Introduction to Data Mining

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A Brief History

- Historically, we had operational databases, ex: for accounts, customers, personnel of a bank
- Data collection is now very easy and storage is very cheap
- Enterprises are in a data collection frenzy hoping that they can use that later on
- Data warehouses:
  - Integrating historical data from multiple sources
  - For high level decision making
- Data Mining

Overview of Data Mining

- Why do we need data mining?
  - Data collection is easy, and huge amounts of data is collected everyday into flat files, databases and data warehouses
  - We have lots of data but this data needs to be turned into knowledge
  - Data mining technology tries to extract useful knowledge from huge collections of data

Overview of Data Mining

- Data mining definition: Extraction of interesting information from large data sources
- The extracted information should be
  - Implicit
  - Non-trivial
  - Previously unknown
  - and potentially useful
- Query processing, simple statistics are not data mining
- Databases + Statistics + Machine Learning = Data Mining

Overview of Data Mining

- Data mining applications
  - Market basket analysis
  - CRM (loyalty detection, churn detection)
  - Fraud detection
  - Stream mining
  - Web mining
  - Mining of bioinformatics data

Overview of Data Mining

- Retail market, as a case study:
  - What type of data is collected?
  - What type of knowledge do we need about customers?
  - Is it useful to know the customer buying patterns?
  - Is it useful to segment the customers?

Overview of Data Mining

- Advertisement of a product: A case study
  - Send all the customers a brochure
  - Or send a targeted list of customers a brochure
  - Sending a smaller targeted list aims to guarantee a high percentage of response, cutting the mailing cost

Overview of Data Mining

- What complicates things in data mining?
  - Incomplete and noisy data
  - Complex data types
  - Heterogeneous data sources
  - Size of data (need to have distributed, parallel scalable algorithms)

Data Mining Models

- Patterns (Associations, sequences, temporal sequences)
- Clusters (Descriptive)
- Predictive models (Classification)

Associations (As an example of patterns)

- Remember the case study of retail market, and market basket analysis
- Remember the type of data collected
- Associations are among the most popular patterns that can be extracted from transactional data.
- We will explain the properties of associations and how they could be extracted from large collections of transactions efficiently based on the slide of the book : “Data Mining Concepts and Techniques” by Jiawei Han and Micheline Kamber.

What Is Association Mining?

- Association rule mining:
  - Finding frequent patterns, associations, correlations, or causal structures among sets of items or objects in transaction databases, relational databases, and other information repositories.
- Applications:
  - Basket data analysis, cross-marketing, catalog design, clustering, classification, etc.
- Examples.
  - Rule form: "Body $\rightarrow$ Head [support, confidence]".
  - buys(x, "diapers") $\rightarrow$ buys(x, "beers") [0.5%, 60%]
  - major(x, "CS") ^ takes(x, "DB") $\rightarrow$ grade(x, "A") [1%, 75%]

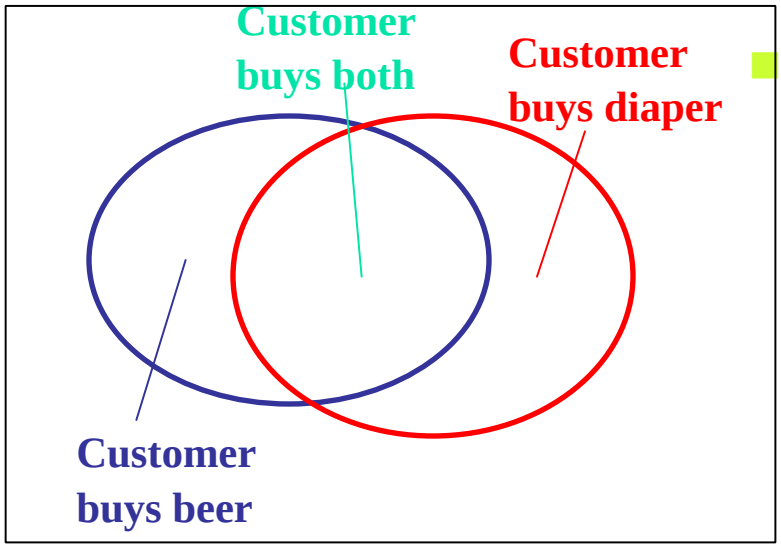
Association Rule: Basic Concepts

- Given:

  (1) database of transactions,

  (2) each transaction is a list of items (purchased by a customer in a visit)
- Find: all rules that correlate the presence of one set of items with that of another set of items
  - E.g., *98% of people who purchase tires and auto accessories also get automotive services done*
- Applications
  - * $\Rightarrow$ *Maintenance Agreement* (What the store should do to boost Maintenance Agreement sales)
  - *Home Electronics* $\Rightarrow$ * (What other products should the store stocks up?)
  - Attached mailing in direct marketing
  - Detecting “ping-pong”ing of patients, faulty “collisions”

Rule Measures: Support and Confidence



Find all the rules $X \& Y \Rightarrow Z$ with minimum confidence and support

- support, *s*, probability that a transaction contains {X & Y & Z}
- confidence, *c*, conditional probability that a transaction having {X & Y} also contains *Z*

Transaction ID	Items Bought
2000	A,B,C
1000	A,C
4000	A,D
5000	B,E,F

Let minimum support 50%, and minimum confidence 50%, we have

- $A \Rightarrow C$ (50%, 66.6%)
- $C \Rightarrow A$ (50%, 100%)

Association Rule Mining: A Road Map

- Boolean vs. quantitative associations (Based on the types of values handled)
  - buys(x, “SQLServer”) ^ buys(x, “DMBook”) → buys(x, “DBMiner”) [0.2%, 60%]
  - age(x, “30..39”) ^ income(x, “42..48K”) → buys(x, “PC”) [1%, 75%]
- Single dimension vs. multiple dimensional associations (see ex. Above)
- Single level vs. multiple-level analysis
  - What brands of beers are associated with what brands of diapers?
- Various extensions
  - Correlation, causality analysis
    - Association does not necessarily imply correlation or causality
  - Maxpatterns and closed itemsets
  - Constraints enforced E.g., small sales (sum < 100) trigger big buys (sum > 1,000)?

Mining Association Rules—An Example

Transaction ID	Items Bought
2000	A,B,C
1000	A,C
4000	A,D
5000	B,E,F

Min. support 50%
Min. confidence 50%

Frequent Itemset	Support
{A}	75%
{B}	50%
{C}	50%
{A,C}	50%

For rule $A \Rightarrow C$:

support = support({A C}) = 50%

confidence = support({A C})/support({A}) = 66.6%

The Apriori principle: (Agrawal and Srikant)

Any subset of a frequent itemset must be frequent

Mining Frequent Itemsets: the Key Step

- Find the *frequent itemsets*: the sets of items that have minimum support
  - A subset of a frequent itemset must also be a frequent itemset
    - i.e., if {*A B*} is a frequent itemset, both {*A*} and {*B*} should be a frequent itemset
  - Iteratively find frequent itemsets with cardinality from 1 to *k (k*-itemset*)*
- Use the frequent itemsets to generate association rules.

The Apriori Algorithm

- Join Step: C_k is generated by joining $L_{k-1}$with itself
- Prune Step: Any (k-1)-itemset that is not frequent cannot be a subset of a frequent k-itemset
- 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 !=∅; 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 $\cup_k L_k$;

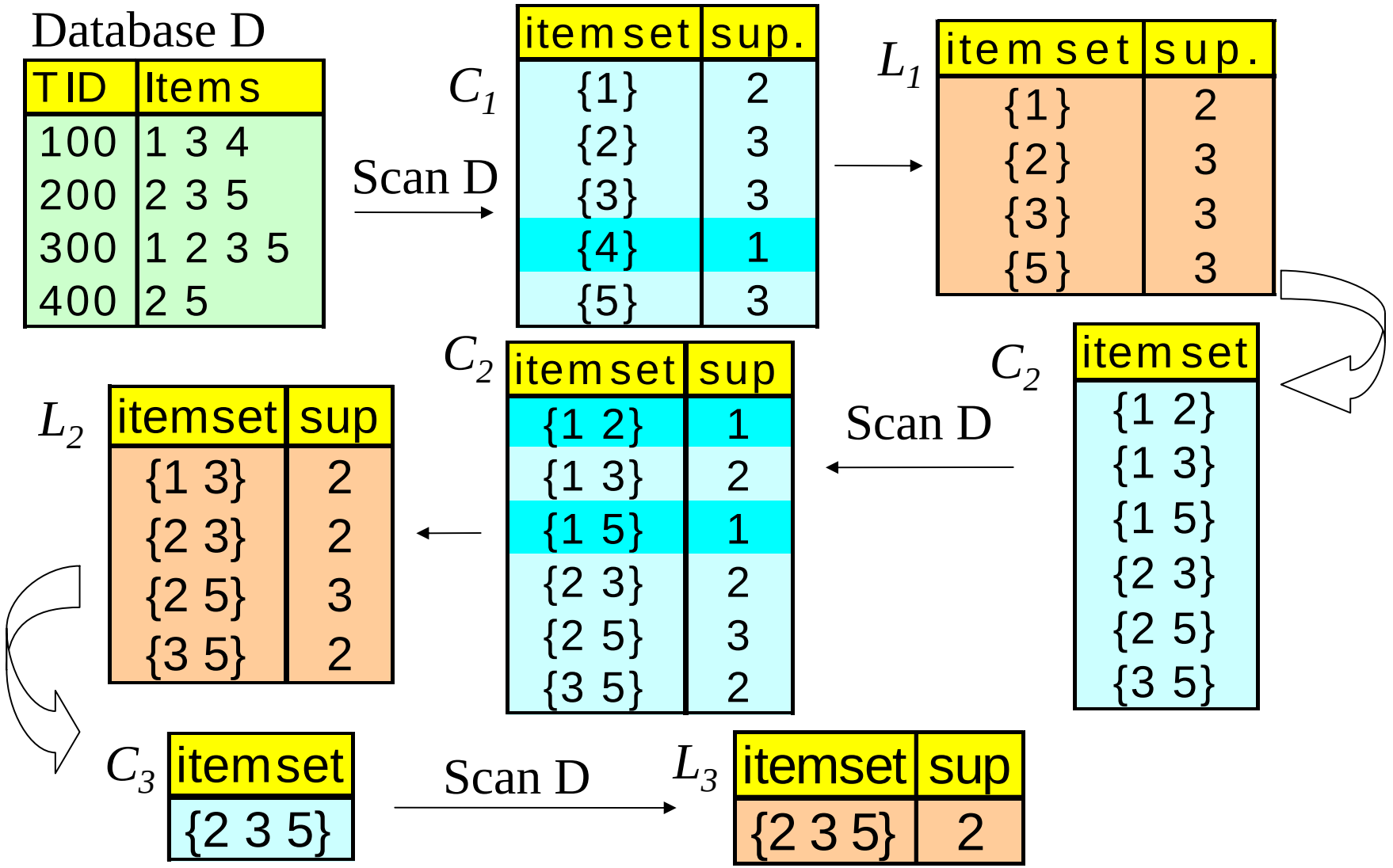
The Apriori Algorithm — Example

Database D

TID	Items
100	1 3 4
200	2 3 5
300	1 2 3 5
400	2 5

- Find frequent sets of items with support 40% or more

The Apriori Algorithm — Example



How to Generate Candidates?

- Suppose the items in L_{k-1} are listed in an order
- Step 1: self-joining L_{k-1}

  insert into C_k

  select $p.item_1, p.item_2, \ldots, p.item_{k-1}, q.item_{k-1}$

  from $L_{k-1}\ p, L_{k-1}\ q$

  where $p.item_1=q.item_1, \ldots, p.item_{k-2}=q.item_{k-2}, p.item_{k-1} < q.item_{k-1}$
- Step 2: pruning

  forall ***itemsets c in*** C_k do

    forall ***(k-1)-subsets s of c*** do

      if *(s is not in* L_{k-1}*)* **then delete** *c* **from** C_k

Example of Generating Candidates

- 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*}

How to Count Supports of Candidates?

- Why counting supports of candidates is a problem?
  - The total number of candidates can be very huge
  - One transaction may contain many candidates
- Method:
  - Candidate itemsets are stored in a *hash-tree*
  - *Leaf* node of hash-tree contains a list of itemsets and counts
  - *Interior* node contains a hash table
  - *Subset function*: finds all the candidates contained in a transaction

How to Generate Candidates?

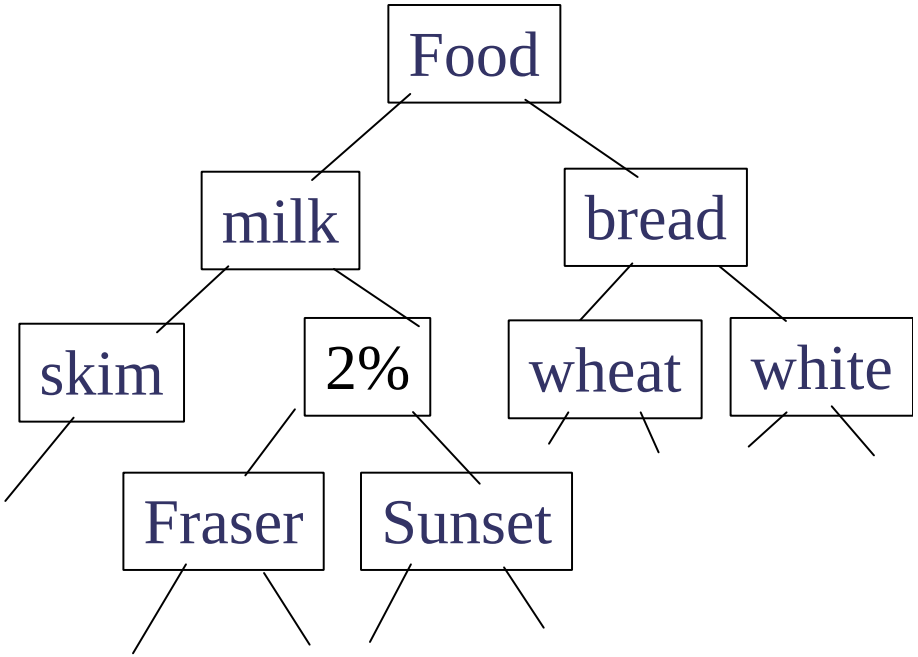
- Assume that you have a relational database for storing customer transactions
- Design simple queries for counting the frequent itemsets
- Design a little system with database interaction for mining associations

Methods to Improve Apriori's Efficiency

- Hash-based itemset counting: A *k*-itemset whose corresponding hashing bucket count is below the threshold cannot be frequent
- Transaction reduction: A transaction that does not contain any frequent k-itemset is useless in subsequent scans
- Partitioning: Any itemset that is potentially frequent in DB must be frequent in at least one of the partitions of DB
- Sampling: mining on a subset of given data, lower support threshold + a method to determine the completeness
- Dynamic itemset counting: add new candidate itemsets only when all of their subsets are estimated to be frequent

Multiple-Level Association Rules

- Items often form hierarchy.
- Items at the lower level are expected to have lower support.
- Rules regarding itemsets at appropriate levels could be quite useful.
- Transaction database can be encoded based on dimensions and levels
- We can explore shared multi-level mining



TID	Items
T1	{111, 121, 211, 221}
T2	{111, 211, 222, 323}
T3	{112, 122, 221, 411}
T4	{111, 121}
T5	{111, 122, 211, 221, 413}

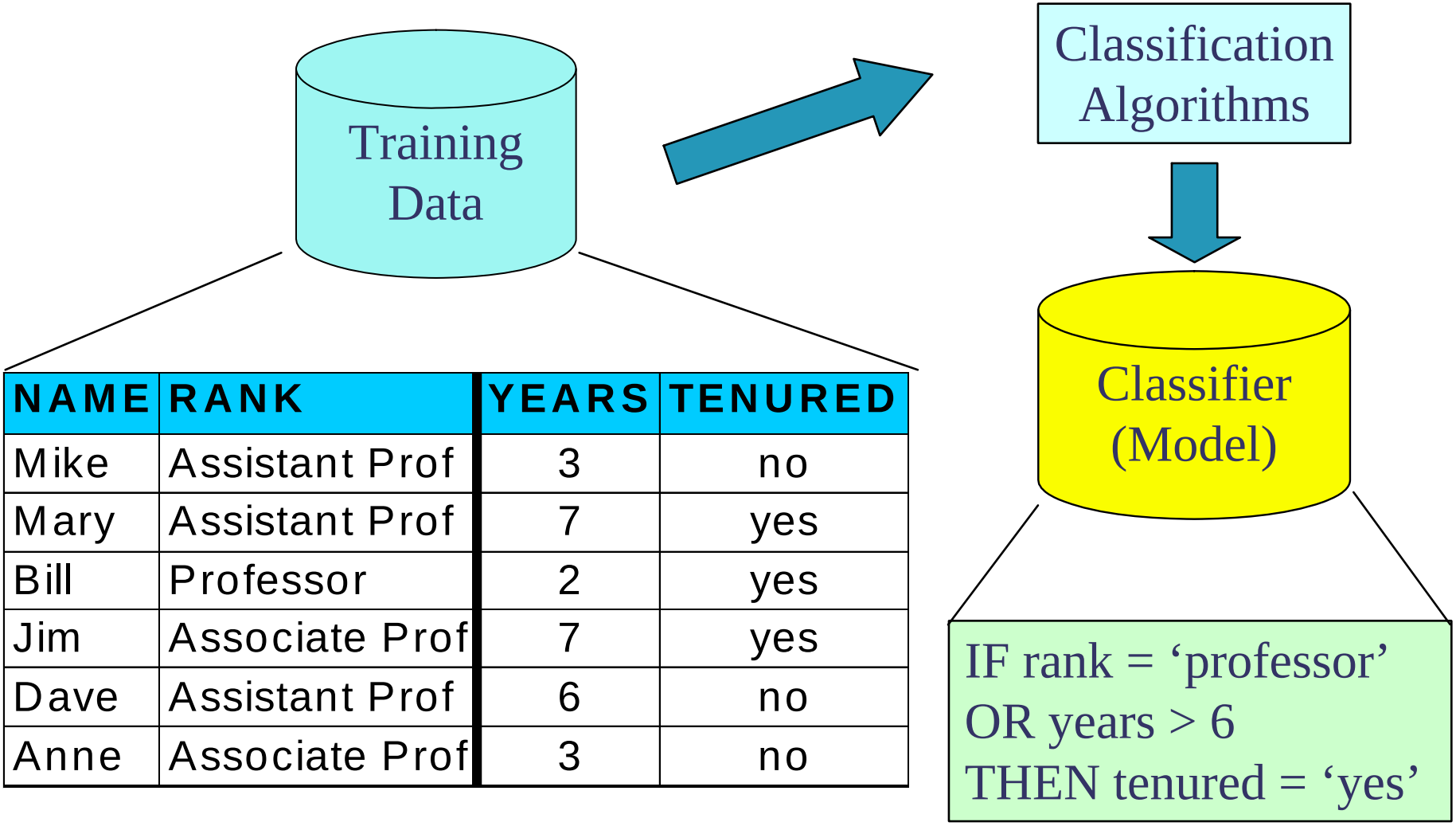
Classification

- Is an example of predictive modelling
- The basic idea is to build a model using past data to predict the class of a new data sample.
- Lets remember the case of targeted mailing of brochures.
- IF we can work on a small well selected sample to profile the future customers who will respond to the mail ad, then we can save the mailing costs.
- The following slides are based on the slides of the book “Data Mining Concepts and Techniques” by Jiawei Han and Micheline Kamber.

Classification—A Two-Step Process

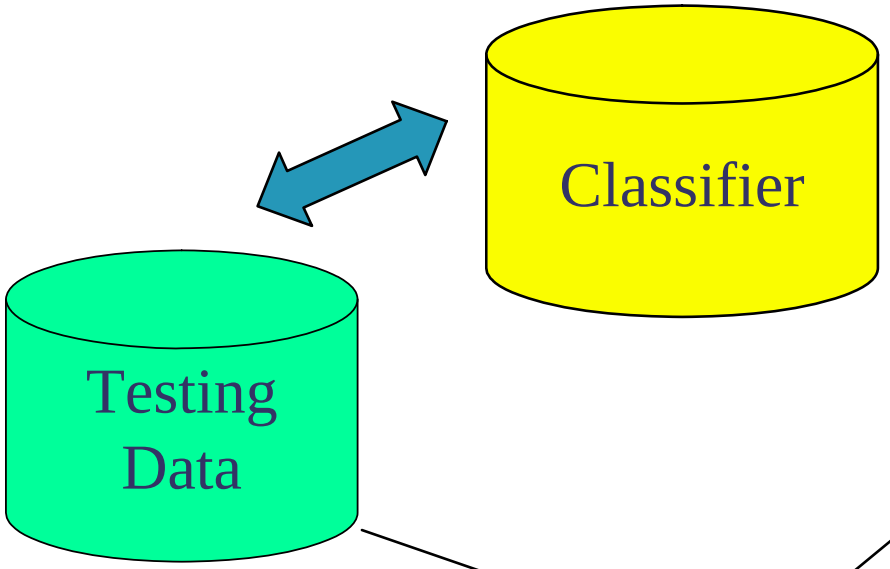
- Model construction: describing a set of predetermined classes
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
  - The set of tuples used for model construction is training set
  - The model is represented as classification rules, decision trees, or mathematical formulae
- Model usage: for classifying future or unknown objects
  - Estimate accuracy of the model
    - The known label of test sample is compared with the classified result from the model
    - Accuracy rate is the percentage of test set samples that are correctly classified by the model
    - Test set is independent of training set, otherwise over-fitting will occur
  - If the accuracy is acceptable, use the model to classify data tuples whose class labels are not known

Classification Process (1): Model Construction



NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Classification Process (2): Use the Model in Prediction



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes

(Jeff, Professor, 4)

Tenured?

Yes

Supervised vs. Unsupervised Learning

- Supervised learning (classification)
  - Supervision: The training data (observations, measurements, etc.) are accompanied by labels indicating the class of the observations
  - New data is classified based on the training set
- Unsupervised learning (clustering)
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

Issues regarding classification and prediction (1): Data Preparation

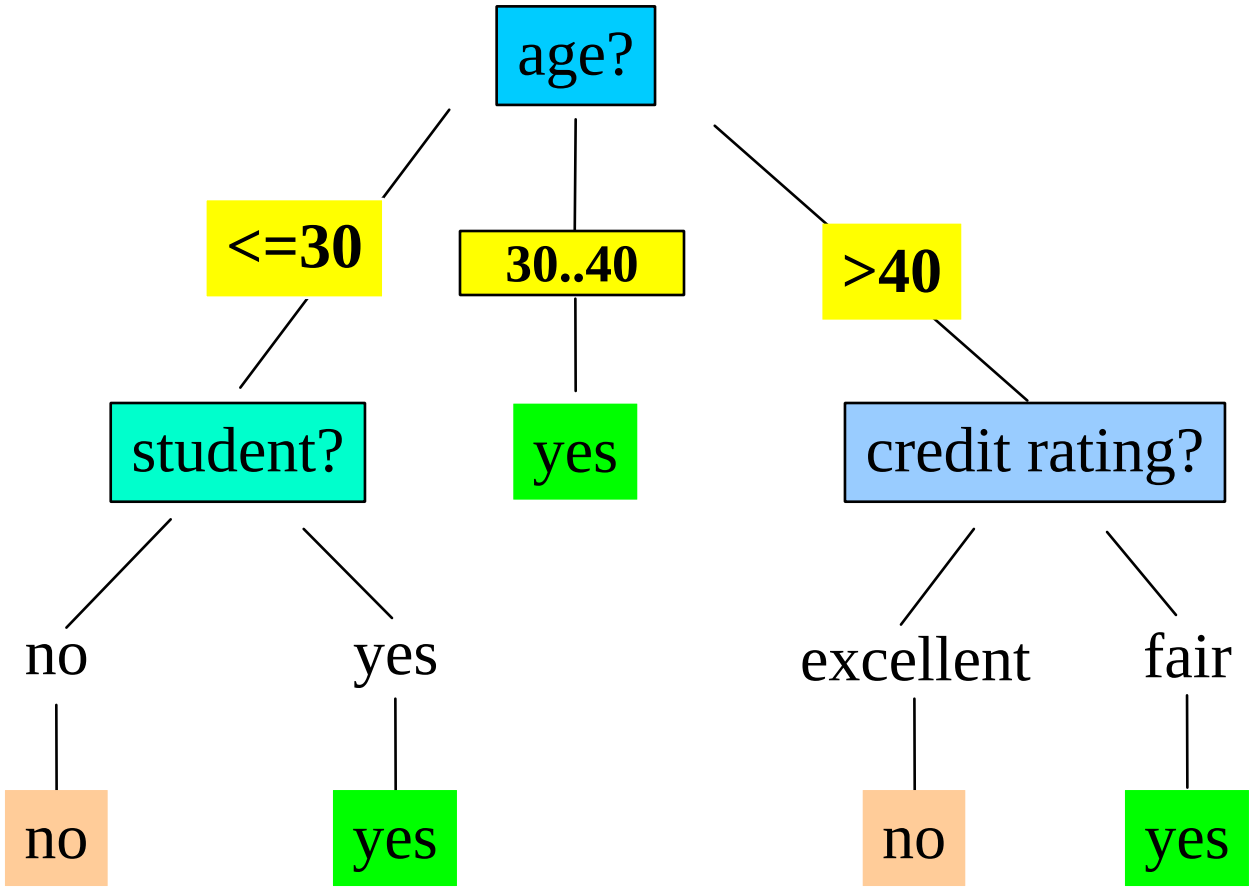
- Data cleaning
  - Pre-process data in order to reduce noise and handle missing values
- Relevance analysis (feature selection)
  - Remove the irrelevant or redundant attributes
- Data transformation
  - Generalize and/or normalize data

Training Dataset

This follows an example from Quinlan's ID3

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
30…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Output: A Decision Tree for "*buys_computer*"



Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

Attribute Selection Measure - Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- S contains s_i tuples of class C_i for i = {1, ..., m}
- information measures info required to classify any arbitrary tuple

$$I(s_1,s_2,\ldots,s_m) = -\sum_{i=1}^{m} \frac{s_i}{s} log_2 \frac{s_i}{s}$$

- entropy of attribute A with values $\{a_1,a_2,\ldots,a_v\}$

$$E(A) = \sum_{j=1}^{v} \frac{s_{1j}+\ldots+s_{mj}}{s} I(s_{1j},\ldots,s_{mj})$$

- information gained by branching on attribute A

$$Gain(A) = I(s_1,s_2,\ldots,s_m) - E(A)$$

Attribute Selection by Information Gain Computation

- Class P: buys_computer = “yes”
- Class N: buys_computer = “no”
- I(p, n) = I(9, 5) =0.940

$$I(s_1,s_2,\ldots,s_m) = -\sum_{i=1}^{m} \frac{s_i}{s} log_2 \frac{s_i}{s}$$

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
30…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Attribute Selection by Information Gain Computation

- Class P: buys_computer = “yes”
- Class N: buys_computer = “no”
- I(p, n) = I(9, 5) =0.940
- Compute the entropy for *age*:

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
30…40	4	0	0
>40	3	2	0.971

$$E(age) = \frac{5}{14} I(2,3) + \frac{4}{14} I(4,0) + \frac{5}{14} I(3,2) = 0.971$$

Hence

$$Gain(age) = I(p,n) - E(age)$$

Similarly

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit\_rating) = 0.048$$

Other Attribute Selection Measures

- Gini index (CART, IBM IntelligentMiner)
  - All attributes are assumed to be continuous-valued
  - Assume there exist several possible split values for each attribute
  - May need other tools, such as clustering, to get the possible split values
  - Can be modified for categorical attributes

Gini Index (IBM IntelligentMiner)

- If a data set *T* contains examples from *n* classes, gini index, *gini*(*T*) is defined as $gini(T) = 1 - \sum_{j=1}^{n} p_j^2$

  where p_j is the relative frequency of class *j* in *T*.
- If a data set *T* is split into two subsets T_1 and T_2 with sizes N_1 and N_2 respectively, the *gini* index of the split data contains examples from *n* classes, the *gini* index *gini*(*T*) is defined as

$$gini_{split}(T) = \frac{N_1}{N} gini(T_1) + \frac{N_2}{N} gini(T_2)$$

- The attribute provides the smallest $gini_{split}(T)$ is chosen to split the node (*need to enumerate all possible splitting points for each attribute*).

Extracting Classification Rules from Trees

- Represent the knowledge in the form of IF-THEN rules
- One rule is created for each path from the root to a leaf
- Each attribute-value pair along a path forms a conjunction
- The leaf node holds the class prediction
- Rules are easier for humans to understand
- Example

  IF *age* = "<=30" AND *student* = "*no*" THEN *buys_computer* = "*no*"

  IF *age* = "<=30" AND *student* = "*yes*" THEN *buys_computer* = "*yes*"

  IF *age* = "31…40" THEN *buys_computer* = "*yes*"

  IF *age* = ">40" AND *credit_rating* = "*excellent*" THEN *buys_computer* = "*yes*"

  IF *age* = "<=30" AND *credit_rating* = "*fair*" THEN *buys_computer* = "*no*"

Avoid Overfitting in Classification

- The generated tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Result is in poor accuracy for unseen samples
- Two approaches to avoid overfitting
  - Prepruning: Halt tree construction early—do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: Remove branches from a “fully grown” tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the “best pruned tree”

Approaches to Determine the Final Tree Size

- Separate training (2/3) and testing (1/3) sets
- Use cross validation, e.g., 10-fold cross validation
- Use all the data for training
  - but apply a statistical test (e.g., chi-square) to estimate whether expanding or pruning a node may improve the entire distribution

Bayesian Classification: Why?

- Probabilistic learning: Calculate explicit probabilities for hypothesis, among the most practical approaches to certain types of learning problems
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct. Prior knowledge can be combined with observed data.
- Probabilistic prediction: Predict multiple hypotheses, weighted by their probabilities
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

Bayesian Theorem: Basics

- Let X be a data sample whose class label is unknown
- Let H be a hypothesis that X belongs to class C
- For classification problems, determine P(H/X): the probability that the hypothesis holds given the observed data sample X
- P(H): prior probability of hypothesis H (i.e. the initial probability before we observe any data, reflects the background knowledge)
- P(X): probability that sample data is observed
- P(X|H) : probability of observing the sample X, given that the hypothesis holds

Bayesian Theorem

- Given training data *X*, *posteriori probability of a hypothesis H, P(H|X)* follows the Bayes theorem

$$P(H \mid X) = \frac{P(X \mid H)P(H)}{P(X)}$$

- Informally, this can be written as

  posterior =likelihood x prior / evidence

- MAP (maximum posteriori) hypothesis

$$h_{MAP} \equiv \arg\max_{h \in H} P(h \mid D) = \arg\max_{h \in H} P(D \mid h)P(h).$$

- Practical difficulty: require initial knowledge of many probabilities, significant computational cost

Naïve Bayesian Classifier

- Each data sample X is represented as a vector $\{x_1, x_2, \ldots, x_n\}$
- There are m classes $C_1, C_2, \ldots, C_m$
- Given unknown data sample X, the classifier will predict that X belongs to class C_i, iff

$$P(C_i|X) > P(C_j|X) \text{ where } 1 \leq j \leq m, I \neq J$$

By Bayes theorem, $P(C_i|X) = P(X|C_i)P(C_i)/ P(X)$

Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent:

$$P(X \mid C_i) = \prod_{k=1}^{n} P(x_k \mid C_i)$$

- The product of occurrence of say 2 elements x_1 and x_2, given the current class is C, is the product of the probabilities of each element taken separately, given the same class $P([y_1,y_2],C) = P(y_1,C) * P(y_2,C)$
- No dependence relation between attributes
- Greatly reduces the computation cost, only count the class distribution.
- Once the probability $P(X|C_i)$ is known, assign X to the class with maximum $P(X|C_i)*P(C_i)$

Training dataset

Class:

C1: buys_computer = 'yes'

C2: buys_computer = 'no'

Data sample

X = (age <= 30, Income = medium, Student = yes Credit_rating = Fair)

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
30…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayesian Classifier: Example

- Compute P(X/Ci) for each class

P(age="<30" | buys_computer="yes") = 2/9=0.222
P(age="<30" | buys_computer="no") = 3/5 =0.6
P(income="medium" | buys_computer="yes")= 4/9 =0.444
P(income="medium" | buys_computer="no") = 2/5 = 0.4
P(student="yes" | buys_computer="yes)= 6/9 =0.667
P(student="yes" | buys_computer="no")= 1/5=0.2
P(credit_rating="fair" | buys_computer="yes")=6/9=0.667
P(credit_rating="fair" | buys_computer="no")=2/5=0.4

X=(age<=30 ,income =medium, student=yes,credit_rating=fair)

P(X|Ci) : P(X|buys_computer="yes")= 0.222 x 0.444 x 0.667 x 0.0.667 =0.044
P(X|buys_computer="no")= 0.6 x 0.4 x 0.2 x 0.4 =0.019
P(X|Ci)*P(Ci) : P(X|buys_computer="yes") * P(buys_computer="yes")=0.028
P(X|buys_computer="no") * P(buys_computer="no")=0.007

X belongs to class "buys_computer=yes"

Naïve Bayesian Classifier: Comments

- Advantages :
  - Easy to implement
  - Good results obtained in most of the cases
- Disadvantages
  - Assumption: class conditional independence , therefore loss of accuracy
  - Practically, dependencies exist among variables
  - E.g., hospitals : patients: Profile : age, family history etc

    Symptoms : fever, cough etc , Disease : lung cancer, diabetes etc , Dependencies among these cannot be modeled by Naïve Bayesian Classifier, use a Bayesian network
- How to deal with these dependencies?
  - Bayesian Belief Networks

k-NN Classifier:

- Learning by analogy,
- Each sample is a point in n-dimensional space
- Given an unknown sample u,
  - search for the k nearest samples
  - Closeness can be defined in Euclidean space
  - Assign the most common class to u.

- Instance based, (Lazy) learning while decision trees are eager
- K-NN requires the whole sample space for classification therefore indexing is needed for efficient search.

Case-based reasoning

- Similar to K-NN,
- When a new case arrives, and identical case is searched
- If not, most similar case is searched
- Depending on the representation, different search techniques are needed, for example graph/subgraph search

Genetic Algorithms

- Incorporate ideas from natural evolution
- Rules are represented as a sequence of bits
  - IF A1 and NOT A2 THEN C2 : 1 0 0
  - Initially generate a sequence of random rules
  - Choose the fittest rules
  - Create offspring by using genetic operations such as
    - crossover (by swapping substrings from pairs of rules)
    - and mutation (inverting randomly selected bits)

Data Mining Tools

- WEKA (Univ of Waikato, NZ)
- Open source implementation of data mining algorithms
- Implemented in Java
- Nice API
- Link : Google WEKA, first entry

Benchmarks

- Important for testing the performance of various algorithms against various datasets
- UCI Machine Learning Repository is a very good data source
- Try a data sample from there and see how you can apply the classification algorithms

Clustering

- A descriptive data mining method
- Groups a given dataset into smaller clusters, where the data inside the clusters are similar to each other while the data belonging to different clusters are dissimilar
- Similar to classification in a sense but this time we do not know the labels of clusters. Therefore it is an unsupervised method.
- Lets go back to the retail market example. How can we segment our customers with respect to their profiles and shopping behaviour.
- The following slides are based on the slides of the book “Data Mining Concepts and Techniques” by Jiawei Han and Micheline Kamber.

What Is Good Clustering?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation.
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns.

Requirements of Clustering in Data Mining

- Scalability
- Ability to deal with different types of attributes
- Discovery of clusters with arbitrary shape
- Able to deal with noise and outliers
- Insensitive to order of input records
- High dimensionality
- Interpretability and usability

Data Structures

- Data matrix

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

Measure the Quality of Clustering

- Dissimilarity/Similarity metric: Similarity is expressed in terms of a distance function, which is typically metric: $d(i, j)$
- There is a separate "quality" function that measures the "goodness" of a cluster.
- The definitions of distance functions are usually very different for interval-scaled, boolean, categorical, ordinal and ratio variables.
- Weights should be associated with different variables based on applications and data semantics.
- It is hard to define "similar enough" or "good enough"
  - the answer is typically highly subjective.

Type of data in clustering analysis

- Interval-scaled variables:
- Binary variables:
- Nominal, ordinal, and ratio variables:
- Variables of mixed types:

Interval-scaled variables

- Standardize data
  - Calculate the mean absolute deviation: $s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + ... + |x_{nf} - m_f|)$

  where $m_f = \frac{1}{n}(x_{1f} + x_{2f} + ... + x_{nf})$.
  - Calculate the standardized measurement (*z-score*) $z_{if} = \frac{x_{if} - m_f}{s_f}$
- Using mean absolute deviation is more robust than using standard deviation

Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

$$d(i,j) = \sqrt[q]{(|x_{i_1} - x_{j_1}|^q + |x_{i_2} - x_{j_2}|^q + ... + |x_{i_p} - x_{j_p}|^q)}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ are two p-dimensional data objects, and q is a positive integer

- If $q = 1$, d is Manhattan distance

$$d(i,j) = |x_{i_1} - x_{j_1}| + |x_{i_2} - x_{j_2}| + ... + |x_{i_p} - x_{j_p}|$$

Similarity and Dissimilarity Between Objects (Cont.)

- *If q = 2*, *d* is Euclidean distance:

$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + ... + |x_{i_p} - x_{j_p}|^2)}$$

  - Properties
    - $d(i,j) \geq 0$
    - $d(i,i) = 0$
    - $d(i,j) = d(j,i)$
    - $d(i,j) \leq d(i,k) + d(k,j)$
- Also one can use weighted distance.

Binary Variables

- A contingency table for binary data

		Object *j*		
		1	0	*sum*
Object *i*	1	a	b	$a+b$
	0	c	d	$c+d$
	sum	$a+c$	$b+d$	p

- Simple matching coefficient (invariant, if the binary variable is *symmetric*):

$$d(i, j) = \frac{b + c}{a + b + c + d}$$

- Jaccard coefficient (noninvariant if the binary variable is *asymmetric*):

$$d(i, j) = \frac{b + c}{a + b + c}$$

Dissimilarity between Binary Variables

- Example

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

- gender is a symmetric attribute
- the remaining attributes are asymmetric binary
- let the values Y and P be set to 1, and the value N be set to 0

$$d(jack, mary) = \frac{0 + 1}{2 + 0 + 1} = 0.33$$

$$d(jack, jim) = \frac{1 + 1}{1 + 1 + 1} = 0.67$$

$$d(jim, mary) = \frac{1 + 2}{1 + 1 + 2} = 0.75$$

Nominal Variables

- A generalization of the binary variable in that it can take more than 2 states, e.g., red, yellow, blue, green
- Method 1: Simple matching
  - *m*: # of matches, *p*: total # of variables

$$d(i, j) = \frac{p - m}{p}$$

- Method 2: use a large number of binary variables
  - creating a new binary variable for each of the *M* nominal states

Ordinal Variables

- An ordinal variable can be discrete or continuous
- order is important, e.g., rank
- Can be treated like interval-scaled
  - replacing x_{if} by their rank $r_{if} \in \{1, \ldots, M_f\}$
  - map the range of each variable onto [0, 1] by replacing *i*-th object in the *f*-th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

  - compute the dissimilarity using methods for interval-scaled variables

Similarity and Dissimilarity Between Objects (Cont.)

- *If q = 2*, *d* is Euclidean distance:

$$d(i,j)=\sqrt{(|x_{i_1}-x_{j_1}|^2+|x_{i_2}-x_{j_2}|^2+...+|x_{i_p}-x_{j_p}|^2)}$$

  - Properties
    - $d(i,j) \geq 0$
    - $d(i,i) = 0$
    - $d(i,j) = d(j,i)$
    - $d(i,j) \leq d(i,k) + d(k,j)$
- Also, one can use weighted distance, parametric

Ratio-Scaled Variables

- Ratio-scaled variable: a positive measurement on a nonlinear scale, approximately at exponential scale, such as Ae^{Bt} or Ae^{-Bt}
- Methods:
  - treat them like interval-scaled variables — *not a good choice! (why?)*
  - apply logarithmic transformation

$$y_{if} = log(x_{if})$$

  - treat them as continuous ordinal data treat their rank as interval-scaled.

Major Clustering Approaches

- Partitioning algorithms: Construct various partitions and then evaluate them by some criterion
- Hierarchcal algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Density-based: based on connectivity and density functions

Partitioning Algorithms: Basic Concept

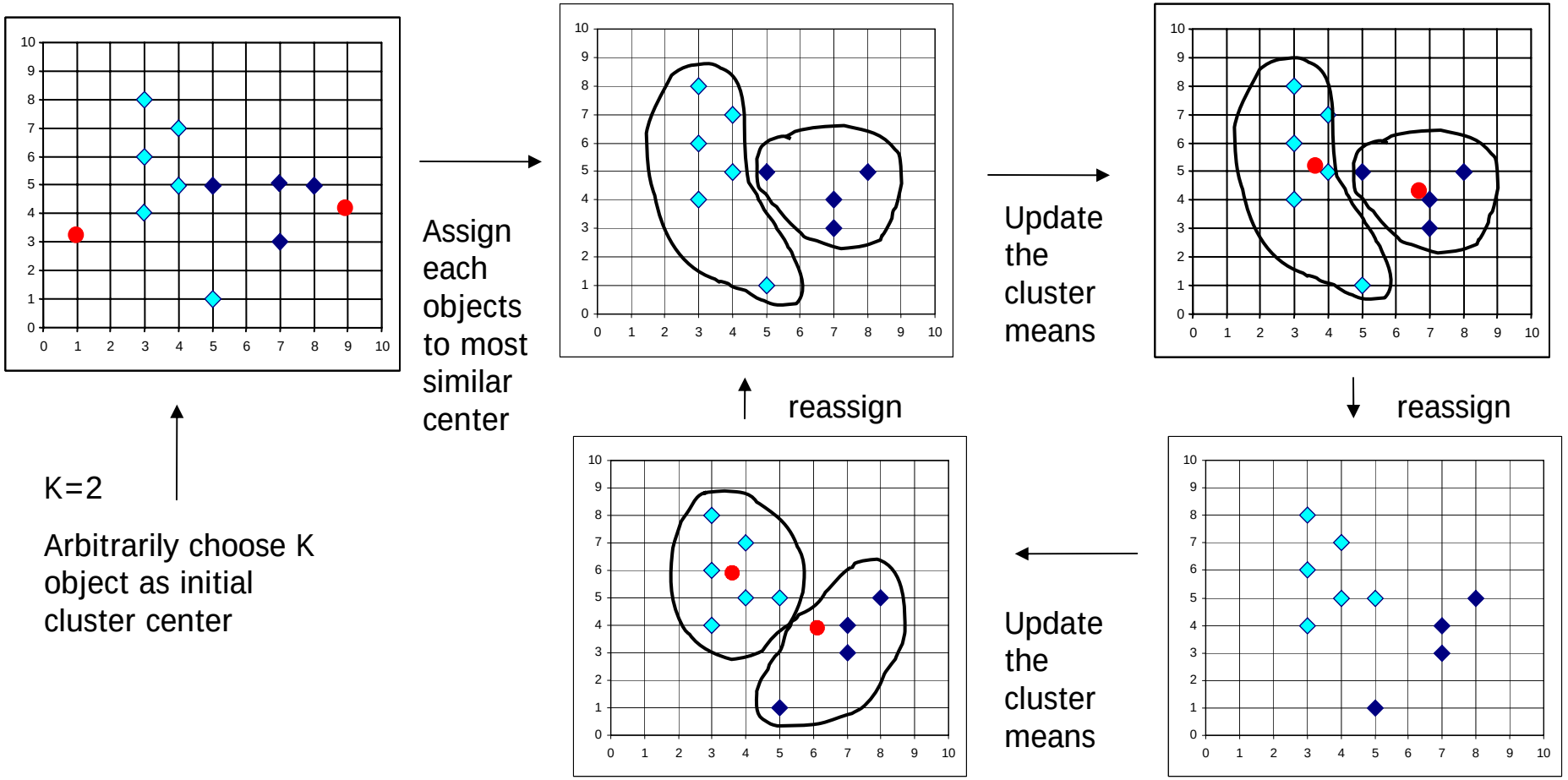
- Partitioning method: Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters
- Given a *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67): 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:
  - Partition objects into *k* nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partition (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 no more new assignment

The *K-Means* Clustering Method

- Example



Comments on the *K-Means* Method

- Strength: *Relatively 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 optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Weakness
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Unable to handle noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*