

Data Mining:


Concepts and Techniques

(3rd ed.)

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Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: Basic Concepts 
- Partitioning Methods
- Density-Based 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

Clustering for Data Understanding and Applications

- Customer reviews clustering (hotel, movies, books, ...)
- 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

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Clustering as a Preprocessing Tool (Utility)

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

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
- Density-based approach:
 - Based on connectivity and density functions
 - Typical methods: DBSACN, OPTICS, DenClue
- Hierarchical approach:
 - Create a hierarchical decomposition of the set of data (or objects) using some criterion
 - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- Grid-based approach:
 - based on a multiple-level granularity structure
 - Typical methods: STING, WaveCluster, CLIQUE

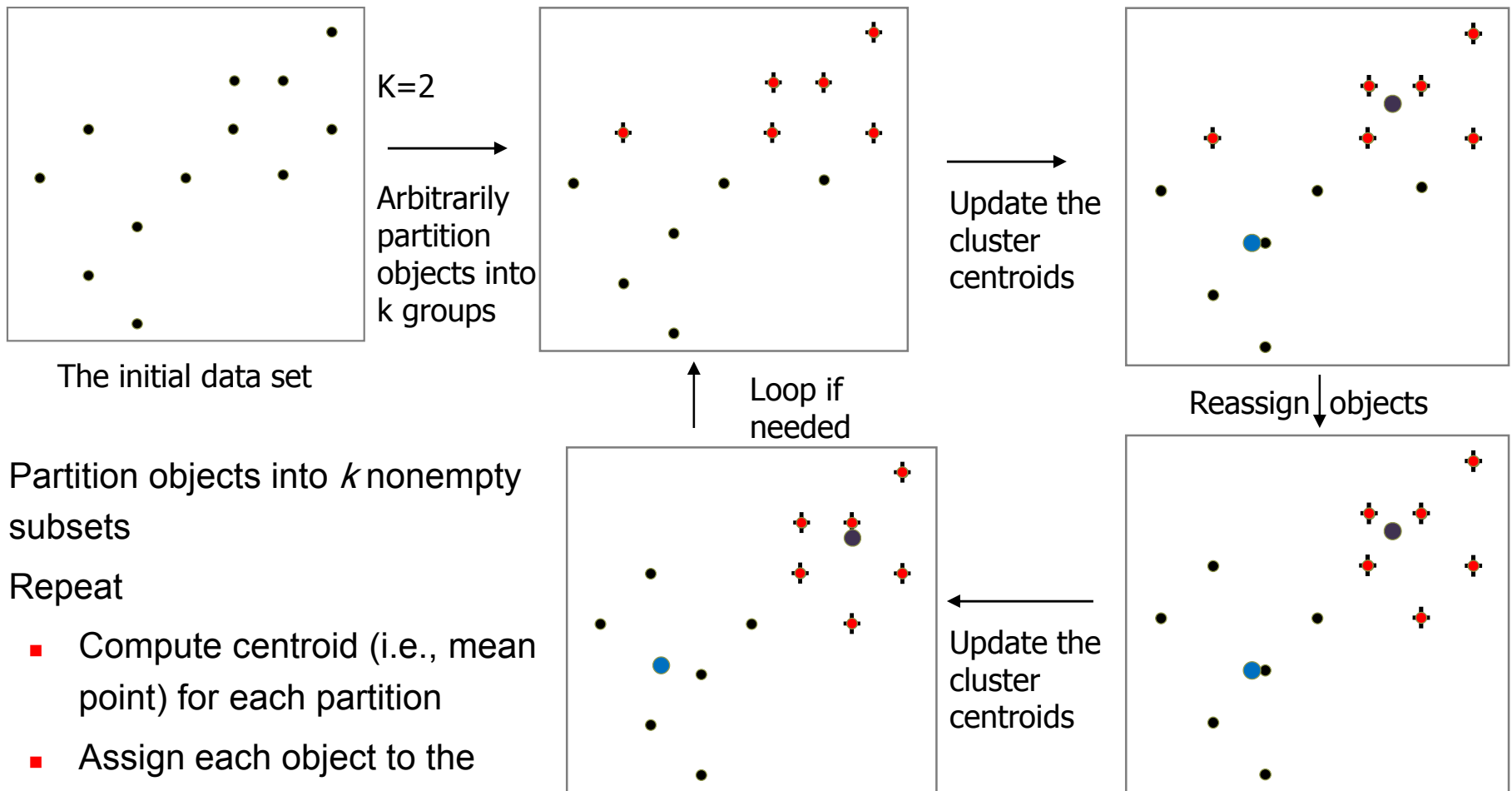
Major Clustering Approaches (II)

- 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

Cluster Analysis: Basic Concepts and Methods

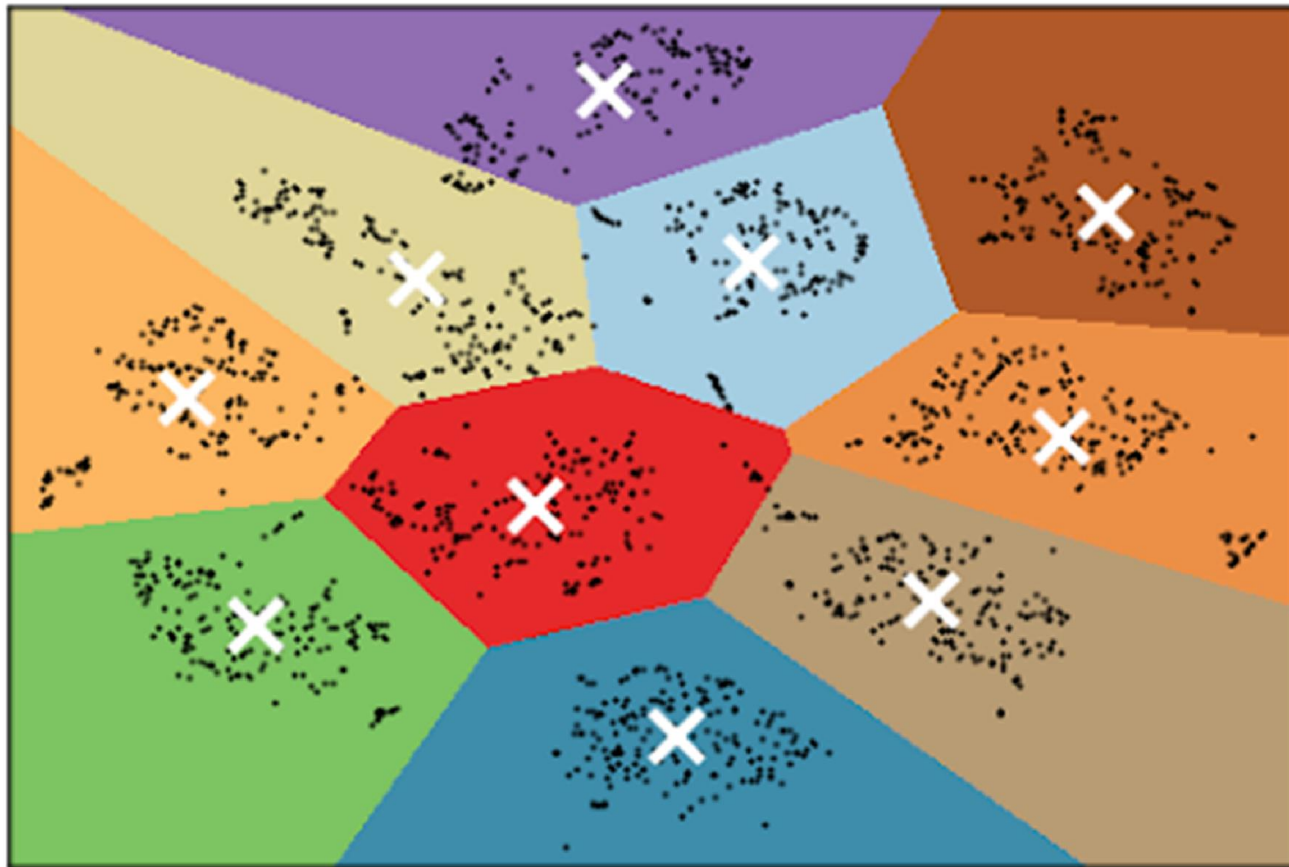
- Cluster Analysis: Basic Concepts
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Review: An Example of *K-Means* Clustering

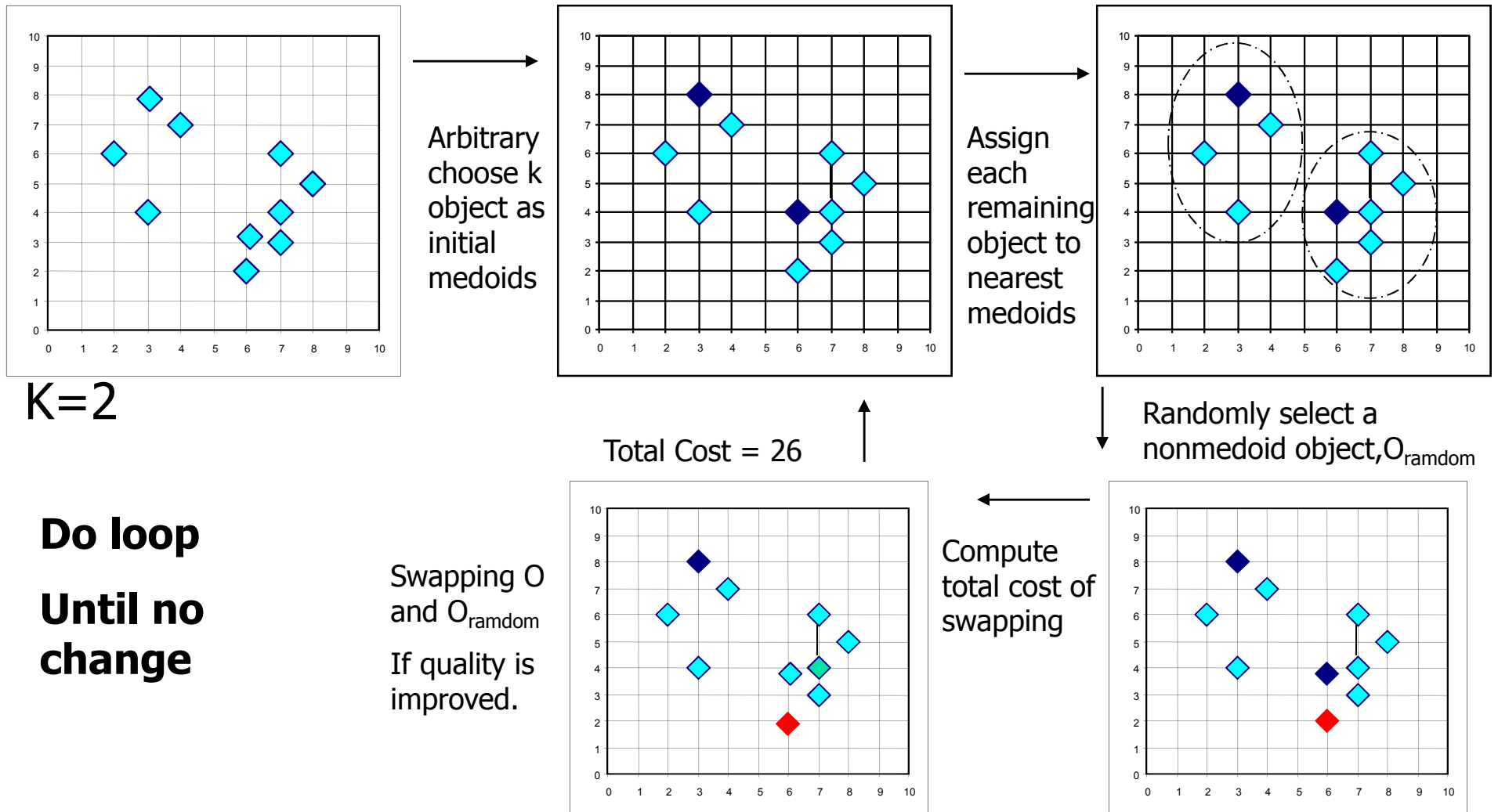


- Partition objects into k nonempty subsets
- Repeat
 - Compute centroid (i.e., mean point) for each partition
 - Assign each object to the cluster of its nearest centroid
- Until Convergence

Review: K-Means Linear Separability

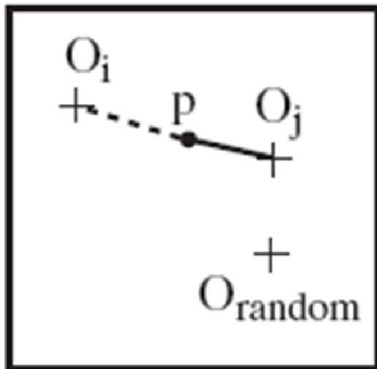


A Typical K-Medoids Algorithm (PAM)

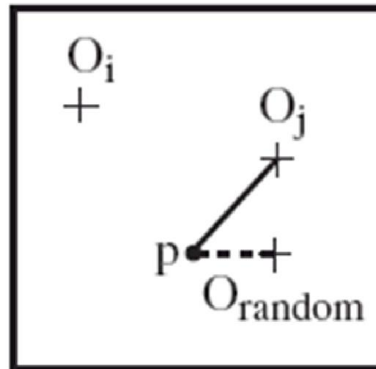


PAM Clustering: Finding the Best Cluster Center

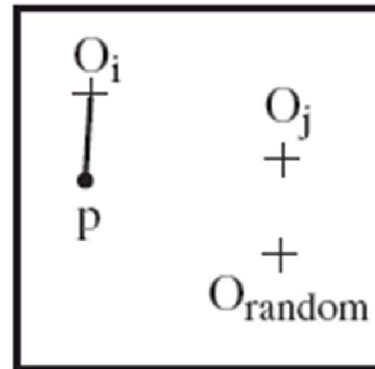
- Case 1: p currently belongs to o_j . If o_j is replaced by o_{random} as a representative object and p is the closest to one of the other representative object o_i , then p is reassigned to o_i



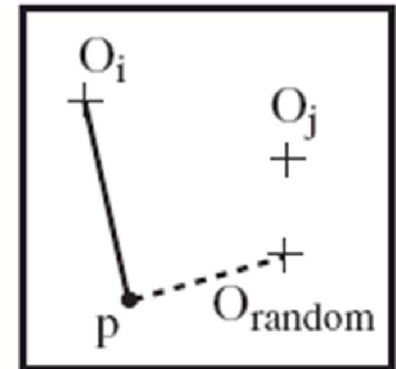
1. Reassigned to O_i



2. Reassigned to O_{random}



3. No change



4. Reassigned to O_{random}

- data object
- + cluster center
- before swapping
- after swapping

What Is the Problem with PAM?

- Pam is more robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean
- Pam works efficiently for small data sets but does not **scale well** for large data sets.
 - $O(k(n-k)^2)$ for each iteration

where n is # of data, k is # of clusters

➔ Sampling-based method

CLARA(Clustering LARge Applications)


***CLARA* (Clustering Large Applications) (1990)**

- *CLARA* (Kaufmann and Rousseeuw in 1990)
 - Built in statistical analysis packages, such as SPlus
 - It draws *multiple samples* of the data set, applies *PAM* on each sample, and gives the best clustering as the output
- Strength: deals with larger data sets than *PAM*
- Weakness:
 - Efficiency depends on the sample size
 - A good clustering based on samples will not necessarily represent a good clustering of the whole data set if the sample is biased

CLARANS (“Randomized” CLARA) (1994)

- *CLARANS* (A Clustering Algorithm based on Randomized Search) (Ng and Han'94)
 - Draws sample of neighbors dynamically
 - The clustering process can be presented as searching a graph where every node is a potential solution, that is, a set of k medoids
 - If the local optimum is found, *it* starts with new randomly selected node in search for a new local optimum
- Advantages: More efficient and scalable than both *PAM* and *CLARA*
- Further improvement: Focusing techniques and spatial access structures (Ester et al.'95)

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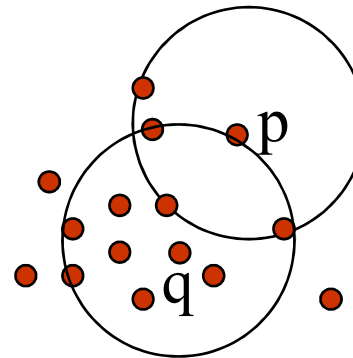
Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
 - Discover clusters of arbitrary shape
 - Handle noise
 - One scan
 - Need density parameters as termination condition
- Several interesting studies:
 - DBSCAN: Ester, et al. (KDD'96)
 - OPTICS: Ankerst, et al (SIGMOD'99).
 - DENCLUE: Hinneburg & D. Keim (KDD'98)
 - CLIQUE: Agrawal, et al. (SIGMOD'98) (more grid-based)

Density-Based Clustering: Basic Concepts

- Two parameters:
 - *Eps*: Maximum radius of the neighbourhood
 - *MinPts*: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: $\{q \text{ belongs to } D \mid \text{dist}(p,q) \leq Eps\}$
- **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:

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



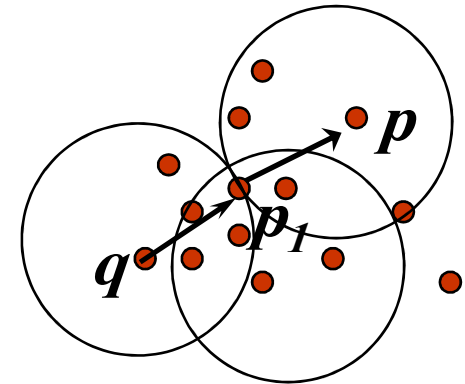
$MinPts = 5$

$Eps = 1 \text{ cm}$

Density-Reachable and Density-Connected

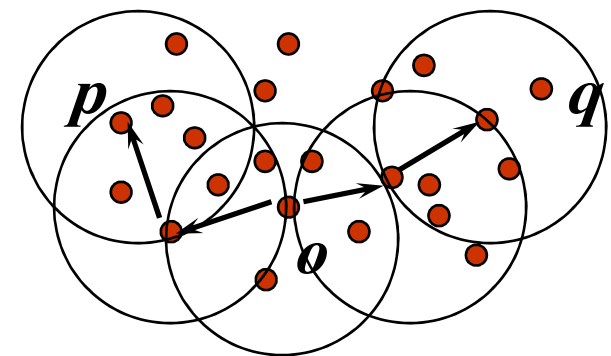
- Density-reachable:

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



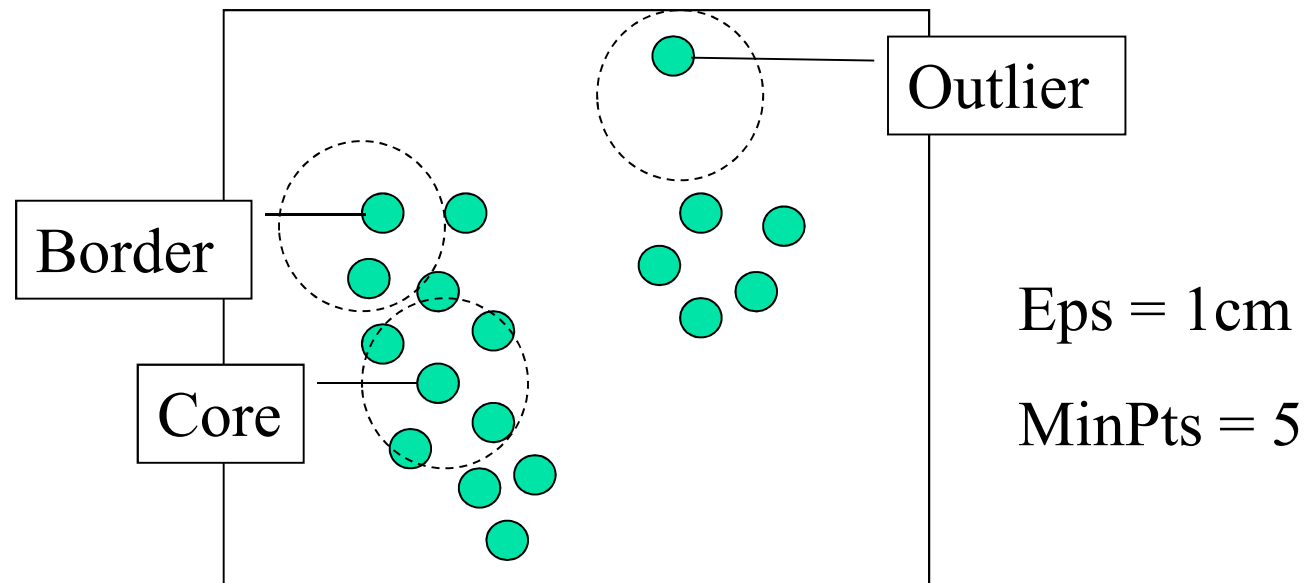
- Density-connected

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



DBSCAN: Density-Based Spatial Clustering of Applications with Noise

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise



DBSCAN: The Algorithm

- Arbitrary select a point p
- Retrieve all points density-reachable from p w.r.t. Eps and $MinPts$
- If p is a core point, a cluster is formed
- If p is a border point, no points are density-reachable from p and DBSCAN visits the next point of the database
- Continue the process until all of the points have been processed

DBSCAN: Sensitive to Parameters

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

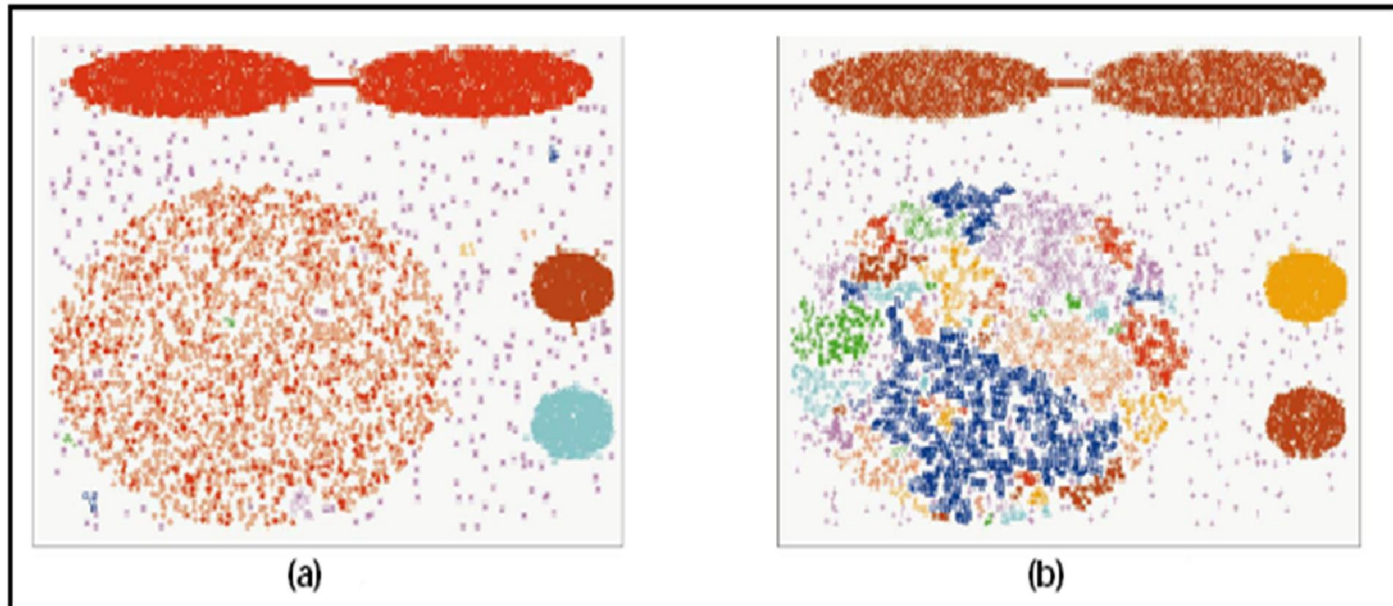
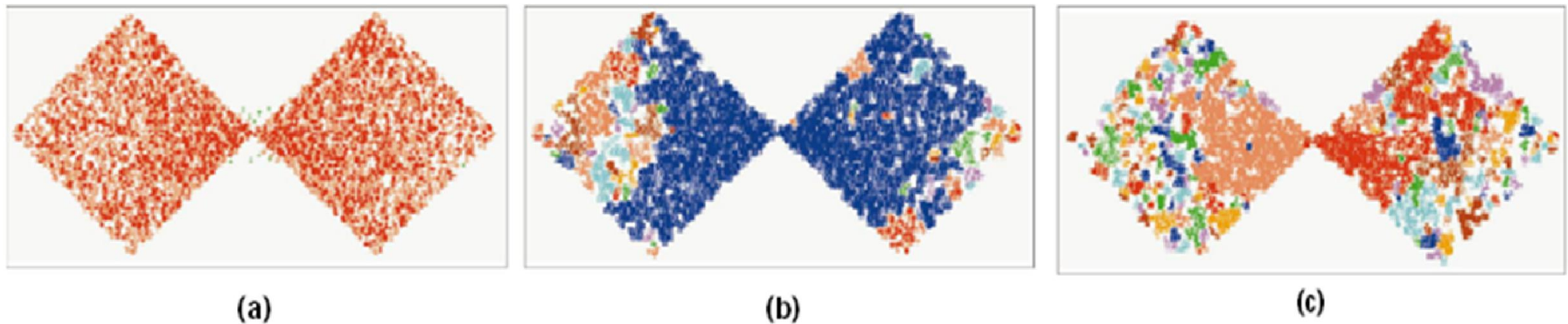


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



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 = number of dimensions

- $N = 20$

- $p = 75\%$

- $M = N(1-p) = 5$

- Complexity: $O(N \log M)$

- Core Distance:

- min eps s.t. point is core

- Reachability Distance

$\text{Max}(\text{core-distance}(o), d(o, p))$

$r(p1, o) = 2.8\text{cm}$. $r(p2, o) = 4\text{cm}$

