Università degli Studi di Milano

Master Degree in Computer Science

Information Management course

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Data Mining:
Concepts and Techniques

(3rd ed.)

— Chapter 10 —

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Cluster Analysis: Concepts and Methods

- Cluster Analysis: Basic Concepts
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- Grid-Based Methods
- Evaluation of Clustering
- Summary

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., *try to learn by extracting regularities in data*)
- 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 research

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 (optimality guarantees + computational effectiveness), and
  - Its ability to discover some or all of the hidden patterns (practical behavior)

Measure the Quality of Clustering

- Dissimilarity/Similarity metric
  - Similarity is expressed in terms of a (typically metric) pairwise distance function *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 global quality function that measures the “goodness” of a cluster.
  - It is hard to define “similar enough” or “good enough” (need to stick to the application!)
    - The answer is typically highly subjective (i.e. don't blame the *algorithm* for *modeling* errors)

Major Clustering Approaches

- 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
  - Agglomerative (bottom-up) or divisive (top-down)
- Density-based approach:
  - Based on connectivity and density functions (keep growing as points are still in the neighborhood of cluster elements)
  - Find arbitrarily shaped clusters
- Grid-based approach:
  - Quantize object space in a grid structure
  - build a multiple-level granularity structure

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Partitioning Algorithms: Basic Concept

Partitioning method:

- given the number of clusters k
- given a dissimilarity measure (partitioning criterion)
- given a database ***D*** of ***n*** objects
- partition it into a set of ***k*** clusters
- such that the sum of dissimilarities with respect to a cluster representative c_i is minimized (e.g. squared distances to the centroid or medoid of cluster C_i)

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

Partitioning Algorithms: Basic Concept

Partitioning method:

- Exact (globally opt) methods: mixed integer programming
- Heuristic methods: *k-means* and *k-medoids* algorithms
- *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center (attibute-wise means) of the cluster
- *k-medoids* or k-medians 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

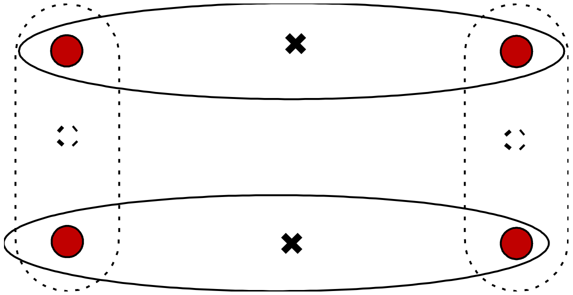
- Given *k*, the *k-means* algorithm is implemented in four steps:
  1) Partition objects into *k* nonempty subsets
  2) Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  3) Assign each object to the cluster with the nearest seed point
  4) Go back to Step 2, stop when the assignment does not 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: $O(ks^2 + k(n-k))$
- Weakness
    - Heuristc; often terminates at a *local optimal*
    - Applicable only to objects in a continuous n-dimensional space
        - Using the k-modes for categorical data
        - Using the k-medoids for a wider range of data
    - Need to give *k,* the *number* of clusters, as input (there are ways to guess meaningful 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

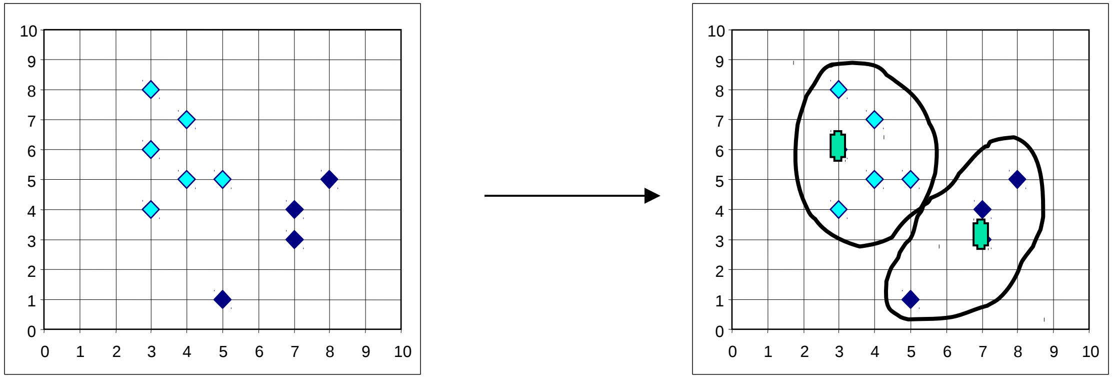
- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means



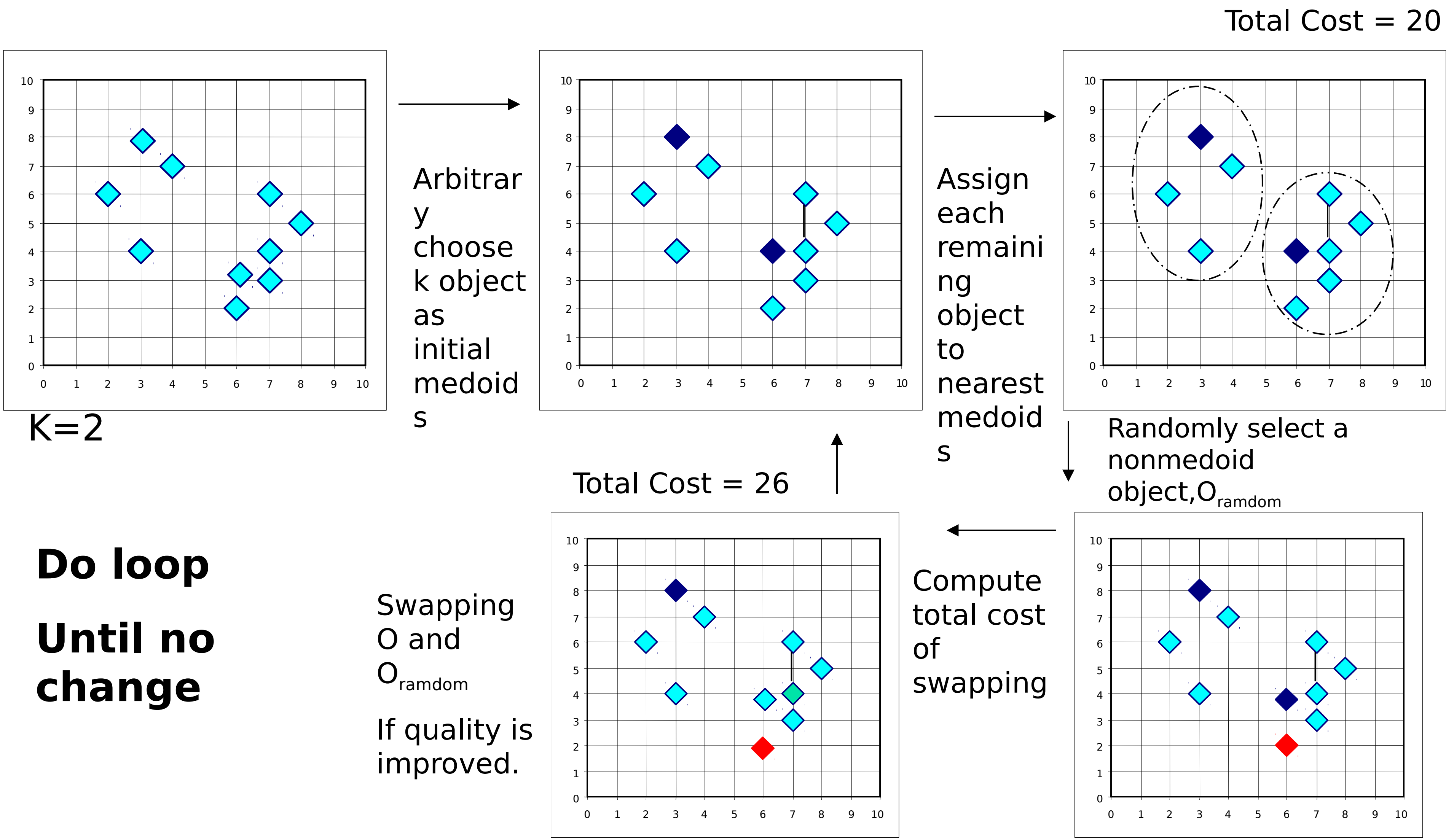
- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

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

Total Cost = 20

Assign each remaining object to nearest medoids

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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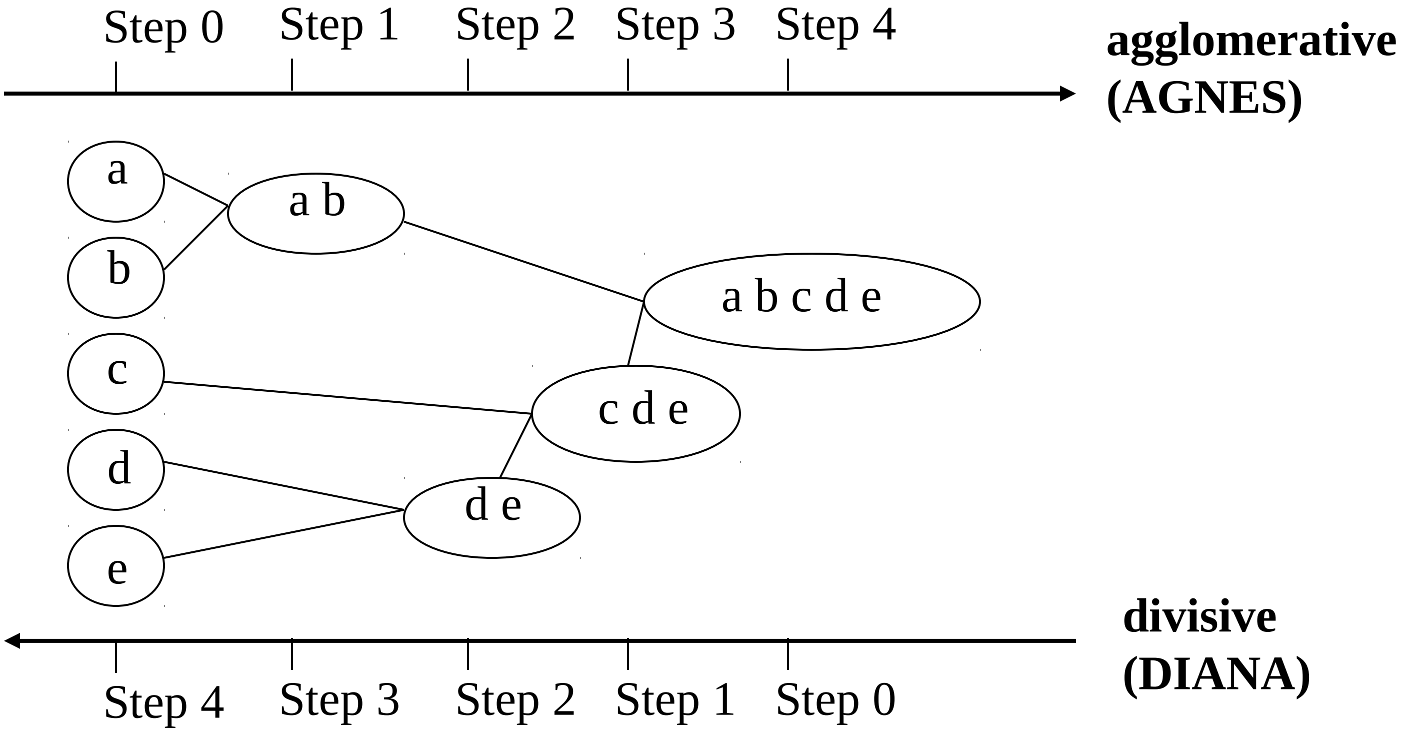
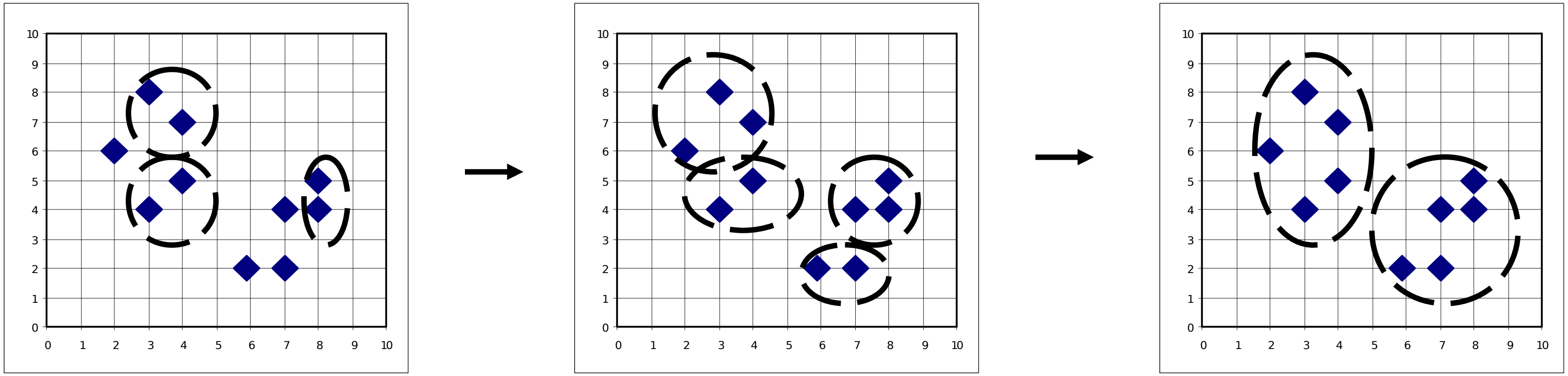
Hierarchical Clustering

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



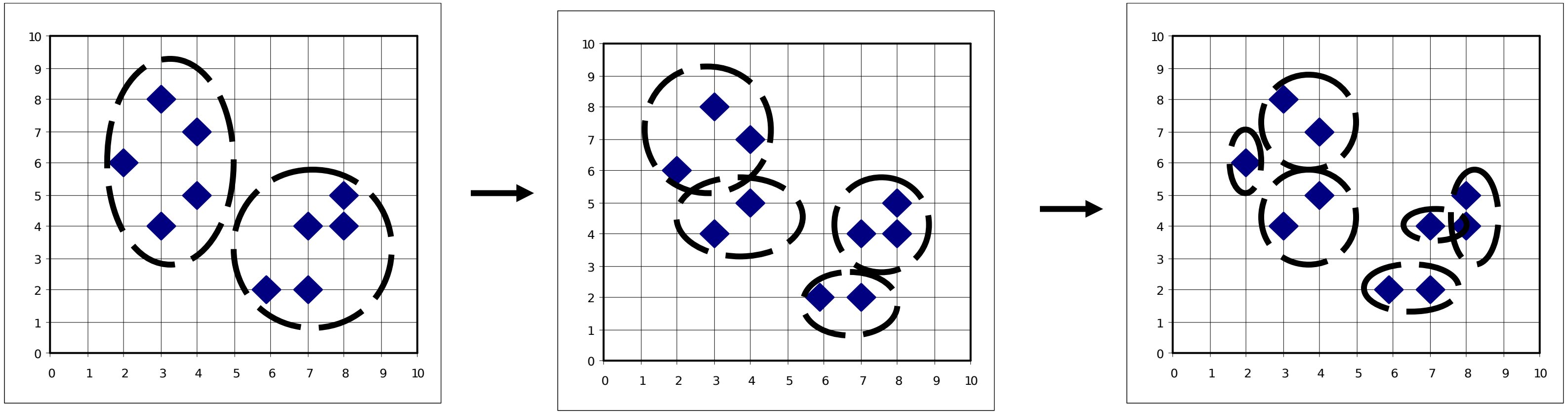
AGNES (AGglomerative NESting)

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



DIANA (DIvisive ANAlysis)

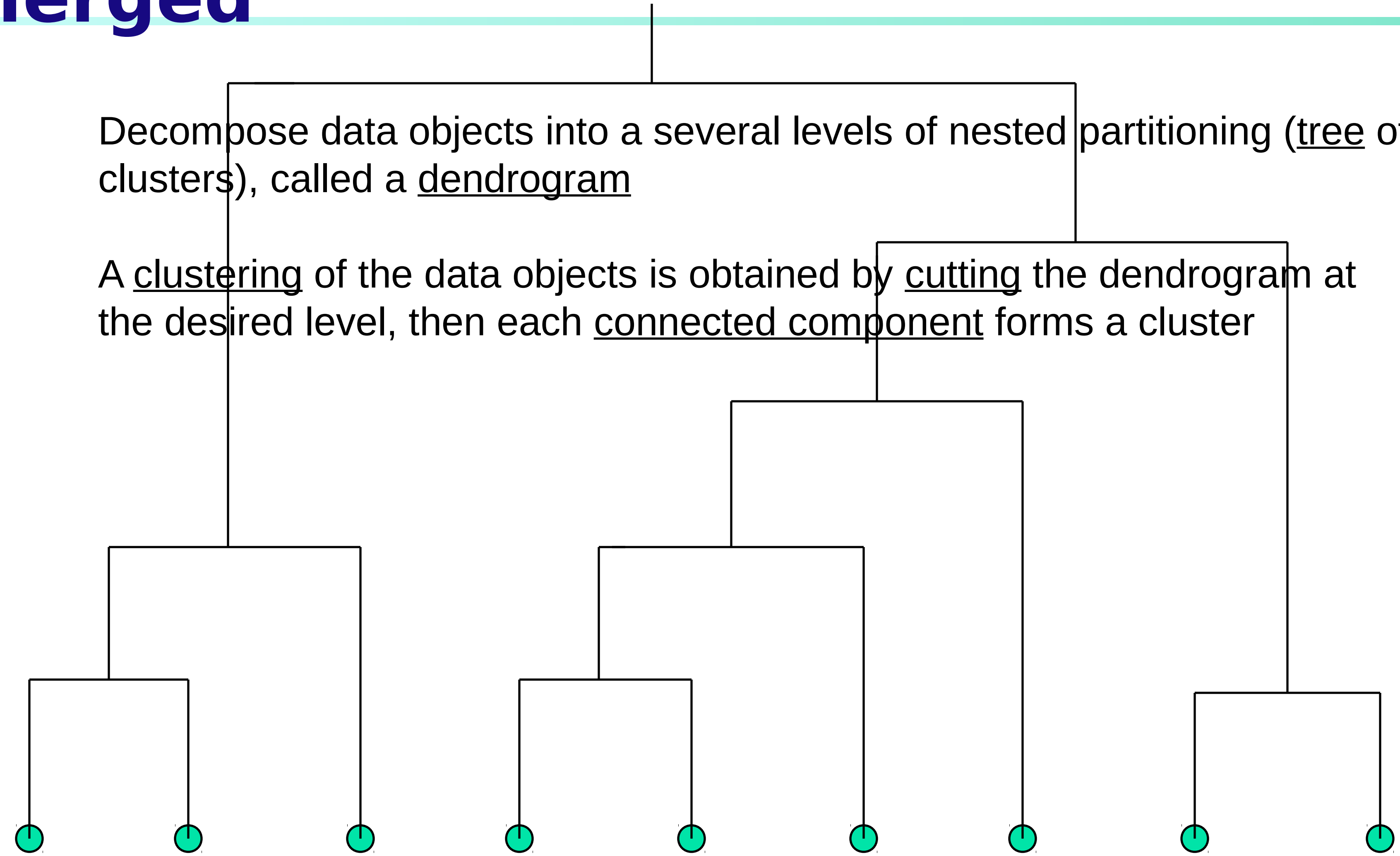
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Inverse order of AGNES
- Eventually each node forms a cluster on its own



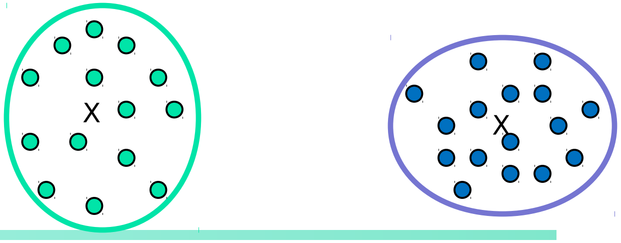
Dendrogram: Shows How Clusters are Merged

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

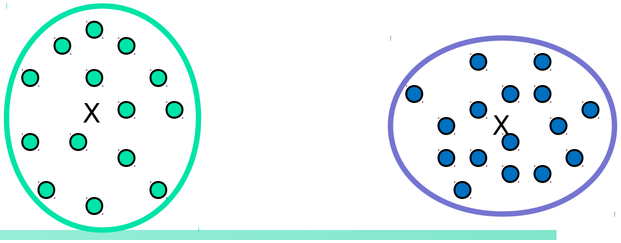


Distance between Clusters



- Single link: smallest distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_j) = $\min_{p \text{ in } Ki,\ q \text{ in } Kj}$ d(p,q)
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_j) = $\max_{p \text{ in } Ki,\ q \text{ in } Kj}$ d(p,q)
- Average: avg distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_j) = $\text{sum}_{p \text{ in } Ki,\ q \text{ in } Kj}$ d(p,q) / (|Ki||Kj|)
- Centroid: distance between the centroids of two clusters, e.g., p = mean(Ki), q = mean(Kj), dist(K_i, K_j) = d(p,q)
- Medoid: distance between the medoids of two clusters, i.e., p = median(Ki), q = median(Kj), dist(K_i, K_j) = d(p,q)

Distance between Clusters



- Algorithms using minimum distance are also called nearest-neighbor clustering algorithms
  - they build minimum spanning trees
  - if clustering is terminated when the minimum inter-cluster distance exceeds a given threshold they are called single-linkage
- Algorithms using maximum distance are also called farthest-neighbor clustering algorithms
  - If clustering is terminated when the maximum inter-cluster distance between nearest clusters exceeds a given threshold they are called complete-linkage

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

- Centroid: the "middle" of a cluster

$$C_m = \frac{\Sigma_{i=1}^{N} \left(t_{ip} \right)}{N}$$

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

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

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

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

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
- Clustering Feature (CF): <n, LS, SS>
  - n: number of points, LS: their sum, SS: their sum of squares
- Easy to compute centroid, radius and diameter from CF
- CFs are additive
- Incrementally construct a CF 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 its inherent clustering structure)
  - Phase 2: use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree

BIRCH (Balanced Iterative Reducing and Clustering Using Hierarchies)

- *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)***

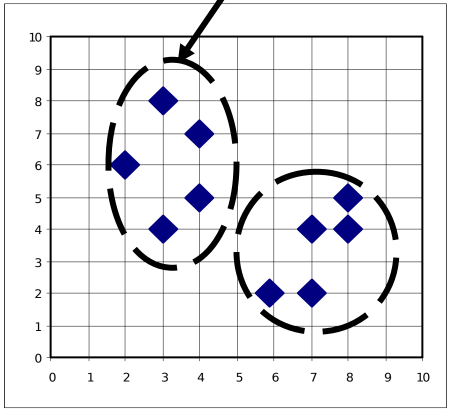
N: **Number of data points**

LS: linear sum of N points:

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

SS: square sum of N points

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



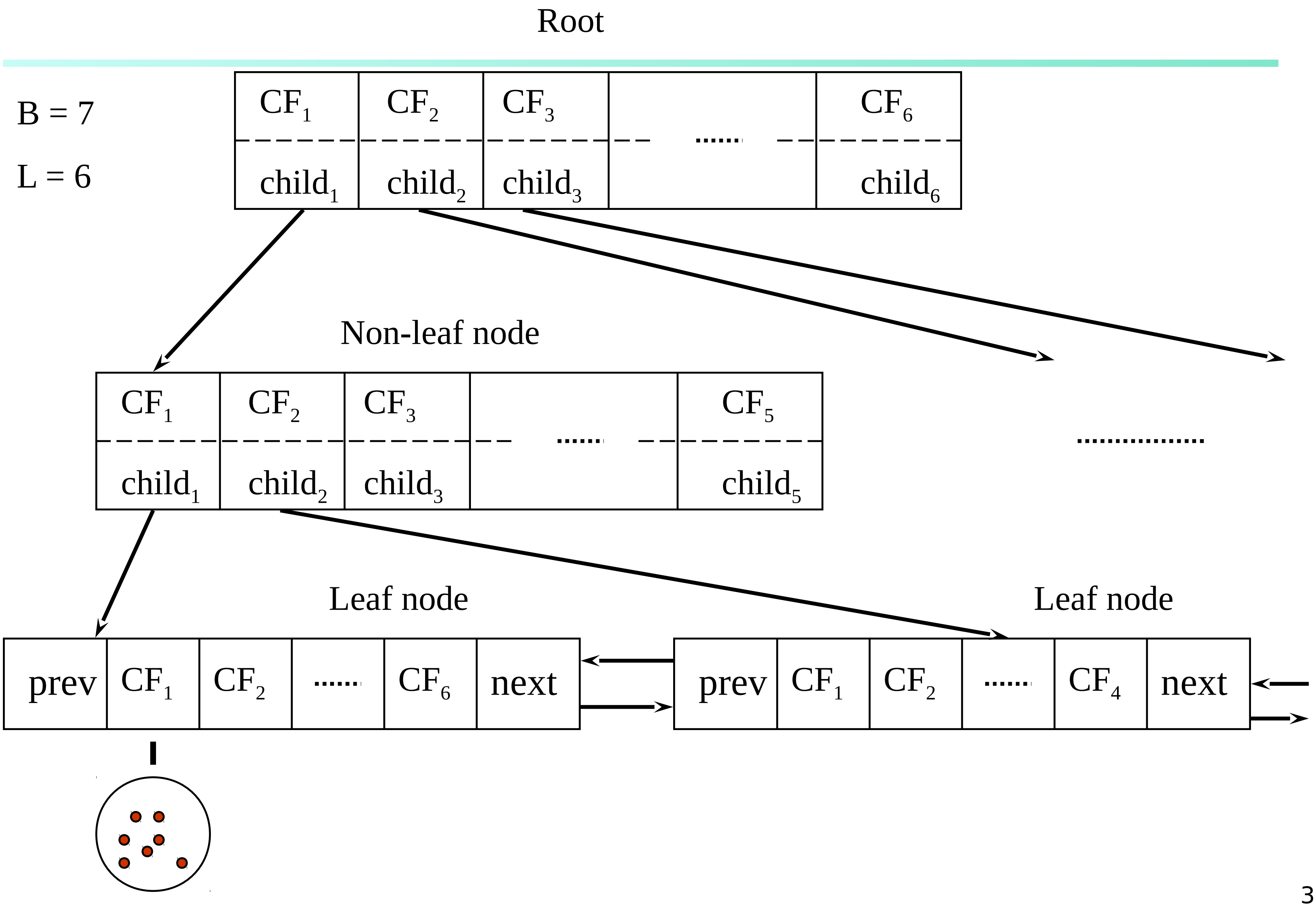
CF = (5, (16;30),(54;190))

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

The CF Tree Structure



Root

B = 7

L = 6

CF_1 | CF_2 | CF_3 | ……. | CF_6

$child_1$ | $child_2$ | $child_3$ | | $child_6$

Non-leaf node

CF_1 | CF_2 | CF_3 | ……. | CF_5

$child_1$ | $child_2$ | $child_3$ | | $child_5$

……………..

Leaf node

prev | CF_1 | CF_2 | ……. | CF_6 | next

Leaf node

prev | CF_1 | CF_2 | ……. | CF_4 | next

The Birch Algorithm

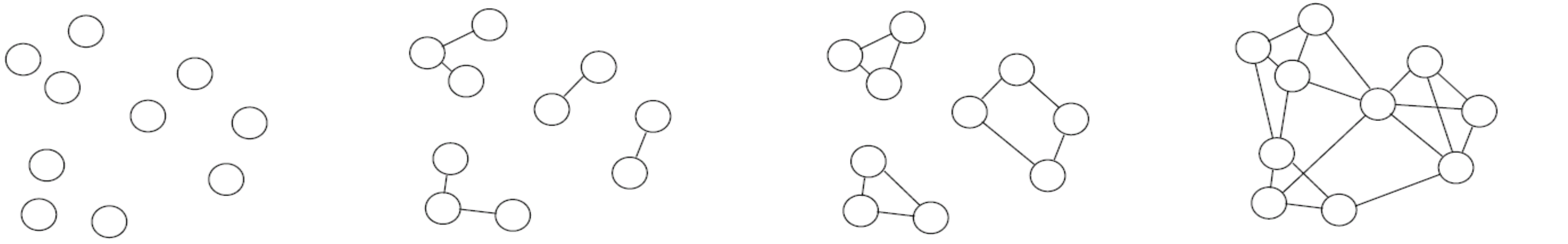
- Cluster Diameter $$\sqrt{\frac{1}{n(n-1)}\sum(x_i-x_j)^2}$$
- For each point in the input
  - Find closest leaf entry
  - Add point to leaf entry and update CF
  - If entry diameter > max_diameter, then split leaf, and possibly parents
- Algorithm is O(n)
- Concerns
  - Sensitive to insertion order 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 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

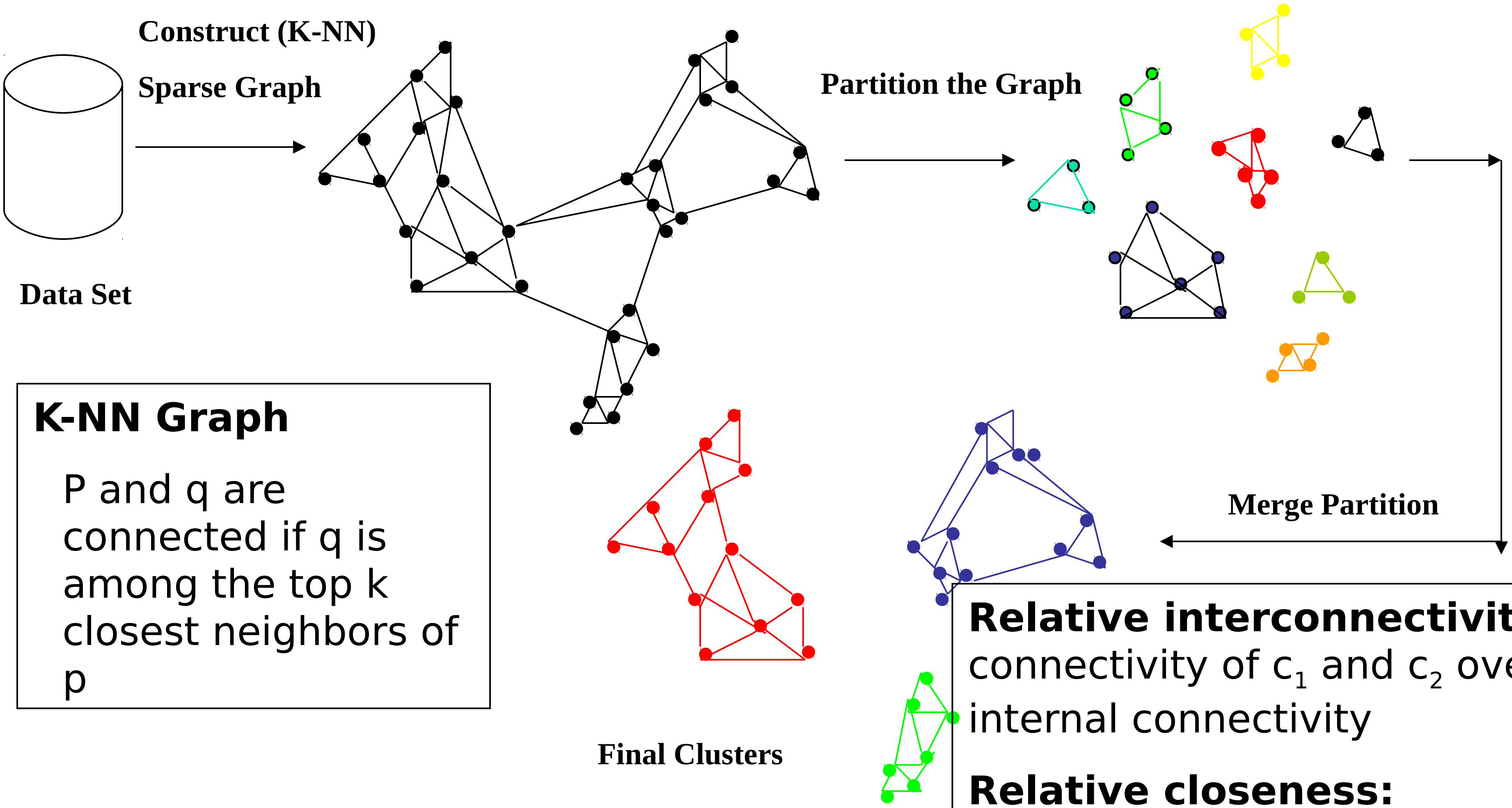
- **Relative closeness** between a pair of clusters C_i *and* C_j *: the absolute closeness* between C_i *and* C_j *normalized w.r.t. the internal closeness of the two clusters* C_i *and* C_j

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

  - $\overline{S}_{EC_{C_i}}$ 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 $\overline{S}_{EC_{\{C_i, C_j\}}}$ is 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 a function combining RI & RC

Overall Framework of CHAMELEON



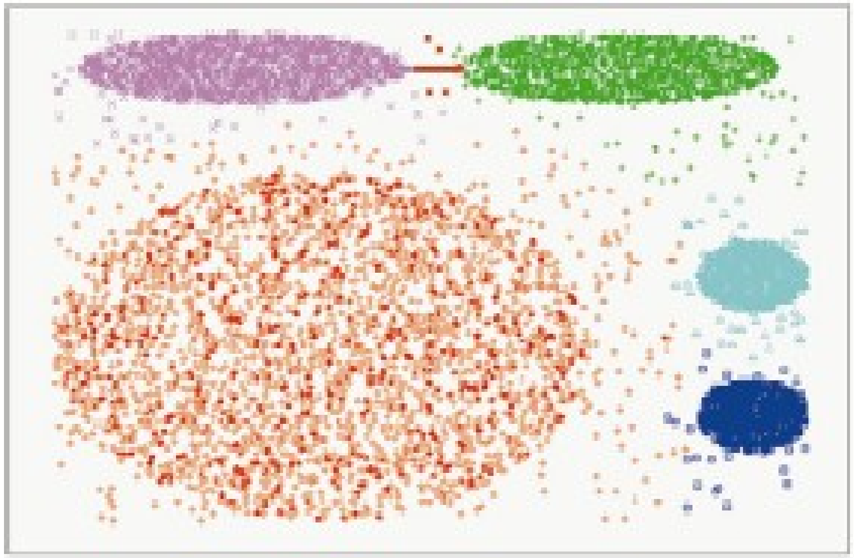
K-NN Graph

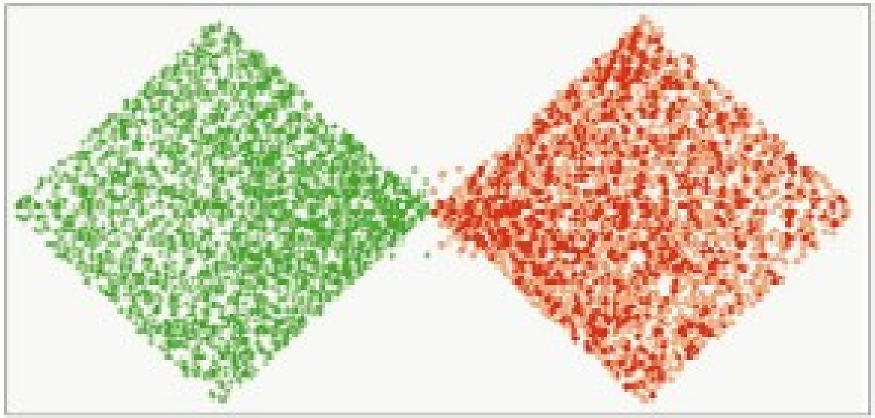
P and q are connected if q is among the top k closest neighbors of p

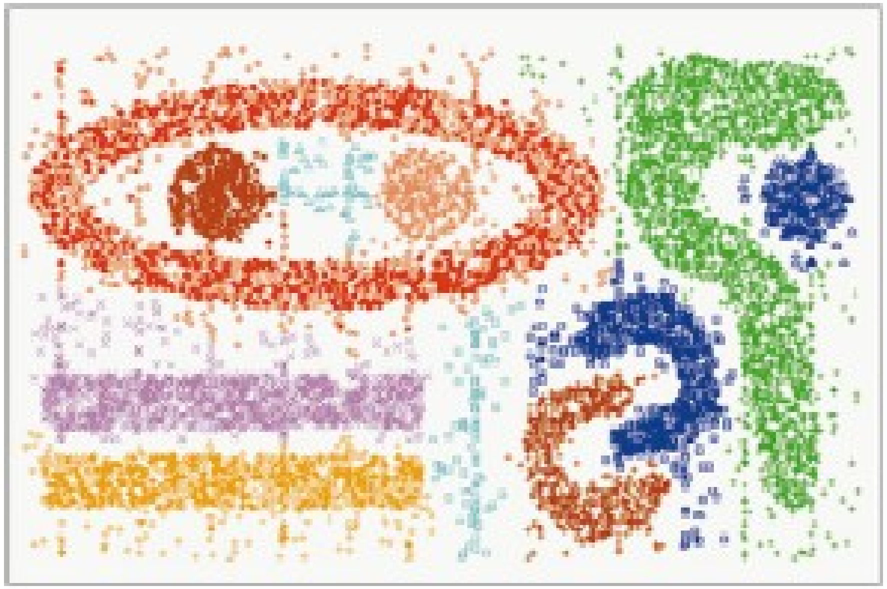
Relative interconnectivity: connectivity of c_1 and c_2 over internal connectivity

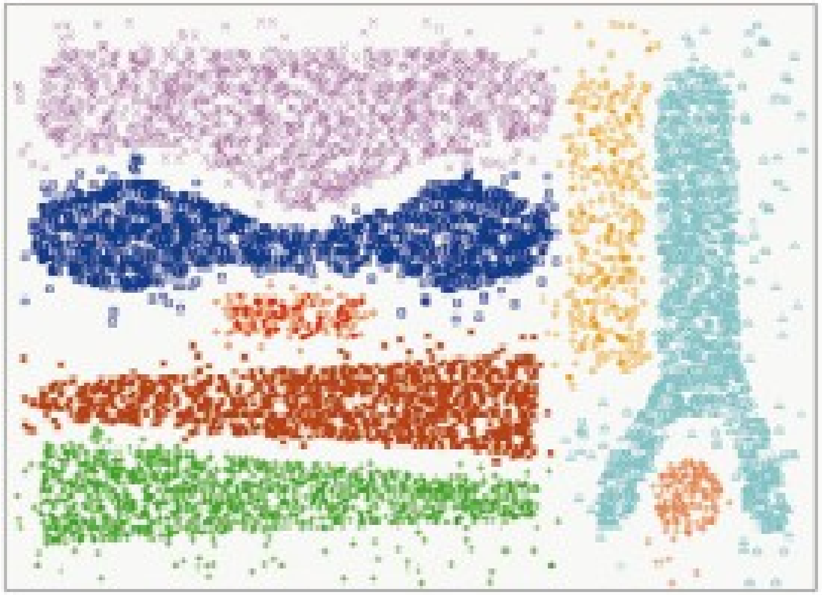
Relative closeness: closeness of c_1 and c_2 over internal closeness

CHAMELEON (Clustering Complex Objects)









Hierarchical Clustering Summary

- Hierarchical clustering strengths
  - Produce at once clustering solutions for different k values
  - Link them, highlighting regularities
- Hierarchical clustering weaknesses
  - Nontrivial to choose a good distance measure
  - Hard to handle missing attribute values
  - Algorithmically (besides theoretically) hard: mainly heuristics in practical settings

Probabilistic Hierarchical Clustering

- Hierarchical (distance-based) clustering strengths …
- Hierarchical (distance-based) clustering weaknesses …
- **Probabilistic** (“fitting”) hierarchical clustering
  - Use probabilistic models to measure distances between clusters
  - Generative model: Regard the set of data objects to be clustered as a sample of the underlying data generation mechanism to be analyzed
  - Easy to understand, same efficiency as algorithmic agglomerative clustering method, can handle partially observed data
- In practice, assume the generative models adopt common distributions functions, e.g., Gaussian distribution or Bernoulli distribution, governed by parameters

Generative Model

- Given a set of 1-D points *X* = {*x*_1, …, *x*_n} for clustering analysis & assuming they are generated by a Gaussian distribution:

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- The probability that a point $x_i \in X$ is generated by the model

$$P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The likelihood that *X* is generated by the model:

$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The task of learning the generative model: find the parameters μ and σ^2 such that

$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}$$

the maximum likelihood

A Probabilistic Hierarchical Clustering Algorithm

- For a set of objects partitioned into *m* clusters $C_1, \ldots, C_m$, the quality can be measured by, $Q(\{C_1,\ldots,C_m\}) = \prod_{i=1}^{m} P(C_i)$

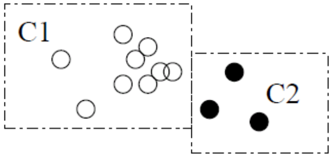
  where *P*() is the maximum likelihood

- If we merge two clusters C_{j1} and C_{j2} into a cluster $C_{j1} \cup C_{j2}$, then, the change in quality of the overall clustering is

$$Q((\{C_1,\ldots,C_m\} - \{C_{j_1}, C_{j_2}\}) \cup \{C_{j_1} \cup C_{j_2}\}) - Q(\{C_1,\ldots,C_m\})$$

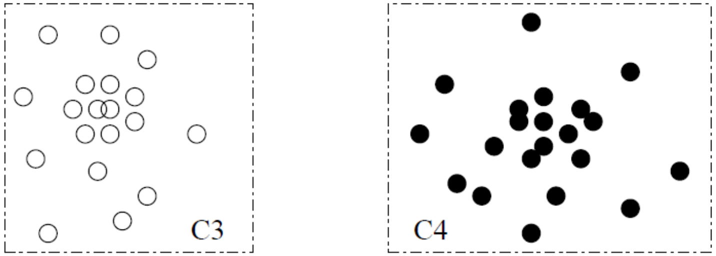
$$= \frac{\prod_{i=1}^{m} P(C_i) \cdot P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - \prod_{i=1}^{m} P(C_i)$$

$$= \prod_{i=1}^{m} P(C_i)\left(\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - 1\right)$$



- Distance between clusters C_1 and C_2:

$$dist(C_i, C_j) = -\log \frac{P(C_1 \cup C_2)}{P(C_1)P(C_2)}$$



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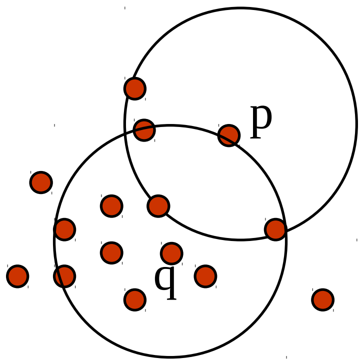
Density-Based Clustering Methods

- 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
- $N_{Eps}(q)$: {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:

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

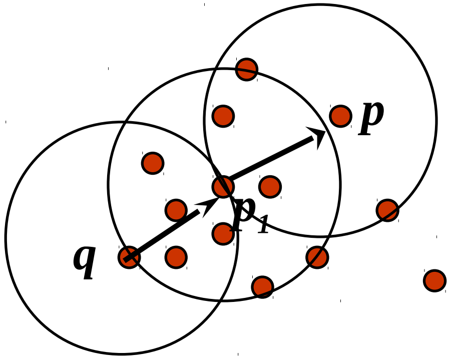


MinPts = 5

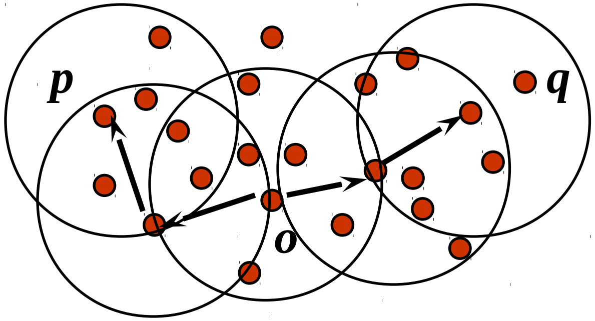
Eps = 1 cm

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

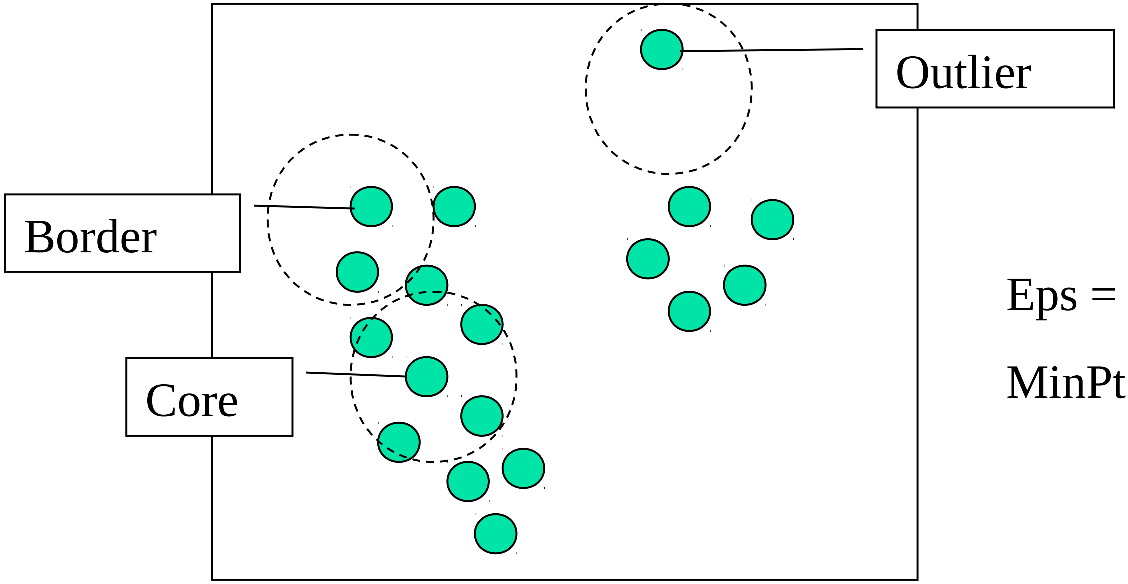


- Density-connected
  - A point *p* is density-connected to a point *q* w.r.t. (*Eps*, *MinPts)* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



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
- Experimentally, discovers clusters of arbitrary shape in spatial databases with noise



Eps = 1cm

MinPts = 5

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

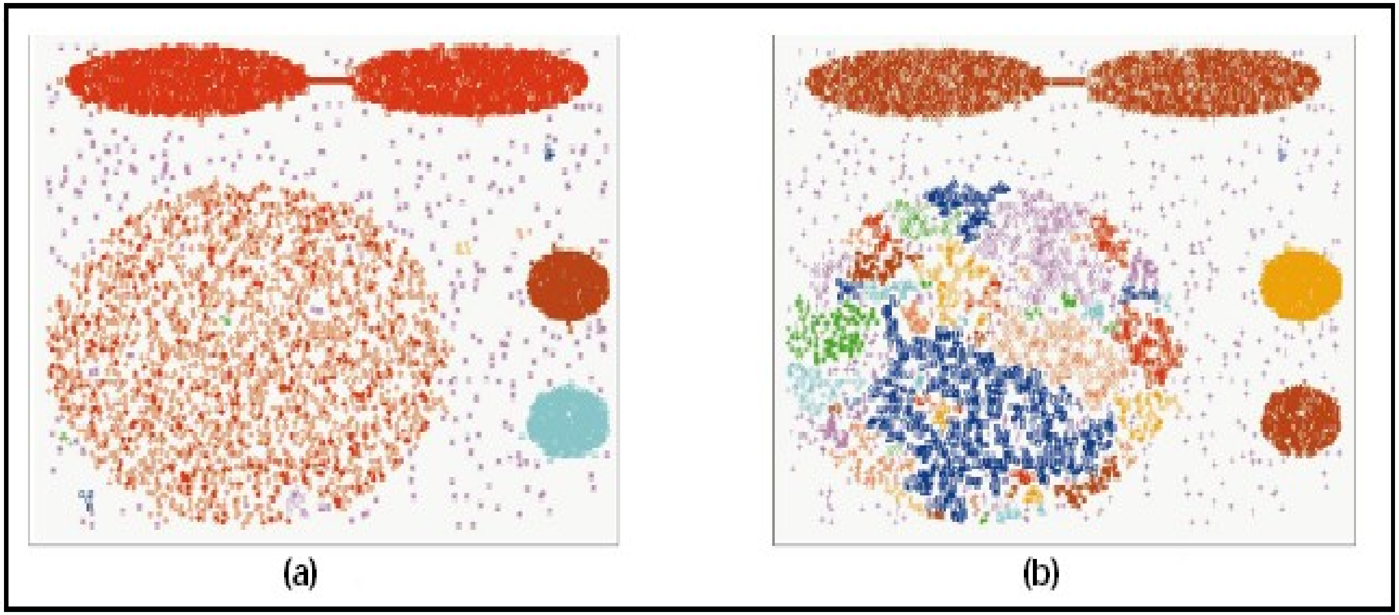


Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

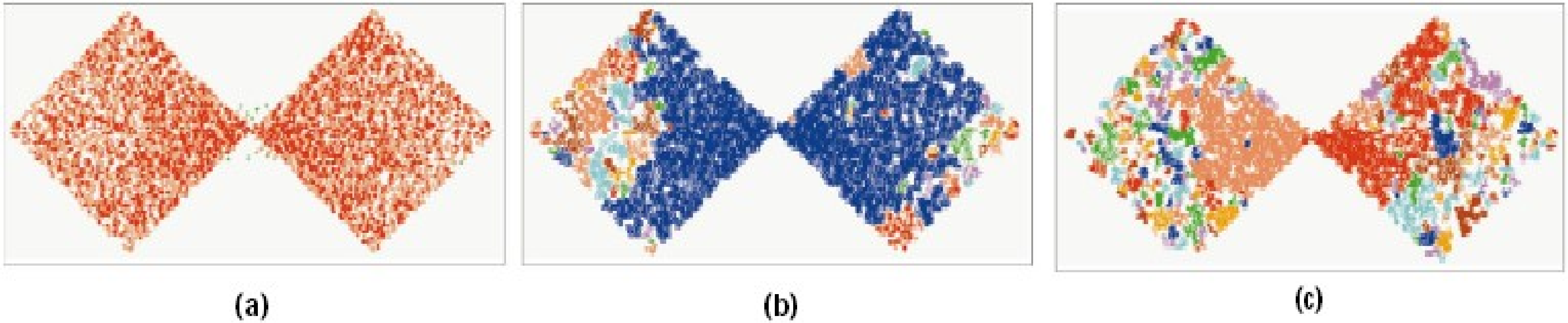


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.

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

DENCLUE: Using Statistical Density Functions

- DENsity-based CLUstEring by Hinneburg & Keim (KDD'98)
- Using statistical density functions:

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

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
  - Uses gaussian *kernel density approximation*

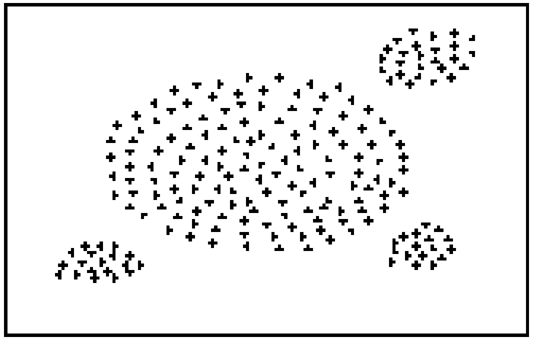
$$f(x)=\frac{1}{ns}\sum_{i=1}^{n}K\left(\frac{x-x_i}{s}\right)$$

  - Clusters can be determined mathematically by identifying density attractors (local maxima of the overall density function)
  - Center defined clusters: assign to each density attractor the points density attracted to it (pick each point and follow the gradient)

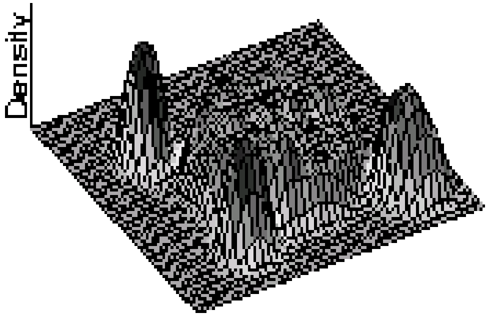
Denclue: Technical Essence

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

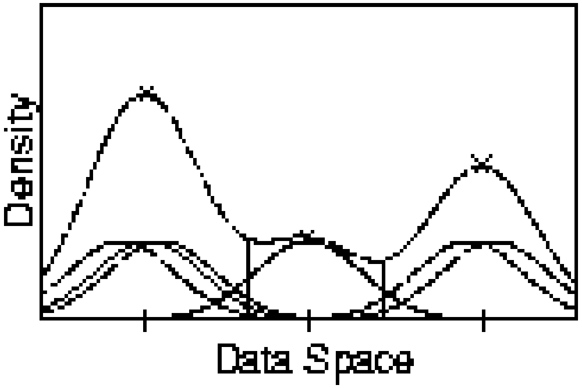
Density Attractor



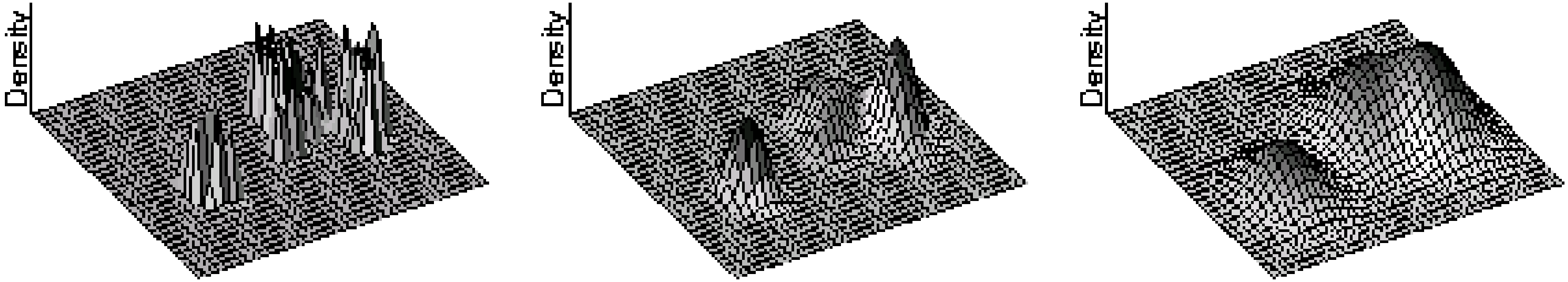
(a) Data Set



(c) Gaussian

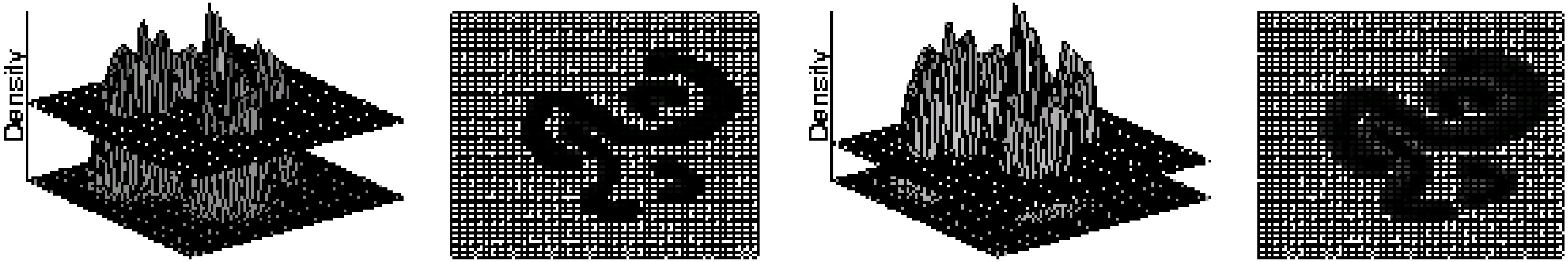


Center-Defined and Arbitrary



(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)
  - WaveCluster by Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
    - A multi-resolution clustering approach using wavelet method
  - CLIQUE: Agrawal, et al. (SIGMOD'98)
    - Both grid-based and subspace clustering

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

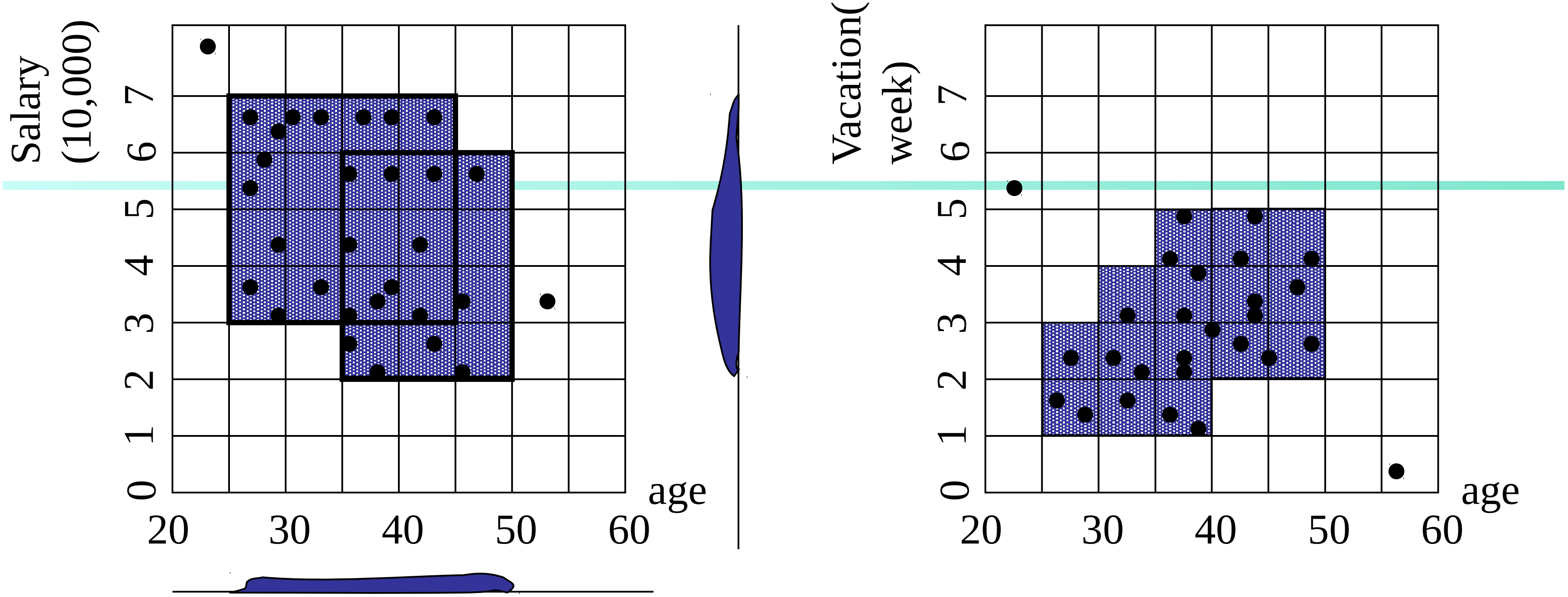
- Remove the irrelevant cells from further consideration
- When finish examining the current layer, proceed to the next lower level
- Repeat this process until the bottom layer is reached
- Advantages:
  - Query-independent, easy to parallelize, incremental update
  - *O(K),* where *K* is the number 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)

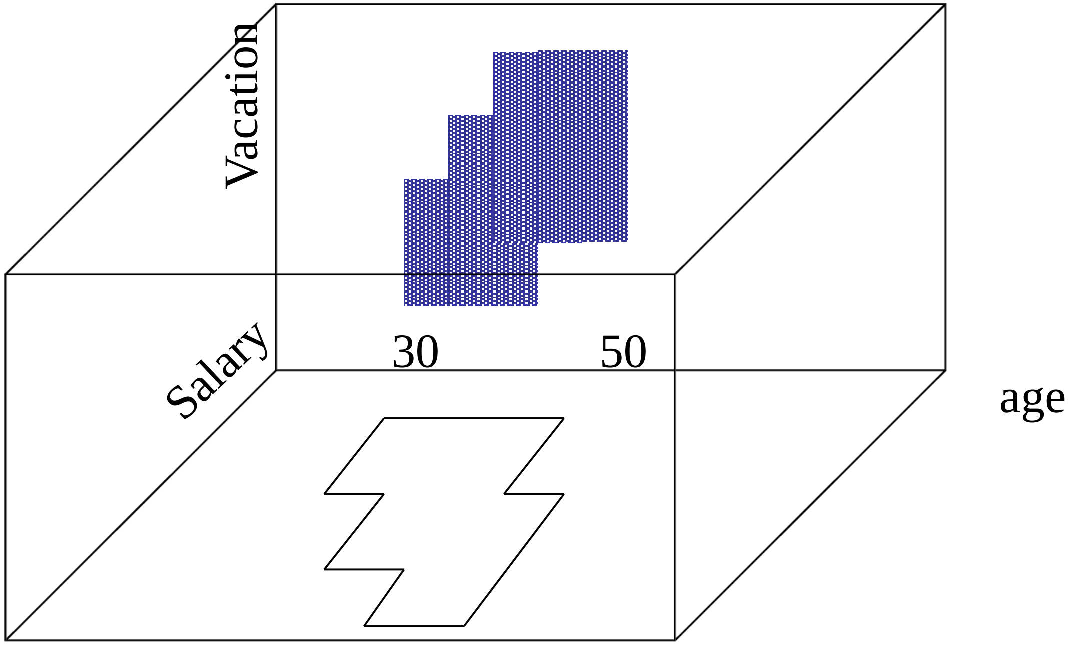
- Agrawal, Gehrke, Gunopulos, Raghavan (SIGMOD’98)
- Automatically identifying subspaces of a high dimensional data space that allow better clustering than original space
- CLIQUE can be considered as both density-based and grid-based
  - It partitions each dimension into the same number of equal length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

τ = 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