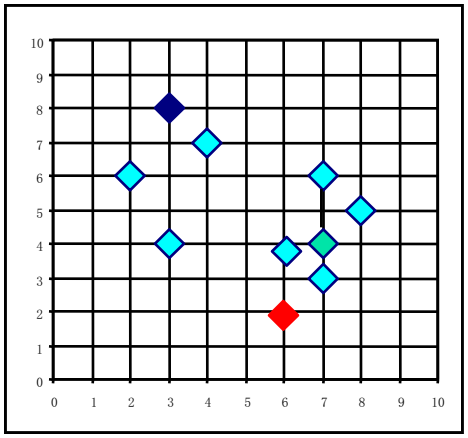


Randomly select a nonmedoid object, O_{ramdom}



Compute total cost of swapping

Total Cost = 26



Swapping O and O_{ramdom}

If quality is improved.

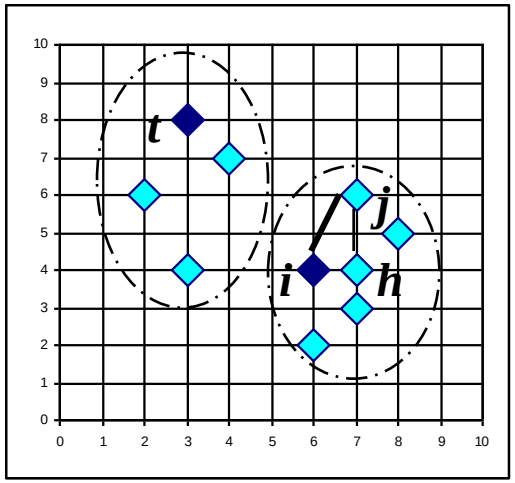
Do loop

Until no change

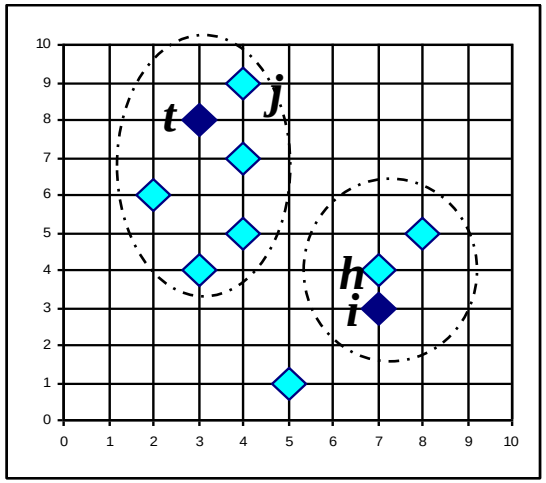
PAM (Partitioning Around Medoids) (1987)

- PAM (Kaufman and Rousseeuw, 1987), built in Splus
- Use real object to represent the cluster
  - Select ***k*** representative objects arbitrarily
  - For each pair of non-selected object ***h*** and selected object ***i***, calculate the total swapping cost TC_{ih}
  - For each pair of ***i*** and ***h***,
    - If $TC_{ih} < 0$, ***i*** is replaced by ***h***
    - Then assign each non-selected object to the most similar representative object
  - repeat steps 2-3 until there is no change

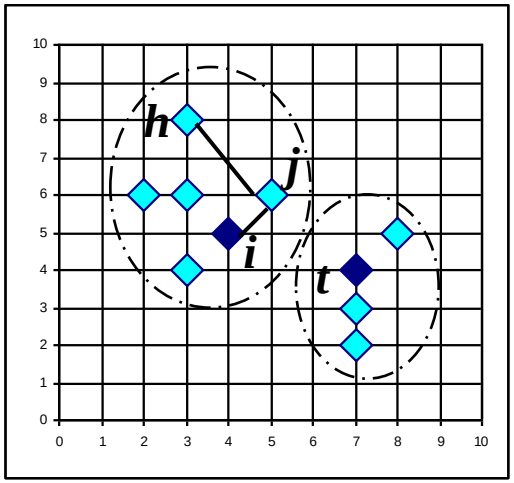
PAM Clustering: Total swapping cost $TC_{ih}=\sum_j C_{jih}$



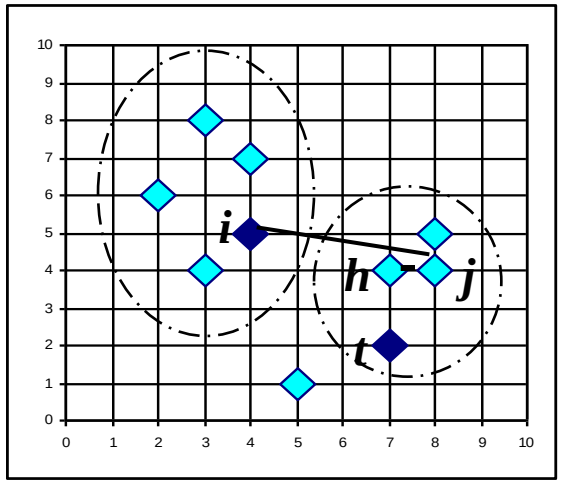
$C_{jih} = d(j, h) - d(j, i)$



$C_{jih} = 0$



$C_{jih} = d(j, t) - d(j, i)$



$C_{jih} = d(j, h) - d(j, t)$

What Is the Problem with PAM?

- Pam is more robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean
- Pam works efficiently for small data sets but does not **scale well** for large data sets.
  - $O(k(n-k)^2)$ for each iteration

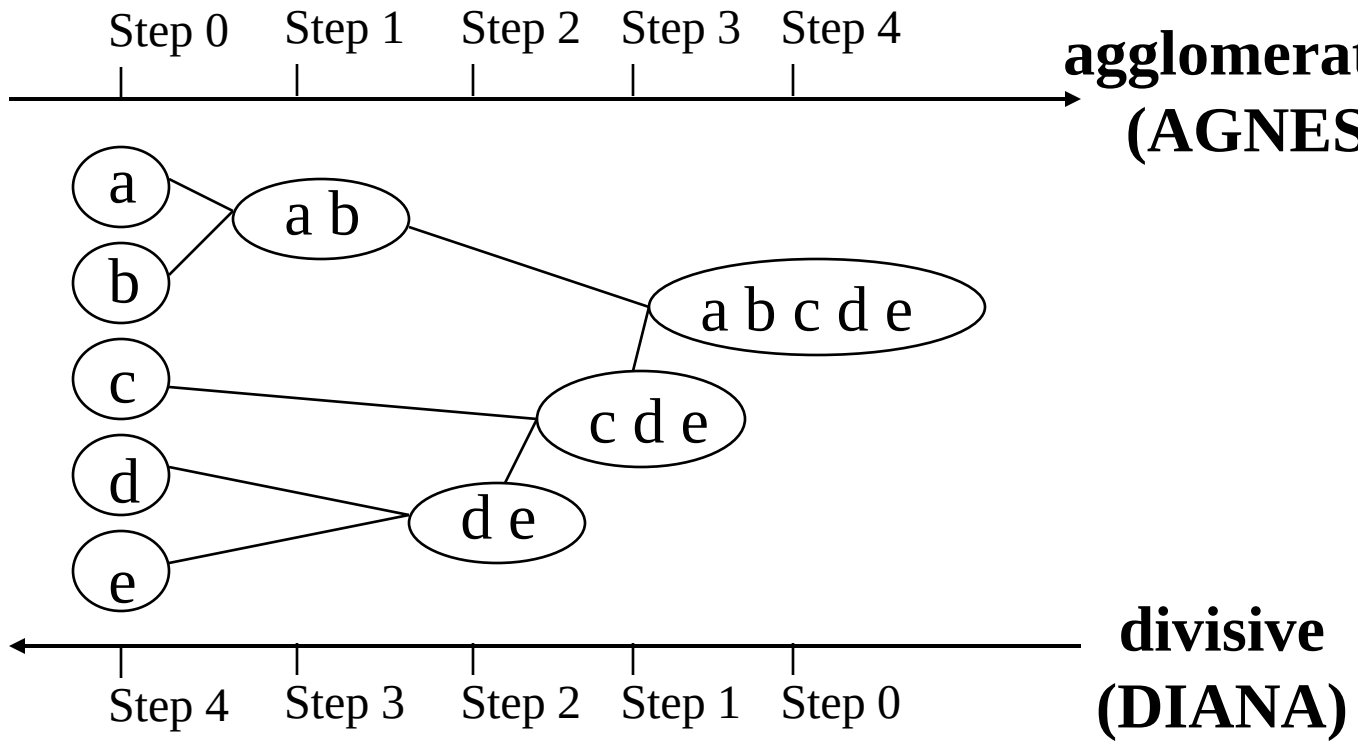
    where n is # of data,k is # of clusters

➔Sampling based method,

CLARA(Clustering LARge Applications)

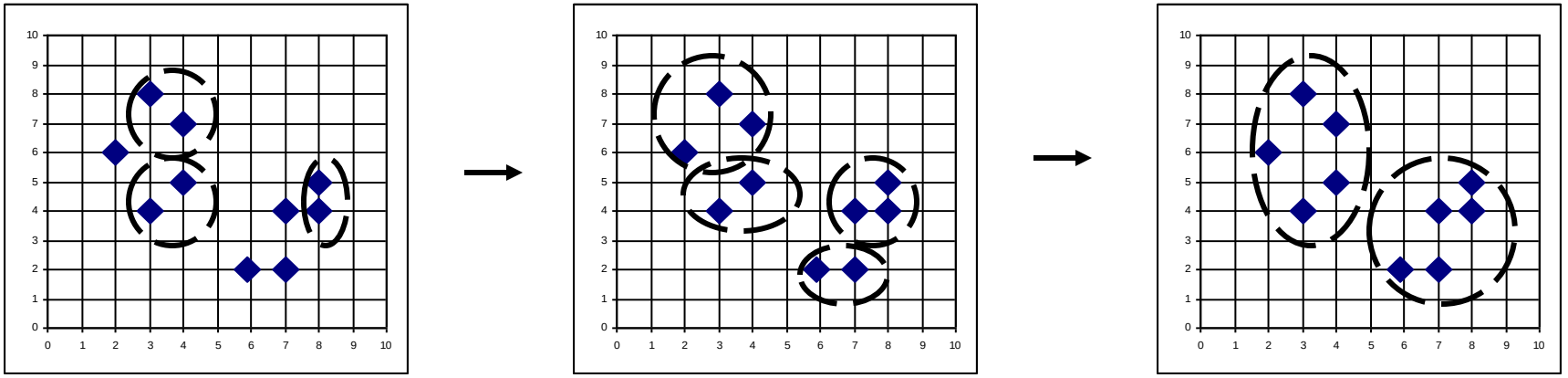
Hierarchical Clustering

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

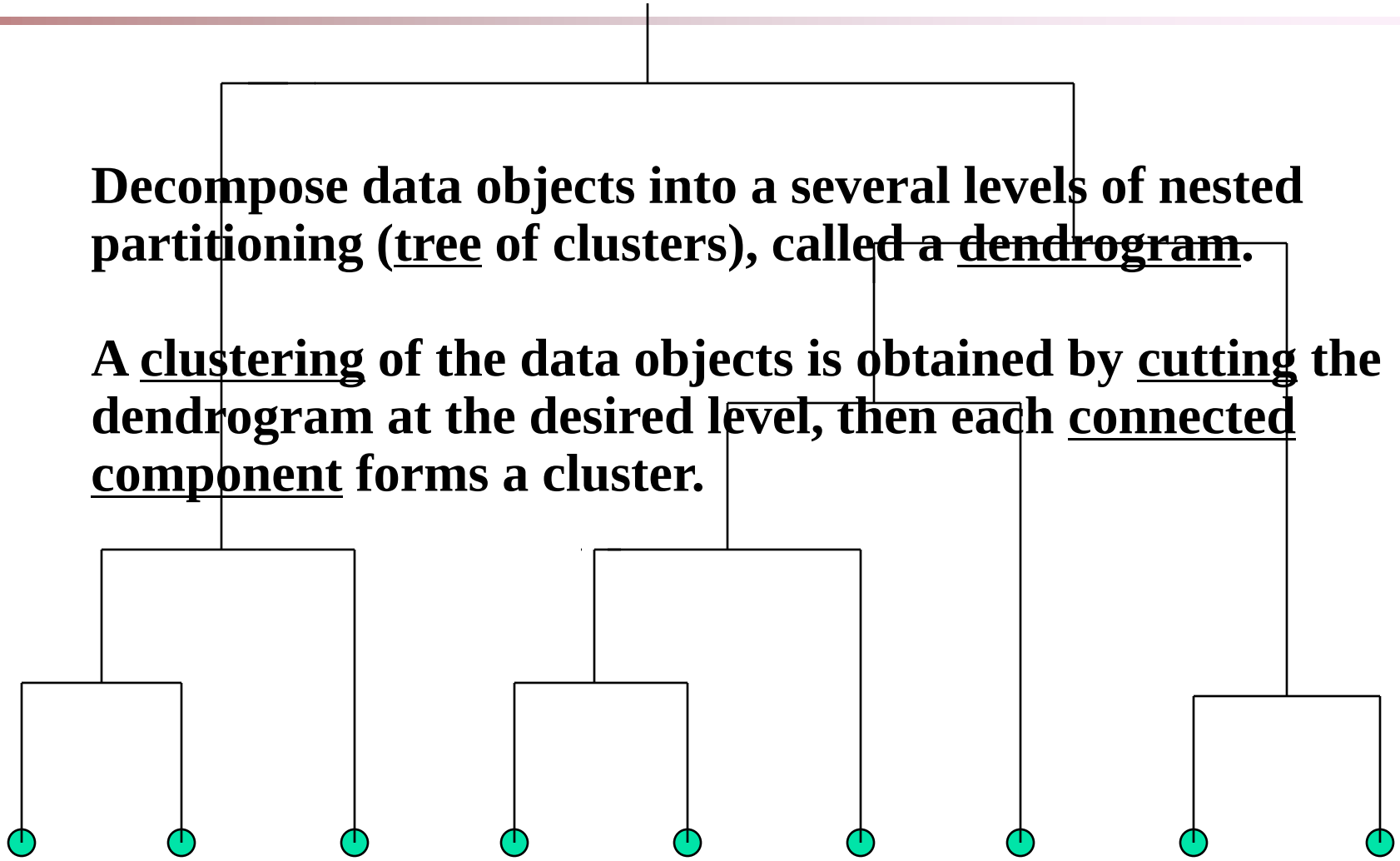


AGNES (Agglomerative Nesting)

- 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

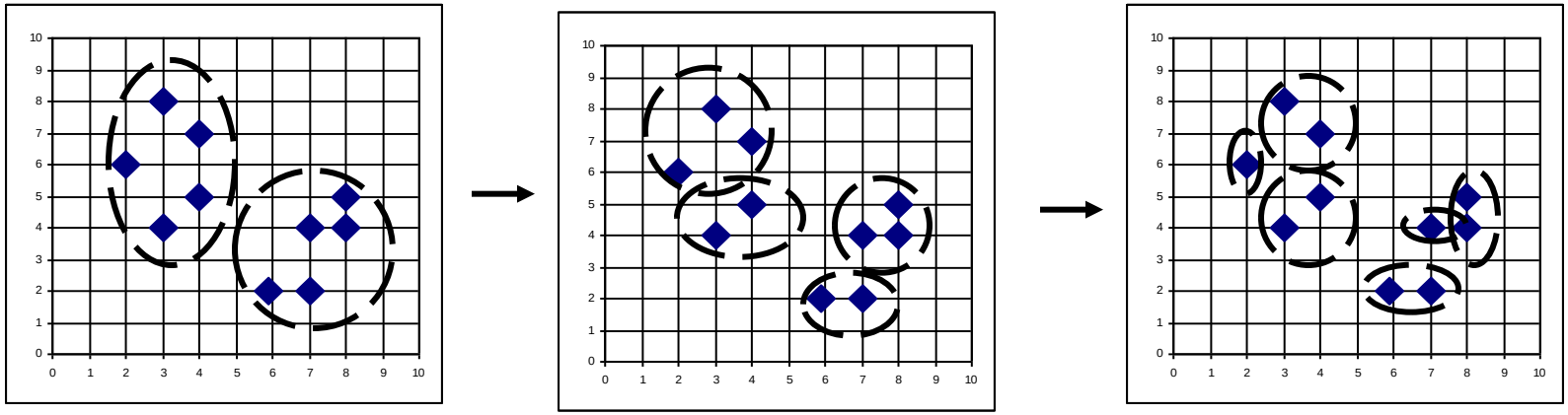


Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram.

A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster.

DIANA (Divisive Analysis)

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



Recent 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
  - ROCK (1999): clustering categorical data by neighbor and link analysis
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98) (more grid-based)

Grid-Based Clustering Method

- Using multi-resolution grid data structure
- Several interesting methods
  - STING (a STatistical INformation Grid approach) by Wang, Yang and Muntz (1997)
  - WaveCluster by Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
    - A multi-resolution clustering approach using wavelet method
  - CLIQUE: Agrawal, et al. (SIGMOD'98)
    - On high-dimensional data (thus put in the section of clustering high-dimensional data

Model-Based Clustering

- What is model-based clustering?
  - Attempt to optimize the fit between the given data and some mathematical model
  - Based on the assumption: Data are generated by a mixture of underlying probability distribution
- Typical methods
  - Statistical approach
    - EM (Expectation maximization), AutoClass
  - Machine learning approach
    - COBWEB, CLASSIT
  - Neural network approach
    - SOM (Self-Organizing Feature Map)

EM — Expectation Maximization

- EM — A popular iterative refinement algorithm
- An extension to k-means
  - Assign each object to a cluster according to a weight (prob. distribution)
  - New means are computed based on weighted measures
- General idea
  - Starts with an initial estimate of the parameter vector
  - Iteratively rescores the patterns against the mixture density produced by the parameter vector
  - The rescored patterns are used to update the parameter updates
  - Patterns belonging to the same cluster, if they are placed by their scores in a particular component
- Algorithm converges fast but may not be in global optima

The EM (Expectation Maximization) Algorithm

- Initially, randomly assign k cluster centers
- Iteratively refine the clusters based on two steps
  - Expectation step: assign each data point X_i to cluster C_i with the following probability

$$P(X_i \in C_k) = p(C_k|X_i) = \frac{p(C_k)p(X_i|C_k)}{p(X_i)},$$

  - Maximization step:
    - Estimation of model parameters

$$m_k = \frac{1}{N}\Sigma_{i=1}^{N}\frac{X_i P(X_i \in C_k)}{\Sigma_j P(X_i \in C_j)}.$$

Conceptual Clustering

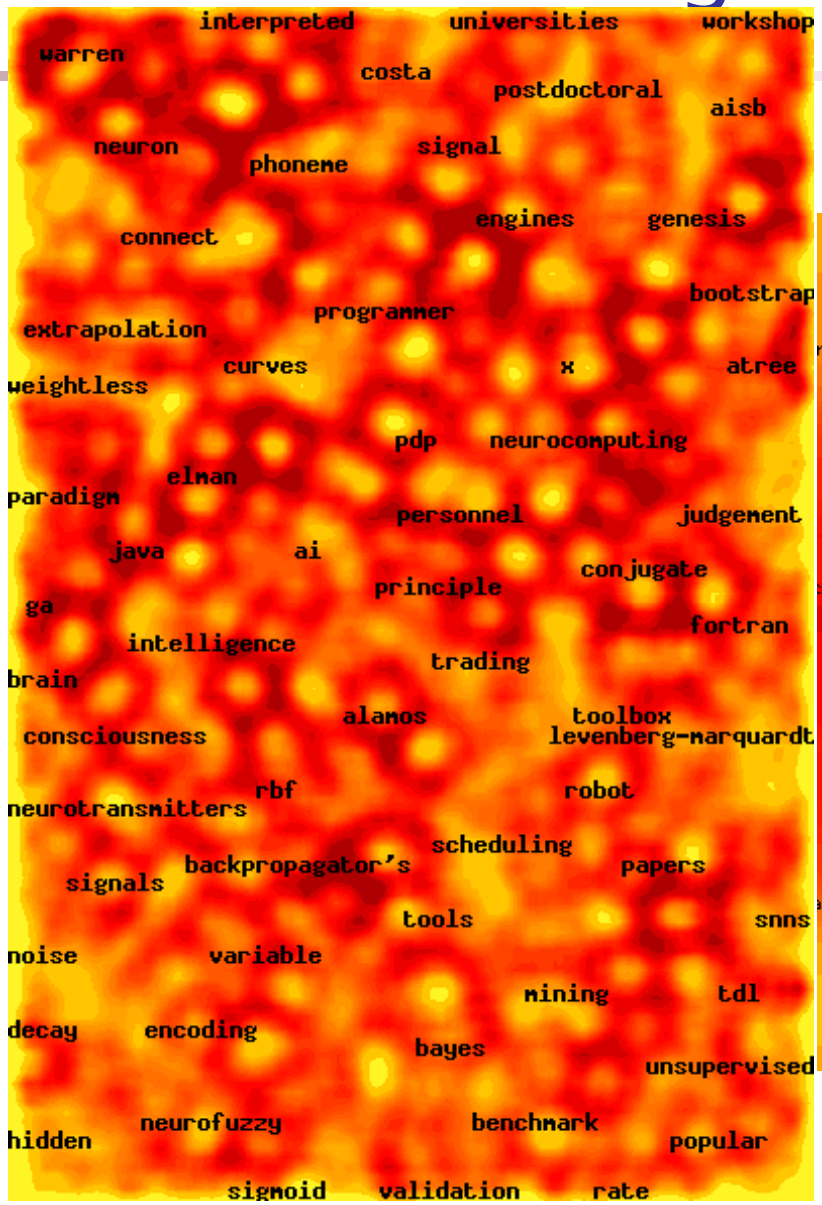
- Conceptual clustering
  - A form of clustering in machine learning
  - Produces a classification scheme for a set of unlabeled objects
  - Finds characteristic description for each concept (class)
- COBWEB (Fisher'87)
  - A popular a simple method of incremental conceptual learning
  - Creates a hierarchical clustering in the form of a classification tree
  - Each node refers to a concept and contains a probabilistic description of that concept

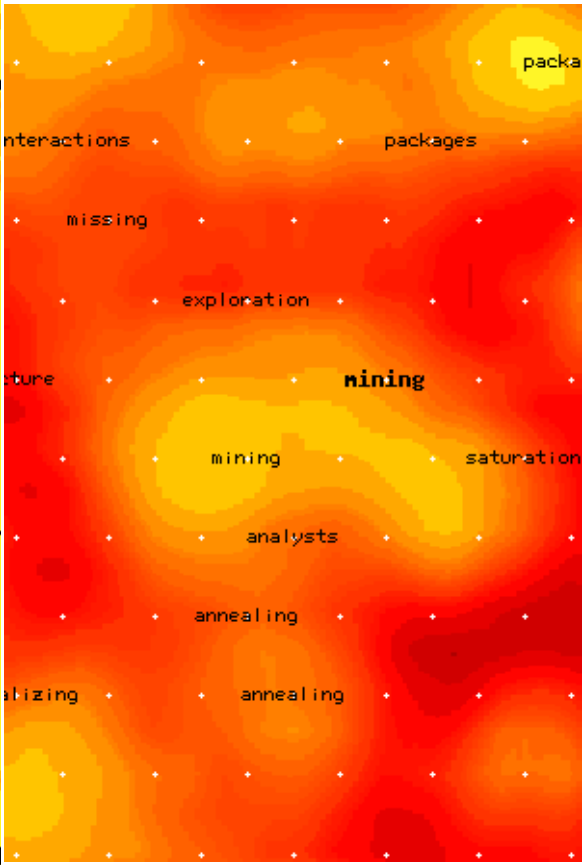
Self-Organizing Feature Map (SOM)

- SOMs, also called topological ordered maps, or Kohonen Self-Organizing Feature Map (KSOMs)
- It maps all the points in a high-dimensional source space into a 2 to 3-d target space, s.t., the distance and proximity relationship (i.e., topology) are preserved as much as possible
- Similar to k-means: cluster centers tend to lie in a low-dimensional manifold in the feature space
- Clustering is performed by having several units competing for the current object
  - The unit whose weight vector is closest to the current object wins
  - The winner and its neighbors learn by having their weights adjusted
- SOMs are believed to resemble processing that can occur in the brain
- Useful for visualizing high-dimensional data in 2- or 3-D space

Web Document Clustering Using SOM

- The result of SOM clustering of 12088 Web articles
- The picture on the right: drilling down on the keyword "mining"
- Based on websom.hut.fi Web page





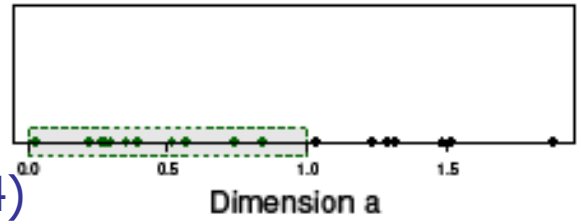
Clustering High-Dimensional Data

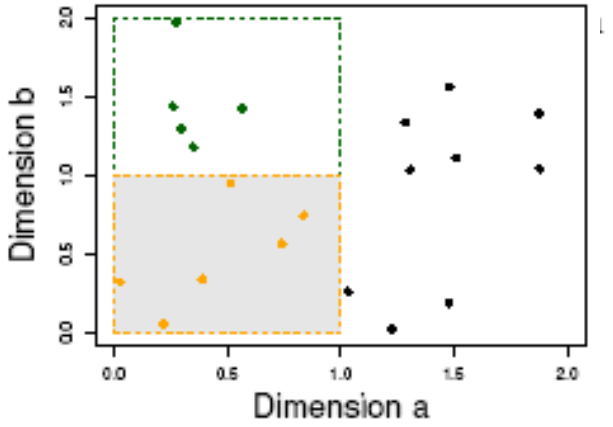
- Clustering high-dimensional data
  - Many applications: text documents, DNA micro-array data
  - Major challenges:
    - Many irrelevant dimensions may mask clusters
    - Distance measure becomes meaningless—due to equi-distance
    - Clusters may exist only in some subspaces
- Methods
  - Feature transformation: only effective if most dimensions are relevant
    - PCA & SVD useful only when features are highly correlated/redundant
  - Feature selection: wrapper or filter approaches
    - useful to find a subspace where the data have nice clusters
  - Subspace-clustering: find clusters in all the possible subspaces
    - CLIQUE, ProClus, and frequent pattern-based clustering

The Curse of Dimensionality

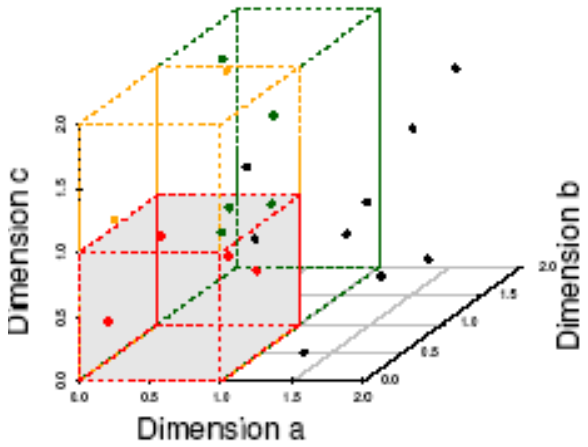
(graphs adapted from Parsons et al. KDD Explorations 2004)

- Data in only one dimension is relatively packed
- Adding a dimension "stretch" the points across that dimension, making them further apart
- Adding more dimensions will make the points further apart—high dimensional data is extremely sparse
- Distance measure becomes meaningless—due to equi-distance





(b) 6 Objects in One Unit Bin



(c) 4 Objects in One Unit Bin

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

Problems and Challenges

- Considerable progress has been made in scalable clustering methods
  - Partitioning: k-means, k-medoids, CLARANS
  - Hierarchical: BIRCH, ROCK, CHAMELEON
  - Density-based: DBSCAN, OPTICS, DenClue
  - Grid-based: STING, WaveCluster, CLIQUE
  - Model-based: EM, Cobweb, SOM
  - Frequent pattern-based: pCluster
  - Constraint-based: COD, constrained-clustering
- Current clustering techniques do not address all the requirements adequately, still an active area of research