UNIT-IV

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

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

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

Types of Data in Cluster Analysis

- Data Matrix: This represents n objects, such as persons, with p variables (also called measurements or attributes), such as age, height, weight and so on.
  - The structure is in the form of a relational table, or n-by-p matrix (n objects x p variables).

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

Dissimilarity Matrix: This stores a collection of proximities that are available for all pairs of n objects.

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

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 $s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + ... + |x_{nf} - m_f|)$
  - Calculate the mean absolute deviation:

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

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

- *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

- 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

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

- Can be treated like interval-scaled
  - replacing x_{if} by their rank
  - 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?)*
  - 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 $z_{if} = \frac{r_{if} - 1}{M_f - 1}$

- and treat z_{if} as interval-scaled

A Categorization of Major Clustering Methods

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

Partitioning Methods

- Partitioning method: 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 4 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 (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.

Comments on the *K-Means* Method

- Strength
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t << n$.
  - 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

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)

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 $\boldsymbol{TC_{ih}}$
  - 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

***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

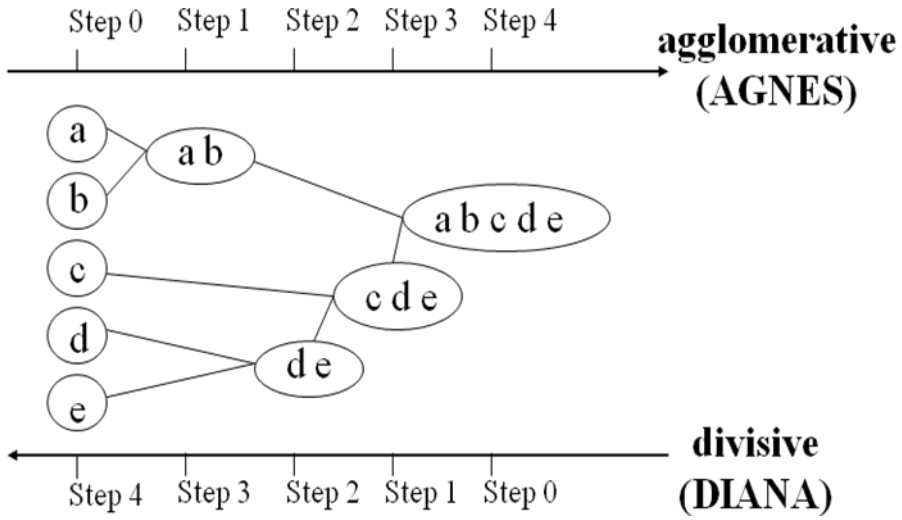
- A good clustering based on samples will not necessarily represent a good clustering of the whole data set if the sample is biased

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

- *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)

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

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

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

BIRCH:-

- 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

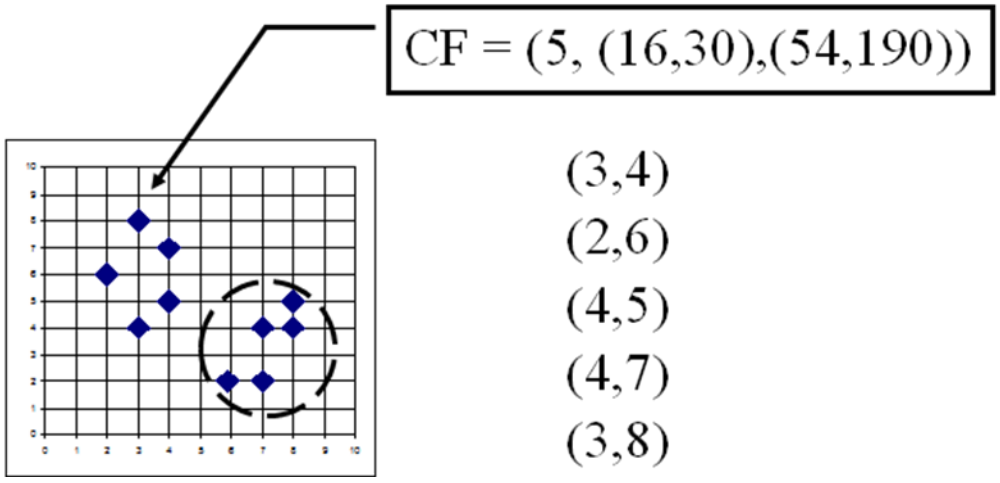
Clustering Feature Vector

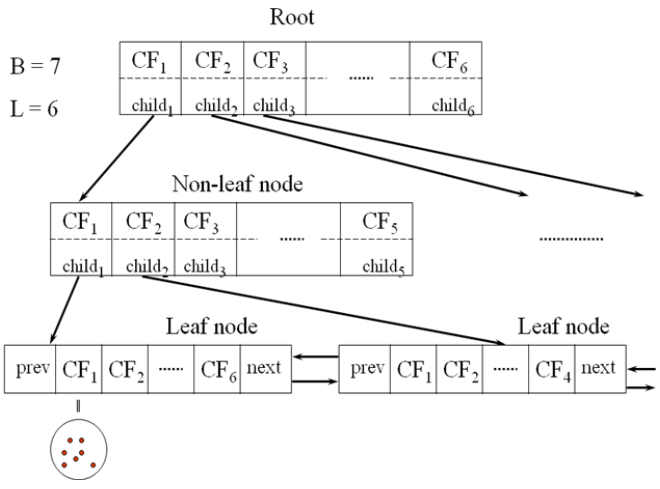
Clustering Feature: $CF = (N, \overrightarrow{LS}, SS)$

N: **Number of data points**

$LS: \sum_{i=1}^{N} = \overrightarrow{X_i}$

$SS: \sum_{i=1}^{N} = \overrightarrow{X_i^2}$





Clustering Categorical Data: ROCK

- ROCK: Robust Clustering using linKs,

  by S. Guha, R. Rastogi, K. Shim (ICDE'99).

  Use links to measure similarity/proximity

  - Computational complexity: $O(n^2 + nm_m m_a + n^2 \log n)$

- Basic ideas:

  - Similarity function and neighbors: $Sim(T_1, T_2) = \frac{|T_1 \cap T_2|}{|T_1 \cup T_2|}$

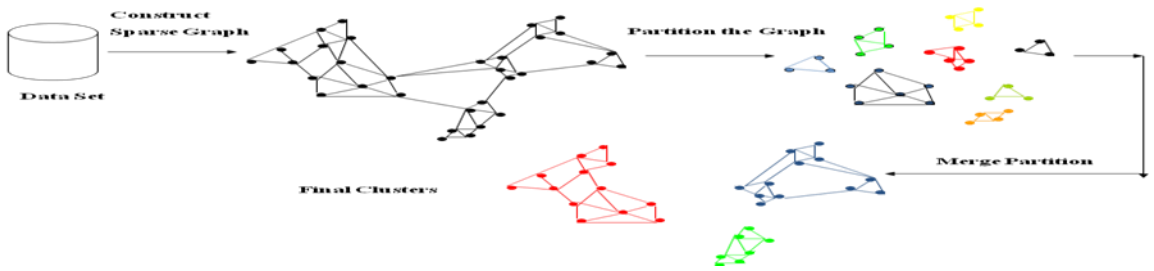
Let T_1 = {1,2,3}, T_2={3,4,5}

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

CHAMELEON

- CHAMELEON: hierarchical clustering using dynamic modeling, 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
- 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

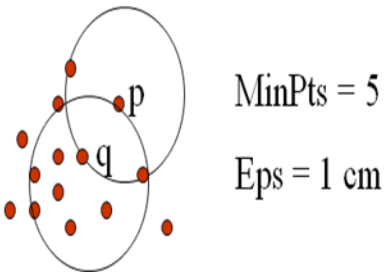
Overall Framework of CHAMELEON



Density-Based Clustering Methods

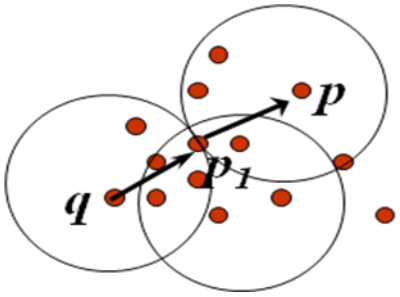
- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  -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

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



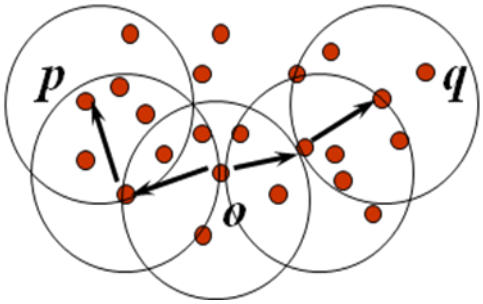
Density-reachable:

- 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



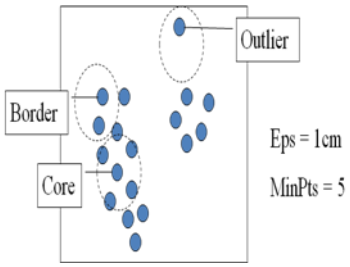
- Density-connected

- 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*.



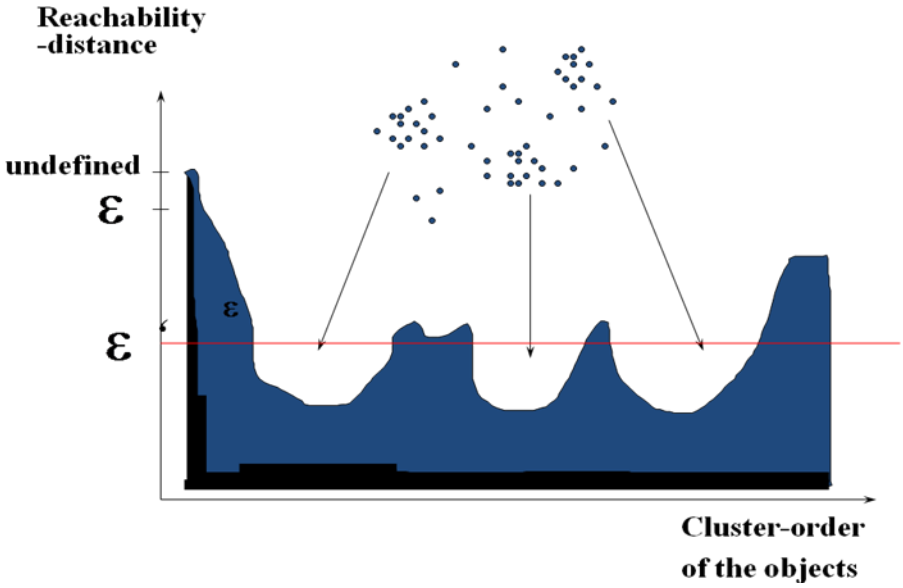
DBSCAN: Density Based Spatial Clustering of Applications with Noise

- 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



OPTICS: A Cluster-Ordering Method

- 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

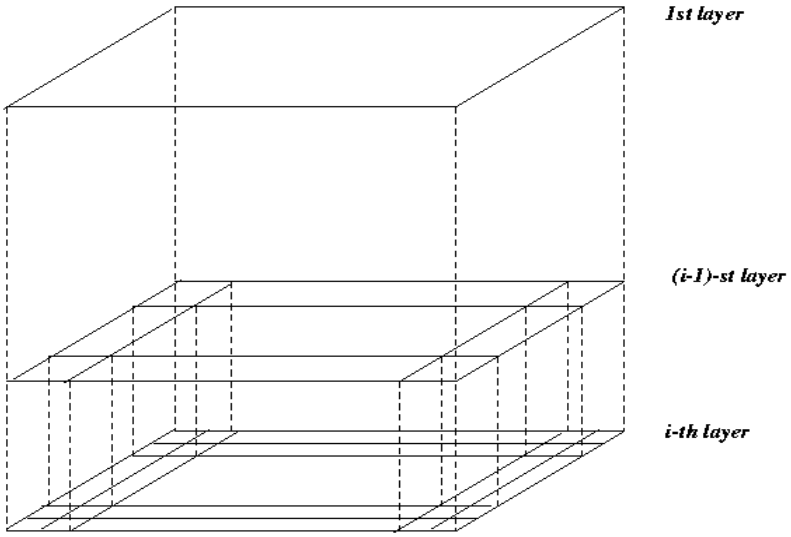


Grid-Based Clustering Method

- 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)

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

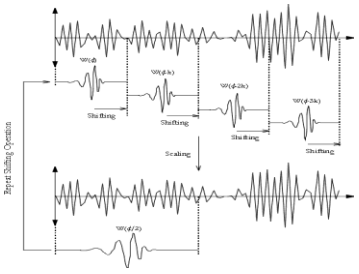


  - Each cell at a high level is partitioned into a number of smaller cells in the next lower level
  - Statistical info of each cell is calculated and stored beforehand and is used to answer queries
  - Parameters of higher level cells can be easily calculated from parameters of lower level cell
    - *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
  - 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

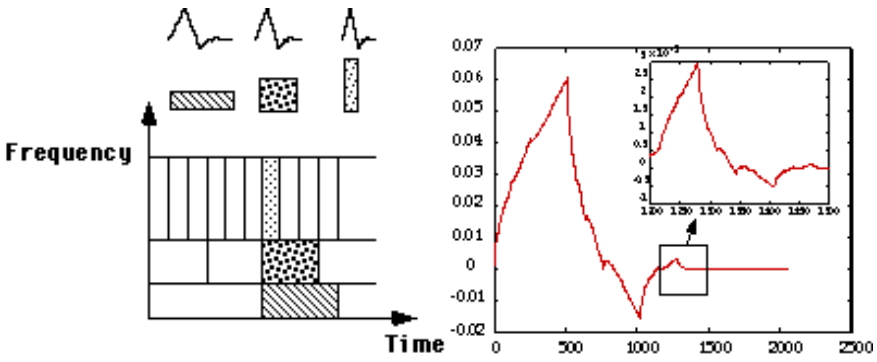
WaveCluster:

- 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.



- 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



Quantization

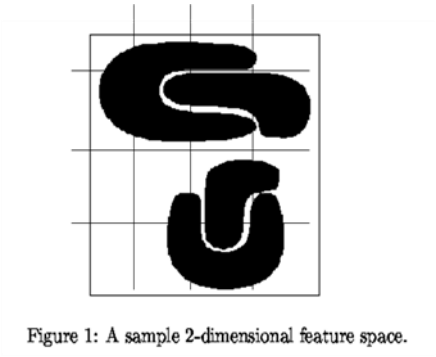
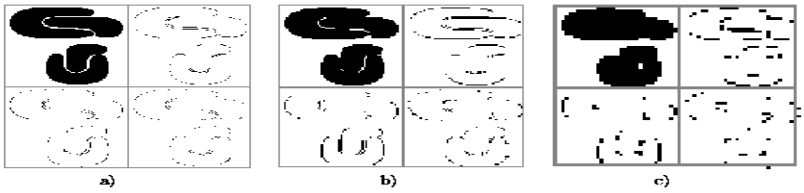


Figure 1: A sample 2-dimensional feature space.

Transformation



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

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