CSE 5243 INTRO. TO DATA MINING

Classification (Basic Concepts) Huan Sun, CSE@The Ohio State University

Slides adapted from UIUC CS412, Fall 2017, by Prof. Jiawei Han

Classification: Basic Concepts

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

This class

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

Next class

2

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

3

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})

ID3 algorithm: how it works

https://www.youtube.com/watch?v=_XhOdSLIE5c

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:

7

- If one of the stopping conditions is satisfied: STOP
- Else: Split (child_node, {subset})

ID3 algorithm: how it works

https://www.youtube.com/watch?v=_XhOdSLIE5c

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 \rightarrow higher uncertainty

• Lower entropy \rightarrow 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 _i	n _i	l(p _i , n _i)
<=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

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

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

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

Similarly,

Gain(income) = 0.029Gain(student) = 0.151Gain(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 $D = \{red data tuples\}$

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.





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:





Non-homogeneous,

High degree of impurity

Homogeneous,

Low degree of impurity

Measures of Node Impurity

Entropy:
$$H(Y) = -\sum_{i=1}^{m} p_i \log(p_i)$$
 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.

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)
<u>v</u> | D, | D, |

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

GainRatio(A) = Gain(A)/SplitInfo(A)

.

\Box Ex.

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

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

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
Gi	ni = ?

Binary Attributes: Computing Gini Index

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

Gini=?





	Parent
C1	6
C2	6
Gini	= 0.500

Gini(N1) = $1 - (5/7)^2 - (2/7)^2$ = 0.194

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

Binary Attributes: Computing Gini Index

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

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



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	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									

Continuous Attributes: Computing Gini Index or Information Gain

To discretize the attribute values	Tid	Refund	Marital Status	Taxable Income	Cheat
Use Binary Decisions based on one splitting value	1	Yes	Single	125K	No
	2	No	Married	100K	No
Several Choices for the splitting value	3	No	Single	70K	No
Number of possible splitting values = Number of distinct values -1	4	Yes	Married	120K	No
Typically, the midpoint between each pair of adjacent values is considered as a	5	No	Divorced	95K	Yes
possible split point	6	No	Married	60K	No
(a+a,)/2 is the midpoint between the values of a and a	7	Yes	Divorced	220K	No
$= (\mathbf{u}_i \cdot \mathbf{u}_{i+1})/2 \text{ is the interpolation between the values of \mathbf{u}_i and \mathbf{u}_{i+1}$			Single	85K	Yes
	9	No	Married	75K	No
Each splitting value has a count matrix associated with it	10	No	Single	90K	Yes
Class counts in each of the partitions, A < v and A \ge v		Та	axable	1	

Income

> 80K?

Yes

No

- □ 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.

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



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



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



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



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



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



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



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)	N	o Yes		S	Yes		Yes		No		No		No			No
	-			_				_		_	Ta	xabl	e Inc	com	e	_						
Stop 1.	Sorted Value	s►	60		70 7		7	75 85		5	90) 9		100		12	20	125			220
Slep 1:	Possible Splitting Values			65 7		7	72		80 8		87 92		2	97		110		122		172		
	-			<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	
		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:	Gini			0.4	00	0.3	575	0.3	343	0.4	17	0.4	00	<u>0.3</u>	<u>800</u>	0.3	43	0.3	575	0.4	00	
															ł	•						

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

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 expected information requirement and choose the split position that has the least value

		Cheat	No		No)	N	0	Ye	S	Ye	s	Ye	es	N	ю	N	lo	N	lo		No
				-			<u> </u>	÷		<u> </u>	Та	xabl	e In	com	е			_			-	
Stop 1.	Sorted Valu	es→	60		70)	7	5	85	5	9(D	9	5	1(00	1	20	1	25		220
Sieb I:	Possible Splitting Value	es→		6	5	7	2	8	0	8	7	9	2	9	7	11	10	1:	22	17	72	
				<=	>	<=	>	<=	>	<=	۸	<=	٨	<=	>	<=	>	<=	۸	<=	>	
Stars O		Yes		0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	
ътер ∠:		No		1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	
Step 3:		Info			?		?		?	4	?		?		?		?		?		?	
lf Informc	ition Gain is used	Sin	nilarly	to	cal	culo	atin	a C	Gini	inc	lex	, fo	r e	ach	sp	litti	ng	" valı	Je,	" com	וטמו	te Info
for attrib	ute selection,		7					J	Ι	nfo	Taxa	ble-1	Incon	ne (1):):	$=\sum_{i=1}^{2}$		$\frac{D_j}{D}$	$\times I$	nfo	(D_j)	,)

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)	N	0	Ye	s	Ye	s	Ye	es	N	0	N	0	N	lo		No
	-		Taxable Inco					com	ne													
Stop 1.	Sorted Value	s►	60		70)	7	5	85	;	9(D	9	5	10	00	12	20	12	25		220
Slep 1:	Possible Splitting Value	s		6	5	7	2	8	0	8	57	9	2	9	7	1'	0	12	22	17	2	
	-			<=	>	<=	>	<=	>	<=	>	<=	٧	<=	>	<=	>	<=	v	<=	۷	
		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:	•	Gini		0.4	00	0.3	75	0.3	843	0.4	117	0.4	100	<u>0.3</u>	<u>300</u>	0.3	43	0.3	575	0.4	00	

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

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		Nc)	N	0	Ye	S	Ye	s	Ye	es	N	0	N	lo	N	lo		No
			Taxable Inco						com	ie											
Stop 1.	Sorted Values	60		70)	7	5	85	5	9(0	9	5	10	00	12	20	12	25	 	220
Slep 1:	Possible Splitting Values		6	5	7	2	8	0	8	7	9	2	9	7	11	10	12	22	17	2	
			<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	
	Yes		0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	
Step 2:	No	1	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	
Step 3:	Gini		0.4	100	0.3	575	0.3	343	0.4	17	0.4	00	<u>0.3</u>	<u>300</u>	0.3	43	0.3	575	0.4	00	
		-							-												

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.

Computing Gini Index or expected information requirement

For each attribute,

only scan the data

tuples once

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

	Che	at No		No)	N	0	Ye	S	Ye	s	Ye	s	N	0	N	0	N	lo		No
			_			_	_		_	Та	xabl	e In	com	e		_				_	
Stop 1.	Sorted Values—	→ 60		70)	7	5	85	;	9()	9	5	10	00	12	20	12	25		220
Slep 1:	Possible Splitting Values—	→	6	5	7	2	8	0	8	7	9	2	9	7	11	0	12	22	17	2	
			<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	
	Yes	s	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:	Gini		0.4	00	0.3	575	0.3	43	0.4	17	0.4	00	<u>0.3</u>	<u>300</u>	0.3	43	0.3	575	0.4	00	
					-		-				-								-		

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. Another Impurity Measure: Misclassification Error

 \Box Classification error at a node t:

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

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

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

C1	0
C2	6

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

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

Comparison among Impurity Measure

For a 2-class problem:



Other Attribute Selection Measures

- \Box <u>CHAID</u>: a popular decision tree algorithm, measure based on χ^2 test for independence
- <u>C-SEP</u>: performs better than info. gain and gini index in certain cases
- \Box <u>G-statistic</u>: has a close approximation to χ^2 distribution
- □ <u>MDL (Minimal Description Length) principle</u> (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., <u>http://www2.cs.uregina.ca/~dbd/cs831/notes/ml/dtrees/c4.5/tutorial.html</u>

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

45

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

Given m classes, an entry, CM_{i,i} 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	¬С	
С	ТР	FN	Р
¬C	FP	TN	Ν
	P'	N'	All

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

Accuracy = (TP + TN)/All

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

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=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 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 ₁	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
		60	250

Accuracy = 80%Cost = 3910

Model M ₂	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	250	45
	-	5	200

Accuracy = 90%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
ACTUALCLASS	Class=Yes	a <mark>(TP)</mark>	b <mark>(FN)</mark>
	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	¬С	
С	ΤР	FN	Ρ
¬C	FP	TN	Ν
	P'	N'	All

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

Accuracy = (TP + TN)/AII

Class Imbalance Problem:

- One class may be rare, e.g. fraud, or HIVpositive
- 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

- **\square** 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
- <u>Random sampling</u>: 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
 - **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 ≈ 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

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?

ROC Curve

(TP,FP):

- (0,0): declare everything
 to be negative class
- (1,1): declare everything
 to be positive class
- □ (1,0): 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
 - \square M₁ is better for small FPR
 - \square M₂ is better for large FPR
- Area Under the ROC curve
 - Ideal:
 - Area = 1
 - Random guess (diagonal line):
 - Area = 0.5

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

63