# Data Mining Classification: Basic Concepts, Decision Trees, and Model Evaluation

Lecture Notes for Chapter 4

Introduction to Data Mining
by
Tan, Steinbach, Kumar

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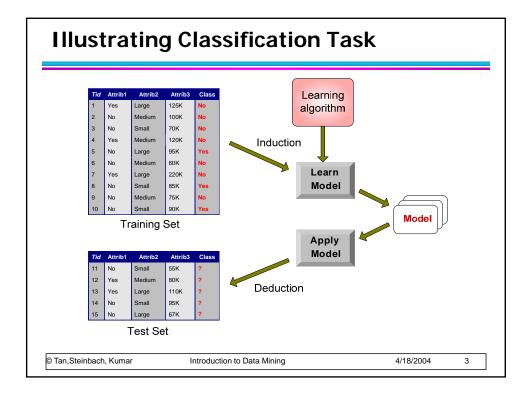
#### **Classification: Definition**

- Given a collection of records (training set)
  - Each record contains a set of attributes, one of the attributes is the class.
- Find a model for class attribute as a function of the values of other attributes.
- Goal: <u>previously unseen</u> records should be assigned a class as accurately as possible.
  - A test set is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.

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# **Examples of Classification Task**

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent

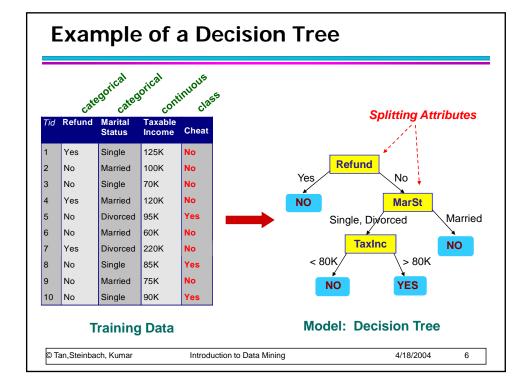


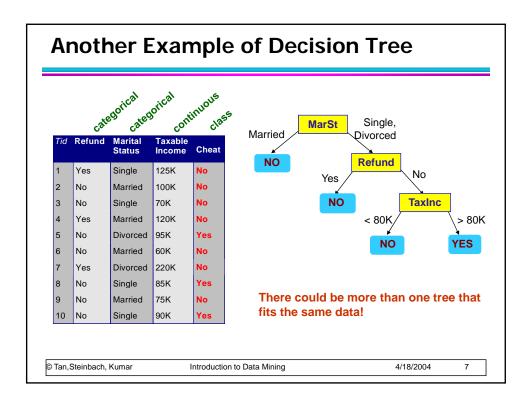
- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil
- Categorizing news stories as finance, weather, entertainment, sports, etc

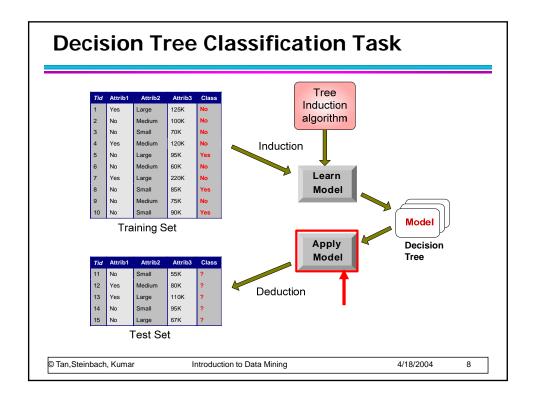
# **Classification Techniques**

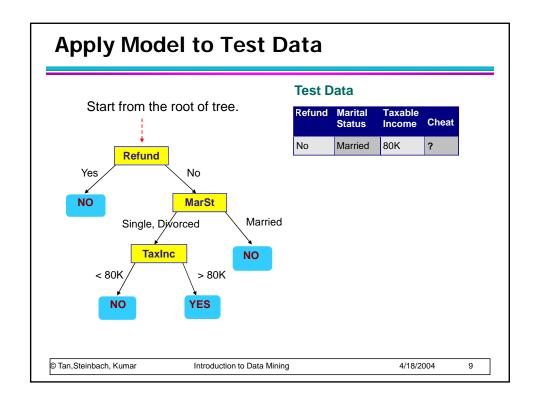
- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines

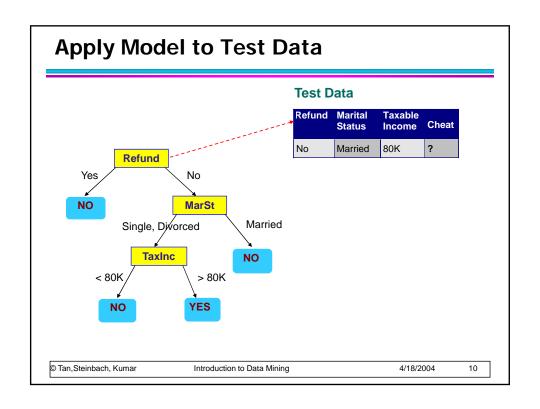
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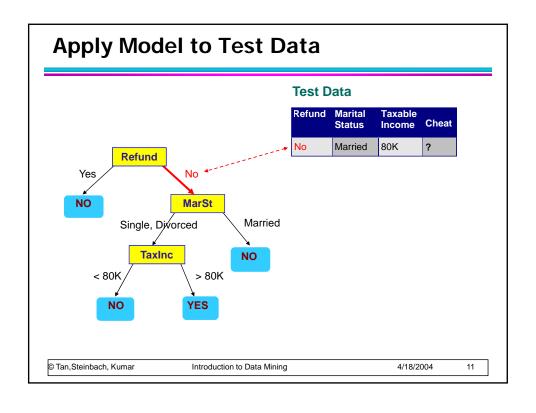


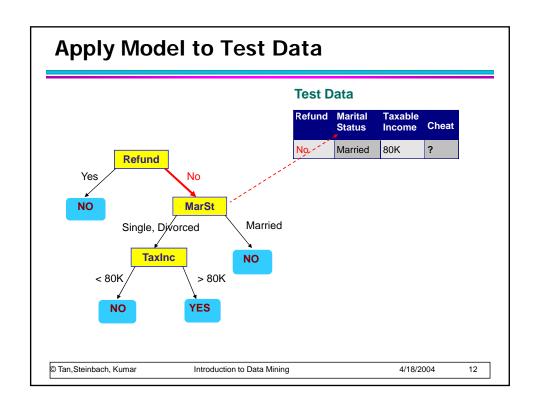


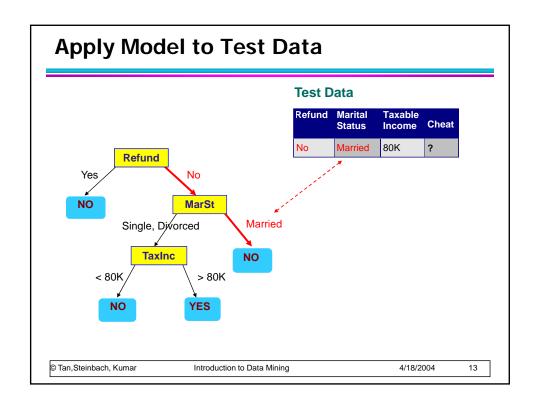


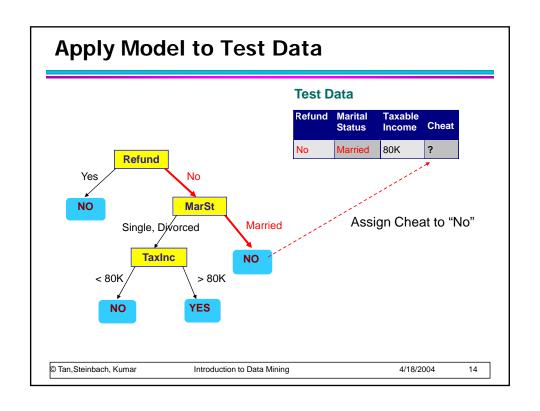


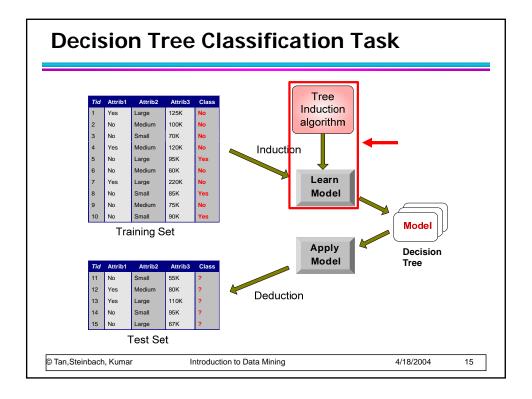








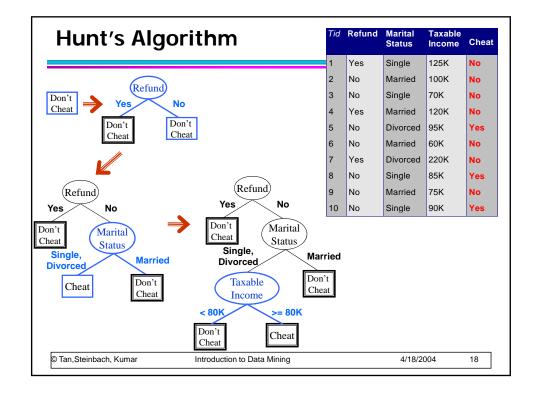




#### **Decision Tree Induction**

- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ,SPRINT

#### **General Structure of Hunt's Algorithm** Let D<sub>t</sub> be the set of training records Cheat that reach a node t Single 125K General Procedure: No Married 100K 70K No Single If D₁ contains records that Yes 120K Married belong the same class y, then t 95K No Divorced is a leaf node labeled as y, No Married 60K No If D, is an empty set, then t is a Yes Divorced 220K No leaf node labeled by the default No Single Yes No Married 75K No Single 90K If D<sub>t</sub> contains records that belong to more than one class, $D_t$ use an attribute test to split the data into smaller subsets. ? Recursively apply the procedure to each subset. © Tan,Steinbach, Kumar Introduction to Data Mining 4/18/2004 17



#### **Tree Induction**

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - ◆How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

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#### **Tree Induction**

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# **How to Specify Test Condition?**

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

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# **Splitting Based on Nominal Attributes**

 Multi-way split: Use as many partitions as distinct values.



Binary split: Divides values into two subsets.
 Need to find optimal partitioning.



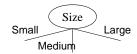
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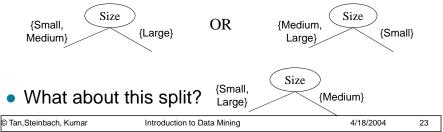
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## **Splitting Based on Ordinal Attributes**

Multi-way split: Use as many partitions as distinct values.



Binary split: Divides values into two subsets.
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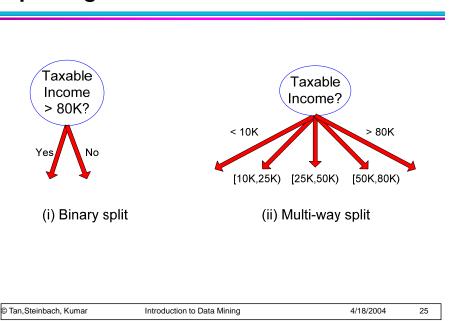
# **Splitting Based on Continuous Attributes**

- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Static discretize once at the beginning
    - Dynamic ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: (A < v) or (A ≥ v)
    - consider all possible splits and finds the best cut

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can be more compute intensive

# **Splitting Based on Continuous Attributes**



#### **Tree Induction**

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
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    - How to specify the attribute test condition?
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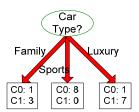
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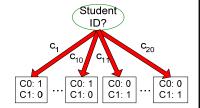
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# How to determine the Best Split

Before Splitting: 10 records of class 0, 10 records of class 1







Which test condition is the best?

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# How to determine the Best Split

- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

C0: 5 C1: 5

C0: 9 C1: 1

Non-homogeneous, High degree of impurity Homogeneous,
Low degree of impurity

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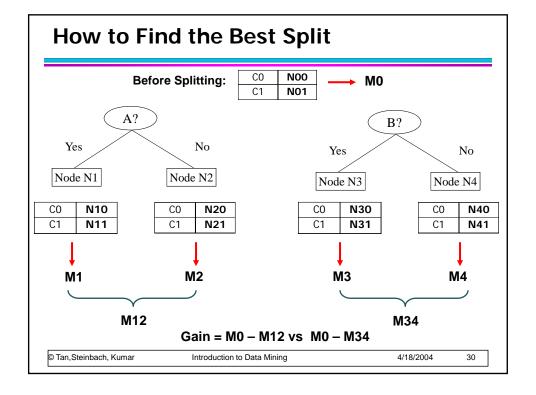
# **Measures of Node Impurity**

- Gini Index
- Entropy
- Misclassification error

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# Measure of Impurity: GINI

• Gini Index for a given node t:

$$GINI(t) = 1 - \sum_{j} [p(j|t)]^{2}$$

(NOTE:  $p(j \mid t)$  is the relative frequency of class j at node t).

- Maximum (1 1/n<sub>c</sub>) when records are equally distributed among all classes, implying least interesting information
- Minimum (0.0) when all records belong to one class, implying most interesting information

C1	0
C2	6
Gini=0.000	

C1	1	
C2	5	
Gini=0.278		





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# **Examples for computing GINI**

$$GINI(t) = 1 - \sum_{j} [p(j|t)]^{2}$$

$$P(C1) = 0/6 = 0$$
  $P(C2) = 6/6 = 1$   
 $Gini = 1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$ 

$$P(C1) = 1/6$$
  $P(C2) = 5/6$   
 $Gini = 1 - (1/6)^2 - (5/6)^2 = 0.278$ 

$$P(C1) = 2/6$$
  $P(C2) = 4/6$   
 $Gini = 1 - (2/6)^2 - (4/6)^2 = 0.444$ 

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## **Splitting Based on GINI**

- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

where,  $n_i$  = number of records at child i, n = number of records at node p.

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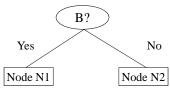
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#### **Binary Attributes: Computing GINI Index**

- Splits into two partitions
- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



	Parent
C1	6
C2	6
Gini = 0.500	

Gini(N1) =  $1 - (5/7)^2 - (2/7)^2$ 

= 0.408

Gini(N2) =  $1 - (1/5)^2 - (4/5)^2$ = 0.32

	N1	N2
C1	5	1
C2	2	4
Gini=0.371		

Gini(Children) = 7/12 \* 0.408 + 5/12 \* 0.32 = 0.371

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#### **Categorical Attributes: Computing Gini Index**

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split

	CarType		
	Family Sports Luxury		
C1	1	2	1
C2	4	1	1
Gini	0.393		

Two-way split (find best partition of values)

	CarType	
	{Sports, Luxury} {Family	
C1	3	1
C2	2 4	
Gini	0.400	

	CarType	
	{Sports}	{Family, Luxury}
C1	2	2
C2	1 5	
Gini	0.419	

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#### **Continuous Attributes: Computing Gini Index**

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible splitting values
     Number of distinct values
- Each splitting value has a count matrix associated with it
  - Class counts in each of the partitions, A < v and A ≥ v</li>
- Simple method to choose best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient!
     Repetition of work.





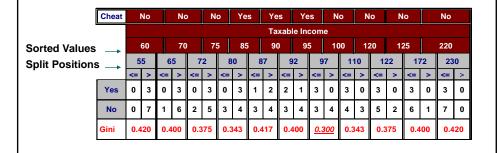
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# Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index



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## **Alternative Splitting Criteria based on INFO**

Entropy at a given node t:

$$Entropy(t) = -\sum_{j} p(j \mid t) \log p(j \mid t)$$

(NOTE:  $p(j \mid t)$  is the relative frequency of class j at node t).

- Measures homogeneity of a node.
  - Maximum (log n<sub>c</sub>) when records are equally distributed among all classes implying least information
  - Minimum (0.0) when all records belong to one class, implying most information
- Entropy based computations are similar to the GINI index computations

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# **Examples for computing Entropy**

$$Entropy(t) = -\sum_{j} p(j | t) \log_{2} p(j | t)$$

$$P(C1) = 0/6 = 0$$
  $P(C2) = 6/6 = 1$   
Entropy =  $-0 \log 0 - 1 \log 1 = -0 - 0 = 0$ 

$$P(C1) = 1/6$$
  $P(C2) = 5/6$   
Entropy = - (1/6)  $log_2$  (1/6) - (5/6)  $log_2$  (5/6) = 0.65

$$P(C1) = 2/6$$
  $P(C2) = 4/6$ 

Entropy = 
$$-(2/6) \log_2(2/6) - (4/6) \log_2(4/6) = 0.92$$

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# **Splitting Based on INFO...**

Information Gain:

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} Entropy(i)\right)$$

Parent Node, p is split into k partitions;

n<sub>i</sub> is number of records in partition i

- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
- Used in ID3 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

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#### Splitting Based on INFO...

Gain Ratio:

$$\boxed{GainRATIO_{split} = \frac{GAIN_{split}}{SplitINFO}} \boxed{SplitINFO = -\sum_{i=1}^{k} \frac{n_{i}}{n} \log \frac{n_{i}}{n}}$$

Parent Node, p is split into k partitions n<sub>i</sub> is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain

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## **Splitting Criteria based on Classification Error**

Classification error at a node t :

$$Error(t) = 1 - \max_{i} P(i \mid t)$$

- Measures misclassification error made by a node.
  - Maximum (1 1/n<sub>c</sub>) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

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# **Examples for Computing Error**

$$Error(t) = 1 - \max_{i} P(i \mid t)$$

C1	0
C2	6

$$P(C1) = 0/6 = 0$$
  $P(C2) = 6/6 = 1$   
 $Error = 1 - max(0, 1) = 1 - 1 = 0$ 

$$P(C1) = 1/6$$
  $P(C2) = 5/6$   
Error = 1 - max (1/6, 5/6) = 1 - 5/6 = 1/6

$$P(C1) = 2/6$$
  $P(C2) = 4/6$ 

Error =  $1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$ 

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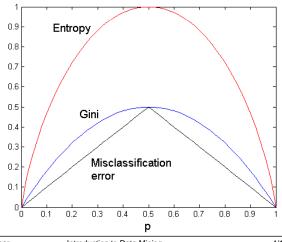
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# **Comparison among Splitting Criteria**

# For a 2-class problem:



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#### **Tree Induction**

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - ◆How to determine the best split?
  - Determine when to stop splitting

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# **Stopping Criteria for Tree Induction**

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (to be discussed later)

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#### **Decision Tree Based Classification**

- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets

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## Example: C4.5

- Simple depth-first construction.
- Uses Information Gain
- Sorts Continuous Attributes at each node.
- Needs entire data to fit in memory.
- Unsuitable for Large Datasets.
  - Needs out-of-core sorting.
- You can download the software from: http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.qz

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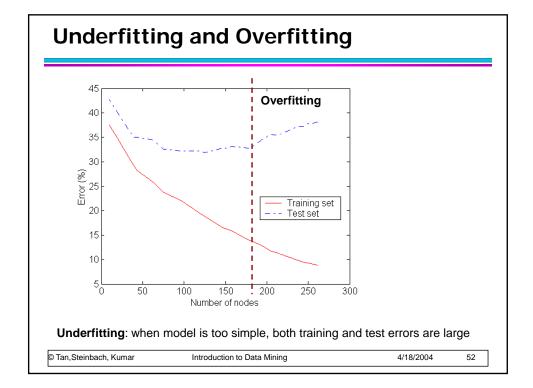
## **Practical Issues of Classification**

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

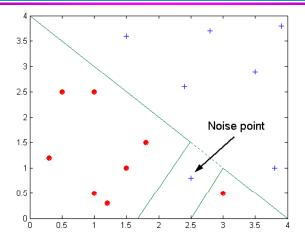
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#### Decision boundary is distorted by noise point

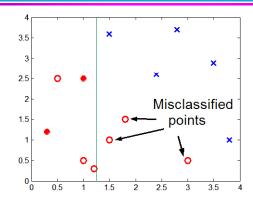
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# **Overfitting due to Insufficient Examples**



Lack of data points in the lower half of the diagram makes it difficult to predict correctly the class labels of that region

- Insufficient number of training records in the region causes the decision tree to predict the test examples using other training records that are irrelevant to the classification task

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## **How to Address Overfitting**

#### Pre-Pruning (Early Stopping Rule)

- Stop the algorithm before it becomes a fully-grown tree
- Typical stopping conditions for a node:
  - Stop if all instances belong to the same class
  - Stop if all the attribute values are the same
- More restrictive conditions:
  - Stop if number of instances is less than some user-specified threshold
  - Stop if class distribution of instances are independent of the available features (e.g., using  $\chi^2$  test)
  - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

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#### **How to Address Overfitting...**

#### Post-pruning

- Grow decision tree to its entirety
- 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
- Can use MDL for post-pruning

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# **Handling Missing Attribute Values**

- Missing values affect decision tree construction in three different ways:
  - Affects how impurity measures are computed
  - Affects how to distribute instance with missing value to child nodes
  - Affects how a test instance with missing value is classified

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#### Other Issues

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication

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## **Data Fragmentation**

- Number of instances gets smaller as you traverse down the tree
- Number of instances at the leaf nodes could be too small to make any statistically significant decision

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# **Search Strategy**

- Finding an optimal decision tree is NP-hard
- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Other strategies?
  - Bottom-up
  - Bi-directional

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#### **Expressiveness**

- Decision tree provides expressive representation for learning discrete-valued function
  - But they do not generalize well to certain types of Boolean functions
    - Example: parity function:
      - Class = 1 if there is an even number of Boolean attributes with truth value = True
      - Class = 0 if there is an odd number of Boolean attributes with truth value = True
    - For accurate modeling, must have a complete tree
- Not expressive enough for modeling continuous variables
  - Particularly when test condition involves only a single attribute at-a-time

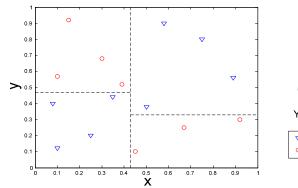
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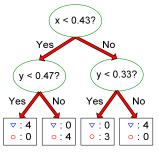
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# **Decision Boundary**



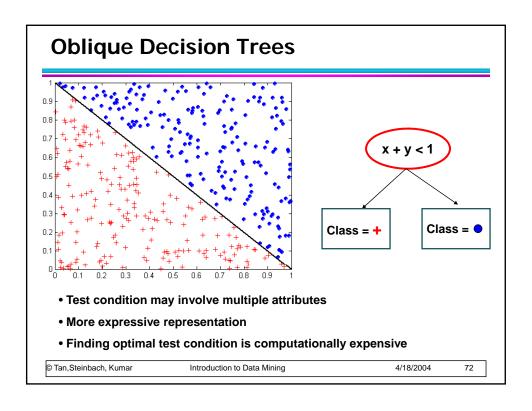


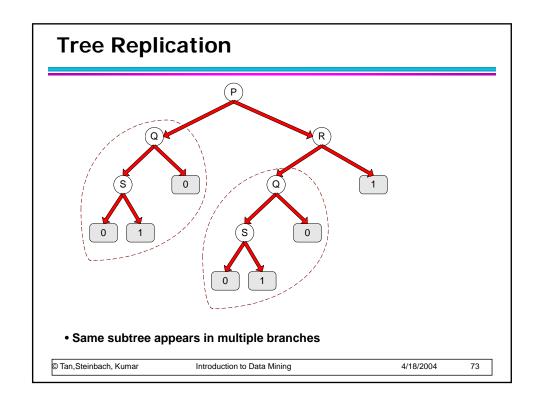
- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

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#### **Model Evaluation**

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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#### **Model Evaluation**

- Metrics for Performance Evaluation
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#### **Metrics for Performance Evaluation**

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL	Class=Yes	а	b
CLASS	Class=No	С	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

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#### **Metrics for Performance Evaluation...**

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL	Class=Yes	a (TP)	b (FN)
CLASS	Class=No	c (FP)	d (TN)

Most widely-used metric:

Accuracy = 
$$\frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

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## **Limitation of Accuracy**

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

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#### **Cost Matrix**

	PREDICTED CLASS		
	C(i j)	Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	C(Yes Yes)	C(No Yes)
	Class=No	C(Yes No)	C(No No)

C(i|j): Cost of misclassifying class j example as class i

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# **Computing Cost of Classification**

Cost Matrix	PREDICTED CLASS		
	C(i j)	+	-
ACTUAL CLASS	+	-1	100
	-	1	0

Model M <sub>1</sub>	PREDICTED CLASS		
ACTUAL CLASS		+	•
	+	150	40
	•	60	250

Model M <sub>2</sub>	PREDICTED CLASS		
ACTUAL CLASS		+	
	+	250	45
	-	5	200

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#### **Cost-Sensitive Measures**

Precision (p) = 
$$\frac{a}{a+c}$$

Recall (r) = 
$$\frac{a}{a+b}$$

F-measure (F) = 
$$\frac{2rp}{r+p}$$
 =  $\frac{2a}{2a+b+c}$ 

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

Weighted Accuracy = 
$$\frac{w_1 a + w_2 d}{w_1 a + w_2 b + w_2 c + w_2 d}$$

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#### **Model Evaluation**

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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0.3

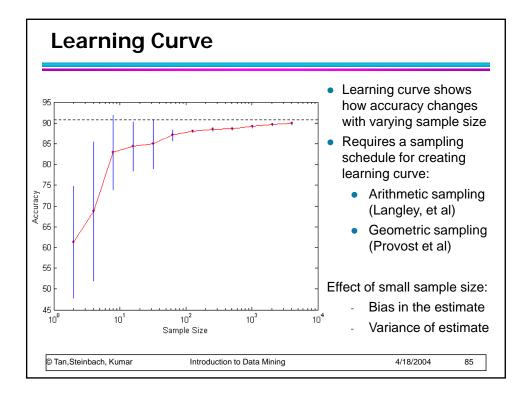
#### **Methods for Performance Evaluation**

- How to obtain a reliable estimate of performance?
- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

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#### **Methods of Estimation**

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

#### **Model Evaluation**

- Metrics for Performance Evaluation
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## **ROC (Receiver Operating Characteristic)**

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TPR (on the y-axis) against FPR (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - changing the threshold of algorithm, sample distribution or cost matrix changes the location of the point

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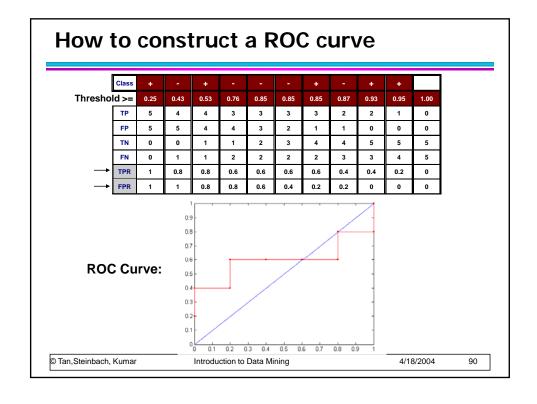
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#### How to construct a ROC curve

Instance	P(+ A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

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#### **ROC Curve** (TPR,FPR): • (0,0): declare everything 0.9 to be negative class 0.0 • (1,1): declare everything 0.7 to be positive class Positive 6.0 • (1,0): ideal ا <sub>0.4</sub> 0.3 Diagonal line: 0.2 - Random guessing Below diagonal line: 0.5 0.6 • prediction is opposite of the true class © Tan, Steinbach, Kumar Introduction to Data Mining 4/18/2004

