Web Mining
(網路探勘)

Supervised Learning
(監督式學習)

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課程大綱（Syllabus)

週次	日期	內容（Subject/Topics）
1	101/09/12	Introduction to Web Mining (網路探勘導論)
2	101/09/19	Association Rules and Sequential Patterns (關聯規則和序列模式)
3	101/09/26	Supervised Learning (監督式學習)
4	101/10/03	Unsupervised Learning (非監督式學習)
5	101/10/10	國慶紀念日(放假一天)
6	101/10/17	Paper Reading and Discussion (論文研讀與討論)
7	101/10/24	Partially Supervised Learning (部分監督式學習)
8	101/10/31	Information Retrieval and Web Search (資訊檢索與網路搜尋)
9	101/11/07	Social Network Analysis (社會網路分析)

課程大綱 (Syllabus)

週次	日期	內容（Subject/Topics）
10	101/11/14	Midterm Presentation (期中報告)
11	101/11/21	Web Crawling (網路爬行)
12	101/11/28	Structured Data Extraction (結構化資料擷取)
13	101/12/05	Information Integration (資訊整合)
14	101/12/12	Opinion Mining and Sentiment Analysis (意見探勘與情感分析)
15	101/12/19	Paper Reading and Discussion (論文研讀與討論)
16	101/12/26	Web Usage Mining (網路使用挖掘)
17	102/01/02	Project Presentation 1 (期末報告1)
18	102/01/09	Project Presentation 2 (期末報告2)

A Taxonomy for Data Mining Tasks

Data Mining	Learning Method	Popular Algorithms
Prediction	Supervised	Classification and Regression Trees, ANN, SVM, Genetic Algorithms
Classification	Supervised	Decision trees, ANN/MLP, SVM, Rough sets, Genetic Algorithms
Regression	Supervised	Linear/Nonlinear Regression, Regression trees, ANN/MLP, SVM
Association	Unsupervised	Apriory, OneR, ZeroR, Eclat
Link analysis	Unsupervised	Expectation Maximization, Apriory Algorithm, Graph-based Matching
Sequence analysis	Unsupervised	Apriory Algorithm, FP-Growth technique
Clustering	Unsupervised	K-means, ANN/SOM
Outlier analysis	Unsupervised	K-means, Expectation Maximization (EM)

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

Supervised Learning 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

Source: Han & Kamber (2006)

Classification Techniques

- Decision tree analysis
- Statistical analysis
- Neural networks
- Support vector machines
- Case-based reasoning
- Bayesian classifiers
- Genetic algorithms
- Rough sets

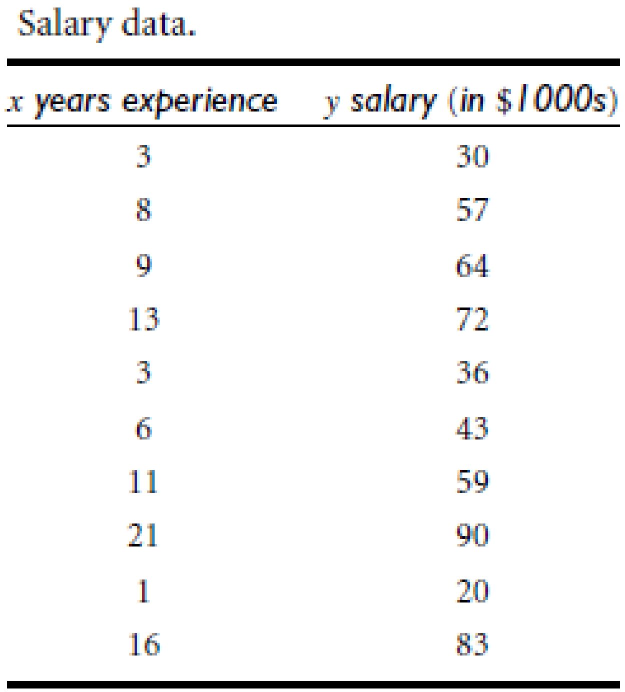
Example of Classification

- Loan Application Data
  - Which loan applicants are "safe" and which are "risky" for the bank?
  - "Safe" or "risky" for load application data
- Marketing Data
  - Whether a customer with a given profile will buy a new computer?
  - "yes" or "no" for marketing data
- **Classification**
  - Data analysis task
  - A model or **Classifier** is constructed to predict categorical labels
    - Labels: "safe" or "risky"; "yes" or "no"; "treatment A", "treatment B", "treatment C"

Source: Han & Kamber (2006)

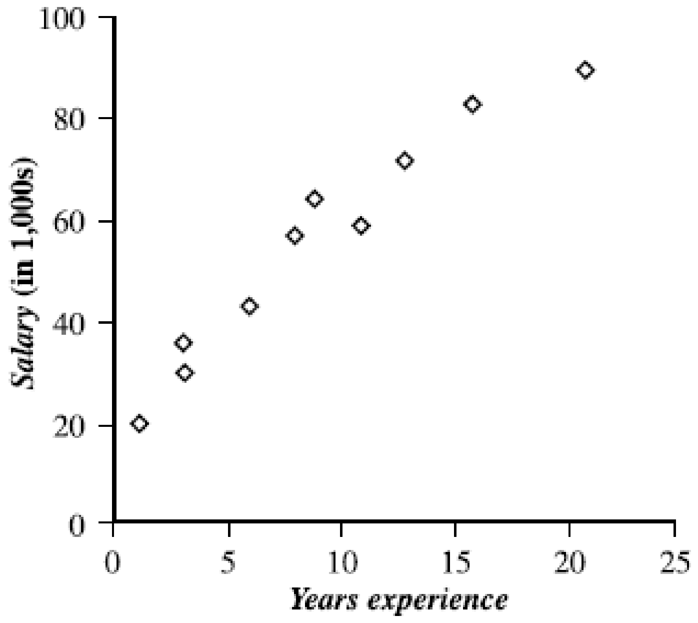
Prediction Methods

- Linear Regression
- Nonlinear Regression
- Other Regression Methods



Salary data.

x years experience	*y salary (in $1000s)*
3	30
8	57
9	64
13	72
3	36
6	43
11	59
21	90
1	20
16	83



Classification and Prediction

- Classification and prediction are two forms of data analysis that can be used to extract models describing important data classes or to predict future data trends.
- Classification
  - Effective and scalable methods have been developed for decision trees induction, Naive Bayesian classification, Bayesian belief network, rule-based classifier, Backpropagation, Support Vector Machine (SVM), associative classification, nearest neighbor classifiers, and case-based reasoning, and other classification methods such as genetic algorithms, rough set and fuzzy set approaches.
- Prediction
  - Linear, nonlinear, and generalized linear models of regression can be used for prediction. Many nonlinear problems can be converted to linear problems by performing transformations on the predictor variables. Regression trees and model trees are also used for prediction.

Source: Han & Kamber (2006)

Classification vs. Prediction

- Classification
  - predicts categorical class labels (discrete or nominal)
  - classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data
- Prediction
  - models continuous-valued functions
    - i.e., predicts unknown or missing values
- Typical applications
  - Credit approval
  - Target marketing
  - Medical diagnosis
  - Fraud detection

Source: Han & Kamber (2006)

Classification—A Two-Step Process

1. 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
2. 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

Issues Regarding Classification and Prediction: Data Preparation

- Data cleaning
  - Preprocess data in order to reduce noise and handle missing values
- Relevance analysis (feature selection)
  - Remove the irrelevant or redundant attributes
  - Attribute subset selection
    - Feature Selection in machine learning
- Data transformation
  - Generalize and/or normalize data
  - Example
    - Income: low, medium, high

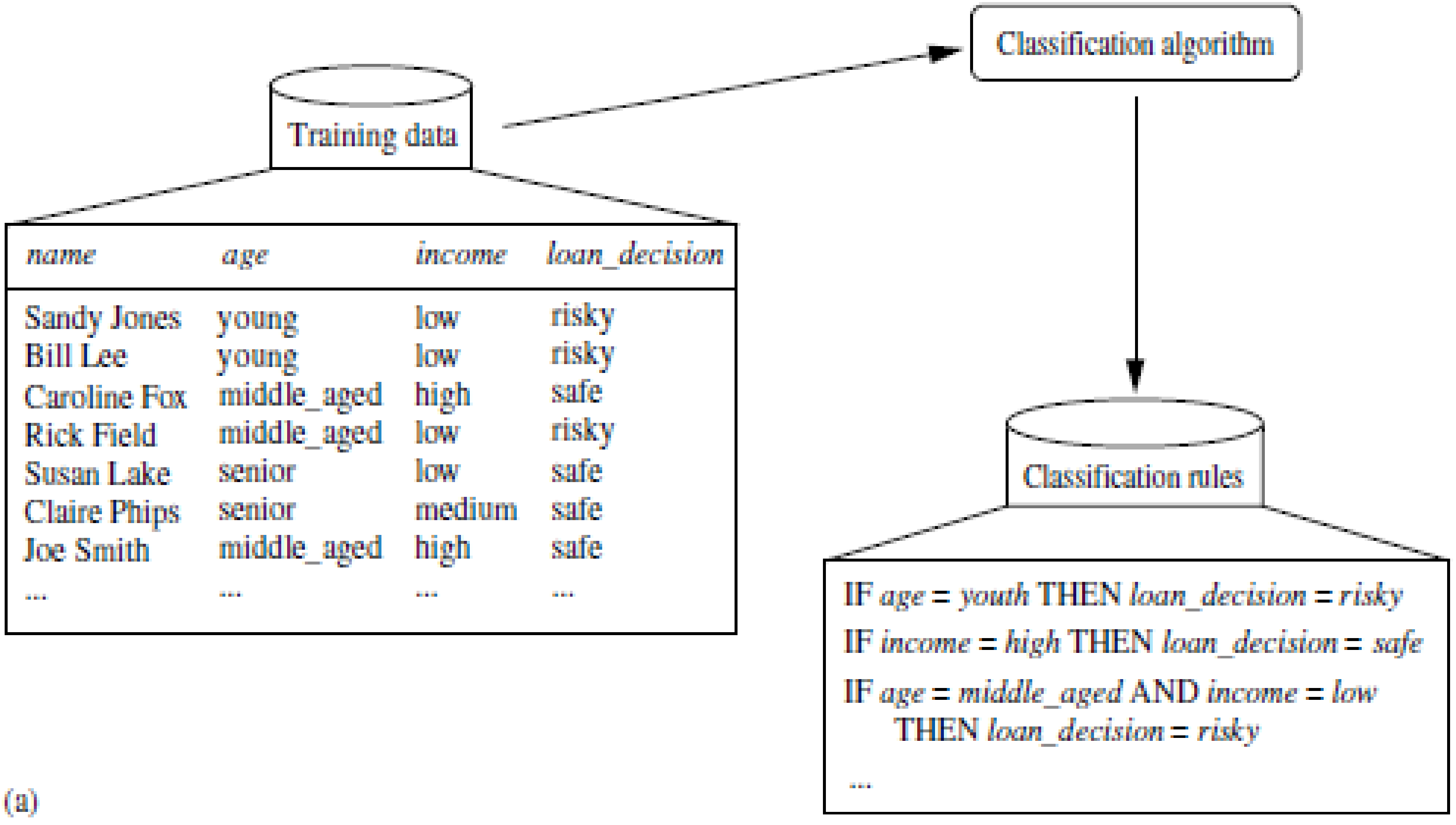
Issues:
Evaluating Classification and Prediction Methods

- Accuracy
  - classifier accuracy: predicting class label
  - predictor accuracy: guessing value of predicted attributes
  - estimation techniques: cross-validation and bootstrapping
- Speed
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- Robustness
  - handling noise and missing values
- Scalability
  - ability to construct the classifier or predictor efficiently given large amounts of data
- Interpretability
  - understanding and insight provided by the model

Source: Han & Kamber (2006)

Data Classification Process 1: Learning (Training) Step (a) Learning: Training data are analyzed by classification algorithm

$y = f(X)$



name	*age*	*income*	*loan_decision*
Sandy Jones	young	low	risky
Bill Lee	young	low	risky
Caroline Fox	middle_aged	high	safe
Rick Field	middle_aged	low	risky
Susan Lake	senior	low	safe
Claire Phips	senior	medium	safe
Joe Smith	middle_aged	high	safe
...	...	...	...

IF *age* = *youth* THEN *loan_decision* = *risky*

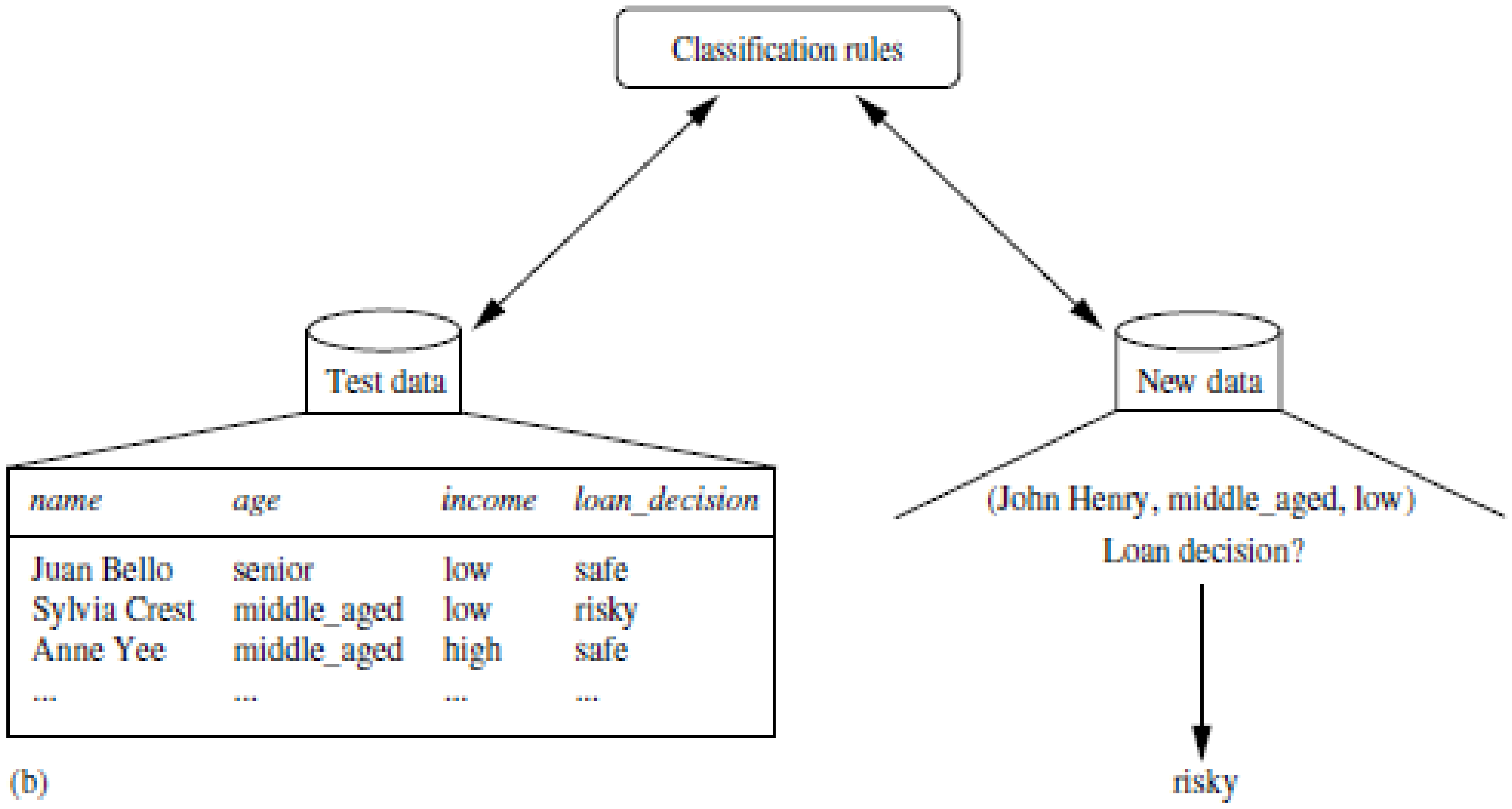
IF *income* = *high* THEN *loan_decision* = *safe*

IF *age* = *middle_aged* AND *income* = *low*
THEN *loan_decision* = *risky*

...

Source: Han & Kamber (2006)

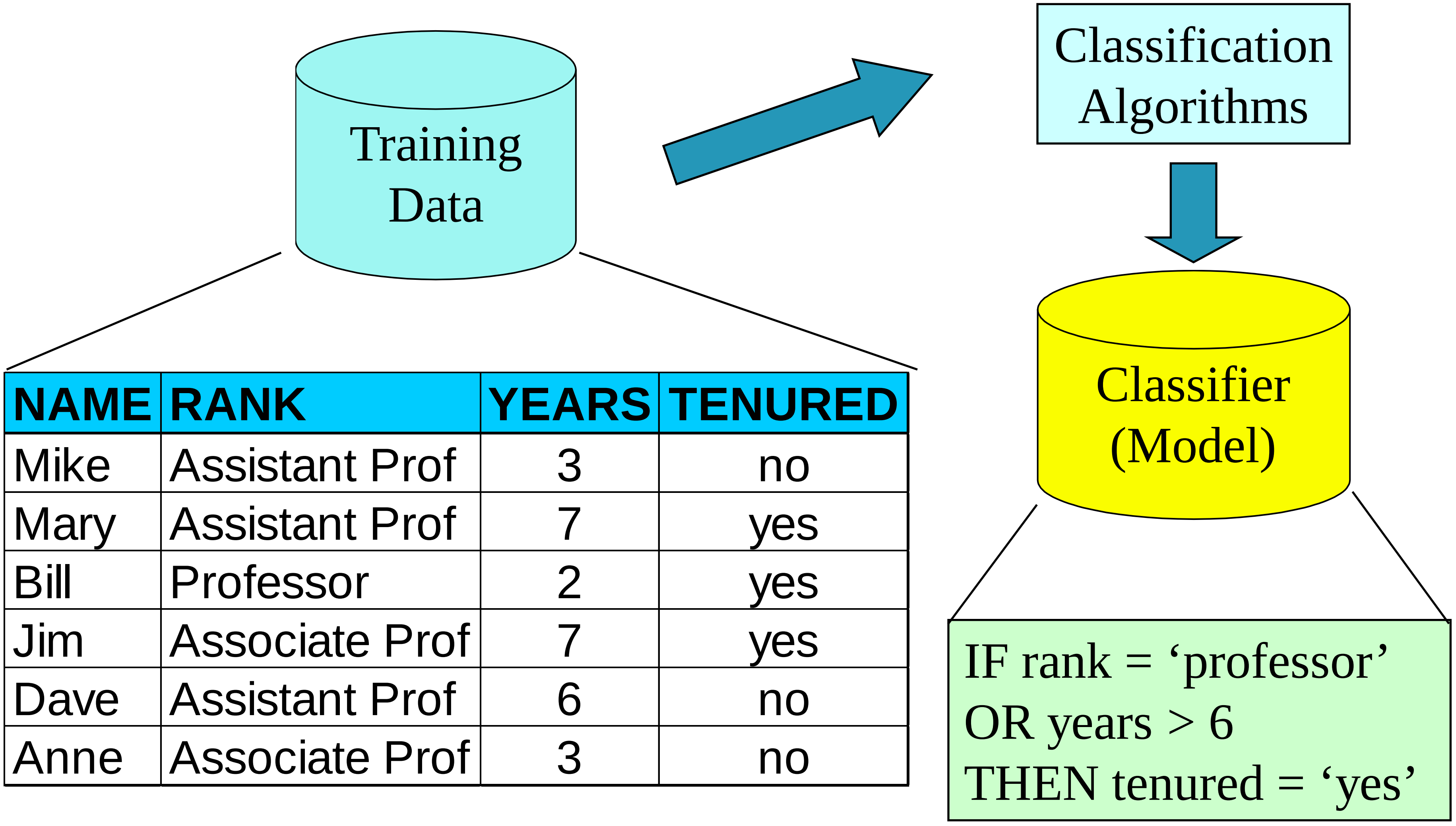
Data Classification Process 2
(b) Classification: Test data are used to estimate the accuracy of the classification rules.



name	*age*	*income*	*loan_decision*
Juan Bello	senior	low	safe
Sylvia Crest	middle_aged	low	risky
Anne Yee	middle_aged	high	safe
...	...	...	...

Source: Han & Kamber (2006)

Process (1): Model Construction

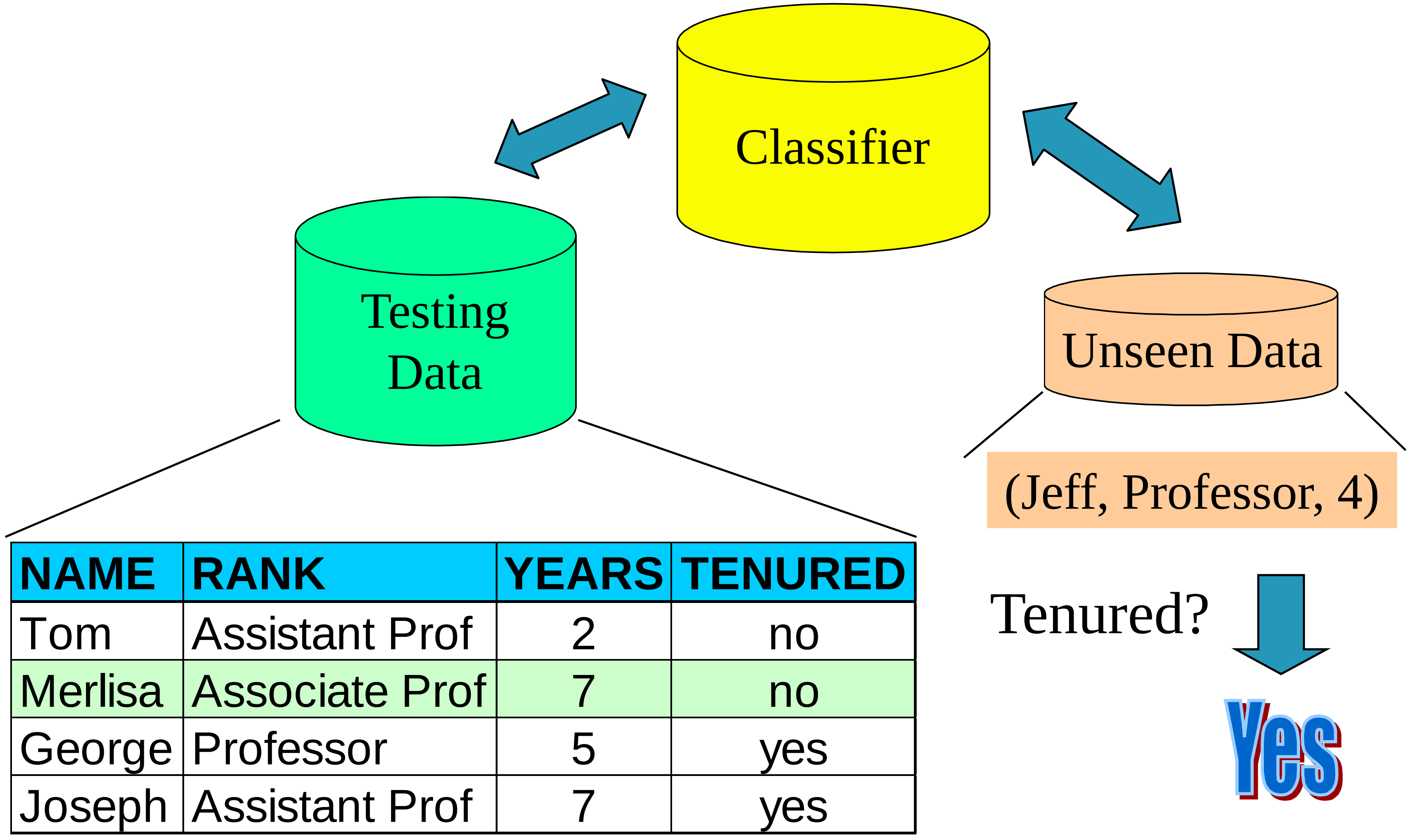


NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

IF rank = ‘professor’
OR years > 6
THEN tenured = ‘yes’

Source: Han & Kamber (2006)

Process (2): Using 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

Source: Han & Kamber (2006)

Decision Trees

A general algorithm for decision tree building

- Employs the divide and conquer method
- Recursively divides a training set until each division consists of examples from one class
    1. Create a root node and assign all of the training data to it
    2. Select the best splitting attribute
    3. Add a branch to the root node for each value of the split. Split the data into mutually exclusive subsets along the lines of the specific split
    4. Repeat the steps 2 and 3 for each and every leaf node until the stopping criteria is reached

Decision Trees

- DT algorithms mainly differ on
  - Splitting criteria
    - Which variable to split first?
    - What values to use to split?
    - How many splits to form for each node?
  - Stopping criteria
    - When to stop building the tree
  - Pruning (generalization method)
    - Pre-pruning versus post-pruning
- Most popular DT algorithms include
  - ID3, C4.5, C5; CART; CHAID; M5

Decision Trees

- Alternative splitting criteria
  - Gini index determines the purity of a specific class as a result of a decision to branch along a particular attribute/value
    - Used in CART
  - Information gain uses entropy to measure the extent of uncertainty or randomness of a particular attribute/value split
    - Used in ID3, C4.5, C5
  - Chi-square statistics (used in CHAID)

Classification by Decision Tree Induction
Training Dataset

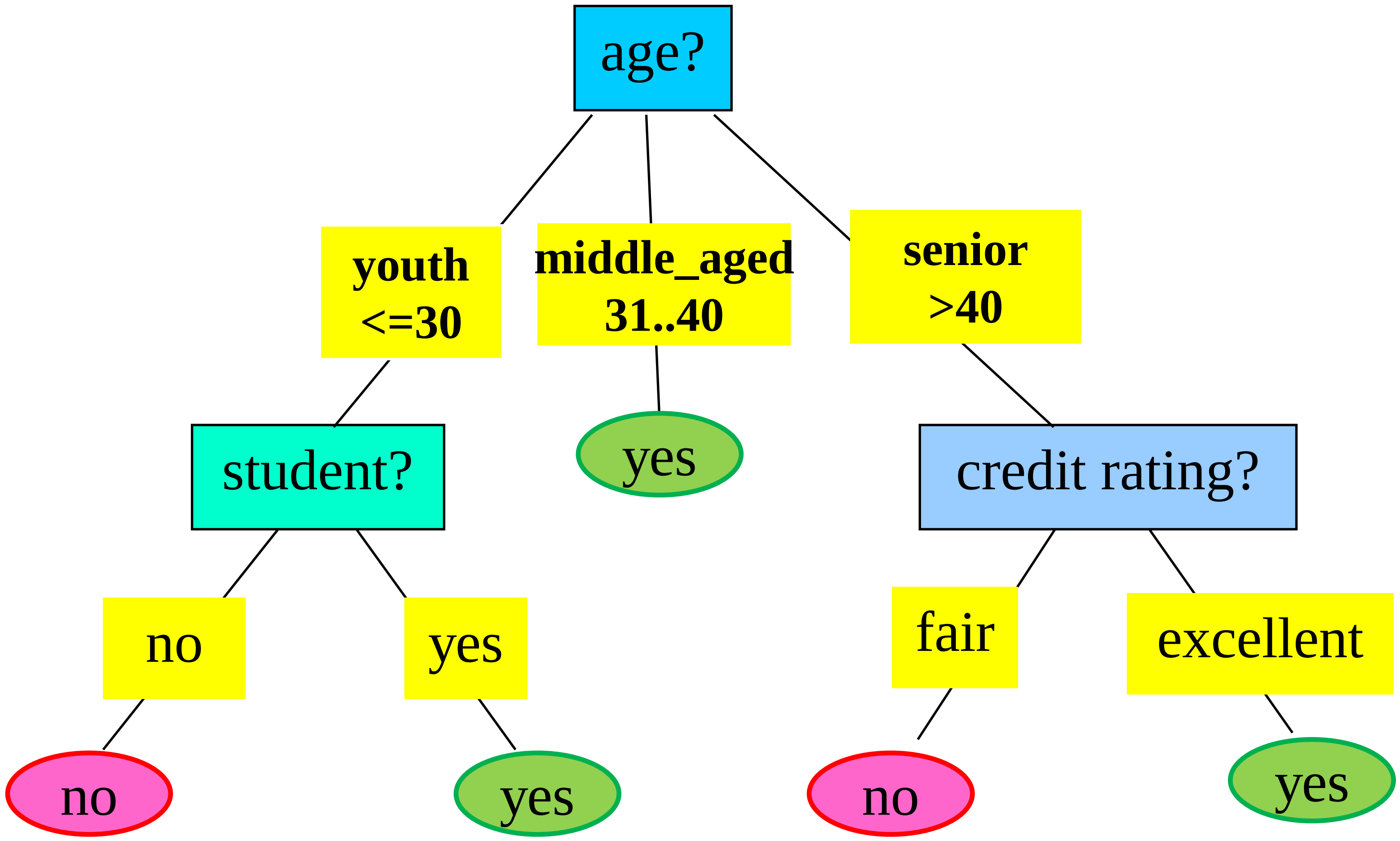
age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent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

This follows an example of Quinlan's ID3 (Playing Tennis)

Source: Han & Kamber (2006)

Classification by Decision Tree Induction

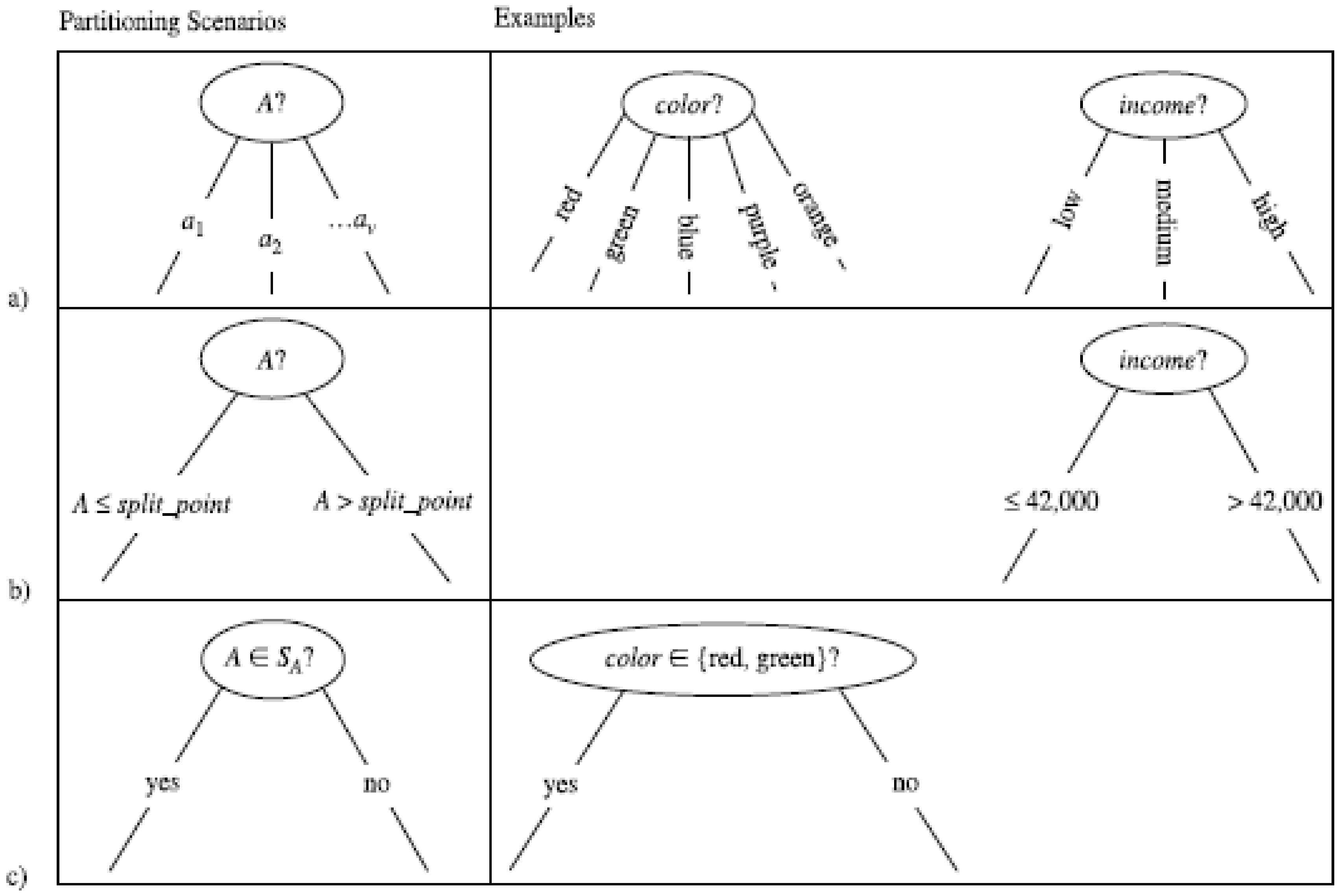
Output: A Decision Tree for "*buys_computer*"



buys_computer="yes" or buys_computer="no"

Source: Han & Kamber (2006)

Three possibilities for partitioning tuples based on the splitting Criterion



Source: Han & Kamber (2006)

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

Source: Han & Kamber (2006)

Attribute Selection Measure

- Information Gain
- Gain Ratio
- Gini Index

Attribute Selection Measure

- Notation: Let *D, the data partition, be a training set of* class-labeled tuples.
  Suppose the class label attribute has *m distinct values defining m* distinct classes, *C_i (for i = 1, … , m).*
  Let *$C_{i,D}$ be the set of tuples of class C_i in D.*
  Let |D| and *| $C_{i,D}$ | denote the number of tuples in D and $C_{i,D}$, respectively.*
- *Example:*
  - *Class: buys_computer= "yes" or "no"*
  - *Two distinct classes (m=2)*
    - *Class C_i (i=1,2):*
      C_1 = "yes",
      C_2 = "no"

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

- Select the attribute with the highest information gain
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i, estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times I(D_j)$$

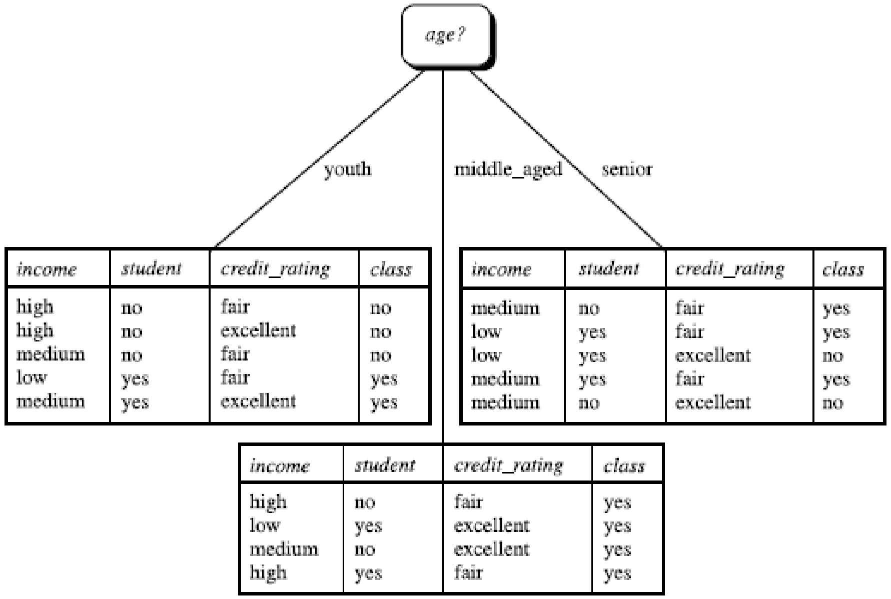
- Information gained by branching on attribute A

$$Gain(A) = Info(D) - Info_A(D)$$

Source: Han & Kamber (2006)

Class-labeled training tuples from the *AllElectronics customer database*

RID	*age*	*income*	*student*	*credit_rating*	*Class: buys_computer*
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no



income	*student*	*credit_rating*	*class*
high	no	fair	no
high	no	excellent	no
medium	no	fair	no
low	yes	fair	yes
medium	yes	excellent	yes

income	*student*	*credit_rating*	*class*
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
medium	no	excellent	no

income	*student*	*credit_rating*	*class*
high	no	fair	yes
low	yes	excellent	yes
medium	no	excellent	yes
high	yes	fair	yes

The attribute age has the highest information gain and therefore becomes the splitting attribute at the root node of the decision tree

Attribute Selection: Information Gain

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

$$Info_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
31…40	4	0	0
>40	3	2	0.971

$\frac{5}{14}I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's. Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…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

Similarly,

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

Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right)$$

  – GainRatio(A) = Gain(A)/SplitInfo(A)
- Ex. $SplitInfo_A(D) = -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) = 0.926$
  – gain_ratio(income) = 0.029/0.926 = 0.031
- The attribute with the maximum gain ratio is selected as the splitting attribute

Gini index (CART, IBM IntelligentMiner)

- If a data set *D* contains examples from *n* classes, gini index, *gini*(*D*) is defined as

$$gini(D) = 1 - \sum_{j=1}^{n} p_j^2$$

where p_j is the relative frequency of class *j* in *D*

- If a data set *D* is split on A into two subsets D_1 and D_2, the *gini* index *gini*(*D*) is defined as

$$gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$$

- Reduction in Impurity:

$$\Delta gini(A) = gini(D) - gini_A(D)$$

- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

Gini index (CART, IBM IntelligentMiner)

- Ex. D has 9 tuples in buys_computer = “yes” and 5 in “no”

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute income partitions D into 10 in D_1: {low, medium} and 4 in D_2

$$gini_{income \in \{low, medium\}}(D) = \left(\frac{10}{14}\right)Gini(D_1) + \left(\frac{4}{14}\right)Gini(D_1)$$

$$= \frac{10}{14}(1 - (\frac{6}{10})^2 - (\frac{4}{10})^2) + \frac{4}{14}(1 - (\frac{1}{4})^2 - (\frac{3}{4})^2)$$

$$= 0.450$$

$$= Gini_{income \ \in \ \{high\}}(D)$$

but $gini_{\{medium,high\}}$ is 0.30 and thus the best since it is the lowest

- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

Comparing Attribute Selection Measures

- The three measures, in general, return good results but
  - Information gain:
    - biased towards multivalued attributes
  - Gain ratio:
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - Gini index:
    - biased to multivalued attributes
    - has difficulty when # of classes is large
    - tends to favor tests that result in equal-sized partitions and purity in both partitions

Classification in Large Databases

- Classification—a classical problem extensively studied by statisticians and machine learning researchers
- Scalability: Classifying data sets with millions of examples and hundreds of attributes with reasonable speed
- Why decision tree induction in data mining?
  - relatively faster learning speed (than other classification methods)
  - convertible to simple and easy to understand classification rules
  - can use SQL queries for accessing databases
  - comparable classification accuracy with other methods

SVM—Support Vector Machines

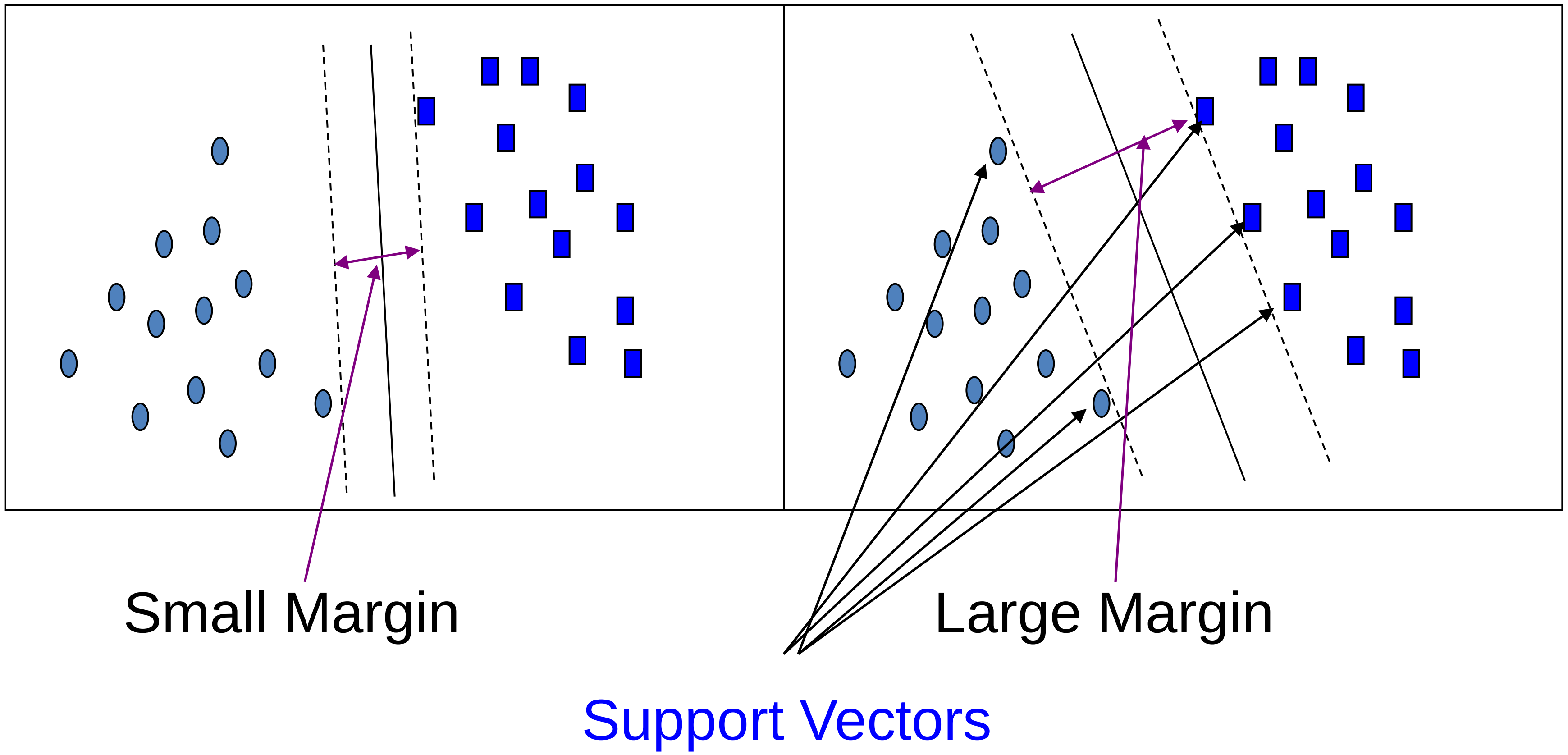
- A new classification method for both linear and nonlinear data
- It uses a nonlinear mapping to transform the original training data into a higher dimension
- With the new dimension, it searches for the linear optimal separating hyperplane (i.e., "decision boundary")
- With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane
- SVM finds this hyperplane using support vectors ("essential" training tuples) and margins (defined by the support vectors)

SVM—History and Applications

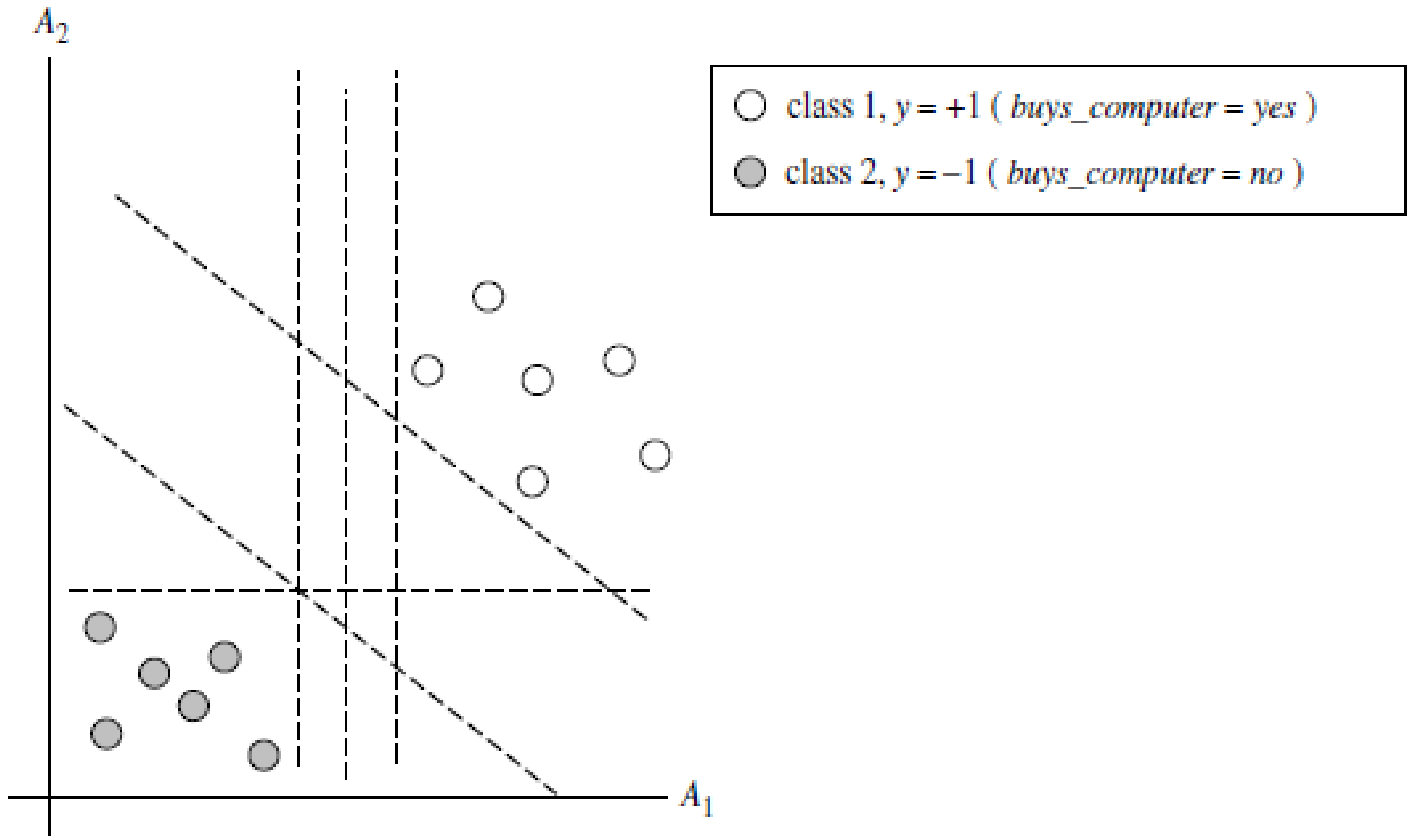
- Vapnik and colleagues (1992)—groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Features: training can be slow but accuracy is high owing to their ability to model complex nonlinear decision boundaries (margin maximization)
- Used both for classification and prediction
- Applications:
  - handwritten digit recognition, object recognition, speaker identification, benchmarking time-series prediction tests, document classification

Source: Han & Kamber (2006)

SVM—General Philosophy



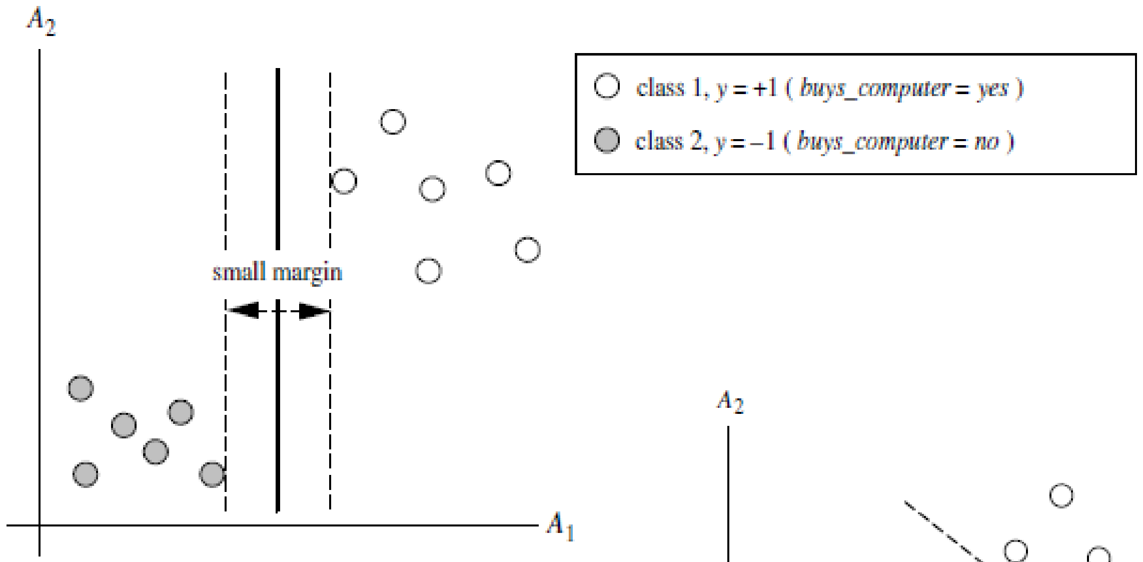
Classification (SVM)

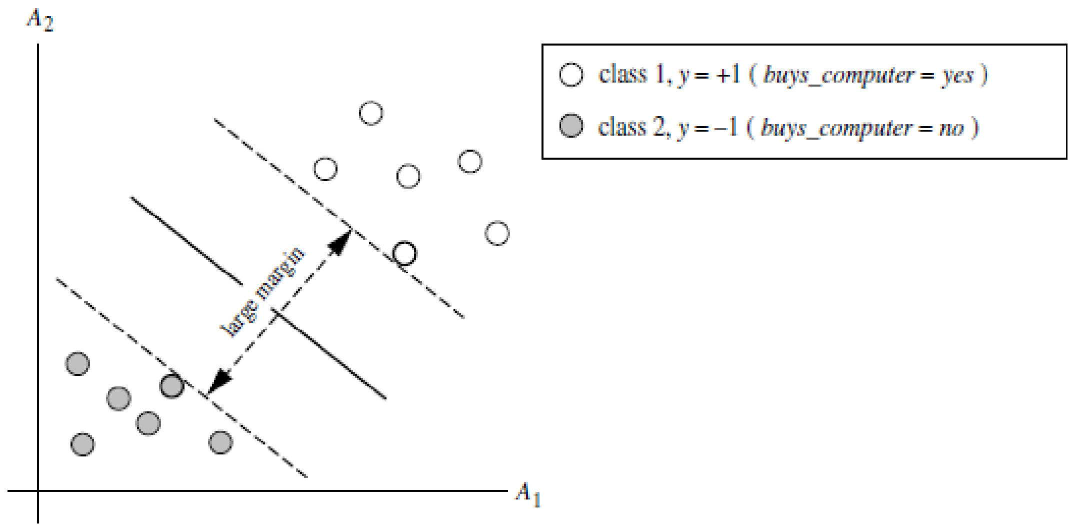


A_2
○ class 1, $y = +1$ (*buys_computer* = *yes*)
● class 2, $y = -1$ (*buys_computer* = *no*)
A_1

The 2-D training data are linearly separable. There are an infinite number of (possible) separating hyperplanes or “decision boundaries.”Which one is best?

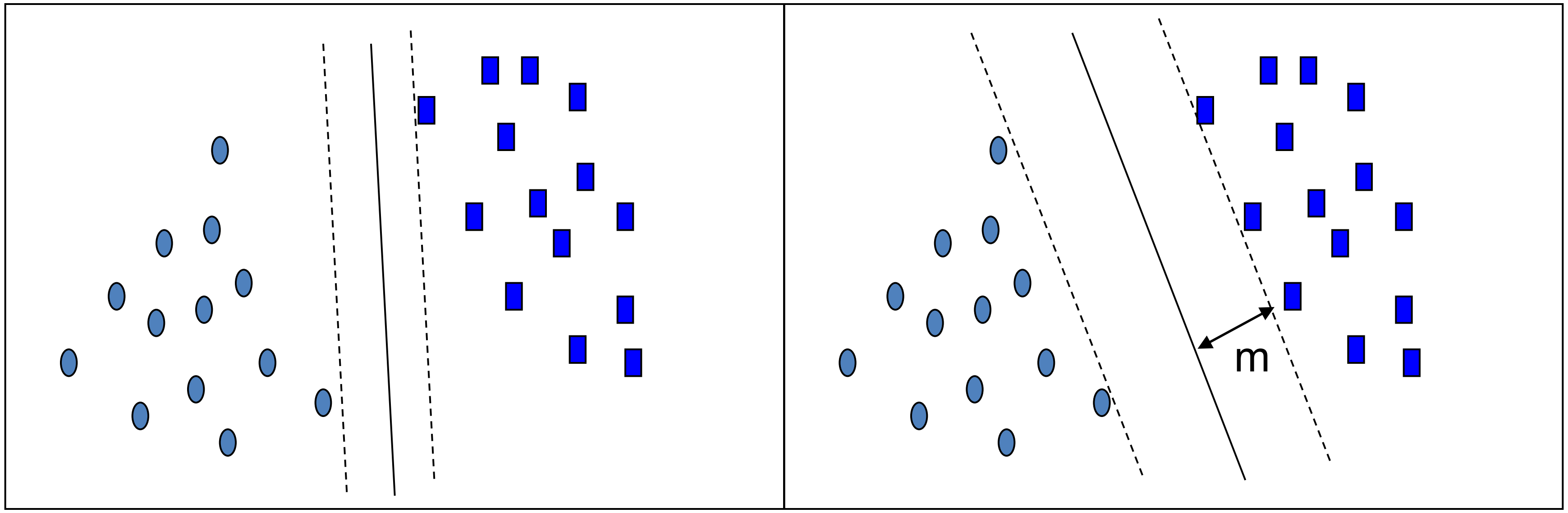
Classification (SVM)


A_2
small margin
A_1
○ class 1, $y = +1$ (*buys_computer = yes*)
● class 2, $y = -1$ (*buys_computer = no*)


A_2
large margin
A_1
○ class 1, $y = +1$ (*buys_computer = yes*)
● class 2, $y = -1$ (*buys_computer = no*)

Which one is better? The one with the larger margin should have greater generalization accuracy.

SVM—When Data Is Linearly Separable



Let data D be ($\mathbf{X}_1$, y_1), …, ($\mathbf{X}_{|D|}$, $y_{|D|}$), where $\mathbf{X}_i$ is the set of training tuples associated with the class labels y_i

There are infinite lines (hyperplanes) separating the two classes but we want to find the best one (the one that minimizes classification error on unseen data)

SVM searches for the hyperplane with the largest margin, i.e., **maximum marginal hyperplane** (MMH)

Source: Han & Kamber (2006)

SVM—Linearly Separable

- A separating hyperplane can be written as

  $\mathbf{W} \bullet \mathbf{X} + b = 0$

  where $\mathbf{W}=\{w_1, w_2, \ldots, w_n\}$ is a weight vector and b a scalar (bias)
- For 2-D it can be written as

  $w_0 + w_1 x_1 + w_2 x_2 = 0$
- The hyperplane defining the sides of the margin:

  H_1: $w_0 + w_1 x_1 + w_2 x_2 \geq 1$ for $y_i = +1$, and

  H_2: $w_0 + w_1 x_1 + w_2 x_2 \leq -1$ for $y_i = -1$
- Any training tuples that fall on hyperplanes H_1 or H_2 (i.e., the sides defining the margin) are **support vectors**
- This becomes a **constrained (convex) quadratic optimization** problem: Quadratic objective function and linear constraints → *Quadratic Programming (QP)* → Lagrangian multipliers

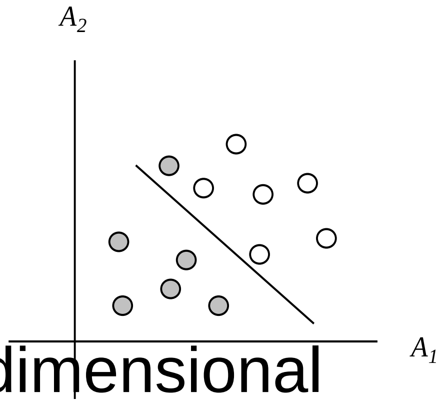
Source: Han & Kamber (2006)

Why Is SVM Effective on High Dimensional Data?

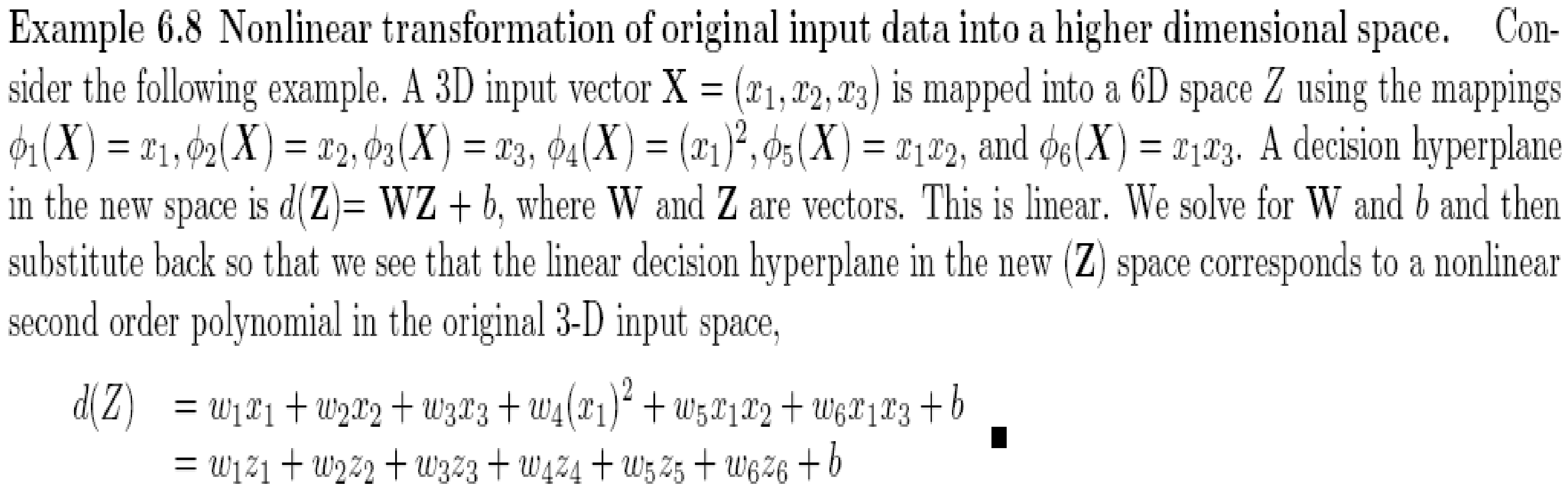
- The complexity of trained classifier is characterized by the # of support vectors rather than the dimensionality of the data
- The support vectors are the essential or critical training examples — they lie closest to the decision boundary (MMH)
- If all other training examples are removed and the training is repeated, the same separating hyperplane would be found
- The number of support vectors found can be used to compute an (upper) bound on the expected error rate of the SVM classifier, which is independent of the data dimensionality
- Thus, an SVM with a small number of support vectors can have good generalization, even when the dimensionality of the data is high

Source: Han & Kamber (2006)

SVM—Linearly Inseparable



- Transform the original input data into a higher dimensional space

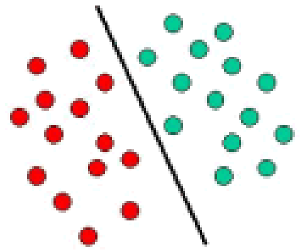


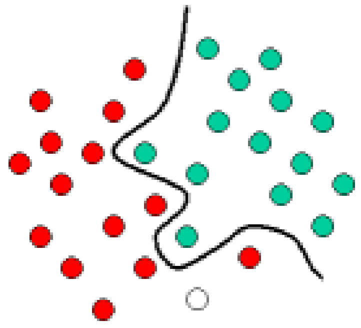
Example 6.8 Nonlinear transformation of original input data into a higher dimensional space. Consider the following example. A 3D input vector $\mathbf{X} = (x_1, x_2, x_3)$ is mapped into a 6D space Z using the mappings $\phi_1(X) = x_1, \phi_2(X) = x_2, \phi_3(X) = x_3$, $\phi_4(X) = (x_1)^2, \phi_5(X) = x_1x_2$, and $\phi_6(X) = x_1x_3$. A decision hyperplane in the new space is $d(\mathbf{Z}) = \mathbf{WZ} + b$, where $\mathbf{W}$ and $\mathbf{Z}$ are vectors. This is linear. We solve for $\mathbf{W}$ and b and then substitute back so that we see that the linear decision hyperplane in the new $(\mathbf{Z})$ space corresponds to a nonlinear second order polynomial in the original 3-D input space,

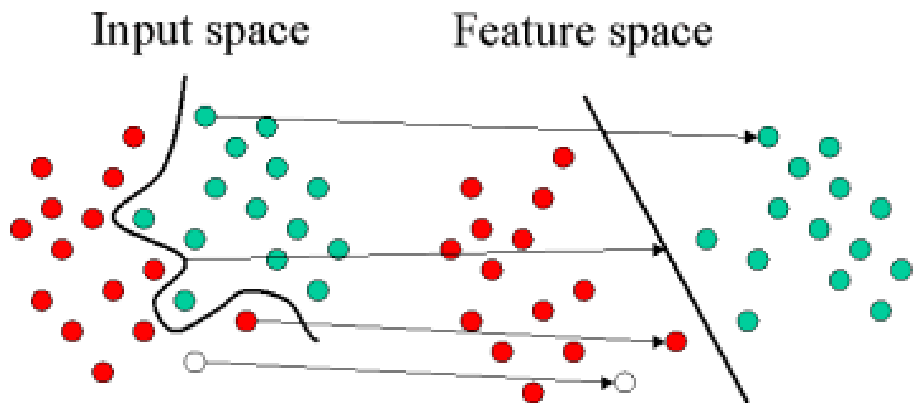
$$\begin{aligned} d(Z) &= w_1x_1 + w_2x_2 + w_3x_3 + w_4(x_1)^2 + w_5x_1x_2 + w_6x_1x_3 + b \\ &= w_1z_1 + w_2z_2 + w_3z_3 + w_4z_4 + w_5z_5 + w_6z_6 + b \end{aligned} \quad ■$$

- Search for a linear separating hyperplane in the new space

Mapping Input Space to Feature Space







Source: http://www.statsoft.com/textbook/support-vector-machines/

SVM—Kernel functions

- Instead of computing the dot product on the transformed data tuples, it is mathematically equivalent to instead applying a kernel function K($\mathbf{X}_i$, $\mathbf{X}_j$) to the original data, i.e., K($\mathbf{X}_i$, $\mathbf{X}_j$) = Φ($\mathbf{X}_i$) Φ($\mathbf{X}_j$)
- Typical Kernel Functions

$$\text{Polynomial kernel of degree } h: \quad K(X_i, X_j) = (X_i \cdot X_j + 1)^h$$

$$\text{Gaussian radial basis function kernel}: \quad K(X_i, X_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$$

$$\text{Sigmoid kernel}: \quad K(X_i, X_j) = \tanh(\kappa X_i \cdot X_j - \delta)$$

- SVM can also be used for classifying multiple (> 2) classes and for regression analysis (with additional user parameters)

SVM vs. Neural Network

- SVM
  - Relatively new concept
  - Deterministic algorithm
  - Nice Generalization properties
  - Hard to learn – learned in batch mode using quadratic programming techniques
  - Using kernels can learn very complex functions

- Neural Network
  - Relatively old
  - Nondeterministic algorithm
  - Generalizes well but doesn't have strong mathematical foundation
  - Can easily be learned in incremental fashion
  - To learn complex functions—use multilayer perceptron (not that trivial)

SVM Related Links

- SVM Website
  - http://www.kernel-machines.org/
- Representative implementations
  - LIBSVM
    - an efficient implementation of SVM, multi-class classifications, nu-SVM, one-class SVM, including also various interfaces with java, python, etc.
  - SVM-light
    - simpler but performance is not better than LIBSVM, support only binary classification and only C language
  - SVM-torch
    - another recent implementation also written in C.

Accuracy of Classification Models

- In classification problems, the primary source for accuracy estimation is the confusion matrix

		True Class	
		Positive	Negative
Predicted Class	Positive	True Positive Count (TP)	False Positive Count (FP)
	Negative	False Negative Count (FN)	True Negative Count (TN)

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

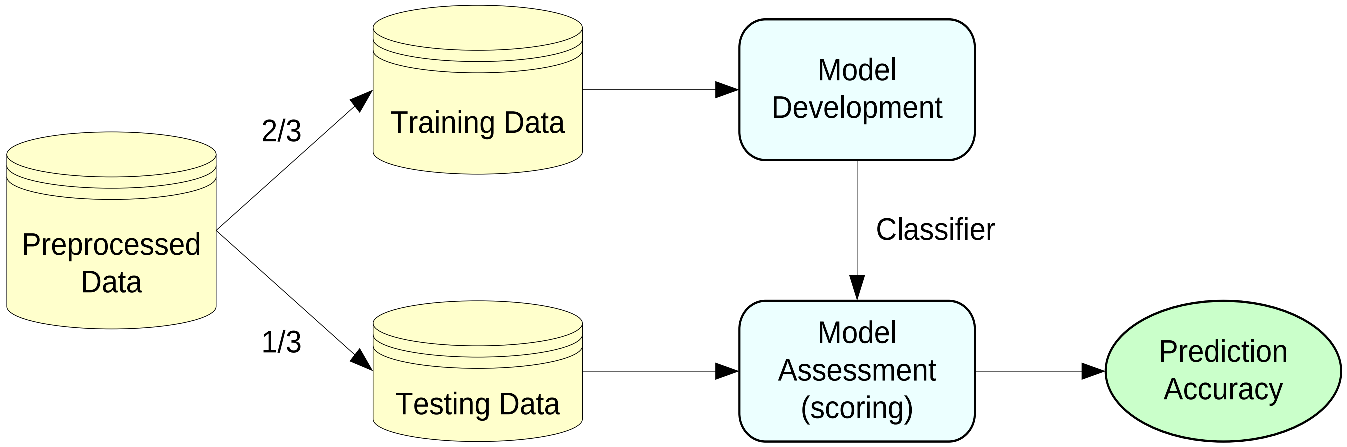
$$True\ Positive\ Rate = \frac{TP}{TP + FN}$$

$$True\ Negative\ Rate = \frac{TN}{TN + FP}$$

$$Precision = \frac{TP}{TP + FP} \qquad Recall = \frac{TP}{TP + FN}$$

Estimation Methodologies for Classification

- Simple split (or holdout or test sample estimation)
  - Split the data into 2 mutually exclusive sets training (~70%) and testing (30%)

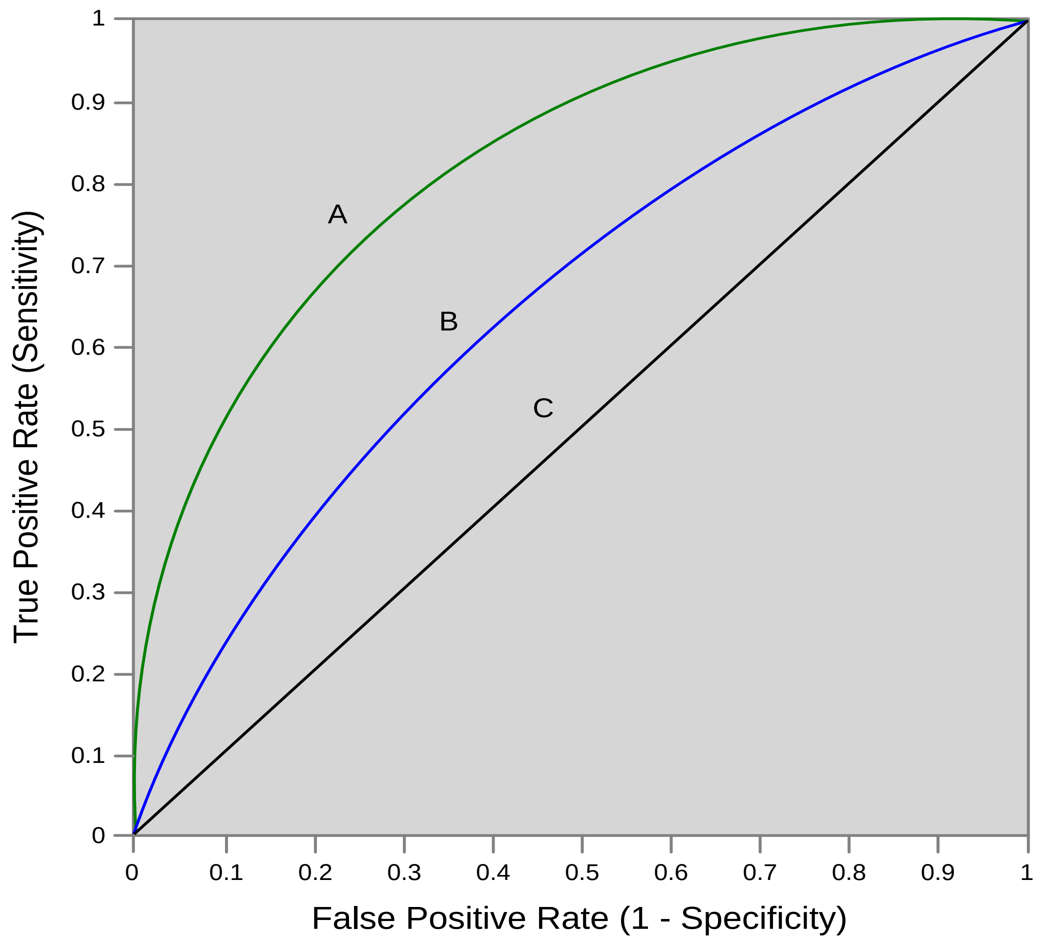


  - For ANN, the data is split into three sub-sets (training [~60%], validation [~20%], testing [~20%])

Estimation Methodologies for Classification

- *k*-Fold Cross Validation (rotation estimation)
  - Split the data into *k* mutually exclusive subsets
  - Use each subset as testing while using the rest of the subsets as training
  - Repeat the experimentation for *k* times
  - Aggregate the test results for true estimation of prediction accuracy training
- Other estimation methodologies
  - Leave-one-out, bootstrapping, jackknifing
  - Area under the ROC curve

Estimation Methodologies for Classification – ROC Curve



Evaluating classification methods

- **Predictive accuracy**

$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}}$$

- Efficiency
  - time to construct the model
  - time to use the model
- Robustness: handling noise and missing values
- Scalability: efficiency in disk-resident databases
- Interpretability:
  - understandable and insight provided by the model
- Compactness of the model: size of the tree, or the number of rules.

Evaluation methods

- **Holdout set**: The available data set *D* is divided into two disjoint subsets,
  - the *training set* D_{train} (for learning a model)
  - the *test set* D_{test} (for testing the model)
- **Important:** training set should not be used in testing and the test set should not be used in learning.
  - Unseen test set provides a unbiased estimate of accuracy.
- The test set is also called the holdout set. (the examples in the original data set *D* are all labeled with classes.)
- This method is mainly used when the data set *D* is large.

Evaluation methods (cont…)

- **n-fold cross-validation**: The available data is partitioned into *n* equal-size disjoint subsets.
- Use each subset as the test set and combine the rest *n*-1 subsets as the training set to learn a classifier.
- The procedure is run *n* times, which give *n* accuracies.
- The final estimated accuracy of learning is the average of the *n* accuracies.
- 10-fold and 5-fold cross-validations are commonly used.
- This method is used when the available data is not large.

Evaluation methods (cont…)

- **Leave-one-out cross-validation**: This method is used when the data set is very small.
- It is a special case of cross-validation
- Each fold of the cross validation has only a single test example and all the rest of the data is used in training.
- If the original data has *m* examples, this is *m*-fold cross-validation

Evaluation methods (cont…)

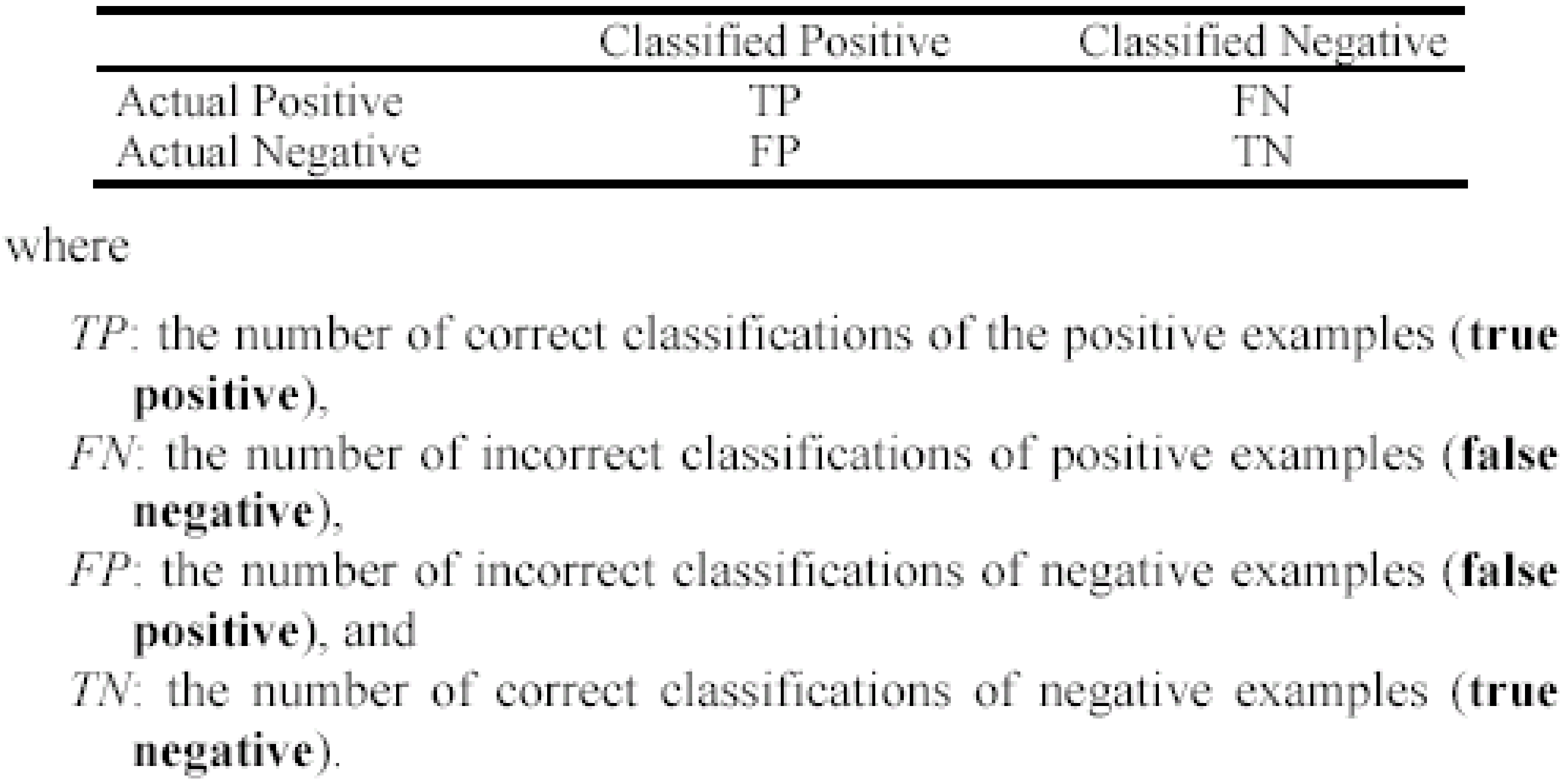
- **Validation set**: the available data is divided into three subsets,
  - a training set,
  - a validation set and
  - a test set.
- A validation set is used frequently for estimating parameters in learning algorithms.
- In such cases, the values that give the best accuracy on the validation set are used as the final parameter values.
- Cross-validation can be used for parameter estimating as well.

Classification measures

- Accuracy is only one measure (error = 1-accuracy).
- **Accuracy is not suitable in some applications**.
- In text mining, we may only be interested in the documents of a particular topic, which are only a small portion of a big document collection.
- In classification involving skewed or highly imbalanced data, e.g., network intrusion and financial fraud detections, we are interested only in the minority class.
  - High accuracy does not mean any intrusion is detected.
  - E.g., 1% intrusion. Achieve 99% accuracy by doing nothing.
- The class of interest is commonly called the **positive class**, and the rest **negative classes**.

Precision and **recall** measures

- Used in information retrieval and text classification.
- We use a confusion matrix to introduce them.



	Classified Positive	Classified Negative
Actual Positive	TP	FN
Actual Negative	FP	TN

where

TP: the number of correct classifications of the positive examples (**true positive**),
FN: the number of incorrect classifications of positive examples (**false negative**),
FP: the number of incorrect classifications of negative examples (**false positive**), and
TN: the number of correct classifications of negative examples (**true negative**).

Precision and recall measures (cont…)

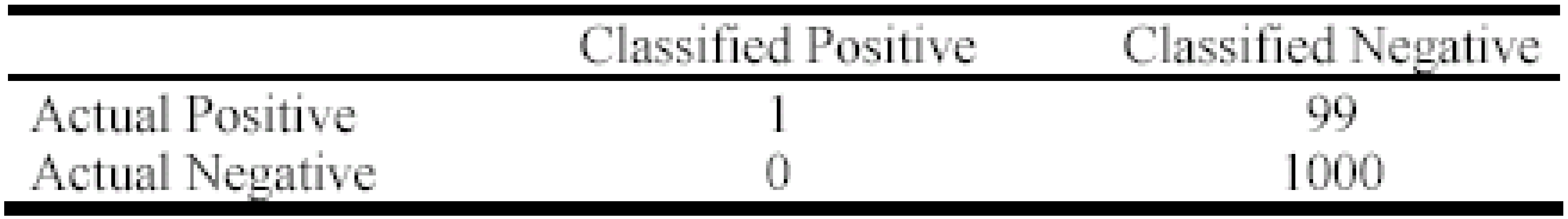
	Classified Positive	Classified Negative
Actual Positive	TP	FN
Actual Negative	FP	TN

$$p = \frac{TP}{TP + FP}. \qquad r = \frac{TP}{TP + FN}.$$

Precision *p* is the number of correctly classified positive examples divided by the total number of examples that are classified as positive.

Recall *r* is the number of correctly classified positive examples divided by the total number of actual positive examples in the test set.

An example



	Classified Positive	Classified Negative
Actual Positive	1	99
Actual Negative	0	1000

- This confusion matrix gives
  - precision p = 100% and
  - recall r = 1%

  because we only classified one positive example correctly and no negative examples wrongly.
- Note: precision and recall only measure classification on the positive class.

F_1-value (also called F_1-score)

- It is hard to compare two classifiers using two measures. F_1 score combines precision and recall into one measure

$$F_1 = \frac{2pr}{p + r}$$

F_1-score is the harmonic mean of precision and recall.

$$F_1 = \frac{2}{\frac{1}{p} + \frac{1}{r}}$$

- The harmonic mean of two numbers tends to be closer to the smaller of the two.
- For F_1-value to be large, both *p* and *r* much be large.

Summary

- Machine Learning
  - Supervised Learning
  - Unsupervised Learning
- Classification and Prediction
- Decision Tree
- Support Vector Machine (SVM)
- Evaluation (Accuracy of Classification Model)

References

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