# Week 3 Classification (Part I)

Seokho Chi Professor | Ph.D. SNU Construction Innovation Lab



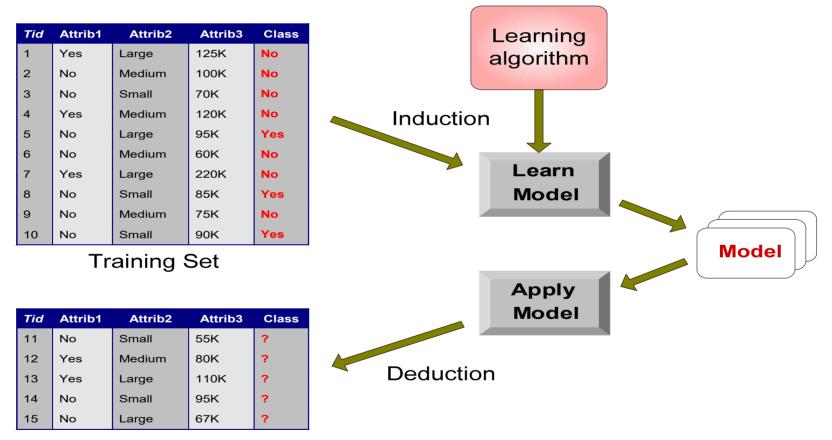
Source: Tan, Kumar, Steinback (2006)



## **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: previously unseen 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.

## Illustrating the Classification Task



Test Set

## Examples of Classification Task

양성종양

악성종양

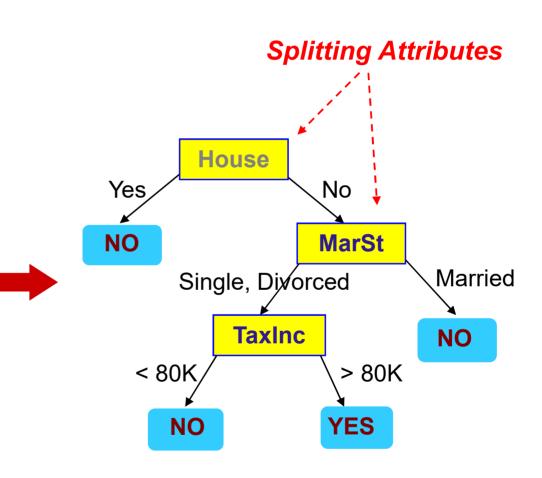
- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent
- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil
- Categorizing news stories as finance, weather, entertainment, sports, etc

## **Classification Techniques**

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

## Example of a Decision Tree



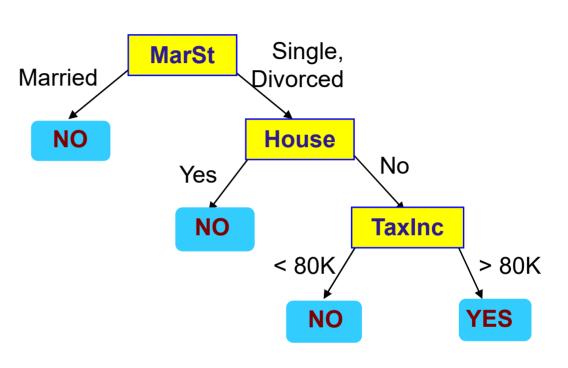


#### **Model: Decision Tree**

**Training Data** 

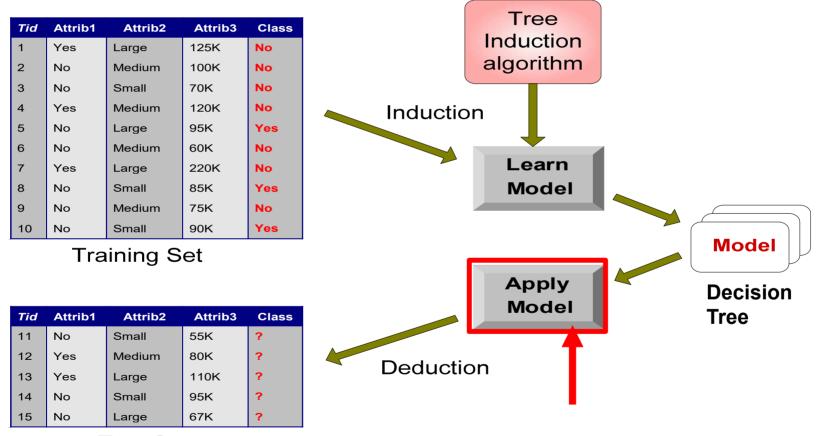
## Another Example of Decision Tree



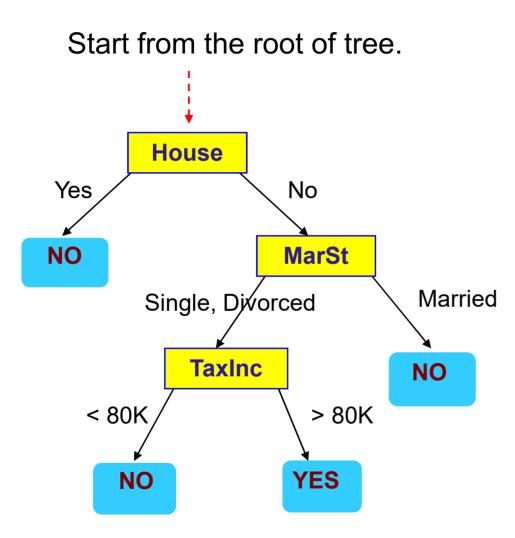


### There could be more than one tree that fits the same data!

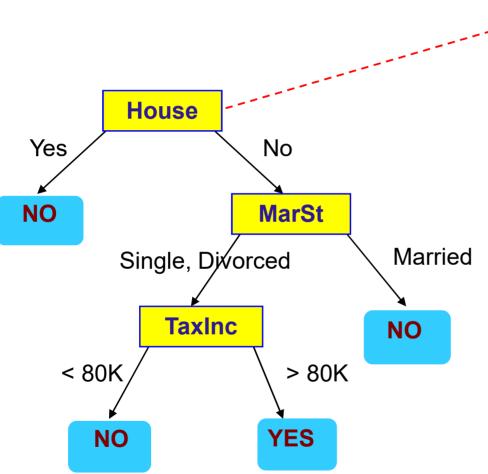
### **Decision Tree Classification Task**



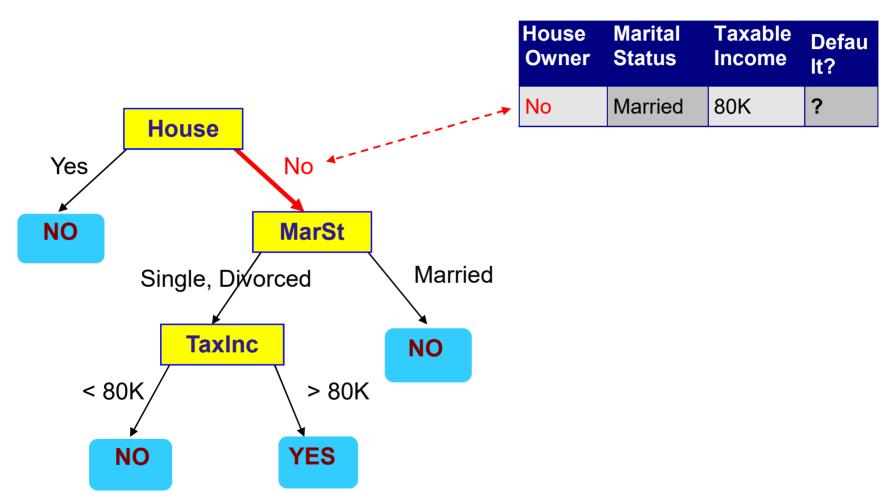
Test Set

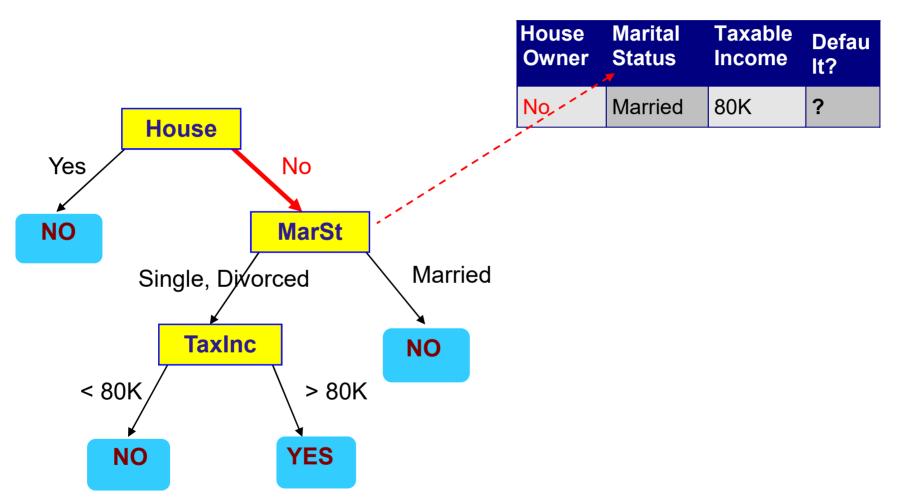


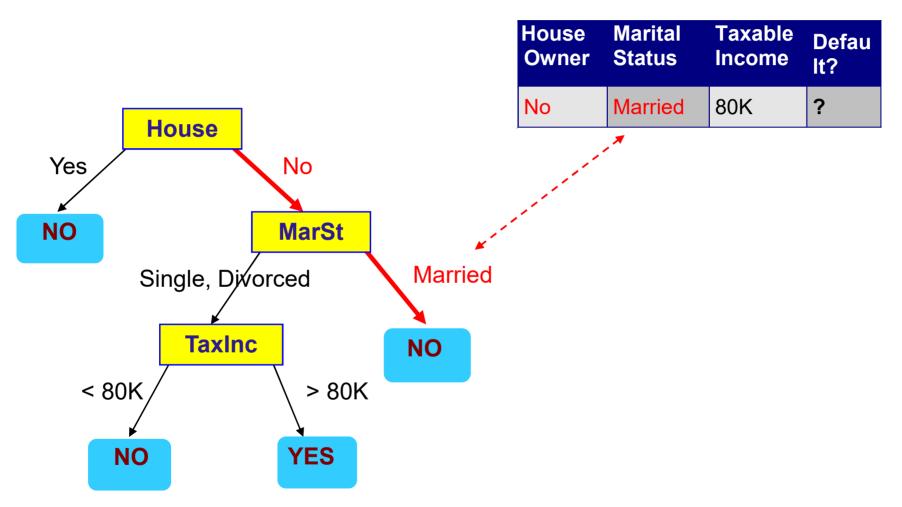
House		Taxable	Defau
Owner		Income	It?
No	Married	80K	?

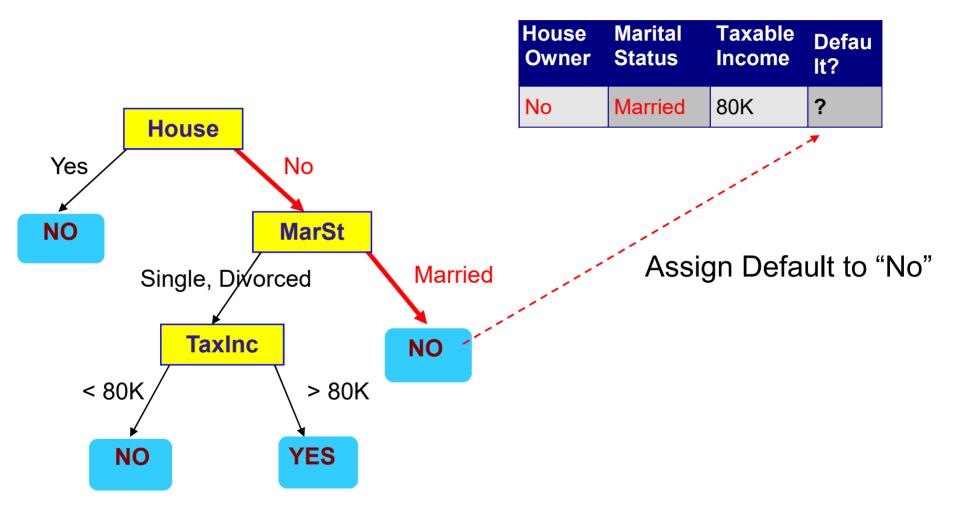


House Owner	Marital Status	_	Defau lt?
No	Married	80K	?

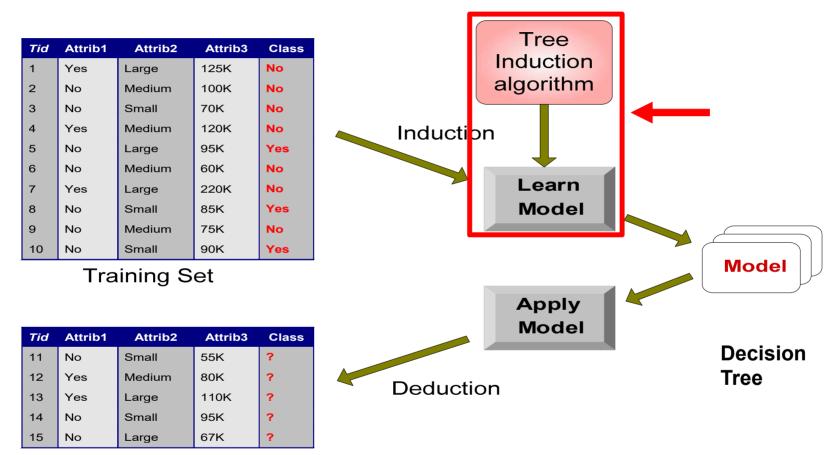








### **Decision Tree Classification Task**



Test Set

## **Decision Tree Induction**

- Greedy strategy
  - Tree is constructed in a top-down recursive divide-andconquer(분할하여 각각의 문제들을 해결) manner
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - 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

## **Tree Induction**

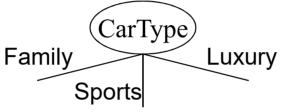
- Greedy strategy
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

## How to Specify Test Condition?

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

## Splitting Based on Nominal Attributes

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

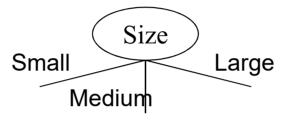


Binary split: Divides values into two subsets.
 Need to find optimal partitioning.

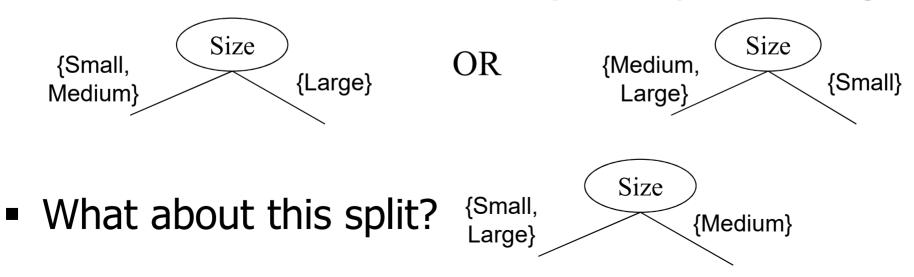


## Splitting Based on Ordinal Attributes

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

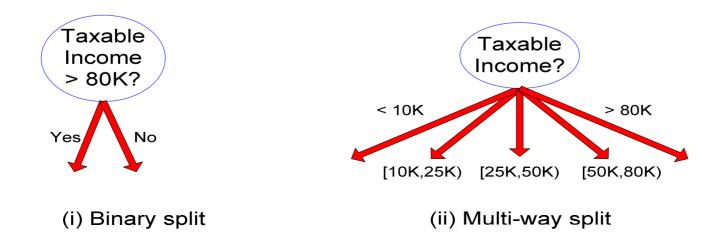


Binary split: Divides values into two subsets.
 Need to find optimal partitioning.



## Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Discretize once at the beginning
    - Equal interval bucketing, equal frequency bucketing, clustering
  - Binary Decision: (A < v) or  $(A \ge v)$ 
    - Consider all possible splits and finds the best cut
    - Can be more compute intensive

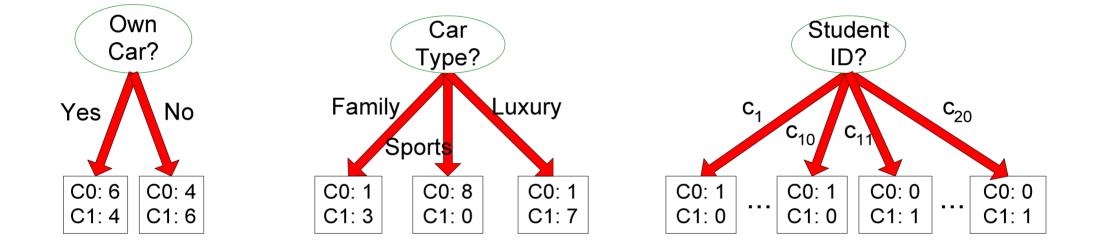


## Tree Induction

- 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

### How to determine the Best Split?

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



Which test condition is the best?

# How to determine the Best Split? (cont.)

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

0: 5 1: 5		C0: 9 C1:	-
	1		

Non-homogeneous,

High degree of impurity

Homogeneous (대표성),

Low degree of impurity (명확성)

Best split : determined by measuring impurity of nodes!

## Measures of Node Impurity

Node  $N_1$ 

Count

Information

$$I(s_1, s_2, \dots, s_m) = -\sum_{i=1}^m \frac{S_i}{s} \log 2 \frac{S_i}{s}$$

Gini Index

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

$$Gini(S_1, S_2, \ldots, S_m) = 1 - \sum_{i=1}^m \left(\frac{S_i}{S}\right)^2$$

Classification error

$$Error(s_1, s_2, \dots, s_m) = 1 - \max(\frac{s_i}{s})$$

## Measures for Selecting the Best Split: Information Gain

\*Best selecting is determined by the degree of impurity of the child nodes

- S contains s<sub>i</sub> records of class C<sub>i</sub> for i = {1, ..., m}
- Information: impurity measure required to classify a given sample (small is better)  $\int_{M}^{m} S_{i} \log S_{i}$

$$V(s_1, s_2, ..., s_m) = -\sum_{i=1}^m \frac{s_i}{s} \log 2 \frac{s_i}{s}$$

- Entropy: summation of information values of subsets partitioned by attribute A (small is better)  $E(A) = \sum_{j=1}^{\nu} \frac{s_{1j} + ... + s_{mj}}{s} I(s_{1j},...,s_{mj})$
- Information Gain: information before splitting entropy (large is better, how impurity decreased by attribute A)

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

Select the attribute with the highest information gain

## Example

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

## (1) Splitting Based on Information Gain

- 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 (splitting by 5(low entropy) is better than splitting by 2)
  - To overcome, do adjustment by considering the ratio of sample numbers
     of each node to the entire samples(전체 중 이 노드가 차지하는 비중)
  - Gain Ratio for C4.5, etc.
  - GINI Index for CART, SLIQ, SPRINT, etc.

#### Splitting Based on INFO...

• Gain Ratio:

$$GainRATIO = \frac{GAIN}{SplitINFO}$$
$$SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

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

## Measure of Impurity: GINI

• Gini Index for a given node t :

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

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

- Maximum (1  $1/n_c$ ) 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

Gini=	0.000	Gini=	0.278	Gini=	0.444	Gini=	0.500
C2	6	C2	5	C2	4	C2	3
C1	0	C1	1	C1	2	C1	3

Lower is better

## Examples for computing GINI

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

C1	0
C2	6

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

C1	1
C2	5

$$P(C1) = 1/6$$
  $P(C2) = 5/6$   
Gini = 1 - (1/6)<sup>2</sup> - (5/6)<sup>2</sup> = 0.278

C1	2
C2	4

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

# (2) Splitting Based on GINI

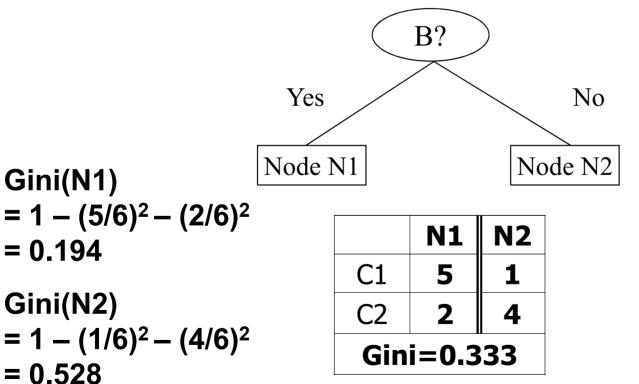
- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

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

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

# Binary Attributes: Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  - Larger and purer partitions are sought for
  - If you pick B as an attribute  $\rightarrow$



	Parent	
C1	6	
C2	6	
Gini = 0.500		

Gini (Children) = 7/12 \* 0.194 + 5/12 \* 0.528 = 0.333

### 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  $\geq$  v
- 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.

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Singl Tax	able	Yes
Income > 80K?				
Yes No				

#### (3) Splitting 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  $1/n_{\rm c})$  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

## **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 = 1Error = 1 - max (0, 1) = 1 - 1 = 0

C1	1
C2	5

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

C1	2
C2	4

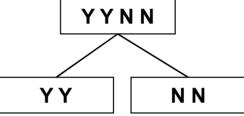
P(C1) = 2/6 P(C2) = 4/6Error = 1 - max (2/6, 4/6) = 1 - 4/6 = 1/3

# 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

# Stopping Criteria for Tree Induction

Stop expanding a node when all the records belong to the same class



 Stop expanding a node when there is no remaining attribute for further partitioning

- Early termination (to be discussed later)
  - Become to be huge  $\rightarrow$  Rather negative effect

#### **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

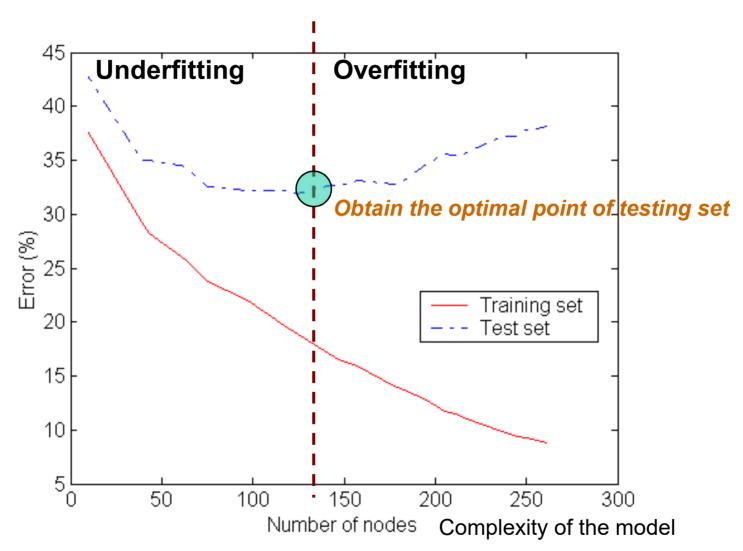
# Example: C4.5

- Uses information gain
- Sorts continuous attributes at each node
- Unsuitable for large datasets
- You can download the software from: <u>http://www.rulequest.com/Personal/</u>
- See5: commercial version (free demo available): <a href="http://www.rulequest.com">http://www.rulequest.com</a>

#### **Practical Issues of Classification**

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

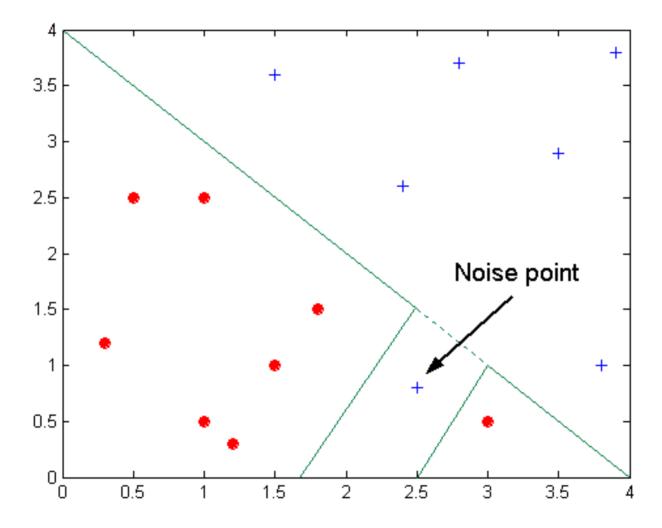
# Underfitting and Overfitting



**Underfitting**: too simple  $\rightarrow$  both training and test errors are large **Overfitting**: too complex  $\rightarrow$  generalization errors (errors on testing) are large (data fragmentation)

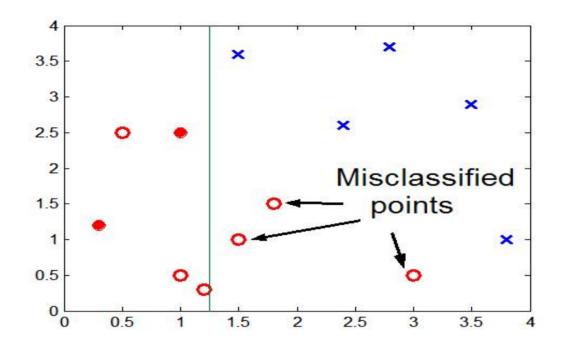
Occam's Razor: Given two models of similar generalization errors, the simpler model is preferred.

#### Overfitting due to Noise



Create tree models with noise samples (Decision boundary is distorted by noise point)

#### Overfitting due to Insufficient Examples



Tree models are development with insufficient samples

(Lack of data points makes it difficult to predict correctly the class labels of a region)

# 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 there is no remaining attribute for further partitioning
  - More restrictive conditions
    - Stop if number of instances is less than some user-specified threshold
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain)
    - Stop if the tree reaches generalization error threshold (pessimistic error estimate, <u>Minimum Description Length Principle</u>, etc.)

*Optimistic: training error = testing error | Pessimistic: training error < testing error* 

#### 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 or impurity 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

# Handling Missing Attribute Values

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

# **Computing Impurity Measure**

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	?	Single	90K	Yes
Missing value				

Before Splitting:

Information(Parent) =  $-0.3 \log(0.3) - (0.7) \log(0.7) = 0.8813$ 

	Class = Yes	
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

#### **Split on Refund:**

Information(Refund=Yes) = 0

Information(Refund=No)

 $= -(2/6)\log(2/6) - (4/6)\log(4/6) = 0.9183$ 

Entropy(Refund)

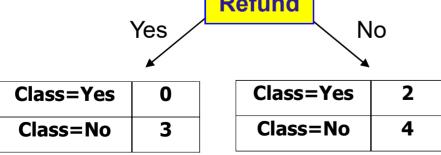
= 0.3 (0) + 0.6 (0.9183) = 0.551

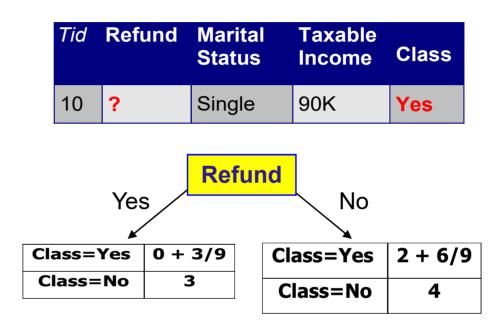
Gain = 0.9 × (0.8813 – 0.551) = 0.3303

Do not consider missing values and adjust with weight (0.9)

#### **Distribute Instances**

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
Refund				





**Probability that Refund=Yes is 3/9** 

**Probability that Refund=No is 6/9** 

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

#### Model Evaluation

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

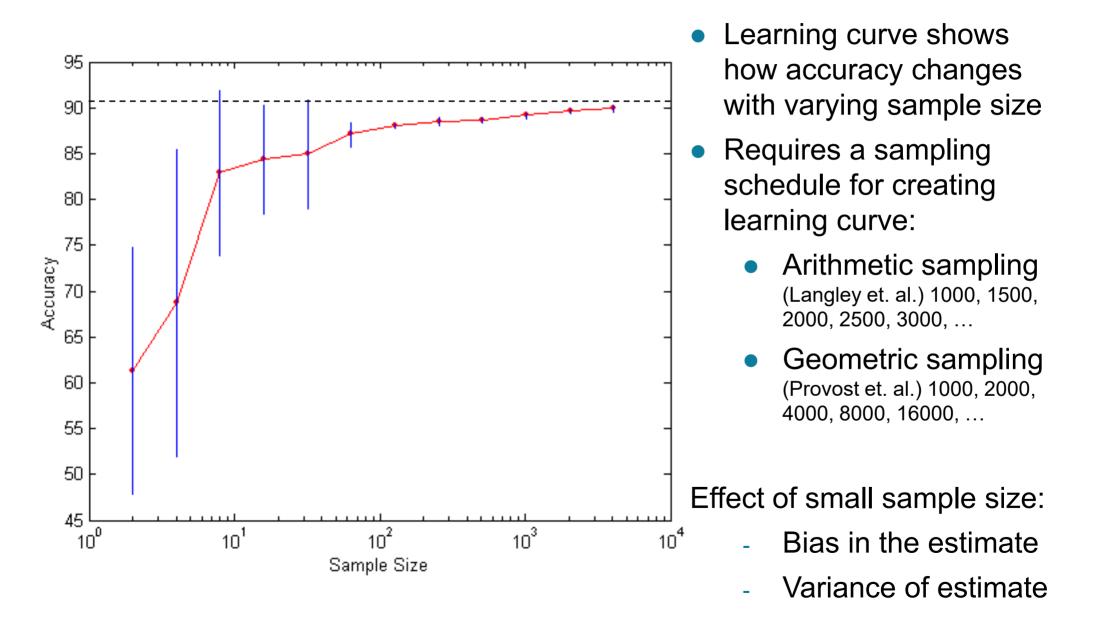
#### Model Evaluation

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

# Methods for Performance Evaluation

- Classification performance of a model may depend on other factors besides the learning algorithms
  - Class distribution
  - Sampling approaches
  - Size of training and test sets

# Learning Curve



# Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing (independent each other)
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets

Limited testing samples, results are affected by the distribution

Good generalization and representativeness, but high computation and still small # of testing samples

- k-fold: train on k-1 partitions, test on the remaining one
   (10-fold: training 90%, testing 10%, then repeat this 10 times)
- Bootstrap
  - Previous: no replacement  $\rightarrow$  no duplicate records
  - Sampling with replacement
  - Probability to be selected to Bootstrap :  $1-(1-1/N)^N \approx 1-e^{-1}=0.632$
  - Records not included in the bootstrap sample  $\rightarrow$  test set

#### Model Evaluation

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

# Metrics for Performance Evaluation

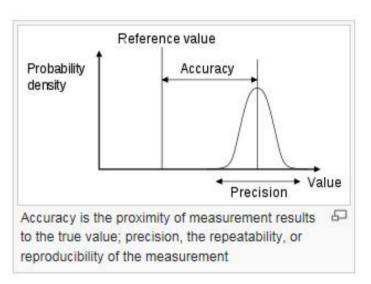
- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	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)

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

Precision (Positive Prediction Value) = TP / (TP + FP) A retrieved document is relevant Recall (Sensitivity) = TP / (TP + FN) A relevant document is retrieved

# 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 (e.g., safety accident)

#### Cost Matrix

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

C(i|j): Cost of misclassifying class j example as class i higher cost  $\rightarrow$  higher concern

# **Computing Cost of Classification**

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

Accuracy = 80%Cost = -1\*150 + 100\* 40 + 1\*60= 3910 Accuracy = 90% Cost = 4255

#### Model Evaluation

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

# 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) → answer is P
- Performance of each classifier represented as a point on the ROC curve

**FPR** 

P(Actually False 중

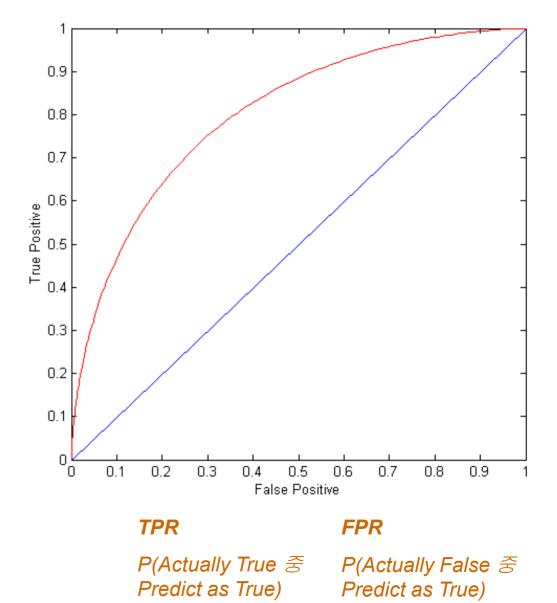
Predict as True)

$$TPR = \frac{TP}{TP + FN} \quad \begin{array}{c} TPR \\ P(Actually True \ \ensuremath{\mathfrak{FPR}}\ \ \ensuremath{\mathfrak{FPR}}\ \ = \frac{FP}{TN + FP} \end{array}$$

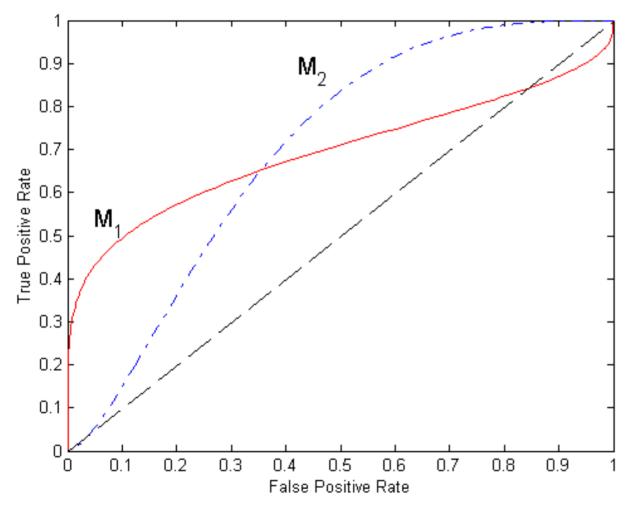
# **ROC Curve**

(TPR,FPR):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal
- (0,1): worst
- Diagonal line:
  - Random guessing(reference line)
  - Below diagonal line:
    - prediction is opposite of the true class



#### Using ROC for Model Comparison



- No model consistently outperform the other
  - M<sub>1</sub> is better for small FPR
  - M<sub>2</sub> is better for large FPR

# Test of Significance

- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances

- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in performance measure be explained as a result of random fluctuations in the test set?

# **Comparing Performance of 2 Models**

- Given the models M1 and M2, which is better?
  - M1 is tested on D1 (size=n1), found error rate =  $e_1$
  - M2 is tested on D2 (size=n2), found error rate =  $e_2$
  - Assume D1 and D2 are independent
  - If n1 and n2 are sufficiently large, then

$$e_1 \sim N(\mu_1, \sigma_1)$$
$$e_2 \sim N(\mu_2, \sigma_2)$$

# **Comparing Performance of 2 Models**

- To test if performance difference is statistically significant: d = e1 – e2
  - Since D1 and D2 are independent, their variance adds up:

$$\hat{\sigma}_{d}^{2} = \sigma_{1}^{2} + \sigma_{2}^{2} \cong \hat{\sigma}_{1}^{2} + \hat{\sigma}_{2}^{2}$$
$$= \frac{e1(1 - e1)}{n1} + \frac{e2(1 - e2)}{n2}$$

– At (1- $\alpha$ ) confidence level,

$$d_t = d \pm Z_{\alpha/2} \hat{\sigma}_d$$

# For this Example

2-sided (tailed) test: deviations of the estimated parameter in either direction are considered (normal distribution)

1-sided: only deviations in one direction are considered (pvalue)

- Given: M1: n1 = 30, e1 = 0.15
   M2: n2 = 5000, e2 = 0.25
- d = |e2 e1| = 0.1 (2-sided test)

$$\hat{\sigma}_d^2 = \frac{0.15(1 - 0.15)}{30} + \frac{0.25(1 - 0.25)}{5000} = 0.0043$$

• At 95% confidence level,  $Z_{\alpha/2}$ =1.96

$$d_{t} = 0.100 \pm 1.96 \times \sqrt{0.0043} = 0.100 \pm 0.128$$
[-0.028, 0.228]

=> Interval contains 0 => difference may not be statistically significant