CS6220: DATA MINING TECHNIQUES

Matrix Data: Clustering: Part 1

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February 10, 2016

Announcements

- Homework 1 grades out
- Re-grading policy:
  - If you have doubts in your grading, please submit a regrading form (via emails to both TAs and CC to the Instructor) indicating clearly the reason why you think it should be regraded
  - The deadline of the regrading form should be submitted within one week after you receive your score
  - We will regrade the whole homework/exam

Methods to Learn

	Matrix Data	Text Data	Set Data	Sequence Data	Time Series	Graph & Network	Images
Classification	Decision Tree; Naïve Bayes; Logistic Regression SVM; kNN			HMM		Label Propagation	Neural Network
Clustering	**K-means; hierarchical clustering; DBSCAN**; Mixture Models; kernel k-means*	PLSA				SCAN; Spectral Clustering	
Frequent Pattern Mining			Apriori; FP-growth	GSP; PrefixSpan			
Prediction	Linear Regression				Autoregression	Collaborative Filtering	
Similarity Search					DTW	P-PageRank	
Ranking						PageRank	

Matrix Data: Clustering: Part 1

- Cluster Analysis: Basic Concepts
- Partitioning Methods
- Hierarchical Methods
- Density-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., *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_i is the centroid or medoid of cluster C_i)

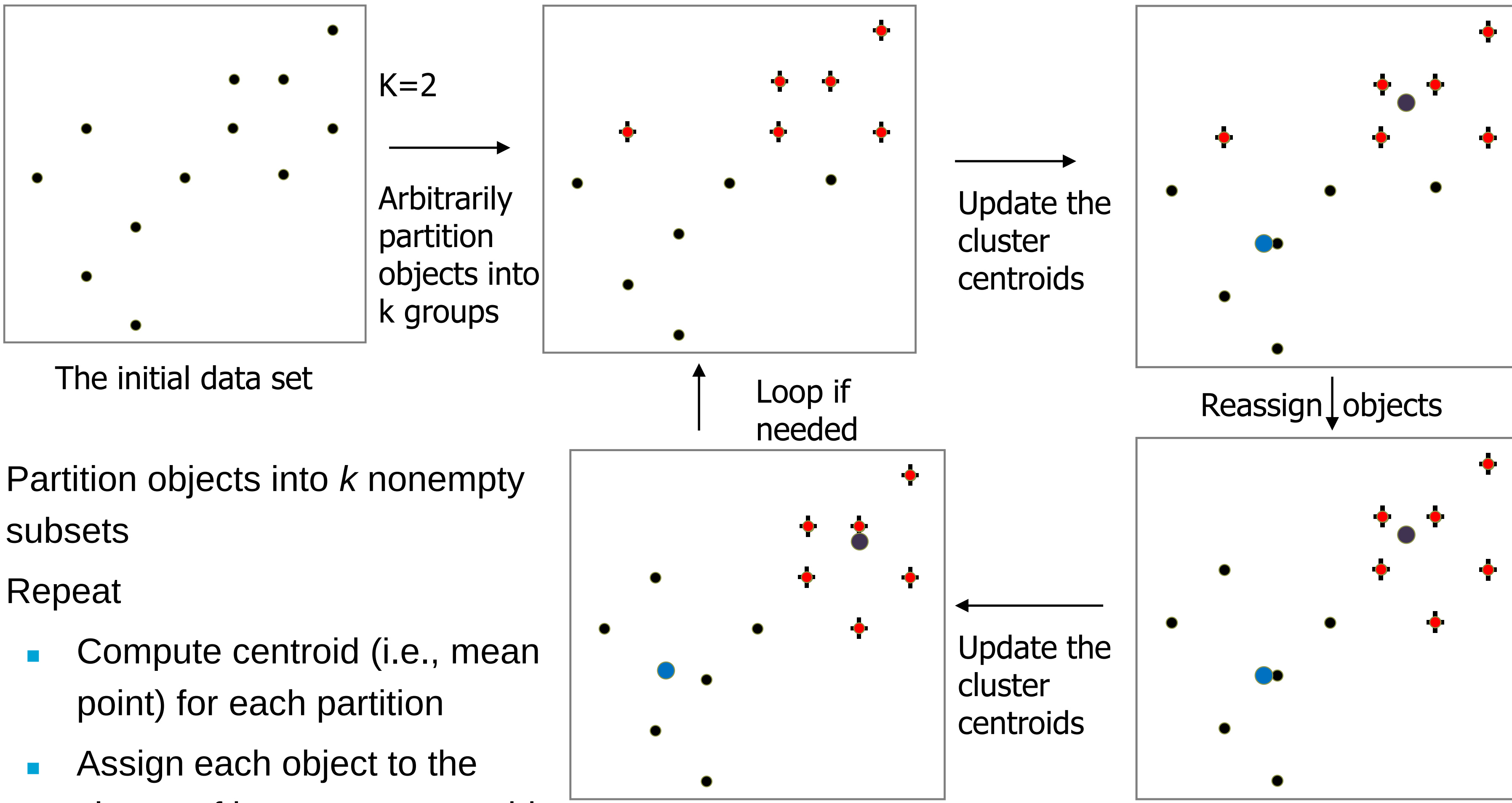
$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (d(p, c_i))^2$$

- 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:
  - 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

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

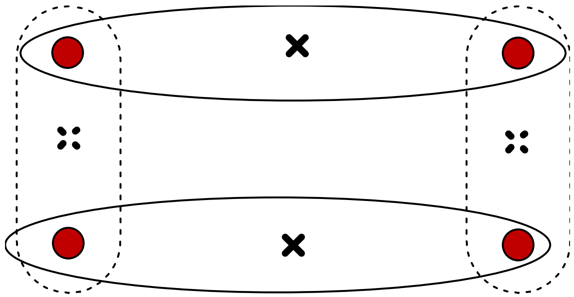
- Iterations
  - Step 1: Fix centers c_j, find assignment w_{ij} that minimizes J
    - => $w_{ij} = 1, if\ ||x_i - c_j||^2$ is the smallest
  - Step 2: Fix assignment w_{ij}, find centers that minimize J
    - => first derivative of J = 0
    - => $\frac{\partial J}{\partial c_j} = -2 \sum_i w_{ij}(x_i - c_j) = 0$
    - =>$c_j = \frac{\sum_i w_{ij} x_i}{\sum_i w_{ij}}$
      - 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

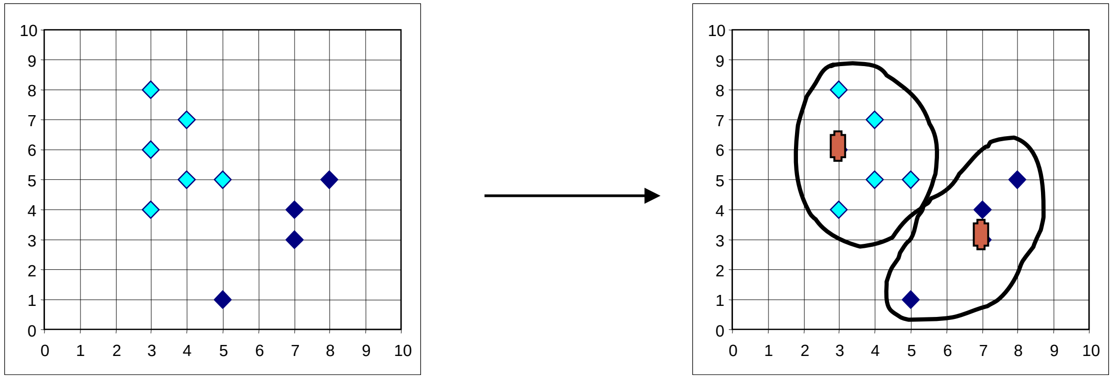
- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means



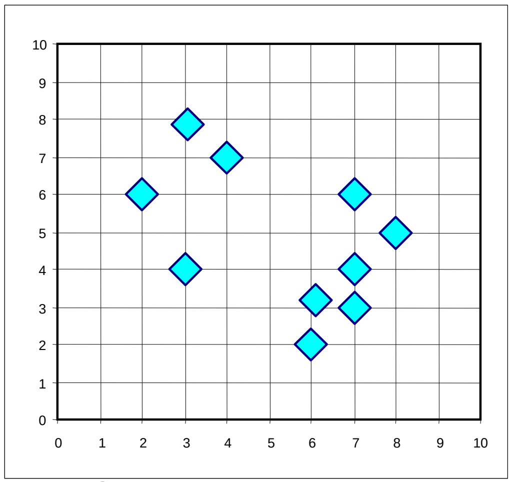
- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

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

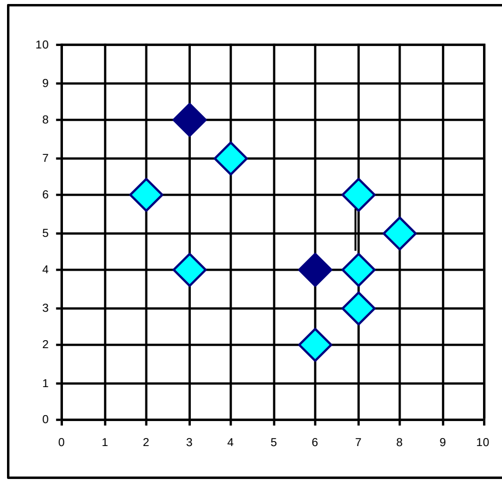


PAM: A Typical K-Medoids Algorithm



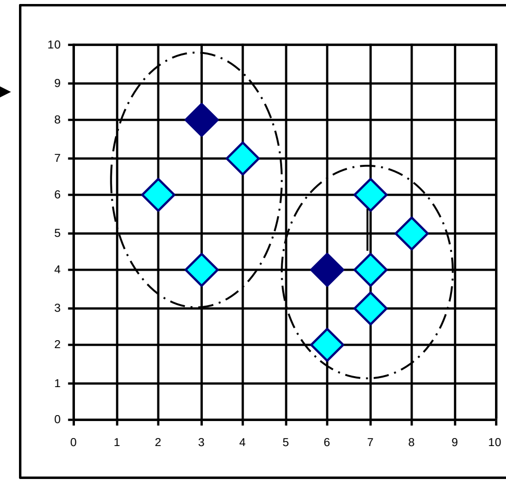
K=2

Arbitrary choose k object as initial medoids

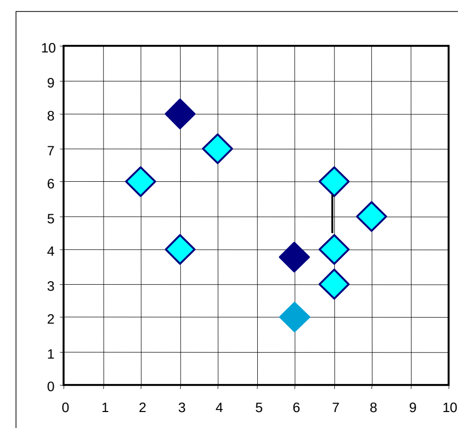


Assign each remaining object to nearest medoids

Total Cost = 20

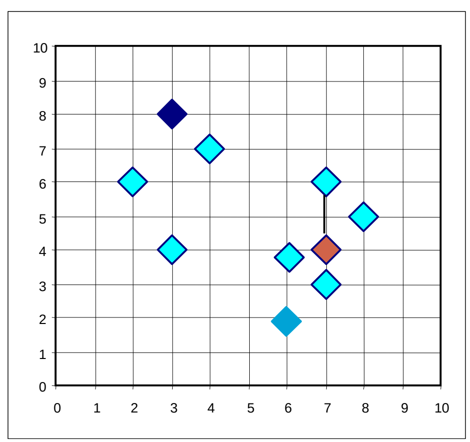


Randomly select a nonmedoid object,O_{ramdom}



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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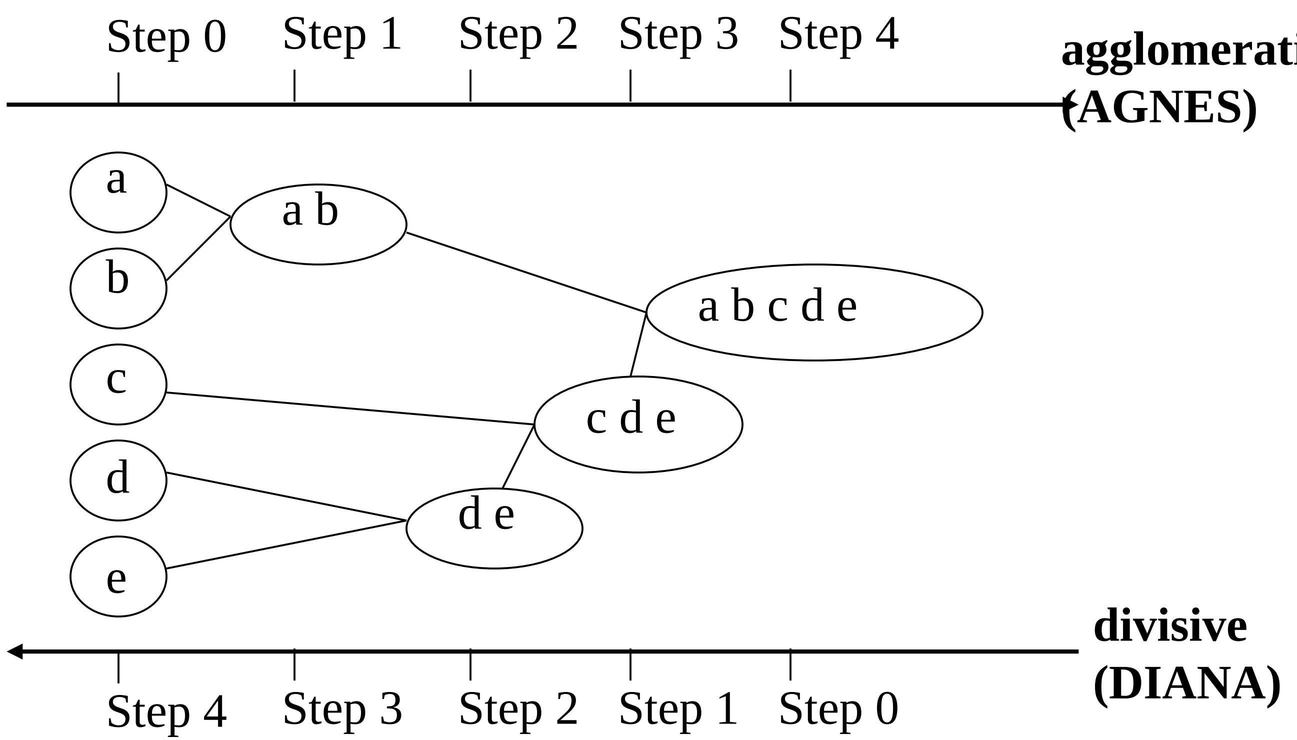
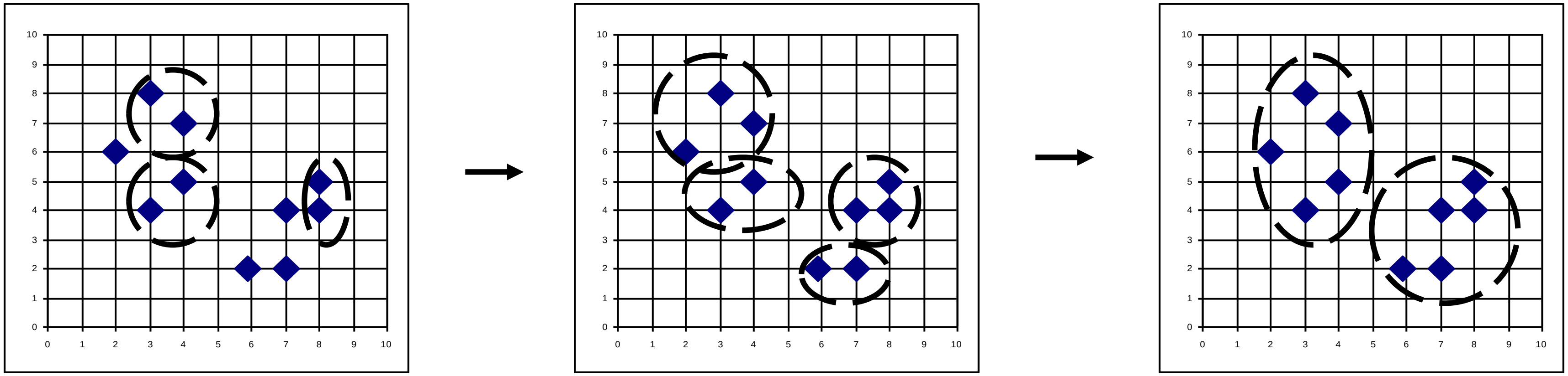
Hierarchical Clustering

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



AGNES (Agglomerative Nesting)

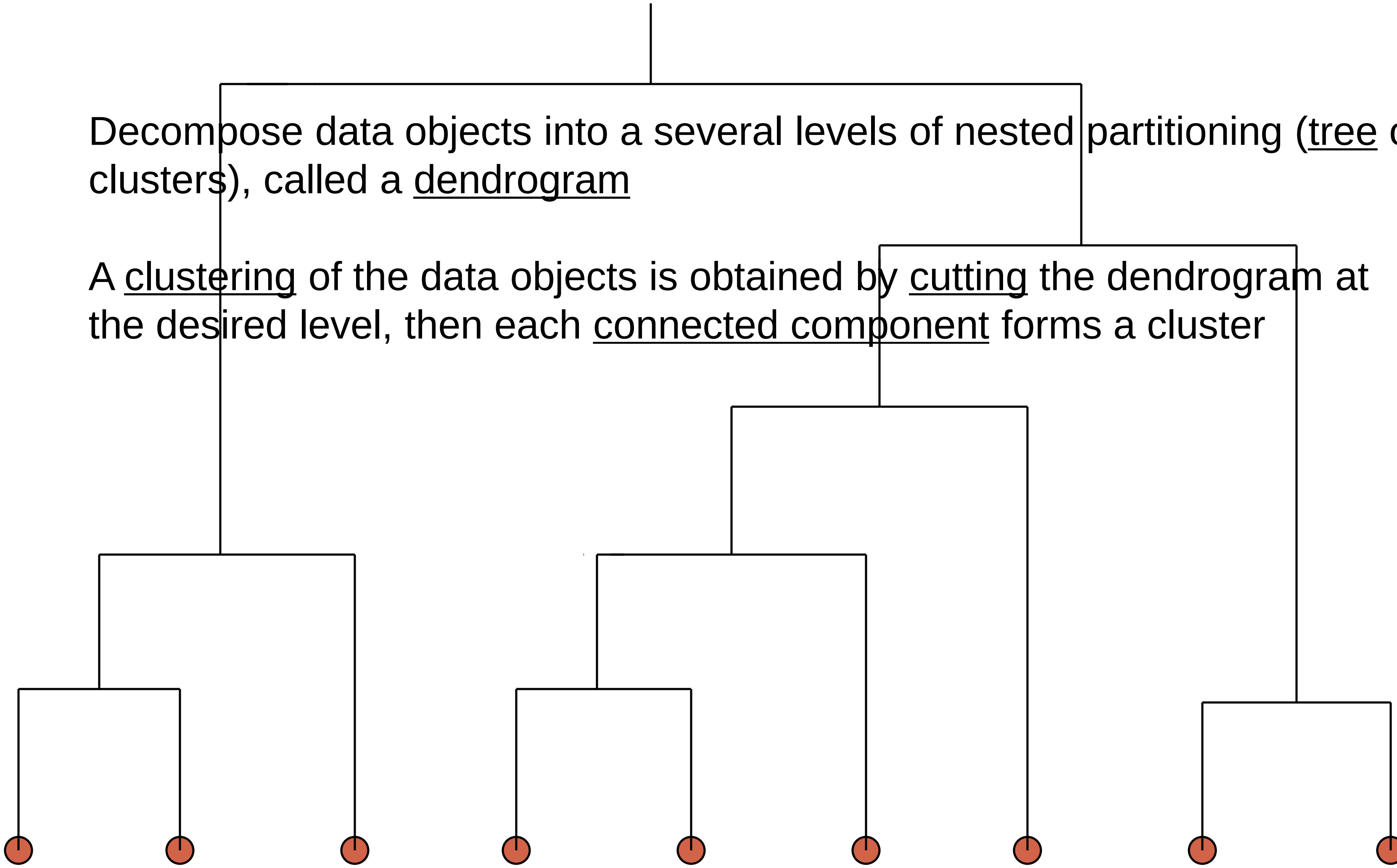
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the **single-link** method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



Dendrogram: Shows How Clusters are Merged

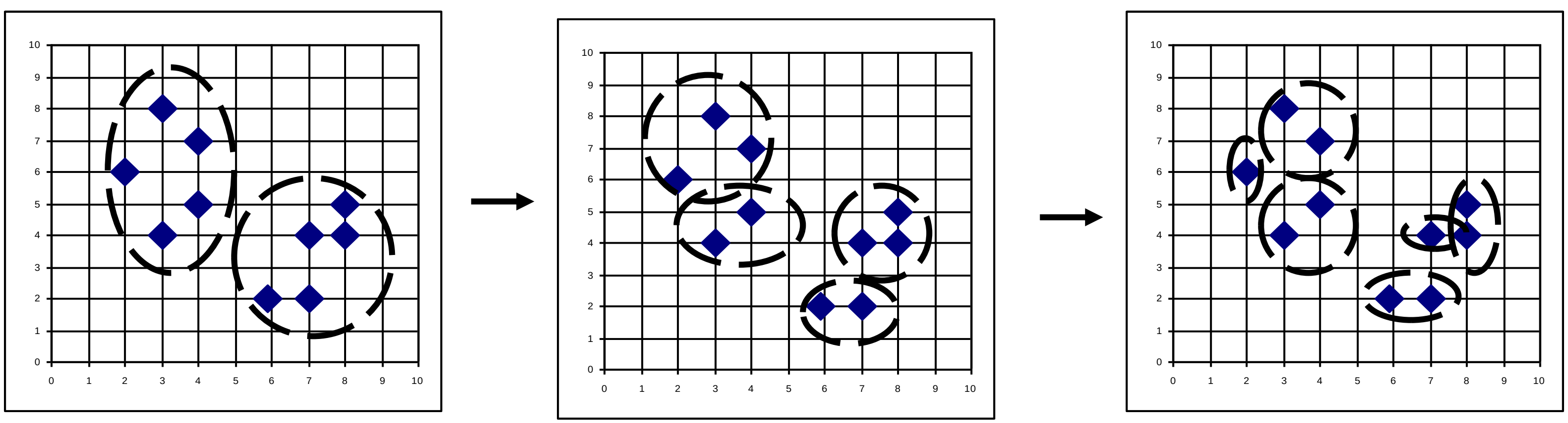
Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram

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

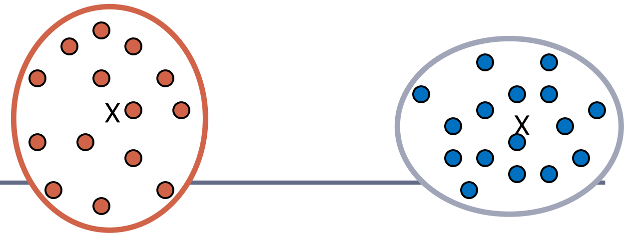


DIANA (Divisive Analysis)

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



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

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

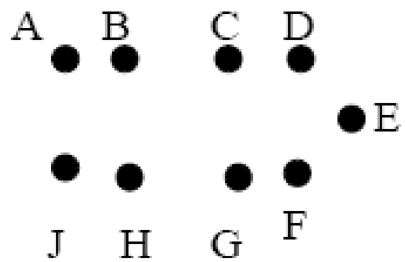
- Radius: square root of average distance from any point of the cluster to its centroid

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

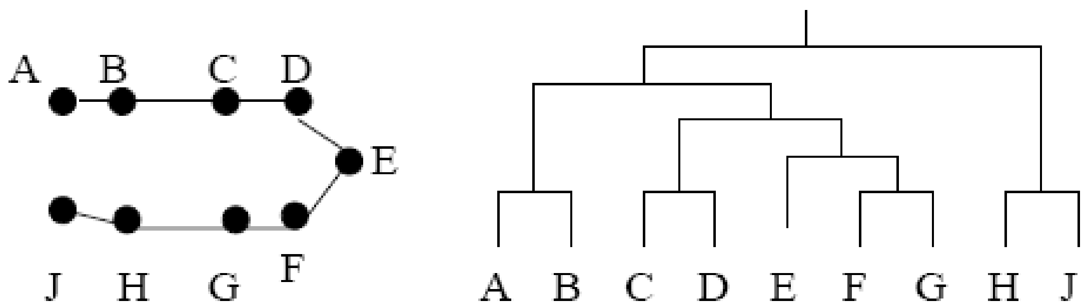
- Diameter: square root of average mean squared distance between all pairs of points in the cluster

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

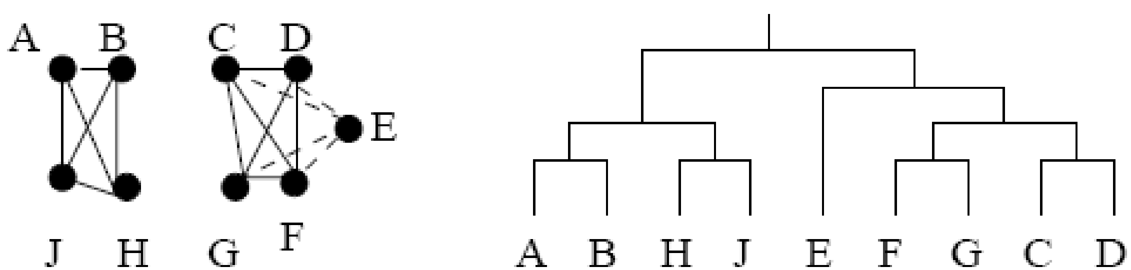
Example: Single Link vs. Complete Link



(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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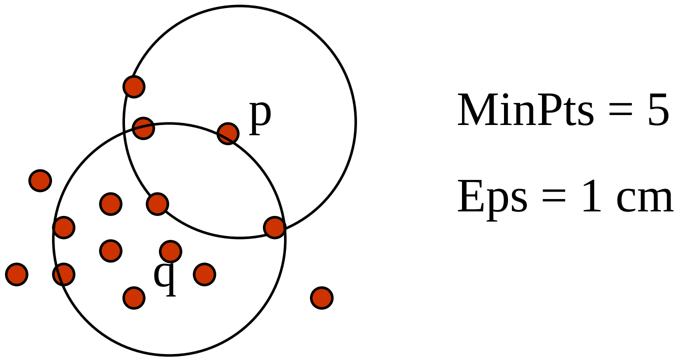
Density-Based Clustering Methods

- 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

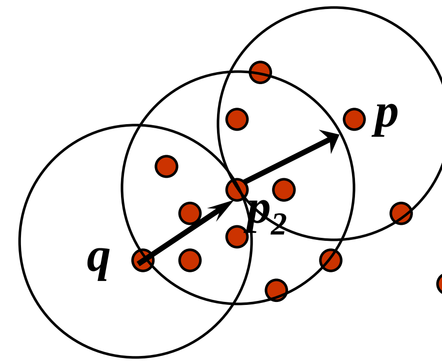
- Two parameters:
  - *Eps*: Maximum radius of the neighborhood
  - *MinPts*: Minimum number of points in an Eps-neighborhood of that point
- $N_{Eps}(q)$: {p belongs to D | dist(p,q) ≤ Eps}
- Directly density-reachable: A point *p* is directly density-reachable from a point *q* w.r.t. *Eps*, *MinPts*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

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

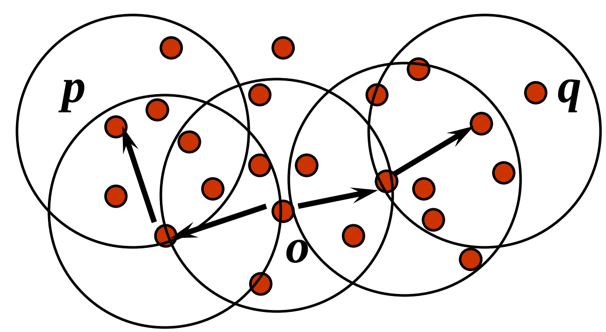


Density-Reachable and Density-Connected

- 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

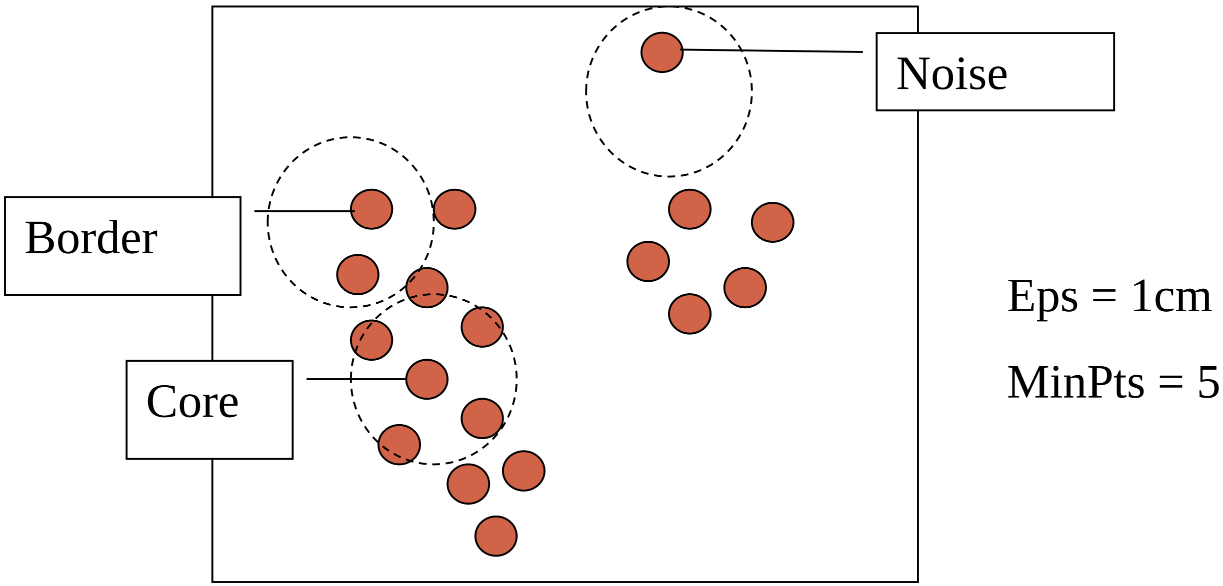


- Density-connected
  - A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



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.

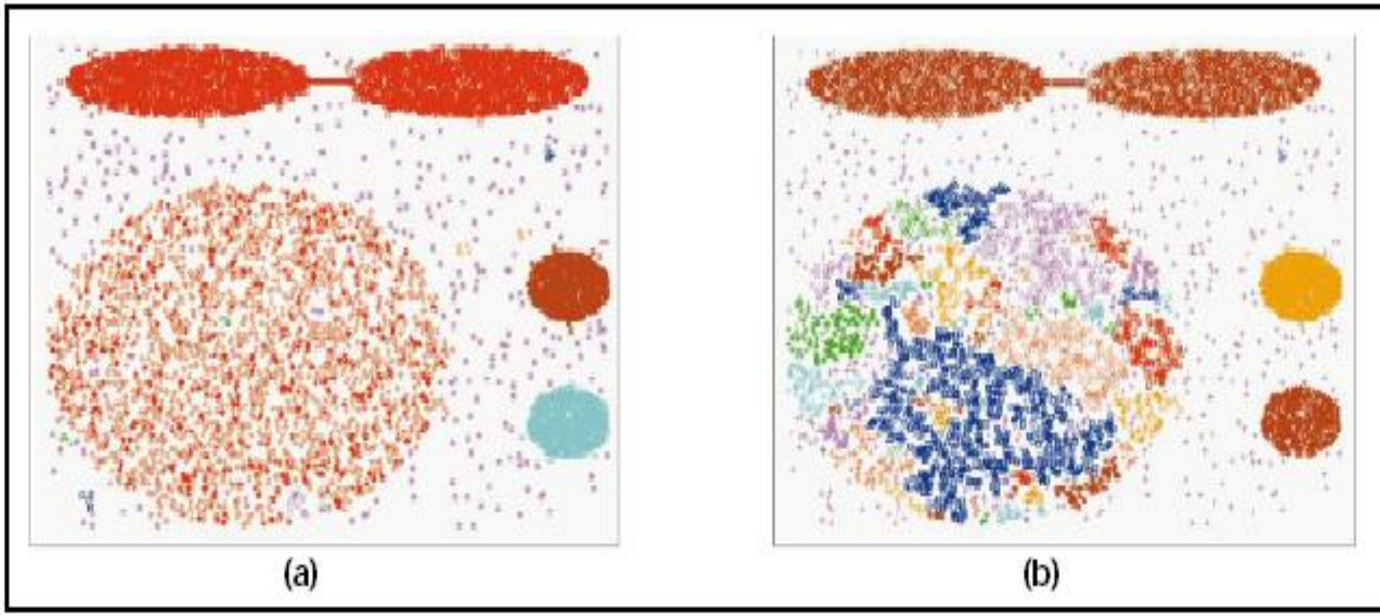
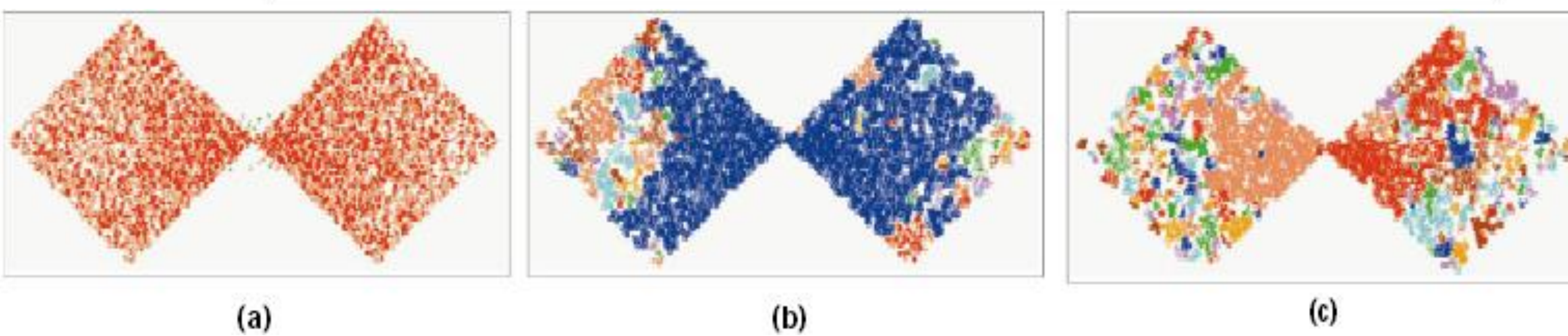


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



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

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

- 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

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

Core Distance & Reachability Distance

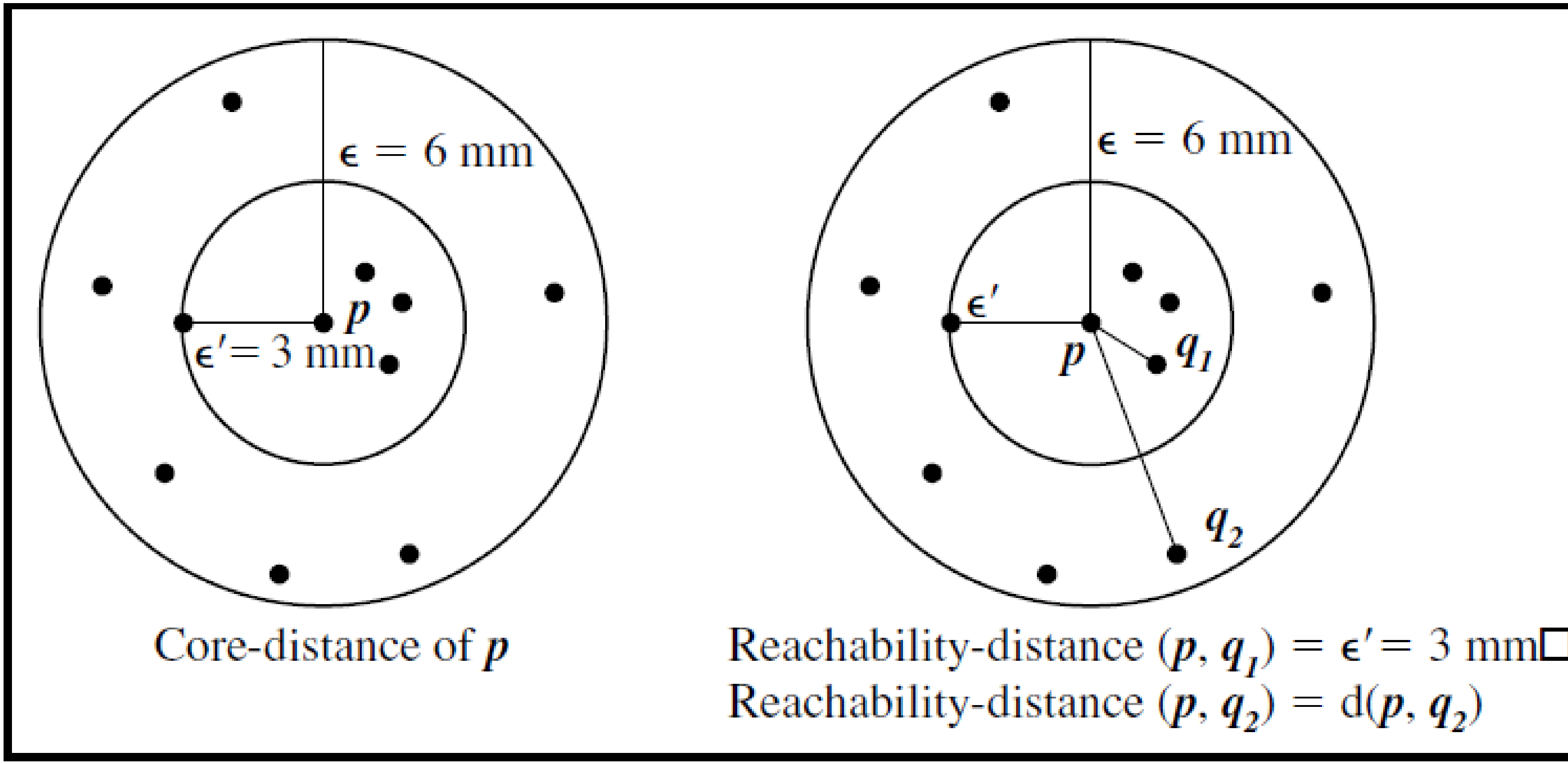
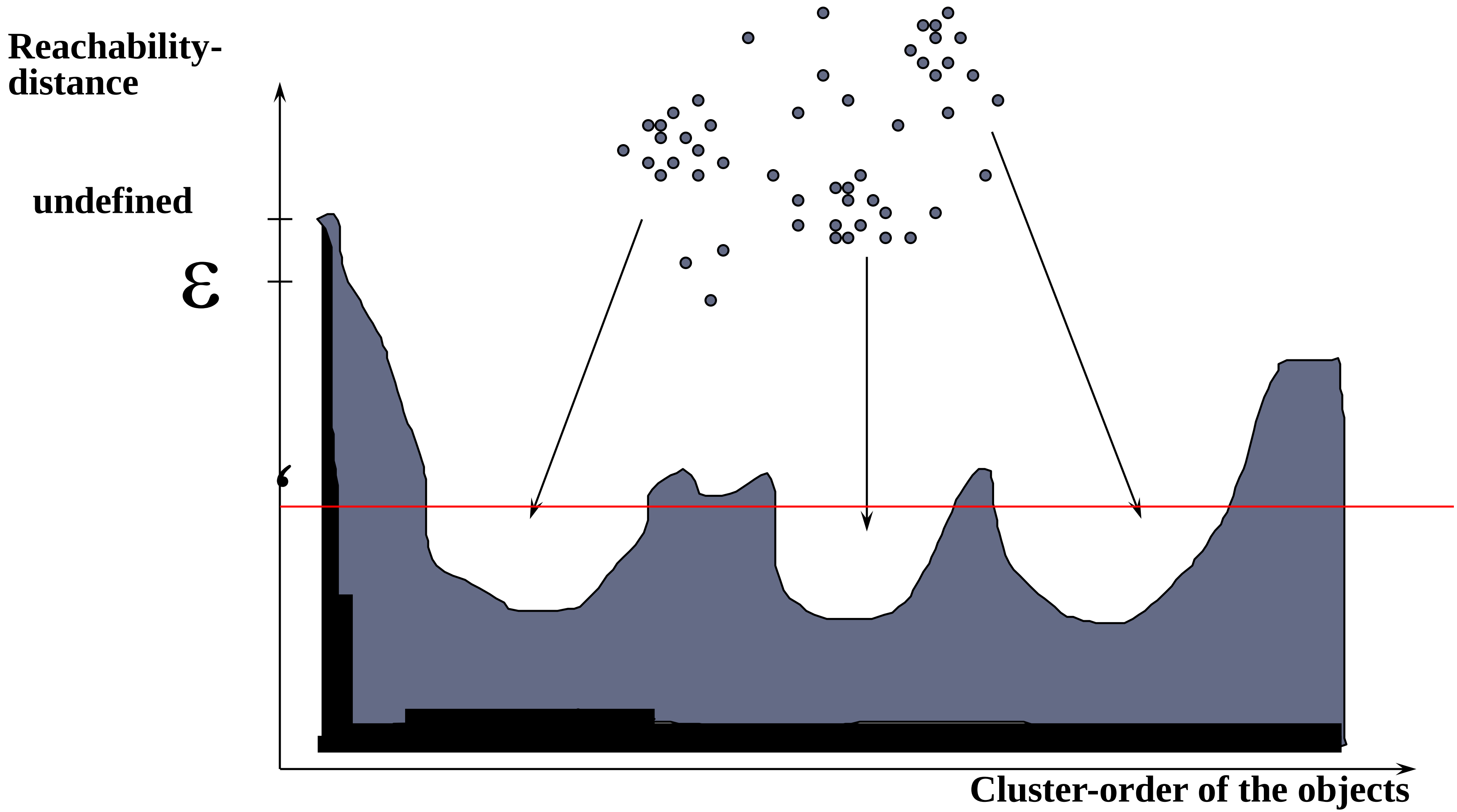


Figure 10.16: OPTICS terminology. Based on [ABKS99].

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

Output of OPTICS: cluster-ordering

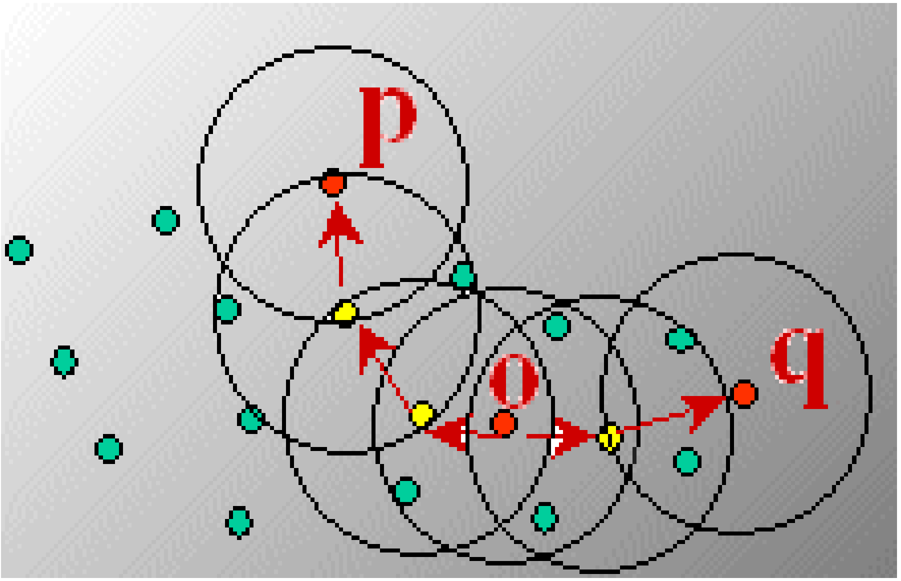


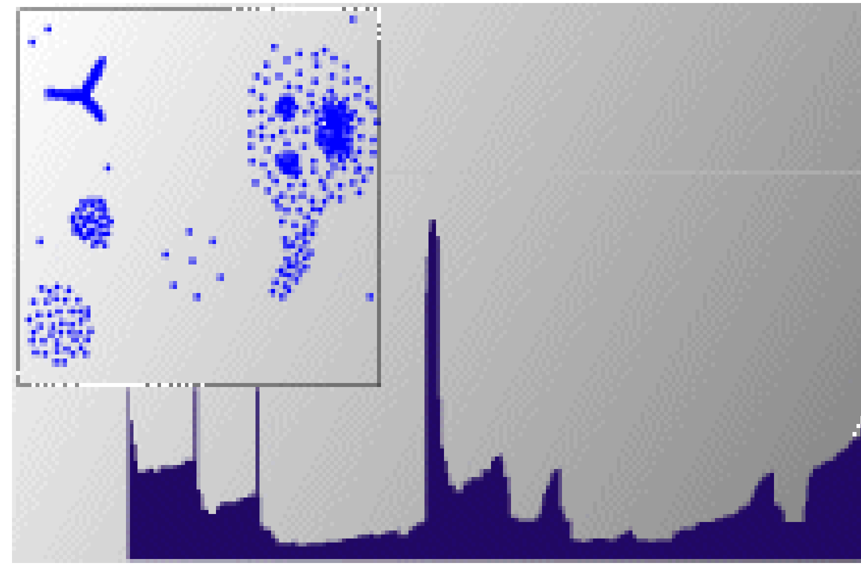
Extract DBSCAN-Clusters

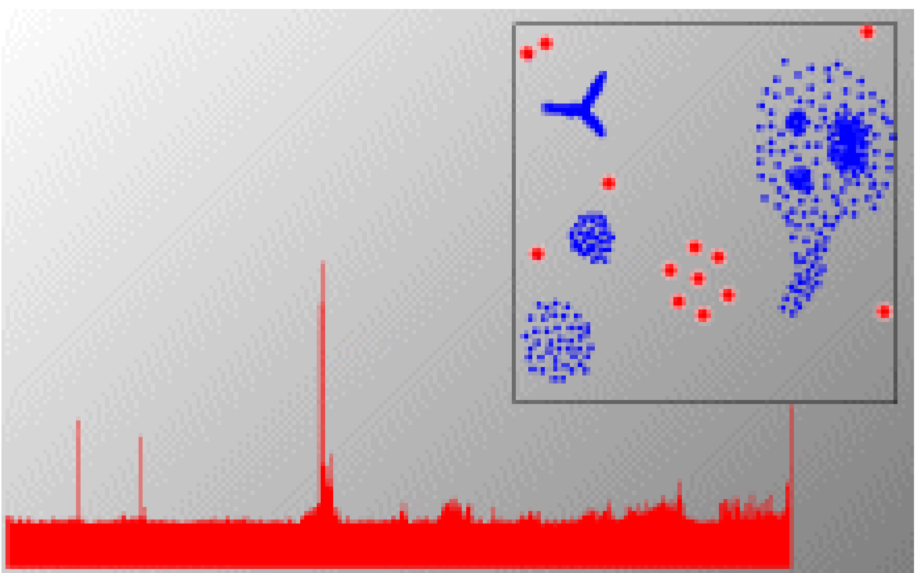
```
ExtractDBSCAN-Clustering (ClusterOrderedObjs,ε', MinPts)
// Precondition: ε' ≤ generating dist ε for ClusterOrderedObjs
   ClusterId := NOISE;
   FOR i FROM 1 TO ClusterOrderedObjs.size DO
      Object := ClusterOrderedObjs.get(i);
      IF Object.reachability_distance > ε' THEN
         // UNDEFINED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

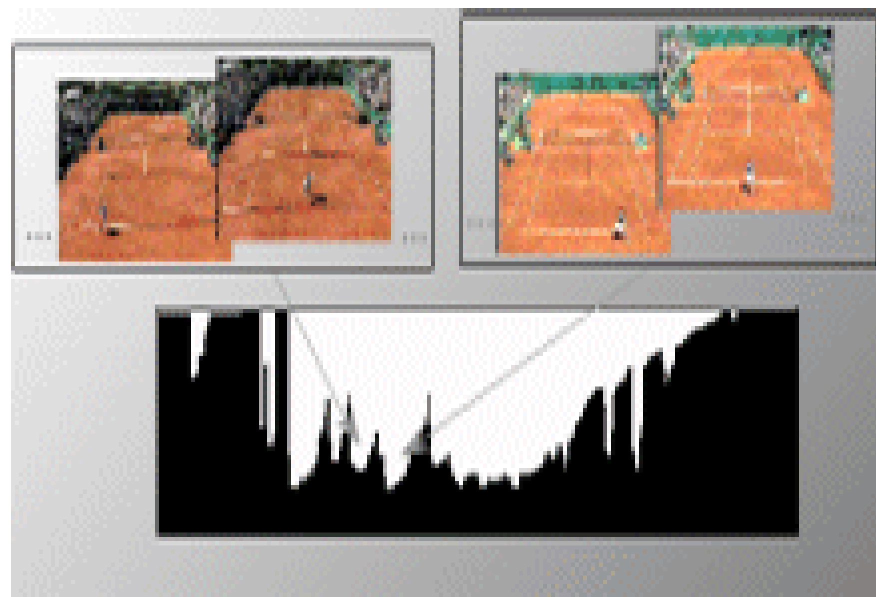
Density-Based Clustering: OPTICS & Applications

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

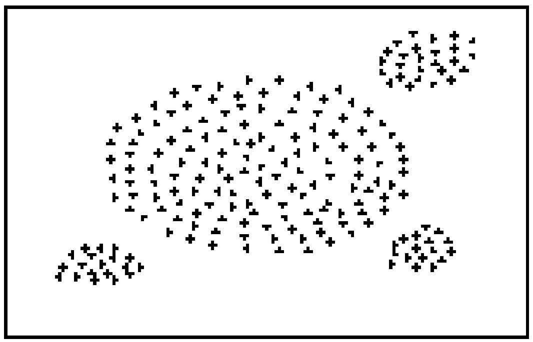
- Major features
  - Solid mathematical foundation
  - Good for data sets with large amounts of noise
  - Allows a compact mathematical description of arbitrarily shaped clusters in high-dimensional data sets
  - Significant faster than existing algorithm (e.g., DBSCAN)
  - But needs a large number of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

Denclue: Technical Essence

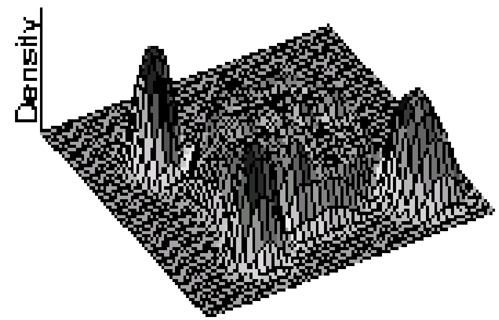
- Overall density of the data space can be calculated as the sum of the influence function of all data points
  - Influence function: describes the impact of a data point within its neighborhood
- Clusters can be determined mathematically by identifying density attractors
  - Density attractors are local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

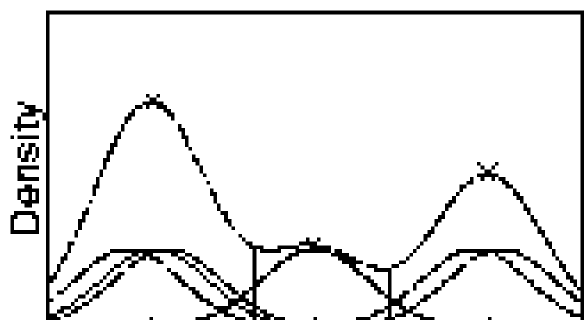
Can be detected by hill-climbing procedure of finding local maximums



(a) Data Set



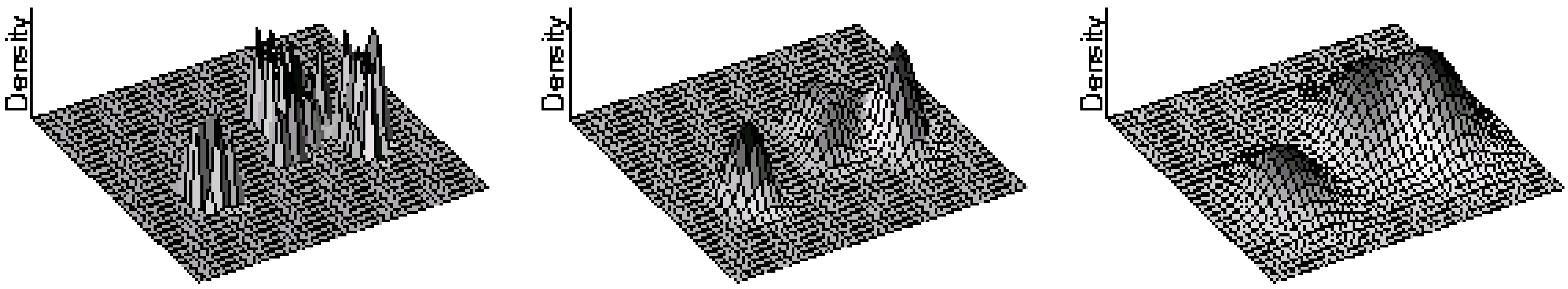
(c) Gaussian



Noise Threshold

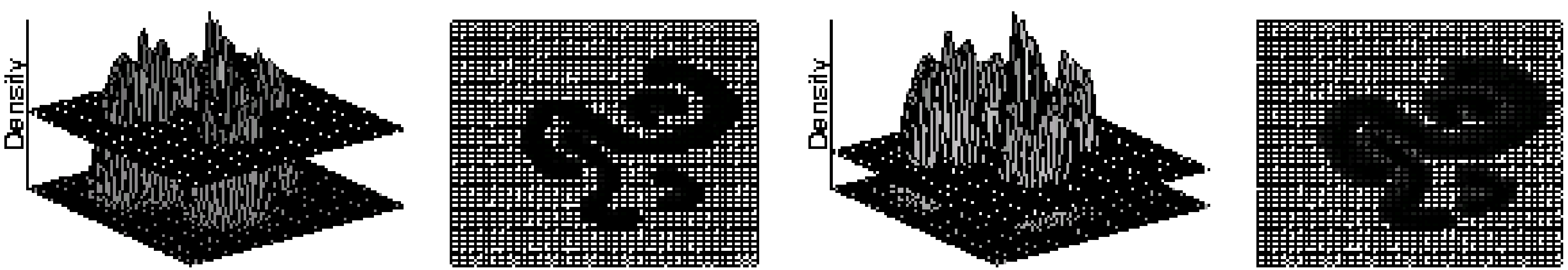
- Noise Threshold ξ
  - Avoid trivial local maximum points
  - A point can be a density attractor only if $\hat{f}(x) \geq \xi$

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

Matrix Data: Clustering: Part 1

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

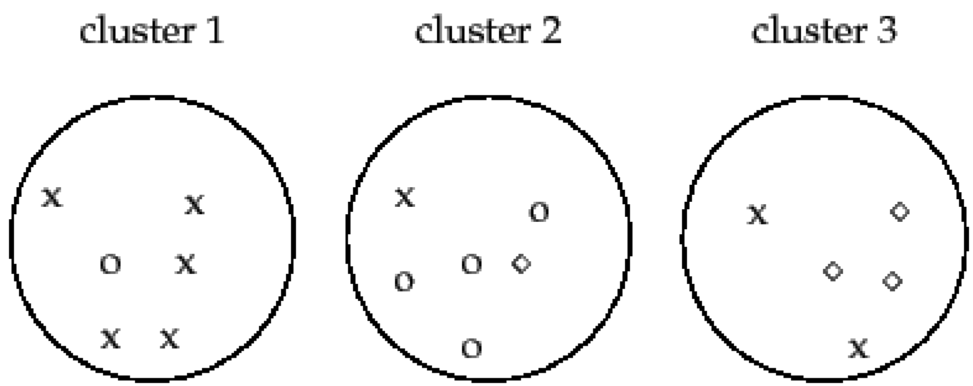
Measuring Clustering Quality

- Two methods: extrinsic vs. intrinsic
- Extrinsic: supervised, i.e., the ground truth is available
  - Compare a clustering against the ground truth using certain clustering quality measure
  - Ex. Purity, BCubed precision and recall metrics, normalized mutual information
- Intrinsic: unsupervised, i.e., the ground truth is unavailable
  - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are
  - Ex. Silhouette coefficient

Purity

- Let $\boldsymbol{C} = \{c_1, \dots, c_K\}$ be the output clustering result, $\boldsymbol{\Omega} = \{\omega_1, \dots, \omega_K\}$ be the ground truth clustering result (ground truth class)
  - c_k and w_k are sets of data points
  - $purity(C, \Omega) = \frac{1}{N} \sum_k \max_j |c_k \cap \omega_j|$

Example



▶ **Figure 16.1** Purity as an external evaluation criterion for cluster quality. Majority class and number of members of the majority class for the three clusters are: x, 5 (cluster 1); o, 4 (cluster 2); and ⋄, 3 (cluster 3). Purity is $(1/17) \times (5+4+3) \approx 0.71$.

- Clustering output: cluster 1, cluster 2, and cluster 3
- Ground truth clustering result: ×'s, ◊'s, and ○'s.

- cluster 1 vs. ×'s, cluster 2 vs. ○'s, and cluster 3 vs. ◊'s

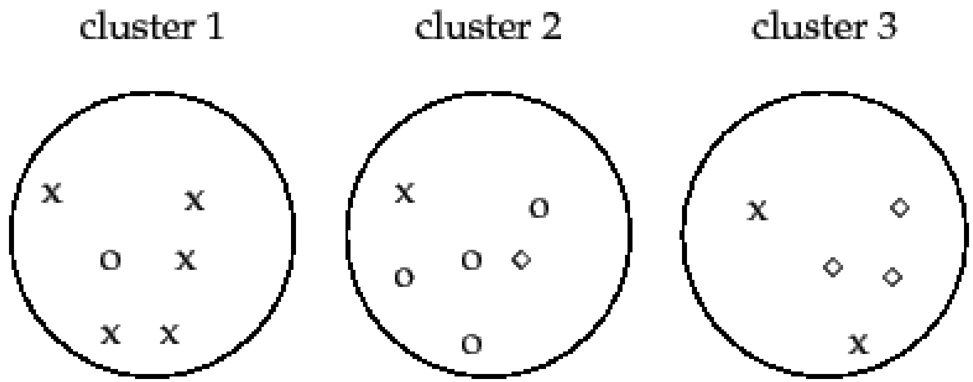
Normalized Mutual Information

- $NMI(\Omega, C) = \dfrac{I(\Omega,C)}{\sqrt{H(\Omega)H(C)}}$
  - $I(\Omega, C) = \sum_k \sum_j P(\omega_k \cap c_j) \log \dfrac{P(\omega_k \cap c_j)}{P(\omega_k)P(c_j)}$

    $= \sum_k \sum_j \dfrac{|\omega_k \cap c_j|}{N} \log \dfrac{N|\omega_k \cap c_j|}{|\omega_k||c_j|}$

  - $H(\Omega) = -\sum_k \dfrac{|\omega_k|}{N} \log \dfrac{|\omega_k|}{N}$

Example



	Cluster 1	Cluster 2	Cluster 3	sum
crosses	5	1	2	8
circles	1	4	0	5
diamonds	0	1	3	4
sum	6	6	5	N=17

$|\omega_k \cap c_j|$

$|\omega_k|$

$|c_j|$

Precision and Recall

- P = TP/(TP+FP)
- R = TP/(TP+FN)
- F-measure: 2P*R/(P+R)

- Consider pairs of data points:
  - hopefully, two data points that are in the same cluster will be clustered into the same cluster (TP), and two data points that are in different clusters will be clustered into different clusters (TN).

	Same cluster	Different clusters
Same class	TP	FN
Different classes	FP	TN

Example

Data points	Output clustering	Ground truth clustering (class)
a	1	2
b	1	2
c	2	2
d	2	1

- # pairs of data points: 6
  - (a, b): same class, same cluster
  - (a, c): same class, different cluster
  - (a, d): different class, different cluster
  - (b, c): same class, different cluster
  - (b, d): different class, different cluster
  - (3,4): different class, same cluster

TP = 1
FP = 1
FN = 2
TN = 2

Matrix Data: Clustering: Part 1

- Cluster Analysis: Basic Concepts
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Summary

- Cluster analysis groups objects based on their similarity and has wide applications; Measure of similarity can be computed for various types of data
- 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
- Clustering evaluation

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