

Chapter 8: Clustering

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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

- 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

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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.

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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)

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

- Dissimilarity matrix

- (one mode)

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

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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.

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Type of data in clustering analysis

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

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Interval-valued variables

- Standardize data
 - Calculate the mean absolute deviation:

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

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

- 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

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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*:

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

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

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

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

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Similarity and Dissimilarity Between Objects (Cont.)

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

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

- 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 dissimilarity measures

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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):

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

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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

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

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

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

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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

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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 $r_{if} \in \{1, \dots, M_f\}$
 - 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

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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

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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

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

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Major Clustering Approaches

- Partitioning algorithms: Construct various partitions and then evaluate them by some criterion
- Hierarchy algorithms: 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

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Partitioning Algorithms: Basic Concept

- 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

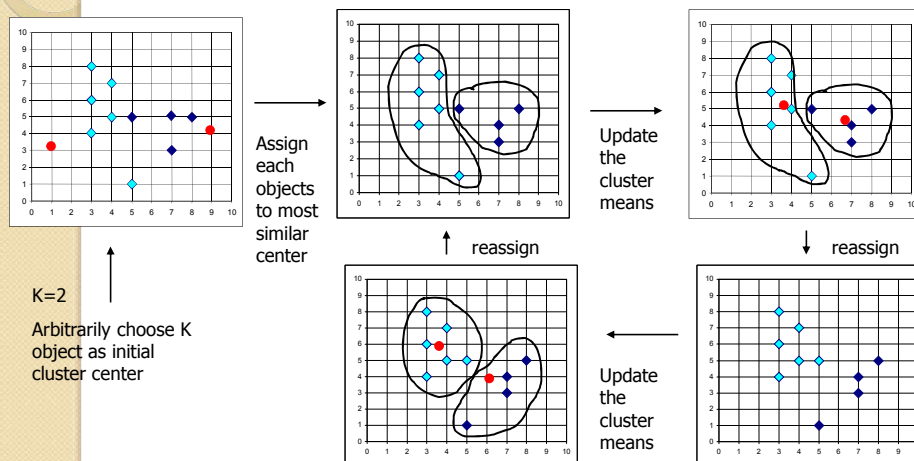
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The *K*-Means Clustering Method

- 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

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The *K*-Means Clustering Method



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Comments on the *K-Means* Method

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

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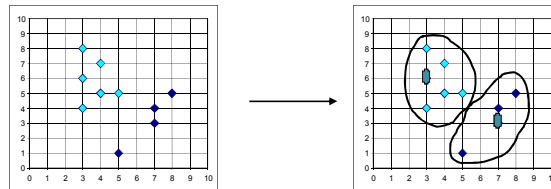
Variations of the *K-Means* Method

- 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

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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.



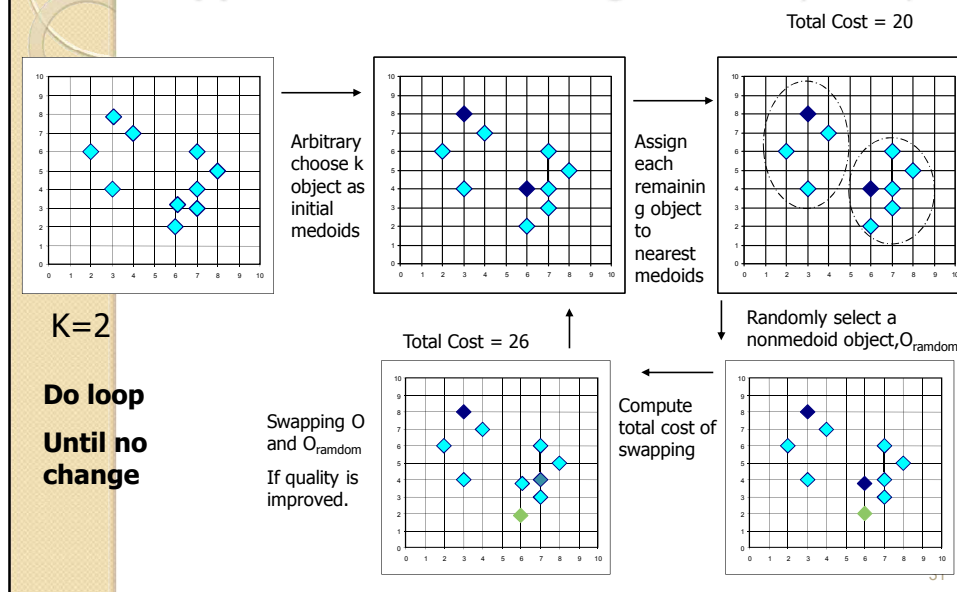
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The K-Medoids Clustering Method

- Find *representative* objects, called 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)

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Typical k-medoids algorithm (PAM)

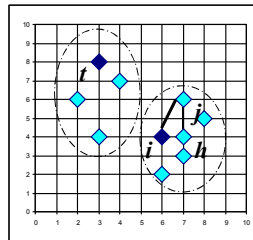


PAM (Partitioning Around Medoids) (1987)

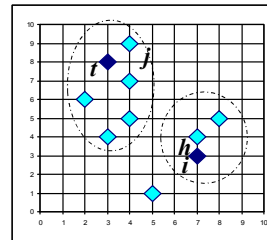
- PAM (Kaufman and Rousseeuw, 1987), built in Splus
- Use real object to represent the cluster
 - Select k representative objects arbitrarily
 - For each pair of non-selected object h and selected object i , calculate the total swapping cost TC_{ih}
 - For each pair of i and h ,
 - If $TC_{ih} < 0$, 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

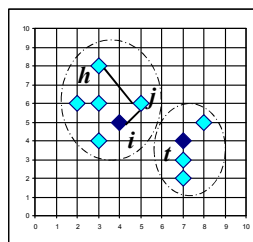
$$TC_{ih} = \sum_j C_{jih}$$



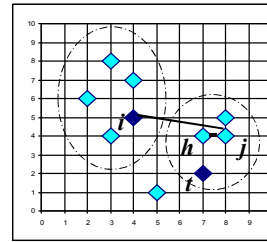
$$C_{jih} = d(j, h) - d(j, i)$$



$$C_{jih} = 0$$



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



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

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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)

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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

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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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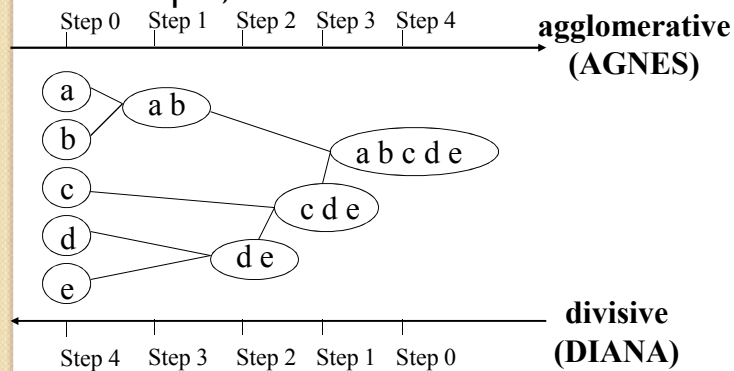
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Hierarchical Clustering

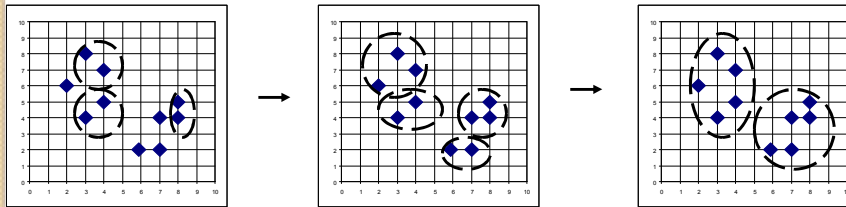
- Use distance matrix as clustering criteria. This method does not require the number of clusters k as an input, but needs a termination condition



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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

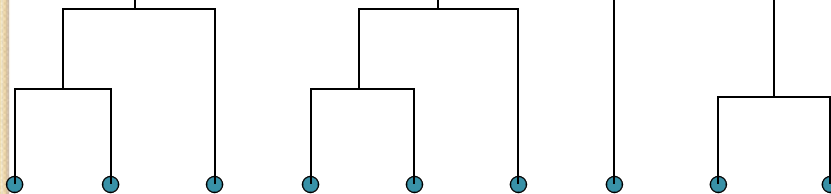


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A Dendrogram Shows How the Clusters are Merged Hierarchically

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

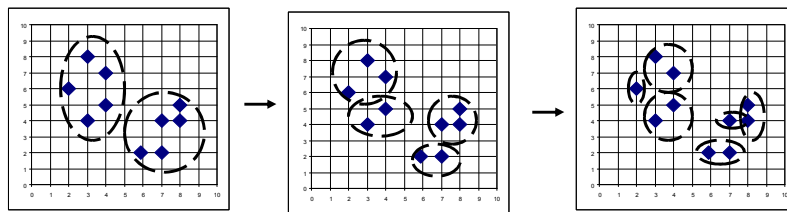
A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster.



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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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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.

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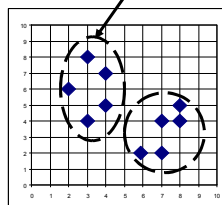
Clustering Feature Vector

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

N : Number of data points

$$LS: \sum_{i=1}^N \vec{X}_i$$

$$SS: \sum_{i=1}^N \vec{X}_i^2$$



$CF = (5, (16,30),(54,190))$

(3,4)

(2,6)

(4,5)

(4,7)

(3,8)

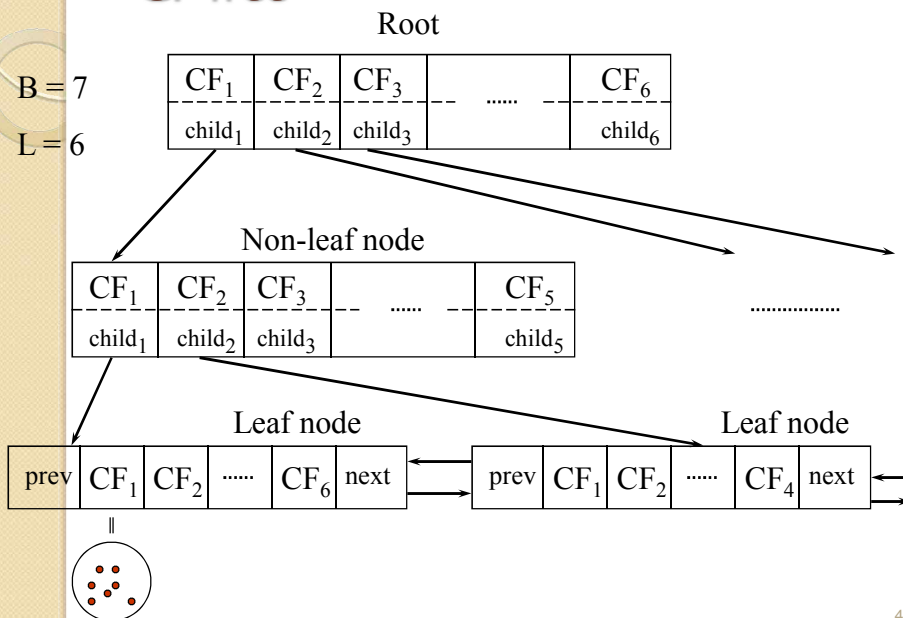
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CF-Tree in BIRCH

- 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

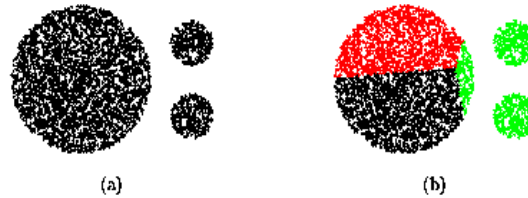
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CF Tree



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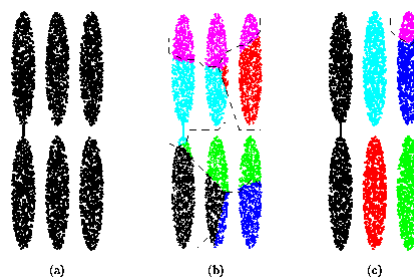
CURE (Clustering Using Representatives)



- 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



- 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

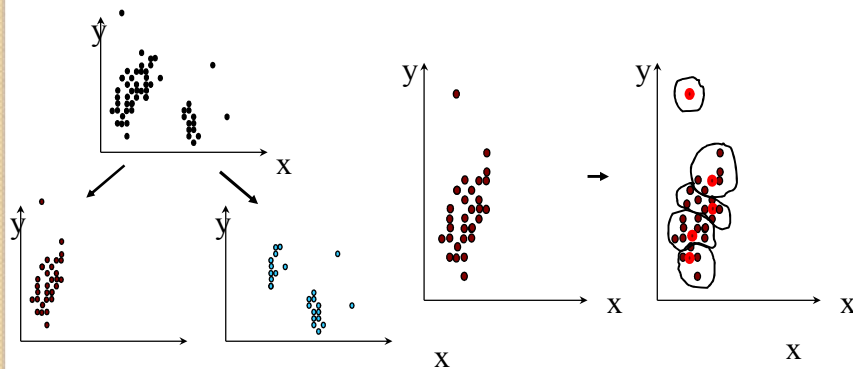
- Draw random sample s .
- Partition sample to p partitions with size s/p
- Partially cluster partitions into s/pq clusters
- Eliminate outliers
 - By random sampling
 - If a cluster grows too slow, eliminate it.
- Cluster partial clusters.
- Label data in disk

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Data Partitioning and Clustering

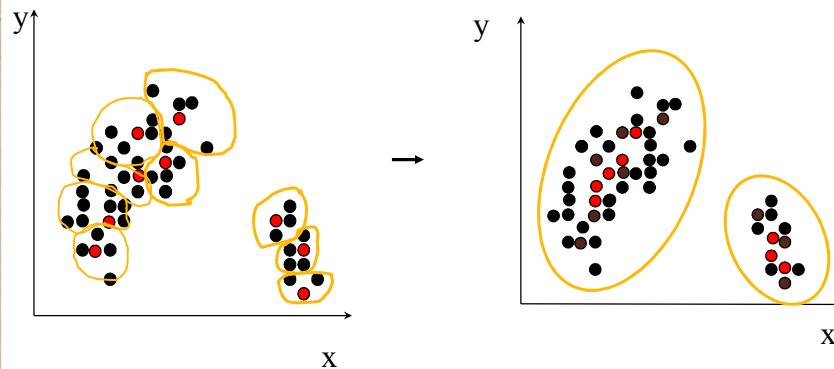
- $s = 50$
- $p = 2$
- $s/p = 25$

■ $s/pq = 5$



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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

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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: $Sim(T_1, T_2) = \frac{|T_1 \cap T_2|}{|T_1 \cup T_2|}$
Let $T_1 = \{1,2,3\}$, $T_2 = \{3,4,5\}$

$$Sim(T_1, T_2) = \frac{|\{3\}|}{|\{1,2,3,4,5\}|} = \frac{1}{5} = 0.2$$

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Rock: Algorithm

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

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

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

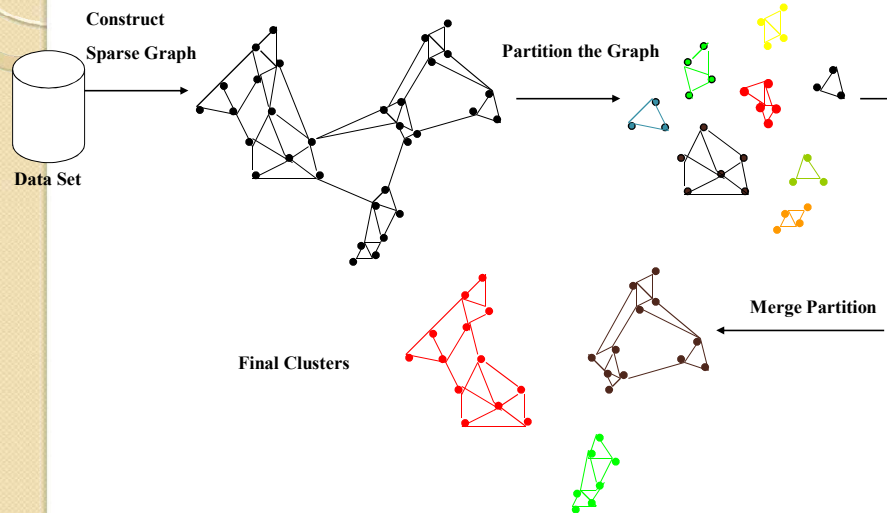
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CHAMELEON (Hierarchical clustering using dynamic modeling)

- 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

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Overall Framework of CHAMELEON



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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)

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Density Concepts

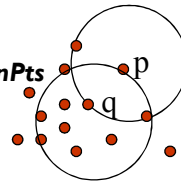
- Core object (CO)—object with at least 'M' objects within a radius 'E-neighborhood'
- Directly density reachable (DDR)—x is CO, y is in x's 'E-neighborhood'
- Density reachable—there exists a chain of DDR objects from x to y
- Density based cluster—density connected objects maximum w.r.t. reachability

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Density-Based Clustering: Background

- Two parameters:
 - Eps**: Maximum radius of the neighbourhood
 - MinPts**: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: $\{q \text{ belongs to } D \mid \text{dist}(p,q) \leq Eps\}$
- 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:

$$|N_{Eps}(q)| \geq \text{MinPts}$$



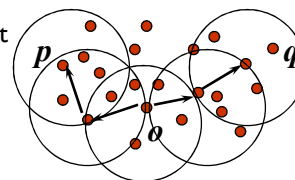
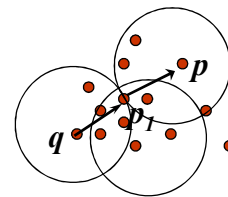
MinPts = 5

Eps = 1 cm

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Density-Based Clustering: Background (II)

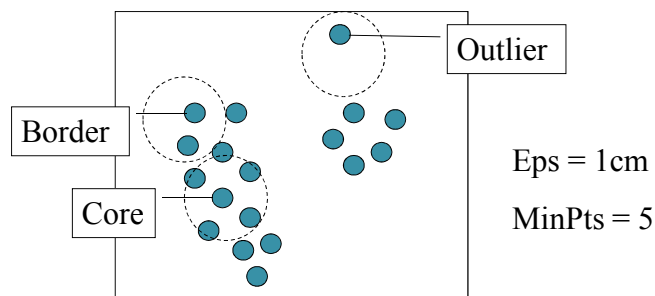
- Density-reachable:
 - A point p is density-reachable from a point q wrt. **Eps**, **MinPts** if there is a chain of points $p_1, \dots, p_n, p_1 = q, p_n = p$ such that p_{i+1} is directly density-reachable from p_i
- Density-connected
 - A point p is density-connected to a point q wrt. **Eps**, **MinPts**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



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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



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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.

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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

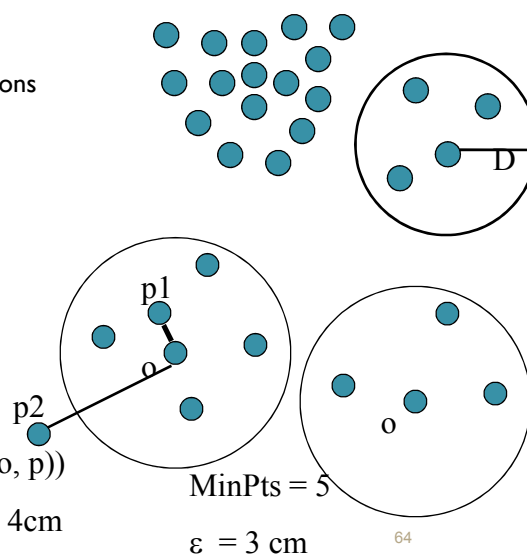
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OPTICS: Some Extension from DBSCAN

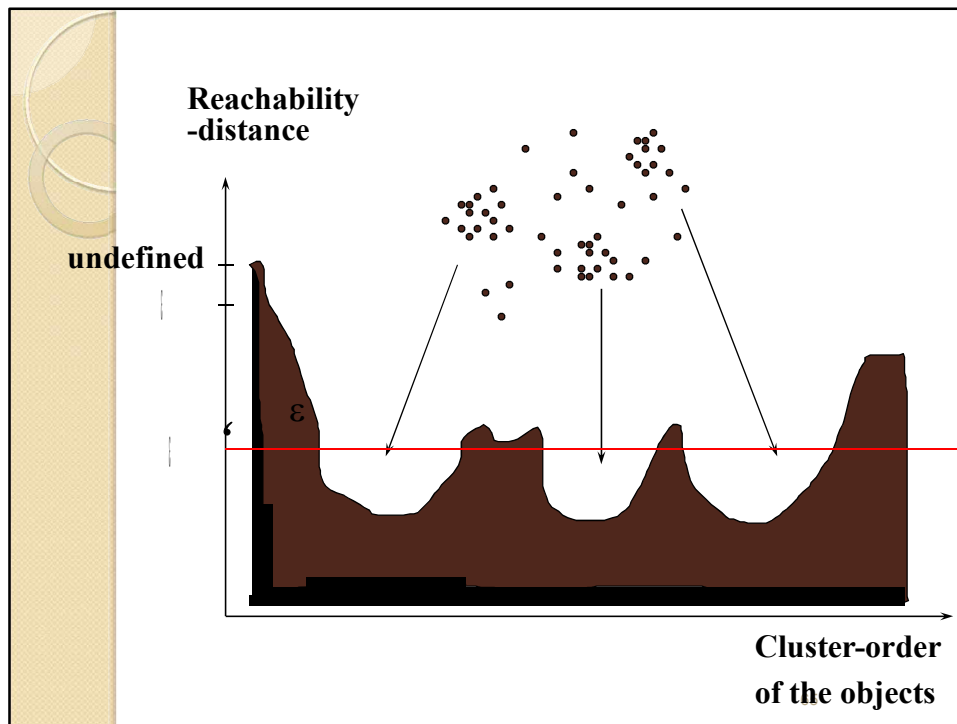
- Index-based:
 - k = number of dimensions
 - $N = 20$
 - $p = 75\%$
 - $M = N(1-p) = 5$
- Complexity: $O(kN^2)$
- Core Distance
- Reachability Distance

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

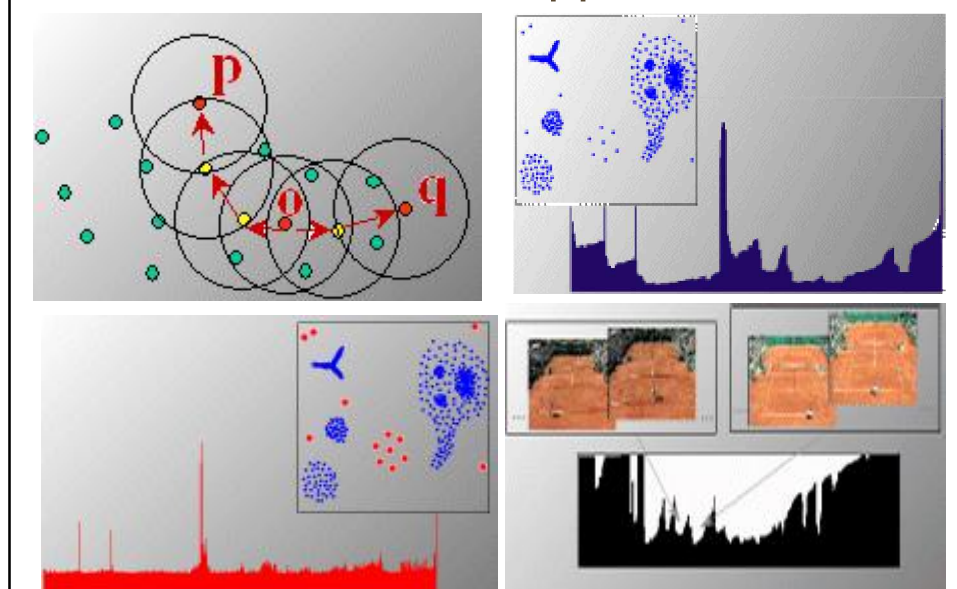
$r(p1, o) = 2.8\text{cm}$. $r(p2, o) = 4\text{cm}$



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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

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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.

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Gradient: The steepness of a slope

- Example

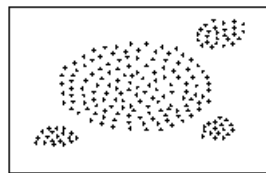
$$f_{\text{Gaussian}}(x, y) = e^{-\frac{d(x, y)^2}{2\sigma^2}}$$

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

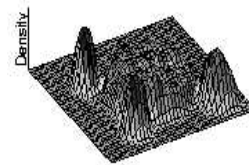
$$\nabla f_{\text{Gaussian}}^D(x, x_i) = \sum_{i=1}^N (x_i - x) \cdot e^{-\frac{d(x, x_i)^2}{2\sigma^2}}$$

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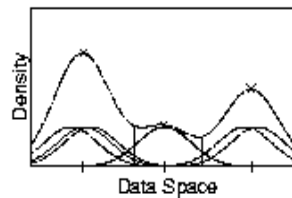
Density Attractor



(a) Data Set



(c) Gaussian



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Center-Defined and Arbitrary

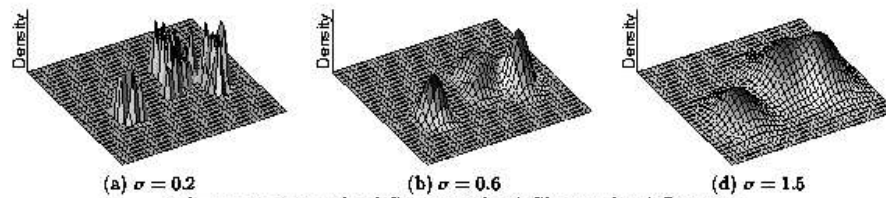


Figure 3: Example of Center-Defined Clusters for different σ

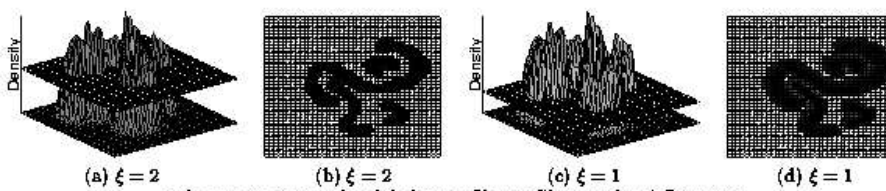


Figure 4: Example of Arbitrary-Shape Clusters for different ξ

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Cluster Analysis

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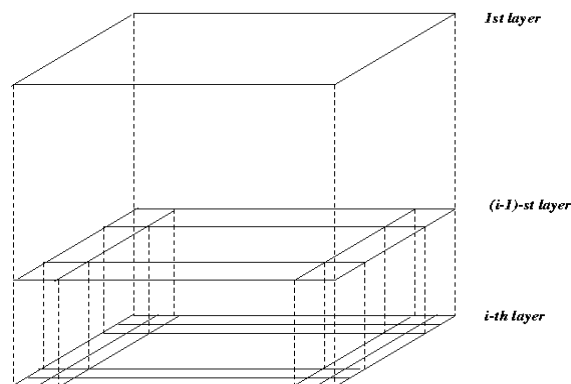
Grid-Based Clustering Method

- 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 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

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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

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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.

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WaveCluster (1998)

- How to apply wavelet transform to find clusters
 - Summarizes 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

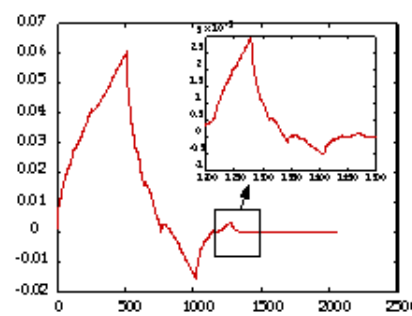
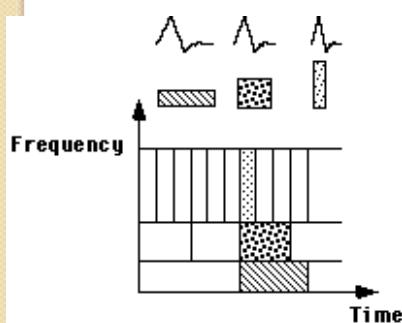
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Wavelet Transform

- 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

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What Is Wavelet (2)?



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Quantization

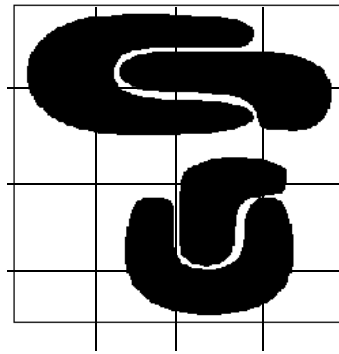
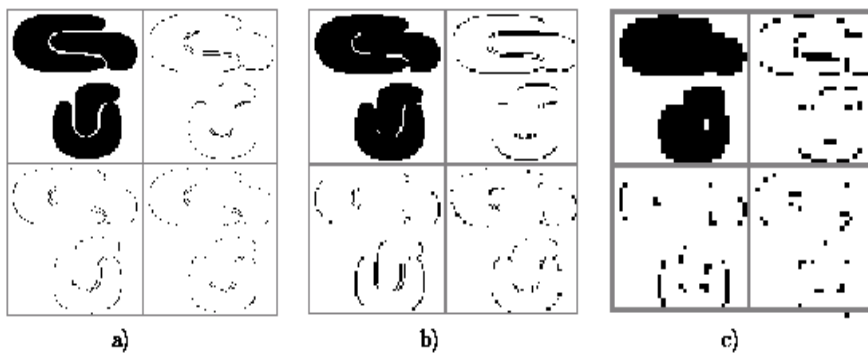


Figure 1: A sample 2-dimensional feature space.

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Transformation



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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

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CLIQUE (Clustering In QUEst)

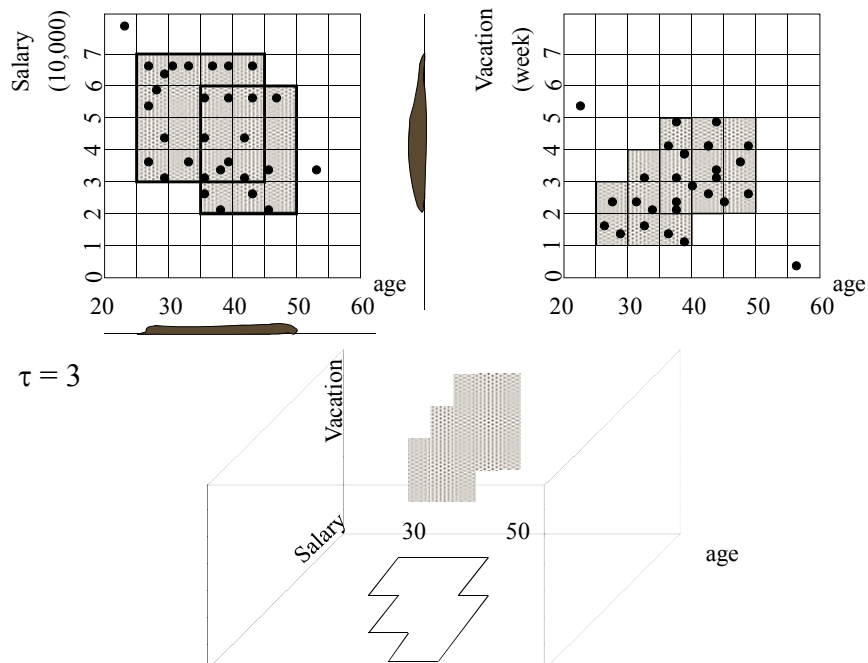
- Agrawal, Gehrke, Gunopulos, Raghavan (SIGMOD'98).
- Automatically identifying subspaces of a high dimensional data space that allow better clustering than original space
- CLIQUE can be considered as both density-based and grid-based
 - It partitions each dimension into the same number of equal length 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

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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

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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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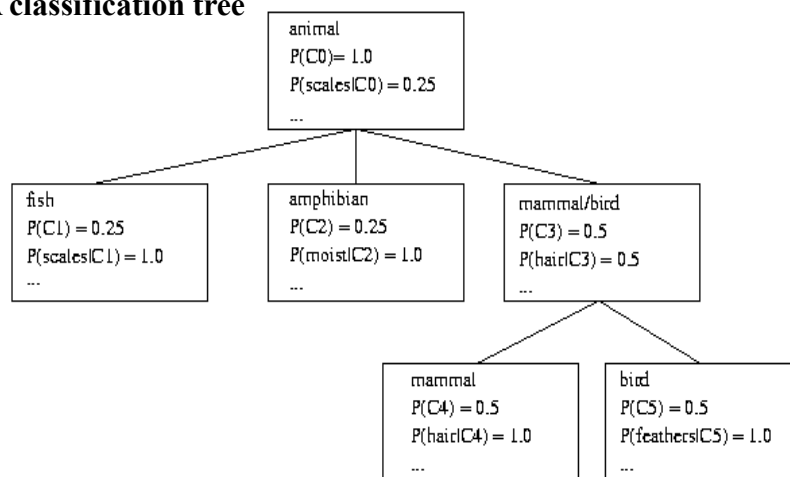
Model-Based Clustering Methods

- 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



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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

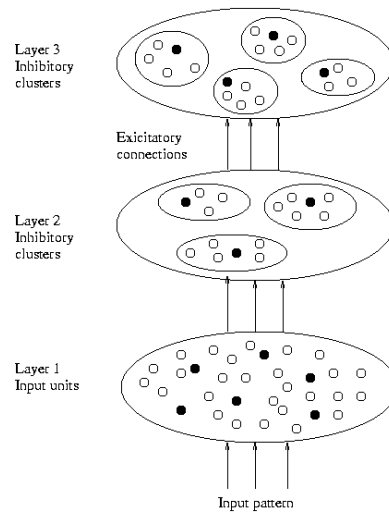
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Other Model-Based Clustering Methods

- 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 distance 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

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Model-Based Clustering Methods



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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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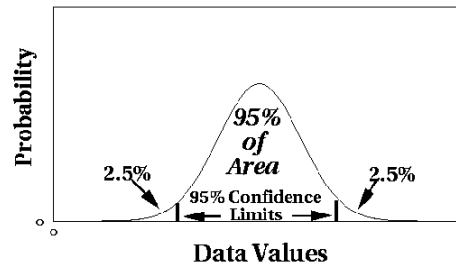
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What Is Outlier Discovery?

- 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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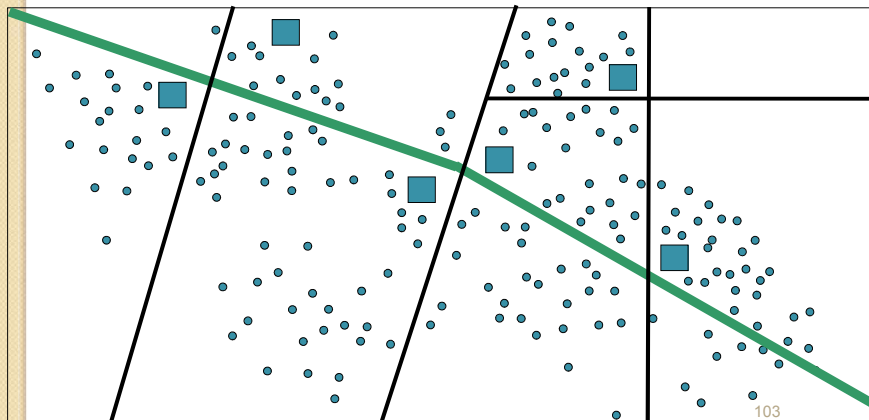
Problems and Challenges

- 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 address all the requirements adequately
- Constraint-based clustering analysis: Constraints exist in data space (bridges and highways) or in user queries

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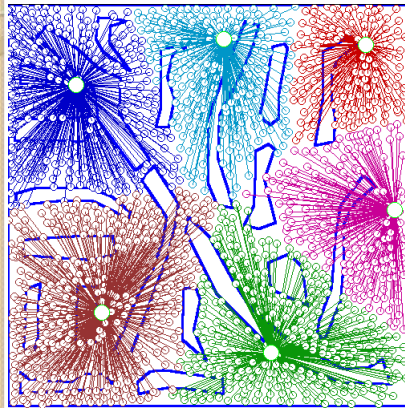
Constraint-Based Clustering Analysis

- 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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References (1)

- R. Agrawal, J. Gehrke, D. Gunopulos, and P. Raghavan. Automatic subspace clustering of high dimensional data for data mining applications. SIGMOD'98
- M. R. Anderberg. Cluster Analysis for Applications. Academic Press, 1973.
- M. Ankerst, M. Breunig, H.-P. Kriegel, and J. Sander. Optics: Ordering points to identify the clustering structure, SIGMOD'99.
- P. Arabie, L. J. Hubert, and G. De Soete. Clustering and Classification. World Scientific, 1996
- M. Ester, H.-P. Kriegel, J. Sander, and X. Xu. A density-based algorithm for discovering clusters in large spatial databases. KDD'96.
- M. Ester, H.-P. Kriegel, and X. Xu. Knowledge discovery in large spatial databases: Focusing techniques for efficient class identification. SSD'95.
- D. Fisher. Knowledge acquisition via incremental conceptual clustering. Machine Learning, 2:139-172, 1987.
- D. Gibson, J. Kleinberg, and P. Raghavan. Clustering categorical data: An approach based on dynamic systems. In Proc. VLDB'98.
- S. Guha, R. Rastogi, and K. Shim. Cure: An efficient clustering algorithm for large databases. SIGMOD'98.
- A. K. Jain and R. C. Dubes. Algorithms for Clustering Data. Printice Hall, 1988.

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References (2)

- L. Kaufman and P. J. Rousseeuw. Finding Groups in Data: an Introduction to Cluster Analysis. John Wiley & Sons, 1990.
- E. Knorr and R. Ng. Algorithms for mining distance-based outliers in large datasets. VLDB'98.
- G. J. McLachlan and K. E. Basford. Mixture Models: Inference and Applications to Clustering. John Wiley and Sons, 1988.
- P. Michaud. Clustering techniques. Future Generation Computer systems, 13, 1997.
- R. Ng and J. Han. Efficient and effective clustering method for spatial data mining. VLDB'94.
- E. Schikuta. Grid clustering: An efficient hierarchical clustering method for very large data sets. Proc. 1996 Int. Conf. on Pattern Recognition, 101-105.
- G. Sheikholeslami, S. Chatterjee, and A. Zhang. WaveCluster: A multi-resolution clustering approach for very large spatial databases. VLDB'98.
- W. Wang, Yang, R. Muntz, STING: A Statistical Information grid Approach to Spatial Data Mining, VLDB'97.
- T. Zhang, R. Ramakrishnan, and M. Livny. BIRCH : an efficient data clustering method for very large databases. SIGMOD'96.

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