## Classification: Basic Concepts and Decision Trees

# A programming task



#### 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.

#### Illustrating Classification Task



**Test Set** 

## 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 Using Distance

- Place items in class to which they are "closest".
- Must determine distance between an item and a class.
- Classes represented by
  - Centroid: Central value.
  - Medoid: Representative point.
  - Individual points
- Algorithm: KNN

## KNearest Neighbor (KNN):

- Training set includes classes.
- Examine K items near item to be classified.
- New item placed in class with the most number of close items.
- O(q) for each tuple to be classified.
  (Here q is the size of the training set.)

#### KNN



#### Classification Techniques

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

#### Example of a Decision Tree





**Training Data** 

**Model: Decision Tree** 

#### Another Example of Decision Tree

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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	Single	90K	Yes

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

#### Decision Tree Classification Task



**Test Set** 



Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?





#### Refund Marital **Taxable** Cheat **Status** Income ? Married 80K No Refund Yes No NO **MarSt** Married Single, Divorced **TaxInc** NO < 80K > 80K YES NO







#### Decision Tree Classification Task

Tid    1    2    3    4    5    6    7    8    9	Attrib1 Yes No Yes No Yes No No No	Attrib2 Large Medium Small Medium Large Medium Large Small Medium	Attrib3 125K 100K 70K 120K 95K 60K 220K 85K 75K	Class No No No Yes No Yes No
No Med Yes Larg No Sma No Med No Sma	Med Larg Sma Med Sma	ium e II ium II	60K 220K 85K 75K 90K	No No Yes No Yes
Tid	I ra	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

#### 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 that reach a node t
- General Procedure:
  - If D<sub>t</sub> contains records that belong the same class y<sub>t</sub>, then t is a leaf node labeled as y<sub>t</sub>
  - If D<sub>t</sub> is an empty set, then t is a leaf node labeled by the default class, y<sub>d</sub>
  - If D<sub>t</sub> contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

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	Single	90K	Yes





#### 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

#### 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

## 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
  - 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 $(A \ge v)$

- consider all possible splits and finds the best cut
- 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

- 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

#### Greedy approach:

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

Non-homogeneous, High degree of impurity C0: 9 C1: 1

Homogeneous,

Low degree of impurity

## Measures of Node Impurity

Gini Index

Entropy

Misclassification error

#### How to Find the Best Split



## Measure of Impurity: GINI

Gini Index for a given node t :

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

(NOTE: p(j | 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



## Examples for computing GINI

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

C1	0
C2	6

J		
P(C1) = 0/6 = 0	P(C2)	= 6/6 = 1
Gini = 1 – P(C1) <sup>2</sup>	<sup>2</sup> – 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) = 4/6Gini = 1 - (2/6)<sup>2</sup> - (4/6)<sup>2</sup> = 0.444

## 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.



### 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

Two-way split (find best partition of values)

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

	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

- 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</p>
- 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	Single	90K	Yes



# 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

	Cheat		No		Nc	)	N	0	Ye	s	Ye	s	Ye	s	N	0	N	0	N	0		No	
•											Ta	xabl	e In	com	е								
Sorted Values		(	60		70	)	7	5	85	5	90	)	9	5	10	00	12	20	12	25		220	
Split Positions	5	5	5	6	5	7	2	8	0	8	7	9	2	9	7	11	0	12	22	17	<b>'</b> 2	23	0
•		<=	<b>N</b>	<=	۷	<=	^	<=	٨	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
	Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
	No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
	Gini	0.4	20	0.4	00	0.3	<b>575</b>	0.3	343	0.4	17	0.4	00	<u>0.:</u>	<u>300</u>	0.3	43	0.3	575	0.4	00	0.4	20

# Alternative Splitting Criteria based on INFO

Entropy at a given node t:

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

(NOTE: p(j | 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

# Examples for computing Entropy

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

C1	0
C2	6

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

C1	1
C2	5

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

C1	2
C2	4

P(C1) = 2/6 P(C2) = 4/6 Entropy =  $-(2/6) \log_2 (2/6) - (4/6) \log_2 (4/6) = 0.92$ 

#### 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.

#### Splitting Based on INFO...

#### Gain Ratio:

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

Parent Node, p is split into k partitions  $n_i$  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

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

## 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

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

# Comparison among Splitting Criteria

#### For a 2-class problem:



#### Misclassification Error vs Gini



	Parent
C1	7
C2	3
Gini	= 0.42

Gini(N1) = 1 - (3/3)<sup>2</sup> - (0/3)<sup>2</sup> = 0

Gini(N2) = 1 - (4/7)<sup>2</sup> - (3/7)<sup>2</sup> = 0.489

Gini(Children) = 3/10 \* 0 + 7/10 \* 0.489 = 0.342

#### 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 all the records have similar attribute values

Early termination (to be discussed later)

#### 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 from: <u>http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.</u> gz

#### Practical Issues of Classification

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

# Underfitting and Overfitting (Example)



500 circular and 500 triangular data points.

Circular points:  $0.5 \le \operatorname{sqrt}(x_1^2 + x_2^2) \le 1$ 

Triangular points:  $sqrt(x_1^2+x_2^2) > 0.5$  or  $sqrt(x_1^2+x_2^2) < 1$ 

## Underfitting and Overfitting



Underfitting: when model is too simple, both training and test errors are large

#### Overfitting due to Noise



#### Decision boundary is distorted by noise point

# 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

## Notes on Overfitting

Overfitting results in decision trees that are more complex than necessary

Training error no longer provides a good estimate of how well the tree will perform on previously unseen records

Need new ways for estimating errors

#### Estimating Generalization Errors

- **Re-substitution errors:** error on training ( $\Sigma$  e(t)) **\Box** Generalization errors: error on testing ( $\Sigma$  e'(t))
- Methods for estimating generalization errors:
  - Optimistic approach: e'(t) = e(t)
  - Pessimistic approach:
    - For each leaf node: e'(t) = (e(t)+0.5)
    - Total errors:  $e'(T) = e(T) + N \times 0.5$  (N: number of leaf nodes)
    - For a tree with 30 leaf nodes and 10 errors on training п. (out of 1000 instances): Training error = 10/1000 = 1%

Generalization error =  $(10 + 30 \times 0.5)/1000 = 2.5\%$ 

- Reduced error pruning (REP):
  - uses validation data set to estimate generalization п error

#### Occam's Razor

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
- For complex models, there is a greater chance that it was fitted accidentally by errors in data
- Therefore, one should include model complexity when evaluating a model

# Minimum Description Length (MDL)



- □ Cost(Model,Data) = Cost(Data|Model) + Cost(Model)
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- Cost(Data|Model) encodes the misclassification errors.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding.

#### 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 χ<sup>2</sup> test)
  - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

#### 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

## Example of Post-Pruning



### Examples of Post-pruning

- Optimistic error?
  Don't prune for both cases
- Pessimistic error?

Don't prune case 1, prune case 2

Reduced error pruning?

![](_page_65_Figure_5.jpeg)

![](_page_65_Figure_6.jpeg)

![](_page_65_Figure_7.jpeg)

# 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

## 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
		Missin	g	

value

**Before Splitting:** 

Entropy(Parent)

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

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

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

Entropy(Refund=Yes) = 0

Entropy(Refund=No)

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

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

Gain = 0.9 × (0.8813 – 0.551) = 0.3303

#### Distribute Instances

Tid	Refund	Marita Status	 ;	Taxable Income	CI	ass	
1	Yes	Single		125K	No	C	
2	No	Marrie	d	100K	No	C	
3	No	Single		70K	No	c	
4	Yes	Marrie	d	120K No		C	
5	No	Divorc	ed	I 95K		Yes	
6	No	Marrie	d	60K	No	C	
7	Yes	Divorc	ed	d 220K		No	
8	No	Single		85K	Ye	es	
9	No	Marrie	d	75K	No	C	
Yes No							
Class	=Yes	0	C	Cheat=Y	es	2	
Class=No		3		Cheat=N	4		

![](_page_68_Figure_2.jpeg)

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

#### Classify Instances

![](_page_69_Figure_1.jpeg)

#### Scalable Decision Tree Induction Methods

#### SLIQ (EDBT'96 — Mehta et al.)

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