


# Chapter 6. Classification and Prediction

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- What is classification? What is prediction? 
- Issues regarding classification and prediction
- Classification by decision tree induction
- Bayesian classification
- Rule-based classification
- Prediction
- Accuracy and error measures
- Summary

# Classification vs. Prediction

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- **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

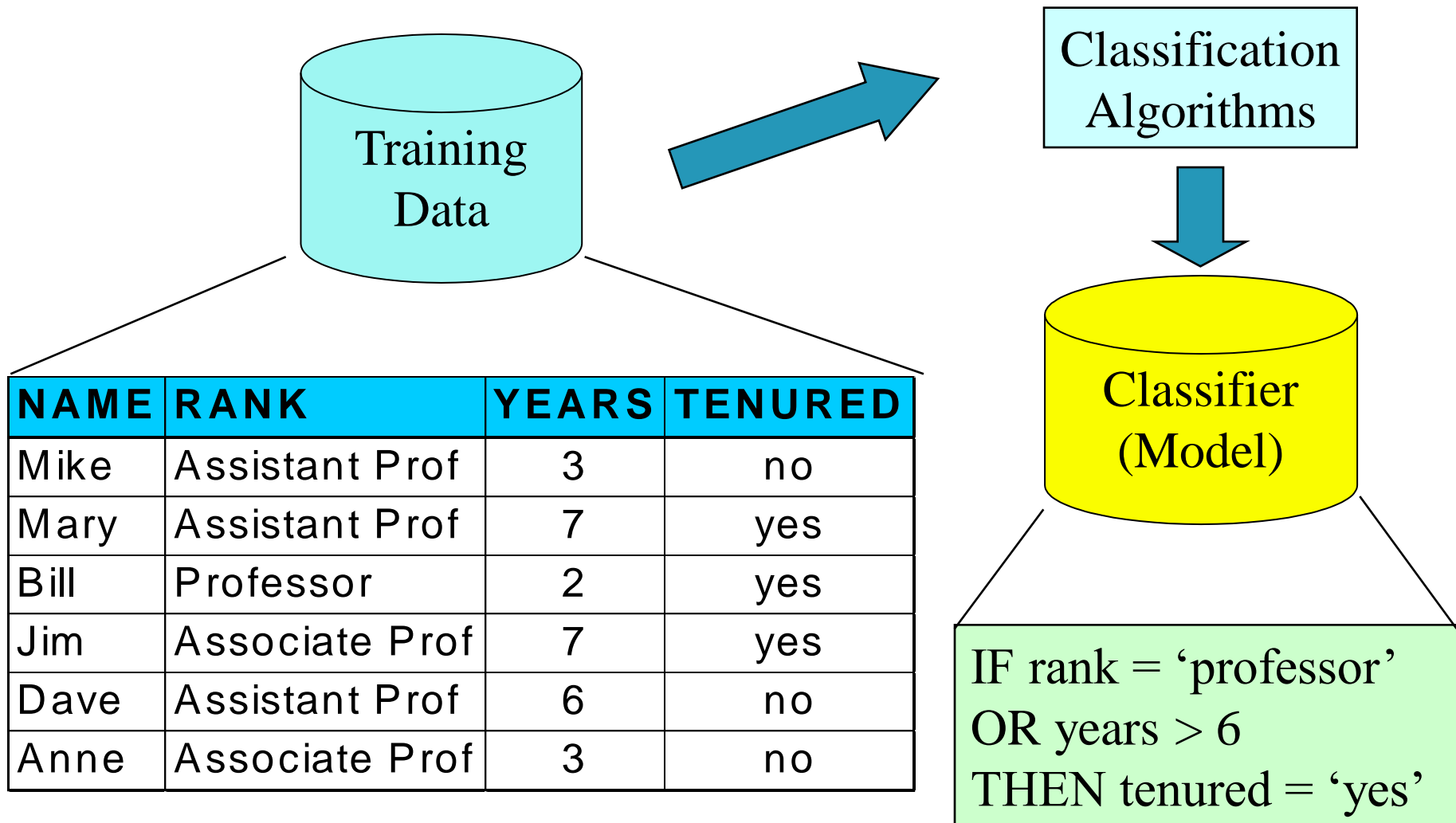
- Credit approval
- Target marketing
- Medical diagnosis
- Fraud detection

# Classification—A Two-Step Process

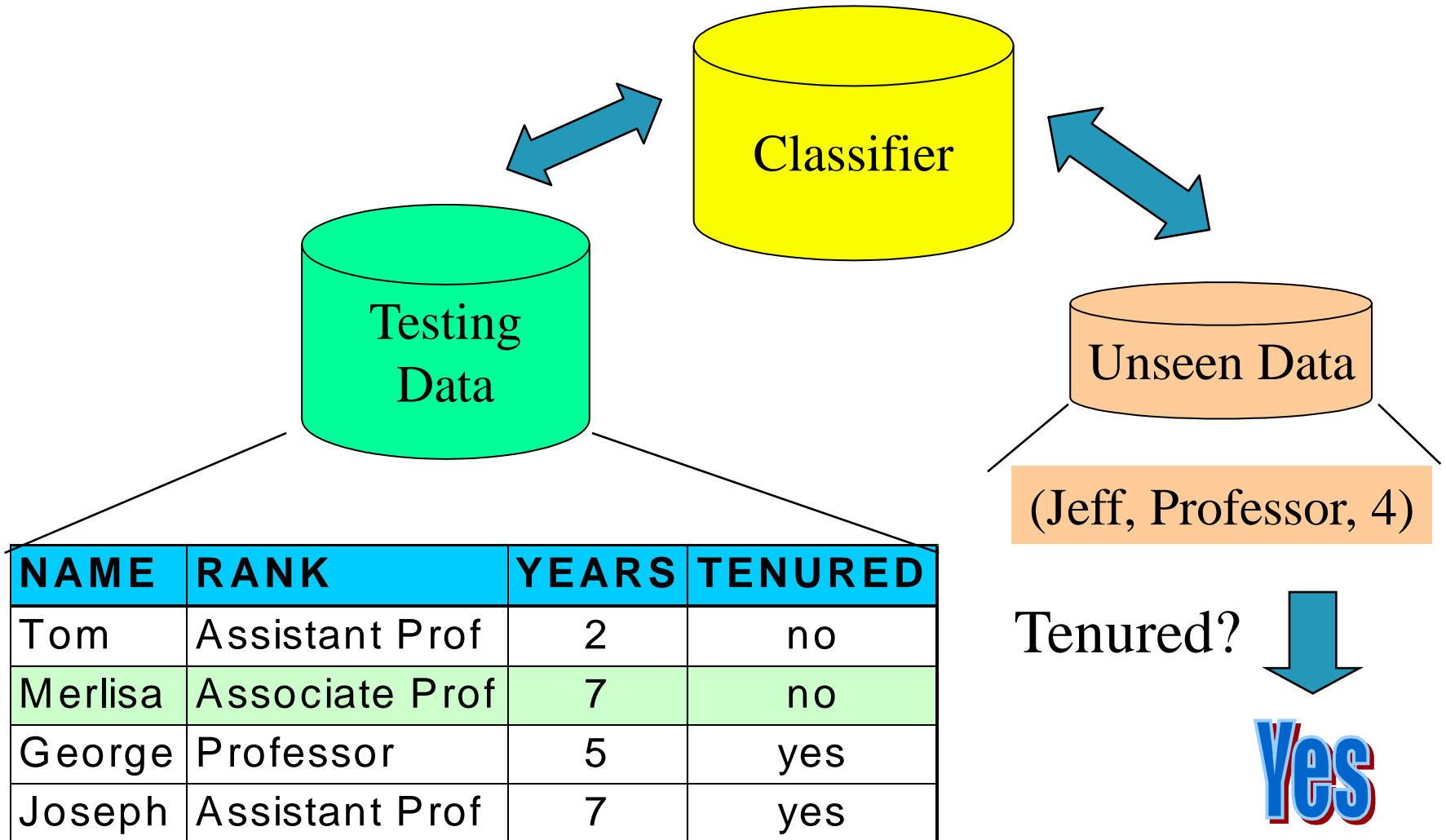
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- **Model construction**: describing a set of predetermined classes
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the **class label attribute**
  - The set of tuples used for model construction is **training set**
  - 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

# Process (1): Model Construction



# Process (2): Using the Model in Prediction



# Supervised vs. Unsupervised Learning

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- 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: Data Preparation

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- Data cleaning
  - Preprocess 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

# Issues: Evaluating Classification Methods

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- Accuracy
  - classifier accuracy: predicting class label
  - predictor accuracy: guessing value of predicted attributes
- Speed
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- Robustness: handling noise and missing values
- Scalability: efficiency in disk-resident databases
- Interpretability
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules



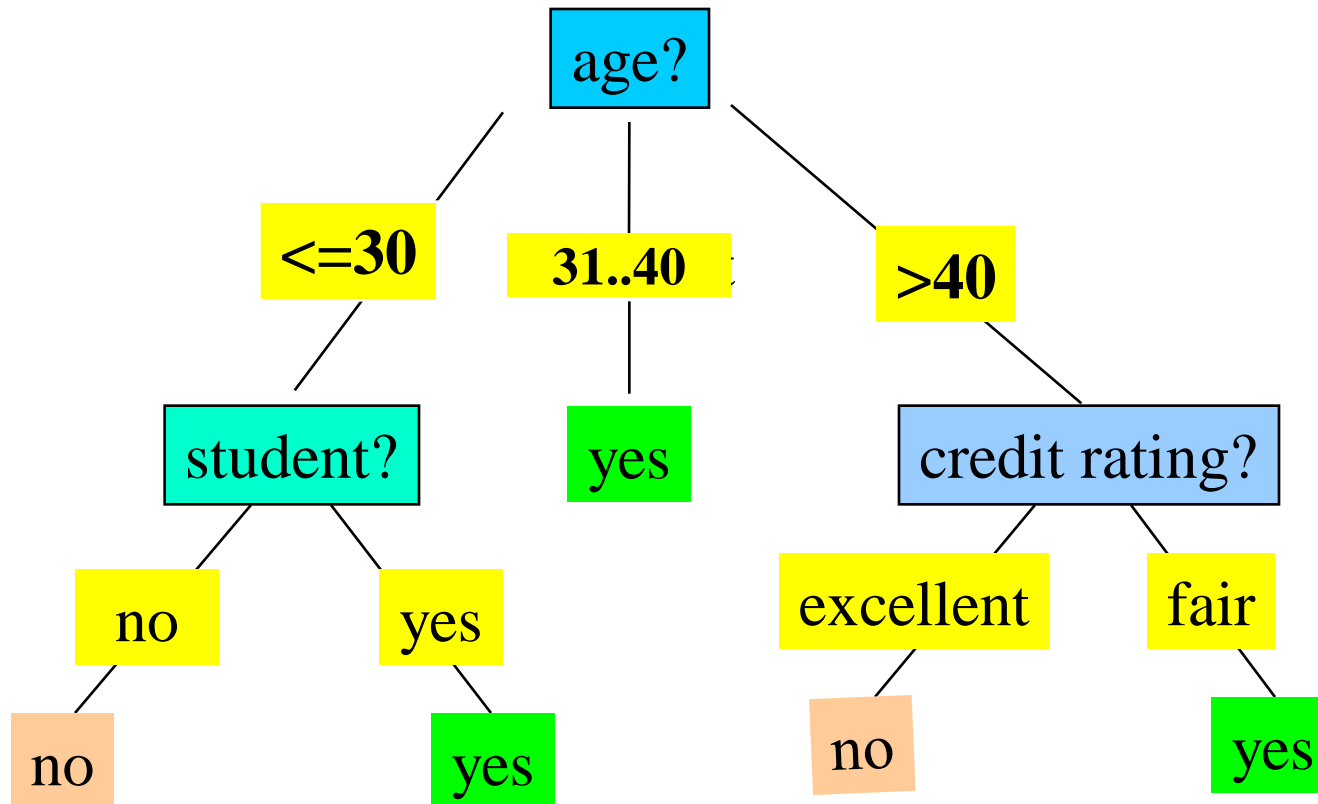
# Decision Tree Induction: Training Dataset

This follows an example of Quinlan's ID3

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

# Output: A Decision Tree for "*buys\_computer*"

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# Algorithm for Decision Tree Induction

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- 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

# Algorithm for Decision Tree Induction

- Algorithm: `Generate_decision_tree`. Generate a decision tree from the given data
- Input: The training samples , represented by discrete valued attributes, the set of candidate attributes, `attribute_list`.
- Output: A decision tree.
- Method:
  - (1) create a node `N`;
  - (2) **if** *samples* are all of the same class , `C` **then**
  - (3) return `N` as a leaf node labelled with the class `C`;

# Algorithm for Decision Tree Induction

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- (4) **if** attribute\_list is empty then
- (5)     return N as a leaf node labelled with the most common class in samples; // majority voting
- (6) select test\_attribute , the attribute among attribute\_list with the highest information gain;
- (7) label node N with the test\_attribute;
- (8) **for each** known value  $a_i$  of test attribute // partition the samples
- (9)     grow a branch from node N for the condition test\_attribute =  $a_i$
- (10)     let  $s_i$  be the set of samples in *samples* for which test attribute =  $a_i$

# Algorithm for Decision Tree Induction

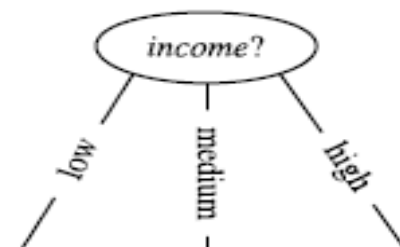
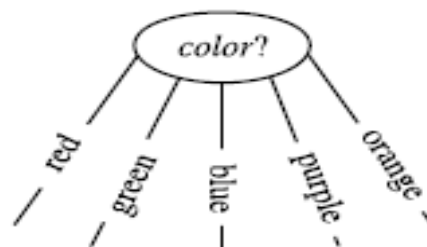
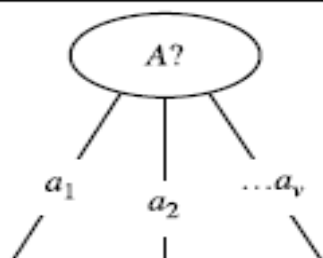
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- (11) **if**  $s_i$  is empty then
- (12)       attach a leaf labelled with the most  
            common class in samples ;
- (13) **else**   attach a node returned by  
            Generate\_decision\_tree  
            ( $s_i$ , attribute\_list, test\_attribute)

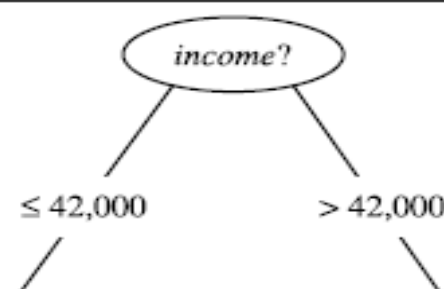
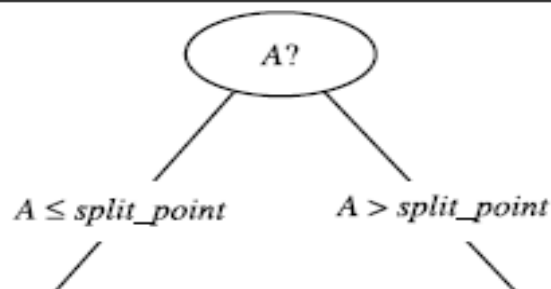
## Partitioning Scenarios

## Examples

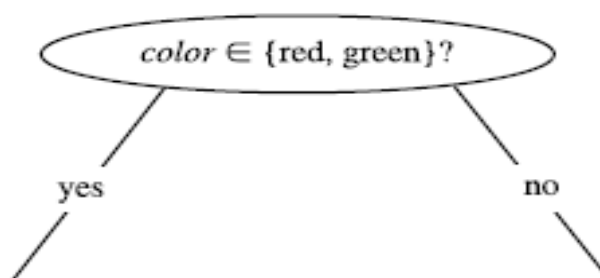
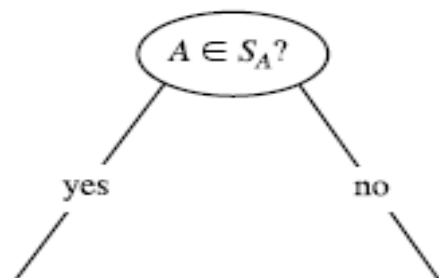
a)



b)



c)



- 4 Three possibilities for partitioning tuples based on the splitting criterion, shown with examples. Let  $A$  be the splitting attribute. (a) If  $A$  is discrete-valued, then one branch is grown for each known value of  $A$ . (b) If  $A$  is continuous-valued, then two branches are grown, corresponding to  $A \leq \text{split\_point}$  and  $A > \text{split\_point}$ . (c) If  $A$  is discrete-valued and a binary tree must be produced, then the test is of the form  $A \in S_A$ , where  $S_A$  is the splitting subset for  $A$ .

# 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  $A$

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



# Attribute Selection: Information Gain

- Class P: buys\_computer = "yes"
- Class N: buys\_computer = "no"

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

age	$p_i$	$n_i$	$I(p_i, n_i)$
$\leq 30$	2	3	0.971
31...40	4	0	0
$> 40$	3	2	0.971

age	income	student	credit_rating	buys_computer
$\leq 30$	high	no	fair	no
$\leq 30$	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
$\leq 30$	medium	no	fair	no
$\leq 30$	low	yes	fair	yes
$> 40$	medium	yes	fair	yes
$\leq 30$	medium	yes	excellent	yes
31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
$> 40$	medium	no	excellent	no

$$\begin{aligned}
 Info_{age}(D) &= \frac{5}{14} \times \left( -\frac{2}{5} \log_2 \frac{2}{5} - \frac{3}{5} \log_2 \frac{3}{5} \right) \\
 &\quad + \frac{4}{14} \times \left( -\frac{4}{4} \log_2 \frac{4}{4} - \frac{0}{4} \log_2 \frac{0}{4} \right) \\
 &\quad + \frac{5}{14} \times \left( -\frac{3}{5} \log_2 \frac{3}{5} - \frac{2}{5} \log_2 \frac{2}{5} \right) \\
 &= 0.694 \text{ bits.}
 \end{aligned}$$

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

$$Gain(income) = 0.029$$

$$Gain(student) = 0.151$$

$$Gain(credit\_rating) = 0.048$$

# 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  $D_2$   
$$gini_{income \in \{low, medium\}}(D) = \left(\frac{10}{14}\right)Gini(D_1) + \left(\frac{4}{14}\right)Gini(D_2)$$
$$= \frac{10}{14}\left(1 - \left(\frac{6}{10}\right)^2 - \left(\frac{4}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{1}{4}\right)^2 - \left(\frac{3}{4}\right)^2\right)$$
$$= 0.450$$
$$= Gini_{income \in \{high\}}(D)$$

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

# Overfitting and Tree Pruning

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- Overfitting:
  - Overfitting results in decision trees that are more complex than necessary
- An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - 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

# Post pruning

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- Trim the nodes of the decision tree in a bottom-up fashion
- If generalization error improves after trimming, replace sub-tree by a leaf node.
- Class label of leaf node is determined from majority class of instances in the sub-tree

# Classification in Large Databases

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- 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

# Scalable Decision Tree Induction Methods in Data Mining Studies

## ■ SLIQ

- builds an index for each attribute and only class list and the current attribute list reside in memory.
- Handles disk resident data sets using disk resident attribute list and memory resident class list.
- Memory restriction is there when the training set is too large.
- When a class list becomes too large performance of SLIQ decreases.

## ■ SPRINT

- constructs an attribute list data structure .
- SPRINT removes all memory restrictions.
- Designed to be easily parallelized.

# Scalable Decision Tree Induction Methods in Data Mining Studies

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- **PUBLIC**
  - integrates tree splitting and tree pruning: stop growing the tree earlier
- **RainForest**
  - separates the scalability aspects from the criteria that determine the quality of the tree
  - builds an AVC-list (attribute, value, class label)
  - Rain forest report a speed up over SPRINT.

# Bayesian Classification: Why?

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- A statistical classifier: performs *probabilistic prediction*, *i.e.*, predicts class membership probabilities
- Foundation: Based on Bayes' Theorem.
- Performance: A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct — prior knowledge can be combined with observed data
- 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

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- Let  $\mathbf{X}$  be a data sample ("*evidence*"): class label is unknown
- Let  $H$  be a *hypothesis* that  $X$  belongs to class  $C$
- Classification is to determine  $P(H|\mathbf{X})$ , the probability that the hypothesis holds given the observed data sample  $\mathbf{X}$
- $P(H)$  (*prior probability*), the initial probability
  - E.g.,  $\mathbf{X}$  will buy computer, regardless of age, income, ...
- $P(\mathbf{X})$ : probability that sample data is observed
- $P(\mathbf{X}|H)$  (*posteriori probability*), the probability of observing the sample  $\mathbf{X}$ , given that the hypothesis holds
  - E.g., Given that  $\mathbf{X}$  will buy computer, the prob. that  $X$  is 31..40, medium income

# Bayesian Theorem

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

$$P(H | \mathbf{X}) = \frac{P(\mathbf{X} | H)P(H)}{P(\mathbf{X})}$$

- Informally, this can be written as  
posteriori = likelihood x prior/evidence
- Predicts  $\mathbf{X}$  belongs to  $C_i$  iff the probability  $P(C_i|\mathbf{X})$  is the highest among all the  $P(C_k|X)$  for all the  $k$  classes
- Practical difficulty: require initial knowledge of many probabilities, significant computational cost

# Towards Naïve Bayesian Classifier

- Let  $D$  be a training set of tuples and their associated class labels, and each tuple is represented by an  $n$ -D attribute vector  $\mathbf{X} = (x_1, x_2, \dots, x_n)$
- Suppose there are  $m$  classes  $C_1, C_2, \dots, C_m$ .
- Classification is to derive the maximum posteriori, i.e., the maximal  $P(C_i|\mathbf{X})$
- This can be derived from Bayes' theorem

$$P(C_i|\mathbf{X}) = \frac{P(\mathbf{X}|C_i)P(C_i)}{P(\mathbf{X})}$$

- Since  $P(\mathbf{X})$  is constant for all classes, only

$$P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$$

needs to be maximized

# Derivation of Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes):

$$P(\mathbf{X} | C_i) = \prod_{k=1}^n P(x_k | C_i) = P(x_1 | C_i) \times P(x_2 | C_i) \times \dots \times P(x_n | C_i)$$

- This greatly reduces the computation cost: Only counts the class distribution
- If  $A_k$  is categorical,  $P(x_k | C_i)$  is the # of tuples in  $C_i$  having value  $x_k$  for  $A_k$  divided by  $|C_i, D|$  (# of tuples of  $C_i$  in  $D$ )
- If  $A_k$  is continuous-valued,  $P(x_k | C_i)$  is usually computed based on Gaussian distribution with a mean  $\mu$  and standard deviation  $\sigma$

$$g(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

and  $P(x_k | C_i)$  is

$$P(\mathbf{X} | C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i})$$

# Naïve Bayesian Classifier: 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	comp
<=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

# Naïve Bayesian Classifier: An Example

- $P(C_i)$ :  
 $P(\text{buys\_computer} = \text{"yes"}) = 9/14 = 0.643$   
 $P(\text{buys\_computer} = \text{"no"}) = 5/14 = 0.357$
- Compute  $P(X|C_i)$  for each class  
 $P(\text{age} = \text{"<=30"} \mid \text{buys\_computer} = \text{"yes"}) = 2/9 = 0.222$   
 $P(\text{age} = \text{"<= 30"} \mid \text{buys\_computer} = \text{"no"}) = 3/5 = 0.6$   
 $P(\text{income} = \text{"medium"} \mid \text{buys\_computer} = \text{"yes"}) = 4/9 = 0.444$   
 $P(\text{income} = \text{"medium"} \mid \text{buys\_computer} = \text{"no"}) = 2/5 = 0.4$   
 $P(\text{student} = \text{"yes"} \mid \text{buys\_computer} = \text{"yes"}) = 6/9 = 0.667$   
 $P(\text{student} = \text{"yes"} \mid \text{buys\_computer} = \text{"no"}) = 1/5 = 0.2$   
 $P(\text{credit\_rating} = \text{"fair"} \mid \text{buys\_computer} = \text{"yes"}) = 6/9 = 0.667$   
 $P(\text{credit\_rating} = \text{"fair"} \mid \text{buys\_computer} = \text{"no"}) = 2/5 = 0.4$
- **$X = (\text{age} \leq 30, \text{income} = \text{medium}, \text{student} = \text{yes}, \text{credit\_rating} = \text{fair})$**   
  
 $P(X|C_i) : P(X|\text{buys\_computer} = \text{"yes"}) = 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044$   
 $P(X|\text{buys\_computer} = \text{"no"}) = 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019$   
 $P(X|C_i) * P(C_i) : P(X|\text{buys\_computer} = \text{"yes"}) * P(\text{buys\_computer} = \text{"yes"}) = 0.028$   
 $P(X|\text{buys\_computer} = \text{"no"}) * P(\text{buys\_computer} = \text{"no"}) = 0.007$

**Therefore, X belongs to class ("buys\_computer = yes")**

## Example - 2

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	false	N
sunny	hot	high	true	N
overcast	hot	high	false	P
rain	mild	high	false	P
rain	cool	normal	false	P
rain	cool	normal	true	N
overcast	cool	normal	true	P
sunny	mild	high	false	N
sunny	cool	normal	false	P
rain	mild	normal	false	P
sunny	mild	normal	true	P
overcast	mild	high	true	P
overcast	hot	normal	false	P
rain	mild	high	true	N

An unseen sample

$X = \langle \text{rain, hot, high, false} \rangle$

# Play-tennis example: estimating

$$P(x_i | C)$$

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	false	N
sunny	hot	high	true	N
overcast	hot	high	false	P
rain	mild	high	false	P
rain	cool	normal	false	P
rain	cool	normal	true	N
overcast	cool	normal	true	P
sunny	mild	high	false	N
sunny	cool	normal	false	P
rain	mild	normal	false	P
sunny	mild	normal	true	P
overcast	mild	high	true	P
overcast	hot	normal	false	P
rain	mild	high	true	N

$$P(p) = 9/14$$

$$P(n) = 5/14$$

## outlook

$$P(\text{sunny} | p) = 2/9$$

$$P(\text{sunny} | n) = 3/5$$

$$P(\text{overcast} | p) = 4/9$$

$$P(\text{overcast} | n) = 0$$

$$P(\text{rain} | p) = 3/9$$

$$P(\text{rain} | n) = 2/5$$

## temperature

$$P(\text{hot} | p) = 2/9$$

$$P(\text{hot} | n) = 2/5$$

$$P(\text{mild} | p) = 4/9$$

$$P(\text{mild} | n) = 2/5$$

$$P(\text{cool} | p) = 3/9$$

$$P(\text{cool} | n) = 1/5$$

## humidity

$$P(\text{high} | p) = 3/9$$

$$P(\text{high} | n) = 4/5$$

$$P(\text{normal} | p) = 6/9$$

$$P(\text{normal} | n) = 2/5$$

## windy

$$P(\text{true} | p) = 3/9$$

$$P(\text{true} | n) = 3/5$$



# Play-tennis example: classifying X

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- An unseen sample  $X = \langle \text{rain}, \text{hot}, \text{high}, \text{false} \rangle$
- $P(X|p) \cdot P(p) =$   
 $P(\text{rain}|p) \cdot P(\text{hot}|p) \cdot P(\text{high}|p) \cdot P(\text{false}|p) \cdot P(p) =$   
 $3/9 \cdot 2/9 \cdot 3/9 \cdot 6/9 \cdot 9/14 = 0.010582$
- $P(X|n) \cdot P(n) =$   
 $P(\text{rain}|n) \cdot P(\text{hot}|n) \cdot P(\text{high}|n) \cdot P(\text{false}|n) \cdot P(n) =$   
 $2/5 \cdot 2/5 \cdot 4/5 \cdot 2/5 \cdot 5/14 = 0.018286$
- Sample **X** is classified in class **n** (don't play)

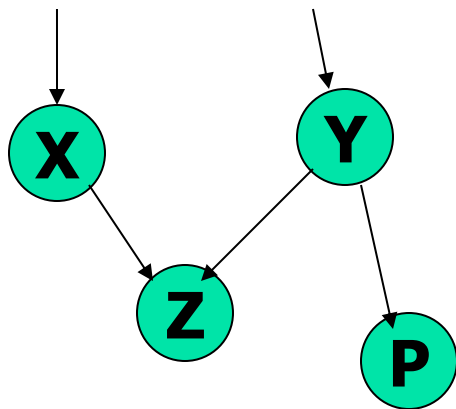
# Naïve Bayesian Classifier: Comments

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- 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
- How to deal with these dependencies?
  - Bayesian Belief Networks

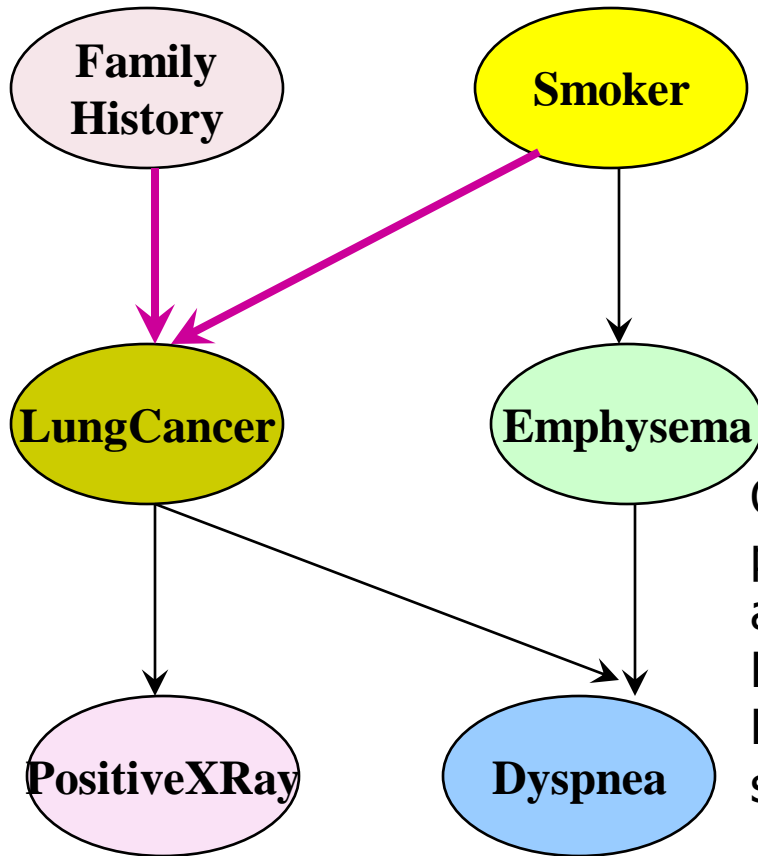
# Bayesian Belief Networks

- Bayesian belief network allows a *subset* of the variables conditionally independent
- A graphical model of casual relationships
  - Represents dependency among the variables
  - Gives a specification of joint probability distribution



- ☐ Nodes: random variables
- ☐ Links: dependency
- ☐ X and Y are the parents of Z, and Y is the parent of P
- ☐ No dependency between Z and P
- ☐ Has no loops or cycles

# Bayesian Belief Network: An Example



The **conditional probability table (CPT)** for variable LungCancer:

	(FH, S)	(FH, ~S)	(~FH, S)	(~FH, ~S)
LC	0.8	0.5	0.7	0.1
~LC	0.2	0.5	0.3	0.9

CPT shows the conditional probability for each possible combination of its parents. The CPT for a variable Z specifies the conditional distribution  $P(Z/\text{Parents}(Z))$ .


$P(\text{Lungcancer}=\text{"yes"} \mid \text{FamilyHistory} = \text{"yes"} , \text{smoker}=\text{"yes"})=0.8$

**Bayesian Belief Networks** Derivation of the probability of a particular combination of values of  $\mathbf{X}$ , from CPT:

$$P(x_1, \dots, x_n) = \prod_{i=1}^n P(x_i \mid \text{Parents}(X_i))$$

# Chapter 6. Classification and Prediction

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- What is classification? What is prediction?
- Issues regarding classification and prediction
- Classification by decision tree induction
- Bayesian classification
- Rule-based classification
- Prediction 
- Accuracy and error measures
- Summary

# What Is Prediction?

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- (Numerical) prediction is similar to classification
  - construct a model
  - use model to predict continuous or ordered value for a given input
- Prediction is different from classification
  - Classification refers to predict categorical class label
  - Prediction models continuous-valued functions
- Major method for prediction: regression
  - model the relationship between one or more *independent* or **predictor** variables and a *dependent* or **response** variable
- Regression analysis
  - Linear and multiple regression
  - Non-linear regression
  - Other regression methods: generalized linear model, Poisson regression, log-linear models, regression trees

# Linear Regression

- Linear regression: involves a response variable  $y$  and a single predictor variable  $x$

$$y = w_0 + w_1 x$$

where  $w_0$  (y-intercept) and  $w_1$  (slope) are regression coefficients

- Method of least squares: estimates the best-fitting straight line

$$w_1 = \frac{\sum_{i=1}^{|D|} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{|D|} (x_i - \bar{x})^2} \quad w_0 = \bar{y} - w_1 \bar{x}$$

- Multiple linear regression: involves more than one predictor variable
  - Training data is of the form  $(\mathbf{X}_1, y_1), (\mathbf{X}_2, y_2), \dots, (\mathbf{X}_{|D|}, y_{|D|})$
  - Ex. For 2-D data, we may have:  $y = w_0 + w_1 x_1 + w_2 x_2$
  - Solvable by extension of least square method
  - Many nonlinear functions can be transformed into the above

# Regression - Example

- Table shows a set of paired data where X is the number of years of work experience of a college graduate and y is the corresponding salary of the graduate.
- $Y = 23.6 + 3.5X$
- Predict the salary for a graduate with 10 yrs of experience.
- $Y = 58.6\$$

<b>X</b> <b>Years</b> <b>Experience</b>	<b>Y</b> <b>Salary (in \$</b> <b>1000s)</b>
3	30
8	57
9	64
13	72
3	36
6	43
11	59
21	90
1	20
16	83



# Nonlinear Regression

- Some nonlinear models can be modeled by a polynomial function
- A polynomial regression model can be transformed into linear regression model. For example,

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

convertible to linear with new variables:  $x_2 = x^2$ ,  $x_3 = x^3$

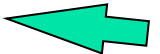
$$y = w_0 + w_1 x + w_2 x_2 + w_3 x_3$$

- Other functions, such as power function, can also be transformed to linear model
- Some models are intractable nonlinear (e.g., sum of exponential terms)
  - possible to obtain least square estimates through extensive calculation on more complex formulae

# Chapter 6. Classification and Prediction

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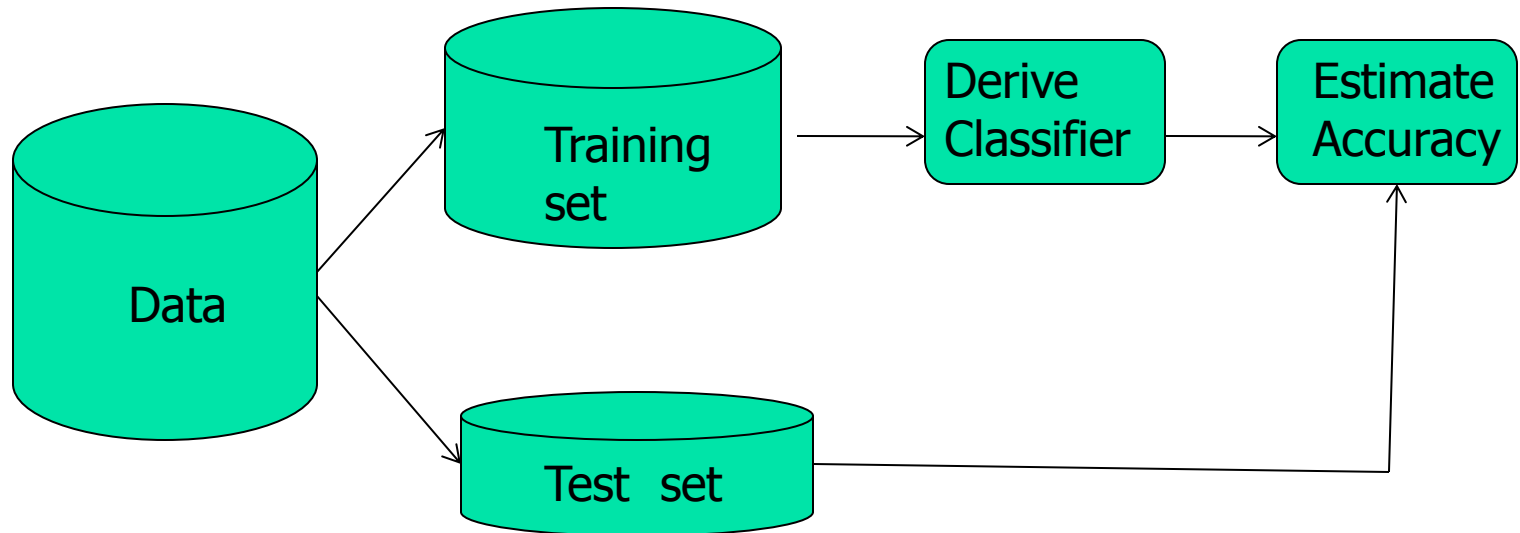
- What is classification? What is prediction?
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# Evaluating the Accuracy of a Classifier or Predictor (I)

- Holdout method

- Given data is randomly partitioned into two independent sets
  - Training set (e.g., 2/3) for model construction
  - Test set (e.g., 1/3) for accuracy estimation



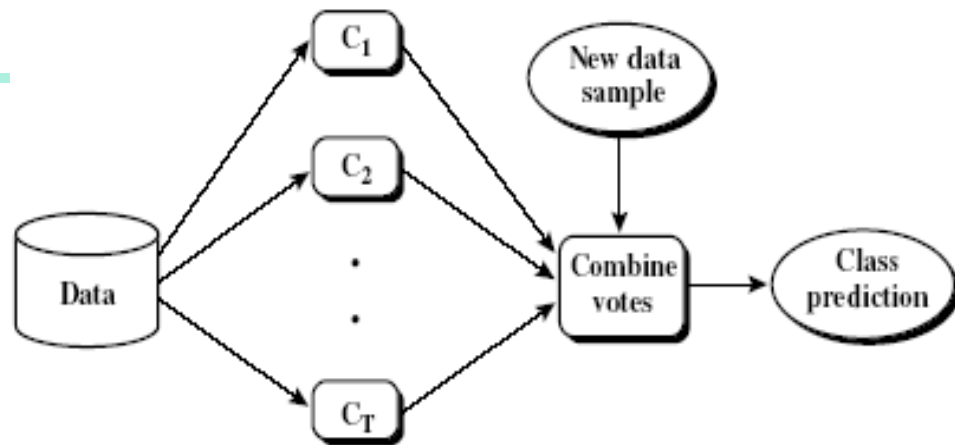
- Random sampling: a variation of holdout
  - Repeat holdout  $k$  times, accuracy = avg. of the accuracies obtained

# Evaluating the Accuracy of a Classifier or Predictor (I)

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- Cross-validation ( $k$ -fold, where  $k = 10$  is most popular)
  - Randomly partition the data into  $k$  *mutually exclusive* subsets, each approximately equal size
  - At  $i$ -th iteration, use  $D_i$  as test set and others as training set
  - The accuracy estimate =
$$\frac{\text{Overall number of correct classifications from the } k \text{ iterations}}{\text{Total number of samples in the initial data}}$$
- Leave-one-out:  $k$  folds where  $k = \#$  of tuples, for small sized data
- Stratified cross-validation: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data.

# Ensemble Methods: Increasing the Accuracy



- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of  $k$  learned models,  $M_1, M_2, \dots, M_k$ , with the aim of creating an improved model  $M^*$
- Popular ensemble methods
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers
  - Ensemble: combining a set of heterogeneous classifiers

# Bagging: Bootstrap Aggregation

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- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set  $D$  of  $d$  tuples, at each iteration  $i$ , a training set  $D_i$  of  $d$  tuples is sampled with replacement from  $D$  (i.e., bootstrap)
  - A classifier model  $M_i$  is learned for each training set  $D_i$
- Classification: classify an unknown sample  $\mathbf{X}$ 
  - Each classifier  $M_i$  returns its class prediction
  - The bagged classifier  $M^*$  counts the votes and assigns the class with the most votes to  $\mathbf{X}$
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy
  - Often significant better than a single classifier derived from  $D$
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction

# Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - Weights are assigned to each training tuple
  - A series of  $k$  classifiers is iteratively learned
  - After a classifier  $M_i$  is learned, the weights are updated to allow the subsequent classifier,  $M_{i+1}$ , to pay more attention to the training tuples that were misclassified by  $M_i$
  - The final  $M^*$  combines the votes of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- The boosting algorithm can be extended for the prediction of continuous values
- Comparing with bagging: boosting tends to achieve greater accuracy, but it also risks overfitting the model to misclassified data

# Classifier Accuracy Measures and Confusion matrix

- t\_pos (Eg "cancer samples" that were correctly classified as such)
- t\_neg ("not\_cancer" samples that were correctly classified as such)
- False positives ("not\_cancer" samples that were incorrectly labeled as "cancer")
- False negative("cancer" samples that were incorrectly labeled as "not\_cancer")
- pos is the number of positive samples
- neg is the number of negative samples

	$C_1$	$C_2$
$C_1$	t_pos	f_neg
$C_2$	f_pos	t_neg



# Classifier Accuracy Measures

classes	buy_computer = yes	buy_computer = no	total	recognition(%)
buy_computer = yes	6954	46	7000	99.34
buy_computer = no	412	2588	3000	86.27
total	7366	2634	10000	95.52

- Accuracy of a classifier  $M$ ,  $\text{acc}(M)$ : percentage of test set tuples that are correctly classified by the model  $M$ 
  - Error rate (misclassification rate) of  $M = 1 - \text{acc}(M)$
  - Given  $m$  classes,  $CM_{i,j}$  an entry in a **confusion matrix**, indicates # of tuples in class  $i$  that are labeled by the classifier as class  $j$
- Alternative accuracy measures (e.g., for cancer diagnosis)
  - sensitivity =  $\text{t-pos}/\text{pos}$  /\* true positive recognition rate \*/
  - specificity =  $\text{t-neg}/\text{neg}$  /\* true negative recognition rate \*/
  - precision =  $\text{t-pos}/(\text{t-pos} + \text{f-pos})$
  - accuracy =  $\text{sensitivity} * \text{pos}/(\text{pos} + \text{neg}) + \text{specificity} * \text{neg}/(\text{pos} + \text{neg})$
  - This model can also be used for cost-benefit analysis

# Predictor Error Measures

- Measure predictor accuracy: measure how far off the predicted value is from the actual known value
- **Loss function:** measures the error betw.  $y_i$  and the predicted value  $y_i'$ 
  - Absolute error:  $|y_i - y_i'|$
  - Squared error:  $(y_i - y_i')^2$
- Test error (generalization error): the average loss over the test set
  - Mean absolute error:  $\frac{\sum_{i=1}^d |y_i - y_i'|}{d}$       Mean squared error:  $\frac{\sum_{i=1}^d (y_i - y_i')^2}{d}$
  - Relative absolute error:  $\frac{\sum_{i=1}^d |y_i - y_i'|}{\sum_{i=1}^d |y_i - \bar{y}|}$       Relative squared error:  $\frac{\sum_{i=1}^d (y_i - y_i')^2}{\sum_{i=1}^d (y_i - \bar{y})^2}$

The mean squared-error exaggerates the presence of outliers

Popularly use (square) root mean-square error, similarly, root relative squared error

