CS 591.03
Data Mining Techniques
Instructor: Abdullah Mueen

LECTURE 6: BASIC CLUSTERING

Chapter 10. Cluster Analysis: Basic Concepts and Methods

What is Cluster Analysis?

Cluster: A collection of data objects
- similar (or related) to one another within the same group
- dissimilar (or unrelated) to the objects in other groups

Cluster analysis (or *clustering*, *data segmentation, …*)
- Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters

Unsupervised learning: no predefined classes (i.e., *learning by observations* vs. learning by examples: supervised)

Typical applications
- As a stand-alone tool to get insight into data distribution
- As a preprocessing step for other algorithms

Applications of Cluster Analysis

Data reduction

- Summarization: Preprocessing for regression, PCA, classification, and association analysis
- Compression: Image processing: vector quantization

Hypothesis generation and testing

Prediction based on groups

- Cluster & find characteristics/patterns for each group

Finding K-nearest Neighbors

- Localizing search to one or a small number of clusters

Outlier detection: Outliers are often viewed as those “far away” from any cluster

Clustering: Application Examples

Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species

Information retrieval: document clustering

Land use: Identification of areas of similar land use in an earth observation database

Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs

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

Climate: understanding earth climate, find patterns of atmospheric and ocean

Economic Science: market resarch

Basic Steps to Develop a Clustering Task

Feature selection
- Select info concerning the task of interest
- Minimal information redundancy

Proximity measure
- Similarity of two feature vectors

Clustering criterion
- Expressed via a cost function or some rules

Clustering algorithms
- Choice of algorithms

Validation of the results
- Validation test (also, *clustering tendency* test)

Interpretation of the results
- Integration with applications

Quality: What Is Good Clustering?

A good clustering method will produce high quality clusters

- high intra-class similarity: cohesive within clusters
- low inter-class similarity: distinctive between clusters

The quality of a clustering method depends on

- the similarity measure used by the method
- its implementation, and
- Its ability to discover some or all of the hidden patterns

Measure the Quality of Clustering

Dissimilarity/Similarity metric

- Similarity is expressed in terms of a distance function, typically metric: $d(i, j)$
- The definitions of distance functions are usually rather different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables
- Weights should be associated with different variables based on applications and data semantics

Quality of clustering:

- There is usually a separate "quality" function that measures the "goodness" of a cluster.
- It is hard to define "similar enough" or "good enough"
  - The answer is typically highly subjective

Considerations for Cluster Analysis

Partitioning criteria

- Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)

Separation of clusters

- Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)

Similarity measure

- Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)

Clustering space

- Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

Requirements and Challenges

Scalability
- Clustering all the data instead of only on samples

Ability to deal with different types of attributes
- Numerical, binary, categorical, ordinal, linked, and mixture of these

Constraint-based clustering
- User may give inputs on constraints
- Use domain knowledge to determine input parameters

Interpretability and usability

Others
- Discovery of clusters with arbitrary shape
- Ability to deal with noisy data
- Incremental clustering and insensitivity to input order
- High dimensionality

Major Clustering Approaches (I)

Partitioning approach:
- Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
- Typical methods: k-means, k-medoids, CLARANS

Hierarchical approach:
- Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Typical methods: Diana, Agnes, BIRCH, CAMELEON

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

Grid-based approach:
- based on a multiple-level granularity structure
- Typical methods: STING, WaveCluster, CLIQUE

Major Clustering Approaches (II)

Model-based:
- A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
- Typical methods: EM, SOM, COBWEB

Frequent pattern-based:
- Based on the analysis of frequent patterns
- Typical methods: p-Cluster

User-guided or constraint-based:
- Clustering by considering user-specified or application-specific constraints
- Typical methods: COD (obstacles), constrained clustering

Link-based clustering:
- Objects are often linked together in various ways
- Massive links can be used to cluster objects: SimRank, LinkClus

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Cluster Analysis: Basic Concepts

Partitioning Methods 

Hierarchical Methods

Density-Based Methods

Grid-Based Methods

Evaluation of Clustering

Summary

Partitioning Algorithms: Basic Concept

Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (d(p, c_i))^2$$

Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion

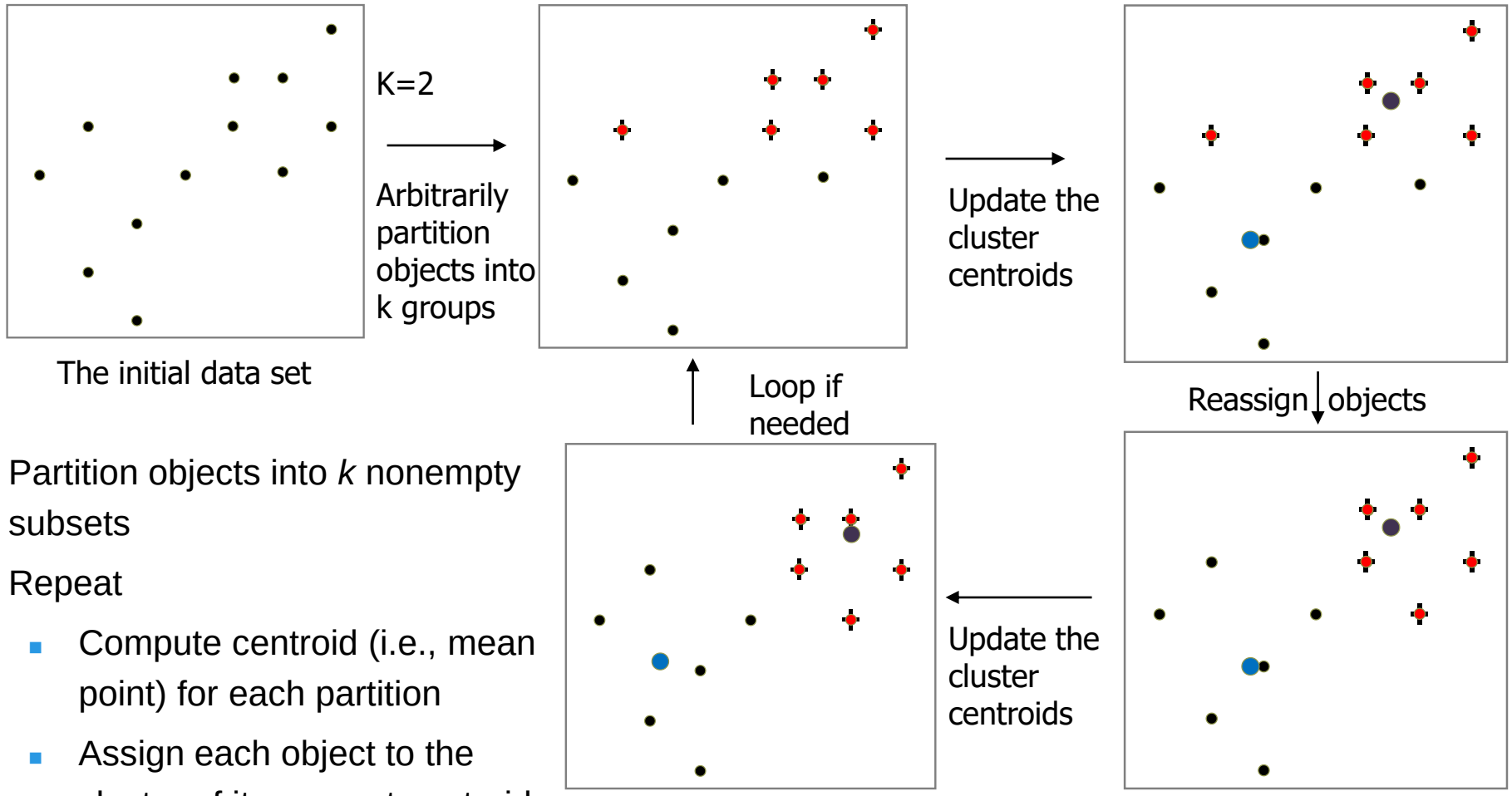
- Global optimal: exhaustively enumerate all partitions
- Heuristic methods: *k-means* and *k-medoids* algorithms
- *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
- *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

The *K-Means* Clustering Method

Given *k*, the *k-means* algorithm is implemented in four steps:

- Partition objects into *k* nonempty subsets
- Compute seed points as the centroids of the clusters of the current partitioning (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 the assignment does not change

An Example of *K-Means* Clustering



- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

Comments on the *K-Means* Method

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

- Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$

Comment: Often terminates at a *local optimal*

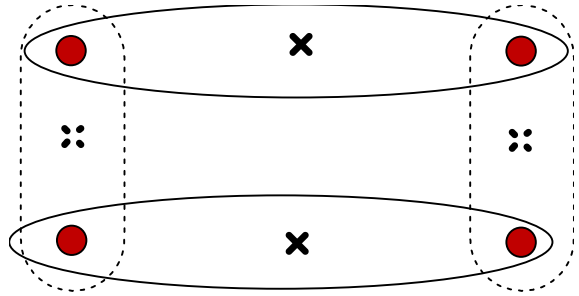
Weakness

- Applicable only to objects in a continuous n-dimensional space
  - Using the k-modes method for categorical data
  - In comparison, k-medoids can be applied to a wide range of data
- Need to specify *k,* the *number* of clusters, in advance (there are ways to automatically determine the best k (see Hastie et al., 2009)
- Sensitive to noisy data and *outliers*
- Not suitable to discover clusters with *non-convex shapes*

Variations of the *K-Means* Method

Most of the 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*

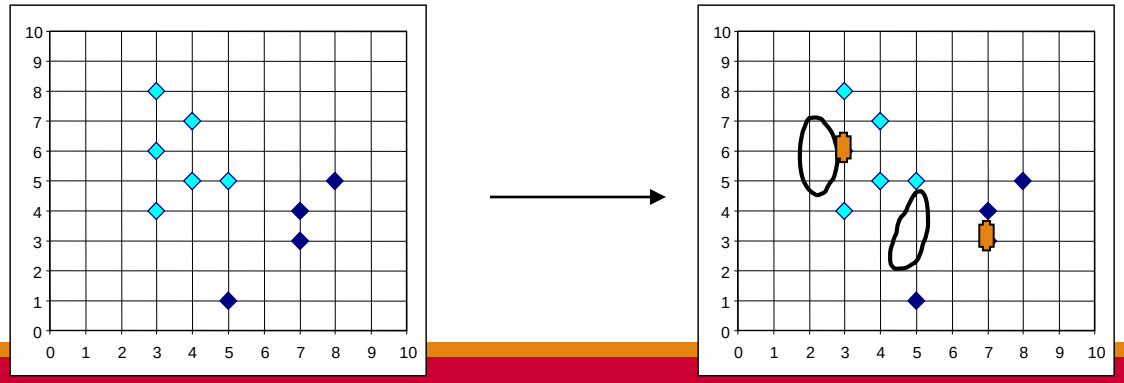
- Replacing means of clusters with modes
- Using new dissimilarity measures to deal with categorical objects
- Using a frequency-based method to update modes of clusters
- A mixture of categorical and numerical data: *k-prototype* method

What Is the Problem of the K-Means Method?

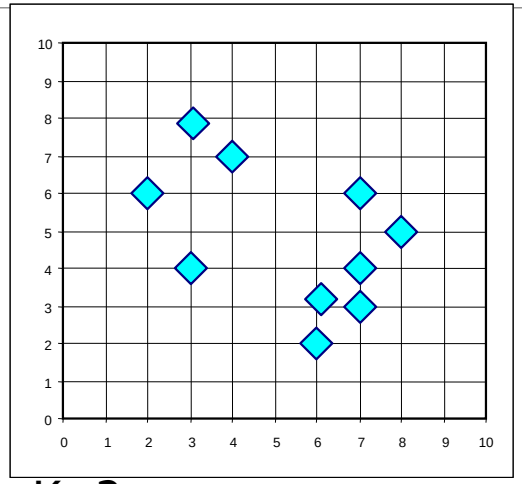
The k-means algorithm is sensitive to outliers !

- Since an object with an extremely large value may substantially distort the distribution of the data

K-Medoids: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster

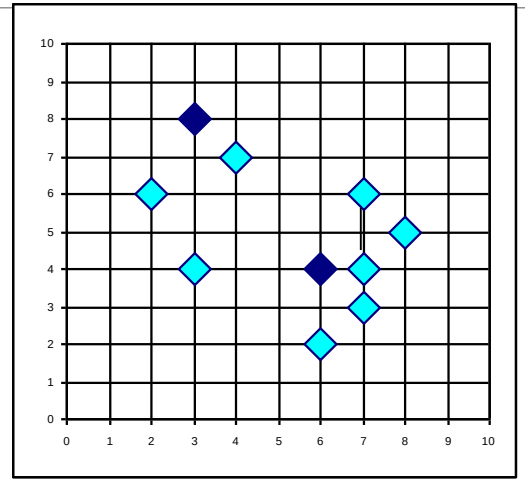


PAM: A Typical K-Medoids Algorithm



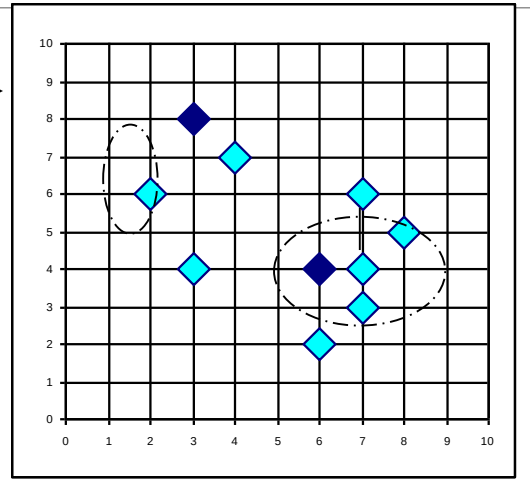
K=2

Arbitrary choose k object as initial medoids

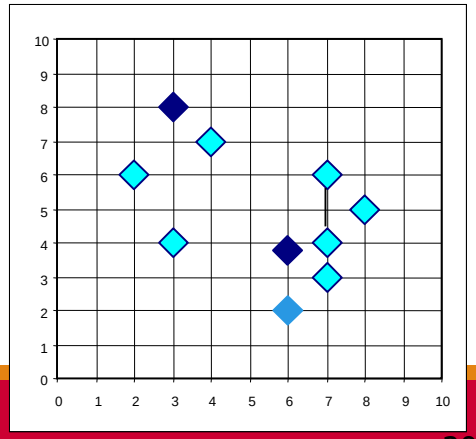


Assign each remaining object to nearest medoids

Total Cost = 20

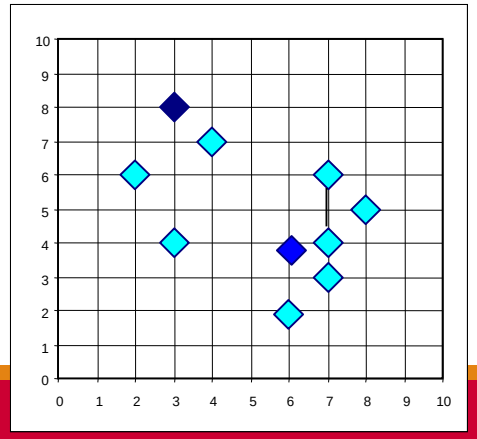


Randomly select a nonmedoid object, O_{ramdom}



Compute total cost of swapping

Total Cost = 26



Swapping O and O_{ramdom}

If quality is improved.

Do loop

Until no change

The K-Medoid Clustering Method

K-Medoids Clustering: Find *representative* objects (medoids) in clusters

- *PAM* (Partitioning Around Medoids, Kaufmann & Rousseeuw 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 (due to the computational complexity)

Efficiency improvement on PAM

- *CLARA* (Kaufmann & Rousseeuw, 1990): PAM on samples
- *CLARANS* (Ng & Han, 1994): Randomized re-sampling

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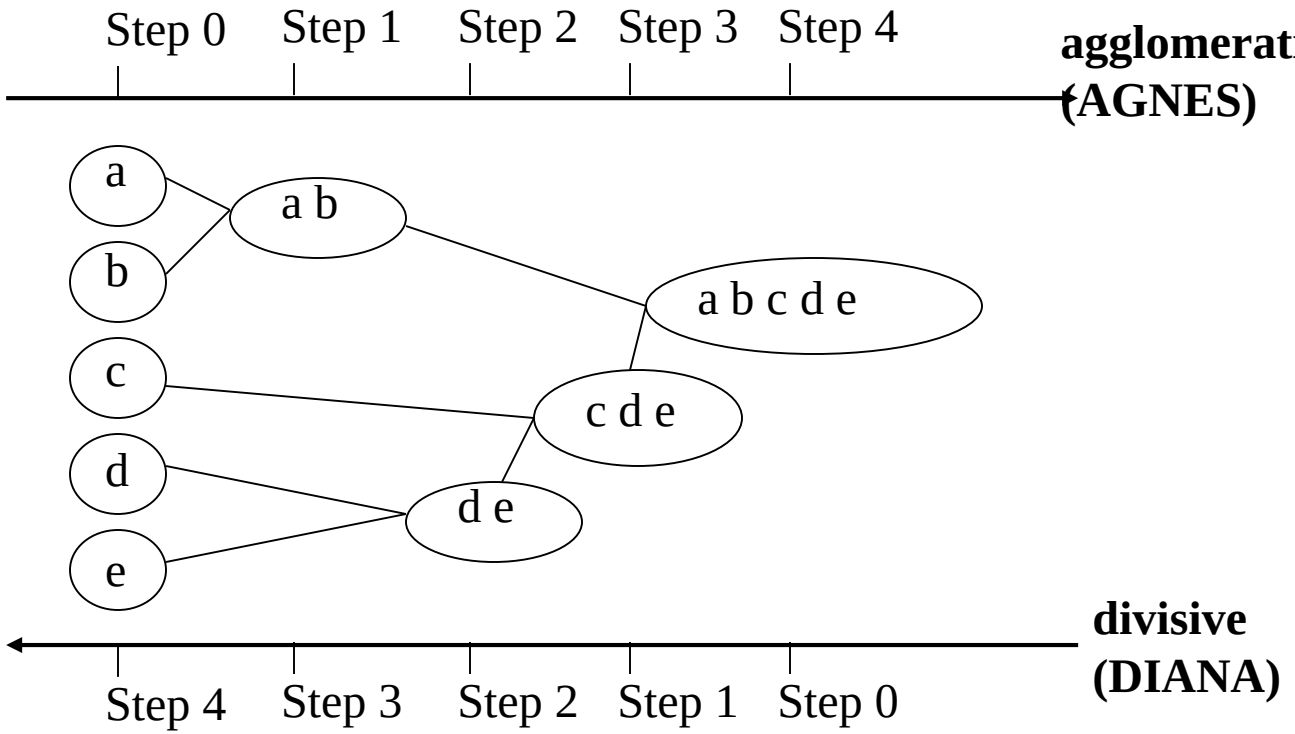
Hierarchical Clustering

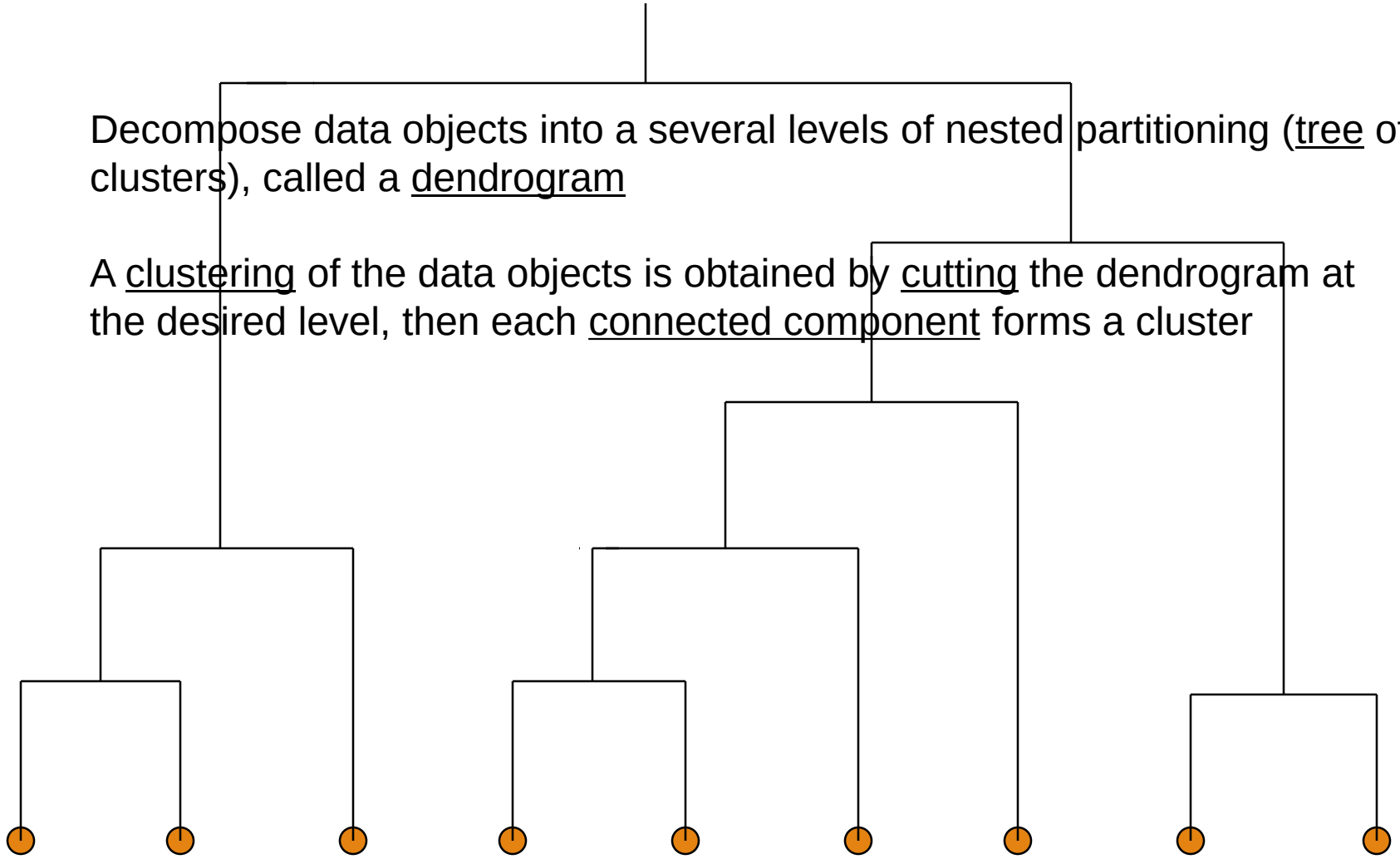
Use distance matrix as clustering criteria. This method does not require the number of clusters ***k*** as an input, but needs a termination condition



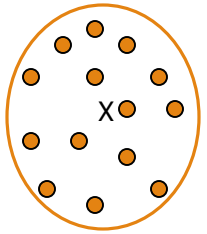
Dendrogram: Shows How Clusters are Merged

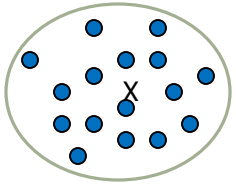
Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram

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



Distance between Clusters





Single link: smallest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = min(t_{ip}, t_{jq})$

Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = max(t_{ip}, t_{jq})$

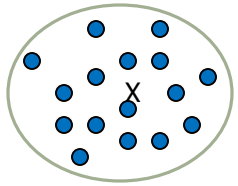
Average: avg distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = avg(t_{ip}, t_{jq})$

Centroid: distance between the centroids of two clusters, i.e., $dist(K_i, K_j) = dist(C_i, C_j)$

Medoid: distance between the medoids of two clusters, i.e., $dist(K_i, K_j) = dist(M_i, M_j)$

- Medoid: a chosen, centrally located object in the cluster

Centroid, Radius and Diameter of a Cluster (for numerical data sets)



Centroid: the "middle" of a cluster

$$C_m = \frac{\sum_{i=1}^{N} (t_{ip})}{N}$$

Radius: square root of average distance from any point of the cluster to its centroid

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

Diameter: square root of average mean squared distance between all pairs of points in the cluster

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

Extensions to Hierarchical Clustering

Major weakness of agglomerative clustering methods

- Can never undo what was done previously
- Do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects

Integration of hierarchical & distance-based clustering

- BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
- CHAMELEON (1999): hierarchical clustering using dynamic modeling

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): ***CF = (N, LS, SS)***

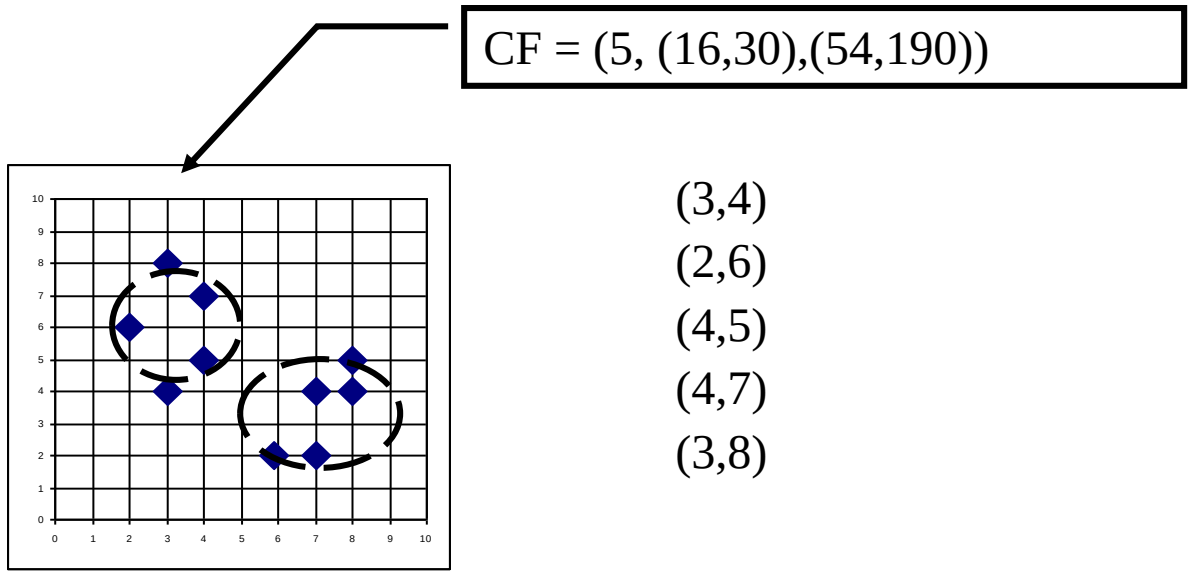
N: **Number of data points**

LS: linear sum of N points:

$$\sum_{i=1}^{N} X_i$$

SS: square sum of N points

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



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

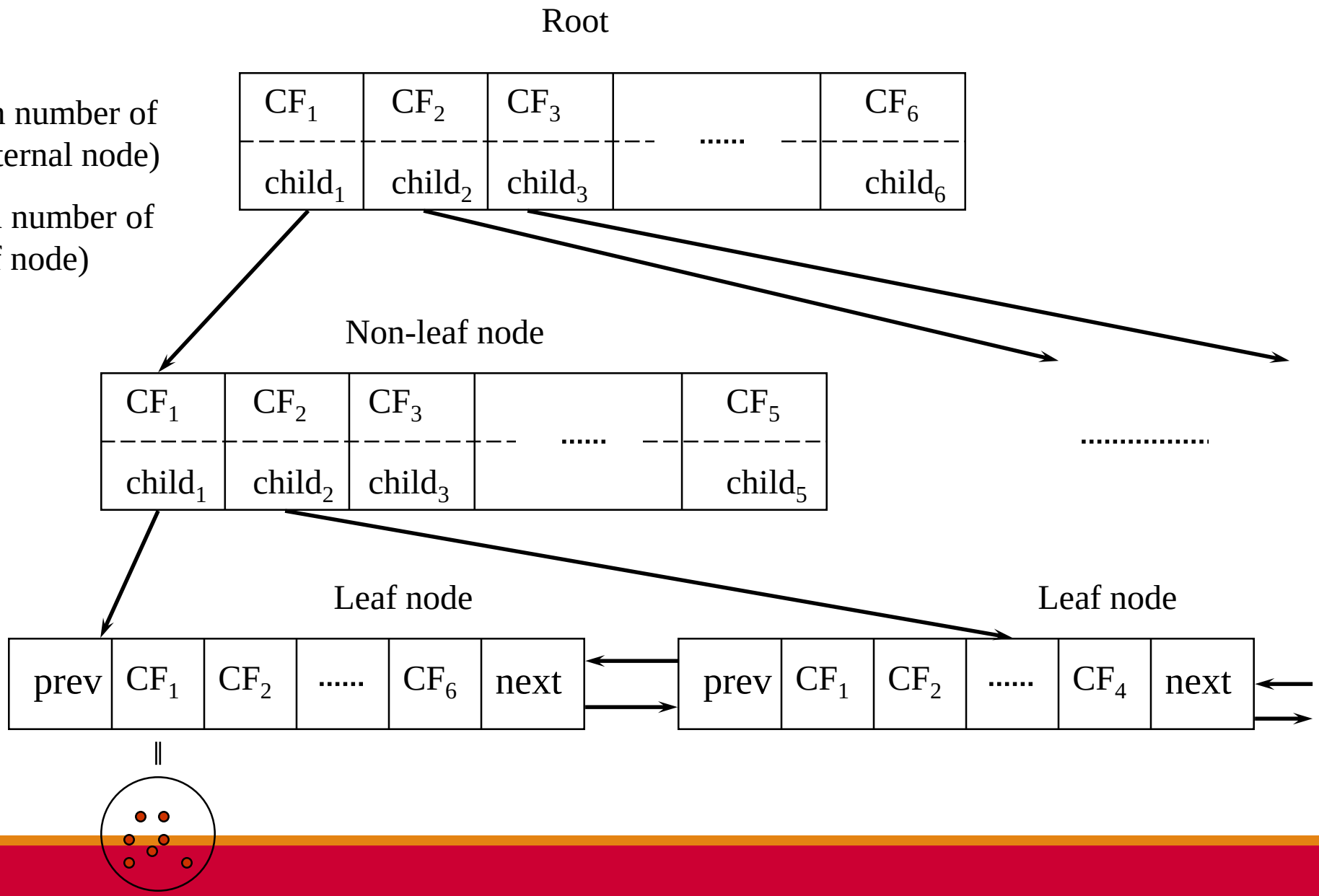
A CF tree has two parameters

- Branching factor: max # of children
- Threshold: max diameter of sub-clusters stored at the leaf nodes

The CF Tree Structure

B = 7 (maximum number of children in an internal node)

L = 6 (maximum number of children in a leaf node)



The Birch Algorithm

Cluster Diameter

$$\sqrt{\frac{1}{n(n-1)}\sum(x_i - x_j)^2}$$

For each point in the input
- Find closest leaf entry
- Add point to leaf entry and update CF
- If entry diameter > max_diameter, then split leaf, and possibly parents

Algorithm is O(n)

Concerns
- Sensitive to insertion order of data points
- Since we fix the size of leaf nodes, so clusters may not be so natural
- Clusters tend to be spherical given the radius and diameter measures

CHAMELEON: Hierarchical Clustering Using Dynamic Modeling (1999)

CHAMELEON: G. Karypis, E. H. Han, and V. Kumar, 1999

Measures the similarity based on a dynamic model

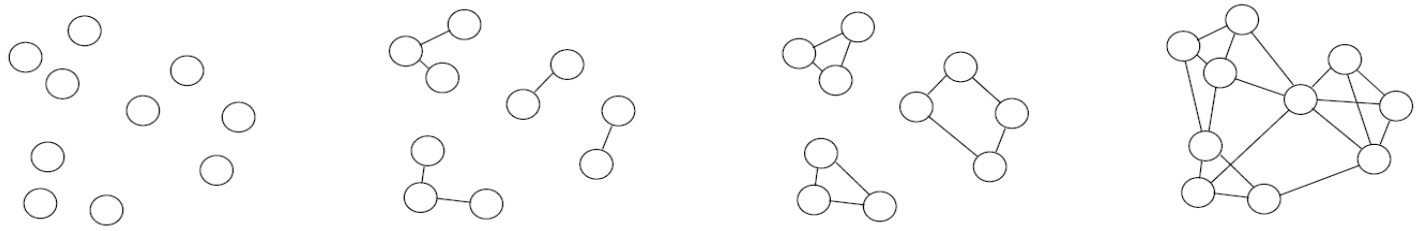
- Two clusters are merged only if the *interconnectivity* and *closeness (proximity)* between two clusters are high *relative to* the internal interconnectivity of the clusters and closeness of items within the clusters

Graph-based, and 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

KNN Graphs & Interconnectivity

k-nearest graphs from an original data in 2D:



(a) Original Data in 2D (b) 1-nearest neighbor graph (c) 2-nearest neighbor graph (d) 3-nearest neighbor graph

$EC_{\{Ci,Cj\}}$.The absolute inter-connectivity between C_i *and* C_j*: the sum* of the weight of the edges that connect vertices in C_i *to vertices in* C_j

Internal inter-connectivity of a cluster C_i : *the size of its min-cut bisector* EC_{Ci} *(i.e., the weighted sum* of edges that partition the graph into two roughly equal parts)

Relative Inter-connectivity (RI):

$$RI(C_i, C_j) = \frac{|EC_{\{C_i,C_j\}}|}{\frac{|EC_{C_i}|+|EC_{C_j}|}{2}}$$

Relative Closeness & Merge of Sub-Clusters

Relative closeness between a pair of clusters C_i *and* C_j *: the absolute closeness* between C_i *and* C_j *normalized w.r.t. the internal closeness of the two clusters* C_i *and* C_j

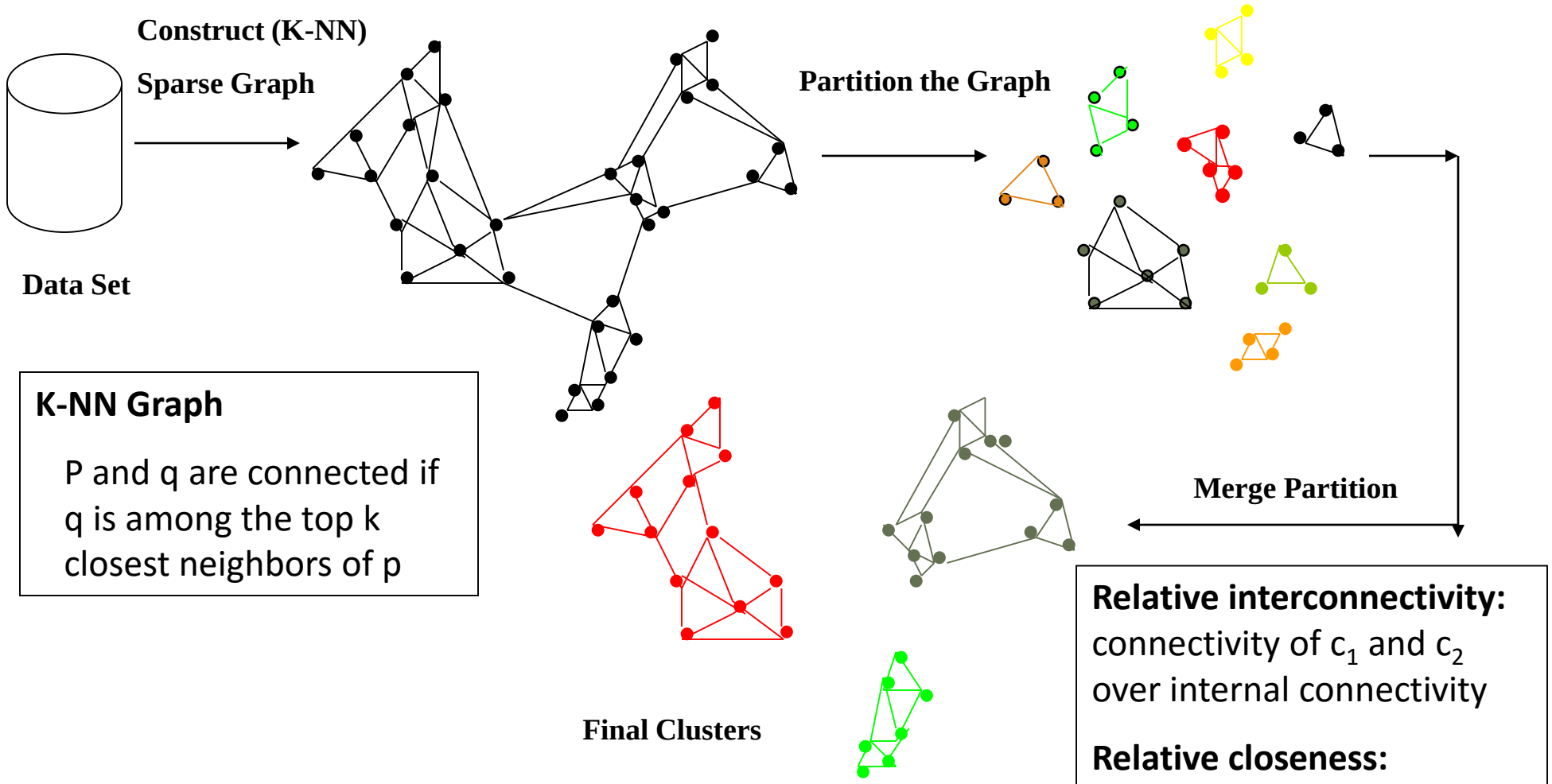
$$RC(C_i, C_j) = \frac{\overline{S}_{EC_{\{C_i, C_j\}}}}{\frac{|C_i|}{|C_i|+|C_j|}\overline{S}_{EC_{C_i}} + \frac{|C_j|}{|C_i|+|C_j|}\overline{S}_{EC_{C_j}}}$$

- $\overline{S}_{EC_{C_i}}$ and $\overline{S}_{EC_{C_j}}$ are the average weights of the edges that belong in the min-cut bisector of clusters C_i *and* C_j, respectively, and $\overline{S}_{EC_{\{C_i, C_j\}}}$ *i*s the average weight of the edges that connect vertices in C_i *to vertices in* C_j

Merge Sub-Clusters:

- Merges only those pairs of clusters whose RI and RC are both above some user-specified thresholds
- Merge those maximizing the function that combines RI and RC

Overall Framework of CHAMELEON



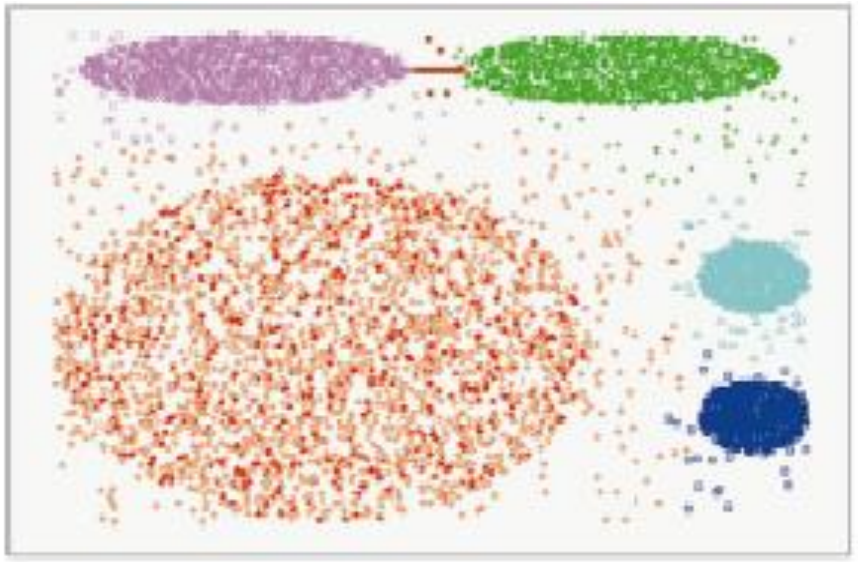
K-NN Graph

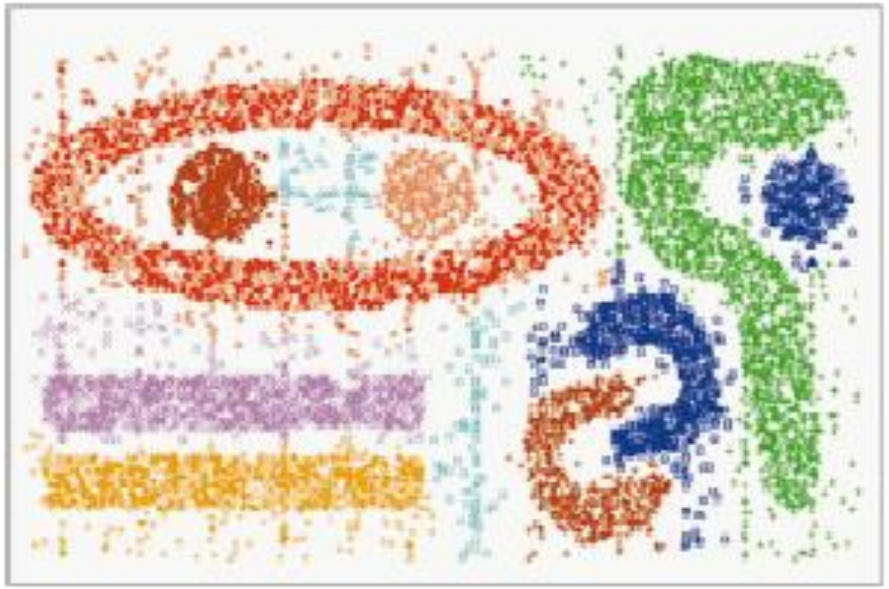
P and q are connected if q is among the top k closest neighbors of p

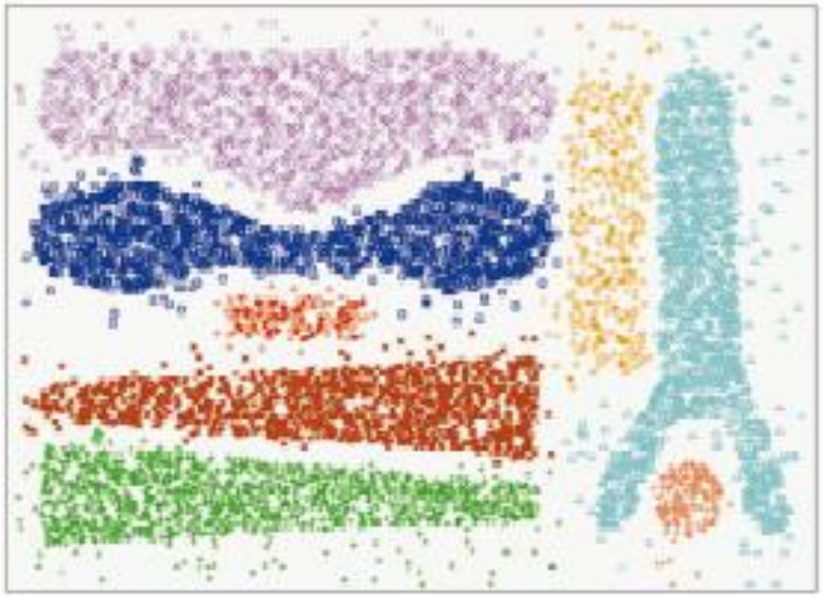
Relative interconnectivity: connectivity of c_1 and c_2 over internal connectivity

Relative closeness: closeness of c_1 and c_2 over internal closeness

CHAMELEON (Clustering Complex Objects)







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Cluster Analysis: Basic Concepts

Partitioning Methods

Hierarchical Methods

Density-Based Methods

Grid-Based Methods

Evaluation of Clustering

Summary

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*:*

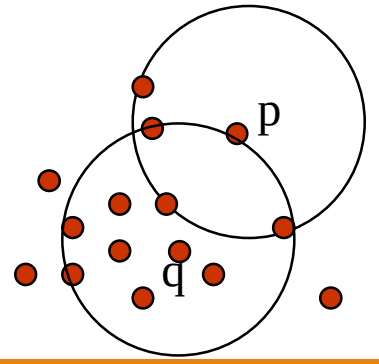
- *Eps*: Maximum radius of the neighbourhood
- *MinPts*: Minimum number of points in an Eps-neighbourhood of that point

$N_{Eps}(q)$: {p belongs to D | 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:

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



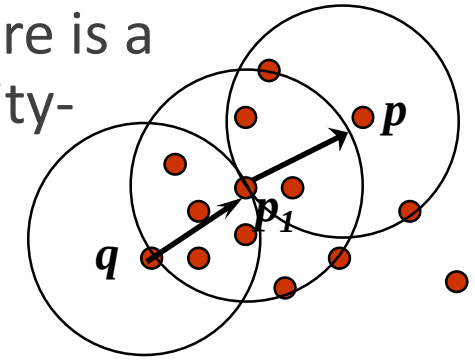
MinPts = 5

Eps = 1 cm

Density-Reachable and Density-Connected

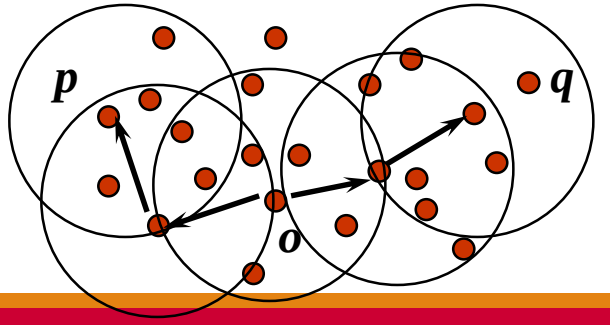
Density-reachable:

- 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

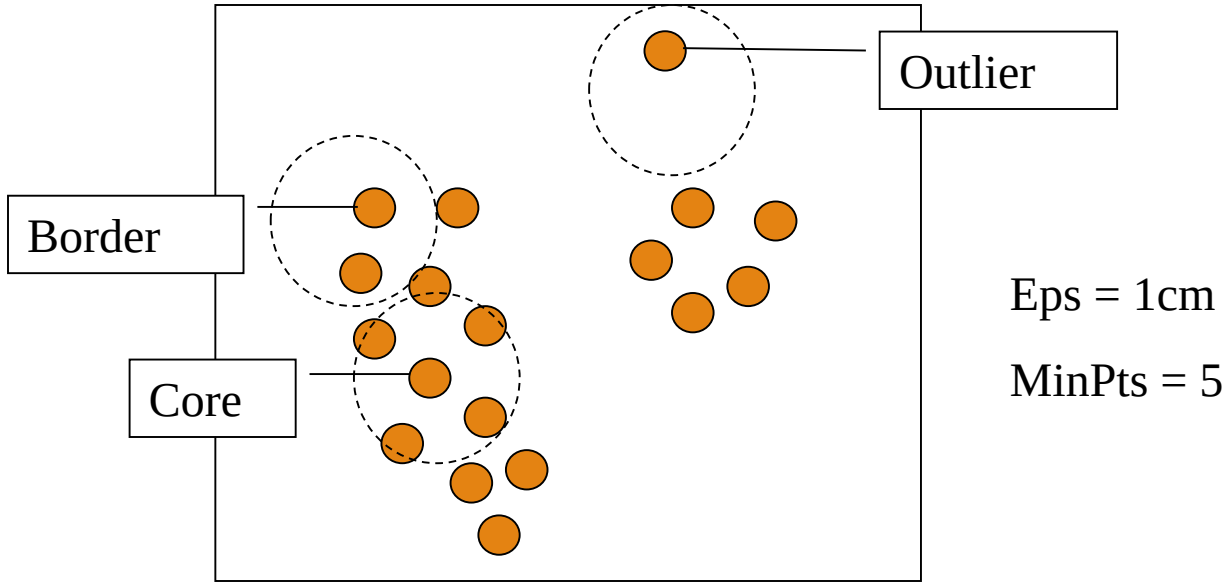
- A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



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

If a spatial index is used, the computational complexity of DBSCAN is O(nlogn), where n is the number of database objects. Otherwise, the complexity is $O(n^2)$

DBSCAN: Sensitive to Parameters

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

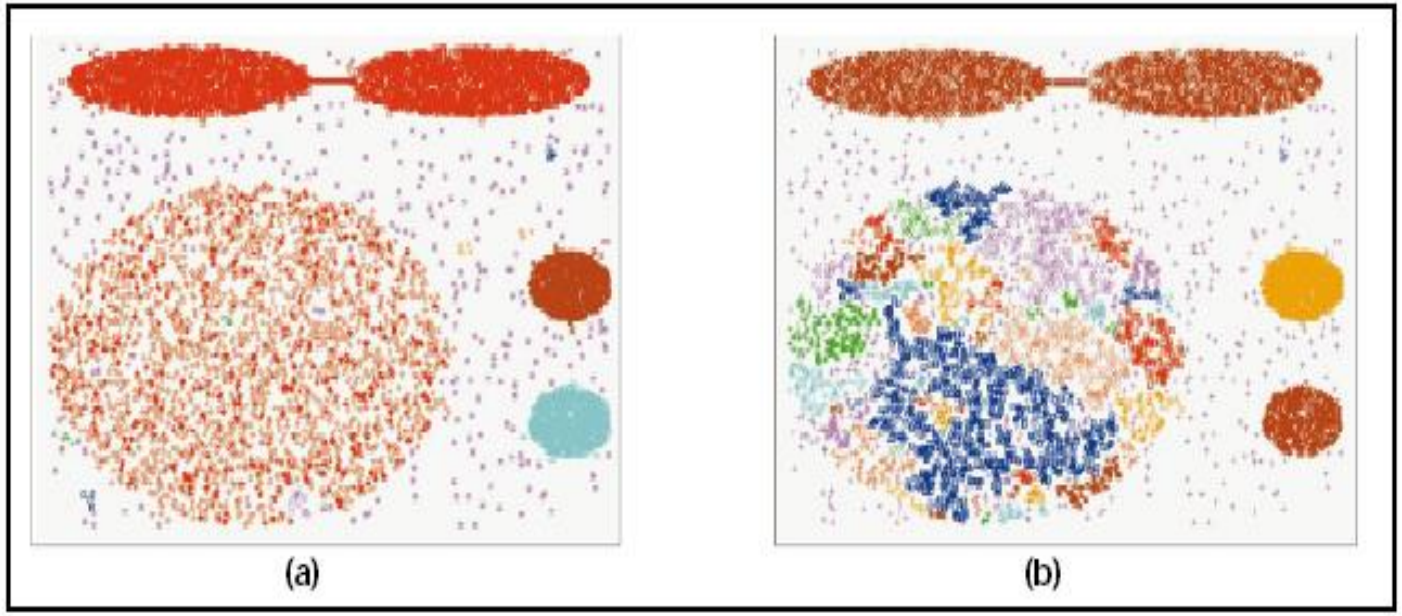
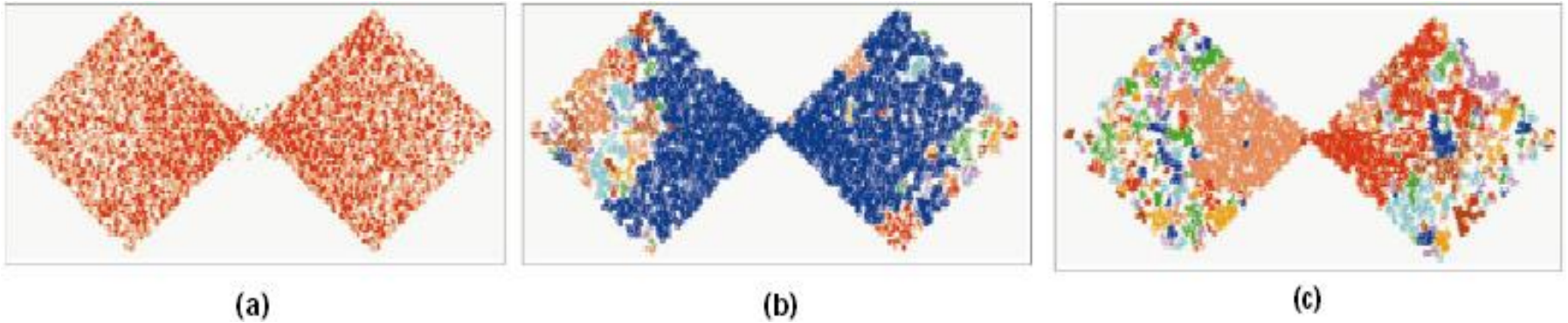


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



DBSCAN online Demo:

http://webdocs.cs.ualberta.ca/~yaling/Cluster/Applet/Code/Cluster.html

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

OPTICS: Some Extension from DBSCAN

Index-based: k = # of dimensions, N: # of points
- Complexity: O(N*logN)

Core Distance of an object p: the smallest value ε such that the ε-neighborhood of p has at least MinPts objects

Let $N_\varepsilon(p)$: ε-neighborhood of p, ε is a distance value

$\text{Core-distance}_{\varepsilon, \text{MinPts}}(p)$ = Undefined if $\text{card}(N_\varepsilon(p)) < \text{MinPts}$

MinPts-distance(p), otherwise

Reachability Distance of object p from core object q is the min radius value that makes p density-reachable from q

$\text{Reachability-distance}_{\varepsilon, \text{MinPts}}(p, q)$ =

Undefined if q is not a core object

max(core-distance(q), distance (q, p)), otherwise

Core Distance & Reachability Distance

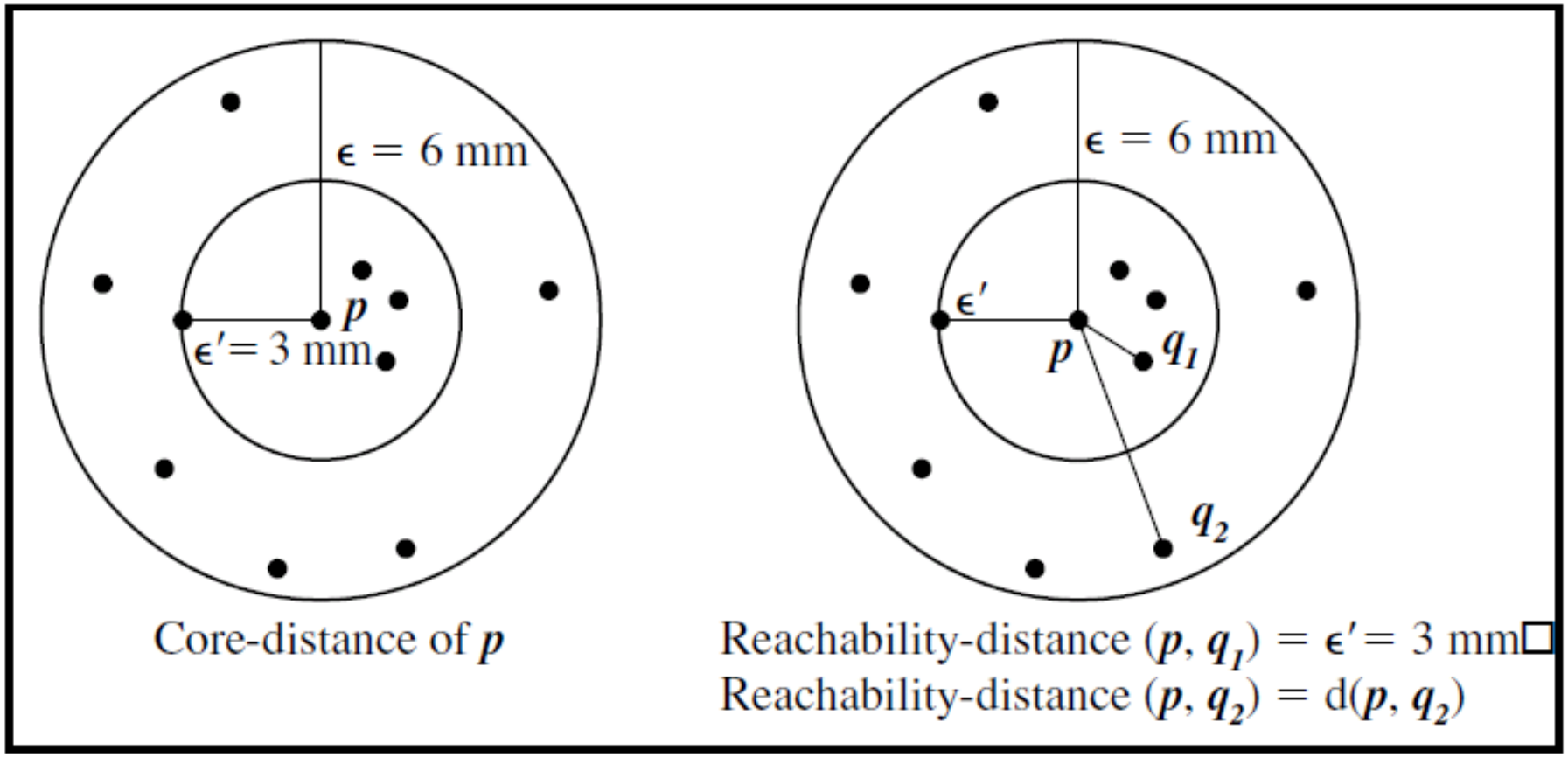
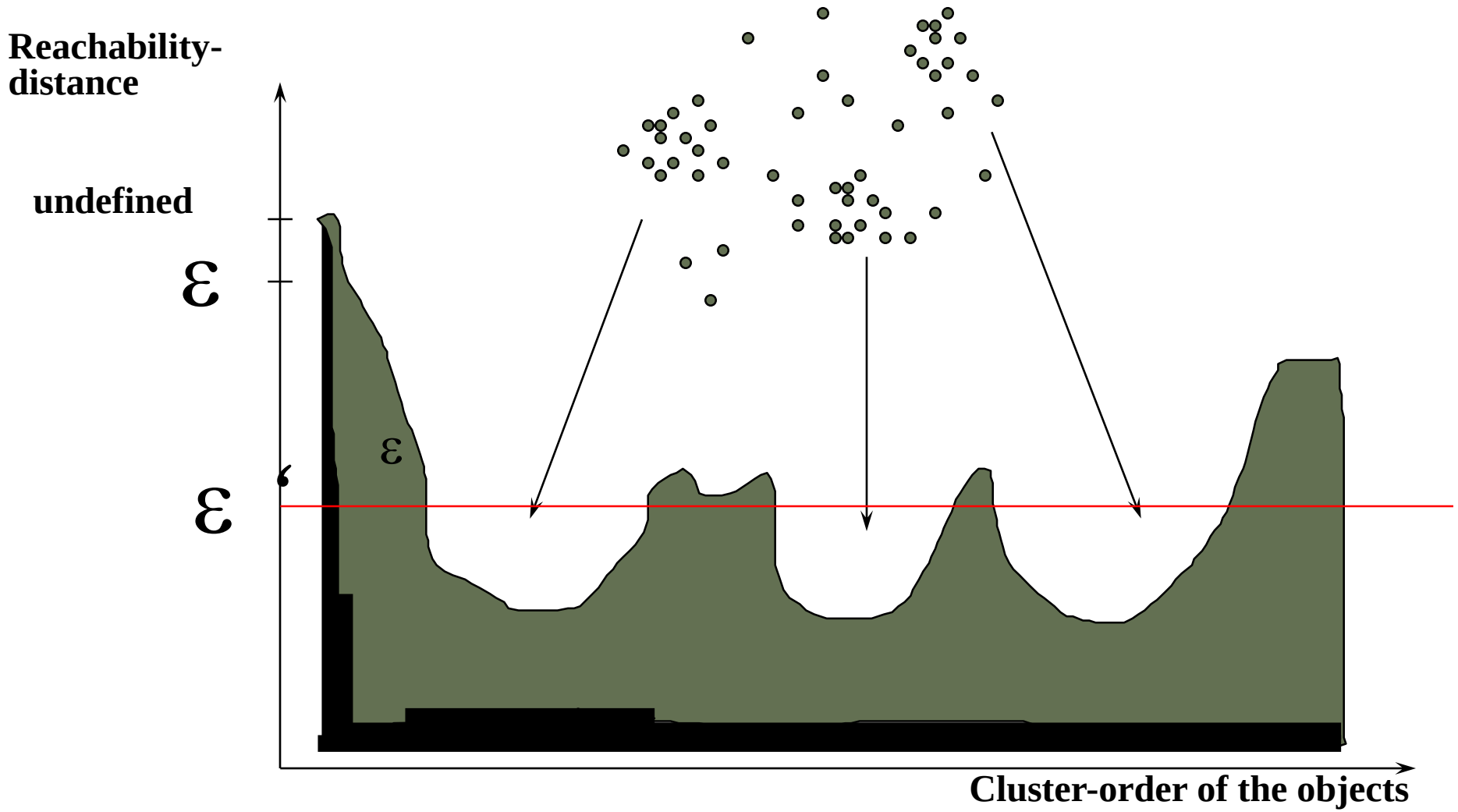
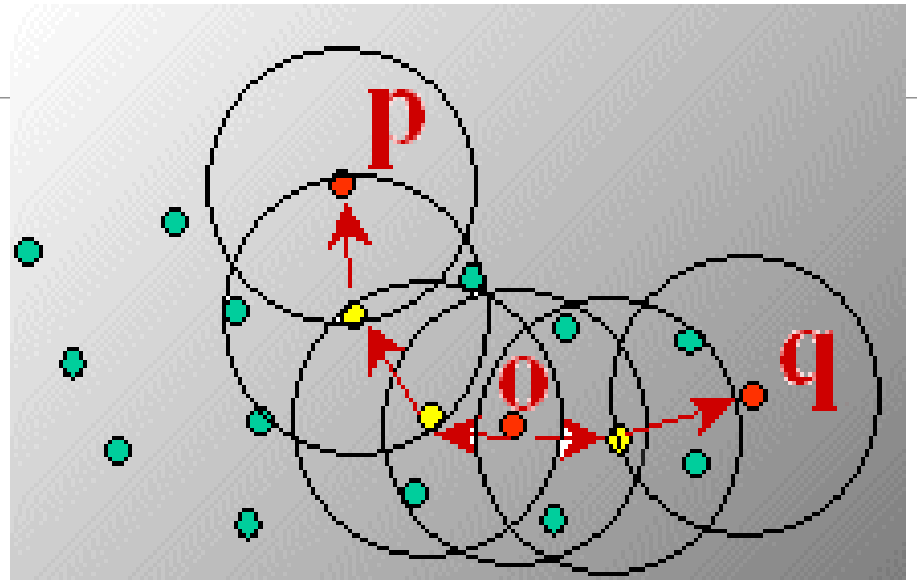


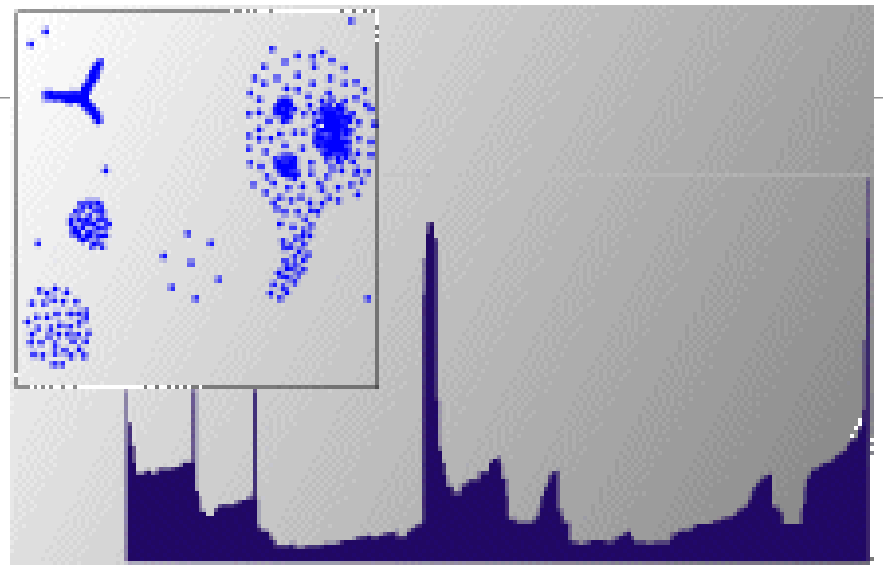
Figure 10.16: OPTICS terminology. Based on [ABKS99].

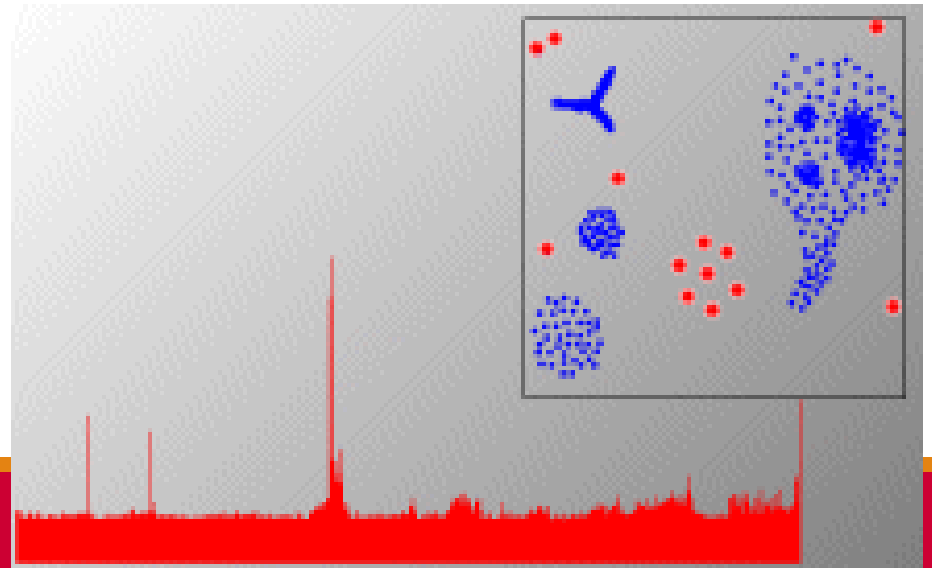

Reachability-
distance
undefined
ε
ε
ε
Cluster-order of the objects

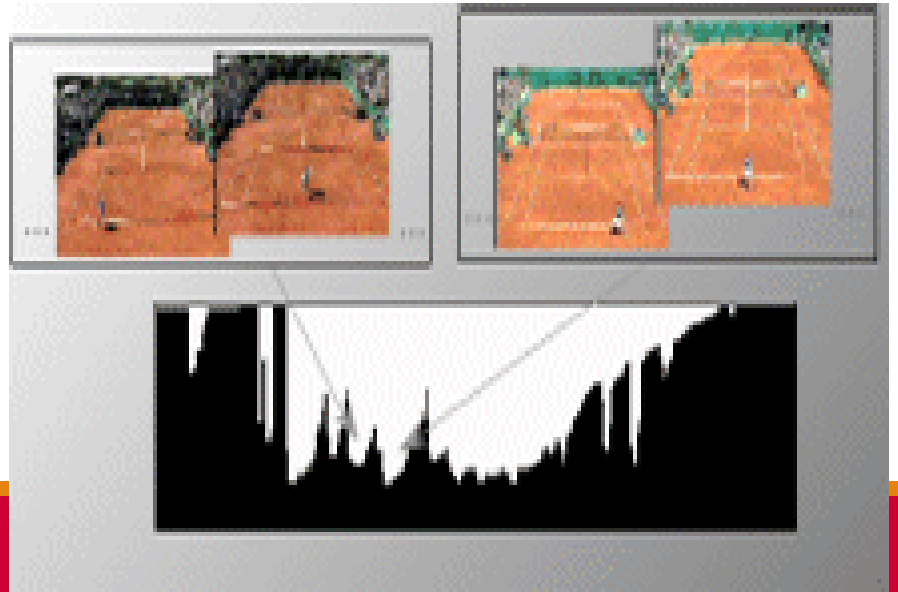
Density-Based Clustering: OPTICS & Applications

demo: http://www.dbs.informatik.uni-muenchen.de/Forschung/KDD/Clustering/OPTICS/Demo









DENCLUE: Using Statistical Density Functions

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

Using statistical density functions:

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

influence of y on x

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

total influence on x

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

gradient of x in the direction of x_i

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 (e.g., DBSCAN)
- But needs a large number of parameters

Denclue: Technical Essence

Uses grid cells but only keeps information about grid cells that do actually contain data points and manages these cells in a tree-based access structure

Influence function: describes the impact of a data point within its neighborhood

Overall density of the data space can be calculated as the sum of the influence function of all data points

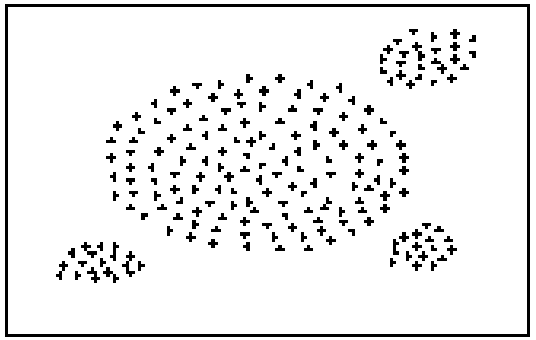
Clusters can be determined mathematically by identifying density attractors

Density attractors are local maximal of the overall density function

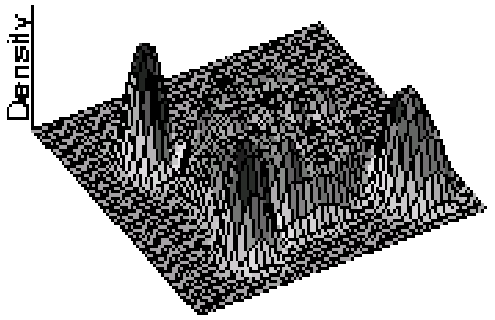
Center defined clusters: assign to each density attractor the points density attracted to it

Arbitrary shaped cluster: merge density attractors that are connected through paths of high density (> threshold)

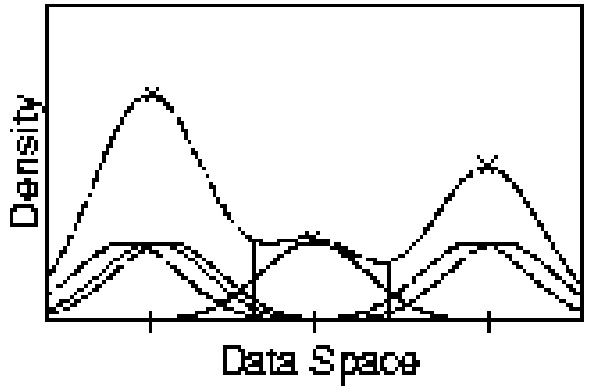
Density Attractor



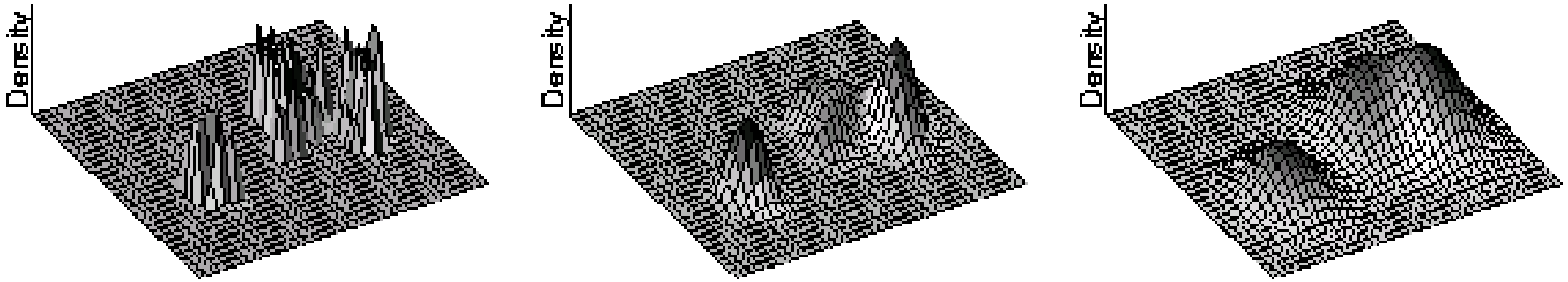
(a) Data Set



(c) Gaussian

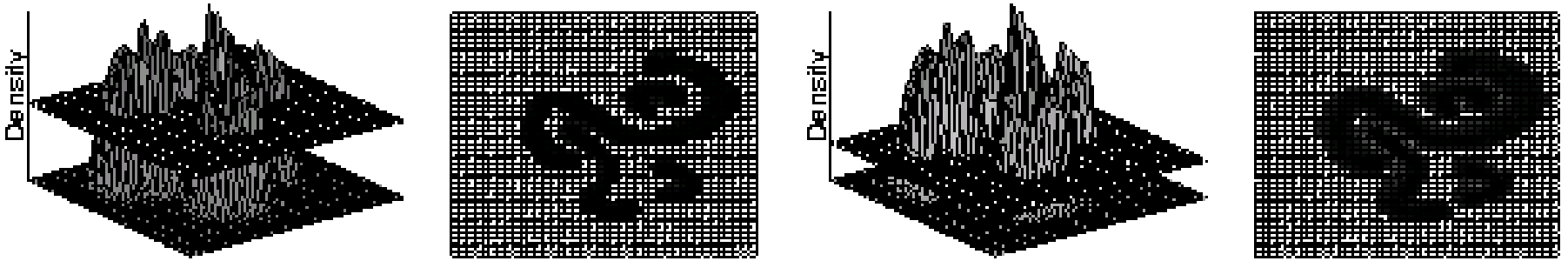


Center-Defined and Arbitrary



(a) $\sigma = 0.2$ (b) $\sigma = 0.6$ (d) $\sigma = 1.5$

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



(a) $\xi = 2$ (b) $\xi = 2$ (c) $\xi = 1$ (d) $\xi = 1$

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

Chapter 10. Cluster Analysis: Basic Concepts and Methods

Cluster Analysis: Basic Concepts

Partitioning Methods

Hierarchical Methods

Density-Based Methods

Grid-Based Methods 

Evaluation of Clustering

Summary

Grid-Based Clustering Method

Using multi-resolution grid data structure

Several interesting methods

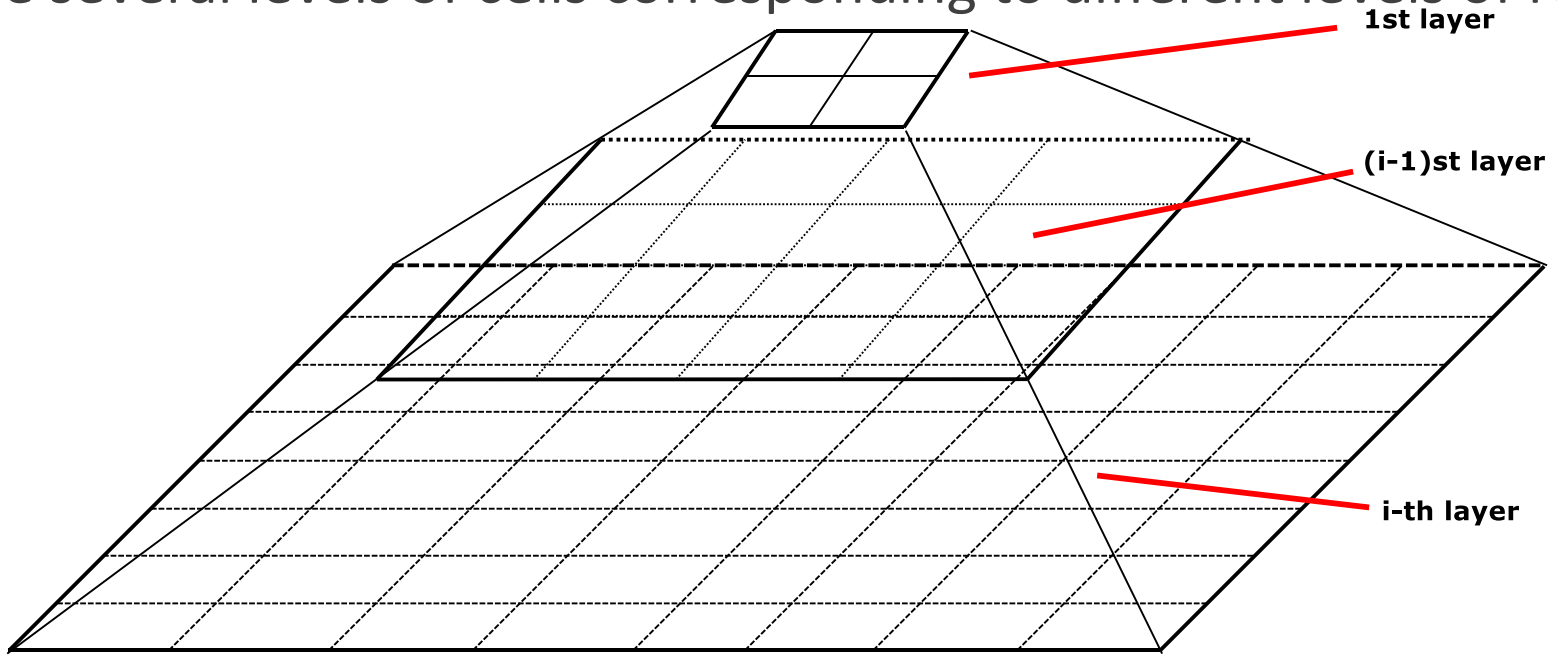
- STING (a STatistical INformation Grid approach) by Wang, Yang and Muntz (1997)
- CLIQUE: Agrawal, et al. (SIGMOD'98)
  - Both grid-based and subspace clustering
- WaveCluster by Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
  - A multi-resolution clustering approach using wavelet method

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



The STING Clustering Method

Each cell at a high level is partitioned into a number of smaller cells in the next lower level

Statistical info of each cell is calculated and stored beforehand and is used to answer queries

Parameters of higher level cells can be easily calculated from parameters of lower level cell

- *count*, *mean*, *s*, *min*, *max*
- type of distribution—*normal*, *uniform*, etc.

Use a top-down approach to answer spatial data queries

Start from a pre-selected layer—typically with a small number of cells

For each cell in the current level compute the confidence interval

STING Algorithm and Its Analysis

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

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.

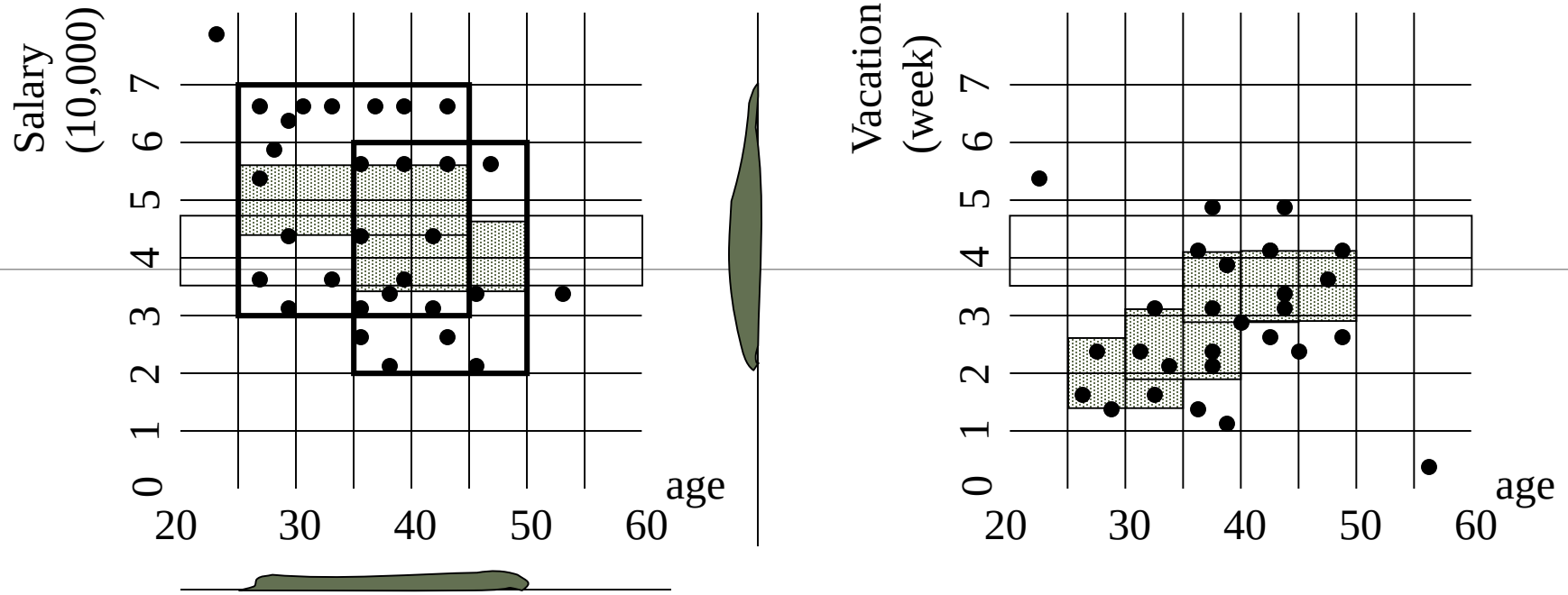
Identify the subspaces that contain clusters using the Apriori principle

Identify clusters

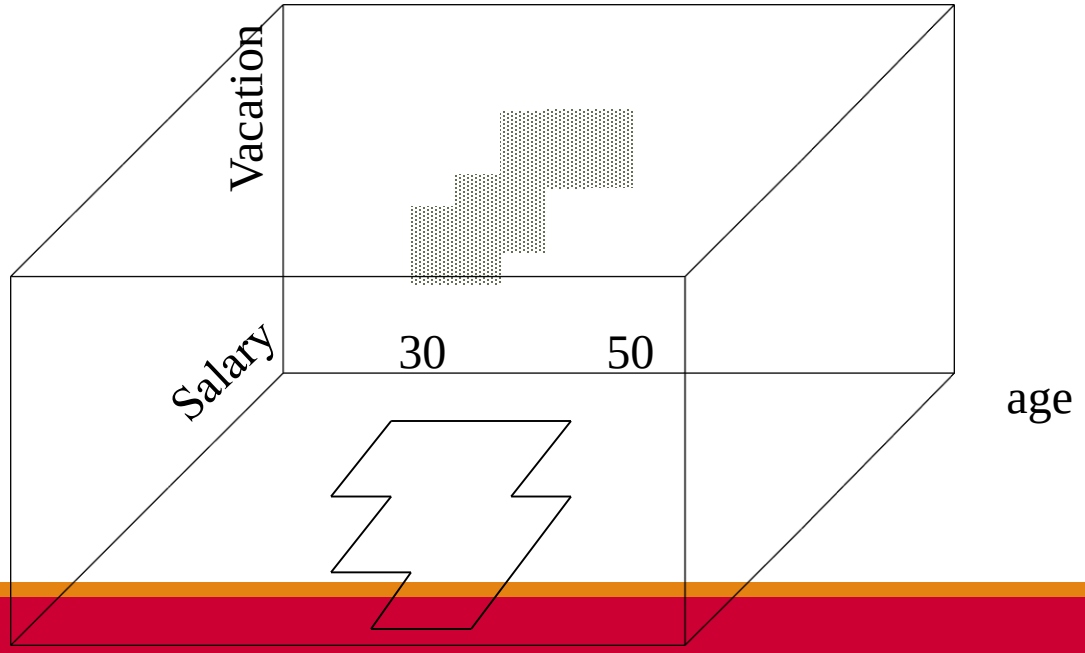
- Determine dense units in all subspaces of interests
- Determine connected dense units in all subspaces of interests.

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


Salary
(10,000)
0 1 2 3 4 5 6 7
20 30 40 50 60
age
Vacation
(week)
0 1 2 3 4 5 6 7
20 30 40 50 60
age

$\tau = 3$


Vacation
Salary
30
50
age

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

Chapter 10. Cluster Analysis: Basic Concepts and Methods

Determine the Number of Clusters

Empirical method

- # of clusters: k ≈√n/2 for a dataset of n points, e.g., n = 200, k = 10

Elbow method

- Use the turning point in the curve of sum of within cluster variance w.r.t the # of clusters

Cross validation method

- Divide a given data set into *m* parts
- Use *m* – 1 parts to obtain a clustering model
- Use the remaining part to test the quality of the clustering
  - E.g., For each point in the test set, find the closest centroid, and use the sum of squared distance between all points in the test set and the closest centroids to measure how well the model fits the test set
- For any k > 0, repeat it *m* times, compare the overall quality measure w.r.t. different *k's*, and find # of clusters that fits the data the best

Measuring Clustering Quality

3 kinds of measures: External, internal and relative

External: supervised, employ criteria not inherent to the dataset

- Compare a clustering against prior or expert-specified knowledge (i.e., the ground truth) using certain clustering quality measure

Internal: unsupervised, criteria derived from data itself

- Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are, e.g., Silhouette coefficient

Relative: directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm

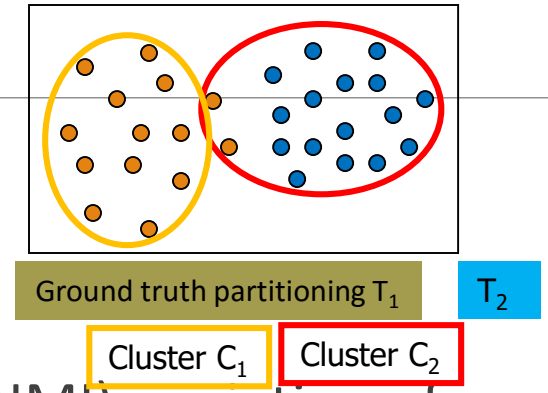
Measuring Clustering Quality: External Methods

Clustering quality measure: *Q(C, T),* for a clustering *C* given the ground truth *T*

Q is good if it satisfies the following **4** essential criteria

- Cluster homogeneity: the purer, the better
- Cluster completeness: should assign objects belong to the same category in the ground truth to the same cluster
- Rag bag: putting a heterogeneous object into a pure cluster should be penalized more than putting it into a *rag bag* (i.e., "miscellaneous" or "other" category)
- Small cluster preservation: splitting a small category into pieces is more harmful than splitting a large category into pieces

Some Commonly Used External Measures



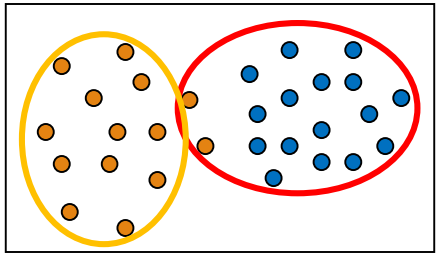
Matching-based measures
- Purity, maximum matching, F-measure

Entropy-Based Measures
- Conditional entropy, normalized mutual information (NMI), variation of information

Pair-wise measures
- Four possibilities: True positive (TP), FN, FP, TN
- Jaccard coefficient, Rand statistic, Fowlkes-Mallow measure

Correlation measures
- Discretized Huber static, normalized discretized Huber static

Entropy-Based Measure (I): Conditional Entropy



Entropy of clustering C:

$$H(\mathcal{C}) = -\sum_{i=1}^{r} p_{C_i} \log p_{C_i} \quad p_{C_i} = \frac{n_i}{n} \text{ the prob. of cluster } C_i$$

Entropy of partitioning T:

$$H(\mathcal{T}) = -\sum_{j=1}^{\kappa} p_{T_i} \log p_{T_j}$$

Entropy of T w.r.t. cluster C_i:

$$H(\mathcal{T}|C_i) = -\sum_{j=1}^{k} (\frac{n_{ij}}{n_i}) \log(\frac{n_{ij}}{n_i})$$

Conditional entropy of T w.r.t. clustering C:

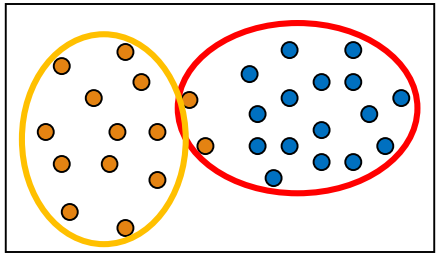
$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r} (\frac{n_i}{n}) H(\mathcal{T}|C_i) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log(\frac{p_{ij}}{p_{C_i}})$$

- The more a cluster's members are split into different partitions, the higher the conditional entropy
- For a perfect clustering, the conditional entropy value is 0, where the worst possible conditional entropy value is log k

$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}(\log p_{ij} - \log p_{C_i}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r}(\log p_{C_i} \sum_{j=1}^{k} p_{ij})$$

$$= -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r}(p_{C_i} \log p_{C_i}) = H(\mathcal{C},\mathcal{T}) - H(\mathcal{C})$$

Entropy-Based Measure (II): Normalized mutual information (NMI)



Mutual information: quantify the amount of shared info between the clustering C and partitioning T:

$$I(\mathcal{C},\mathcal{T}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}\log\left(\frac{p_{ij}}{p_{C_i}\cdot p_{T_j}}\right)$$

It measures the dependency between the observed joint probability p_{ij} of C and T, and the expected joint probability $p_{Ci} * p_{Tj}$ under the independence assumption

When C and T are independent, $p_{ij} = p_{Ci} * p_{Tj}$, I(C, T) = 0. However, there is no upper bound on the mutual information

Normalized mutual information (NMI)

$$NMI(\mathcal{C},\mathcal{T}) = \sqrt{\frac{I(\mathcal{C},\mathcal{T})}{H(\mathcal{C})}\cdot\frac{I(\mathcal{C},\mathcal{T})}{H(\mathcal{T})}} = \frac{I(\mathcal{C},\mathcal{T})}{\sqrt{H(\mathcal{C})\cdot H(\mathcal{T})}}$$

Value range of NMI: [0,1]. Value close to 1 indicates a good clustering

Chapter 10. Cluster Analysis: Basic Concepts and Methods

Cluster Analysis: Basic Concepts

Partitioning Methods

Hierarchical Methods

Density-Based Methods

Grid-Based Methods

Evaluation of Clustering

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

K-means and K-medoids algorithms are popular partitioning-based clustering algorithms

Birch and Chameleon are interesting hierarchical clustering algorithms, and there are also probabilistic hierarchical clustering algorithms

DBSCAN, OPTICS, and DENCLU are interesting density-based algorithms

STING and CLIQUE are grid-based methods, where CLIQUE is also a subspace clustering algorithm

Quality of clustering results can be evaluated in various ways