### CSE 5243 INTRO. TO DATA MINING

Classification (Basic Concepts)

Yu Su, CSE@The Ohio State University

## Classification: Basic Concepts

Classification: Basic Concepts

Decision Tree Induction

Model Evaluation and Selection

Practical Issues of Classification

Bayes Classification Methods

Techniques to Improve Classification Accuracy: Ensemble Methods

This class

Summary

Next class

# Classification: Basic Concepts

□ Classification: Basic Concepts

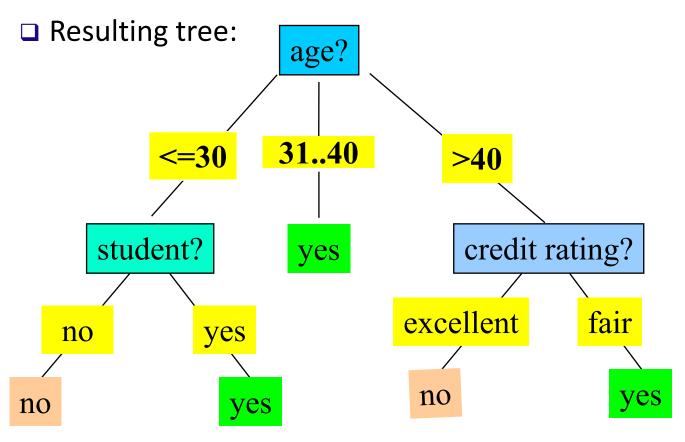
Decision Tree Induction



- Model Evaluation and Selection
- Practical Issues of Classification
- Bayes Classification Methods
- □ Techniques to Improve Classification Accuracy: Ensemble Methods
- Summary

## Decision Tree Induction: An Example

- □ Training data set: Buys\_computer
- ☐ The data set follows an example of Quinlan's ID3 (Playing Tennis)



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

## Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning—majority voting is employed for classifying the leaf
  - There are no samples left

## Algorithm Outline

- Split (node, {data tuples})
  - A <= the best attribute for splitting the {data tuples}</p>
  - Decision attribute for this node <= A</p>
  - For each value of A, create new child node
  - For each child node / subset:
    - If one of the stopping conditions is satisfied: STOP
    - Else: Split (child\_node, {subset})

## Algorithm Outline

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    - Else: Split (child\_node, {subset})

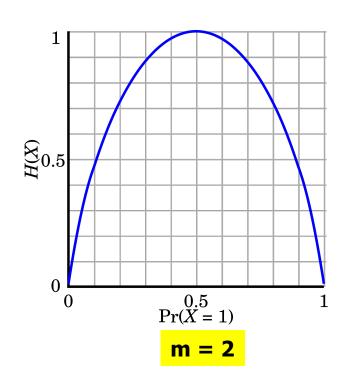
# Brief Review of Entropy

- Entropy (Information Theory)
  - A measure of uncertainty associated with a random number
  - □ Calculation: For a discrete random variable Y taking m distinct values  $\{y_1, y_2, ..., y_m\}$

$$H(Y) = -\sum_{i=1}^{m} p_i \log(p_i) \quad where \ p_i = P(Y = y_i)$$

- Interpretation
  - Higher entropy → higher uncertainty
  - Lower entropy → lower uncertainty
- Conditional entropy

$$H(Y|X) = \sum_{x} p(x)H(Y|X = x)$$



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

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

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

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

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

☐ 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"

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

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

Look at "age":

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

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

### Attribute Selection: Information Gain

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

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

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

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

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

$$Gain(income) = 0.029$$

$$Gain(student) = 0.151$$

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

#### Recursive Procedure

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. After selecting age at the root node, we will create three child nodes.
- 2. One child node is associated with red data tuples.
- 3. How to continue for this child node?

Now, you will make  $D = \{\text{red data tuples}\}\$ 

and then select the best attribute to further split

D.

A recursive procedure.

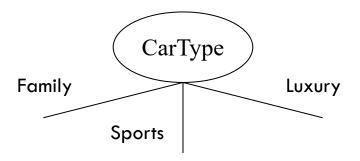
### How to Select Test Attribute?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

- Depends on number of ways to split
  - 2-way split
  - Multi-way split

## Splitting Based on Nominal Attributes

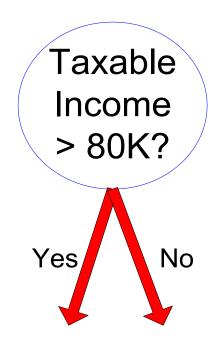
Multi-way split: Use as many partitions as distinct values.



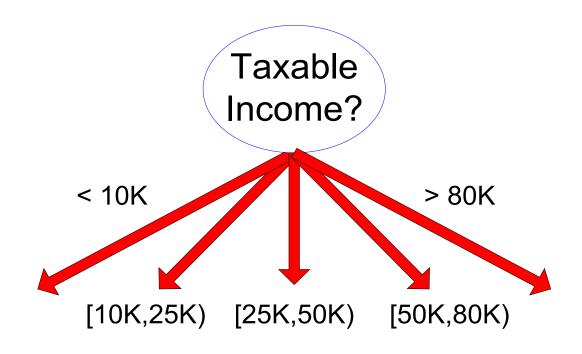
 Binary split: Divides values into two subsets. Need to find optimal partitioning.



### Splitting Based on Continuous Attributes



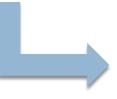
(i) Binary split



(ii) Multi-way split

## How to Determine the Best Split

- Greedy approach:
  - Nodes with homogeneous class distribution are preferred



Ideally, data tuples at that node belong to the same class.

C0: 5

C1: 5

C0: 9

C1: 1

Non-homogeneous,

High degree of impurity

Homogeneous,

Low degree of impurity

### Rethink about Decision Tree Classification

□ 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

# Measures of Node Impurity

□ Entropy:

$$H(Y) = -\sum_{i=1}^{m} p_i \log(p_i) \text{ where } p_i = P(Y = y_i)$$

- Higher entropy => higher uncertainty, higher node impurity
- Why entropy is used in information gain
- □ Gini Index
- Misclassification error

### 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)

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

- The entropy of the partitioning, or the potential information generated by splitting *D* into *v* partitions.
- $\Box$  GainRatio(A) = Gain(A)/SplitInfo(A) (normalizing Information Gain)

### Gain Ratio for Attribute Selection (C4.5)

□ C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)  $\frac{V + D + \cdots + D}{V}$ 

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

- $\Box$  GainRatio(A) = Gain(A)/SplitInfo(A)
- □ Ex.

Gain(income) = 0.029 (from last class, slide 27)

$$SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) = 1.557$$

- $\square$  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)

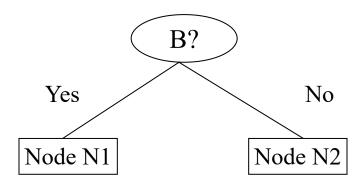
- If a data set D contains examples from n classes, gini index, gini(D) is defined as  $gini(D) = 1 \sum_{j=1}^{n} p_{j}^{2}$ , where  $p_{j}$  is the relative frequency of class j in D
- If a data set D is split on A into two subsets  $D_1$  and  $D_2$ , the gini index after the split is defined as  $gini_A(D) = \frac{|D_1|}{|D|}gini(D_1) + \frac{|D_2|}{|D|}gini(D_2)$
- Reduction in impurity:

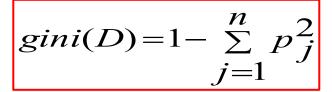
$$\Delta gini(A) = gini(D) - gini_A(D)$$

□ The attribute provides the smallest  $gini_A(D)$  (or, the largest reduction in impurity) is chosen to split the node.

## Binary Attributes: Computing Gini Index

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

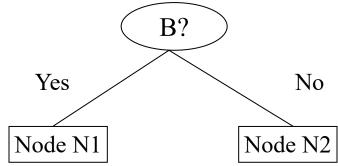




	Parent
C1	6
C2	6
Gini = ?	

## Binary Attributes: Computing Gini Index

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



	<u>B?</u>	
Yes		No
Node N1		Node N2

= 0.194
Gini(N2) = $1 - (1/5)^2 - (4/5)^2$ = $0.528$

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

Gini(N1)

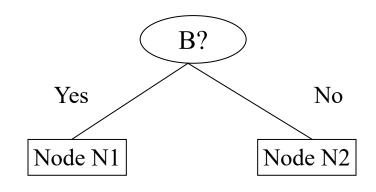
	N1	<b>N2</b>
C1	5	1
C2	2	4
Gini=?		

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

	Parent
C1	6
C2	6
Gini	= 0.500

## Binary Attributes: Computing Gini Index

- Splits into two partitions
- Effect of weighing partitions:
  - Prefer Larger and Purer Partitions.



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

	Parent							
C1	6							
C2	6							
Gini = ?								

Gini(NT)	
$= 1 - (5/7)^2$	$-(2/7)^2$
= 0.194	

Gini(N2)  
= 
$$1 - (1/5)^2 - (4/5)^2$$
  
= 0.528

	N1	N2							
C1	5	1							
C2	2	4							
Gini=0.333									

weighting

### 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	Family Sports Luxury											
<b>C1</b>	1	2	1										
C2	4	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								

#### Continuous Attributes: Computing Gini Index or Information Gain

- To discretize the attribute values
  - Use Binary Decisions based on one splitting value
- Several Choices for the splitting value
  - Number of possible splitting values = Number of distinct values -1
  - 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  $a_{i+1}$
- Each splitting value has a count matrix associated with it
  - $\square$  Class counts in each of the partitions, A < v and A  $\ge$  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.



Taxable Income > 80K?

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values



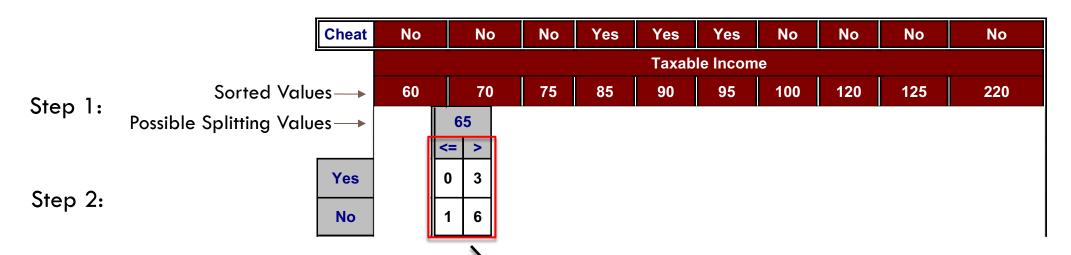
27

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values

Step 2: Linearly scan these values, each time updating the count matrix



For each splitting value, get its count matrix: how many data tuples have:

(a) Taxable income <=65 with class label "Yes", (b) Taxable income <=65 with class label "No", (c) Taxable income >65 with class label "Yes",

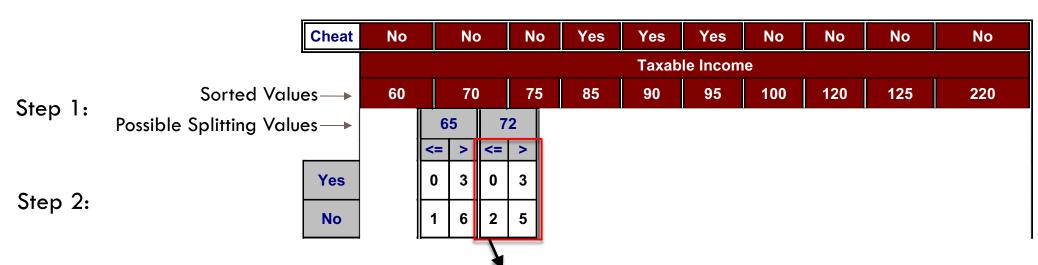
(d) Taxable income >65 with class label "No".

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values

Step 2: Linearly scan these values, each time updating the count matrix



For each splitting value, get its count matrix: how many data tuples have:

(a) Taxable income <=72 with class label "Yes", (b) Taxable income

<=72 with class label "No", (c) Taxable income >72 with class label "Yes",

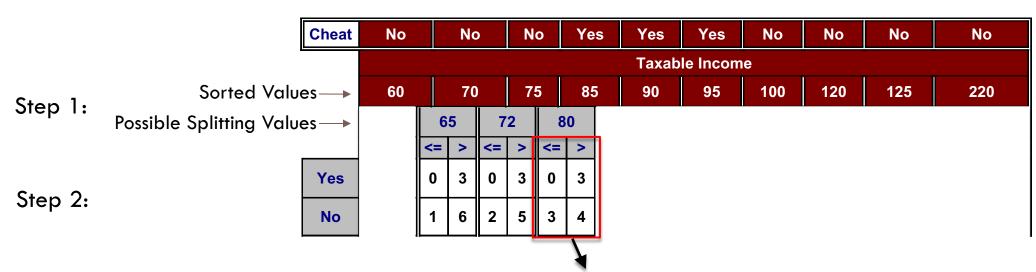
(d) Taxable income >72 with class label "No".

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values

Step 2: Linearly scan these values, each time updating the count matrix



For each splitting value, get its count matrix: how many data tuples have:

(a) Taxable income <=80 with class label "Yes", (b) Taxable income <=80 with class label "No", (c) Taxable income >80 with class label "Yes",

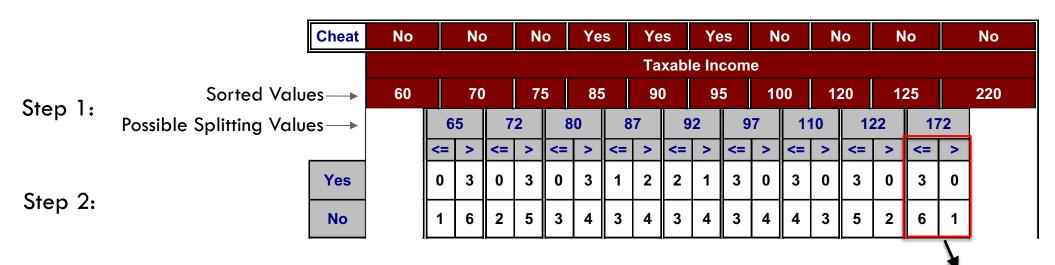
(d) Taxable income >80 with class label "No".

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values

Step 2: Linearly scan these values, each time updating the count matrix

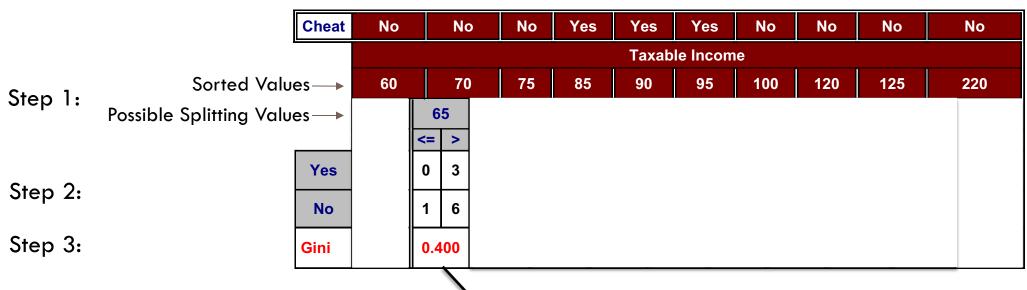


For each splitting value, get its count matrix: how many data tuples have:

(a) Taxable income <=172 with class label "Yes", (b) Taxable income
<=172 with class label "No", (c) Taxable income >172 with class label
"Yes", (d) Taxable income >172 with class label "No".

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

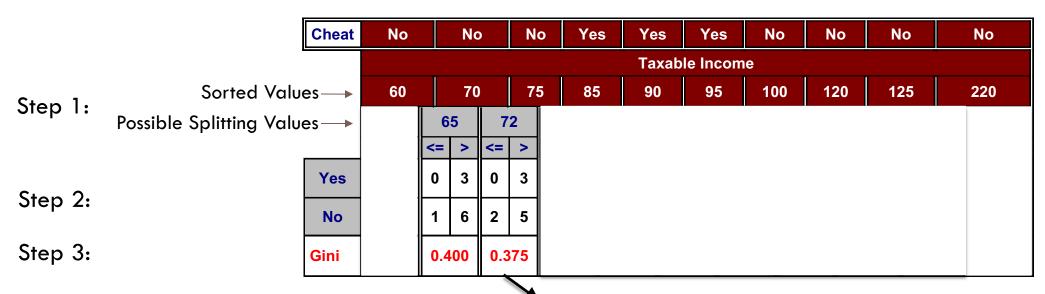


For each splitting value v (e.g., 65), compute its Gini index:

$$gini_{Taxable\_Income}(D) = \frac{|D_1|}{|D|}gini(D_1) + \frac{|D_2|}{|D|}gini(D_2) \quad \text{Here D1 and D2 are two partitions based on v: D1 has taxable income <=v and D2 has >v}$$

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

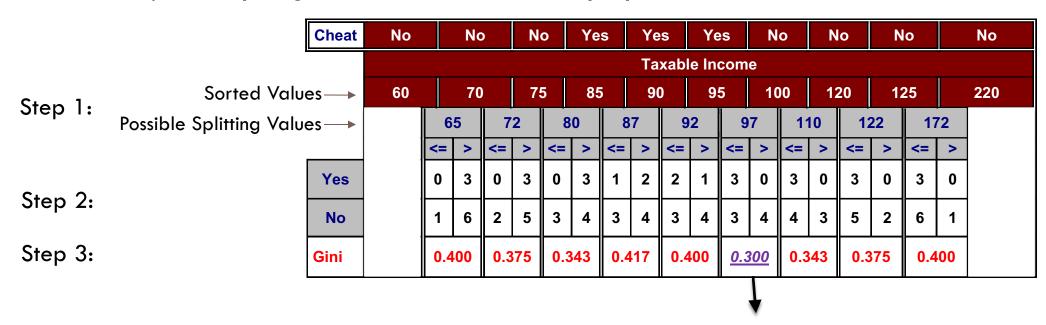


For each splitting value v (e.g., 72), compute its Gini index:

$$gini_{Taxable\_Income}(D) = \frac{|D_1|}{|D|}gini(D_1) + \frac{|D_2|}{|D|}gini(D_2)$$
 Here D1 and D2 are two partitions based on v: D1 has taxable income <=v and D2 has >v

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index



Choose this splitting value (=97) with the least Gini index to discretize Taxable Income

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing expected information requirement and choose the split position that has the least value

		Cheat	No	No No			N	0	Yes		Yes Ye		es N		No		o	No			No	
	•		Taxable Income																			
Step 1: Sorted Value Possible Splitting Value		es <b>→</b>			70		75		5 85		90		9	5 1		00		20	125		220	
		es→			65		72		80		87		2	97		110		122		172		
				<=	>	<=	>	<=	>	<=	>	<b>&lt;=</b>	>	<=	>	<=	>	<b>"</b>	>	<=	>	
C+		Yes		0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	
Step 2:	No		1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1		
Step 3:		Info		7	?	7	?		?		?	7	•	7		•	?	1	?	?	•	

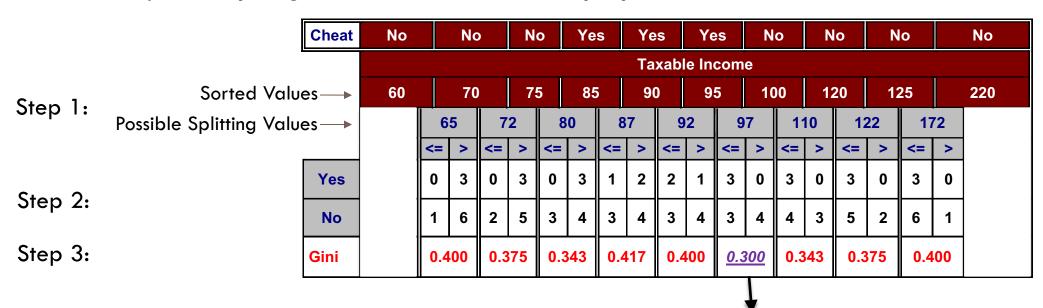
If Information Gain is used for attribute selection,

Similarly to calculating Gini index, for each splitting value, compute Info\_{Taxable Income}:

$$Info_{Taxable-Income}(D) = \sum_{j=1}^{2} \frac{|D_j|}{|D|} \times Info(D_j)$$

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

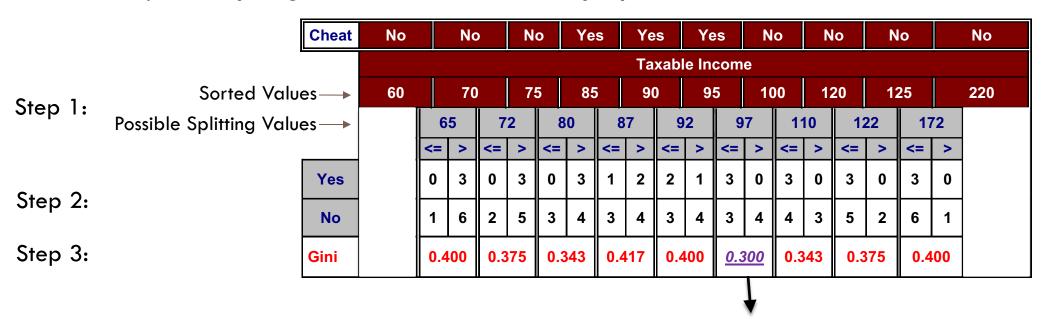


Choose this splitting value (=97 here) with the least Gini index or expected information requirement to discretize Taxable Income

# Continuous Attributes: Computing Gini Index or expected information requirement

#### First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index



At each level of the decision tree, for attribute selection, (1) First, discretize a continuous attribute by deciding the splitting value; (2) Then, compare the discretized attribute with other attributes in terms of Gini Index reduction or Information Gain.

# Continuous Attributes: Computing Gini Index or expected information requirement

#### First decide the splitting value to discretize the attribute:

For efficient computation: for each attribute,

Step 1: Sort the attribute on values

Step 2: Linearly scan these values, each time updating the count matrix

Step 3: Computing Gini index and choose the split position that has the least Gini index

Cheat No No No Yes Yes Yes No No No No **Taxable Income** Sorted Values 70 75 90 95 100 120 125 85 220 Step 1: Possible Splitting Values --> 65 72 80 87 92 97 122 172 110 <= > Yes Step 2: 4 | 3 | No Step 3: 0.400 0.375 0.343 0.417 0.400 0.300 0.343 0.375 0.400 Gini

At each level of the decision tree, for attribute selection, (1) First, discretize a continuous attribute by deciding the splitting value; (2) Then, compare the discretized attribute with other attributes in terms of Gini Index reduction or Information Gain.

For each attribute,

only scan the data

tuples once

## Another Impurity Measure: Misclassification Error

 $\square$  Classification error at a node t:

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

 $\blacksquare$  P(i|t) means the relative frequency of class i at node t.

- Measures misclassification error made by a node.
  - Maximum (1  $1/n_c$ ) when records are equally distributed among all classes, implying most impurity
  - Minimum (0.0) when all records belong to one class, implying least impurity

# Examples for Misclassification Error

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

$$P(C1) = 0/6 = 0$$
  $P(C2) = 6/6 = 1$ 

Error = 
$$1 - \max(0, 1) = 1 - 1 = 0$$

$$P(C1) = 1/6$$
  $P(C2) = 5/6$ 

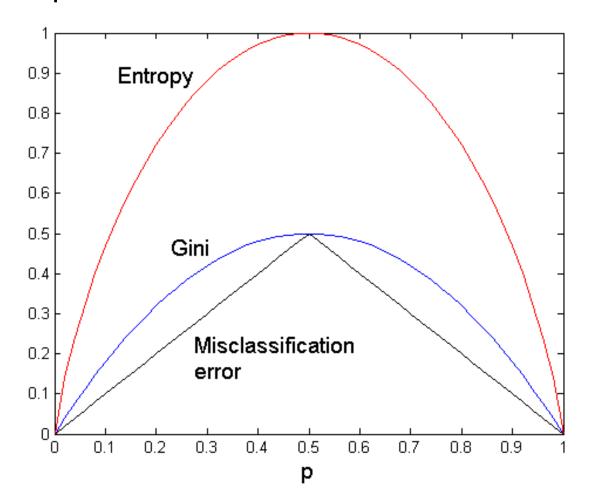
Error = 
$$1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

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

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

# Comparison among Impurity Measure

#### For a 2-class problem:



$$Entropy = -p \log(p) - (1-p) \log(1-p)$$

$$|Gini=1-p^2-(1-p)^2|$$

$$Error = 1 - \max(p, 1 - p)$$

### Other Attribute Selection Measures

- $\Box$  CHAID: a popular decision tree algorithm, measure based on  $\chi^2$  test for independence
- C-SEP: performs better than info. gain and gini index in certain cases
- $\Box$  G-statistic: has a close approximation to  $\chi^2$  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)
  - CART: 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

## 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

- 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 online, e.g., <a href="http://www2.cs.uregina.ca/~dbd/cs831/notes/ml/dtrees/c4.5/tutorial.html">http://www2.cs.uregina.ca/~dbd/cs831/notes/ml/dtrees/c4.5/tutorial.html</a>

# Classification: Basic Concepts

- □ Classification: Basic Concepts
- □ Decision Tree Induction
- □ Model Evaluation and Selection



- Practical Issues of Classification
- Bayes Classification Methods
- □ Techniques to Improve Classification Accuracy: Ensemble Methods
- Summary

## **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?

## 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)

## Classifier Evaluation Metrics: Confusion Matrix

#### **Confusion Matrix:**

Actual class\Predicted class	C <sub>1</sub>	¬ C <sub>1</sub>
C <sub>1</sub>	True Positives (TP)	False Negatives (FN)
¬ C <sub>1</sub>	False Positives (FP)	True Negatives (TN)

#### **Example of Confusion Matrix:**

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

- $\square$  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

A\P	С	¬C	
С	TP	FN	P
¬C	FP	TN	N
	P'	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)/AII

# Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If a 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

# Cost Matrix

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

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

# 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

$$Cost = 3910$$

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

$$Cost = 4255$$

## Cost-Sensitive Measures

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

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

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

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

- 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 = 
$$\frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

## Classifier Evaluation Metrics: Sensitivity and Specificity

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

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

$$Accuracy = (TP + TN)/AII$$

Error rate: 1 — accuracy, orError 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

## Methods for Performance Evaluation

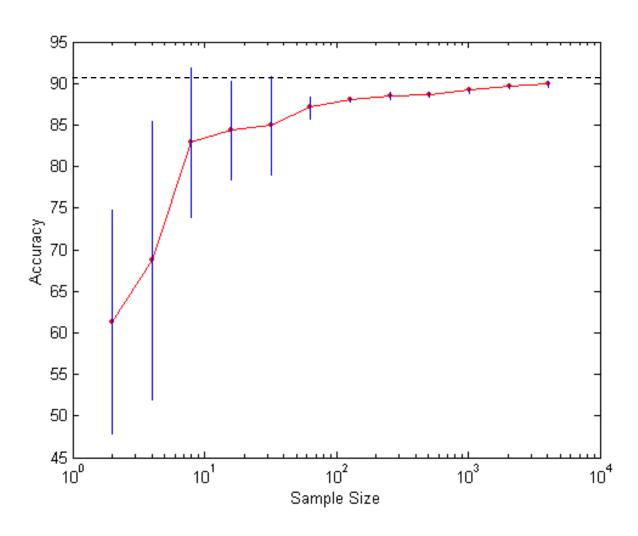
□ How to obtain a reliable estimate of performance?

- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution

Cost of misclassification

■ Size of training and test sets

# Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

#### Effect of small sample size:

- Bias in the estimate
- Variance of estimate

## Methods of Estimation

- □ Holdout
  - $\blacksquare$  E.g., 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

### 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
- $\Box$  Cross-validation (k-fold, where k = 10 is most popular)
  - $\blacksquare$  Randomly partition the data into k mutually exclusive subsets, each approximately equal size
  - $\blacksquare$  At *i*-th iteration, use  $D_i$  as test set and others as training set
  - Leave-one-out: k folds where k = # of tuples, for small sized data
  - \*Stratified cross-validation\*: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

## Evaluating Classifier Accuracy: Bootstrap

#### Bootstrap

- Works well with small data sets
- Samples the given training tuples uniformly with replacement
  - 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  $(1 1/d)^d \approx e^{-1} = 0.368$ )
  - $\square$  Repeat the sampling procedure k times, overall accuracy of the model:

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

## **Model Evaluation**

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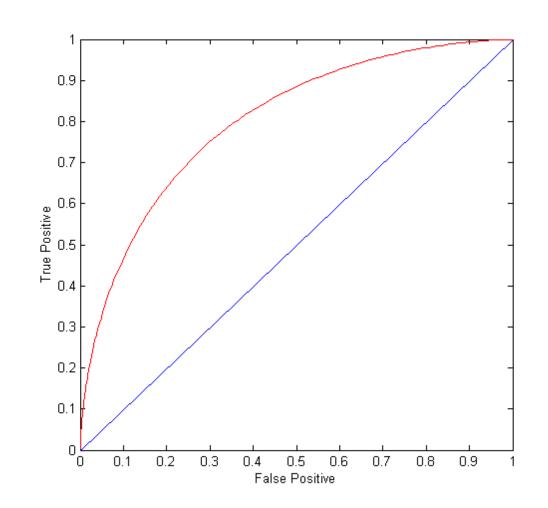
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- □ Methods for Model Comparison
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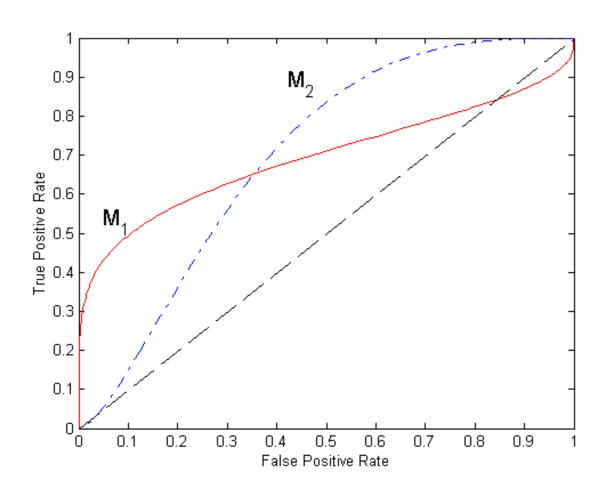
# ROC (Receiver Operating Characteristic) Curve

#### (False Positive Rate, True Positive Rate):

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



# Using ROC for Model Comparison



- No model consistently outperform the other
  - $\bullet$   $M_1$  is better for small FPR
  - M<sub>2</sub> is better for large FPR
- Area Under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess (diagonal line):
    - Area = 0.5

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