CS249: ADVANCED DATA MINING

Vector Data: Clustering: Part I

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Methods to Learn

	Vector Data	Text Data	Recommender System	Graph & Network
Classification	**Decision Tree**; **Naïve Bayes**; **Logistic Regression** **SVM; NN**			Label Propagation
Clustering	**K-means; hierarchical clustering; DBSCAN;** Mixture Models; kernel k-means	PLSA; LDA	Matrix Factorization	SCAN; Spectral Clustering
Prediction	**Linear Regression** **GLM**		Collaborative Filtering	
Ranking				PageRank
Feature Representation		Word embedding		Network embedding

Vector Data: Clustering: Part I

- Clustering Analysis: Basic Concepts
- Partitioning methods
- Hierarchical Methods
- Density-Based Methods
- 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., *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
- 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

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

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

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Partitioning Algorithms: Basic Concept

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

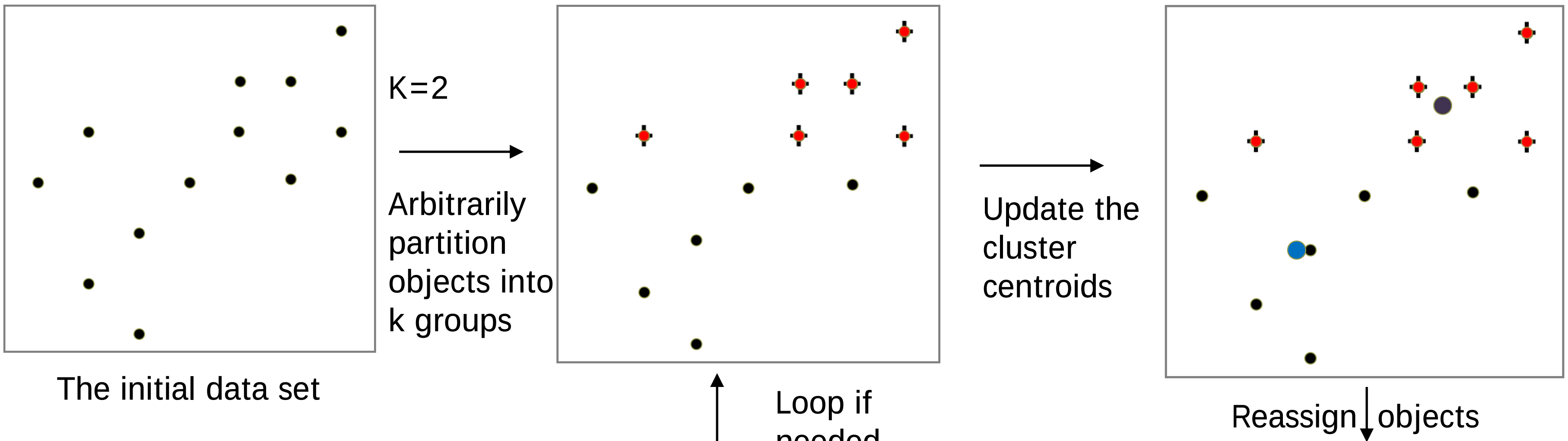
$$J = \Sigma_{j=1}^{k} \Sigma_{p \in C_j} (d(p, c_j))^2$$

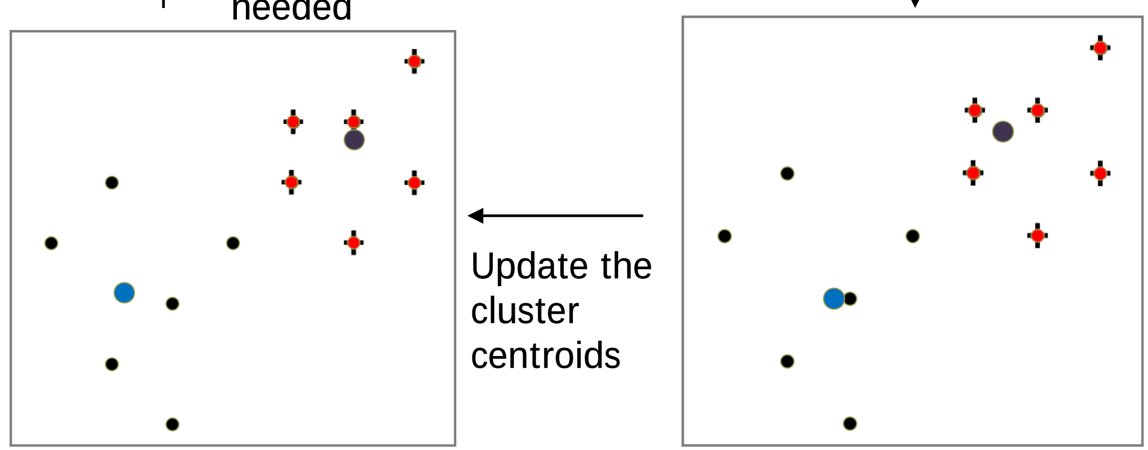
- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of 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:
  - Step 0: Partition objects into *k* nonempty subsets
  - Step 1: 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)
  - Step 2: Assign each object to the cluster with the nearest seed point
  - Step 3: Go back to Step 1, 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

Theory Behind K-Means

- Objective function
  - $J = \sum_{j=1}^{k} \sum_{C(i)=j} ||x_i - c_j||^2$
  - Total within-cluster variance
- Re-arrange the objective function
  - $J = \sum_{j=1}^{k} \sum_{i} w_{ij} ||x_i - c_j||^2$
    - $w_{ij} \in \{0,1\}$
    - $w_{ij} = 1, if\ x_i\ belongs\ to\ cluster\ j; w_{ij} = 0, otherwise$
  - Looking for:
    - The best assignment w_{ij}
    - The best center c_j

Solution of K-Means

- Iterations

$$J = \sum_{j=1}^{k} \sum_{i} w_{ij} ||x_i - c_j||^2$$

  - Step 1: Fix centers c_j, find assignment w_{ij} that minimizes J
    - => $w_{ij} = 1, if\ ||x_i - c_j||^2$ is the smallest

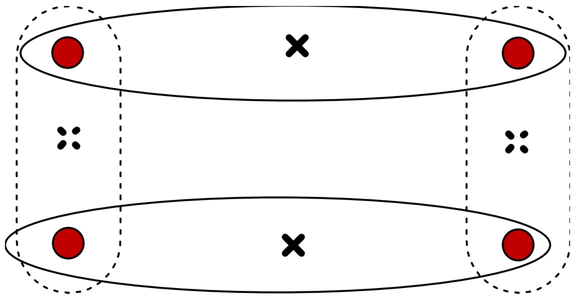
  - Step 2: Fix assignment w_{ij}, find centers that minimize J
    - => first derivative of J = 0
    - => $\frac{\partial J}{\partial c_j} = -2 \sum_i w_{ij}(x_i - c_j) = 0$
    - =>$c_j = \frac{\sum_i w_{ij} x_i}{\sum_i w_{ij}}$
      - Note $\sum_i w_{ij}$ is the total number of objects in cluster j

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.
- 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

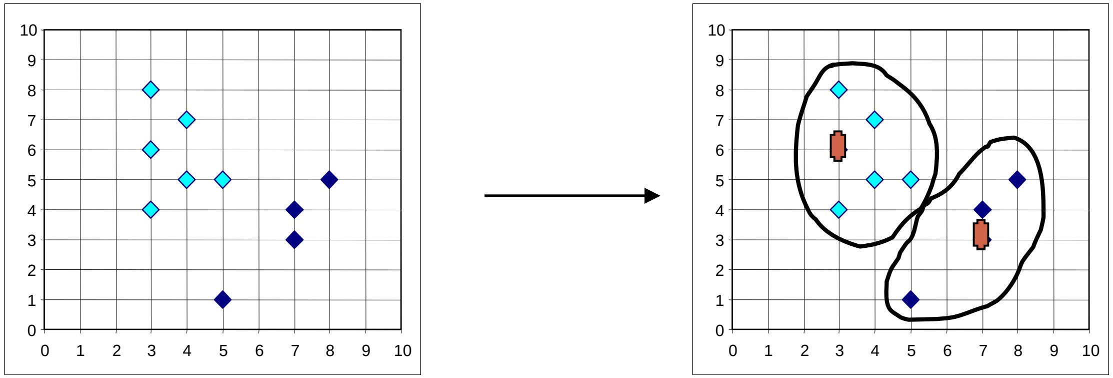
- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means



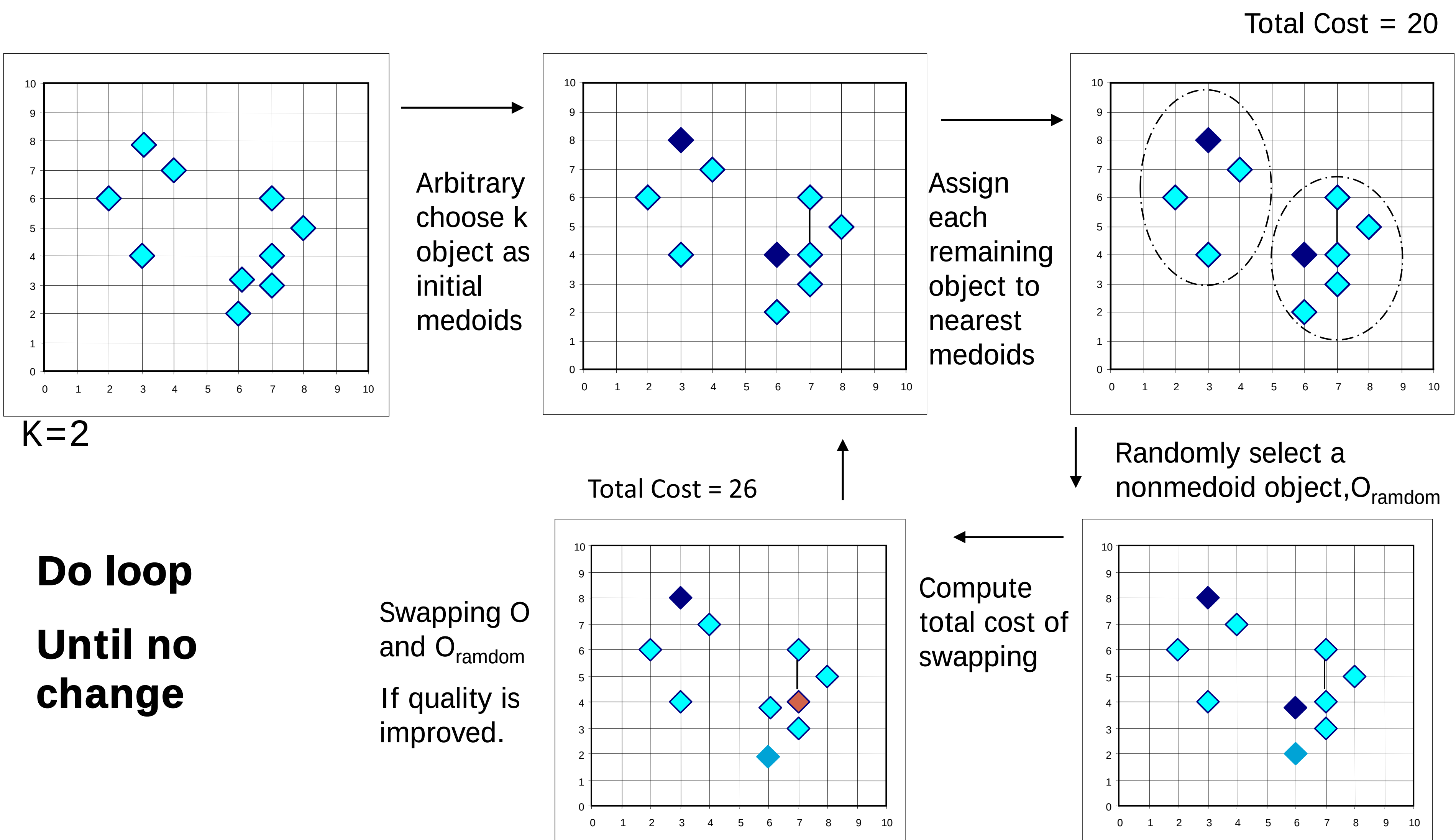
- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

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



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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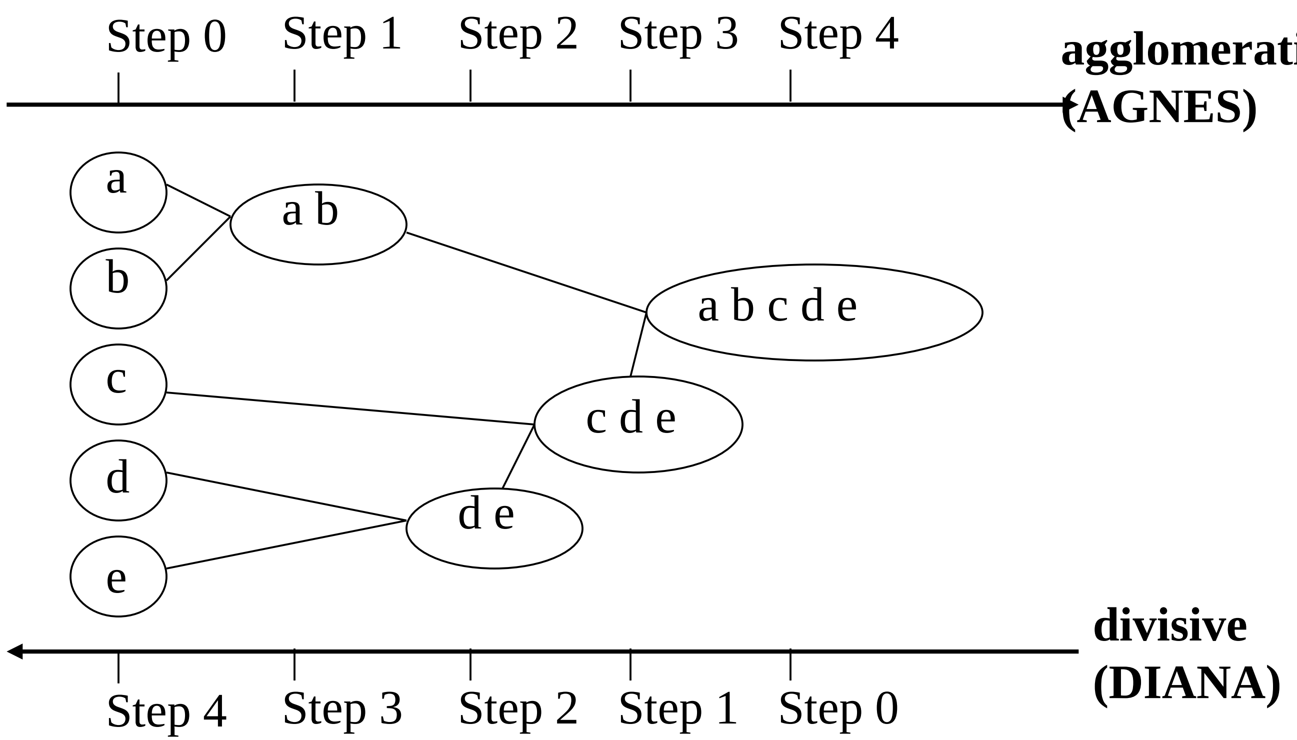
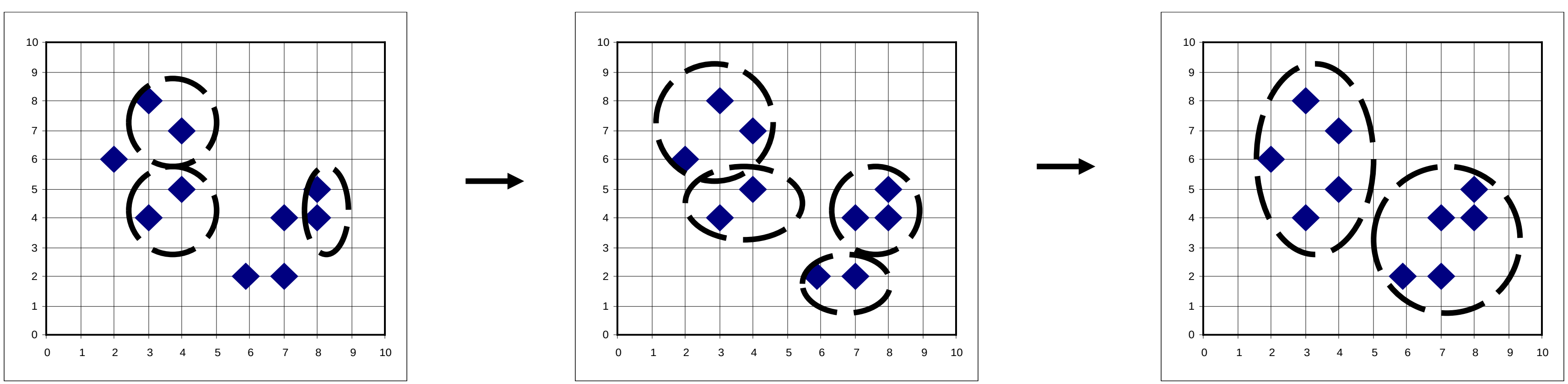
Hierarchical Clustering

- 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)

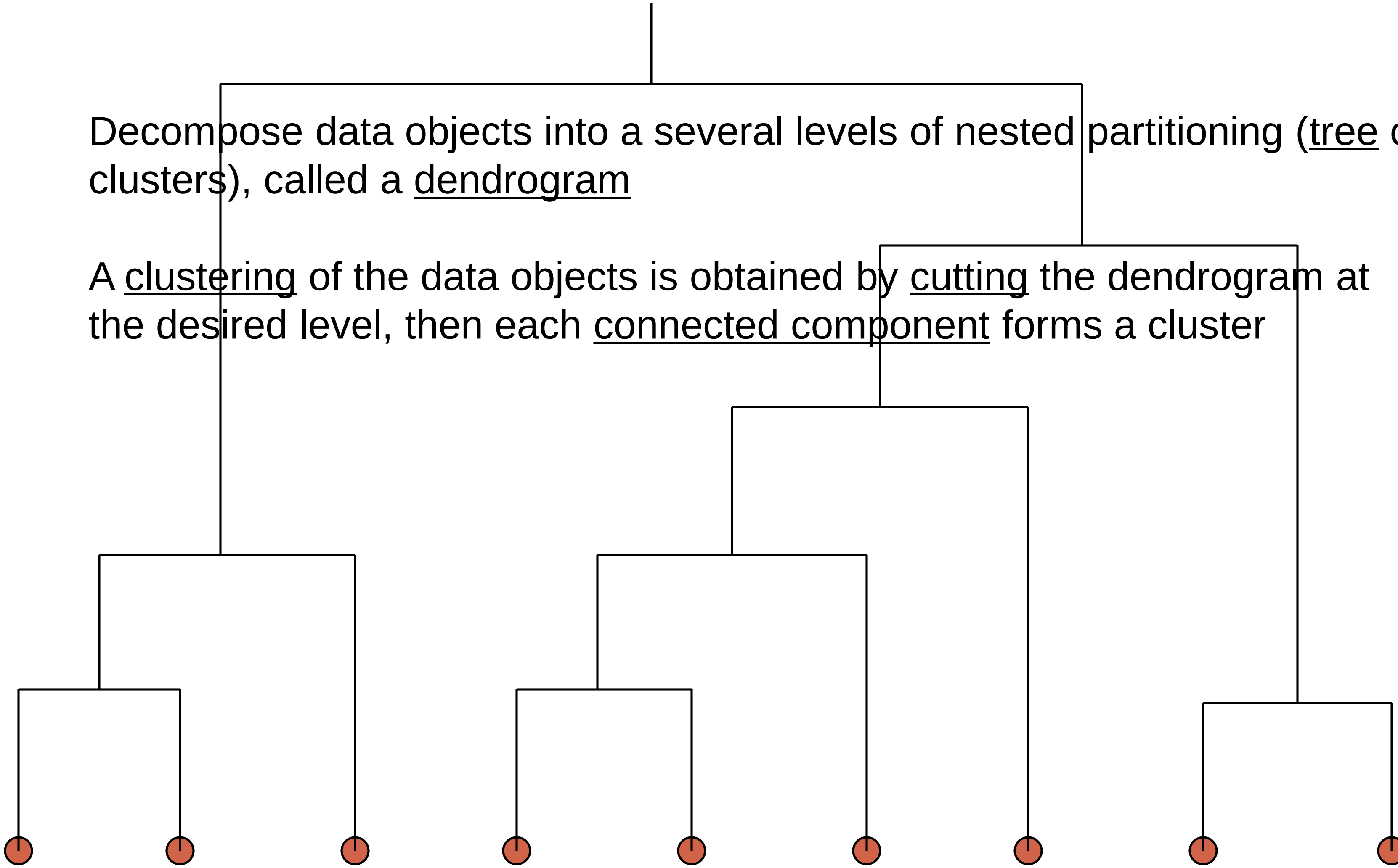
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the **single-link** method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



Dendrogram: Shows How Clusters are Merged

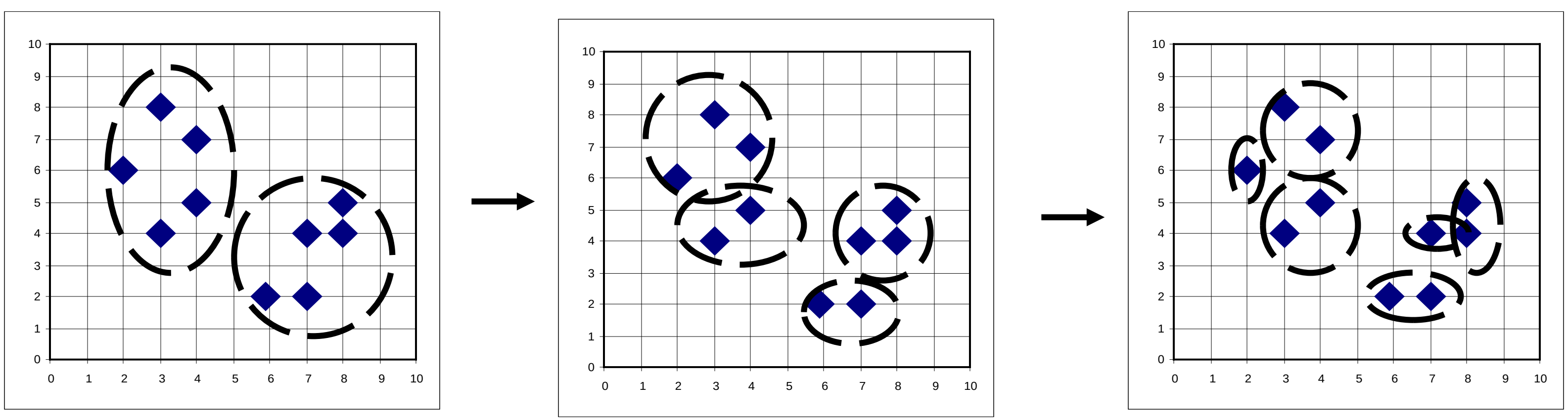
Decompose data objects into a several levels of nested partitioning (<u>tree</u> of clusters), called a <u>dendrogram</u>

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

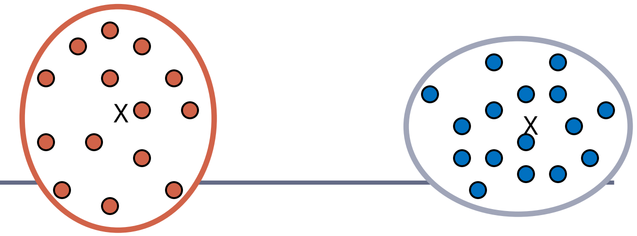


DIANA (Divisive Analysis)

- 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



Distance between Clusters



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

$$C_i = \frac{\sum_{p=1}^{N_i}(t_{ip})}{N_i}$$

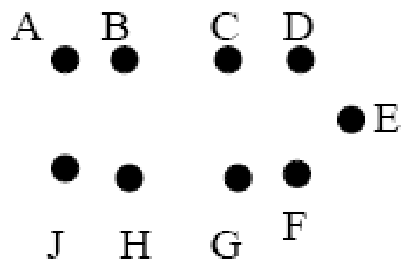
- Radius: square root of average distance from any point of the cluster to its centroid

$$R_i = \sqrt{\frac{\sum_{p=1}^{N_i}(t_{ip} - c_i)^2}{N_i}}$$

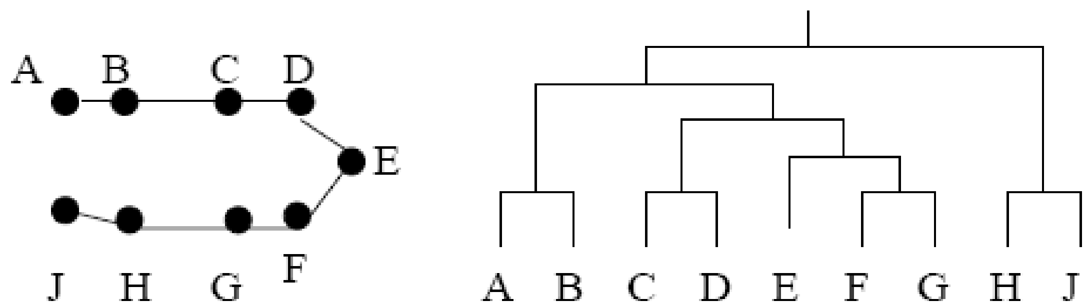
- Diameter: square root of average mean squared distance between all pairs of points in the cluster

$$D_i = \sqrt{\frac{\sum_{p=1}^{N_i}\sum_{q=1}^{N_i}(t_{ip} - t_{iq})^2}{N_i(N_i - 1)}}$$

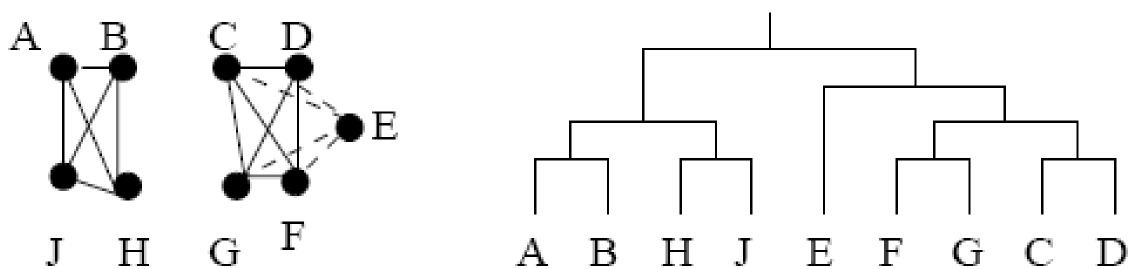
Example: Single Link vs. Complete Link



(a) Data set



(b) Clustering using single linkage



(c) Clustering using complete linkage

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

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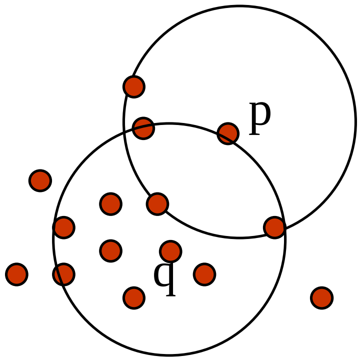
Density-Based Clustering Methods

- 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)

DBSCAN: Basic Concepts

- Two parameters:
  - *Eps*: Maximum radius of the neighborhood
  - *MinPts*: Minimum number of points in an Eps-neighborhood 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:

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

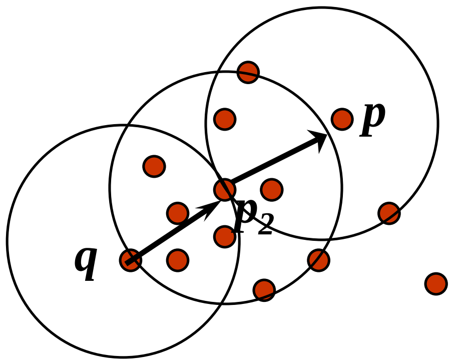


MinPts = 5

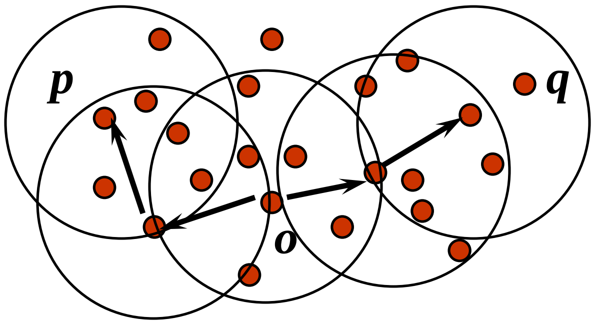
Eps = 1 cm

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

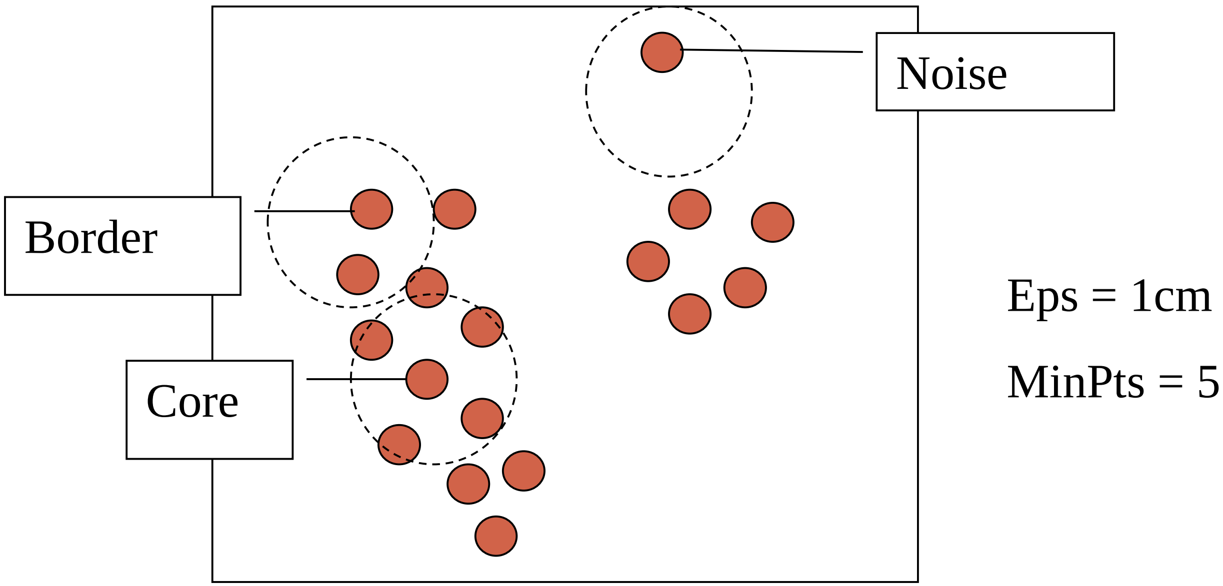


- Density-connected
  - A point p is density-connected to a point q w.r.t. *Eps*, *MinPts* if there is a point o such that both, p and q are density-reachable from o w.r.t. *Eps* and *MinPts*



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
- Noise: object not contained in any cluster is noise
- Discovers clusters of arbitrary shape in spatial databases with noise



DBSCAN: The Algorithm

```
mark all objects as unvisited;
do
    randomly select an unvisited object p;
    mark p as visited;
    if the ε-neighborhood of p has at least MinPts objects
        create a new cluster C, and add p to C;
        let N be the set of objects in the ε-neighborhood of p;
        for each point p′ in N
            if p′ is unvisited
                mark p′ as visited;
                if the ε-neighborhood of p′ has at least MinPts points,
                add those points to N;
            if p′ is not yet a member of any cluster, add p′ to C;
        end for
        output C;
    else mark p as noise;
until no object is unvisited;
```

- *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.

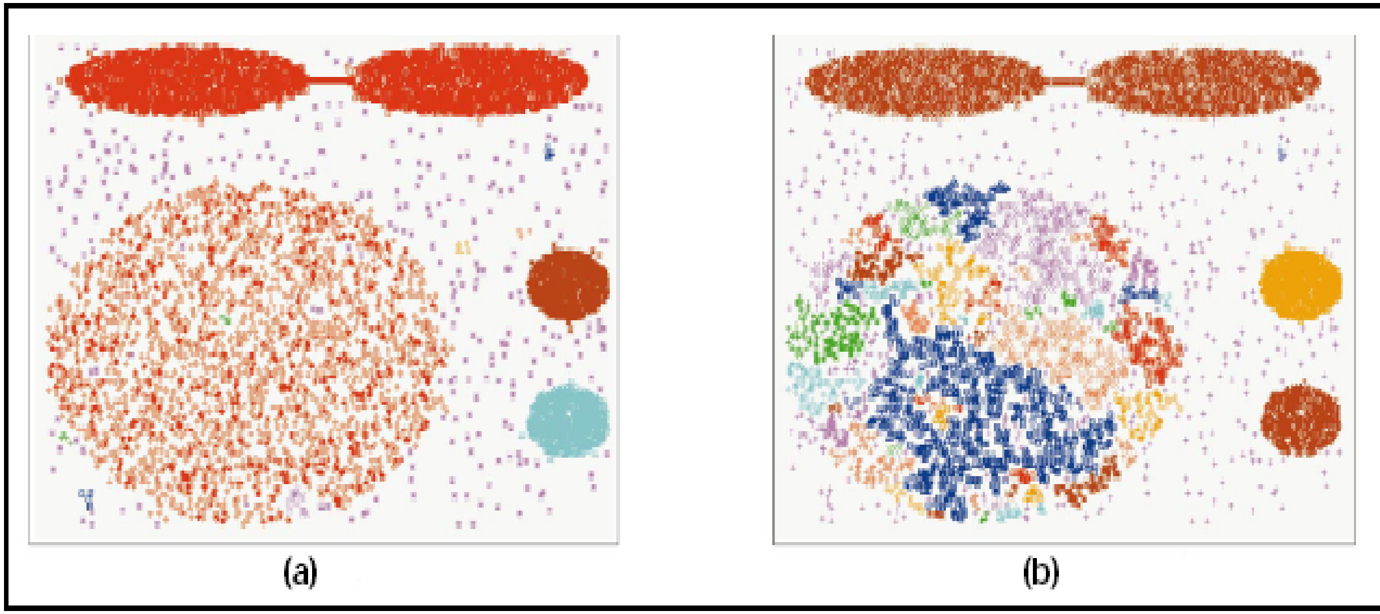
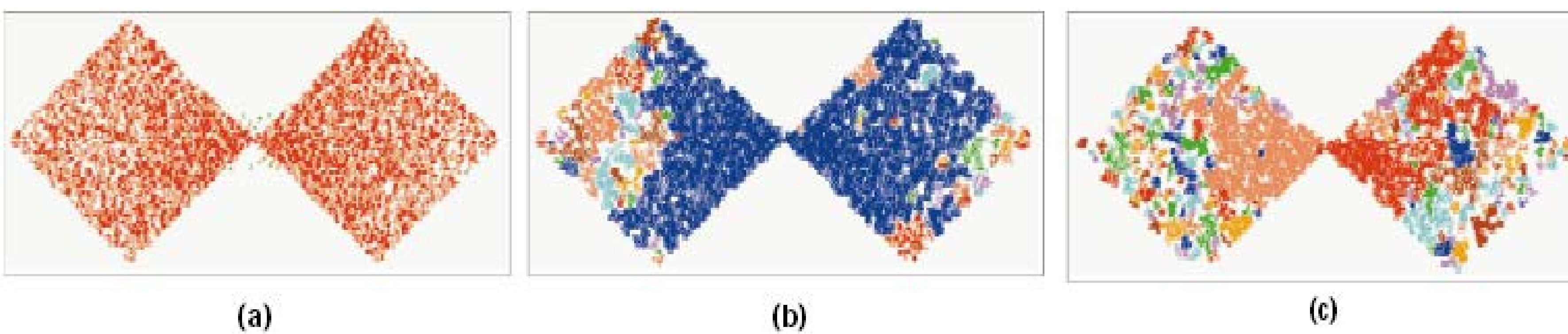


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



DBSCAN online Demo:

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

Questions about Parameters

- Fix Eps, increase MinPts, what will happen?
- Fix MinPts, decrease Eps, what will happen?

*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
  - Index-based time complexity: O(N*logN)

OPTICS: Some Extension from DBSCAN

- 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; $card(N_\varepsilon(p))$: the size of set $N_\varepsilon(p)$
  - Let MinPts-distance(p): the distance from p to its MinPts' neighbor

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

- Reachability Distance of object p from core object q is the min radius value that makes p density-reachable from q
  - Let distance(q,p) be the Euclidean distance between q and p

$$\text{Reachability-distance}_{\varepsilon,\ \text{MinPts}}(p, q) = \begin{cases} \text{Undefined, if } q \text{ is not a core object} \\ \max(\text{core-distance}(q),\ \text{distance}(q, p)), \text{ otherwise} \end{cases}$$

Core Distance & Reachability Distance

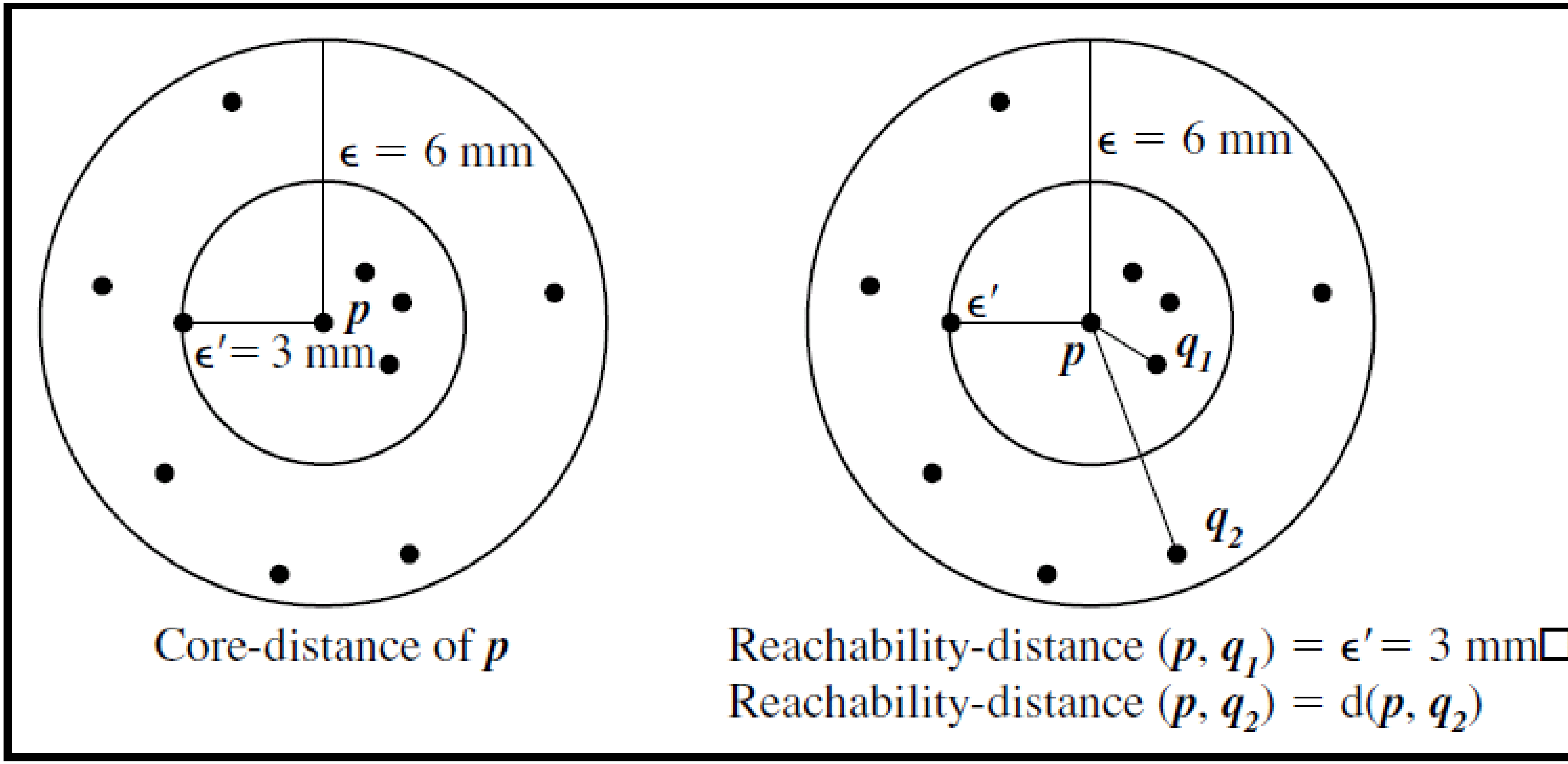
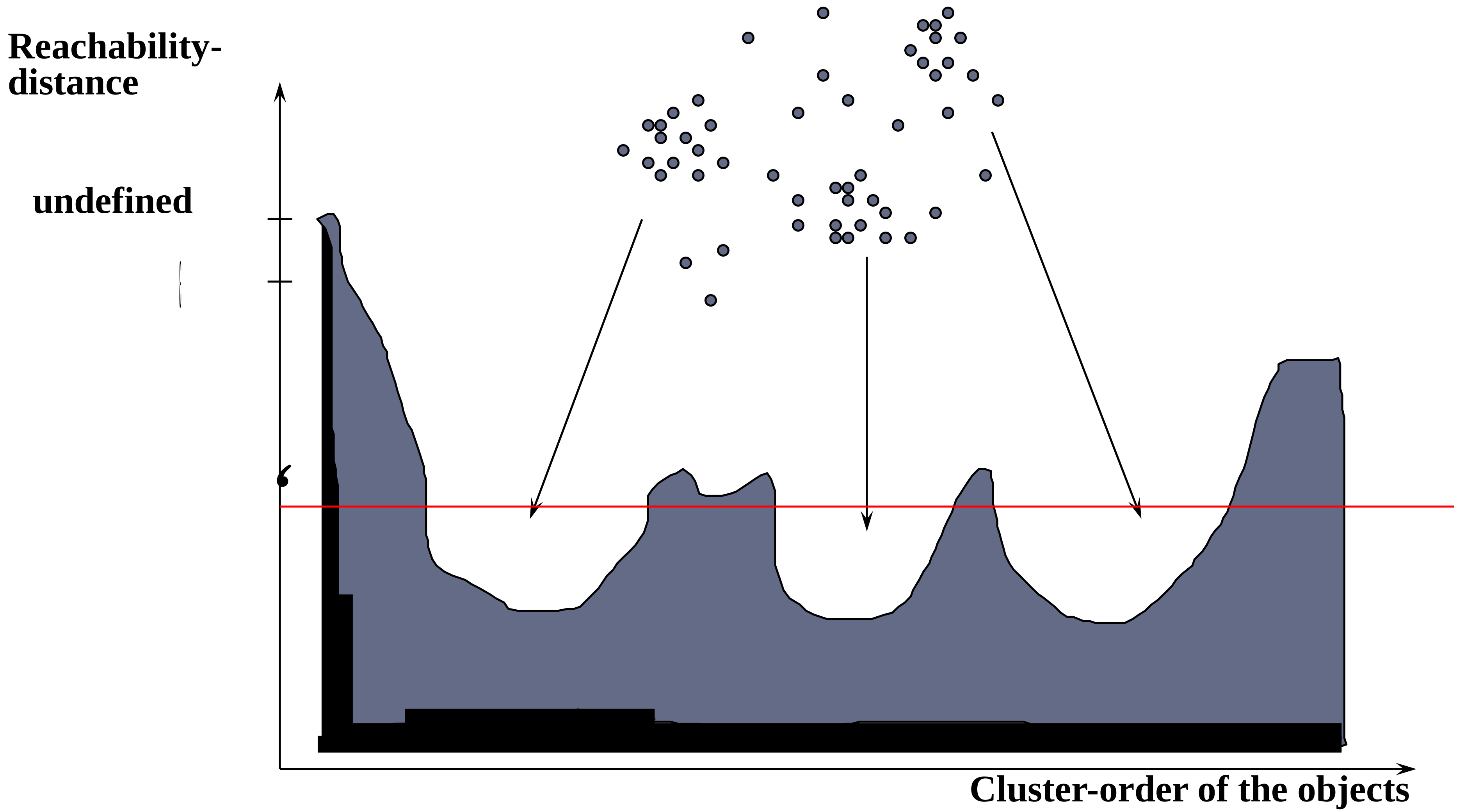


Figure 10.16: OPTICS terminology. Based on [ABKS99].

$$\varepsilon = 6mm, MinPts = 5$$

Output of OPTICS: cluster-ordering

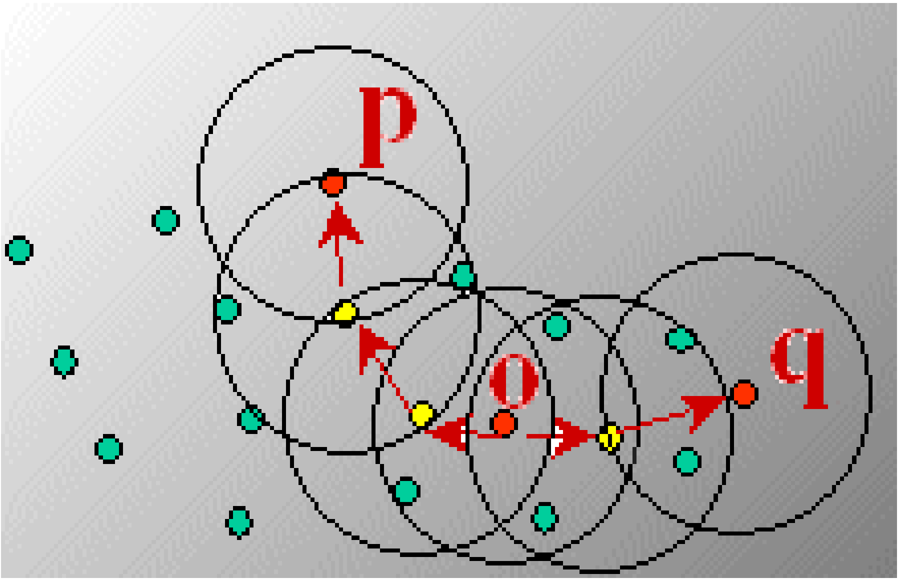


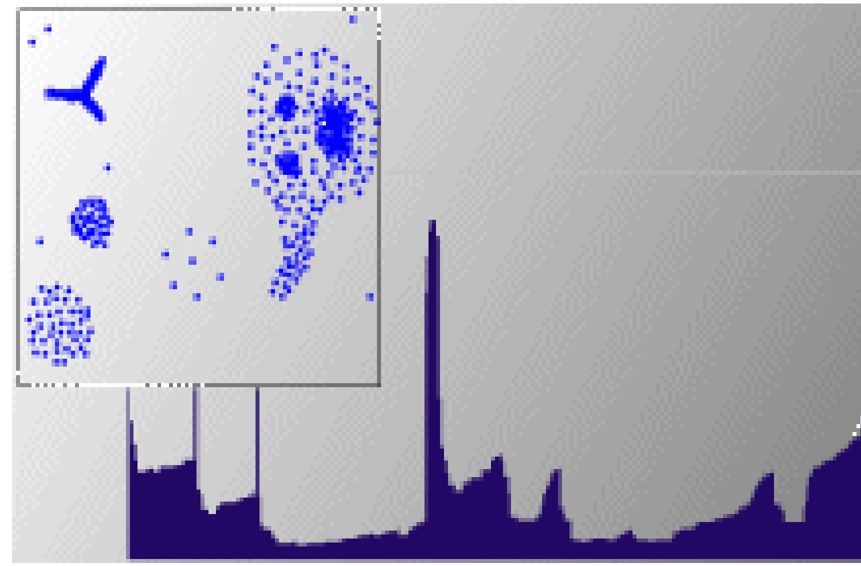
Extract DBSCAN-Clusters

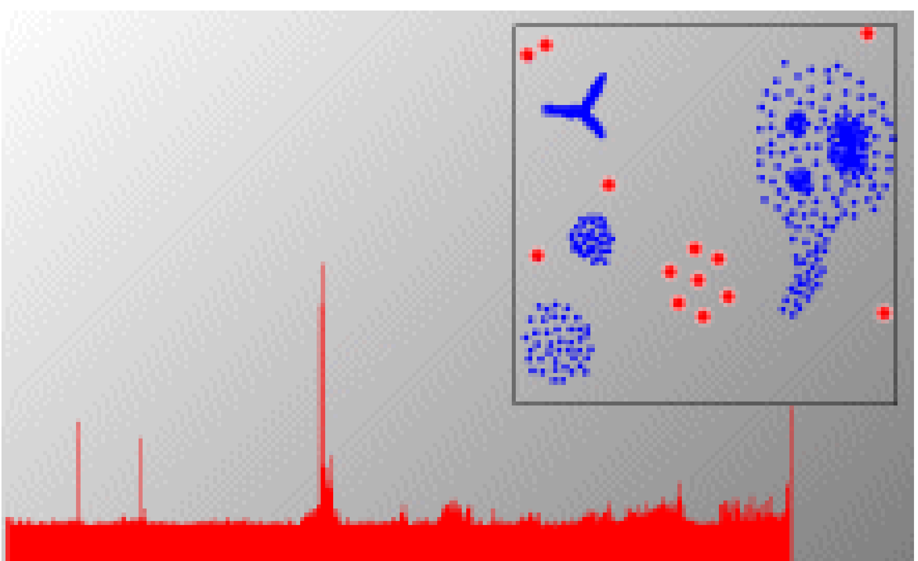
```
ExtractDBSCAN-Clustering (ClusterOrderedObjs,ε', MinPts)
// Precondition: ε' ≤ generating dist ε for ClusterOrderedObjs
  ClusterId := NOISE;
  FOR i FROM 1 TO ClusterOrderedObjs.size DO
    Object := ClusterOrderedObjs.get(i);
    IF Object.reachability_distance > ε' THEN
      // UNDEFINED > ε
      IF Object.core_distance ≤ ε' THEN
        ClusterId := nextId(ClusterId);
        Object.clusterId := ClusterId;
      ELSE
        Object.clusterId := NOISE;
    ELSE    // Object.reachability_distance ≤ ε'
      Object.clusterId := ClusterId;
END; // ExtractDBSCAN-Clustering
```

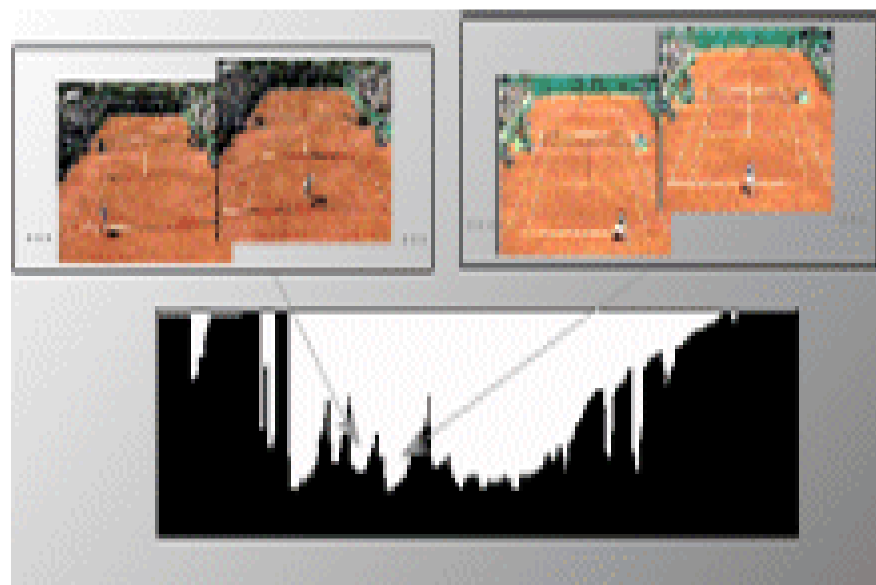
Density-Based Clustering: OPTICS & Applications

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

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

total influence on x

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

gradient of x in the direction of x_i

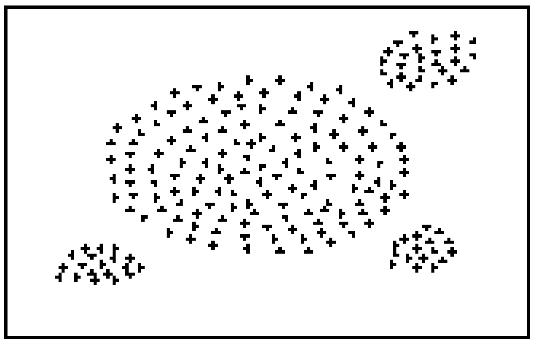
- Major features
  - Solid mathematical foundation
  - Good for data sets with large amounts of noise
  - Allows a compact mathematical description of arbitrarily shaped clusters in high-dimensional data sets
  - Significant faster than existing algorithm (e.g., DBSCAN)
  - But needs a large number of parameters

Denclue: Technical Essence

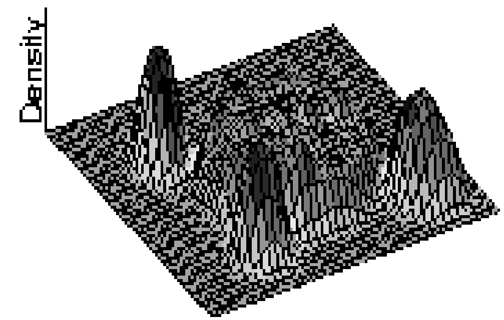
- Overall density of the data space can be calculated as the sum of the influence function of all data points
  - Influence function: describes the impact of a data point within its neighborhood
- Clusters can be determined mathematically by identifying density attractors
  - Density attractors are local 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

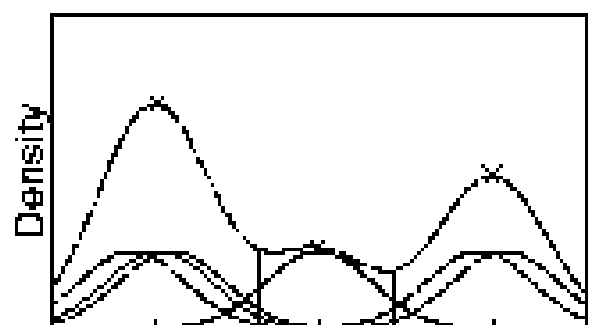
Can be detected by hill-climbing procedure of finding local maximums



(a) Data Set



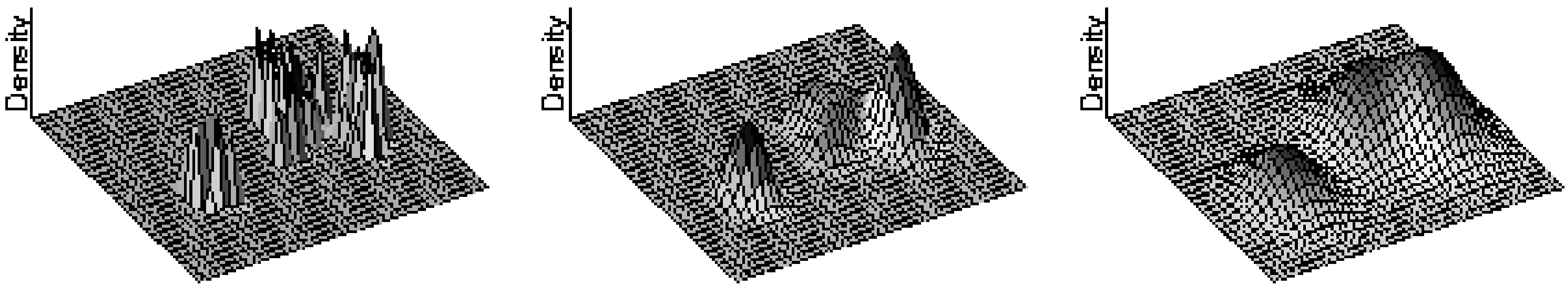
(c) Gaussian



Noise Threshold

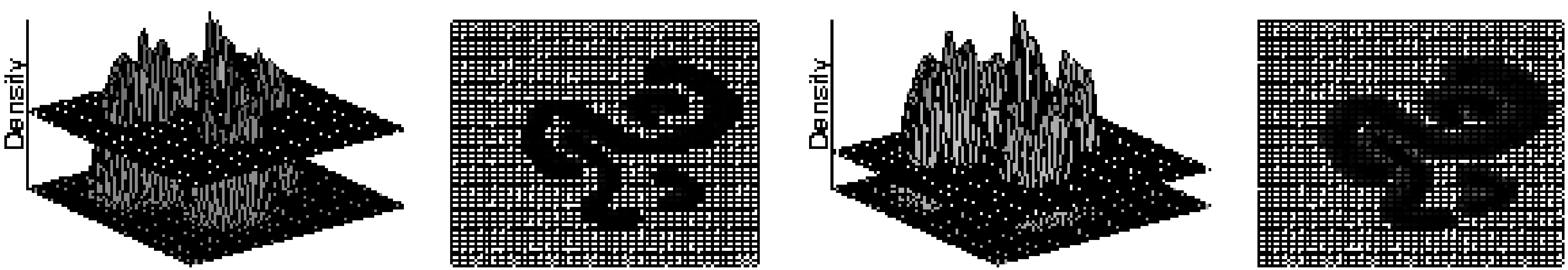
- Noise Threshold ξ
  - Avoid trivial local maximum points
  - A point can be a density attractor only if $\hat{f}(x) \geq \xi$

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

Vector Data: Clustering: Part I

- Clustering Analysis: Basic Concepts
- Partitioning methods
- Hierarchical Methods
- Density-Based Methods
- 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
- K-means and K-medoids algorithms are popular partitioning-based clustering algorithms
- AGNES and DIANA are interesting hierarchical clustering algorithms
- DBSCAN, OPTICS*, and DENCLU* are interesting density-based algorithms

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