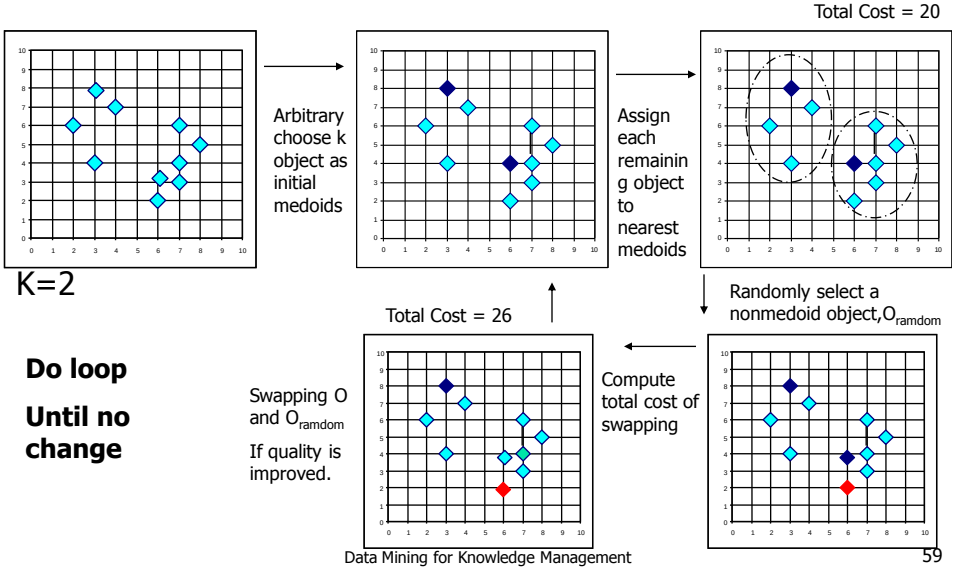
# The *K-Medoids* Clustering Method

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



# A Typical K-Medoids Algorithm (PAM)



# 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



# 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)

# Roadmap

1. What is Cluster Analysis?
2. Types of Data in Cluster Analysis
3. A Categorization of Major Clustering Methods
4. Partitioning Methods
5. Hierarchical Methods
6. Density-Based Methods
7. Grid-Based Methods
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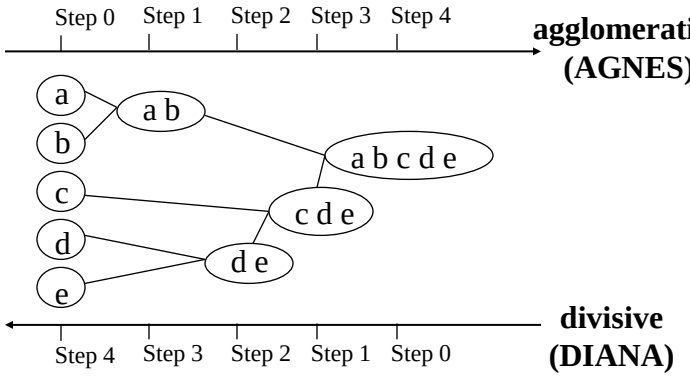
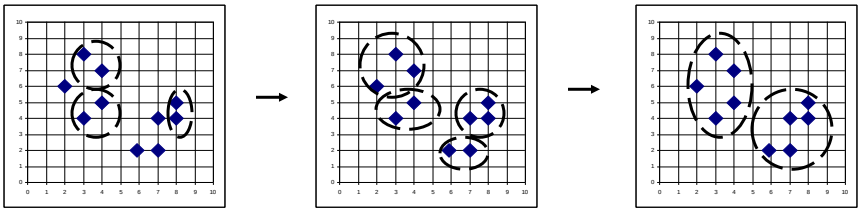
# Hierarchical Clustering

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



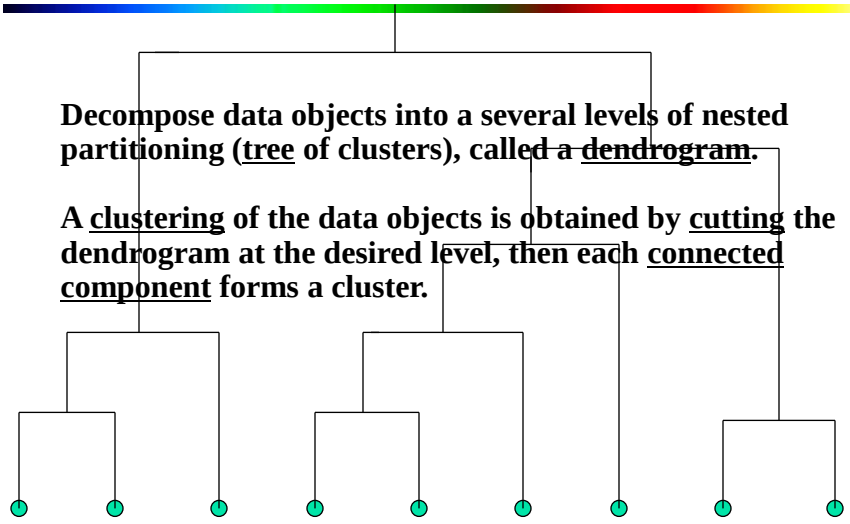
# AGNES (Agglomerative Nesting)

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





# *Dendrogram:* Shows How the Clusters are Merged

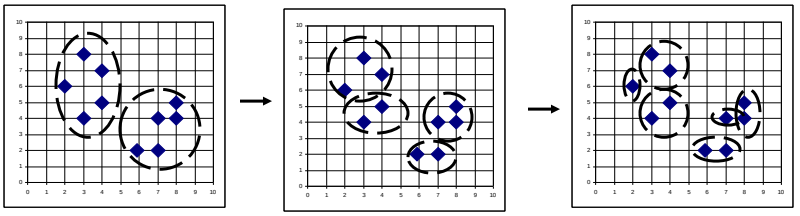


**Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram.**

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

# DIANA (Divisive Analysis)

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





# Recent Hierarchical Clustering Methods

- Major weakness of agglomerative clustering methods
  - do not scale well: time complexity of at least $O(n^2)$, where $n$ is the number of total objects
  - can never undo what was done previously
- Integration of hierarchical with distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
  - ROCK (1999): clustering categorical data by neighbor and link analysis
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

# BIRCH (1996)

- Birch: Balanced Iterative Reducing and Clustering using Hierarchies (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.



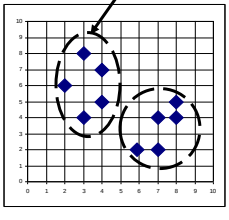
# Clustering Feature Vector in BIRCH

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

$N$: **Number of data points**

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

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



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

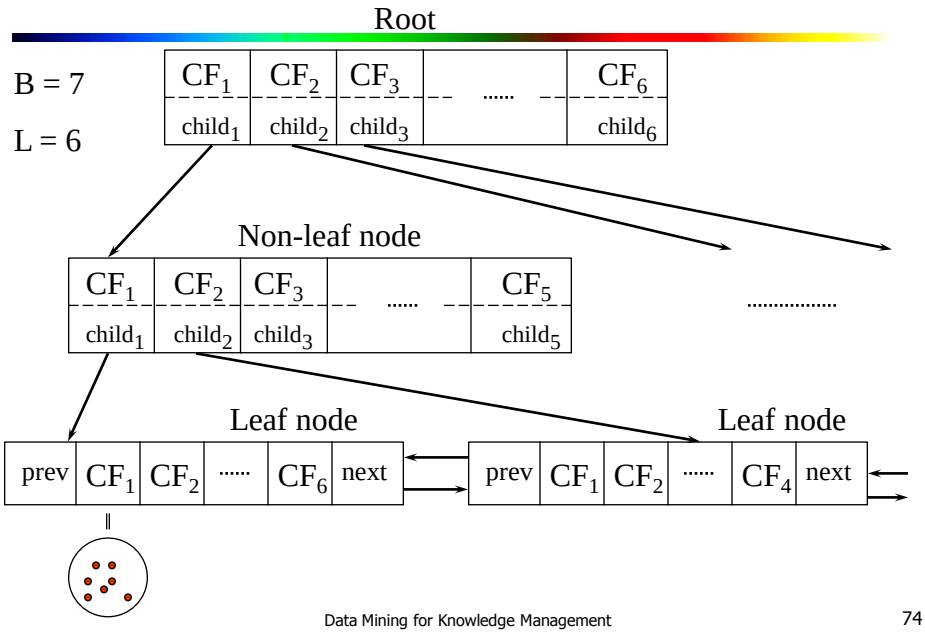
(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

# 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



# The CF Tree Structure



# Clustering Categorical Data: The ROCK Algorithm

- ROCK: RObust Clustering using linKs
  - S. Guha, R. Rastogi & K. Shim, ICDE'99
- Major ideas
  - Not distance-based
  - Use links to measure similarity/proximity
  - Measure similarity between points, as well as between their corresponding neighborhoods
    - two points are closer together if they share some of their neighbors
- Algorithm: sampling-based clustering
  - Draw random sample
  - Cluster with links
  - Label data in disk
  - Computational complexity: $O(n^2 + nm_m m_a + n^2 \log n)$



# Similarity Measure in ROCK

- Traditional measures for categorical data may not work well, e.g., Jaccard coefficient
- Example: Two groups (clusters) of transactions
  - $C_1$. <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - $C_2$. <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}

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  - $C_2$. <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}
- Jaccard co-efficient may lead to wrong clustering result
  - $C_1$: 0.2 ({a, b, c}, {b, d, e}} to 0.5 ({a, b, c}, {a, b, d})
  - $C_1$ & $C_2$: could be as high as 0.5 ({a, b, c}, {a, b, f})
- Jaccard co-efficient-based similarity function: $Sim(T_1, T_2) = \frac{|T_1 \cap T_2|}{|T_1 \cup T_2|}$
  - Ex. Let $T_1$ = {a, b, c}, $T_2$ = {c, d, e}

$$Sim(T_1, T_2) = \frac{|\{c\}|}{|\{a, b, c, d, e\}|} = \frac{1}{5} = 0.2$$



# Link Measure in ROCK

- Links: # of common neighbors
  - $C_1$ <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - $C_2$ <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}

# Link Measure in ROCK

- Links: # of common neighbors
  - $C_1$ <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - $C_2$ <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}

- Let $T_1$ = {a, b, c}, $T_2$ = {c, d, e}, $T_3$ = {a, b, f}



# Link Measure in ROCK

- Links: # of common neighbors
  - $C_1$ <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - $C_2$ <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}

- Let $T_1$ = {a, b, c}, $T_2$ = {c, d, e}, $T_3$ = {a, b, f}
  - link($T_1$, $T_2$) = 4, *since they have 4 common neighbors*
    - {a, c, d}, {a, c, e}, {b, c, d}, {b, c, e}

# Link Measure in ROCK

- Links: # of common neighbors
  - $C_1$ <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - $C_2$ <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}

- Let $T_1$ = {a, b, c}, $T_2$ = {c, d, e}, $T_3$ = {a, b, f}
  - link($T_1$, $T_2$) = 4, *since they have 4 common neighbors*
    - {a, c, d}, {a, c, e}, {b, c, d}, {b, c, e}
  - link($T_1$, $T_3$) = 3, *since they have 3 common neighbors*
    - {a, b, d}, {a, b, e}, {a, b, g}

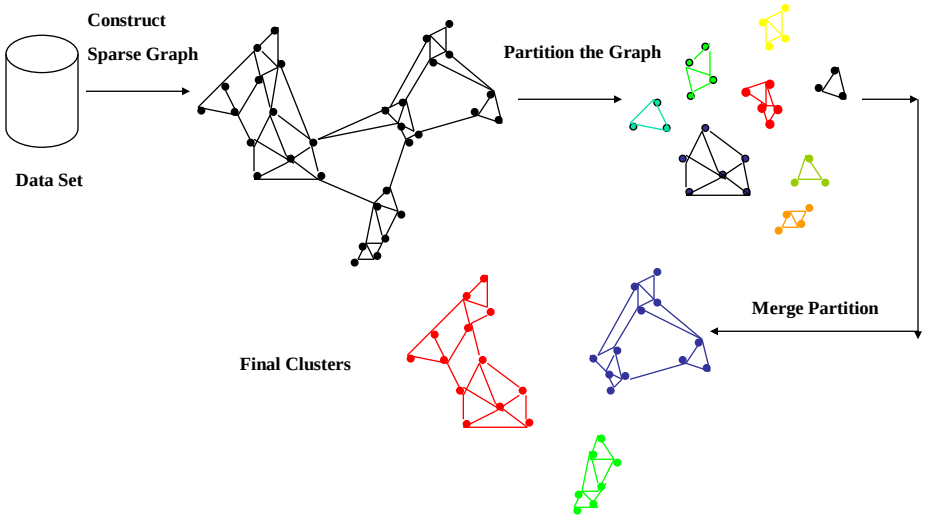
- Thus, link is a better measure than Jaccard coefficient



# CHAMELEON: Hierarchical Clustering Using Dynamic Modeling (1999)

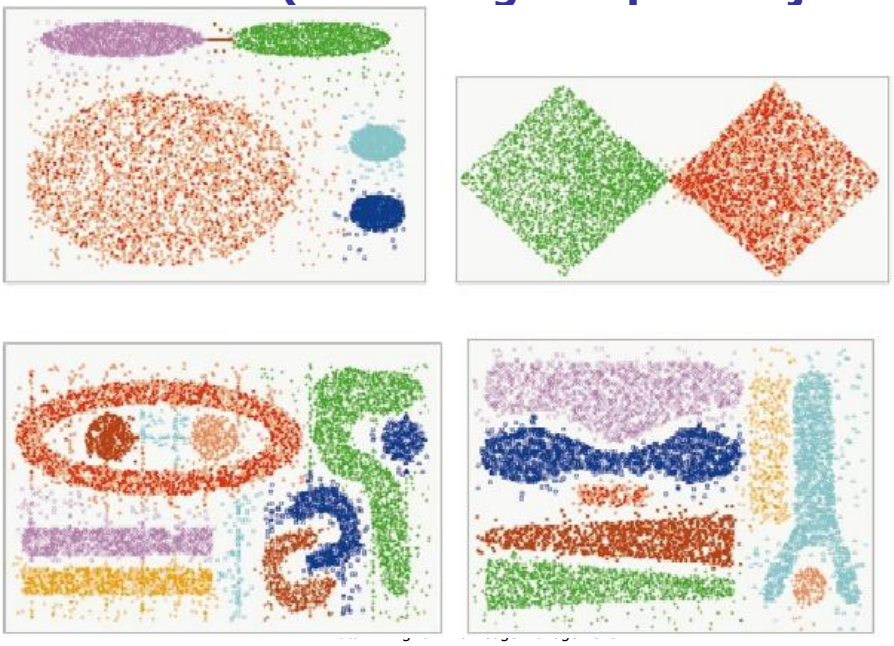
- CHAMELEON: by G. Karypis, E.H. Han, and V. Kumar'99
- Measures the similarity based on a dynamic model
  - Two clusters are merged only if the *interconnectivity* and *closeness (proximity)* between two clusters are high *relative to* the internal interconnectivity of the clusters and closeness of 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






# CHAMELEON (Clustering Complex Objects)



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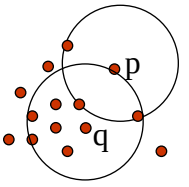
# Density-Based Clustering Methods

- 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) (more grid-based)

# Density-Based Clustering: Basic Concepts

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

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



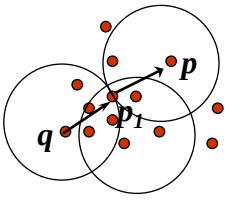

MinPts = 5

Eps = 1 cm

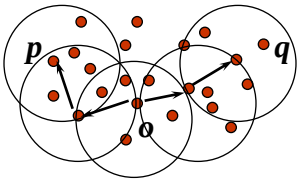


# Density-Reachable and Density-Connected

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

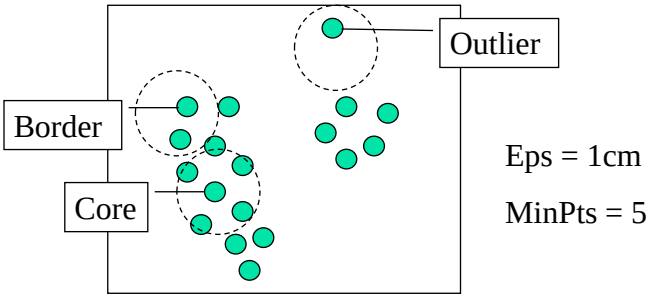



- Density-connected
  - A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



# 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






# DBSCAN: The Algorithm

- Arbitrary select a point *p*
- Retrieve all points density-reachable from *p* w.r.t. *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.

# DBSCAN: Sensitive to Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

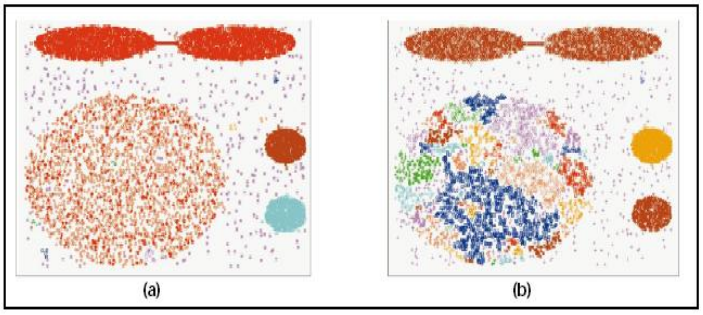
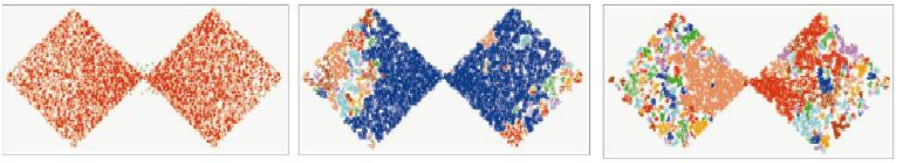



Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



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# Model-Based Clustering

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



# EM — Expectation Maximization

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

# The EM (Expectation Maximization) Algorithm

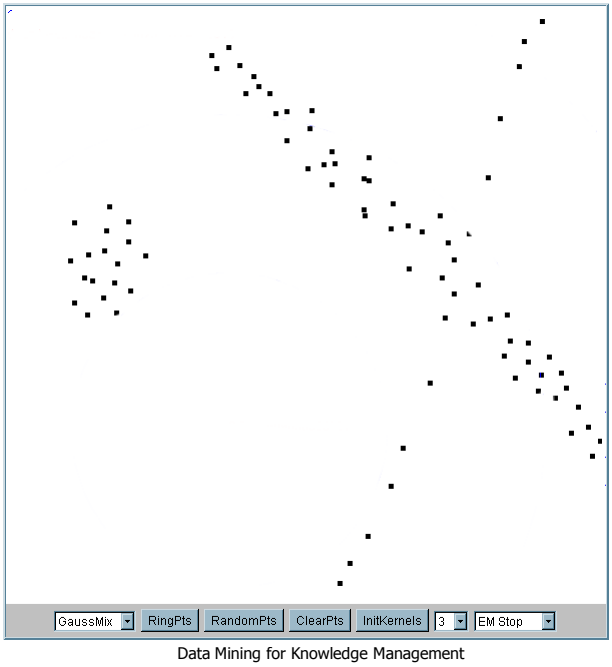
- Initially, randomly assign k cluster centers
- Iteratively refine the clusters based on two steps
  - Expectation step: assign each data point $X_i$ to cluster $C_i$ with the following probability

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

  - Maximization step:
    - Estimation of model parameters

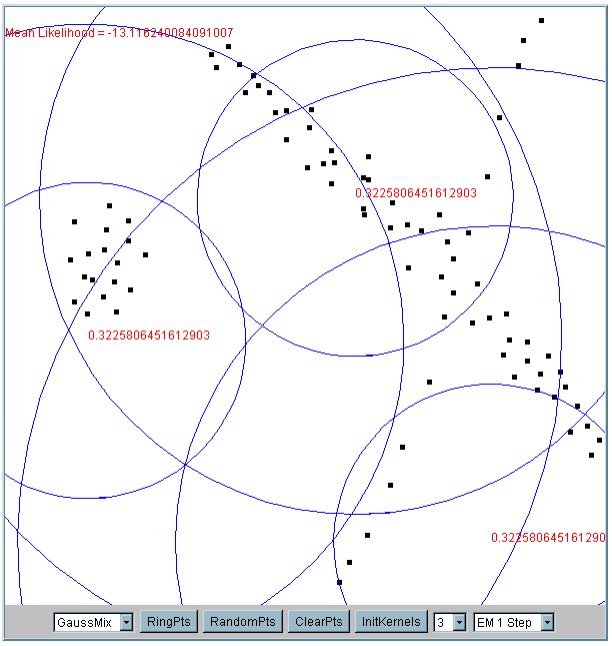
$$m_k = \frac{1}{N}\Sigma_{i=1}^{N}\frac{X_i P(X_i \in C_k)}{\Sigma_j P(X_i \in C_j)}.$$





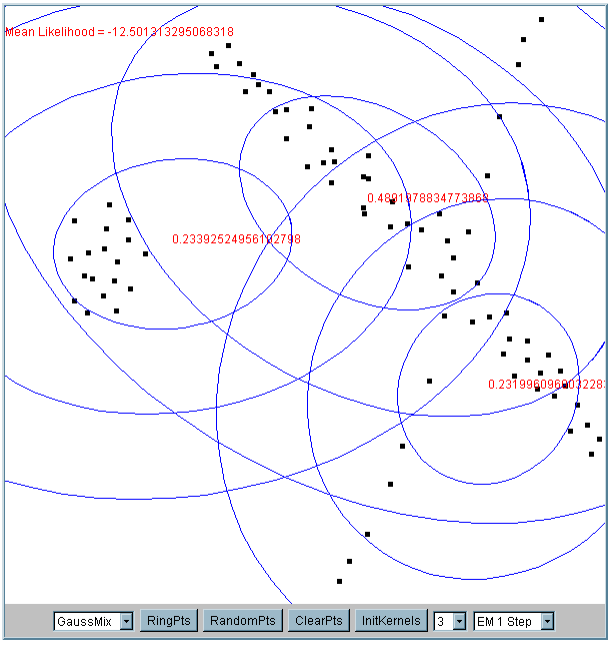
## Iteration 1

The cluster means are randomly assigned

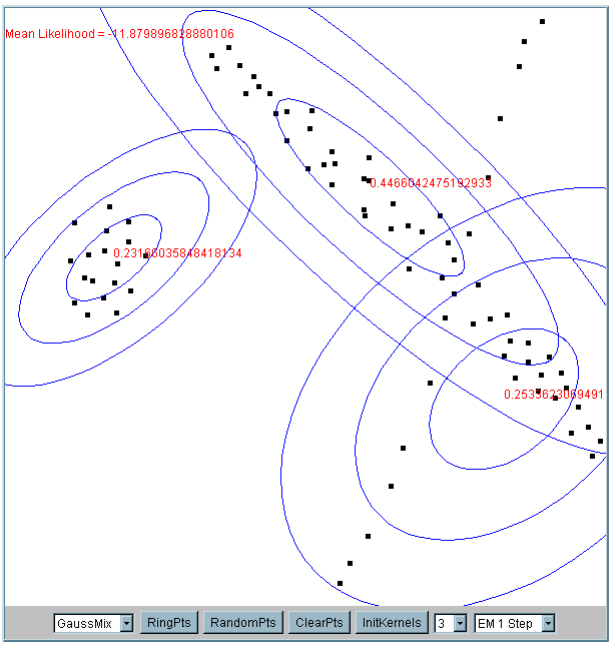





## Iteration 2

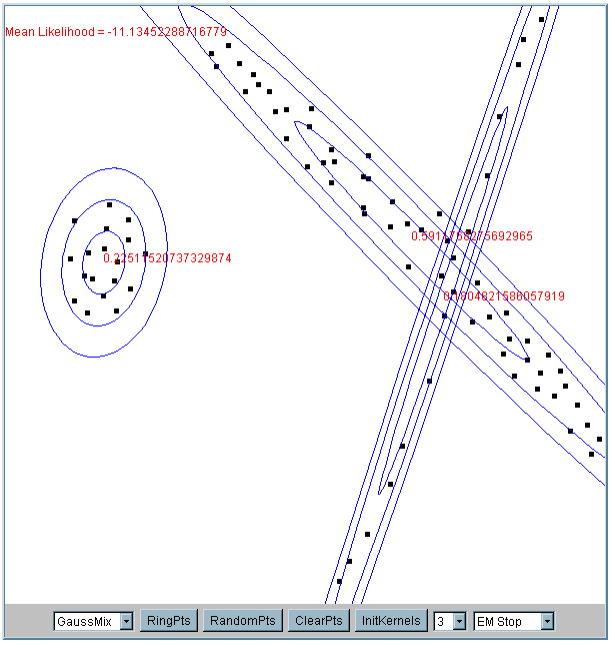


Iteration 5






Iteration 25



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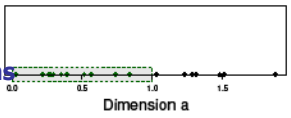
# Clustering High-Dimensional Data

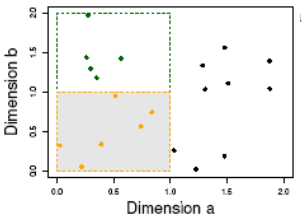
- Clustering high-dimensional data
  - Many applications: text documents, DNA micro-array data
  - Major challenges:
    - Many irrelevant dimensions may mask clusters
    - Distance measure becomes meaningless—due to equi-distance
    - Clusters may exist only in some subspaces
- Methods
  - Feature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

# The Curse of Dimensionality

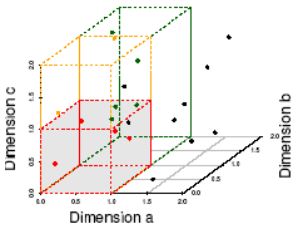
**(graphs adapted from Parsons et al. KDD Explorations 2004)**

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




(b) 6 Objects in One Unit Bin

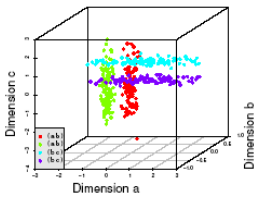



(c) 4 Objects in One Unit Bin

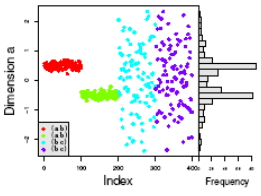


# Why Subspace Clustering?

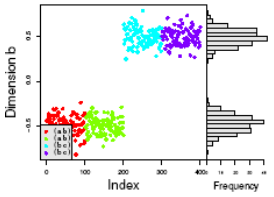
**(adapted from Parsons et al. SIGKDD Explorations 2004)**



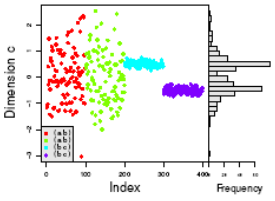

- Clusters may exist only in some subspaces
- Subspace-clustering: find clusters in all the subspaces



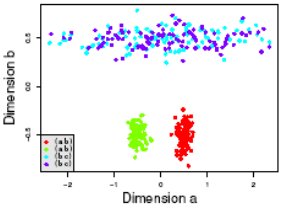

(a) Dimension $a$



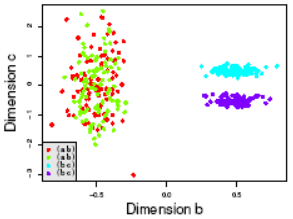

(b) Dimension $b$



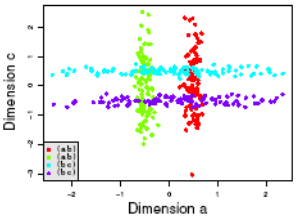

(c) Dimension $c$




(a) Dims $a$ & $b$




(b) Dims $b$ & $c$




(c) Dims $a$ & $c$

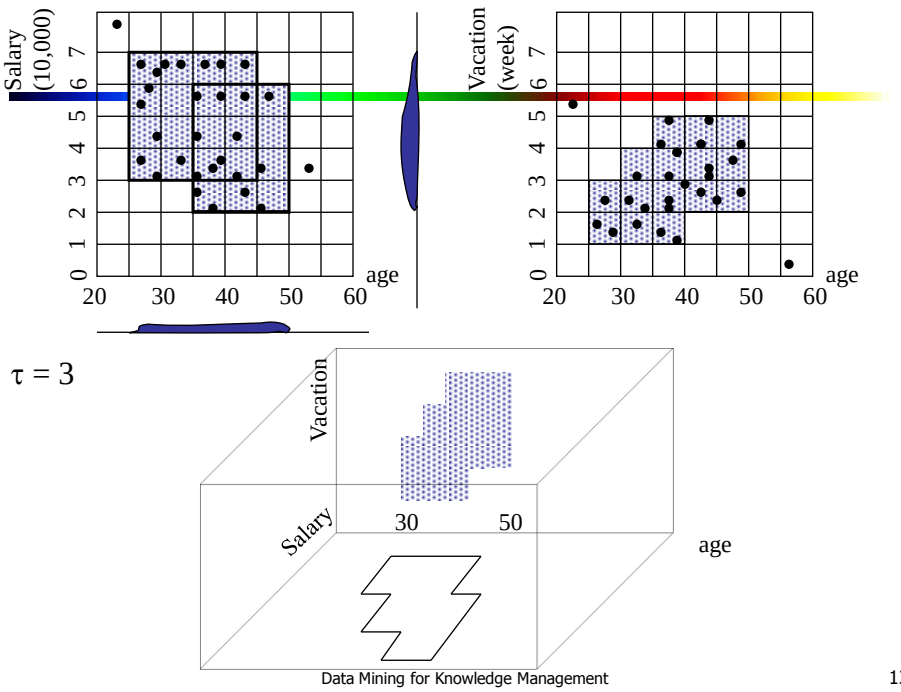
# CLIQUE (Clustering In QUEst)

- 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






# Strength and Weakness of *CLIQUE*

- Strength
  - *automatically* finds subspaces of the highest dimensionality such that high density clusters exist in those subspaces
  - *insensitive* to the order of records in input and does not presume some canonical data distribution
  - 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

# Roadmap

1. What is Cluster Analysis?
2. Types of Data in Cluster Analysis
3. A Categorization of Major Clustering Methods
4. Partitioning Methods
5. Hierarchical Methods
6. Density-Based Methods
7. Grid-Based Methods
8. Model-Based Methods
9. Clustering High-Dimensional Data
10. Constraint-Based Clustering
11. Summary



# Summary

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

# Problems and Challenges

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



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