CS490D:
Introduction to Data Mining
Prof. Chris Clifton

February 22, 2004

Clustering

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

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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

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General Applications of Clustering

- Pattern Recognition
- Spatial Data Analysis
  - create thematic maps in GIS by clustering feature spaces
  - detect spatial clusters and explain them in spatial data mining
- Image Processing
- Economic Science (especially market research)
- WWW
  - Document classification
  - Cluster Weblog data to discover groups of similar access patterns

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Examples of Clustering Applications

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

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What Is Good Clustering?

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

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Requirements of Clustering in Data Mining

- Scalability
- 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
- Insensitive to order of input records
- High dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability

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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)

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

Measure the Quality of Clustering

- Dissimilarity/Similarity metric: Similarity is expressed in terms of a distance function, which is 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 and ratio 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.

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

- <u>Distances</u> are normally used to measure the <u>similarity</u> or <u>dissimilarity</u> between two data objects

- Some popular ones include: *Minkowski distance*:

$$d(i,j) = \sqrt[q]{(|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + ... + |x_{ip} - x_{jp}|^q)}$$

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

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

$$d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + ... + |x_{ip} - x_{jp}|$$

Similarity and Dissimilarity Between Objects (Cont.)

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

$$d(i,j) = \sqrt{(|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + ... + |x_{ip} - x_{jp}|^2)}$$

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

- Simple matching coefficient (invariant, if the binary variable is _symmetric_):

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

- Jaccard coefficient (noninvariant if the binary variable is _asymmetric_):

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

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 $\quad r_{if} \in \{1,..., M_f\}$
  - 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

- <u>Ratio-scaled variable</u>: 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 $d_{ij}^{(f)} = 1$ o.w.
  - 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 $z_{if} = \dfrac{r_{if} - 1}{M_f - 1}$

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Major Clustering Approaches

- <u>Partitioning algorithms</u>: Construct various partitions and then evaluate them by some criterion
- <u>Hierarchy algorithms</u>: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- <u>Density-based</u>: based on connectivity and density functions
- <u>Grid-based</u>: based on a multiple-level granularity structure
- <u>Model-based</u>: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

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Partitioning Algorithms: Basic Concept

- <u>Partitioning method:</u> Construct a partition of a database **D** of **n** objects into a set of **k** clusters

- 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

Assign each objects to most similar center

Update the cluster means

reassign

Update the cluster means

reassign

K=2

Arbitrarily choose K object as initial cluster center
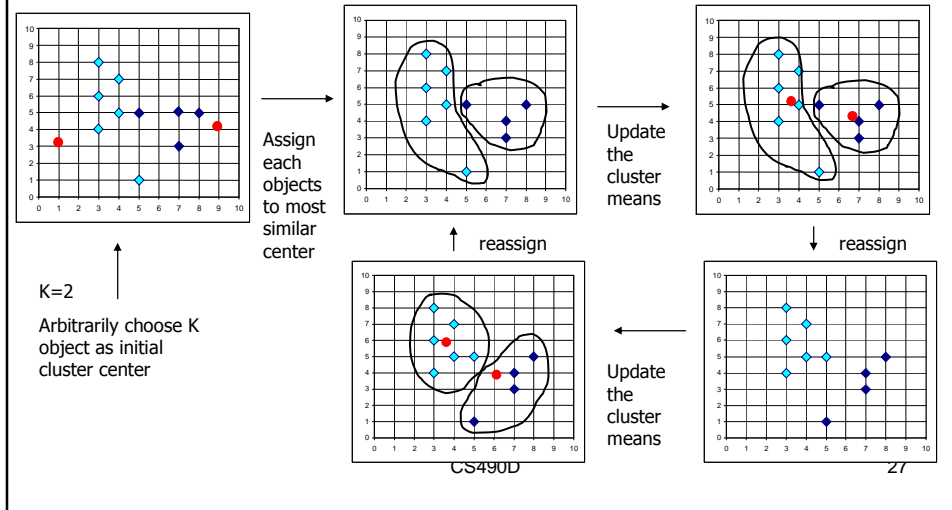
Comments on the *K-Means* Method

- <u>Strength</u>: *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: $O(ks^2 + k(n-k))$
- <u>Comment:</u> Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- <u>Weakness</u>
    - 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 <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

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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.
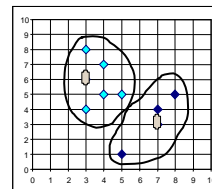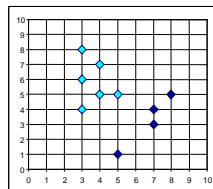
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The *K-Medoids* Clustering Method

- Find *representative* objects, called <u>medoids</u>, 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)

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Typical k-medoids algorithm (PAM)

Total Cost = 20

K=2

Do loop

Until no change

Arbitrary choose k object as initial medoids

Assign each remaining object to nearest medoids

Randomly select a nonmedoid object, O_{ramdom}

Total Cost = 26

Swapping O and O_{ramdom}

If quality is improved.

Compute total cost of swapping
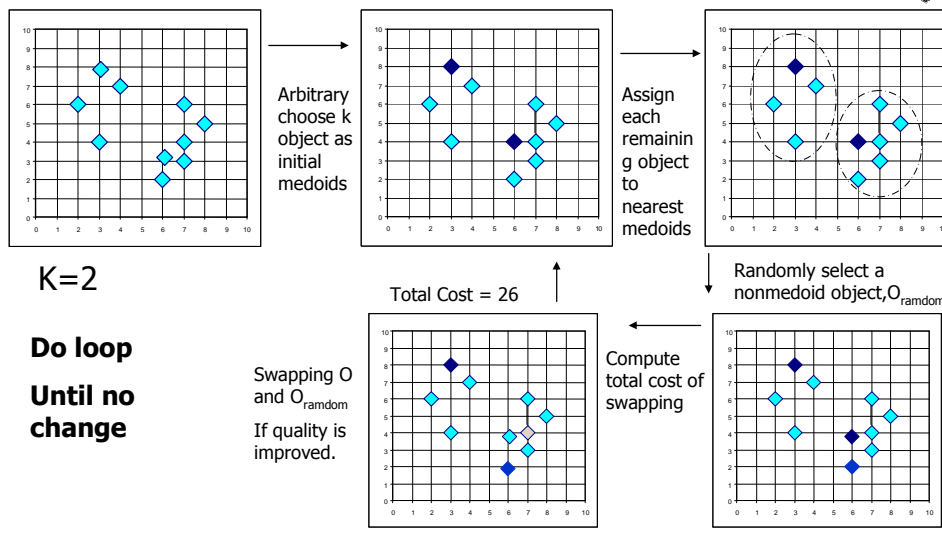
PAM (Partitioning Around Medoids) (1987)

- 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 $TC_{ih}=\Sigma_j C_{jih}$
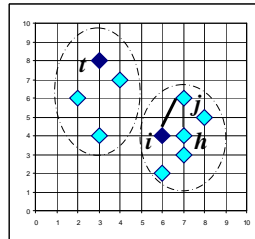
$C_{jih} = d(j, h) - d(j, i)$
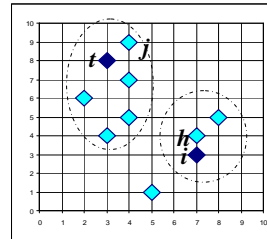
$C_{jih} = 0$
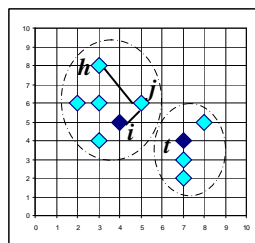
$C_{jih} = d(j, t) - d(j, i)$
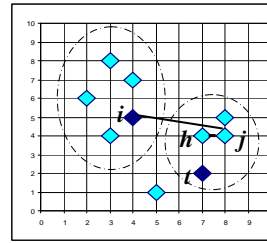
$C_{jih} = d(j, h) - d(j, t)$

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)

CLARA (Clustering Large Applications) (1990)

- *CLARA* (Kaufmann and Rousseeuw in 1990)
    - Built in statistical analysis packages, such as S+
- It draws *multiple samples* of the data set, applies *PAM* on each sample, and gives the best clustering as the output
- Strength: deals with larger data sets than *PAM*
- Weakness:
    - Efficiency depends on the sample size
    - A good clustering based on samples will not necessarily represent a good clustering of the whole data set if the sample is biased

CLARANS ("Randomized" CLARA) *(1994)*

- *CLARANS* (A Clustering Algorithm based on Randomized Search) (Ng and Han'94)
- CLARANS draws sample of neighbors dynamically
- The clustering process can be presented as searching a graph where every node is a potential solution, that is, a set of k medoids
- If the local optimum is found, *CLARANS* starts with new randomly selected node in search for a new local optimum
- It is more efficient and scalable than both *PAM* and *CLARA*
- Focusing techniques and spatial access structures may further improve its performance (Ester et al.'95)

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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

Step 0   Step 1   Step 2   Step 3   Step 4   **agglomerative**
                                                  (AGNES)

a
  a b
b
            a b c d e
c
      c d e
d
   d e
e

divisive
Step 4   Step 3   Step 2   Step 1   Step 0   **(DIANA)**
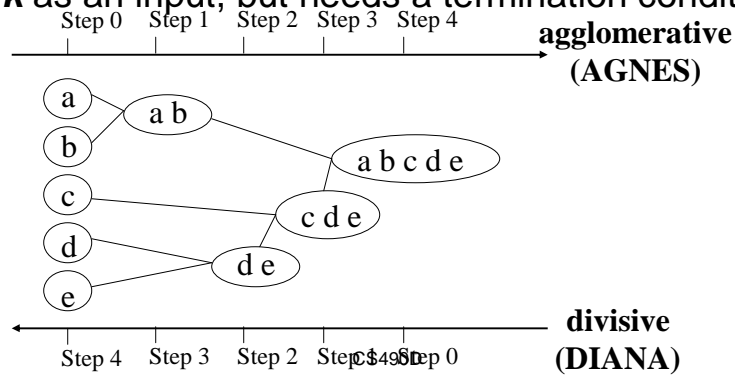
AGNES (Agglomerative Nesting)

- 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

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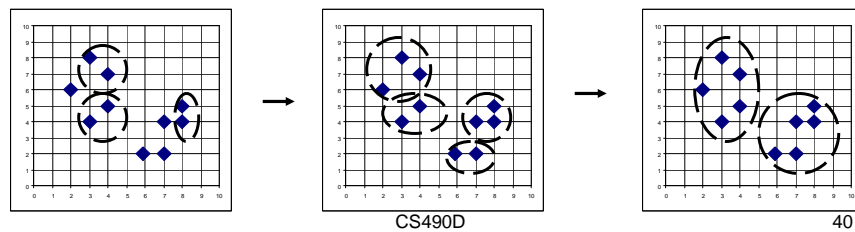
A Dendrogram Shows How the Clusters are Merged Hierarchically

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.
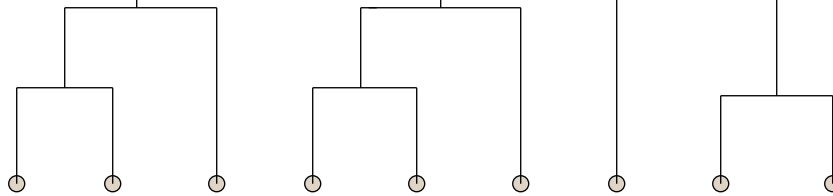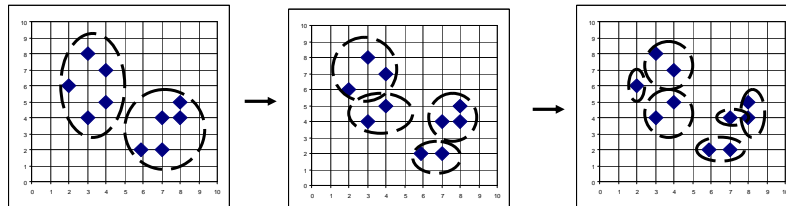
DIANA (Divisive Analysis)

- 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

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March 1, 2004
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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

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BIRCH (1996)

- Birch: Balanced Iterative Reducing and Clustering using Hierarchies, by Zhang, Ramakrishnan, Livny (SIGMOD'96)
- Incrementally construct a CF (Clustering Feature) tree, a hierarchical data structure for multiphase clustering
    - Phase 1: scan DB to build an initial in-memory CF tree (a multi-level compression of the data that tries to preserve the inherent clustering structure of the data)
    - Phase 2: use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree
- *Scales linearly*: finds a good clustering with a single scan and improves the quality with a few additional scans
- *Weakness:* handles only numeric data, and sensitive to the order of the data record.

Clustering Feature Vector

Clustering Feature: $CF = (N, \vec{LS}, SS)$

N: **Number of data points**

$LS: \sum^{N}_{i=1} = \vec{X_i}$

$SS: \sum^{N}_{i=1} = \vec{X_i}^2$
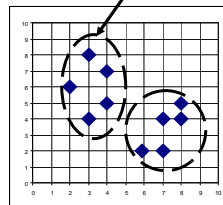
$CF = (5, (16,30),(54,190))$

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

CF-Tree in BIRCH

- Clustering feature:
  - summary of the statistics for a given subcluster: the 0-th, 1st and 2nd moments of the subcluster from the statistical point of view.
  - registers crucial measurements for computing cluster and utilizes storage efficiently
- A CF tree is a height-balanced tree that stores the clustering features for a hierarchical clustering
  - A nonleaf node in a tree has descendants or "children"
  - The nonleaf nodes store sums of the CFs of their children
- A CF tree has two parameters
  - Branching factor: specify the maximum number of children.
  - threshold: max diameter of sub-clusters stored at the leaf nodes

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CF Tree

Root

$B = 7$

$L = 6$

CF_1	CF_2	CF_3	......	CF_6
child$_1$	child$_2$	child$_3$		child$_6$

Non-leaf node

CF_1	CF_2	CF_3	......	CF_5
child$_1$	child$_2$	child$_3$		child$_5$

....

Leaf node   Leaf node

prev	CF_1	CF_2	......	CF_6	next

prev	CF_1	CF_2	......	CF_4	next
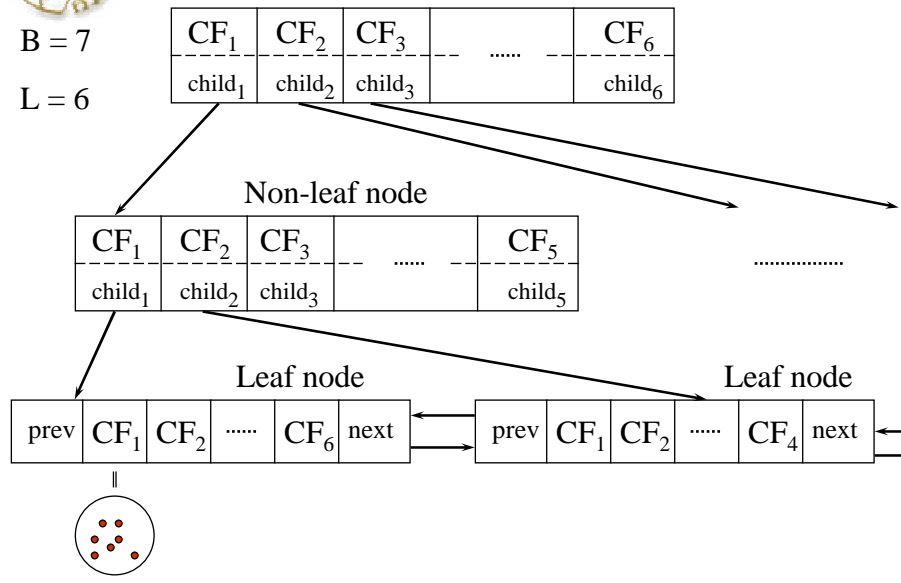
CURE (Clustering Using REpresentatives)
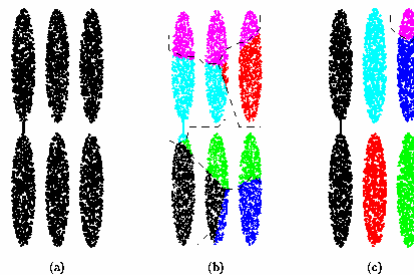

(a)   (b)
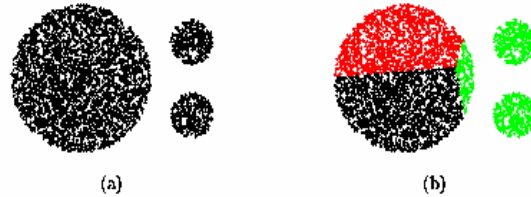
- CURE: proposed by Guha, Rastogi & Shim, 1998
  - Stops the creation of a cluster hierarchy if a level consists of k clusters
  - Uses multiple representative points to evaluate the distance between clusters, adjusts well to arbitrary shaped clusters and avoids single-link effect

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Drawbacks of Distance-Based Method

(a)   (b)   (c)

- Drawbacks of square-error based clustering method
  - Consider only one point as representative of a cluster
  - Good only for convex shaped, similar size and density, and if k can be reasonably estimated

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Cure: The Algorithm

- Draw random sample *s*.
- Partition sample to *p* partitions with size *s/p*
- Partially cluster partitions into *s/pq* clusters
- Eliminate outliers
  - By random sampling
  - If a cluster grows too slow, eliminate it.
- Cluster partial clusters.
- Label data in disk

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Data Partitioning and Clustering

- s = 50
- p = 2
- s/p = 25

■s/pq = 5

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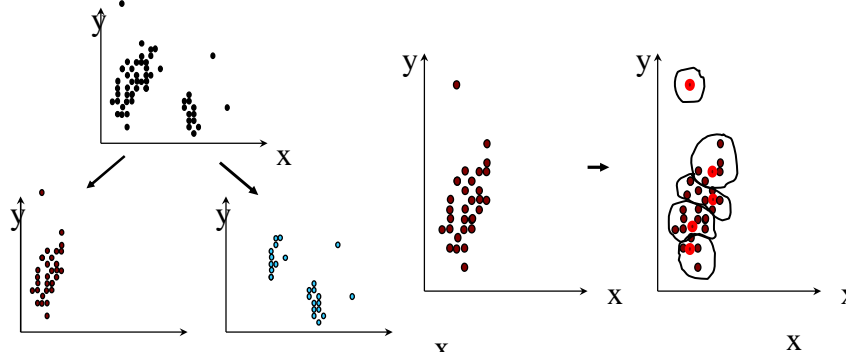
Cure: Shrinking Representative Points
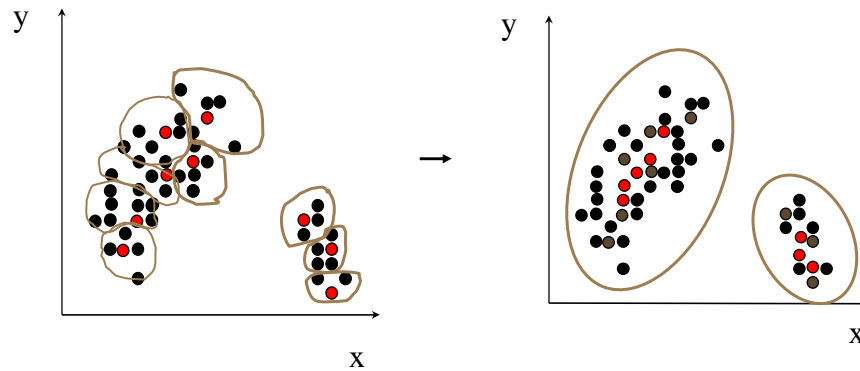
- Shrink the multiple representative points towards the gravity center by a fraction of α.
- Multiple representatives capture the shape of the cluster

Clustering Categorical Data: ROCK

- ROCK: Robust Clustering using linKs, by S. Guha, R. Rastogi, K. Shim (ICDE'99).
    - Use links to measure similarity/proximity
    - Not distance based
    - Computational complexity: $O(n^2 + nm_m m_a + n^2 \log n)$
- Basic ideas:
    - Similarity function and neighbors: $Sim(T_1, T_2) = \dfrac{|T_1 \cap T_2|}{|T_1 \cup T_2|}$

      Let $T_1 = \{1,2,3\}$, $T_2 = \{3,4,5\}$

$$Sim(T1, T2) = \frac{|\{3\}|}{|\{1,2,3,4,5\}|} = \frac{1}{5} = 0.2$$

Rock: Algorithm

- Links: The number of common neighbours for the two points.

$$\{1,2,3\}, \{1,2,4\}, \{1,2,5\}, \{1,3,4\}, \{1,3,5\}$$
$$\{1,4,5\}, \{2,3,4\}, \{2,3,5\}, \{2,4,5\}, \{3,4,5\}$$

$$\{1,2,3\} \xleftarrow{\quad 3 \quad} \{1,2,4\}$$

- Algorithm
  - Draw random sample
  - Cluster with links
  - Label data in disk

CHAMELEON (Hierarchical clustering using dynamic modeling)

- CHAMELEON: by G. Karypis, E.H. Han, and V. Kumar'99

- Measures the similarity based on a dynamic model
  - Two clusters are merged only if the *interconnectivity* and *closeness (proximity)* between two clusters are high *relative to* the internal interconnectivity of the clusters and closeness of items within the clusters
  - **Cure** ignores information about **interconnectivity** of the objects, **Rock** ignores information about the **closeness** of two clusters

- A two-phase algorithm
  1. Use a graph partitioning algorithm: cluster objects into a large number of relatively small sub-clusters
  2. Use an agglomerative hierarchical clustering algorithm: find the genuine clusters by repeatedly combining these sub-clusters

Overall Framework of CHAMELEON
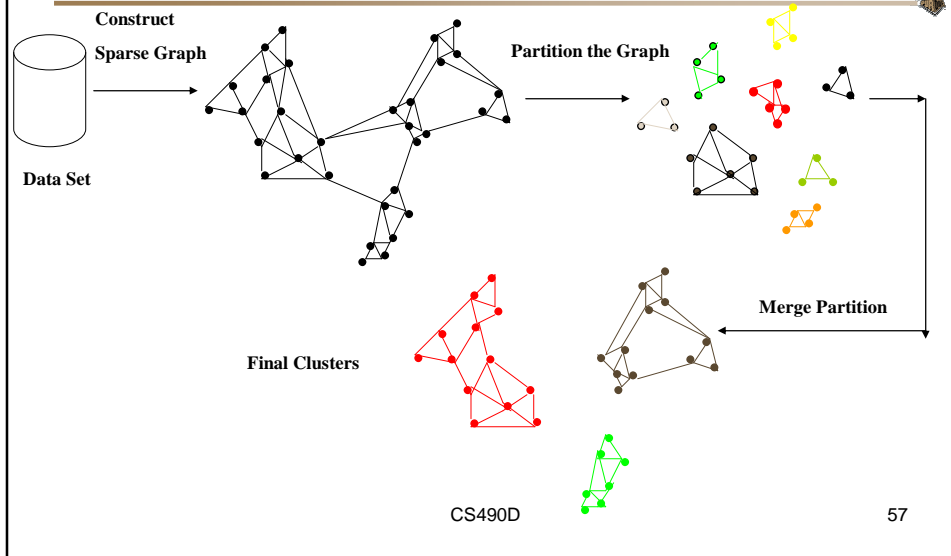
Construct
Sparse Graph

Data Set

Partition the Graph

Merge Partition

Final Clusters

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Cluster Analysis

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

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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)

Density Concepts

- Core object (CO)–object with at least 'M' objects within a radius 'E-neighborhood'

- Directly density reachable (DDR)–x is CO, y is in x's 'E-neighborhood'

- Density reachable–there exists a chain of DDR objects from x to y

- Density based cluster–density connected objects maximum w.r.t. reachability

Density-Based Clustering: Background

- Two parameters**:**
  - **Eps**: Maximum radius of the neighbourhood
  - **MinPts**: Minimum number of points in an Eps-neighbourhood of that point
- **$N_{Eps}(p)$:   {q belongs to D | dist(p,q) <= Eps}**
- Directly density-reachable**:** A point **p** is directly density-reachable from a point **q** wrt. **Eps**, **MinPts** if
  - 1) **p** belongs to $N_{Eps}(q)$
  - 2) core point condition:

    $|N_{Eps}(q)|$ >= **MinPts**

p

q
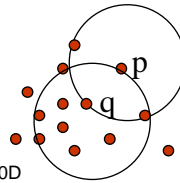
MinPts = 5

Eps = 1 cm

Density-Based Clustering: Background (II)

- Density-reachable:
  - A point *p* is density-reachable from a point *q* wrt. *Eps*, *MinPts* if there is a chain of points p_1, ..., p_n, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i

p

p_1

q

- Density-connected
  - A point *p* is density-connected to a point *q* wrt. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* wrt. *Eps* and *MinPts.*

p

q

o
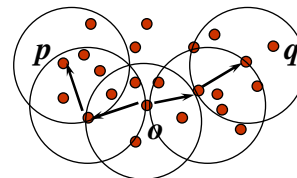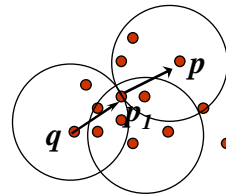
DBSCAN: Density Based Spatial Clustering of Applications with Noise

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise

Outlier

Border

Core

Eps = 1cm
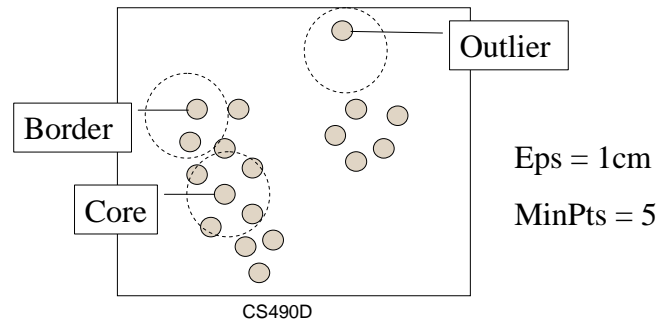
MinPts = 5

DBSCAN: The Algorithm

– Arbitrary select a point *p*

– Retrieve all points density-reachable from *p* wrt *Eps* and *MinPts*.

– If *p* is a core point, a cluster is formed.

– If *p* is a border point, no points are density-reachable from *p* and DBSCAN visits the next point of the database.

– Continue the process until all of the points have been processed.

OPTICS: A Cluster-Ordering Method (1999)

- OPTICS: Ordering Points To Identify the Clustering Structure
  - Ankerst, Breunig, Kriegel, and Sander (SIGMOD'99)
  - Produces a special order of the database wrt its density-based clustering structure
  - This cluster-ordering contains info equiv to the density-based clusterings corresponding to a broad range of parameter settings
  - Good for both automatic and interactive cluster analysis, including finding intrinsic clustering structure
  - Can be represented graphically or using visualization techniques

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OPTICS: Some Extension from DBSCAN

- Index-based:
  - k = number of dimensions
  - N = 20
  - p = 75%
  - M = N(1-p) = 5
  - Complexity: O(kN^2)
- Core Distance

- Reachability Distance

Max (core-distance (o), d (o, p))

r(p1, o) = 2.8cm. r(p2,o) = 4cm

D

p1

o

p2

o

MinPts = 5

ε = 3 cm

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Reachability
-distance

undefined

ε

ε

ε'

Cluster-order
of the objects
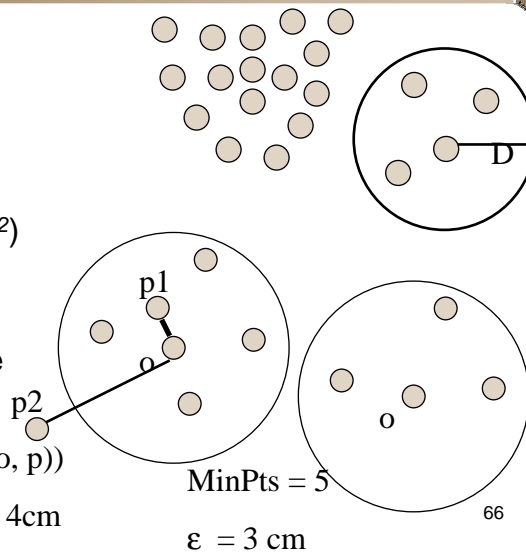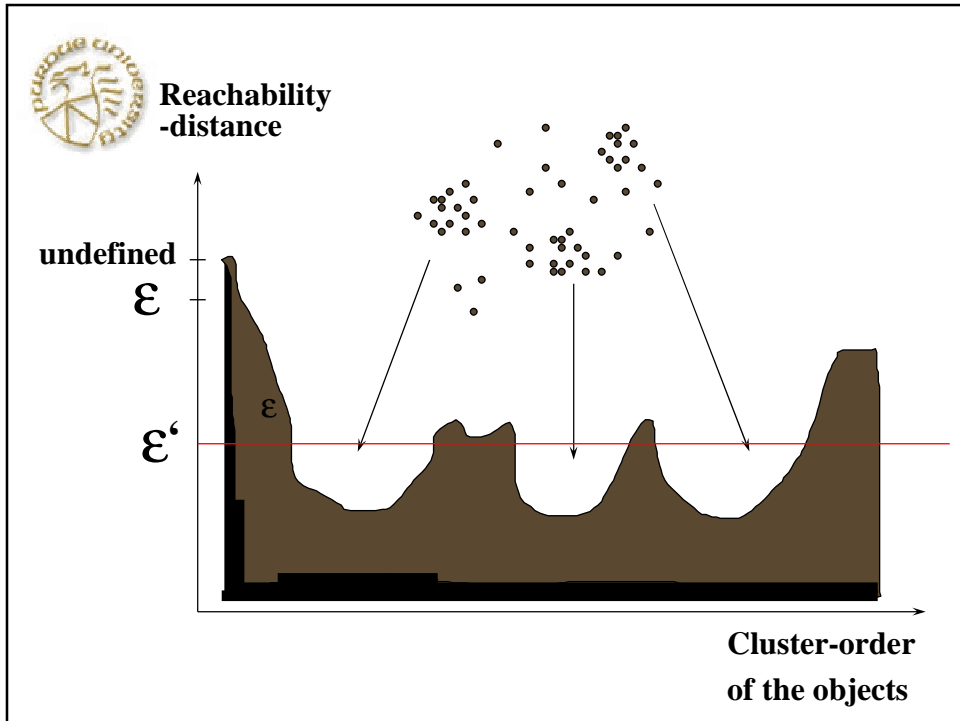
Density-Based Cluster analysis:
OPTICS & Its Applications

DENCLUE: Using density functions

- DENsity-based CLUstEring by Hinneburg & Keim (KDD'98)

- Major features
  - Solid mathematical foundation
  - Good for data sets with large amounts of noise
  - Allows a compact mathematical description of arbitrarily shaped clusters in high-dimensional data sets
  - Significant faster than existing algorithm (faster than DBSCAN by a factor of up to 45)
  - But needs a large number of parameters

Denclue: Technical Essence

- Uses grid cells but only keeps information about grid cells that do actually contain data points and manages these cells in a tree-based access structure.
- Influence function: describes the impact of a data point within its neighborhood.
- Overall density of the data space can be calculated as the sum of the influence function of all data points.
- Clusters can be determined mathematically by identifying density attractors.
- Density attractors are local maximal of the overall density function.

Gradient: The steepness of a slope

- Example

$$f_{Gaussian}(x,y) = e^{-\frac{d(x,y)^2}{2\sigma^2}}$$

$$f_{Gaussian}^{D}(x) = \sum_{i=1}^{N} e^{-\frac{d(x,x_i)^2}{2\sigma^2}}$$

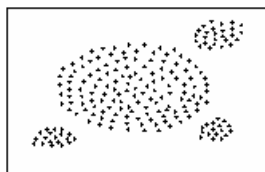$$\nabla f_{Gaussian}^{D}(x,x_i) = \sum_{i=1}^{N} (x_i - x) \cdot e^{-\frac{d(x,x_i)^2}{2\sigma^2}}$$
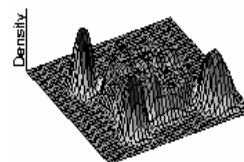
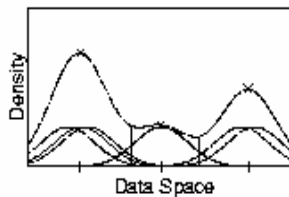CS490D   71

Density Attractor
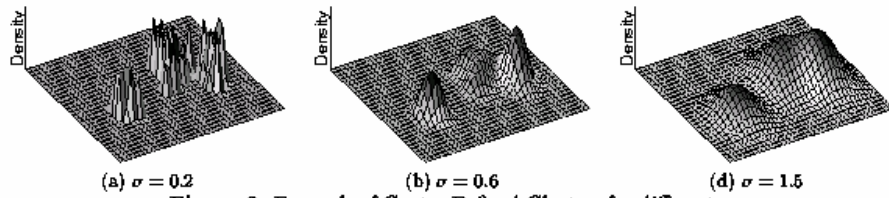

(a) Data Set

(c) Gaussian

Density

Data Space

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Center-Defined and Arbitrary

(a) σ = 0.2   (b) σ = 0.6   (d) σ = 1.5

Figure 3: Example of Center-Defined Clusters for different σ

(a) ξ = 2   (b) ξ = 2   (c) ξ = 1   (d) ξ = 1
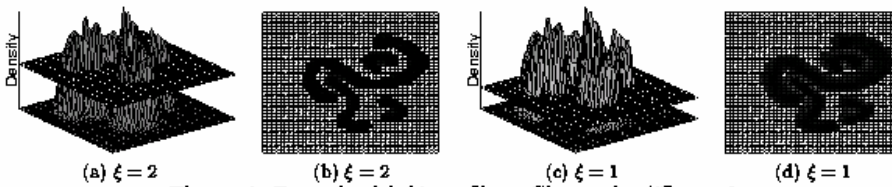
Figure 4: Example of Arbitray-Shape Clusters for different ξ

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PURDUE
UNIVERSITY

CS490D:
Introduction to Data Mining
Prof. Chris Clifton

March 5, 2004

Clustering

Cluster Analysis

- What is Cluster Analysis?
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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
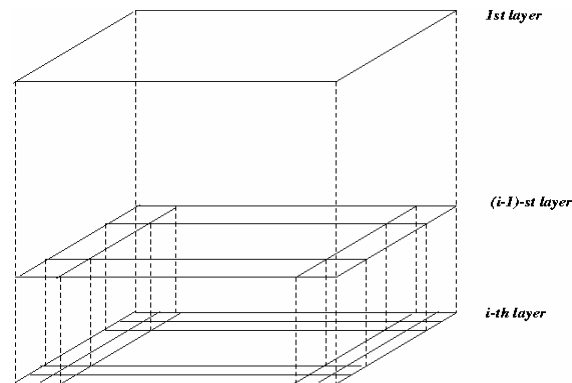 - CLIQUE: Agrawal, et al. (SIGMOD'98)

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STING: A Statistical Information Grid Approach

- Wang, Yang and Muntz (VLDB'97)
- The spatial area area is divided into rectangular cells
- There are several levels of cells corresponding to different levels of resolution

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STING: A Statistical Information Grid Approach (2)

- Each cell at a high level is partitioned into a number of smaller cells in the next lower level
- Statistical info of each cell is calculated and stored beforehand and is used to answer queries
- Parameters of higher level cells can be easily calculated from parameters of lower level cell
  - *count*, *mean*, *s*, *min*, *max*
  - type of distribution—normal, *uniform*, etc.
- Use a top-down approach to answer spatial data queries
- Start from a pre-selected layer—typically with a small number of cells
- For each cell in the current level compute the confidence interval

STING: A Statistical Information Grid Approach (3)

- Remove the irrelevant cells from further consideration
- When finish examining the current layer, proceed to the next lower level
- Repeat this process until the bottom layer is reached
- Advantages:
  - Query-independent, easy to parallelize, incremental update
  - $O(K)$, where K is the number of grid cells at the lowest level
- Disadvantages:
  - All the cluster boundaries are either horizontal or vertical, and no diagonal boundary is detected

WaveCluster (1998)

- Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
- A multi-resolution clustering approach which applies wavelet transform to the feature space
  - A wavelet transform is a signal processing technique that decomposes a signal into different frequency sub-band.
- Both grid-based and density-based
- Input parameters:
  - # of grid cells for each dimension
  - the wavelet, and the # of applications of wavelet transform.

WaveCluster (1998)

- How to apply wavelet transform to find clusters
  - Summaries the data by imposing a multidimensional grid structure onto data space
  - These multidimensional spatial data objects are represented in a n-dimensional feature space
  - Apply wavelet transform on feature space to find the dense regions in the feature space
  - Apply wavelet transform multiple times which result in clusters at different scales from fine to coarse
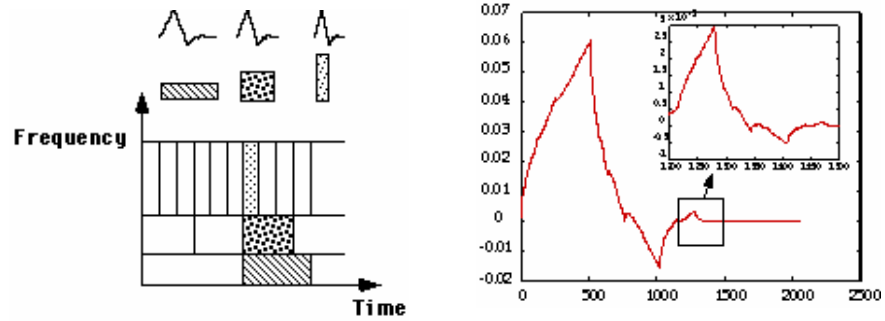
Wavelet Transform

- Decomposes a signal into different frequency subbands. (can be applied to n-dimensional signals)
- Data are transformed to preserve relative distance between objects at different levels of resolution.
- Allows natural clusters to become more distinguishable

What Is Wavelet (2)?

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Quantization

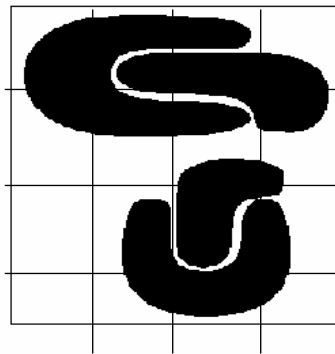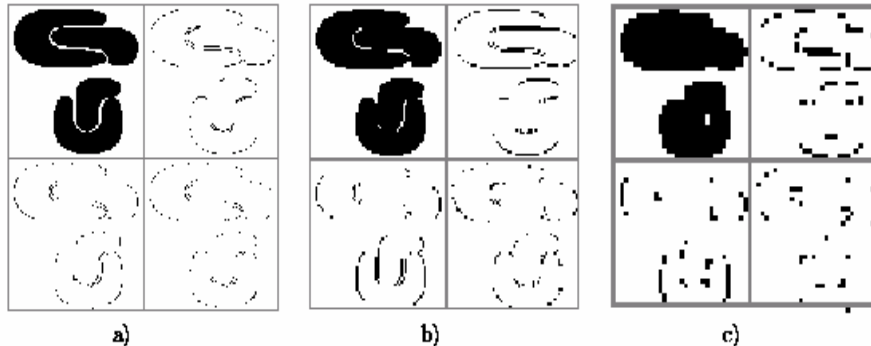Figure 1: A sample 2-dimensional feature space.

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Transformation

a) b) c)

WaveCluster (1998)

- Why is wavelet transformation useful for clustering
  - Unsupervised clustering

    It uses hat-shape filters to emphasize region where points cluster, but simultaneously to suppress weaker information in their boundary
  - Effective removal of outliers
  - Multi-resolution
  - Cost efficiency
- Major features:
  - Complexity $O(N)$
  - Detect arbitrary shaped clusters at different scales
  - Not sensitive to noise, not sensitive to input order
  - Only applicable to low dimensional data

CLIQUE (Clustering In QUEst)

- Agrawal, Gehrke, Gunopulos, Raghavan (SIGMOD'98).
- Automatically identifying subspaces of a high dimensional data space that allow better clustering than original space
- CLIQUE can be considered as both density-based and grid-based
    - It partitions each dimension into the same number of equal length interval
    - It partitions an m-dimensional data space into non-overlapping rectangular units
    - A unit is dense if the fraction of total data points contained in the unit exceeds the input model parameter
    - A cluster is a maximal set of connected dense units within a subspace

CLIQUE: The Major Steps

- Partition the data space and find the number of points that lie inside each cell of the partition.

- Identify the subspaces that contain clusters using the Apriori principle

- Identify clusters:
    - Determine dense units in all subspaces of interests
    - Determine connected dense units in all subspaces of interests.

- Generate minimal description for the clusters
    - Determine maximal regions that cover a cluster of connected dense units for each cluster
    - Determination of minimal cover for each cluster

$\tau = 3$
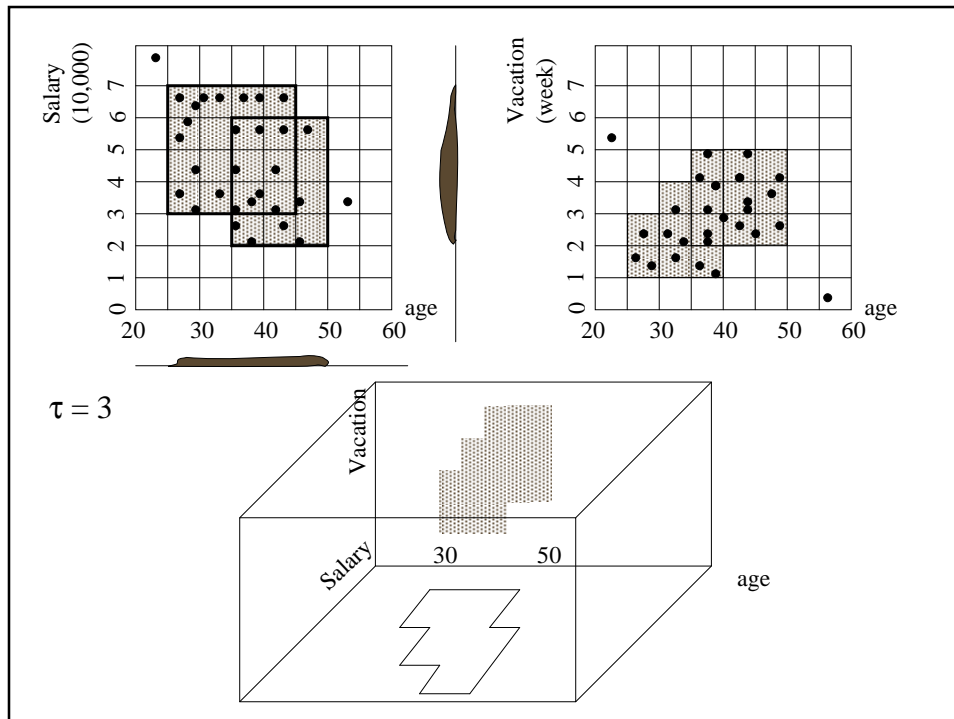
Strength and Weakness of *CLIQUE*

- Strength
    - It *automatically* finds subspaces of the highest dimensionality such that high density clusters exist in those subspaces
    - It is *insensitive* to the order of records in input and does not presume some canonical data distribution
    - It scales *linearly* with the size of input and has good scalability as the number of dimensions in the data increases
- Weakness
    - The accuracy of the clustering result may be degraded at the expense of simplicity of the method

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Cluster Analysis

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Model-Based Clustering Methods

- Attempt to optimize the fit between the data and some mathematical model
- Statistical and AI approach
  - 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
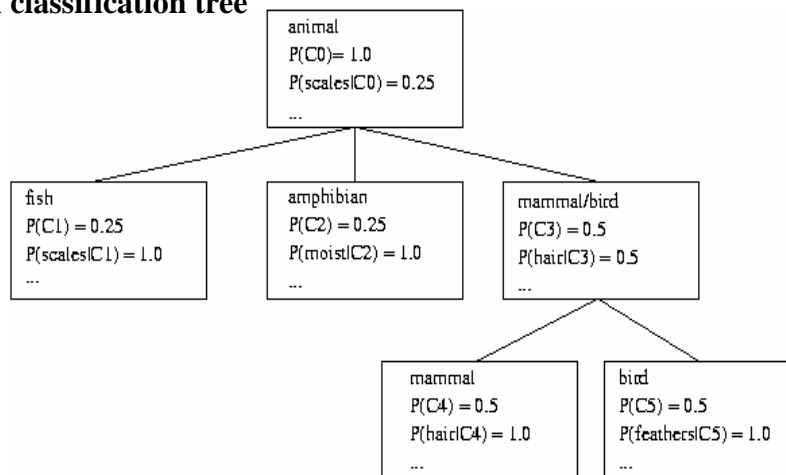   - Each node refers to a concept and contains a probabilistic description of that concept

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COBWEB Clustering Method

A classification tree

```
                        animal
                        P(C0)= 1.0
                        P(scales|C0) = 0.25
                        ...
              /            |              \
   fish              amphibian          mammal/bird
   P(C1) = 0.25      P(C2) = 0.25       P(C3) = 0.5
   P(scales|C1) = 1.0  P(moist|C2) = 1.0   P(hair|C3) = 0.5
   ...               ...                 ...
                                       /          \
                                  mammal           bird
                                  P(C4) = 0.5      P(C5) = 0.5
                                  P(hair|C4) = 1.0  P(feathers|C5) = 1.0
                                  ...              ...
```

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More on Statistical-Based Clustering

- Limitations of COBWEB
  - The assumption that the attributes are independent of each other is often too strong because correlation may exist
  - Not suitable for clustering large database data – skewed tree and expensive probability distributions
- CLASSIT
  - an extension of COBWEB for incremental clustering of continuous data
  - suffers similar problems as COBWEB
- AutoClass (Cheeseman and Stutz, 1996)
  - Uses Bayesian statistical analysis to estimate the number of clusters
  - Popular in industry

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Other Model-Based Clustering Methods

- Neural network approaches
  - Represent each cluster as an exemplar, acting as a "prototype" of the cluster
  - New objects are distributed to the cluster whose exemplar is the most similar according to some dostance measure
- Competitive learning
  - Involves a hierarchical architecture of several units (neurons)
  - Neurons compete in a "winner-takes-all" fashion for the object currently being presented
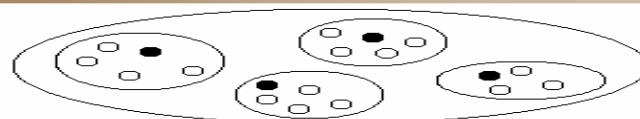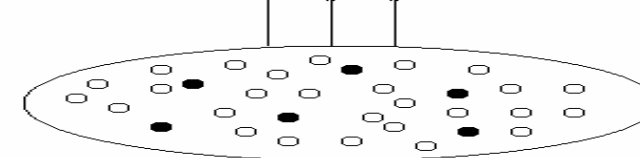
Model-Based Clustering Methods

Self-organizing feature maps (SOMs)

- Clustering is also 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

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What Is Outlier Discovery?

- What are outliers?
  - The set of objects are considerably dissimilar from the remainder of the data
  - Example: Sports: Michael Jordon, Wayne Gretzky, ...
- Problem
  - Find top n outlier points
- Applications:
  - Credit card fraud detection
  - Telecom fraud detection
  - Customer segmentation
  - Medical analysis

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Outlier Discovery: Statistical Approaches
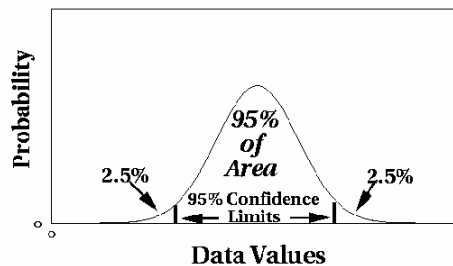
↗ Assume a model underlying distribution that generates data set (e.g. normal distribution)
- Use discordancy tests depending on
  - data distribution
  - distribution parameter (e.g., mean, variance)
  - number of expected outliers
- Drawbacks
  - most tests are for single attribute
  - In many cases, data distribution may not be known

Outlier Discovery: Distance-Based Approach

- Introduced to counter the main limitations imposed by statistical methods
  - We need multi-dimensional analysis without knowing data distribution.
- Distance-based outlier: A DB(p, D)-outlier is an object O in a dataset T such that at least a fraction p of the objects in T lies at a distance greater than D from O
- Algorithms for mining distance-based outliers
  - Index-based algorithm
  - Nested-loop algorithm
  - Cell-based algorithm

Outlier Discovery: Deviation-Based Approach

- Identifies outliers by examining the main characteristics of objects in a group
- Objects that "deviate" from this description are considered outliers
- sequential exception technique
  - simulates the way in which humans can distinguish unusual objects from among a series of supposedly like objects
- OLAP data cube technique
  - uses data cubes to identify regions of anomalies in large multidimensional data

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Problems and Challenges

- Considerable progress has been made in scalable clustering methods
  - Partitioning: k-means, k-medoids, CLARANS
  - Hierarchical: BIRCH, CURE
  - Density-based: DBSCAN, CLIQUE, OPTICS
  - Grid-based: STING, WaveCluster
  - Model-based: Autoclass, Denclue, Cobweb
- Current clustering techniques do not <u>address</u> all the requirements adequately
- Constraint-based clustering analysis: Constraints exist in data space (bridges and highways) or in user queries
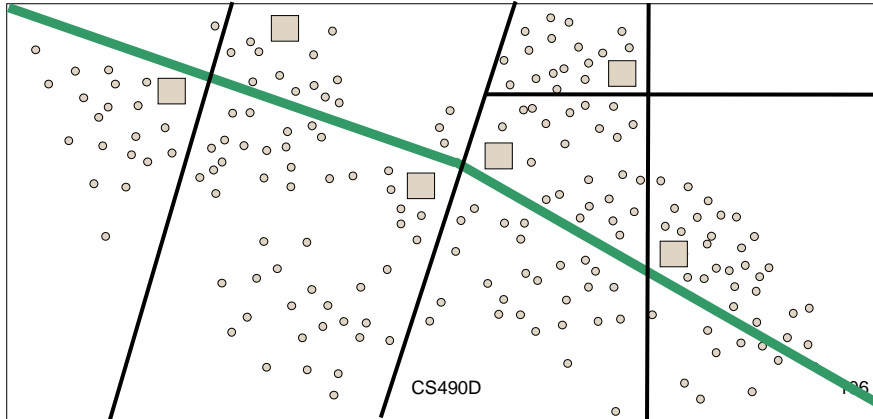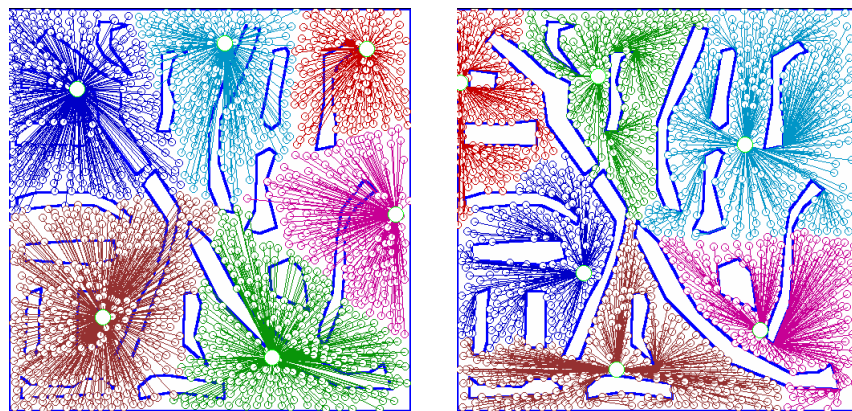
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Constraint-Based Clustering Analysis

- Clustering analysis: less parameters but more user-desired constraints, e.g., an ATM allocation problem

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Clustering With Obstacle Objects

Not Taking obstacles into account   Taking obstacles into account

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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 **constraint-based clustering**

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