

# **Data Mining**

## **Classification: Basic Concepts, Decision Trees, and Model Evaluation**

Lecture Notes for Chapter 4

Introduction to Data Mining  
by

Tan, Steinbach, Kumar

(modified by Predrag Radivojac, 2017)

# 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.

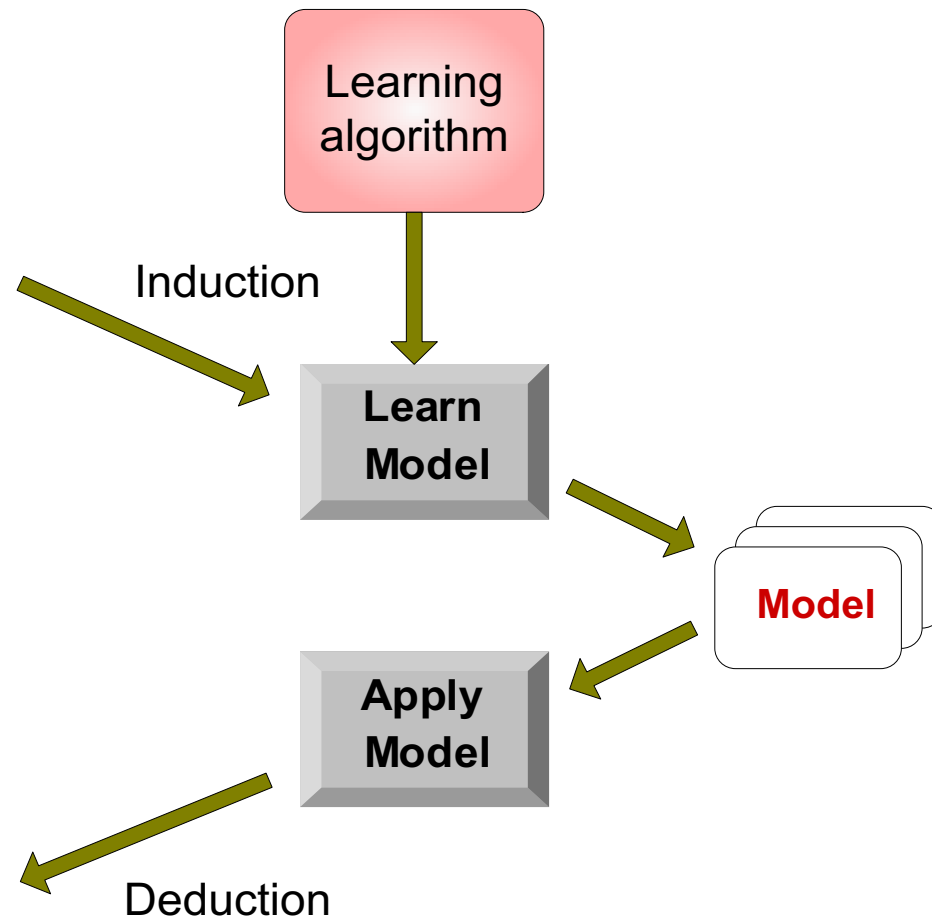
# Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

Tid	Attrib1	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



# Examples of Classification Task

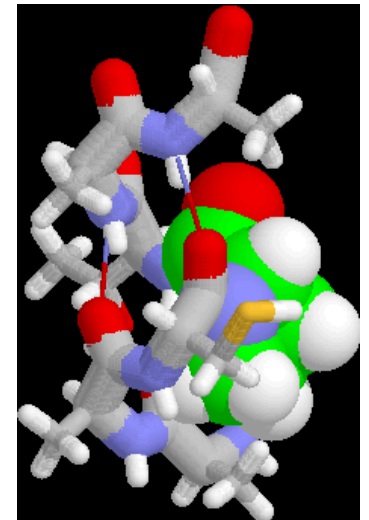
- Predicting tumor cells as benign or malignant

- Classifying credit card transactions as legitimate or fraudulent



- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil

- Categorizing news stories as finance, weather, entertainment, sports, etc



# Classification Techniques

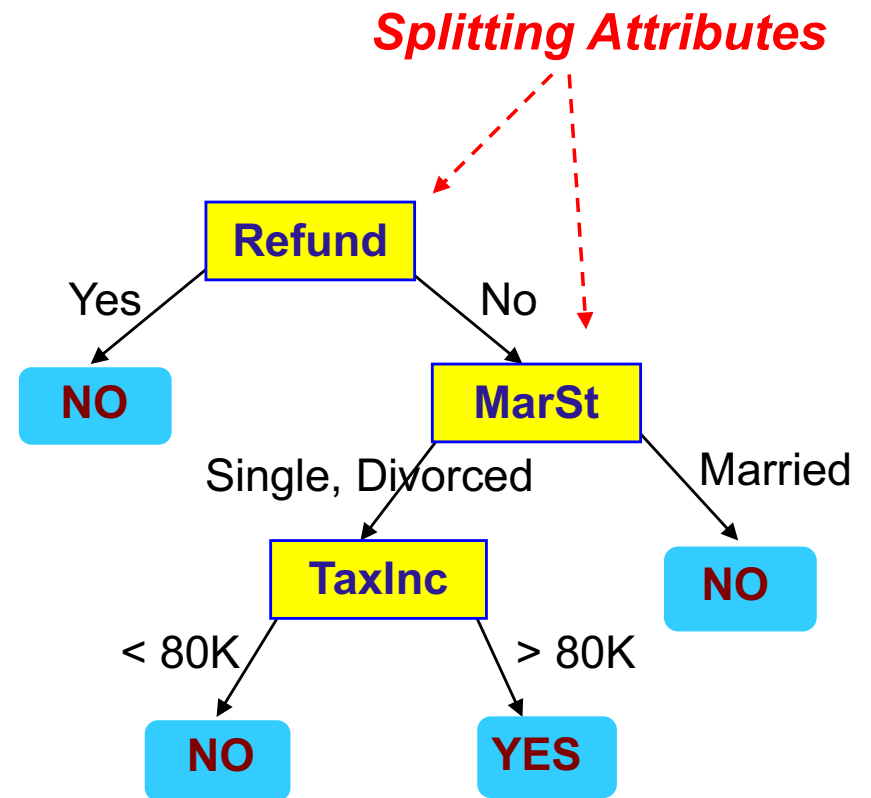
- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines

# Example of a Decision Tree

<i>Tid</i>	<i>Refund</i>	<i>Marital Status</i>	<i>Taxable Income</i>	<i>Cheat</i>
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

*categorical*  
*categorical*  
*continuous*  
*class*

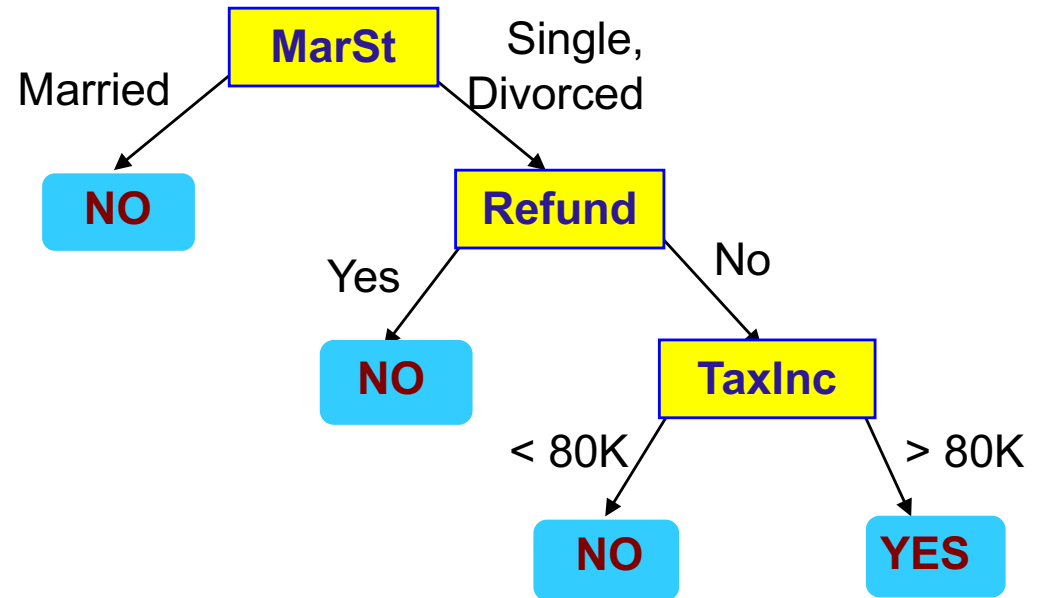
Training Data



Model: Decision Tree

# Another Example of Decision Tree

<i>Tid</i>	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



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

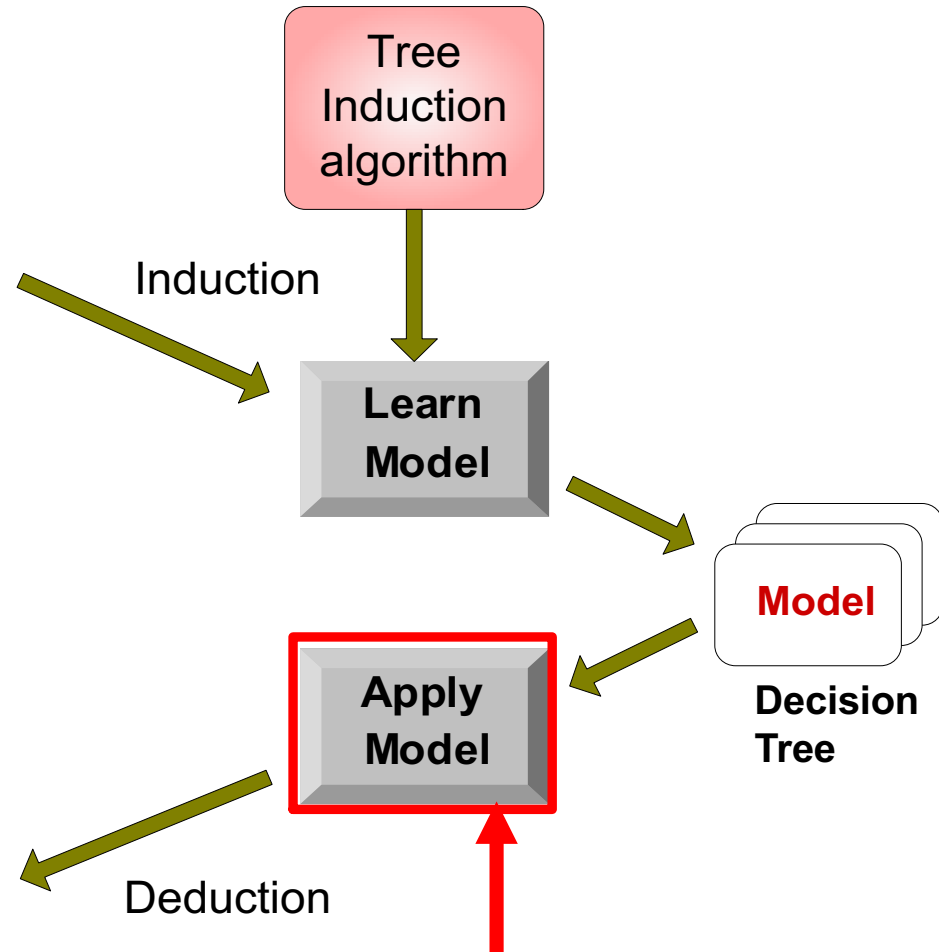
# Decision Tree Classification Task

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Training Set

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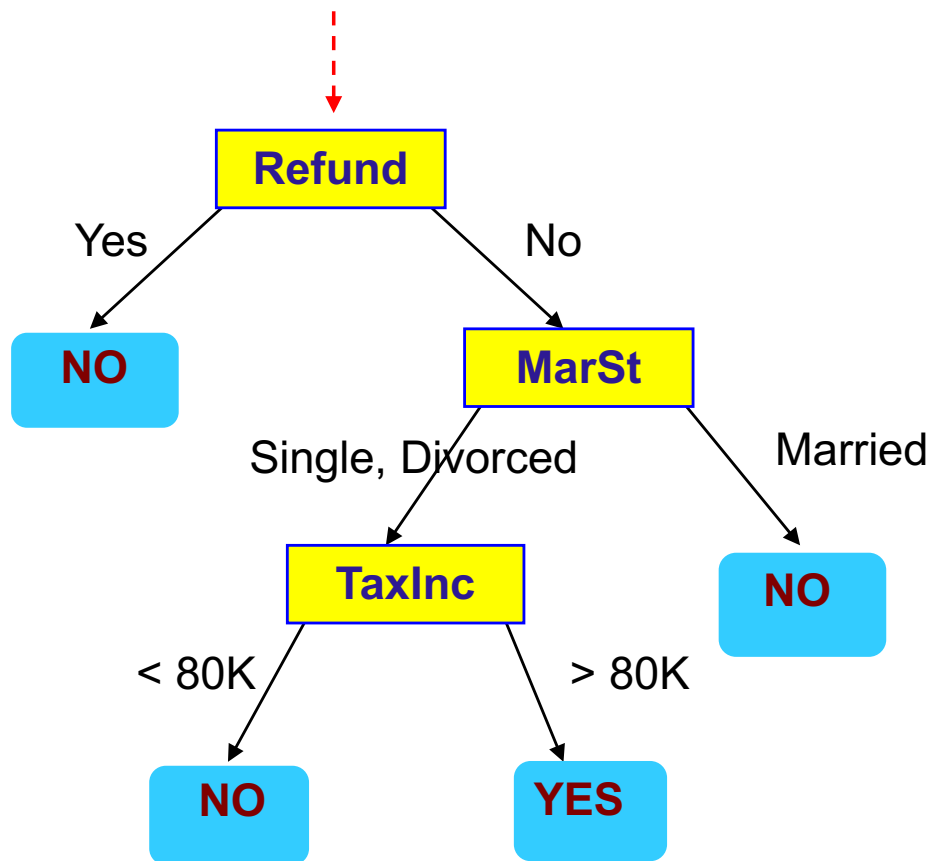
Test Set





# Apply Model to Test Data

Start from the root of tree.



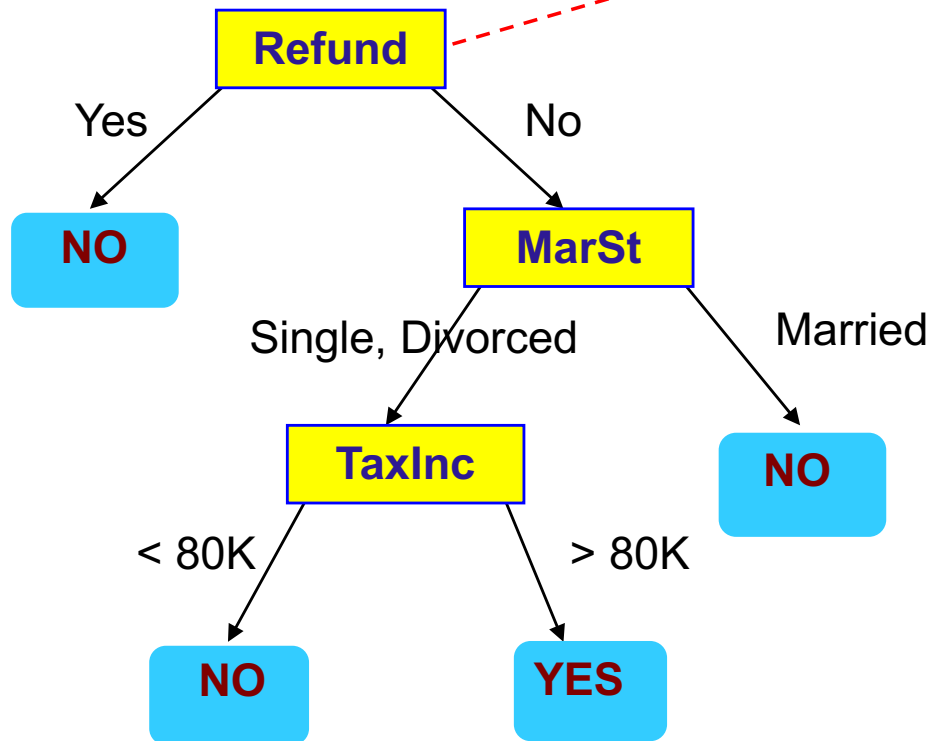
## Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

# Apply Model to Test Data

## Test Data

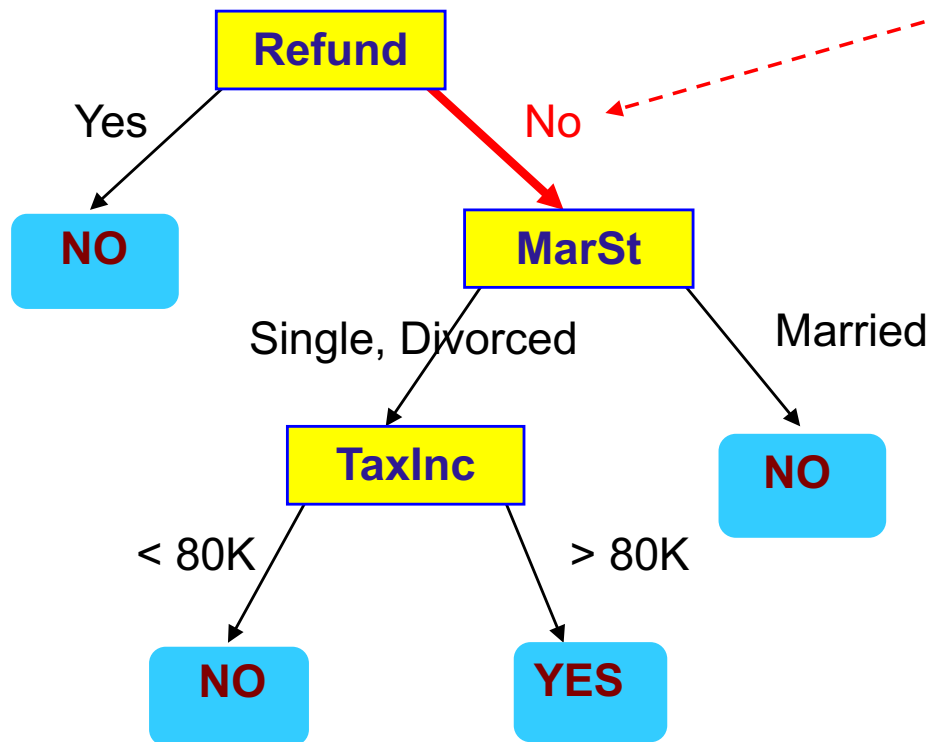
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

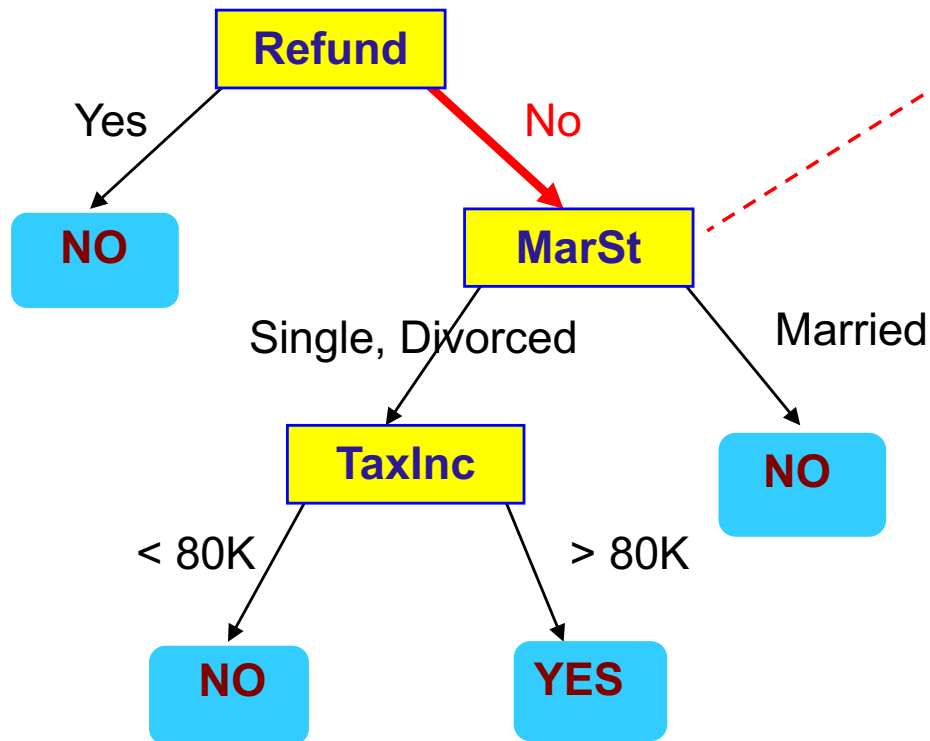
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

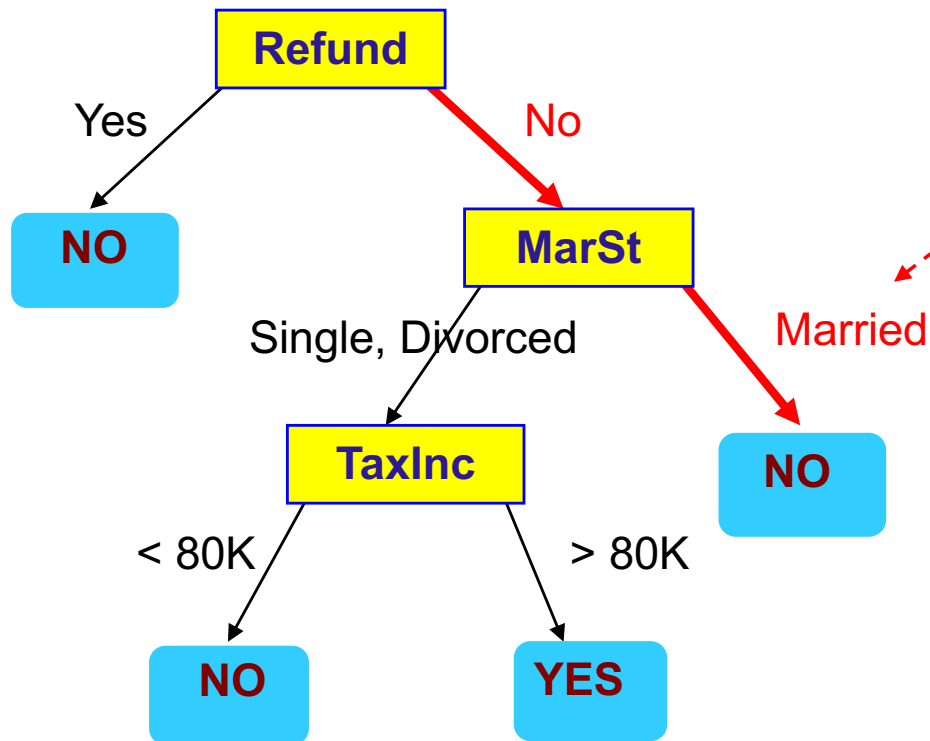
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

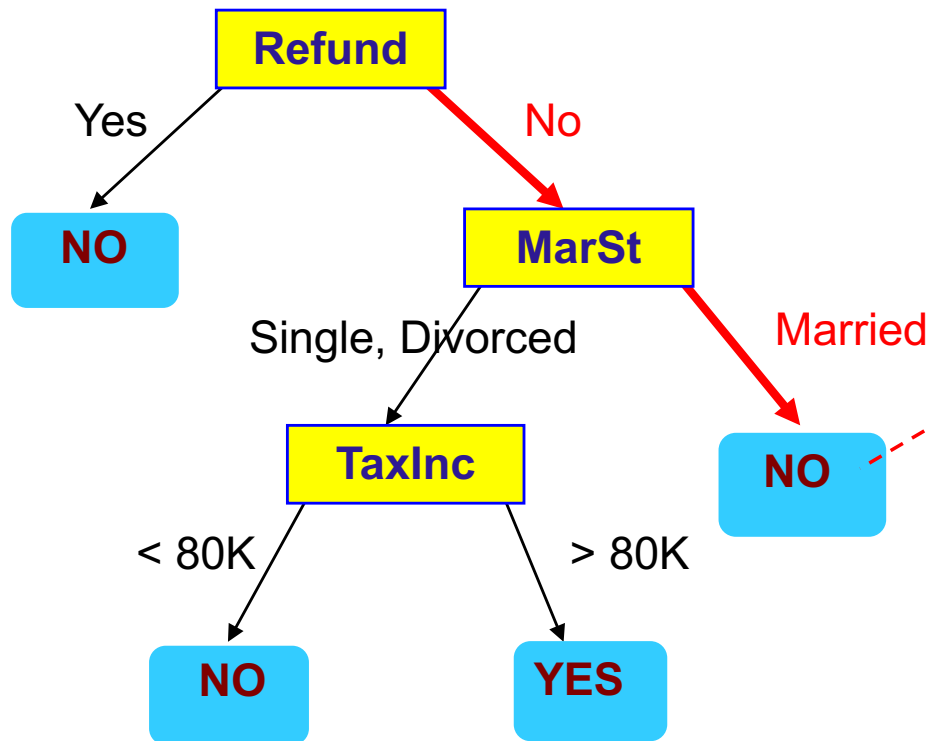
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to "No"

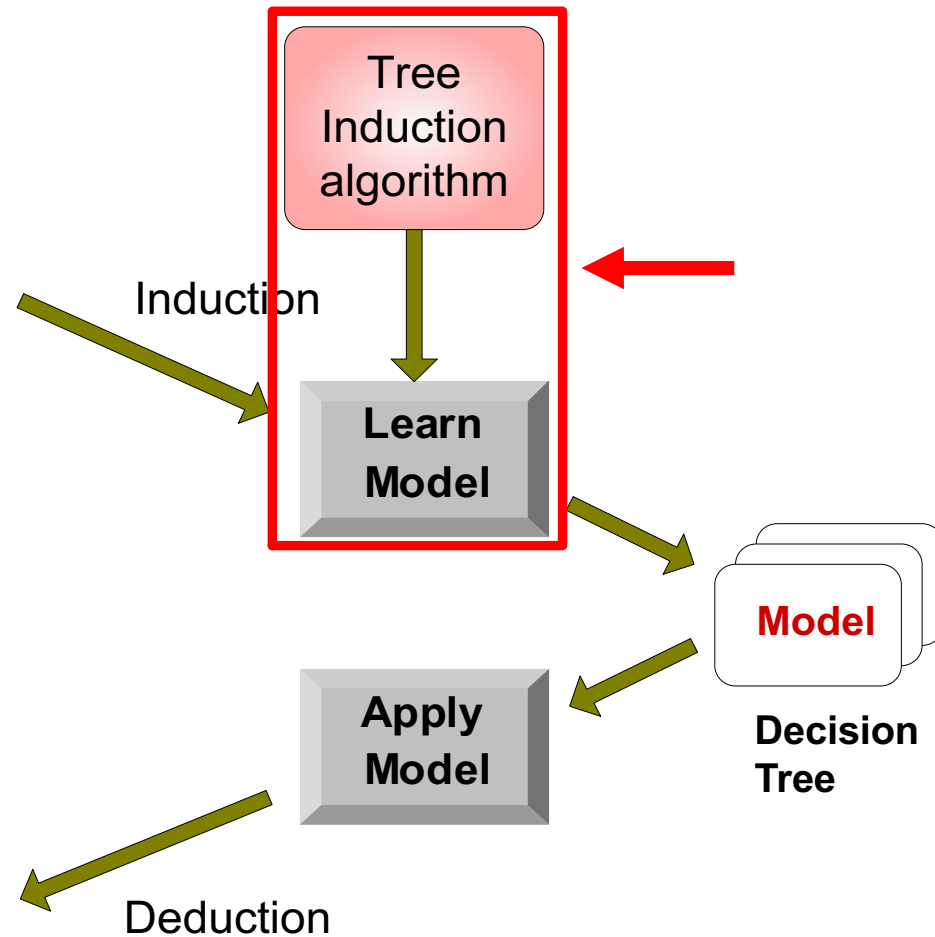
# Decision Tree Classification Task

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Test Set



# Decision Tree Induction

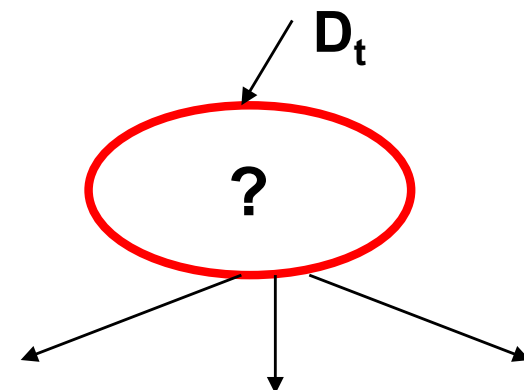
- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ, SPRINT



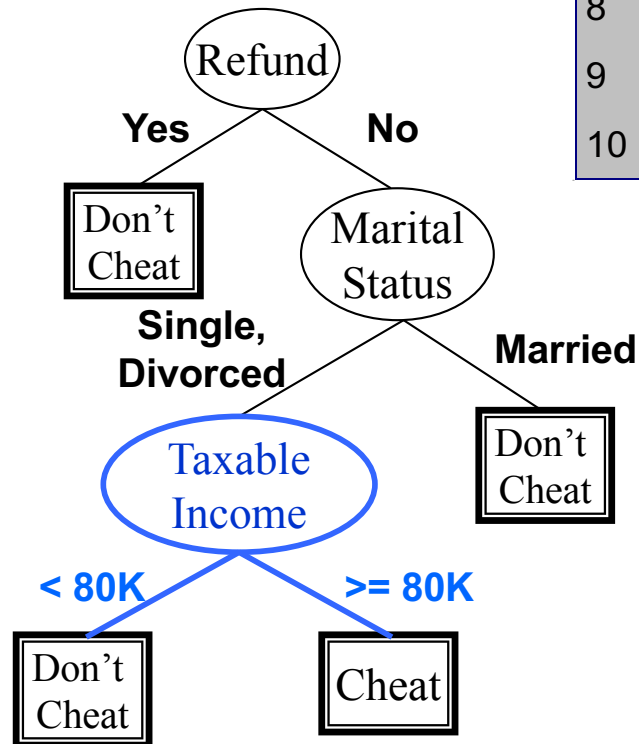
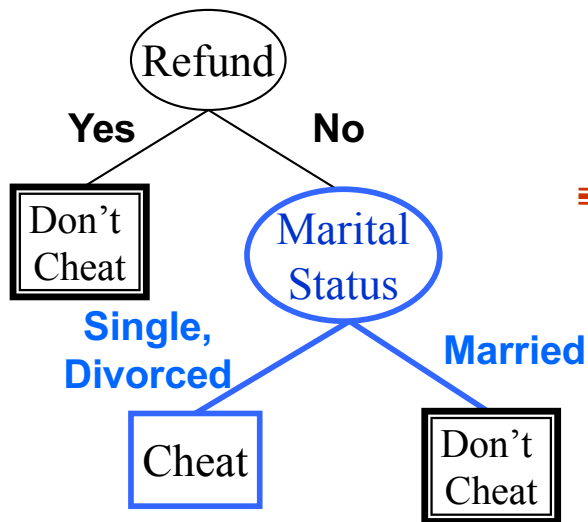
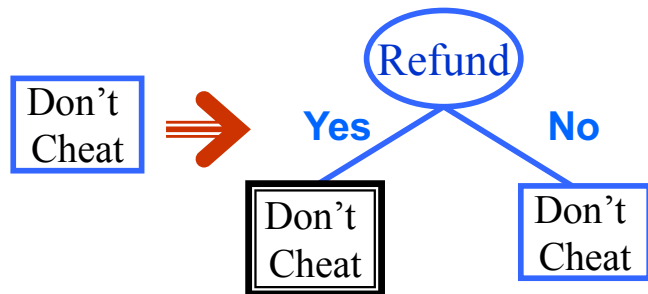
# General Structure of Hunt's Algorithm

- Let  $D_t$  be the set of training records that reach a node  $t$
- General Procedure:
  - If  $D_t$  contains records that belong the same class  $y_t$ , then  $t$  is a leaf node labeled as  $y_t$
  - If  $D_t$  is an empty set, then  $t$  is a leaf node labeled by the default class,  $y_d$
  - If  $D_t$  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.

<i>Tid</i>	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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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



# Hunt's Algorithm



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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

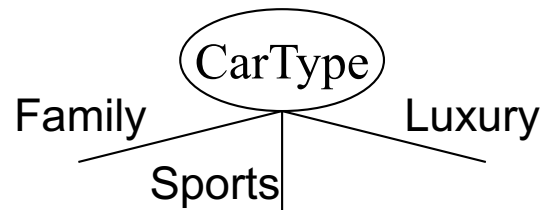
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# How to Specify Test Condition?

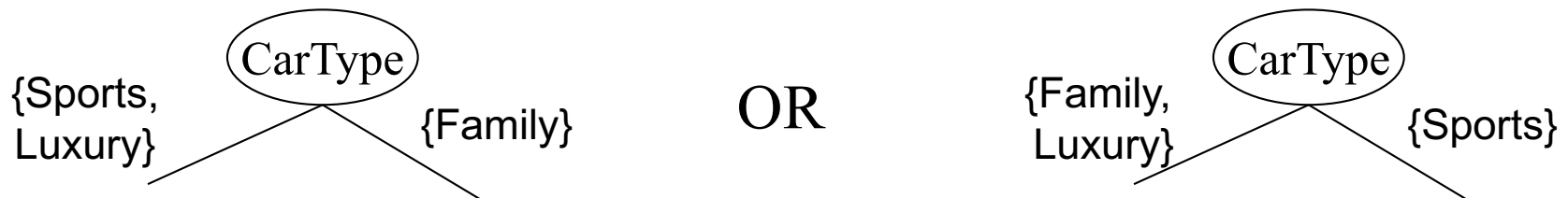
- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

# Splitting Based on Nominal Attributes

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

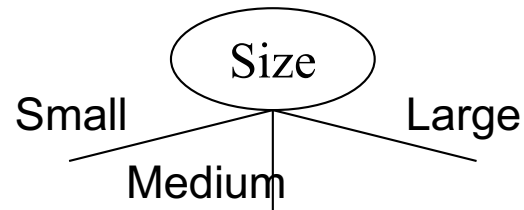


- **Binary split:** Divides values into two subsets.  
Need to find optimal partitioning.

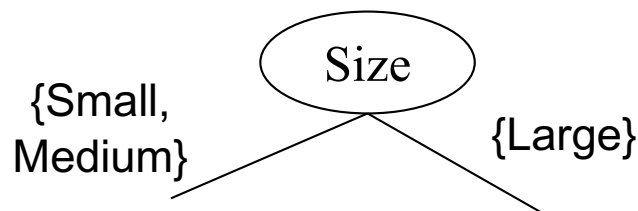


# Splitting Based on Ordinal Attributes

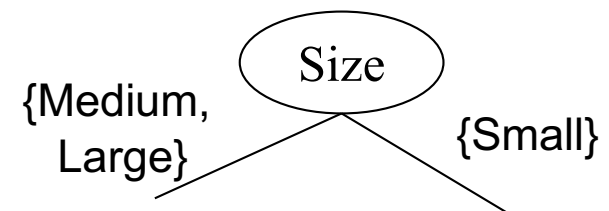
- **Multi-way split:** Use as many partitions as distinct values.



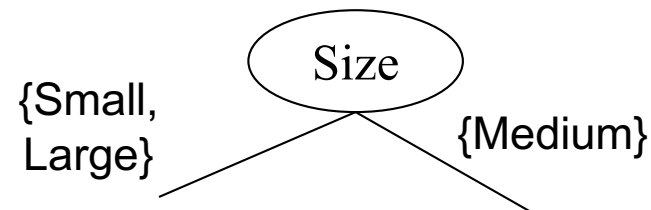
- **Binary split:** Divides values into two subsets.  
Need to find optimal partitioning.



OR



- What about this split?

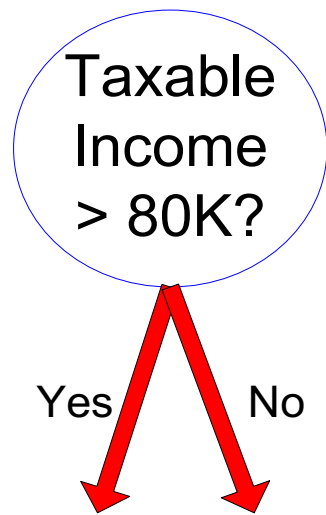


# Splitting Based on Continuous Attributes

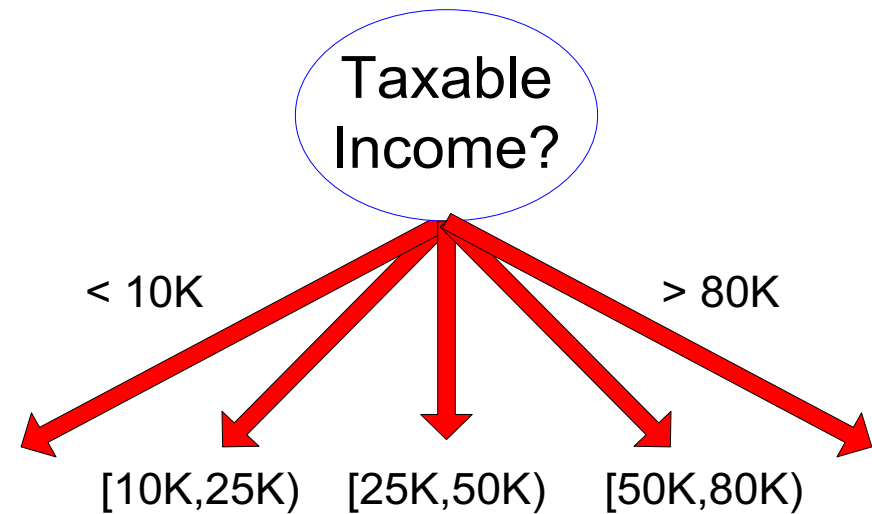
- Different ways of handling
  - **Discretization** to form an ordinal categorical attribute
    - ◆ Static – discretize once at the beginning
    - ◆ Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - **Binary Decision**:  $(A < v)$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



# Splitting Based on Continuous Attributes



(i) Binary split



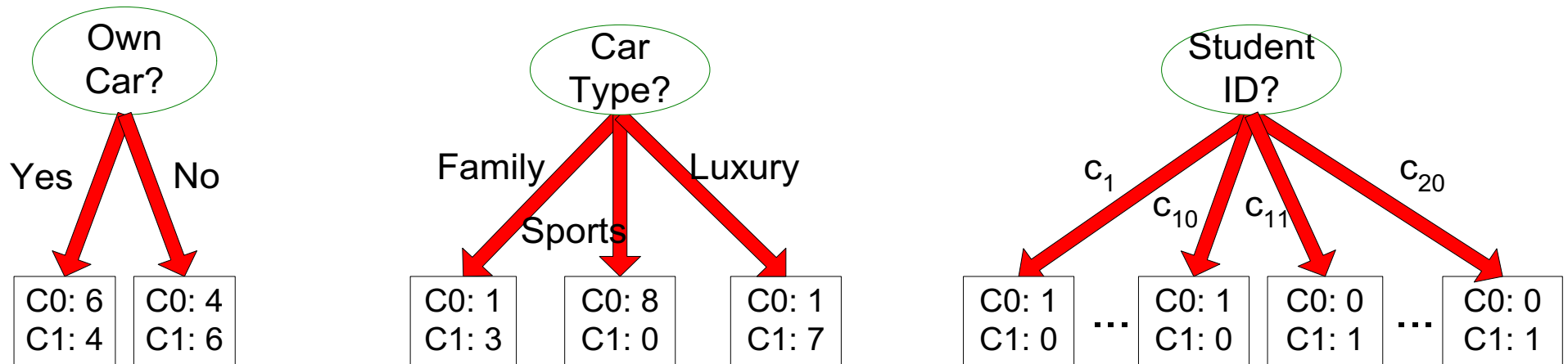
(ii) Multi-way split

# 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:

C0: 5
C1: 5

**Non-homogeneous,  
High degree of impurity**

C0: 9
C1: 1

**Homogeneous,  
Low degree of impurity**

# Measures of Node Impurity

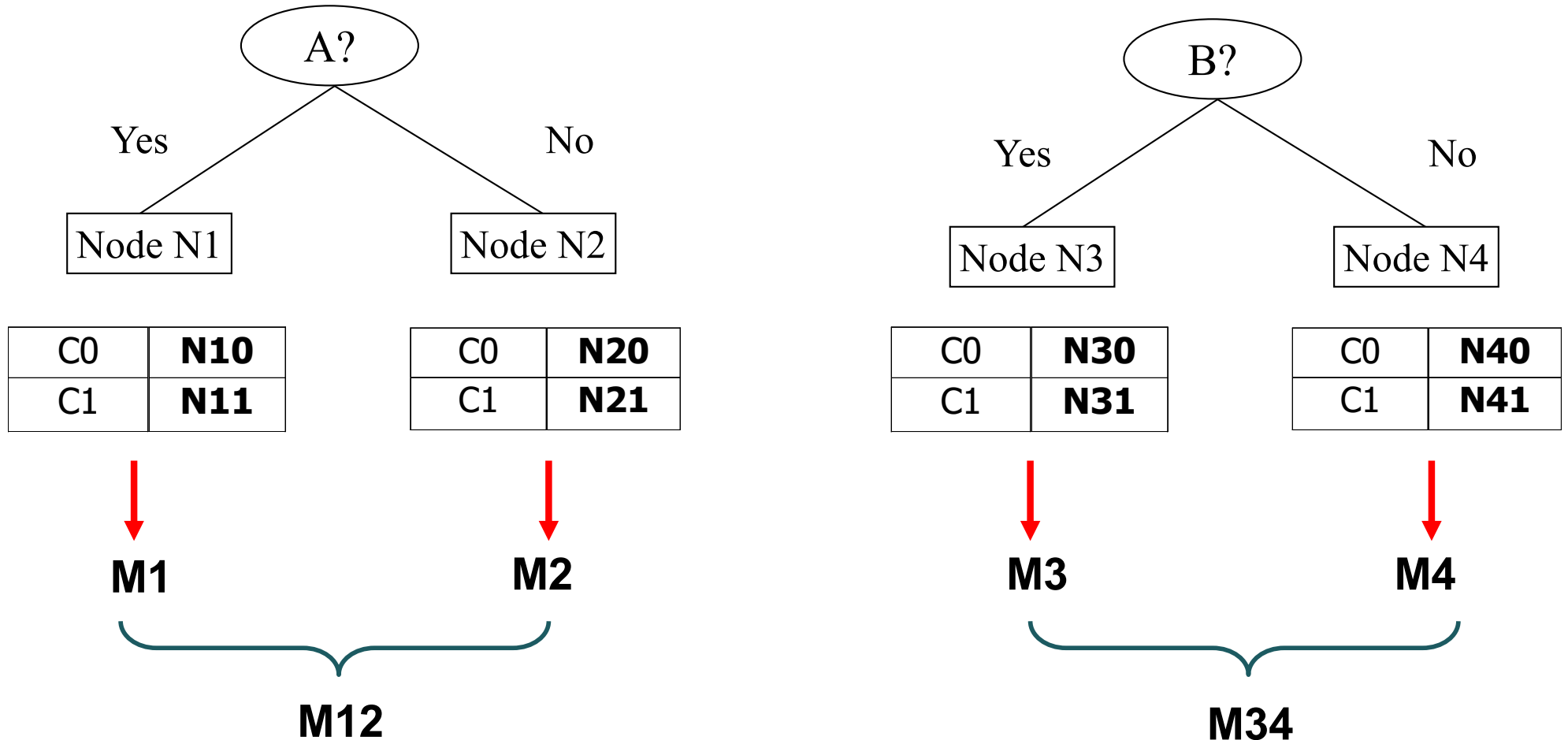
- Gini Index
- Entropy
- Misclassification error

# How to Find the Best Split

Before Splitting:

C0	<b>N00</b>
C1	<b>N01</b>

→ **M0**



$$\text{Gain} = M0 - M12 \text{ vs } M0 - M34$$

# 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  $(1 - 1/n_c)$  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

C1	<b>0</b>
C2	<b>6</b>
<b>Gini=0.000</b>	

C1	<b>1</b>
C2	<b>5</b>
<b>Gini=0.278</b>	

C1	<b>2</b>
C2	<b>4</b>
<b>Gini=0.444</b>	

C1	<b>3</b>
C2	<b>3</b>
<b>Gini=0.500</b>	

# Examples for computing GINI

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

C1	<b>0</b>
C2	<b>6</b>

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

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

C1	<b>1</b>
C2	<b>5</b>

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

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

C1	<b>2</b>
C2	<b>4</b>

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

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



# Splitting Based on GINI

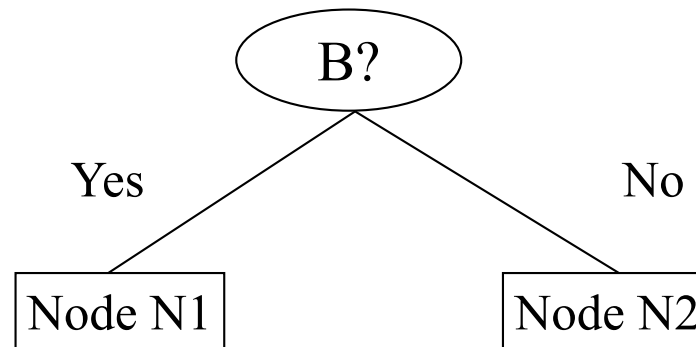
- Used in CART, SLIQ, SPRINT.
- When a node  $p$  is split into  $k$  partitions (children), the quality of split is computed as,

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

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.



$$\begin{aligned}
 \text{Gini}(N1) &= 1 - (5/6)^2 - (2/6)^2 \\
 &= 0.194
 \end{aligned}$$

$$\begin{aligned}
 \text{Gini}(N2) &= 1 - (1/6)^2 - (4/6)^2 \\
 &= 0.528
 \end{aligned}$$

	N1	N2
C1	5	1
C2	2	4
<b>Gini=0.333</b>		

	Parent
C1	6
C2	6
<b>Gini = 0.500</b>	

$$\begin{aligned}
 \text{Gini(Children)} &= 7/12 * 0.194 + \\
 &\quad 5/12 * 0.528 \\
 &= 0.333
 \end{aligned}$$

**This calculation is not correct! Why?**

# Categorical Attributes: Computing Gini Index

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

Multi-way split

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

Two-way split  
(find best partition of values)

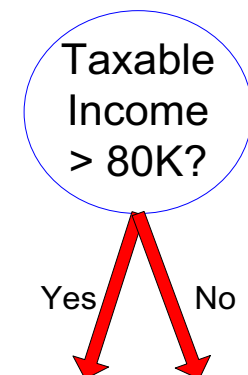
	CarType	
	{Sports, Luxury}	{Family}
C1	3	1
C2	2	4
Gini	0.400	

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

# 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.

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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	No	No	Yes	Yes	Yes	No	No	No	No											
Sorted Values Split Positions	→	Taxable Income																					
		60		70		75		85		90		95		100		120		125		220			
		55		65		72		80		87		92		97		110		122		172		230	
		<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
	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	0.420		0.400		0.375		0.343		0.417		0.400		<u>0.300</u>		0.343		0.375		0.400		0.420	

# 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 ( $\log n_c$ ) 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

$$Entropy(t) = -\sum_j p(j | t) \log_2 p(j | t)$$

C1	<b>0</b>
C2	<b>6</b>

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

$$Entropy = -0 \log 0 - 1 \log 1 = -0 - 0 = 0$$

C1	<b>1</b>
C2	<b>5</b>

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

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

C1	<b>2</b>
C2	<b>4</b>

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

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

# 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;

$n_i$  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:

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

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  $t$  :

$$Error(t) = 1 - \max_i P(i | t)$$

- Measures misclassification error made by a node.
  - ◆ 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

# Examples for Computing Error

$$Error(t) = 1 - \max_i P(i | t)$$

C1	<b>0</b>
C2	<b>6</b>

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

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

C1	<b>1</b>
C2	<b>5</b>

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

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

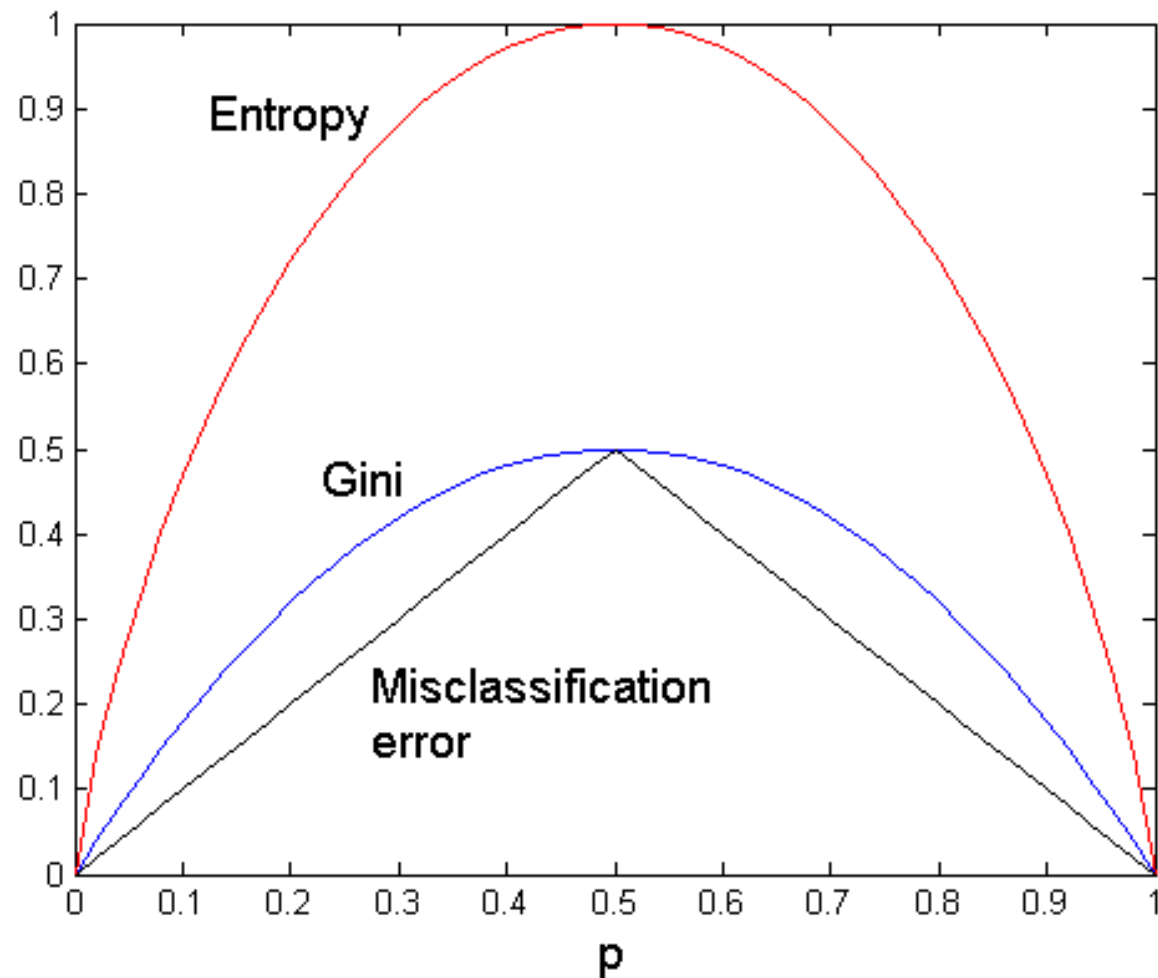
C1	<b>2</b>
C2	<b>4</b>

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

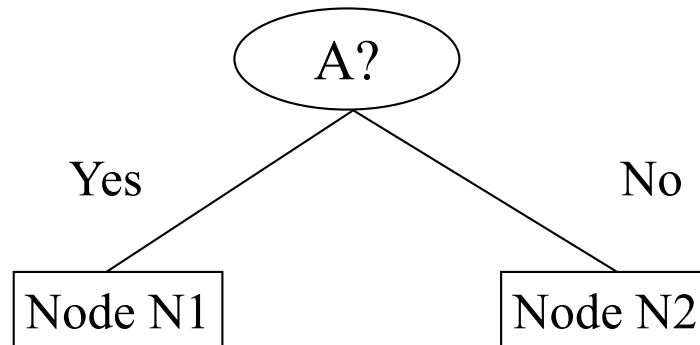
$$Error = 1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$$

# Comparison among Splitting Criteria

For a 2-class problem:



# Misclassification Error vs Gini



	Parent
C1	<b>7</b>
C2	<b>3</b>
<b>Gini = 0.42</b>	

$$\begin{aligned}
 &\text{Gini(N1)} \\
 &= 1 - (3/3)^2 - (0/3)^2 \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 &\text{Gini(N2)} \\
 &= 1 - (4/7)^2 - (3/7)^2 \\
 &= 0.489
 \end{aligned}$$

	N1	N2
C1	<b>3</b>	<b>4</b>
C2	<b>0</b>	<b>3</b>
<b>Gini=0.361</b>		

$$\begin{aligned}
 &\text{Gini(Children)} \\
 &= 3/10 * 0 \\
 &+ 7/10 * 0.489 \\
 &= 0.342
 \end{aligned}$$

**Gini improves !!**

# Tom Mitchell's example

Day	Outlook	Temperature	Humidity	Wind	Play Tennis?
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

# 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

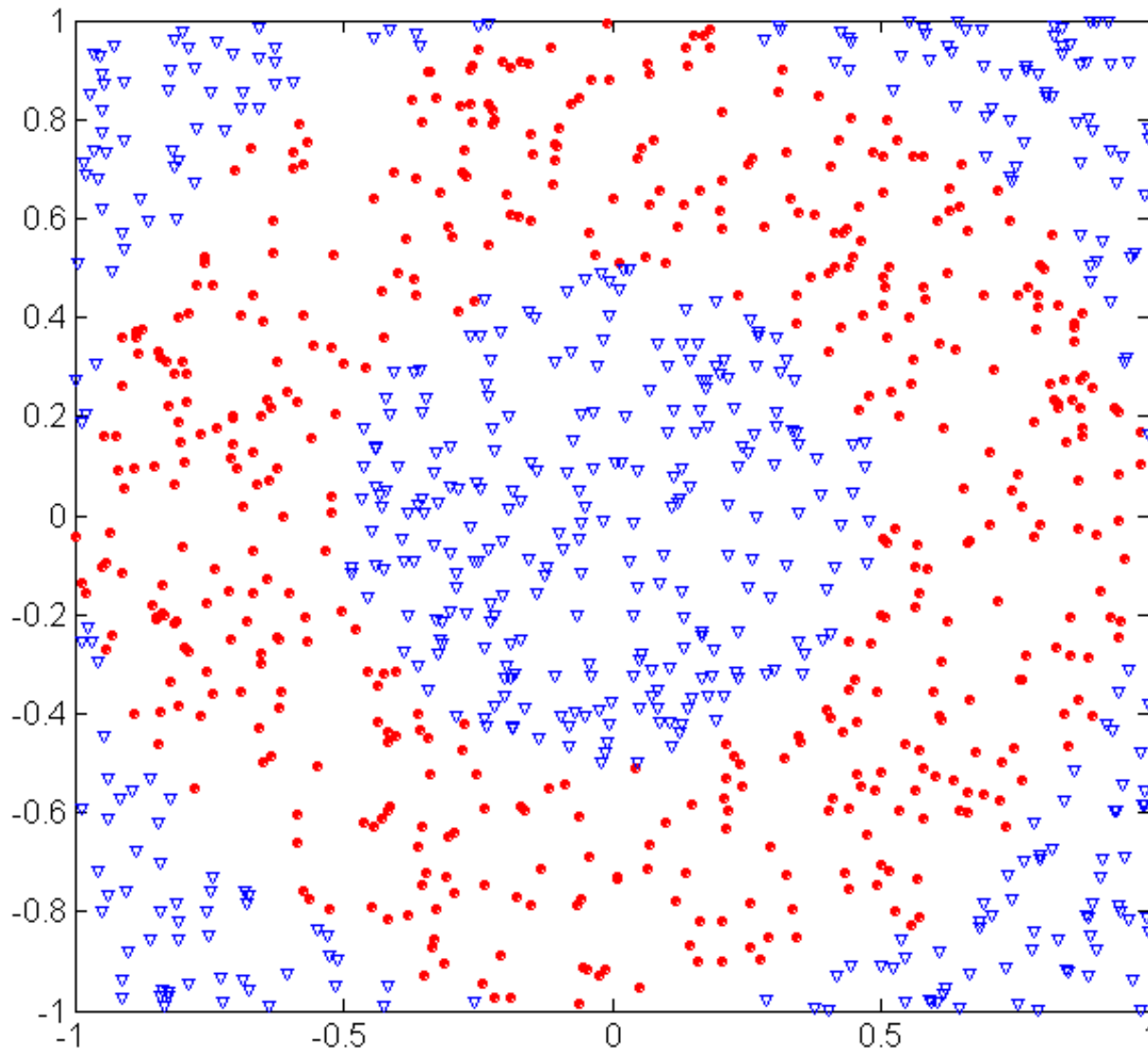
# Example: C4.5

- 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:  
<http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz>
  - not there any longer, but you can Google it

# Practical Issues of Classification

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

# Underfitting and Overfitting (Example)



**500 circular and 500 triangular data points.**

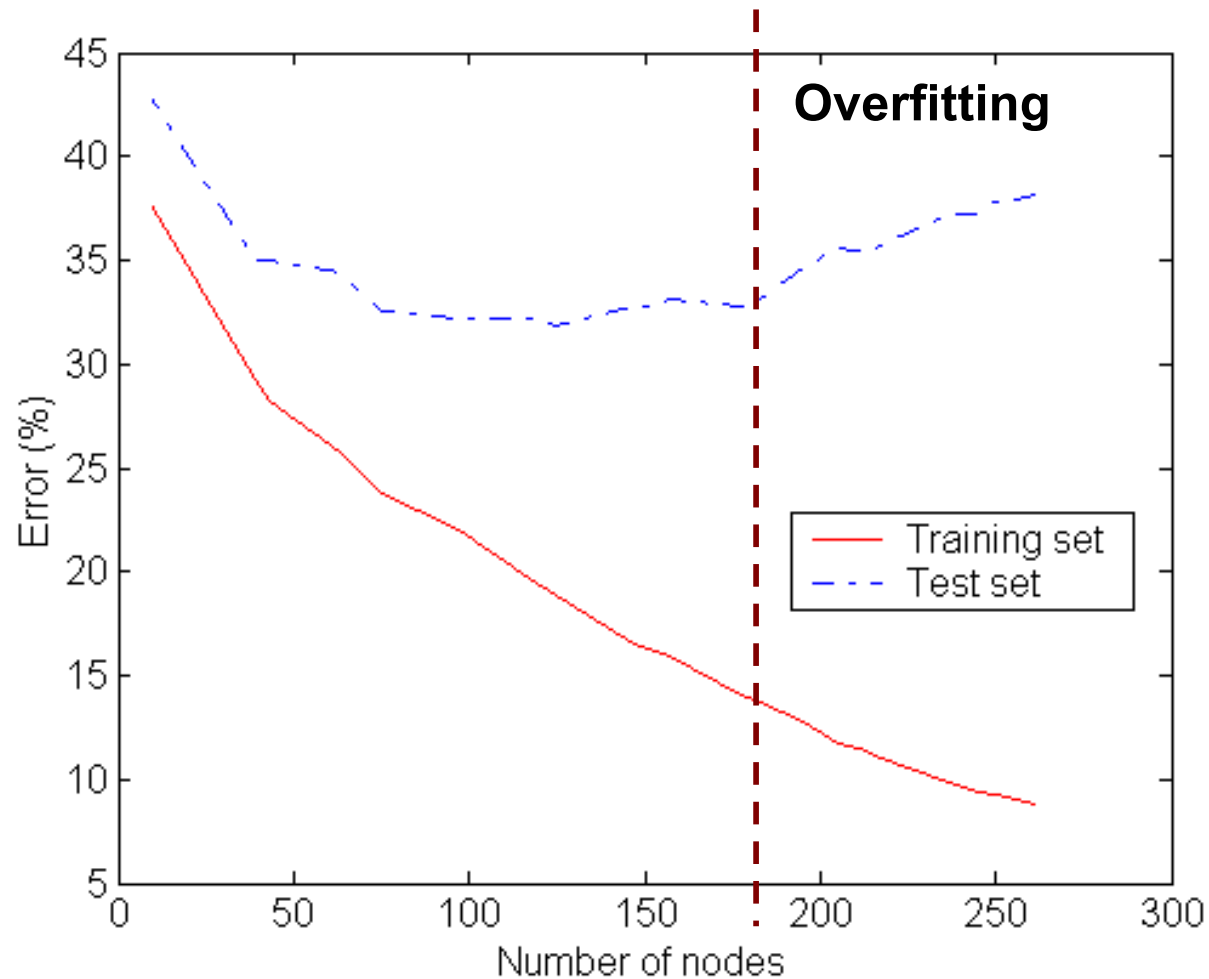
**Circular points:**

$$0.5 \leq \text{sqrt}(x_1^2 + x_2^2) \leq 1$$

**Triangular points:**

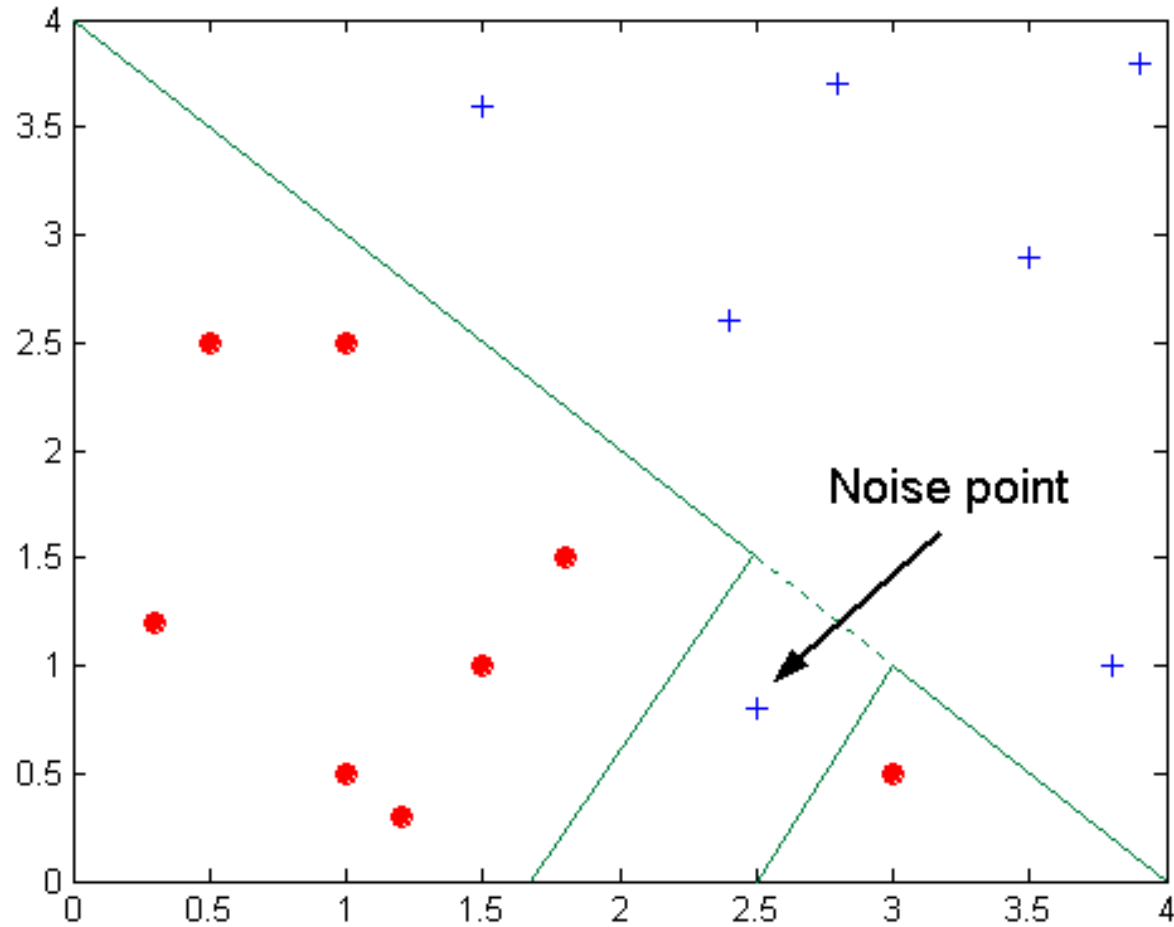
$$\text{sqrt}(x_1^2 + x_2^2) > 0.5 \text{ or } \text{sqrt}(x_1^2 + x_2^2) < 1$$

# Underfitting and Overfitting



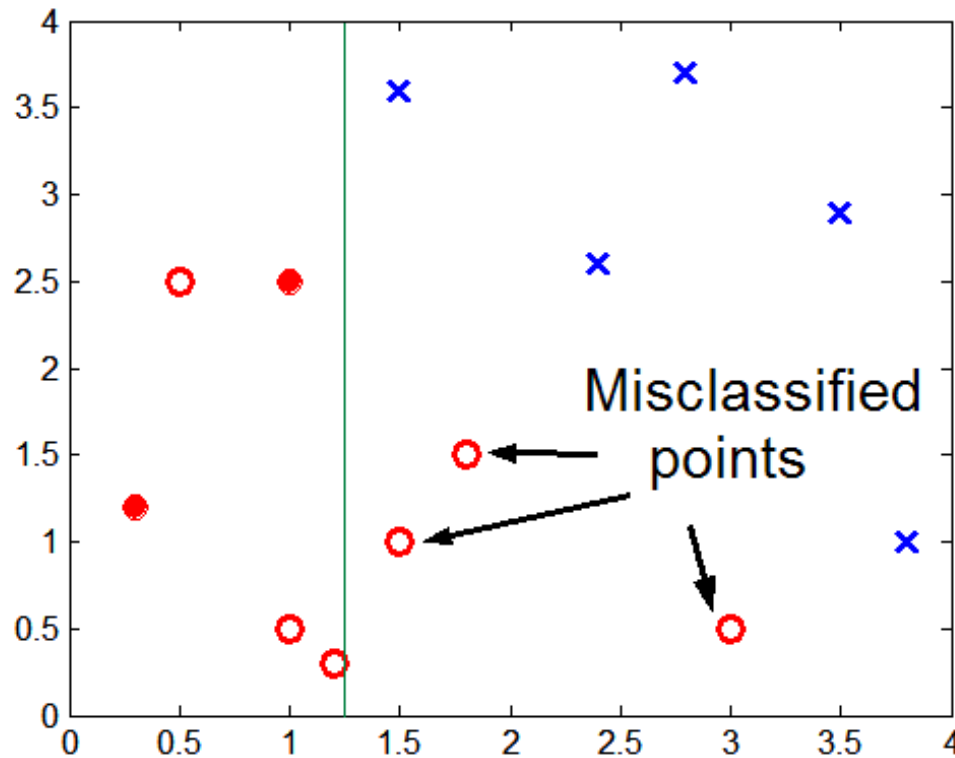
**Underfitting:** when model is too simple, both training and test errors are large

# 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

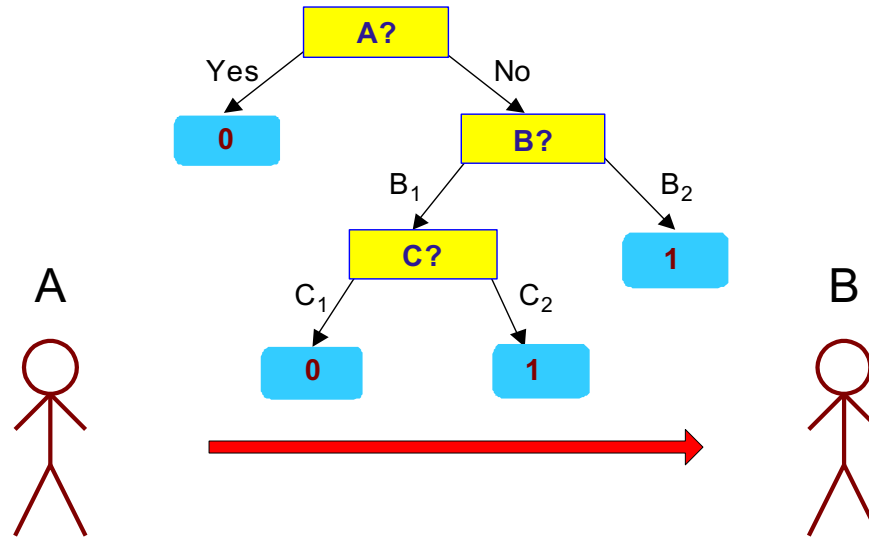
- **Re-substitution errors:** error on training ( $\sum e(t)$  )
- **Generalization errors:** error on testing ( $\sum e'(t)$ )
- Methods for estimating generalization errors:
  - **Optimistic approach:**  $e'(t) = e(t)$
  - **Pessimistic approach:**
    - ◆ For each leaf node:  $e'(t) = (e(t)+0.5)$
    - ◆ 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 (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 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)

X	y
$X_1$	1
$X_2$	0
$X_3$	0
$X_4$	1
...	...
$X_n$	1



X	y
$X_1$	?
$X_2$	?
$X_3$	?
$X_4$	?
...	...
$X_n$	?

- $\text{Cost}(\text{Model}, \text{Data}) = \text{Cost}(\text{Data}|\text{Model}) + \text{Cost}(\text{Model})$ 
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- $\text{Cost}(\text{Data}|\text{Model})$  encodes the misclassification errors.
- $\text{Cost}(\text{Model})$  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  $\chi^2$  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

Class = Yes	20
Class = No	10
Error = 10/30	

Training Error (Before splitting) = 10/30

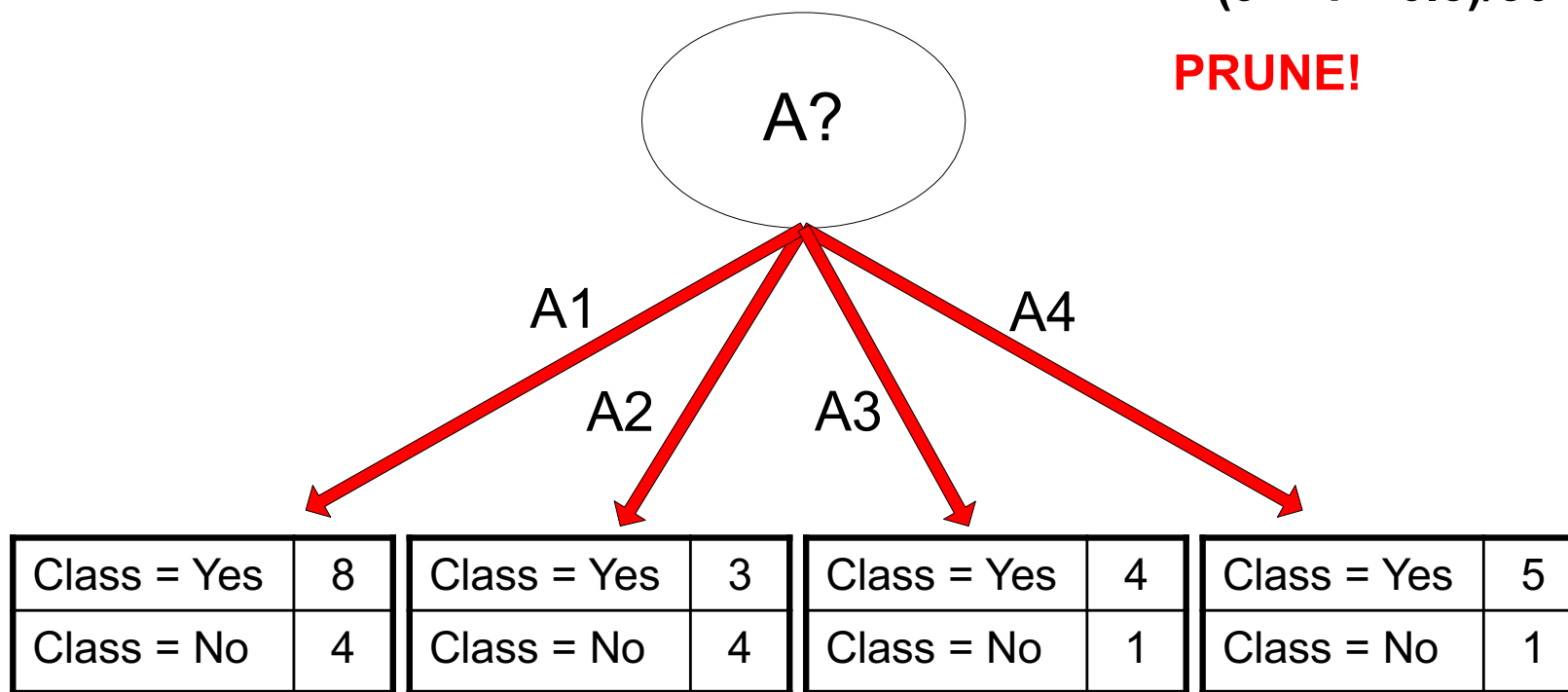
Pessimistic error =  $(10 + 0.5)/30 = 10.5/30$

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

$$= (9 + 4 \times 0.5)/30 = 11/30$$

**PRUNE!**



# Examples of Post-pruning

- Optimistic error?

Don't prune for both cases

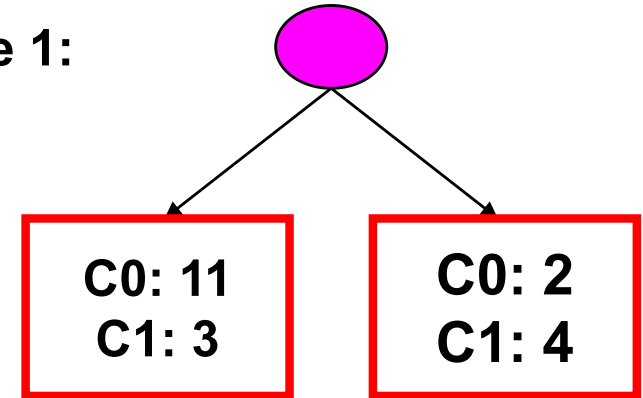
- Pessimistic error?

Don't prune case 1, prune case 2

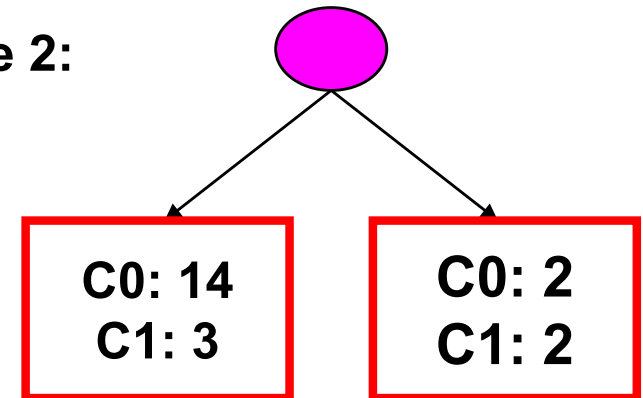
- Reduced error pruning?

Depends on validation set

Case 1:



Case 2:



# 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

Missing  
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)

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

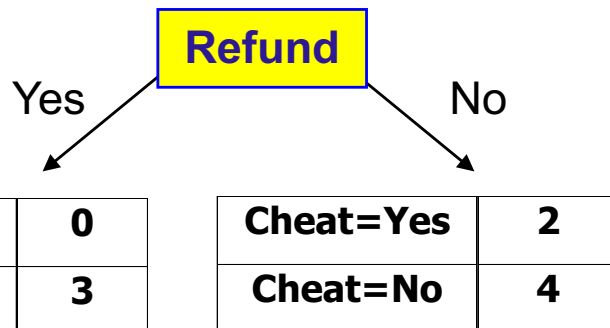
Entropy(Children)

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

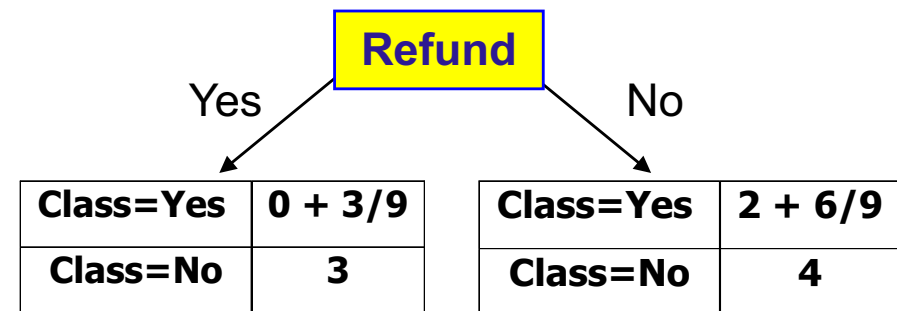
$$\text{Gain} = 0.9 \times (0.8813 - 0.551) = 0.3303$$

# Distribute Instances

<i>Tid</i>	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



<i>Tid</i>	Refund	Marital Status	Taxable Income	Class
10	?	Single	90K	Yes



Probability that Refund=Yes is 3/9

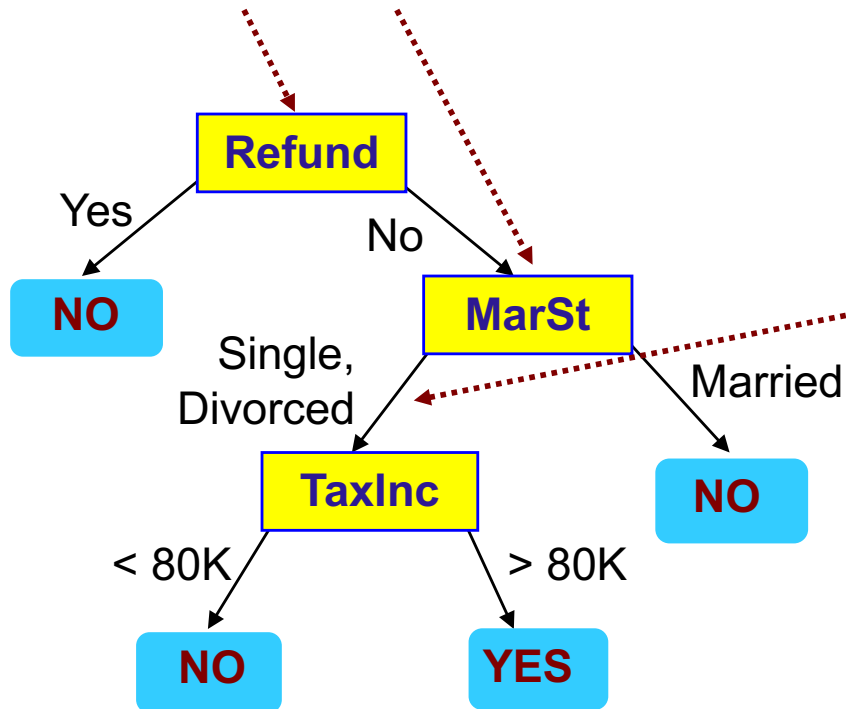
Probability that Refund=No is 6/9

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

# Classify Instances

New record:

<i>Tid</i>	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?



	Married	Single	Divorced	Total
Class=No	3	1	0	4
Class=Yes	6/9	1	1	2.67
Total	3.67	2	1	6.67

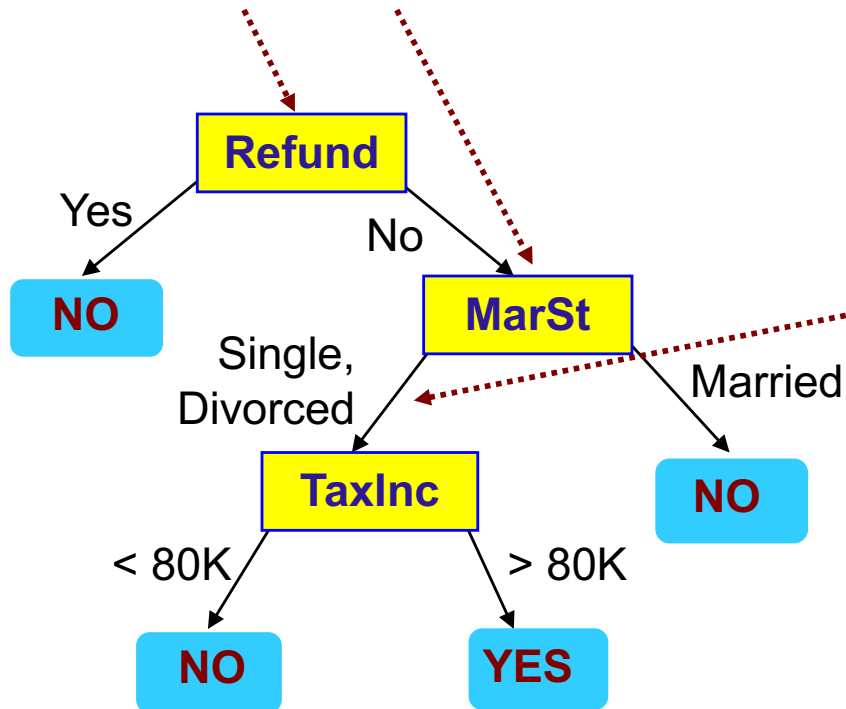
Probability that Marital Status = Married is  $3.67/6.67$

Probability that Marital Status = {Single, Divorced} is  $3/6.67$

# Classify Instances

New record:

<i>Tid</i>	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?



	Married	Single	Divorced	Total
Class=No	3	1	0	4
Class=Yes	0	15/9	1	2.67
Total	3	24/9	1	6.67

Probability that Marital Status = Married is  $3/6.67$

Probability that Marital Status = {Single, Divorced} is  $3.67/6.67$

Corrected table!

# Other Issues

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication

# Data Fragmentation

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

# Search Strategy

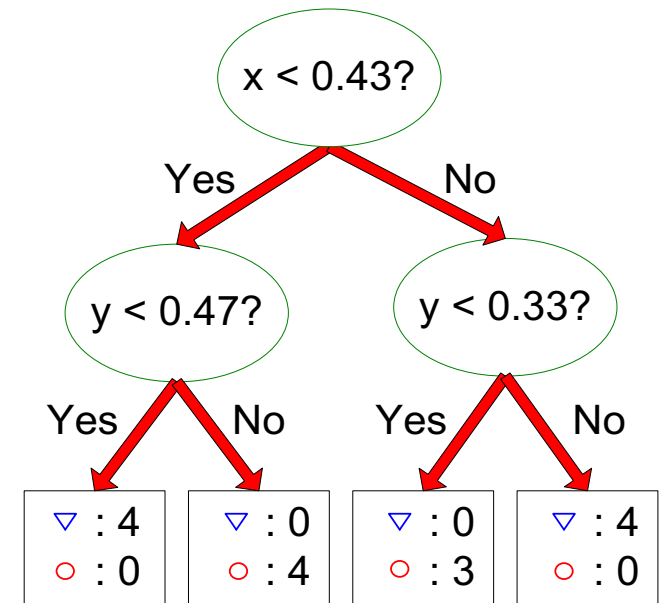
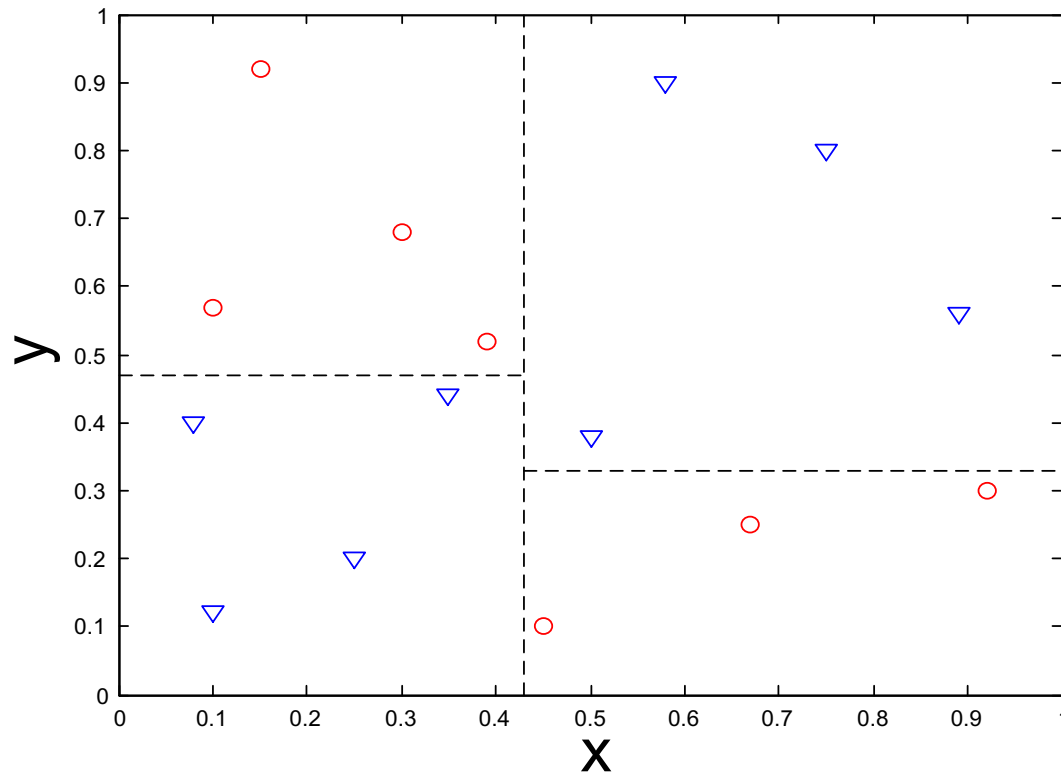
- Finding an optimal decision tree is NP-hard
- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Other strategies?
  - Bottom-up
  - Bi-directional

# Expressiveness

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

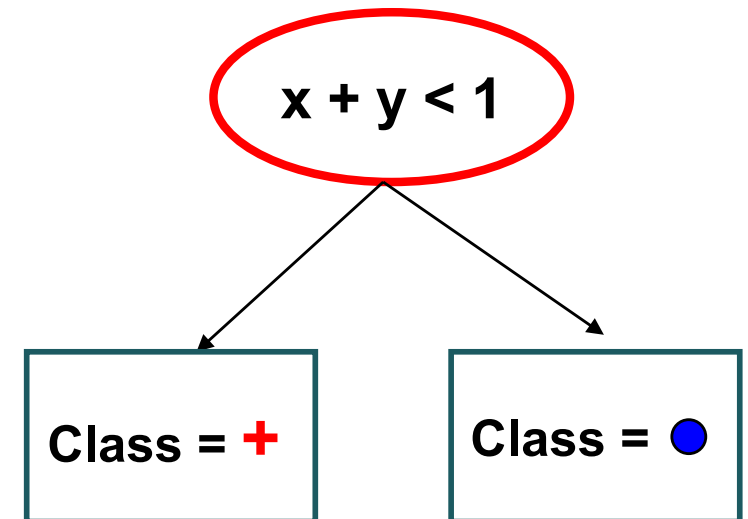
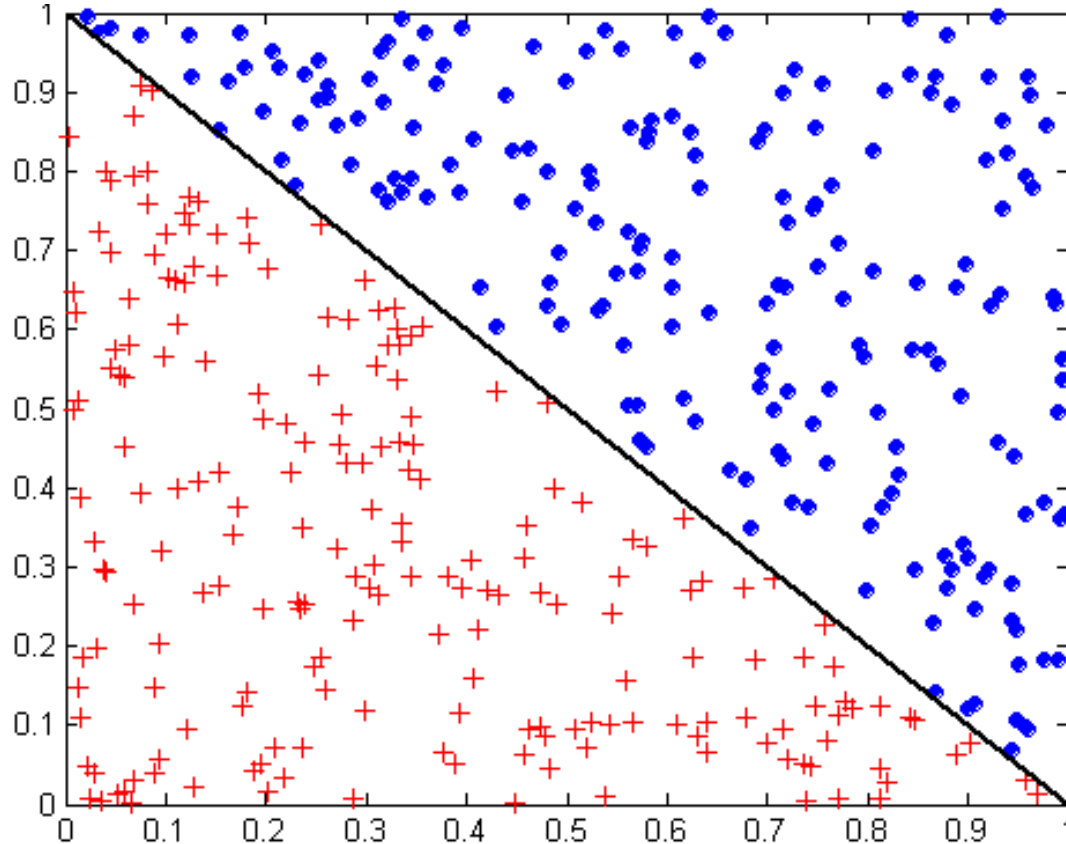


# Decision Boundary



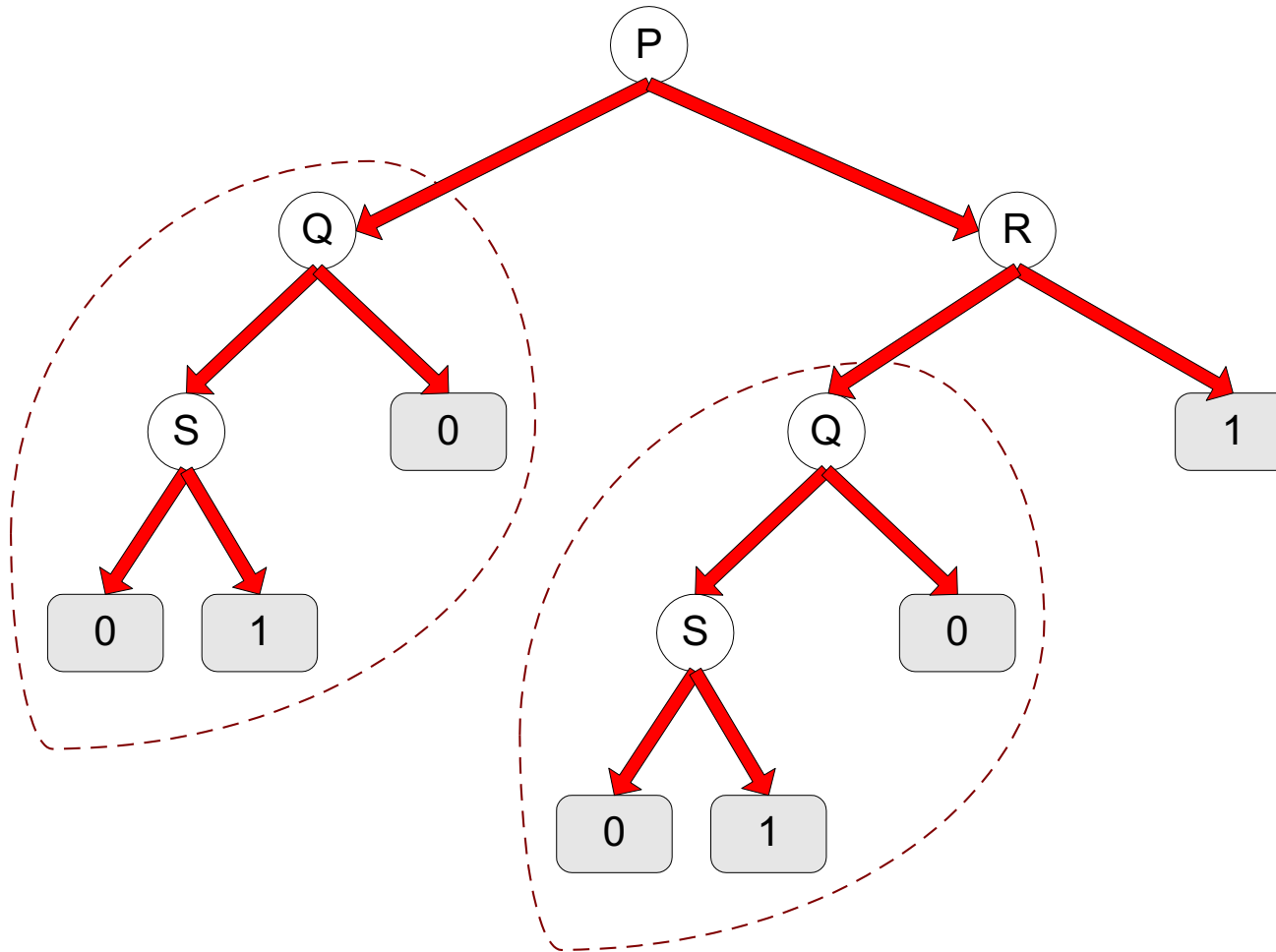
- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at a time

# Oblique Decision Trees



- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive

# Tree Replication



- Same subtree appears in multiple branches

# 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?

# Model Evaluation

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# Metrics for Performance Evaluation

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

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
	Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a
	Class=No	c

a: TP (true positive)  
b: FN (false negative)  
c: FP (false positive)  
d: TN (true negative)

# Metrics for Performance Evaluation...

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

- Most widely-used metric:

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

# 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



# Cost Matrix

	PREDICTED CLASS		
	$C(i j)$	Class=Yes	Class=No
	Class=Yes	$C(\text{Yes} \text{Yes})$	$C(\text{No} \text{Yes})$
	Class=No	$C(\text{Yes} \text{No})$	$C(\text{No} \text{No})$

$C(i|j)$ : Cost of misclassifying 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 vs Accuracy

Count	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d

Accuracy is proportional to cost if

$$1. C(\text{Yes}|\text{No})=C(\text{No}|\text{Yes}) = q$$

$$2. C(\text{Yes}|\text{Yes})=C(\text{No}|\text{No}) = p$$

$$N = a + b + c + d$$

$$\text{Accuracy} = (a + d)/N$$

Cost	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	p	q
	Class=No	q	p

$$\text{Cost} = p (a + d) + q (b + c)$$

$$= p (a + d) + q (N - a - d)$$

$$= q N - (q - p)(a + d)$$

$$= N [q - (q-p) \times \text{Accuracy}]$$

# Cost-Sensitive Measures

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

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

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

- Precision is biased towards  $C(\text{Yes}|\text{Yes})$  &  $C(\text{Yes}|\text{No})$
- Recall is biased towards  $C(\text{Yes}|\text{Yes})$  &  $C(\text{No}|\text{Yes})$
- F-measure is biased towards all except  $C(\text{No}|\text{No})$

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

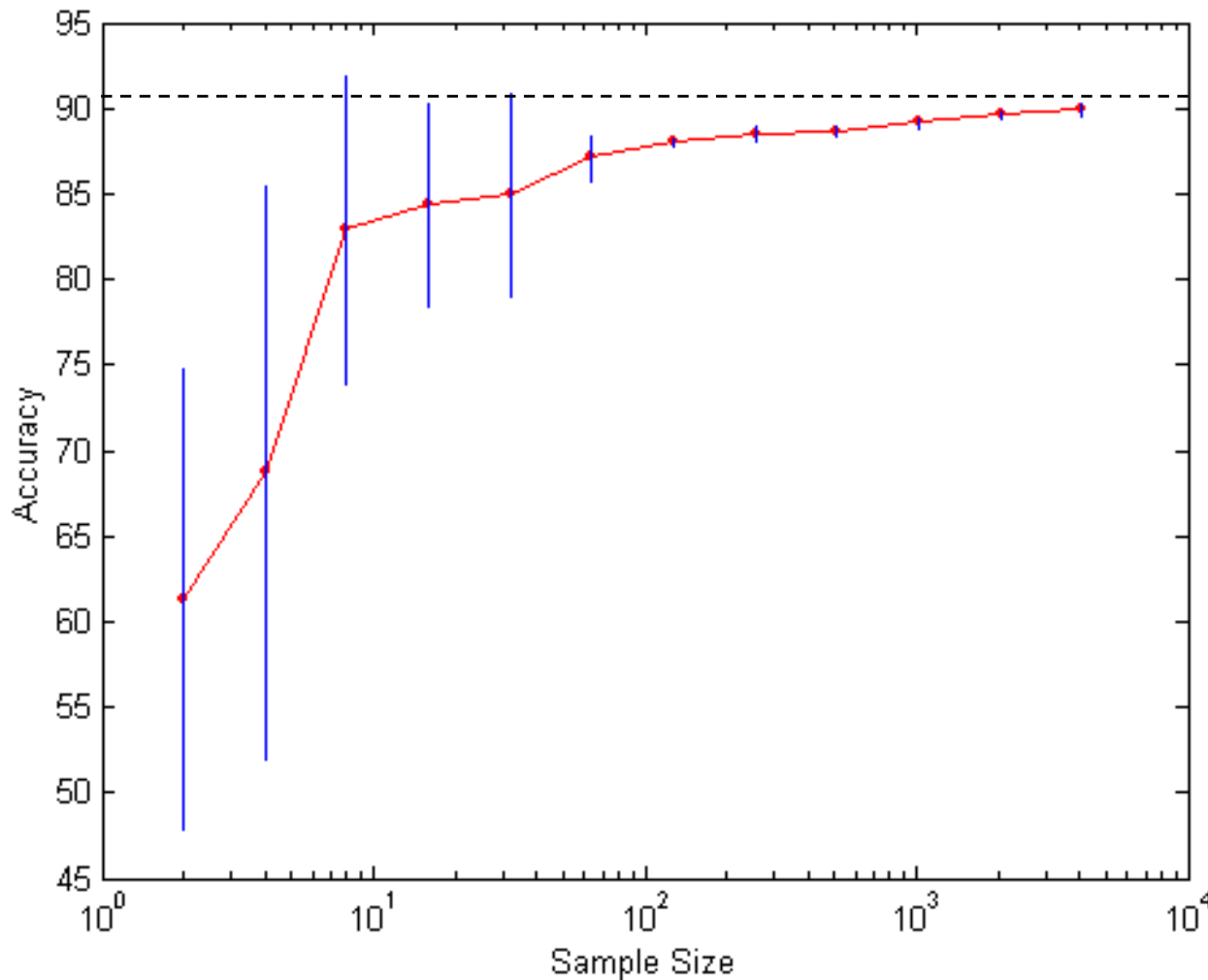
# Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
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# 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
  - Reserve  $2/3$  for training and  $1/3$  for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into  $k$  disjoint subsets
  - $k$ -fold: train on  $k-1$  partitions, test on the remaining one
  - Leave-one-out:  $k=n$
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement



# Model Evaluation

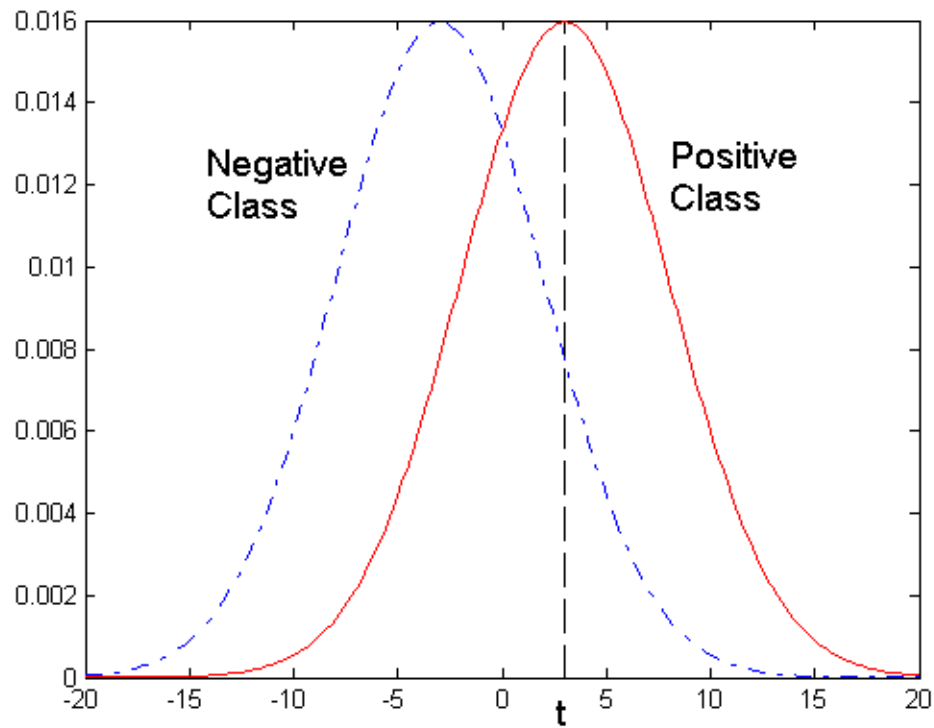
- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
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# ROC (Receiver Operating Characteristic)

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

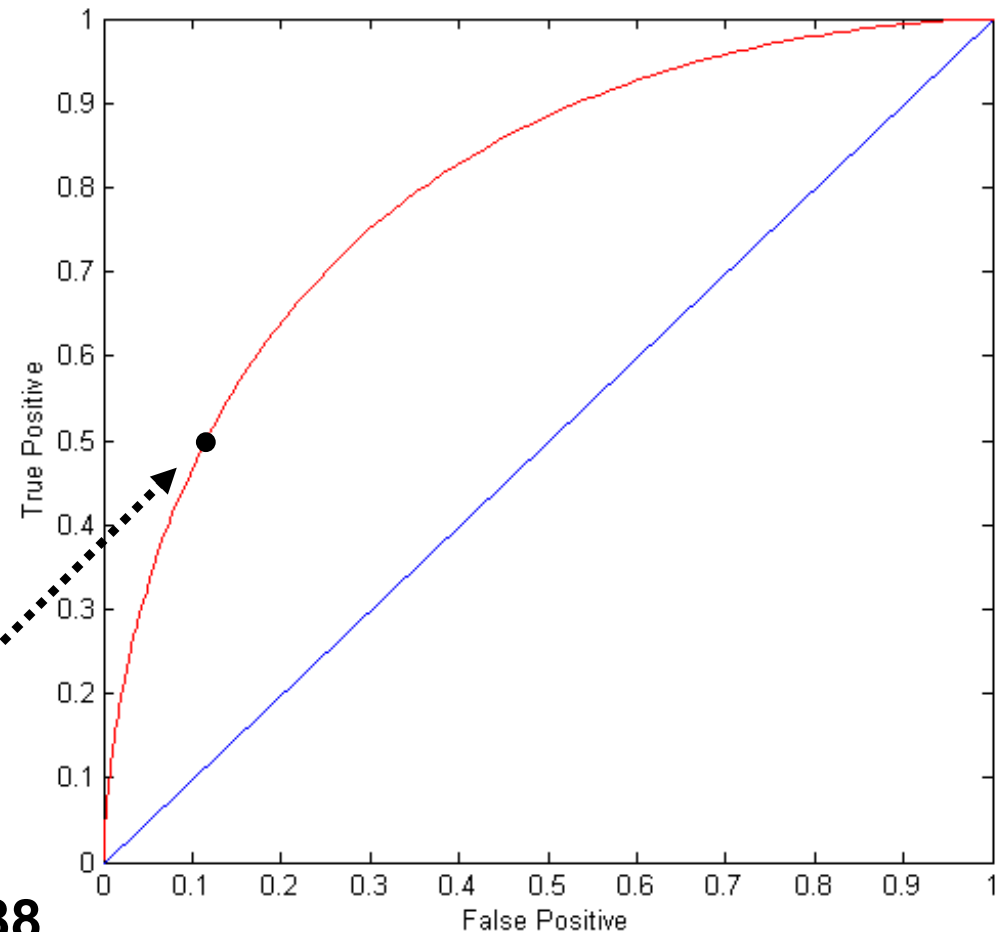
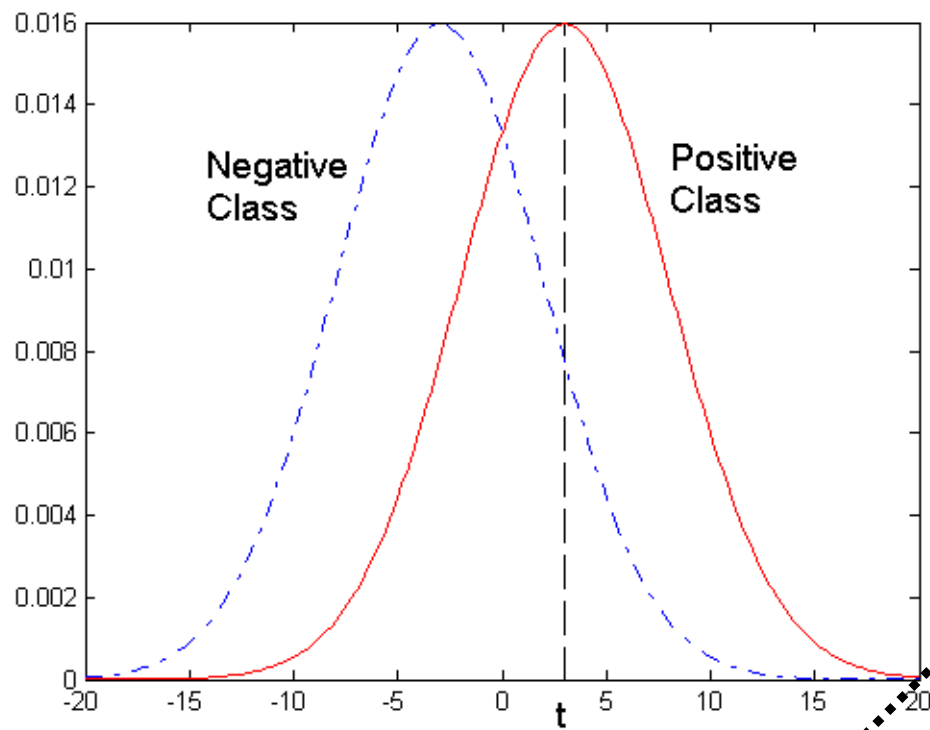
# ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at  $x > t$  is classified as positive



# ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at  $x > t$  is classified as positive



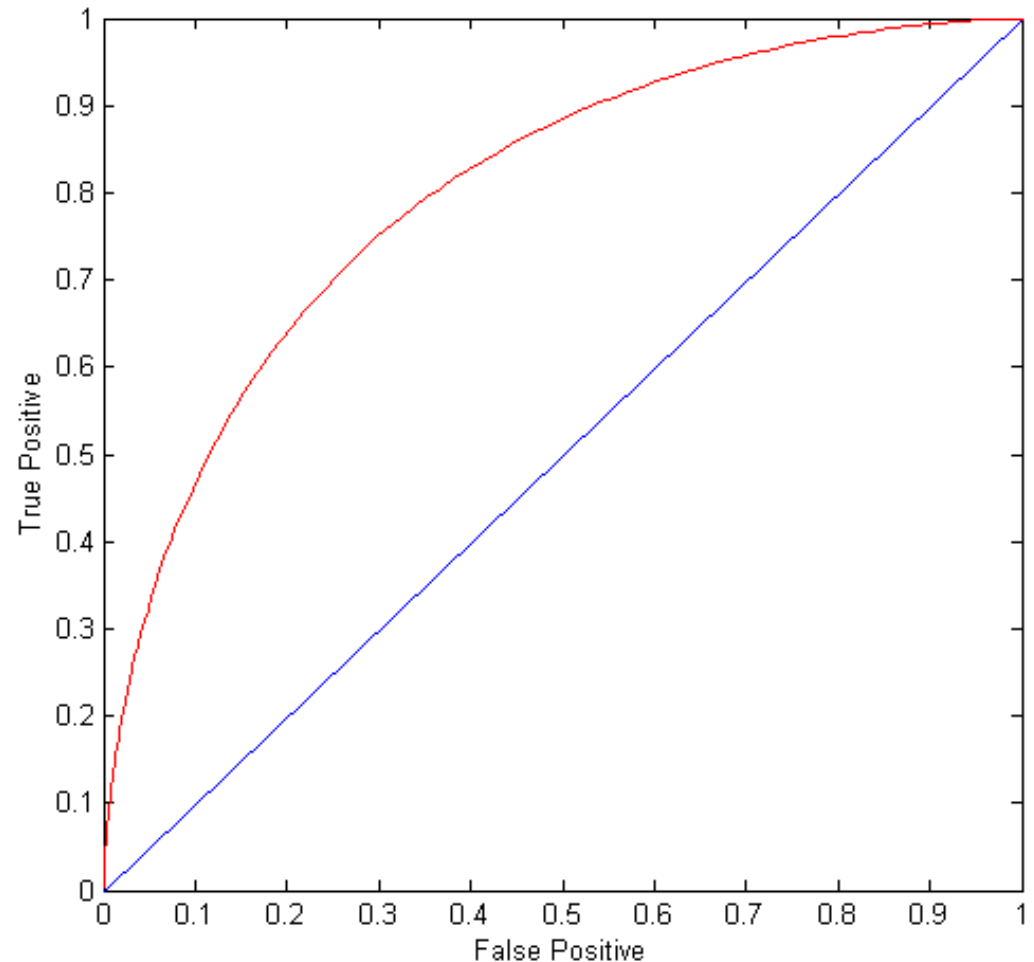
At threshold  $t$ :

TP=0.5, FN=0.5, FP=0.12, FN=0.88

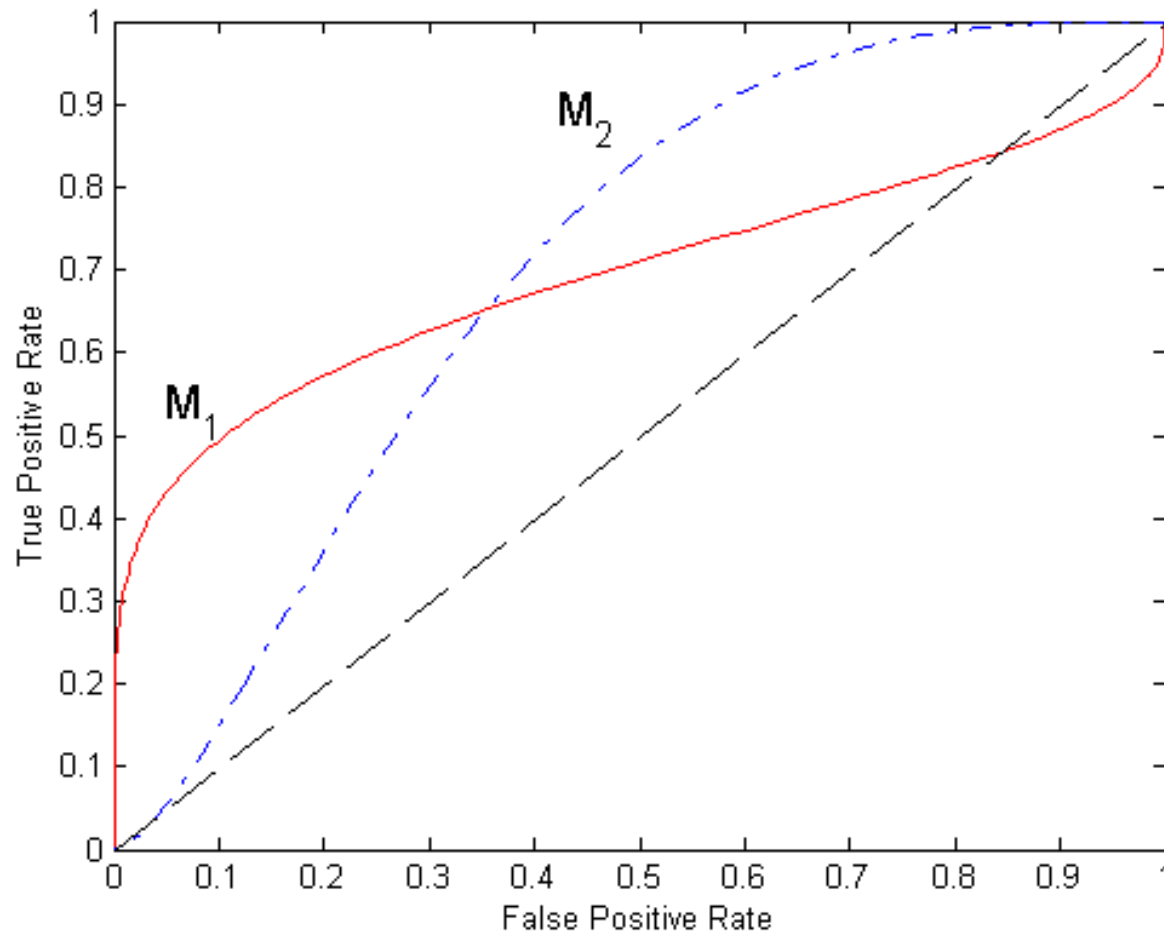
# ROC Curve

(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
  - $M_1$  is better for small FPR
  - $M_2$  is better for large FPR
- Area Under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

# How to Construct an ROC curve

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

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

# How to construct an ROC curve

Class	+	-	+	-	-	-	+	-	+	+	
Threshold $\geq$	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2	1	0
FP	5	5	4	4	3	2	1	1	0	0	0
TN	0	0	1	1	2	3	4	4	5	5	5
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve:

