Unsupervised Learning

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

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- Information retrieval: document clustering
- Land use: Identification of areas of similar land use in an earth observation database
- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults
- Climate: understanding earth climate, find patterns of atmospheric and ocean
- Economic Science: market resarch

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

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

Partitioning Algorithms: Basic Concept

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

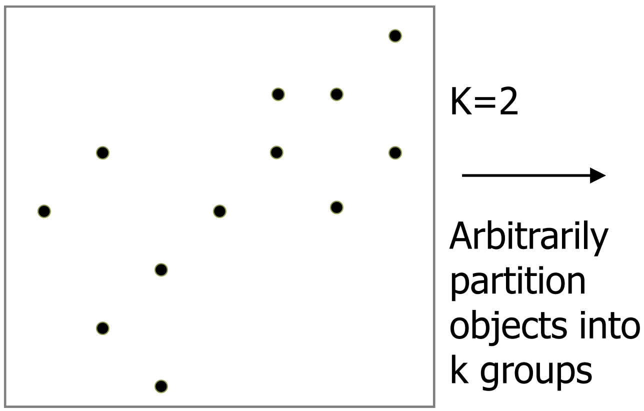
$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (p - c_i)^2$$

- 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* : Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids): Each cluster is represented by one of the objects in the cluster

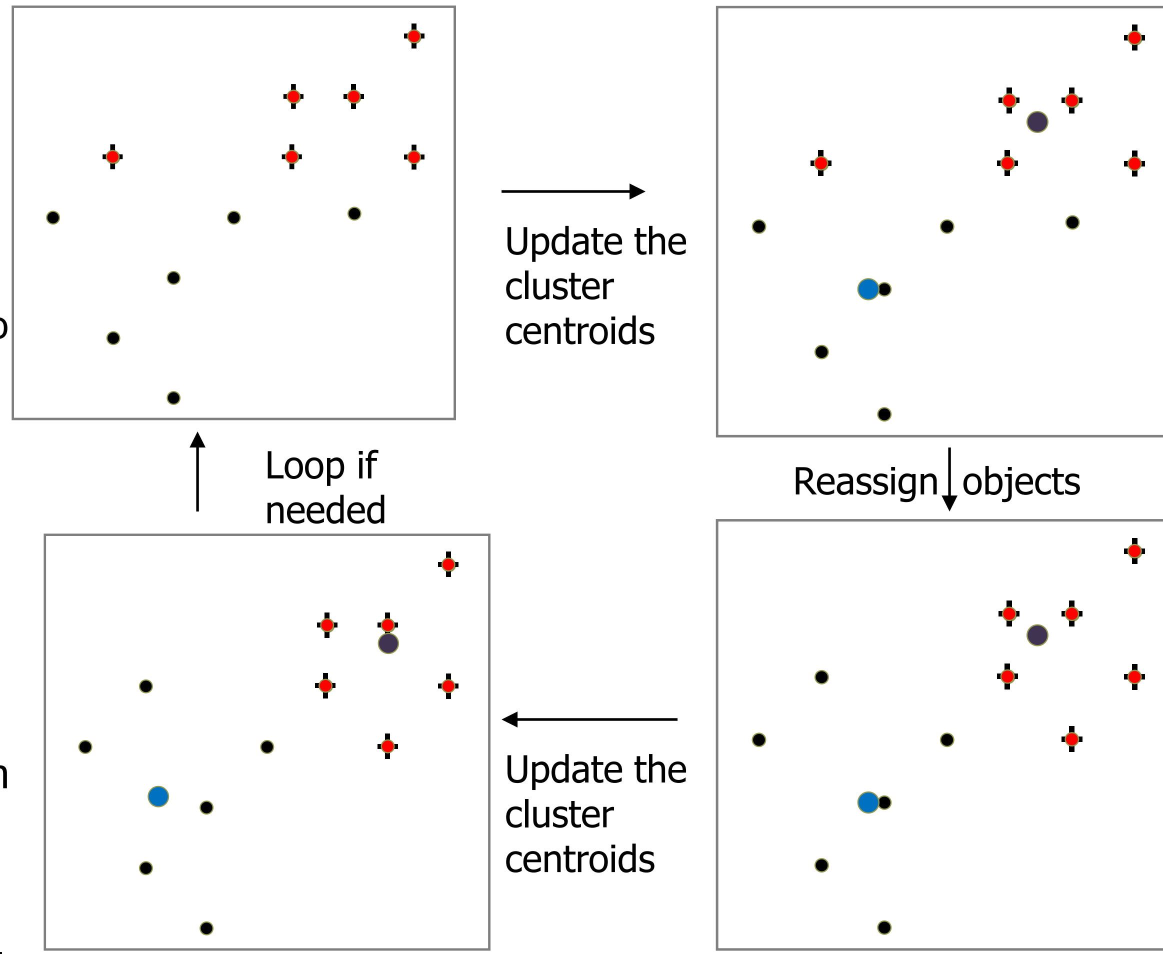
The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in four steps:
  - Partition objects into *k* nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  - Assign each object to the cluster with the nearest seed point
  - Go back to Step 2, stop when the assignment does not change

An Example of *K-Means* Clustering



The initial data set



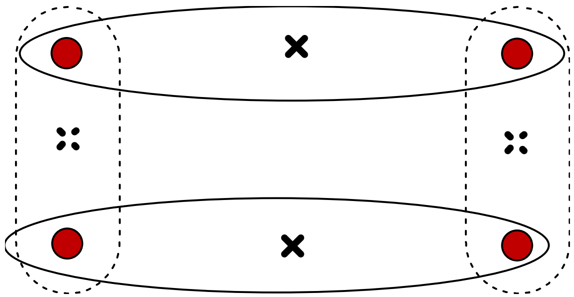
- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

Comments on the *K-Means* Method

- Strength: *Efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, t << n.
    - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- Comment: Often terminates at a *local optimal*.
- Weakness
    - Applicable only to objects in a continuous n-dimensional space
        - Using the k-modes method for categorical data
        - In comparison, k-medoids can be applied to a wide range of data
    - Need to specify *k,* the *number* of clusters, in advance
    - Sensitive to noisy data and *outliers*
    - Not suitable to discover clusters with *non-convex shapes*

Variations of the *K-Means* Method

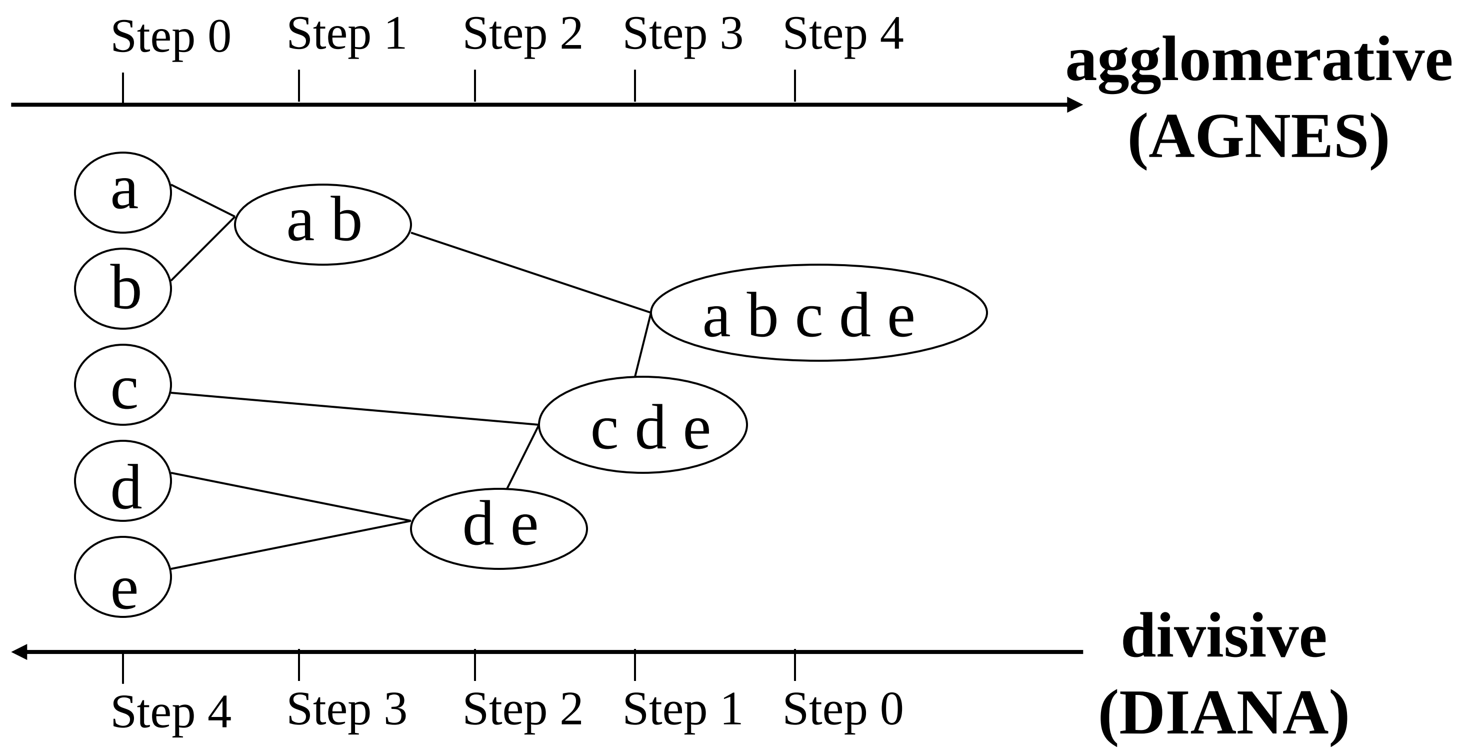
- Most of the variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means



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

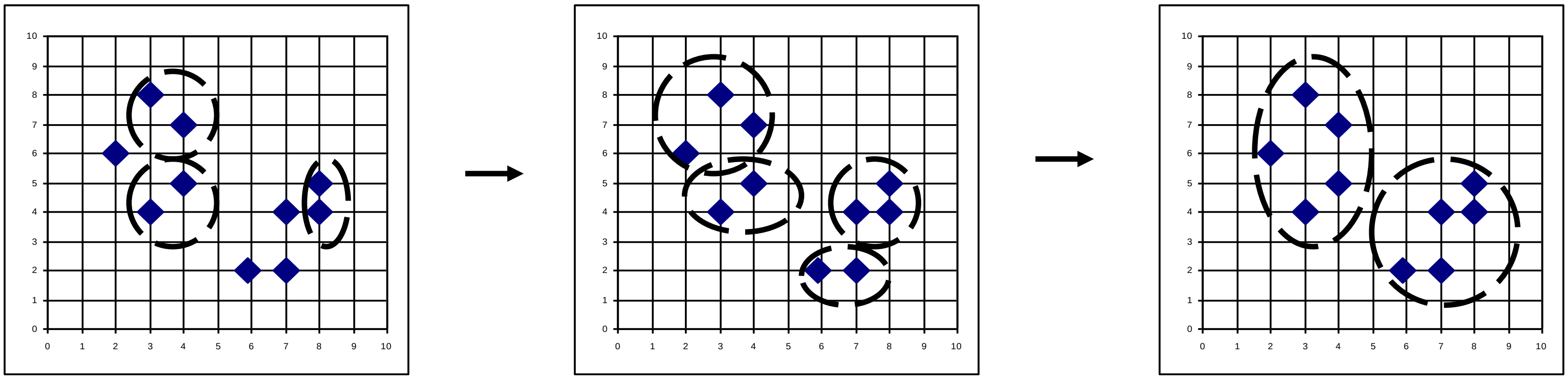
Hierarchical Clustering

- 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)

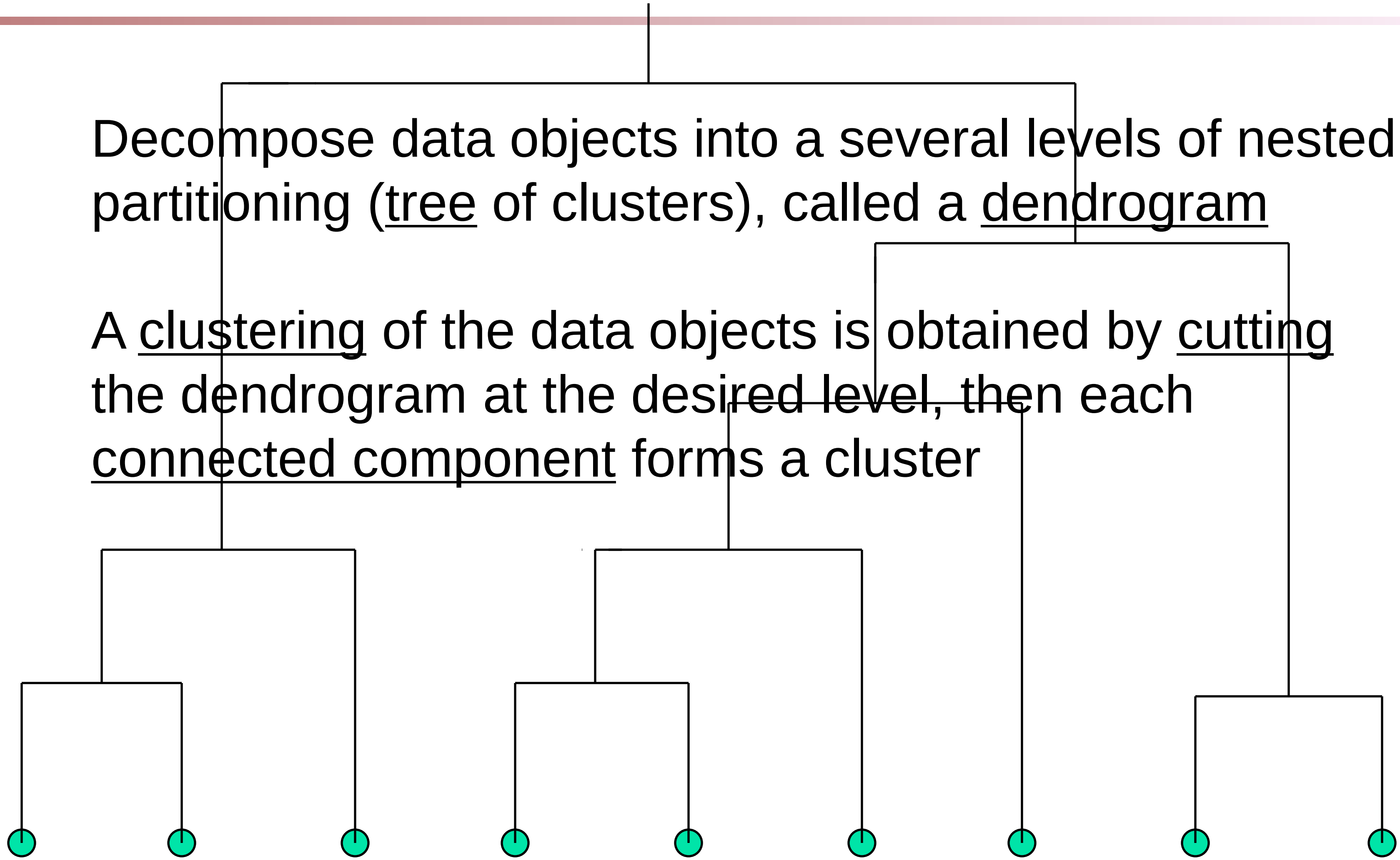
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the **single-link** method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



Dendrogram: Shows How Clusters are Merged

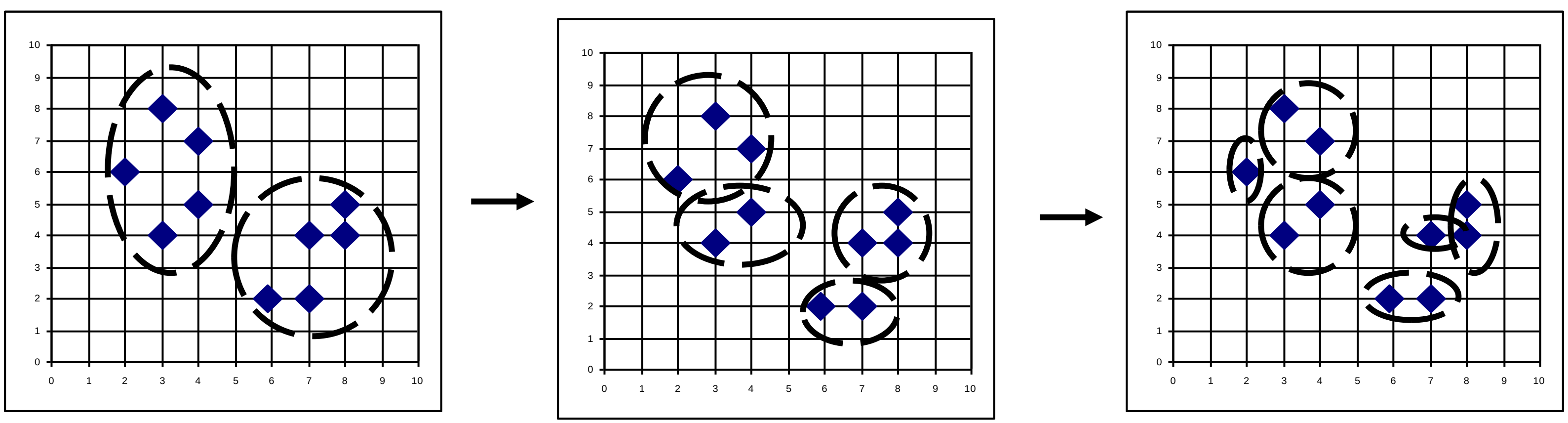
Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram

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

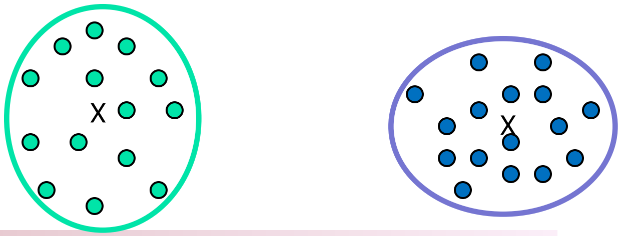


DIANA (Divisive Analysis)

- 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., $dist(K_i, K_j) = min(t_{ip}, t_{jq})$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = max(t_{ip}, t_{jq})$
- Average: avg distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = avg(t_{ip}, t_{jq})$
- Centroid: distance between the centroids of two clusters, i.e., $dist(K_i, K_j) = dist(C_i, C_j)$
- Medoid: distance between the medoids of two clusters, i.e., $dist(K_i, K_j) = dist(M_i, M_j)$
  - Medoid: a chosen, centrally located object in the cluster

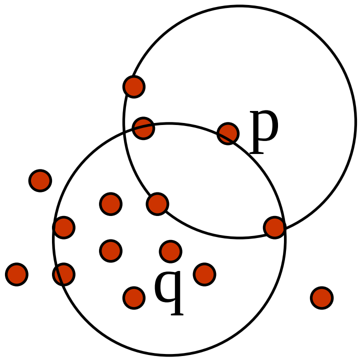
Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape(S or oval shaped)
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - <u>DBSCAN:</u> Ester, et al. (KDD'96)
  - <u>OPTICS</u>: Ankerst, et al (SIGMOD'99).
  - <u>DENCLUE</u>: Hinneburg & D. Keim (KDD'98)
  - <u>CLIQUE</u>: 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 belongs to D | dist(p,q) ≤ Eps}
- Directly density-reachable: A point *p* is directly density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if
  - *p* belongs to $N_{Eps}(q)$
  - core point condition:

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

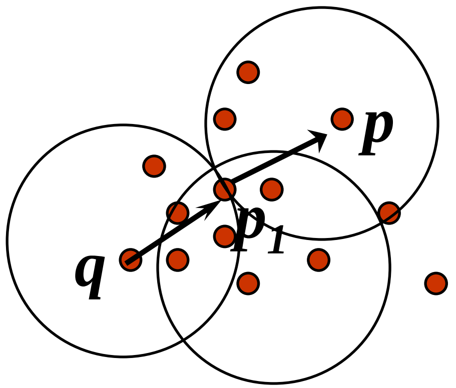


MinPts = 5

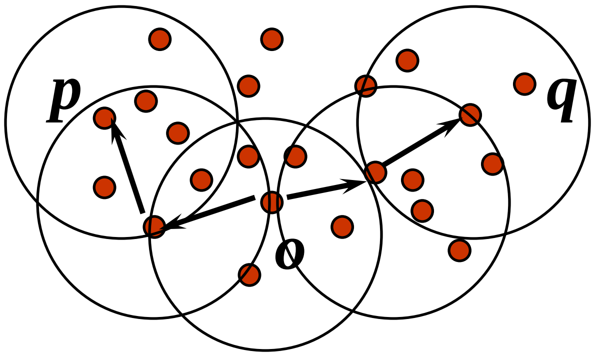
Eps = 1 cm

Density-Reachable and Density-Connected

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

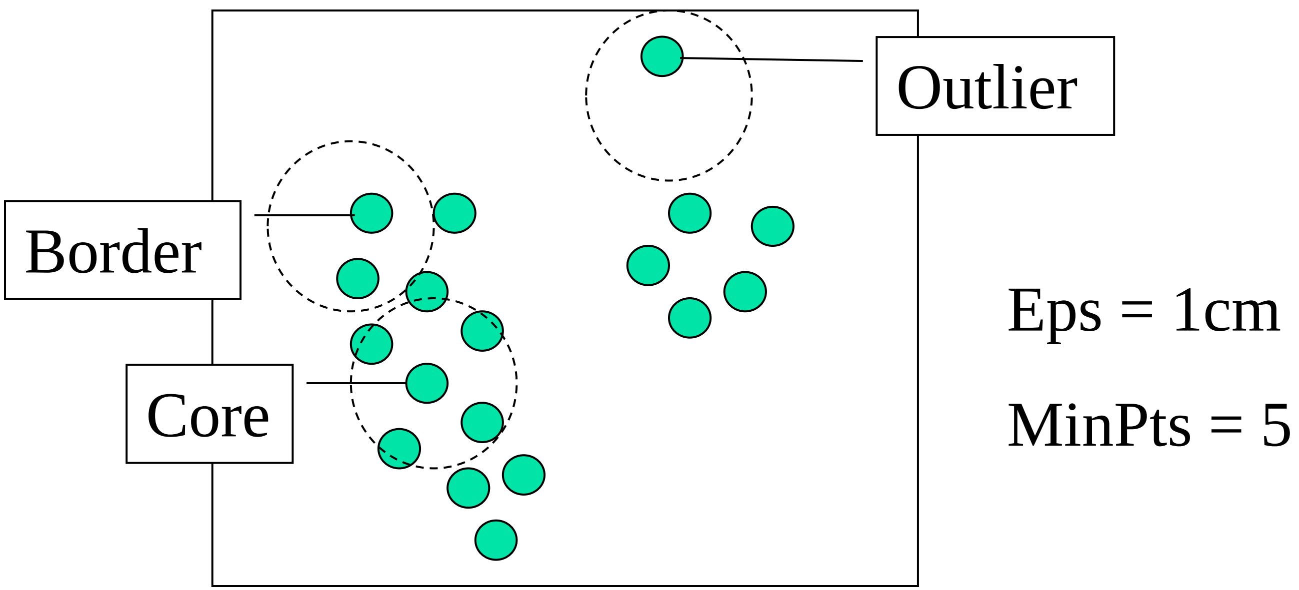


- Density-connected
  - A point p is density-connected to a point q w.r.t. *Eps*, *MinPts* if there is a point o such that both, p and q are density-reachable from o w.r.t. *Eps* and *MinPts*



DBSCAN: Density-Based Spatial Clustering of Applications with Noise

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



Algorithm: DBSCAN: a density-based clustering algorithm.

Input:

- D: a data set containing n objects,
- ϵ: the radius parameter, and
- *MinPts*: the neighborhood density threshold.

Output: A set of density-based clusters.

Method:

(1) mark all objects as unvisited;
(2) **do**
(3)   randomly select an unvisited object $\boldsymbol{p}$;
(4)   mark $\boldsymbol{p}$ as visited;
(5)   **if** the ϵ-neighborhood of $\boldsymbol{p}$ has at least *MinPts* objects
(6)   create a new cluster C, and add $\boldsymbol{p}$ to C;
(7)   let N be the set of objects in the ϵ-neighborhood of $\boldsymbol{p}$;
(8)   **for** each point $\boldsymbol{p}'$ in N
(9)   if $\boldsymbol{p}'$ is unvisited
(10)   mark $\boldsymbol{p}'$ as visited;
(11)   if the ϵ-neighborhood of $\boldsymbol{p}'$ has at least *MinPts* points,
                     add those points to N;
(12)   if $\boldsymbol{p}'$ is not yet a member of any cluster, add $\boldsymbol{p}'$ to C;
(13)   **end for**
(14)   output C;
(15)   **else** mark $\boldsymbol{p}$ as noise;
(16) **until** no object is unvisited;

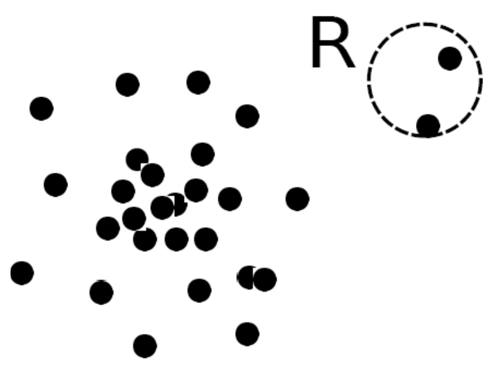
5 DBSCAN algorithm.

DBSCAN: The Algorithm

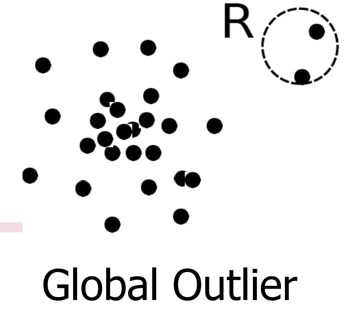
- Arbitrary select a point *p*
- Retrieve all points density-reachable from *p* w.r.t. *Eps* and *MinPts*
- If *p* is a core point, a cluster is formed
- If *p* is a border point, no points are density-reachable from *p* and DBSCAN visits the next point of the database
- Continue the process until all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

What Are Outliers?

- **Outlier**: A data object that **deviates significantly** from the normal objects as if it were **generated by a different mechanism**
  - Ex.: Unusual credit card purchase, sports: Michael Jordon, Wayne Gretzky, ...
- Outliers are different from the noise data
  - Noise is random error or variance in a measured variable
  - Noise should be removed before outlier detection
- Outliers are interesting: It violates the mechanism that generates the normal data
- Outlier detection vs. *novelty detection*: early stage, outlier; but later merged into the model
- Applications:
  - Credit card fraud detection
  - Telecom fraud detection
  - Customer segmentation
  - Medical analysis



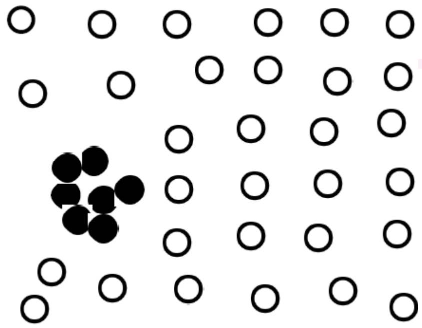
Types of Outliers (I)



- Three kinds: *global, contextual* and *collective* outliers
- **Global outlier** (or point anomaly)
  - Object is O_g if it significantly deviates from the rest of the data set
  - Ex. Intrusion detection in computer networks
  - Issue: Find an appropriate measurement of deviation
- **Contextual outlier** (or *conditional outlier*)
  - Object is O_c if it deviates significantly based on a selected context
  - Ex. 80^o F in Urbana: outlier? (depending on summer or winter?)
  - Attributes of data objects should be divided into two groups
    - Contextual attributes: defines the context, e.g., time & location
    - Behavioral attributes: characteristics of the object, used in outlier evaluation, e.g., temperature
  - Can be viewed as a generalization of *local outliers*—whose density significantly deviates from its local area
  - Issue: How to define or formulate meaningful context?

Types of Outliers (II)

- **Collective Outliers**
  - A subset of data objects *collectively* deviate significantly from the whole data set, even if the individual data objects may not be outliers
  - Applications: E.g., *intrusion detection*:
    - When a number of computers keep sending denial-of-service packages to each other



Collective Outlier

  - Detection of collective outliers
    - Consider not only behavior of individual objects, but also that of groups of objects
    - Need to have the background knowledge on the relationship among data objects, such as a distance or similarity measure on objects.
- A data set may have multiple types of outlier
- One object may belong to more than one type of outlier

Challenges of Outlier Detection

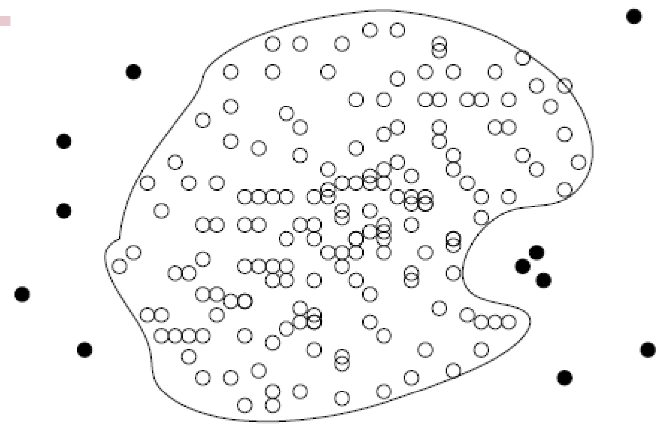
- Modeling normal objects and outliers properly
  - Hard to enumerate all possible normal behaviors in an application
  - The border between normal and outlier objects is often a gray area
- Application-specific outlier detection
  - Choice of distance measure among objects and the model of relationship among objects are often application-dependent
  - E.g., clinic data: a small deviation could be an outlier; while in marketing analysis, larger fluctuations
- Handling noise in outlier detection
  - Noise may distort the normal objects and blur the distinction between normal objects and outliers. It may help hide outliers and reduce the effectiveness of outlier detection
- Understandability
  - Understand why these are outliers: Justification of the detection
  - Specify the degree of an outlier: the unlikelihood of the object being generated by a normal mechanism

Supervised Methods

- Two ways to categorize outlier detection methods:
  - Based on whether user-*labeled* examples of outliers can be obtained:
    - Supervised, semi-supervised vs. unsupervised methods
  - Based on *assumptions about normal data and outliers*:
    - Statistical, proximity-based, and clustering-based methods
- **Outlier Detection I: Supervised Methods**
  - Modeling outlier detection as a classification problem
    - Samples examined by domain experts used for training & testing
  - Methods for Learning a classifier for outlier detection effectively:
    - Model normal objects & report those not matching the model as outliers, or
    - Model outliers and treat those not matching the model as normal
  - Challenges
    - Imbalanced classes, i.e., outliers are rare: Boost the outlier class and make up some artificial outliers
    - Catch as many outliers as possible, i.e., recall is more important than accuracy (i.e., not mislabeling normal objects as outliers)

Classification-Based Method :One-Class Model

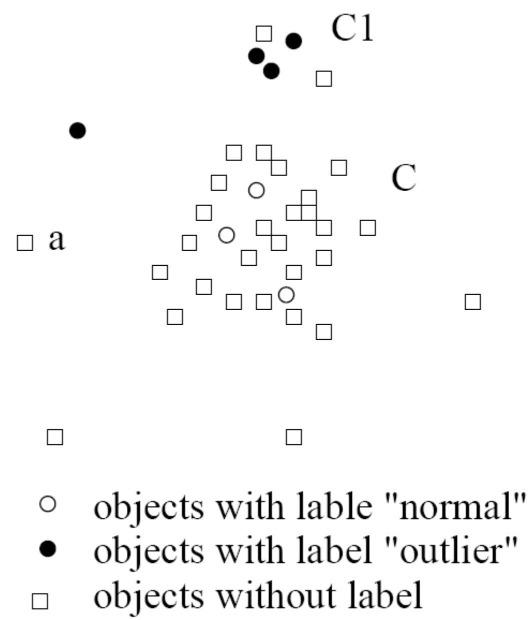
- Idea: Train a classification model that can distinguish "normal" data from outliers
- A brute-force approach: Consider a training set that contains samples labeled as "normal" and others labeled as "outlier"
  - But, the training set is typically heavily biased: # of "normal" samples likely far exceeds # of outlier samples
  - Cannot detect unseen anomaly



- One-class model: A classifier is built to describe only the normal class.
  - Learn the decision boundary of the normal class using classification methods such as SVM
  - Any samples that do not belong to the normal class (not within the decision boundary) are declared as outliers
  - Adv: can detect new outliers that may not appear close to any outlier objects in the training set
  - Extension: Normal objects may belong to multiple classes

Semi-Supervised Methods

- Semi-supervised learning: Combining classification-based and clustering-based methods
- Method
  - Using a clustering-based approach, find a large cluster, C, and a small cluster, C_1
  - Since some objects in C carry the label "normal", treat all objects in C as normal
  - Use the one-class model of this cluster to identify normal objects in outlier detection
  - Since some objects in cluster C_1 carry the label "outlier", declare all objects in C_1 as outliers
  - Any object that does not fall into the model for C (such as *a*) is considered an outlier as well



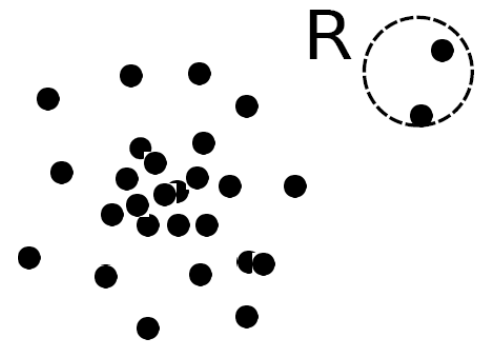
- Comments on classification-based outlier detection methods
  - Strength: Outlier detection is fast
  - Bottleneck: Quality heavily depends on the availability and quality of the training set, but often difficult to obtain representative and high-quality training data

Unsupervised Methods

- Assume the normal objects are somewhat ``clustered'' into multiple groups, each having some distinct features
- An outlier is expected to be far away from any groups of normal objects
- Weakness: Cannot detect collective outlier effectively
  - Normal objects may not share any strong patterns, but the collective outliers may share high similarity in a small area
- Ex. In some intrusion or virus detection, normal activities are diverse
  - Unsupervised methods may have a high false positive rate but still miss many real outliers.
  - Supervised methods can be more effective, e.g., identify attacking some key resources
- Many clustering methods can be adapted for unsupervised methods
  - Find clusters, then outliers: not belonging to any cluster
  - Problem 1: Hard to distinguish noise from outliers
  - Problem 2: Costly since first clustering: but far less outliers than normal objects
    - Newer methods: tackle outliers directly

Clustering-Based Methods

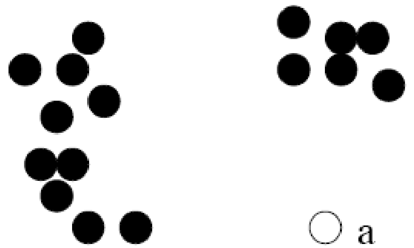
- Normal data belong to large and dense clusters, whereas outliers belong to small or sparse clusters, or do not belong to any clusters



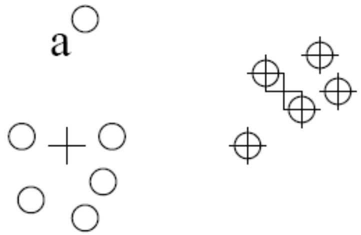
- Example (right figure): two clusters
  - All points not in R form a large cluster
  - The two points in R form a tiny cluster, thus are outliers
- Since there are many clustering methods, there are many clustering-based outlier detection methods as well
- Clustering is expensive: straightforward adaption of a clustering method for outlier detection can be costly and does not scale up well for large data sets

Clustering-Based Outlier Detection

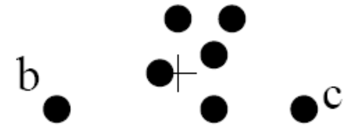
- An object is an outlier if (1) it does not belong to any cluster, (2) there is a large distance between the object and its closest cluster , or (3) it belongs to a small or sparse cluster
- Case I: Not belong to any cluster
  - Identify animals not part of a flock: Using a density-based clustering method such as DBSCAN



- Case 2: Far from its closest cluster
  - Using k-means, partition data points of into clusters
  - For each object o, assign an outlier score based on its distance from its closest center
    - If dist(o, c_o)/avg_dist(c_o) is large, likely an outlier



- Ex. Intrusion detection: Consider the similarity between data points and the clusters in a training data set



  - Use a training set to find patterns of “normal” data, e.g., frequent itemsets in each segment, and cluster similar connections into groups
  - Compare new data points with the clusters mined—Outliers are possible attacks

Mining Frequent Patterns, Association and Correlations: Basic Concepts and Methods

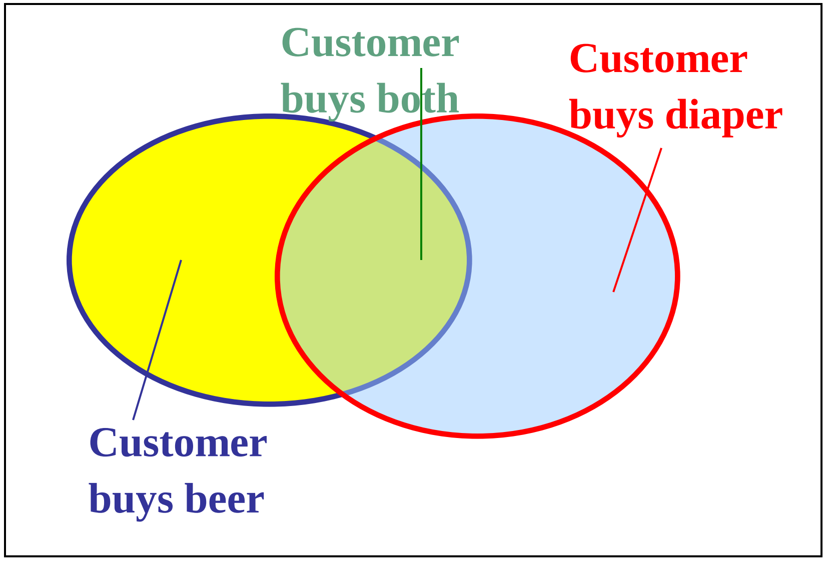
- Frequent pattern: a pattern (a set of items, subsequences, substructures, etc.) that occurs frequently in a data set
- First proposed by Agrawal, Imielinski, and Swami [AIS93] in the context of frequent itemsets and association rule mining
- Motivation: Finding inherent regularities in data
  - What products were often purchased together?— Beer and diapers?!
  - What are the subsequent purchases after buying a PC?
  - What kinds of DNA are sensitive to this new drug?
  - Can we automatically classify web documents?
- Applications
  - Basket data analysis, cross-marketing, catalog design, sale campaign analysis, Web log (click stream) analysis, and DNA sequence analysis.

Why Is Freq. Pattern Mining Important?

- Freq. pattern: An intrinsic and important property of datasets
- Foundation for many essential data mining tasks
  - Association, correlation, and causality analysis
  - Sequential, structural (e.g., sub-graph) patterns
  - Pattern analysis in spatiotemporal, multimedia, time-series, and stream data
  - Classification: discriminative, frequent pattern analysis
  - Cluster analysis: frequent pattern-based clustering
  - Data warehousing: iceberg cube and cube-gradient
  - Semantic data compression: fascicles
  - Broad applications

Basic Concepts: Frequent Patterns

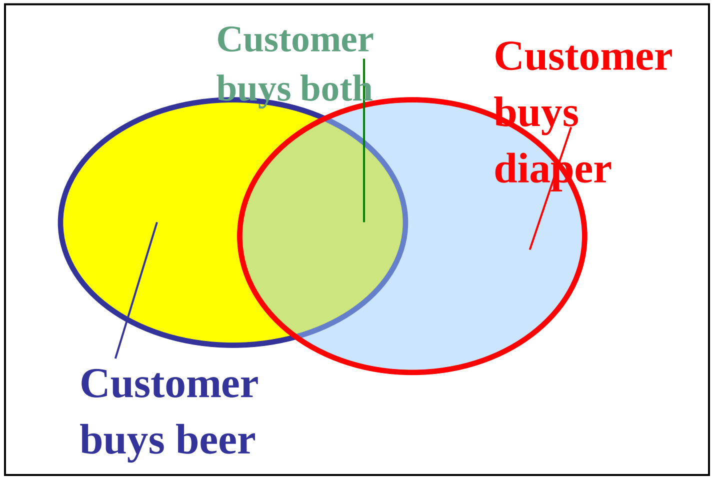
Tid	Items bought
10	Beer, Nuts, Diaper
20	Beer, Coffee, Diaper
30	Beer, Diaper, Eggs
40	Nuts, Eggs, Milk
50	Nuts, Coffee, Diaper, Eggs, Milk



- itemset: A set of one or more items
- k-itemset $X = \{x_1, \ldots, x_k\}$
- *(absolute) support*, or, *support count* of X: Frequency or occurrence of an itemset X
- *(relative) support*, *s*, is the fraction of transactions that contains X (i.e., the probability that a transaction contains X)
- An itemset X is *frequent* if X's support is no less than a *minsup* threshold

Basic Concepts: Association Rules

Tid	Items bought
10	Beer, Nuts, Diaper
20	Beer, Coffee, Diaper
30	Beer, Diaper, Eggs
40	Nuts, Eggs, Milk
50	Nuts, Coffee, Diaper, Eggs, Milk



- Find all the rules *X* → *Y* with minimum support and confidence
  - support, *s*, probability that a transaction contains X ∪ Y
  - confidence, *c*, conditional probability that a transaction having X also contains *Y*

Let minsup = 50%, minconf = 50%

Freq. Pat.: Beer:3, Nuts:3, Diaper:4, Eggs:3, {Beer, Diaper}:3

- Association rules: (many more!)
  - *Beer* → *Diaper* (60%, 100%)
  - *Diaper* → *Beer* (60%, 75%)

Apriori: A Candidate Generation & Test Approach

- Apriori pruning principle: If there is any itemset which is infrequent, its superset should not be generated/tested!

  Method:
  - Initially, scan DB once to get frequent 1-itemset
  - Generate length (k+1) candidate itemsets from length k frequent itemsets
  - Test the candidates against DB
  - Terminate when no frequent or candidate set can be generated

The Apriori Algorithm—An Example

$Sup_{min} = 2$

Database TDB

Tid	Items
10	A, C, D
20	B, C, E
30	A, B, C, E
40	B, E

1st scan →

C_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{D}	1
{E}	3

→ L_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{E}	3

C_2

Itemset
{A, B}
{A, C}
{A, E}
{B, C}
{B, E}
{C, E}

← 2nd scan

C_2

Itemset	sup
{A, B}	1
{A, C}	2
{A, E}	1
{B, C}	2
{B, E}	3
{C, E}	2

← L_2

Itemset	sup
{A, C}	2
{B, C}	2
{B, E}	3
{C, E}	2

C_3

Itemset
{B, C, E}

3rd scan →

L_3

Itemset	sup
{B, C, E}	2

The Apriori Algorithm (Pseudo-Code)

C_k: Candidate itemset of size k
L_k : frequent itemset of size k

L_1 = {frequent items};
for (k = 1; L_k $!=\varnothing$; k++) **do begin**
  C_{k+1} = candidates generated from L_k;
  for each transaction t in database do
    increment the count of all candidates in C_{k+1} that are contained in t
  L_{k+1} = candidates in C_{k+1} with min_support
  end
return $\cup_k L_k$;

Implementation of Apriori

- How to generate candidates?
  - Step 1: self-joining L_k
  - Step 2: pruning
- Example of Candidate-generation
  - L_3={*abc, abd, acd, ace, bcd*}
  - Self-joining: L_3*L_3
    - *abcd* from *abc* and *abd*
    - *acde* from *acd* and *ace*
  - Pruning:
    - *acde* is removed because *ade* is not in L_3
  - C_4 = {*abcd*}