Data Mining:

Classification: Basic Concepts



- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Rule-Based Classification
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy:
 Ensemble Methods
- Summary

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

Prediction Problems: Classification vs. Numeric 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

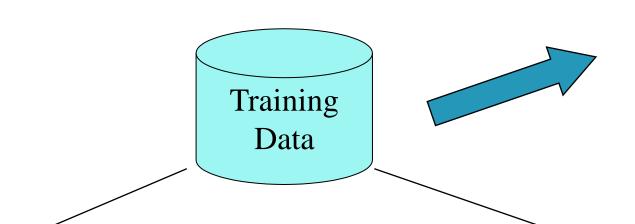
Numeric Prediction

- models continuous-valued functions, i.e., predicts unknown or missing values
- Typical applications
 - Credit/loan approval:
 - Medical diagnosis: if a tumor is cancerous or benign
 - Fraud detection: if a transaction is fraudulent
 - Web page categorization: which category it is

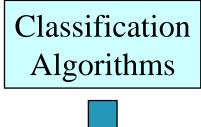
Classification—A Two-Step Process

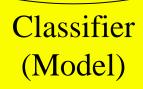
- Model construction: describing a set of predetermined classes
 - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
 - The set of tuples used for model construction is training set
 - The model is represented as classification rules, decision trees, 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 overfitting)
 - If the accuracy is acceptable, use the model to classify new data
- Note: If the test set is used to select models, it is called validation (test) set

Process (1): Model Construction



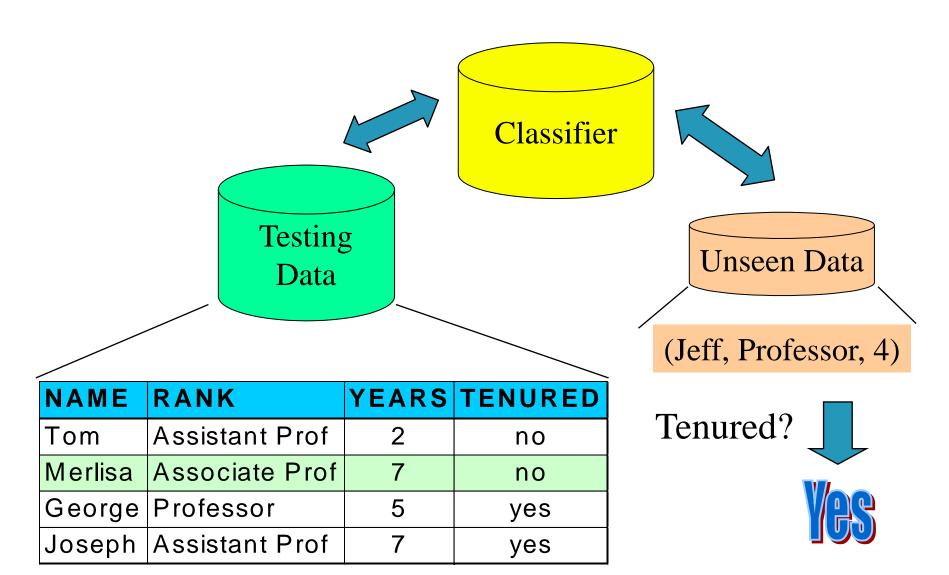
NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no





IF rank = 'professor'
OR years > 6
THEN tenured = 'yes'

Process (2): Using the Model in Prediction



Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction

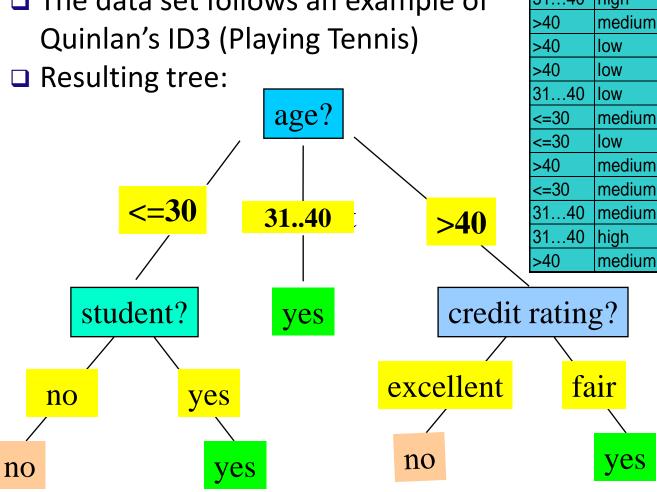


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Decision Tree Induction: An Example

- ☐ Training data set: Buys computer
- ☐ The data set follows an example of





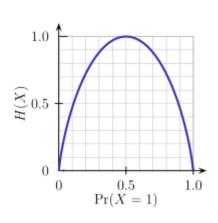
age	income	student	credit_rating	buys_compute
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
 - Tree is constructed in a top-down recursive divide-andconquer 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

Brief Review of Entropy

- Entropy (Information Theory)
 - A measure of uncertainty associated with a random variable
 - Calculation: For a discrete random variable Y taking m distinct values $\{y_1, \dots, y_m\}$,
 - $H(Y) = -\sum_{i=1}^{m} p_i \log(p_i)$, where $p_i = P(Y = y_i)$
 - Interpretation:
 - Higher entropy => higher uncertainty
 - Lower entropy => lower uncertainty
- Conditional Entropy
 - $H(Y|X) = \sum_{x} p(x)H(Y|X = x)$



m = 2

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:

$$Info(D) = -\sum_{i=0}^{m} p_i \log_2(p_i)$$

■ Information needed (after using A to split $D^{i=1}$ into v partitions) to classify D: $v \in D$.

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

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"

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940 + \frac{5}{14}I(3,2) = 0.694$$

age	p _i	n _i	I(p _i , n _i)
<=30	2	3	0.971
3140	4	0	0
>40	3	2	0.971

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

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

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

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

Similarly,

$$Gain(income) = 0.029$$

 $Gain(student) = 0.151$
 $Gain(credit_rating) = 0.048$

Computing Information-Gain for Continuous-Valued Attributes

- Let attribute A be a continuous-valued attribute
- Must determine the best split point for A
 - Sort the value A in increasing order
 - Typically, the midpoint between each pair of adjacent values is considered as a possible split point
 - $(a_i+a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
 - The point with the minimum expected information requirement for A is selected as the split-point for A
- Split:
 - D1 is the set of tuples in D satisfying A ≤ split-point, and D2 is the set of tuples in D satisfying A > split-point

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)

$$SplitInfo_{A}(D) = -\sum_{j=1}^{\nu} \frac{|D_{j}|}{|D|} \times \log_{2}(\frac{|D_{j}|}{|D|})$$

- GainRatio(A) = Gain(A)/SplitInfo(A)
- Ex. $SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2(\frac{4}{14}) \frac{6}{14} \times \log_2(\frac{6}{14}) \frac{4}{14} \times \log_2(\frac{4}{14}) = 1.557$
 - gain_ratio(income) = 0.029/1.557 = 0.019
- 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_i 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)

Computation of Gini Index

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 D₁: {low, medium} and 4 in D₂ $gini_{income \in \{low, medium\}}(D) = \left(\frac{10}{14}\right)Gini(D_1) + \left(\frac{4}{14}\right)Gini(D_2)$

$$= \frac{10}{14} \left(1 - \left(\frac{7}{10} \right)^2 - \left(\frac{3}{10} \right)^2 \right) + \frac{4}{14} \left(1 - \left(\frac{2}{4} \right)^2 - \left(\frac{2}{4} \right)^2 \right)$$

$$= 0.443$$

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

Gini_{low,high} is 0.458; Gini_{medium,high} is 0.450. Thus, split on the {low,medium} (and {high}) since it has the lowest Gini index

- 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

Other Attribute Selection Measures

- CHAID: a popular decision tree algorithm, measure based on χ^2 test for independence
- C-SEP: performs better than info. gain and gini index in certain cases
- G-statistic: has a close approximation to χ^2 distribution
- MDL (Minimal Description Length) principle (i.e., the simplest solution is preferred):
 - The best tree as the one that requires the fewest # of bits to both (1) encode the tree, and (2) encode the exceptions to the tree
- Multivariate splits (partition based on multiple variable combinations)
 - <u>CART</u>: finds multivariate splits based on a linear comb. of attrs.
- Which attribute selection measure is the best?
 - Most give good results, none is significantly superior than others

Overfitting and Tree Pruning

- Overfitting: 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
 - <u>Postpruning</u>: 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"

Enhancements to Basic Decision Tree Induction

Allow for continuous-valued attributes

 Dynamically define new discrete-valued attributes that partition the continuous attribute value into a discrete set of intervals

Handle missing attribute values

- Assign the most common value of the attribute
- Assign probability to each of the possible values

Attribute construction

- Create new attributes based on existing ones that are sparsely represented
- This reduces fragmentation, repetition, and replication

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 is decision tree induction popular?
 - 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
- RainForest (VLDB'98 Gehrke, Ramakrishnan & Ganti)
 - Builds an AVC-list (attribute, value, class label)

Scalability Framework for RainForest

- Separates the scalability aspects from the criteria that determine the quality of the tree
- Builds an AVC-list: AVC (Attribute, Value, Class_label)
- AVC-set (of an attribute X)
 - Projection of training dataset onto the attribute X and class label where counts of individual class label are aggregated
- AVC-group (of a node n)
 - Set of AVC-sets of all predictor attributes at the node n

Rainforest: Training Set and Its AVC Sets

Training Examples

age	income	student	redit_rating	_com
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no
			·	

AVC-set on Age

Age	Buy_Computer		
	yes	no	
<=30	2	3	
3140	4	0	
>40	3	2	

AVC-set on income

income	Buy_Computer		
	yes	no	
high	2	2	
medium	4	2	
low	3	1	

AVC-set on *Student*

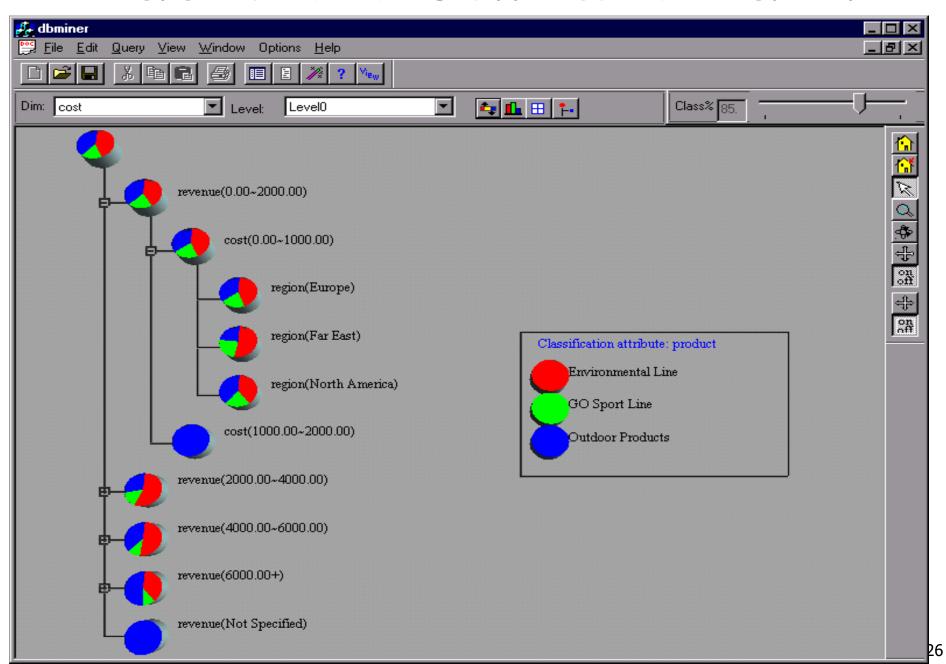
AVC-set on credit_rating

student	Buy_Computer		0 111	Buy_Compute	
	yes	no	Credit rating	yes	no
yes	6	1	fair	6	2
no	3	4	excellent	3	3

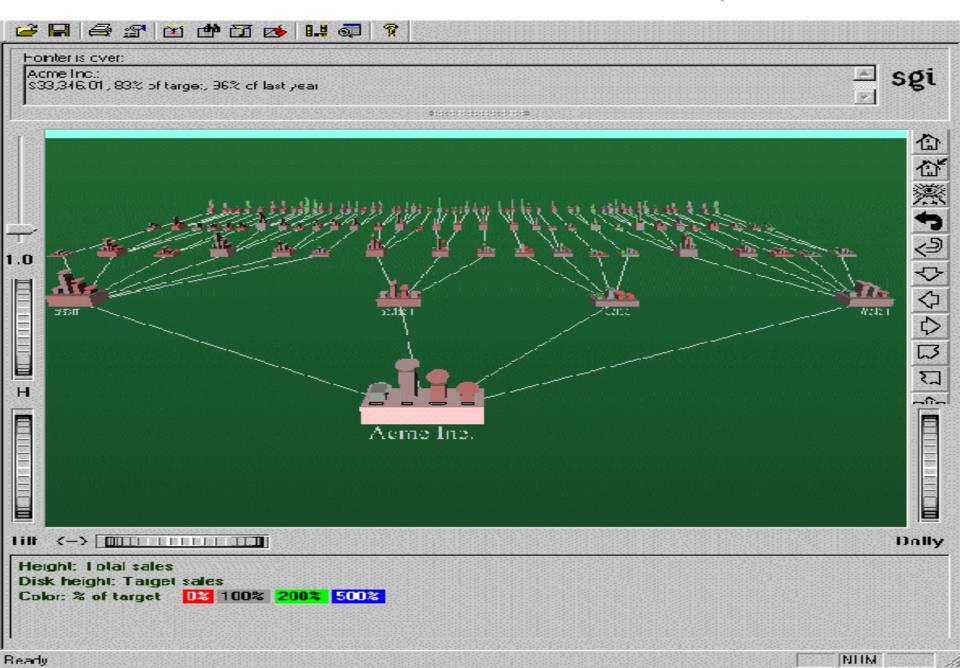
BOAT (Bootstrapped Optimistic Algorithm for Tree Construction)

- Use a statistical technique called bootstrapping to create several smaller samples (subsets), each fits in memory
- Each subset is used to create a tree, resulting in several trees
- These trees are examined and used to construct a new tree T'
 - It turns out that T' is very close to the tree that would be generated using the whole data set together
- Adv: requires only two scans of DB, an incremental alg.

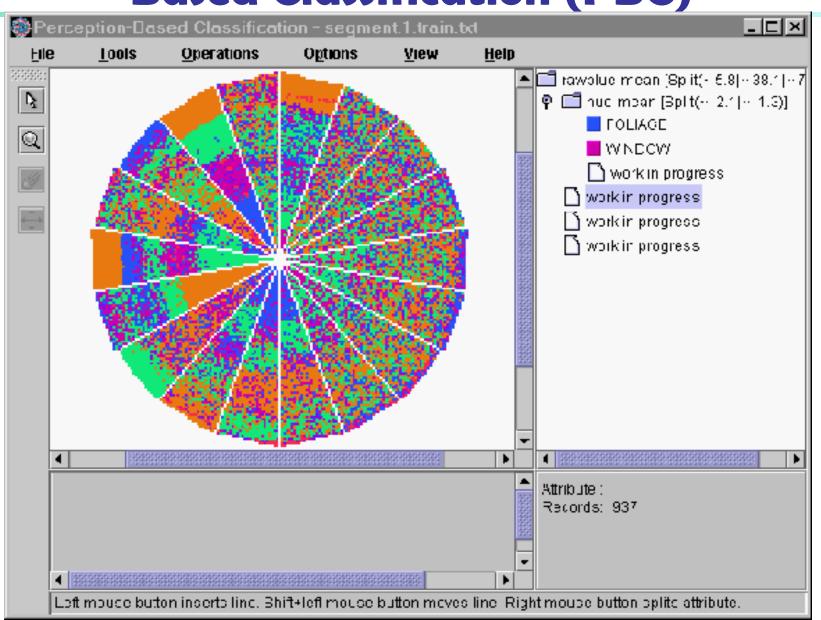
Presentation of Classification Results



Visualization of a Decision Tree in SGI/MineSet 3.0



Interactive Visual Mining by Perception-Based Classification (PBC)



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- Bayes Classification Methods



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Bayesian Classification: Why?

- A statistical classifier: performs probabilistic prediction, i.e., predicts class membership probabilities
- Foundation: Based on Bayes' Theorem.
- <u>Performance:</u> 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

Bayes' Theorem: Basics

- Total probability Theorem: $P(B) = \sum_{i=1}^{M} P(B|A_i)P(A_i)$
- Bayes' Theorem: $P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H)/P(\mathbf{X})$
 - Let 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|X), (i.e., posteriori probability): the probability that the hypothesis holds given the observed data sample X
 - P(H) (prior probability): the initial probability
 - E.g., X will buy computer, regardless of age, income, ...
 - P(X): probability that sample data is observed
 - P(X|H) (likelihood): the probability of observing the sample X, given that the hypothesis holds
 - E.g., Given that X will buy computer, the prob. that X is 31..40, medium income

Prediction Based on Bayes' Theorem

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

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

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

Classification Is to Derive the Maximum Posteriori

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n-D attribute vector
 X = (x₁, x₂, ..., x_n)
- Suppose there are m classes C₁, C₂, ..., C_m.
- Classification is to derive the maximum posteriori, i.e., the maximal P(C_i | 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(X) is constant for all classes, only

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

needs to be maximized

Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes): $P(\mathbf{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i) = P(x_1|C_i) \times P(x_2|C_i) \times ... \times P(x_n|C_i)$
- 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 continous-valued, $P(x_k|C_i)$ is usually computed based on Gaussian distribution with a mean μ and standard deviation σ

and
$$P(\mathbf{x}_k | \mathbf{C}_i)$$
 is
$$g(\mathbf{x}, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2}}$$
$$P(\mathbf{X} | \mathbf{C}_i) = g(\mathbf{x}_k, \mu_{C_i}, \sigma_{C_i})$$

Naïve Bayes Classifier: Training Dataset

Class:

C1:buys_computer = 'yes'

C2:buys_computer = 'no'

Data to be classified:

X = (age <= 30,

Income = medium,

Student = yes

Credit_rating = Fair)

	_	_		
age	income	<u>student</u>	credit_rating	_com
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
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<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayes Classifier: An Example

- P(C_i): P(buys_computer = "yes") = 9/14 = 0.643P(buys_computer = "no") = 5/14 = 0.357
- Compute P(X|C_i) for each class

$$P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6$$

P(student = "yes" | buys_computer = "no") =
$$1/5 = 0.2$$

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

$$P(X|C_i)$$
: $P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = 0.044$

$$P(X|buys_computer = "no") = 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019$$

$$P(X|C_i)*P(C_i): P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028$$

Therefore, X belongs to class ("buys_computer = yes")

excellent

excellent

excellent

excellent

excellent

excellent

yes

yes

yes

no

yes

yes yes

high

high

medium

Avoiding the Zero-Probability Problem

 Naïve Bayesian prediction requires each conditional prob. be non-zero. Otherwise, the predicted prob. will be zero

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

- Ex. Suppose a dataset with 1000 tuples, income=low (0), income= medium (990), and income = high (10)
- Use Laplacian correction (or Laplacian estimator)
 - Adding 1 to each case

Prob(income =
$$low$$
) = $1/1003$

Prob(income = high) =
$$11/1003$$

 The "corrected" prob. estimates are close to their "uncorrected" counterparts

Naïve Bayes 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 Bayes Classifier
- How to deal with these dependencies? Bayesian Belief Networks (Chapter 9)

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Using IF-THEN Rules for Classification

- Represent the knowledge in the form of IF-THEN rules
 - R: IF age = youth AND student = yes THEN buys_computer = yes
 - Rule antecedent/precondition vs. rule consequent
- Assessment of a rule: coverage and accuracy
 - n_{covers} = # of tuples covered by R
 - $n_{correct}$ = # of tuples correctly classified by R coverage(R) = $n_{covers}/|D|$ /* D: training data set */ accuracy(R) = $n_{correct}/n_{covers}$
- If more than one rule are triggered, need conflict resolution
 - Size ordering: assign the highest priority to the triggering rules that has the "toughest" requirement (i.e., with the most attribute tests)
 - Class-based ordering: decreasing order of prevalence or misclassification cost per class
 - Rule-based ordering (decision list): rules are organized into one long priority list, according to some measure of rule quality or by experts

Rule Extraction from a Decision Tree

- Rules are easier to understand than large trees
- 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 holds the class prediction
- Rules are mutually exclusive and exhaustive
- Example: Rule extraction from our buys_computer decision-tree

age?

31..40

yes

>40

excellent

no

credit rating?

fair

ves

<=30

yes

yes

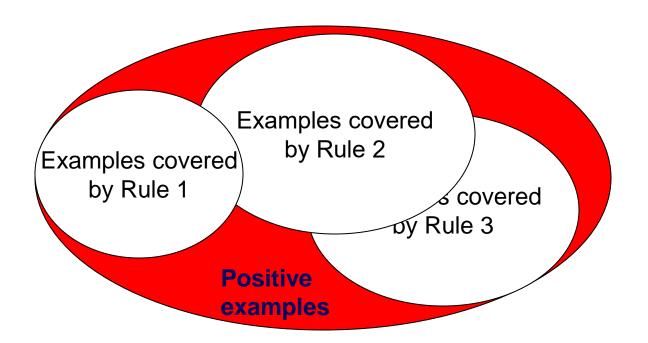
student?

Rule Induction: Sequential Covering Method

- Sequential covering algorithm: Extracts rules directly from training data
- Typical sequential covering algorithms: FOIL, AQ, CN2, RIPPER
- Rules are learned sequentially, each for a given class C_i will cover many tuples of C_i but none (or few) of the tuples of other classes
- Steps:
 - Rules are learned one at a time
 - Each time a rule is learned, the tuples covered by the rules are removed
 - Repeat the process on the remaining tuples until termination condition, e.g., when no more training examples or when the quality of a rule returned is below a user-specified threshold
- Comp. w. decision-tree induction: learning a set of rules simultaneously

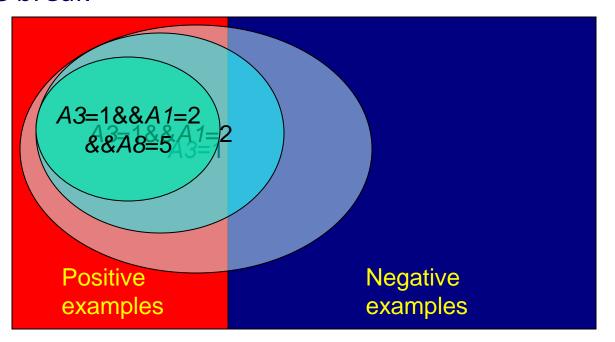
Sequential Covering Algorithm

while (enough target tuples left)
generate a rule
remove positive target tuples satisfying this rule



Rule Generation

To generate a rule
 while(true)
 find the best predicate p
 if foil-gain(p) > threshold then add p to current rule
 else break



How to Learn-One-Rule?

- Start with the most general rule possible: condition = empty
- Adding new attributes by adopting a greedy depth-first strategy
 - Picks the one that most improves the rule quality
- Rule-Quality measures: consider both coverage and accuracy
 - Foil-gain (in FOIL & RIPPER): assesses info_gain by extending condition
 pos'
 pos

$$FOIL_Gain = pos' \times (\log_2 \frac{pos'}{pos' + neg'} - \log_2 \frac{pos}{pos + neg})$$

- favors rules that have high accuracy and cover many positive tuples
- Rule pruning based on an independent set of test tuples

$$FOIL_Prune(R) = \frac{pos - neg}{pos + neg}$$

Pos/neg are # of positive/negative tuples covered by R. If *FOIL_Prune* is higher for the pruned version of R, prune R

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- Techniques to Improve Classification Accuracy:
 Ensemble Methods
- Summary

Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use validation test set of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
 - Holdout method, random subsampling
 - Cross-validation
 - Bootstrap
- Comparing classifiers:
 - Confidence intervals
 - Cost-benefit analysis and ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	¬ C ₁		
C_1	True Positives (TP)	False Negatives (FN)		
¬ C ₁	False Positives (FP)	True Negatives (TN)		

Example of Confusion Matrix:

Actual class\Predicted	buy_computer	buy_computer	Total
class	= yes	= no	
buy_computer = yes	6954	46	7000
buy_computer = no	412	2588	3000
Total	7366	2634	10000

- Given m classes, an entry, $CM_{i,j}$ in a confusion matrix indicates # of tuples in class i that were labeled by the classifier as class j
- May have extra rows/columns to provide totals

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	С	¬C	
С	TP	FN	Р
¬C	FP	TN	N
	Ρ'	N'	All

 Classifier Accuracy, or recognition rate: percentage of test set tuples that are correctly classified

Accuracy = (TP + TN)/AII

Error rate: 1 – accuracy, or Error rate = (FP + FN)/All

Class Imbalance Problem:

- One class may be rare, e.g. fraud, or HIV-positive
- Significant majority of the negative class and minority of the positive class
- Sensitivity: True Positive recognition rate
 - Sensitivity = TP/P
- Specificity: True Negative recognition rate
 - Specificity = TN/N

Classifier Evaluation Metrics: Precision and Recall, and F-measures

Precision: exactness – what % of tuples that the classifier labeled as positive are actually positive

$$precision = \frac{1}{TP + FP}$$

- **Recall:** completeness what % of positive tuples did the classifier label as positive? $recall = \frac{TP}{TP + FN}$
- Perfect score is 1.0
- Inverse relationship between precision & recall
- **F measure** (F_1 or F-score): harmonic mean of precision and recall,

recall,
$$F = \frac{2 \times precision \times recall}{precision + recall}$$

- F_{β} : weighted measure of precision and recall
 - assigns ß times as much weight to recall as to precision

$$F_{\beta} = \frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$$

Classifier Evaluation Metrics: Example

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	90	210	300	30.00 (sensitivity
cancer = no	140	9560	9700	98.56 (specificity)
Total	230	9770	10000	96.40 (accuracy)

$$Recall = 90/300 = 30.00\%$$

Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

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
- 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
 - <u>Leave-one-out</u>: 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

Evaluating Classifier Accuracy: Bootstrap

Bootstrap

- Works well with small data sets
- Samples the given training tuples uniformly with replacement
 - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several bootstrap methods, and a common one is .632 boostrap
 - A data set with d tuples is sampled d times, with replacement, resulting in a training set of d samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since $(1-1/d)^d \approx e^{-1} = 0.368$)
 - Repeat the sampling procedure k times, overall accuracy of the model:

$$Acc(M) = \frac{1}{k} \sum_{i=1}^{k} (0.632 \times Acc(M_i)_{test_set} + 0.368 \times Acc(M_i)_{train_set})$$

Estimating Confidence Intervals: Classifier Models M₁ vs. M₂

- Suppose we have 2 classifiers, M_1 and M_2 , which one is better?
- Use 10-fold cross-validation to obtain $\overline{err}(M_1)$ and $\overline{err}(M_2)$
- These mean error rates are just estimates of error on the true population of future data cases
- What if the difference between the 2 error rates is just attributed to chance?
 - Use a test of statistical significance
 - Obtain confidence limits for our error estimates

Estimating Confidence Intervals: Null Hypothesis

- Perform 10-fold cross-validation
- Assume samples follow a t distribution with k-1 degrees of freedom (here, k=10)
- Use t-test (or Student's t-test)
- Null Hypothesis: $M_1 \& M_2$ are the same
- If we can reject null hypothesis, then
 - we conclude that the difference between M₁ & M₂ is
 statistically significant
 - Chose model with lower error rate

Estimating Confidence Intervals: t-test

- If only 1 test set available: pairwise comparison
 - For ith round of 10-fold cross-validation, the same cross partitioning is used to obtain $err(M_1)_i$ and $err(M_2)_i$
 - Average over 10 rounds to get $\overline{err}(M_1)$ and $\overline{err}(M_2)$
 - t-test computes t-statistic with k-1 degrees of freedom:

$$t = \frac{\overline{err}(M_1) - \overline{err}(M_2)}{\sqrt{var(M_1 - M_2)/k}} \quad \text{where}$$

$$var(M_1 - M_2) = \frac{1}{k} \sum_{i=1}^k \left[err(M_1)_i - err(M_2)_i - (\overline{err}(M_1) - \overline{err}(M_2)) \right]^2$$

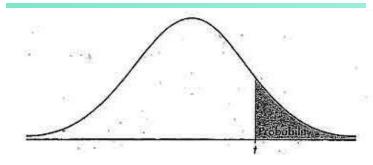
If two test sets available: use non-paired t-test

where
$$var(M_1 - M_2) = \sqrt{\frac{var(M_1)}{k_1} + \frac{var(M_2)}{k_2}},$$

where $k_1 \& k_2$ are # of cross-validation samples used for $M_1 \& M_2$, resp.

Estimating Confidence Intervals: Table for t-distribution

TABLE B: t-DISTRIBUTION CRITICAL VALUES



- Symmetric
- Significance level,
 e.g., sig = 0.05 or
 5% means M₁ & M₂
 are significantly
 different for 95% of
 population
- Confidence limit, z= sig/2

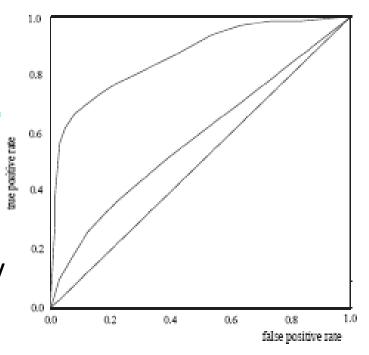
. Tail probability p												
df	.25	.20	.15	.10	.05	.025	.02	.01	.005	.0025	.001	.0005
1	1.000	1.376	1.963	3.078	6.314	12.71	15.89	31.82	63.66	127.3	318.3	636.6
2	.816	1.061	1.386	1.886	2.920	4.303	4.849	6.965	9.925	14.09	22.33	31.60
3	.765	.978	1.250	1.638	2.353	3,182	3,482	4.541	5.841	7.453	10.21	12.92
4	.741	.941	1.190	1.533	2.132	2.776	2.999	3.747	4.604	5.598	7.173	8.610
5	.727	.920	1.156	1.476	2.015	2.571	2.757	3.365	4.032	4.773	5.893	6.869
6	.718	.906	1.134	1.440	1.943	2.447	2.612	3.143	3.707	4.317		5.959
7	.711	.896	1.119	1.415	1.895	2.365	2.517	2.998	3.499	4.029	4.785	5,408
8	.706	.889	1.108	1.397	1.860	2.306	2.449	2.896	3.355	3.833	4.501	5:041
9	.703	.883	1.100	1.383	1.833	2.262	2.398	2.821	3.250	3.690	4.297	4.781
10	.700	.879	1.093	1.372	1.812	2.228	2,359	2.764	3.169	3.581	4.144	4.587
11	.697	.876	1.088	1.363	1.796	2,201	2.328	2.718	3.106	3.497	4.025	4.437
12	.695	.873	1.083	1.356	1.782	2.179	2.303	2.681	3.055	3.428	3.930	4.318
13	.694	.870	1.079	1.350	1.771	2.160	2.282	2.650	3.012	3.372	3.852	4.221
14	.692	.868	1.076	1.345	1.761	2.145	2.264	2.624	2.977	3.326	3.787	4.140
15	.691	.866	1.074	1.341	1.753	2.131	2.249	2.602	2.947	3.286	3.733	4.073
16	.690	.865	1.071	1.337	1.746	2.120	2.235	2.583	2.921	3,252-	3.686	4.015
17	.689	.863	1.069	1.333	1.740	2.110	2.224	2.567	2.898	3.222	3.646	3.965
18	.688	.862	1.067	1.330	1.734	2.101	2.214	2.552	2.878	3.197	3.611	3.922
19	.688	.861	1.066	1.328	1.729	2.093	2.205	2.539	2.861	3.174	3.579	3.883
20	.687	.860	1.064	1.325	1.725	2.086	2.197	2.528	2.845	3.153	3.552	3.850
21	.686	.859	1.063	1.323	1.721	2.080	2.189	2.518	2.831	3.135	3.527	3.819
22	.686	.858	1.061	1.321	1.717	2.074	2,183	2.508	2.819	3.119	3.505	3.792
23	.685	.858	1.060	1.319	1.714	2.069	2.177	2.500	2.807	3.104	3.485	3.768
24	685	.857	1.059	1.318	1.711	2.064	2.172	2.492	2.797	3.091	3.467.	3.745
25	.684	.856	1.058	1.316	1.708	2.060	2.167	2.485	2.787	3.078	3.450	3.725
26	.684	.856	1.058	1.315	1.706	2.056	2.162	2.479	2.779	3.067	3.435	3.707
27	.684	.855	1.057	1.314	1.703	2.052	2.158	2.473	2.771	3.057	3.421	3.690
28	.683	.855	1.056	1.313	1.701	2.048	2.154	2.467	2.763	3.047	3.408	3.674
29	.683	.854	1.055	1.311	1.699	2.045	2.150	2.462	2.756	3.038	3.396	3.659
30	.683	.854	1.055	1.310	1.697	2.042	2.147	2:457	2.750	3.030	3.385	3.646
40	.681	.851	1.050	1.303	1.684	2.021	2.123	2.423	2.704	2.971	3.307	3.551
50	.679	.849	1.047	1.299	1.676	2.009	2.109	2.403	2.678	2.937	3.261	3.496
60	.679	.848	1.045	1.296	1.671	2.000	2.099	2.390	2.660	2.915	3.232	3,460
80	.678	.846	1.043	1.292	1.664	1.990	2.088	2.374	2.639	2.887	3.195	3.416
100	.677	.845	1.042	1.290	1.660	1.984	2.081	2.364	2.626	2.871	3.174	3.390
000	.675	.842	1.037	1.282	1.646	1.962	2.056	2.330	2.581	2.813	3.098	3.300
00	.674	.841	1.036	1.282	1.645	1.960	2.054	2.326	2.576	2.807	3.091	3.291
	50%	60%	70%	80%	90%	95%	96%	98%	99%	99.5%	99.8%	99.9%

Estimating Confidence Intervals: Statistical Significance

- Are M₁ & M₂ significantly different?
 - Compute t. Select significance level (e.g. sig = 5%)
 - Consult table for t-distribution: Find t value corresponding to k-1 degrees of freedom (here, 9)
 - t-distribution is symmetric: typically upper % points of distribution shown \rightarrow look up value for **confidence limit** z=sig/2 (here, 0.025)
 - If t > z or t < -z, then t value lies in rejection region:</p>
 - Reject null hypothesis that mean error rates of M₁ & M₂ are same
 - Conclude: <u>statistically significant</u> difference between M₁
 & M₂
 - Otherwise, conclude that any difference is chance

Model Selection: ROC Curves

- ROC (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



- Vertical axis represents the true positive rate
- Horizontal axis rep. the false positive rate
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0

Issues Affecting Model Selection

Accuracy

classifier accuracy: predicting class label

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

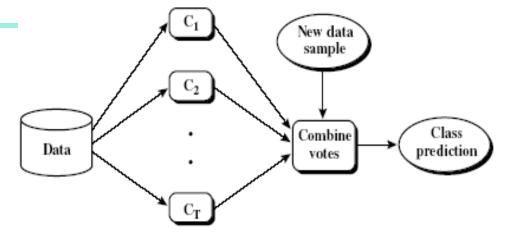
Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Rule-Based Classification
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy:
 Ensemble Methods



Summary

Ensemble Methods: Increasing the Accuracy



- Ensemble methods
 - Use a combination of models to increase accuracy
 - Combine a series of k learned models, M₁, M₂, ..., 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: Boostrap Aggregation

- 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 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 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 significantly 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
- Boosting algorithm can be extended for numeric prediction
- Comparing with bagging: Boosting tends to have greater accuracy, but it also risks overfitting the model to misclassified data

Adaboost (Freund and Schapire, 1997)

- Given a set of d class-labeled tuples, $(X_1, y_1), ..., (X_d, y_d)$
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
 - Tuples from D are sampled (with replacement) to form a training set
 D_i of the same size
 - Each tuple's chance of being selected is based on its weight
 - A classification model M_i is derived from D_i
 - Its error rate is calculated using D_i as a test set
 - If a tuple is misclassified, its weight is increased, o.w. it is decreased
- Error rate: $err(X_j)$ is the misclassification error of tuple X_j . Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_{j}^{d} w_j \times err(\mathbf{X_j})$$

The weight of classifier M_i's vote is

$$\log \frac{1 - error(M_i)}{error(M_i)}$$

Random Forest (Breiman 2001)

Random Forest:

- Each classifier in the ensemble is a decision tree classifier and is generated using a random selection of attributes at each node to determine the split
- During classification, each tree votes and the most popular class is returned
- Two Methods to construct Random Forest:
 - Forest-RI (random input selection): Randomly select, at each node, F
 attributes as candidates for the split at the node. The CART methodology
 is used to grow the trees to maximum size
 - Forest-RC (random linear combinations): Creates new attributes (or features) that are a linear combination of the existing attributes (reduces the correlation between individual classifiers)
- Comparable in accuracy to Adaboost, but more robust to errors and outliers
- Insensitive to the number of attributes selected for consideration at each split, and faster than bagging or boosting

Classification of Class-Imbalanced Data Sets

- Class-imbalance problem: Rare positive example but numerous negative ones, e.g., medical diagnosis, fraud, oil-spill, fault, etc.
- Traditional methods assume a balanced distribution of classes and equal error costs: not suitable for class-imbalanced data
- Typical methods for imbalance data in 2-class classification:
 - Oversampling: re-sampling of data from positive class
 - Under-sampling: randomly eliminate tuples from negative class
 - Threshold-moving: moves the decision threshold, t, so that the rare class tuples are easier to classify, and hence, less chance of costly false negative errors
 - Ensemble techniques: Ensemble multiple classifiers introduced above
- Still difficult for class imbalance problem on multiclass tasks

Classification: Basic Concepts

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- Rule-Based Classification
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- Summary



Summary (I)

- Classification is a form of data analysis that extracts models describing important data classes.
- Effective and scalable methods have been developed for decision tree induction, Naive Bayesian classification, rule-based classification, and many other classification methods.
- **Evaluation metrics** include: accuracy, sensitivity, specificity, precision, recall, F measure, and $F_{\mathcal{B}}$ measure.
- Stratified k-fold cross-validation is recommended for accuracy estimation. Bagging and boosting can be used to increase overall accuracy by learning and combining a series of individual models.

Summary (II)

- Significance tests and ROC curves are useful for model selection.
- There have been numerous comparisons of the different classification methods; the matter remains a research topic
- No single method has been found to be superior over all others for all data sets
- Issues such as accuracy, training time, robustness, scalability, and interpretability must be considered and can involve tradeoffs, further complicating the quest for an overall superior method

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Issues: Evaluating Classification Methods

- 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

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

$$\frac{\sum_{i=1}^{d} |y_i| \Re \dot{B} \text{ lative squared error}}{\sum_{i=1}^{d} |y_i - \overline{y}|}$$

The mean squared-error exaggerates the presence of outliers

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

Scalable Decision Tree Induction Methods

- SLIQ (EDBT'96 Mehta et al.)
 - Builds an index for each attribute and only class list and the current attribute list reside in memory
- SPRINT (VLDB'96 J. Shafer et al.)
 - Constructs an attribute list data structure
- PUBLIC (VLDB'98 Rastogi & Shim)
 - Integrates tree splitting and tree pruning: stop growing the tree earlier
- RainForest (VLDB'98 Gehrke, Ramakrishnan & Ganti)
 - Builds an AVC-list (attribute, value, class label)
- BOAT (PODS'99 Gehrke, Ganti, Ramakrishnan & Loh)
 - Uses bootstrapping to create several small samples

Data Cube-Based Decision-Tree Induction

- Integration of generalization with decision-tree induction (Kamber et al.'97)
- Classification at primitive concept levels
 - E.g., precise temperature, humidity, outlook, etc.
 - Low-level concepts, scattered classes, bushy classificationtrees
 - Semantic interpretation problems
- Cube-based multi-level classification
 - Relevance analysis at multi-levels
 - Information-gain analysis with dimension + level