

Data Mining

Classification: Basic Concepts and Techniques

Lecture Notes for Chapter 3

Introduction to Data Mining, 2nd Edition

by

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Classification: Definition

- Given a collection of records (training set)
 - Each record is by characterized by a tuple (x,y) , where x is the attribute set and y is the class label
 - ◆ x : attribute, predictor, independent variable, input
 - ◆ y : class, response, dependent variable, output
- Task:
 - Learn a model that maps each attribute set x into one of the predefined class labels y

Examples of Classification Task

Task	Attribute set, x	Class label, y
Categorizing email messages	Features extracted from email message header and content	spam or non-spam
Identifying tumor cells	Features extracted from x-rays or MRI scans	malignant or benign cells
Cataloging galaxies	Features extracted from telescope images	Elliptical, spiral, or irregular-shaped galaxies

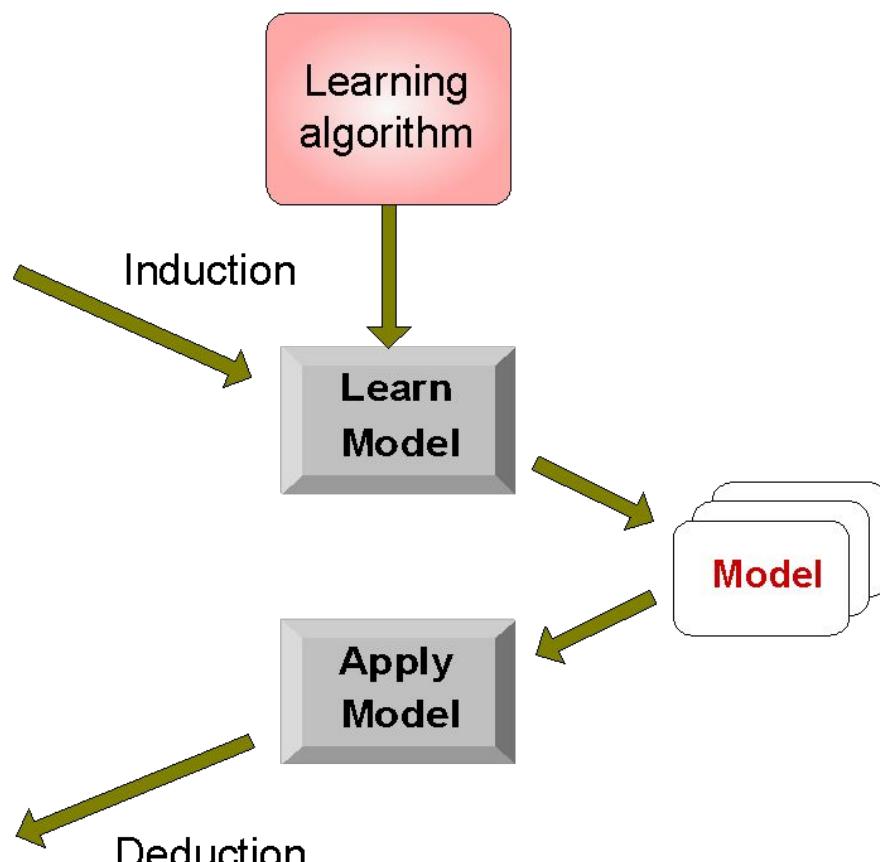
General Approach for Building Classification Model

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

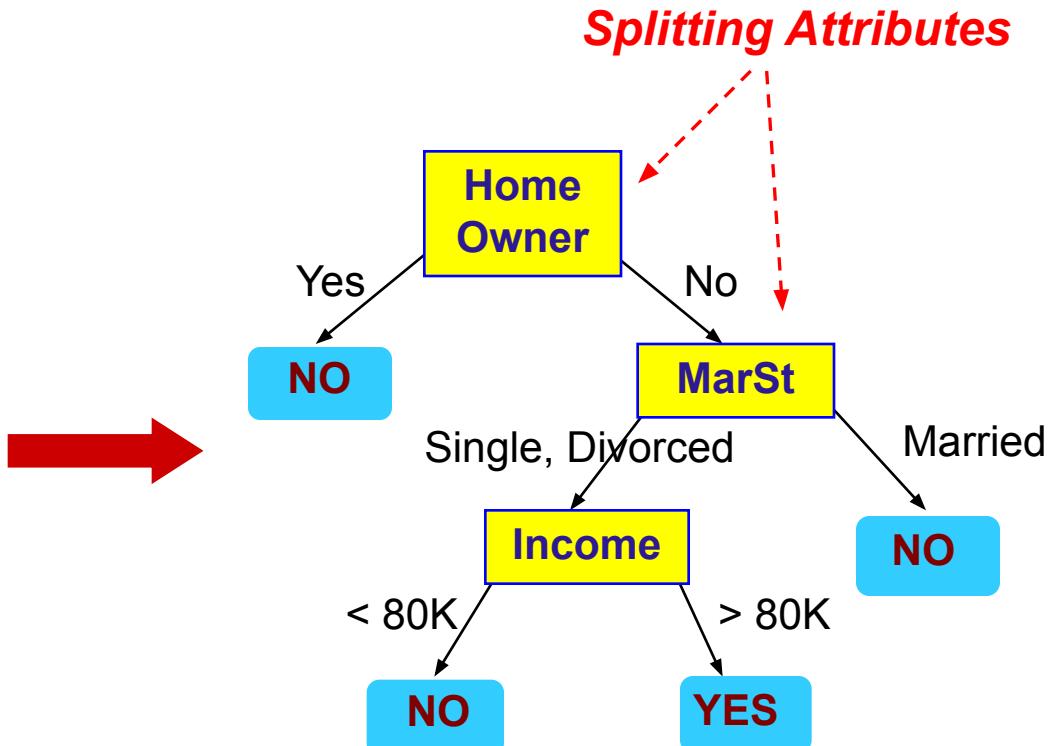


Classification Techniques

- Base Classifiers
 - Decision Tree based Methods
 - Rule-based Methods
 - Nearest-neighbor
 - Neural Networks, Deep Neural Nets
 - Naïve Bayes and Bayesian Belief Networks
 - Support Vector Machines
- Ensemble Classifiers
 - Boosting, Bagging, Random Forests

Example of a Decision Tree

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower	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	No	Single	90K	Yes	

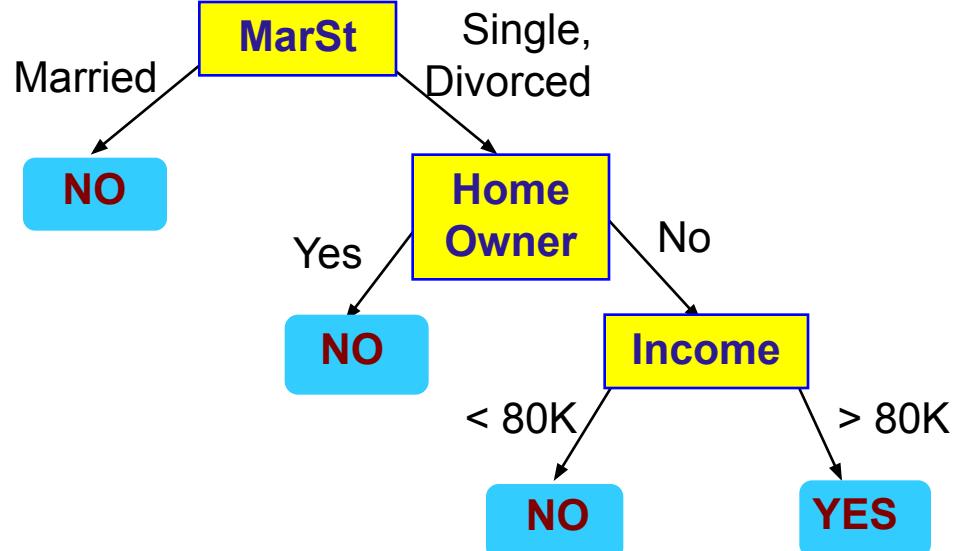


Training Data

Model: Decision Tree

Another Example of Decision Tree

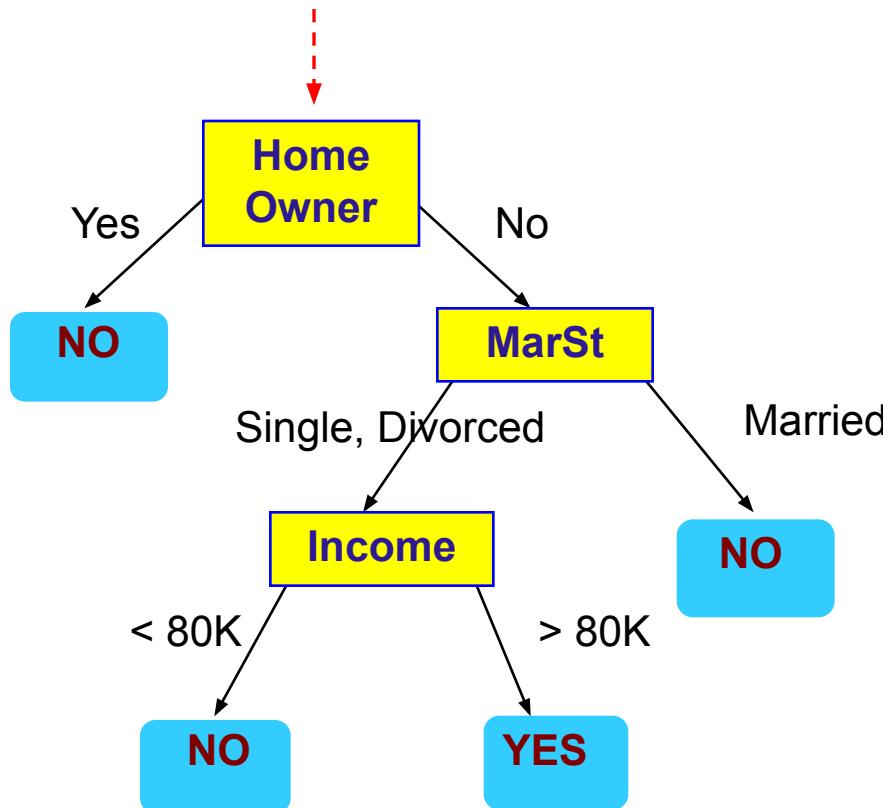
ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower	
				categorical	categorical
1	Yes	Single	125K	No	continuous
2	No	Married	100K	No	class
3	No	Single	70K	No	
4	Yes	Married	120K	No	
5	No	Divorced	95K	Yes	
6	No	Married	60K	No	
7	Yes	Divorced	220K	No	
8	No	Single	85K	Yes	
9	No	Married	75K	No	
10	No	Single	90K	Yes	



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

Apply Model to Test Data

Start from the root of tree.



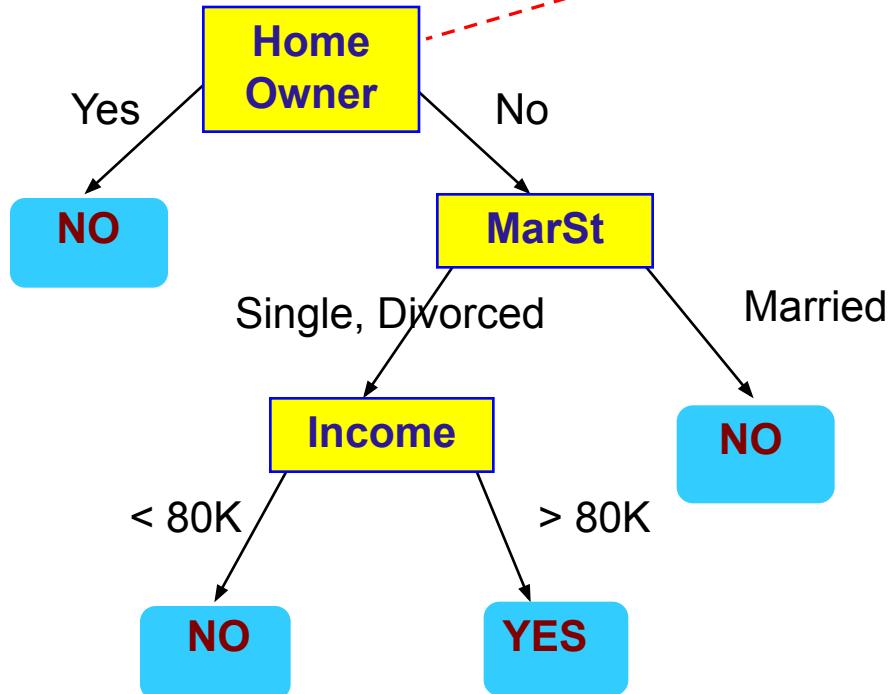
Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?

Apply Model to Test Data

Test Data

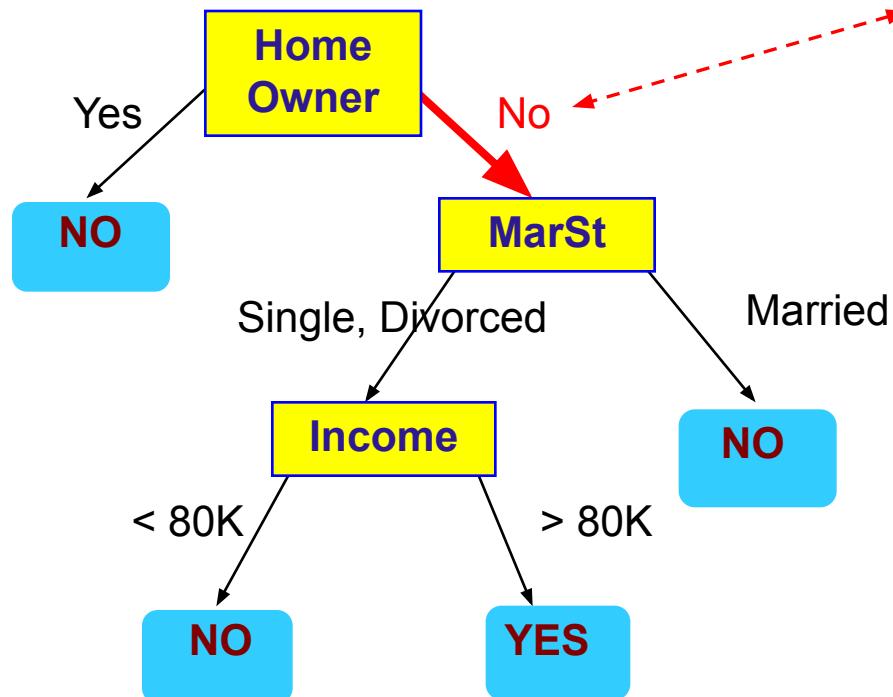
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

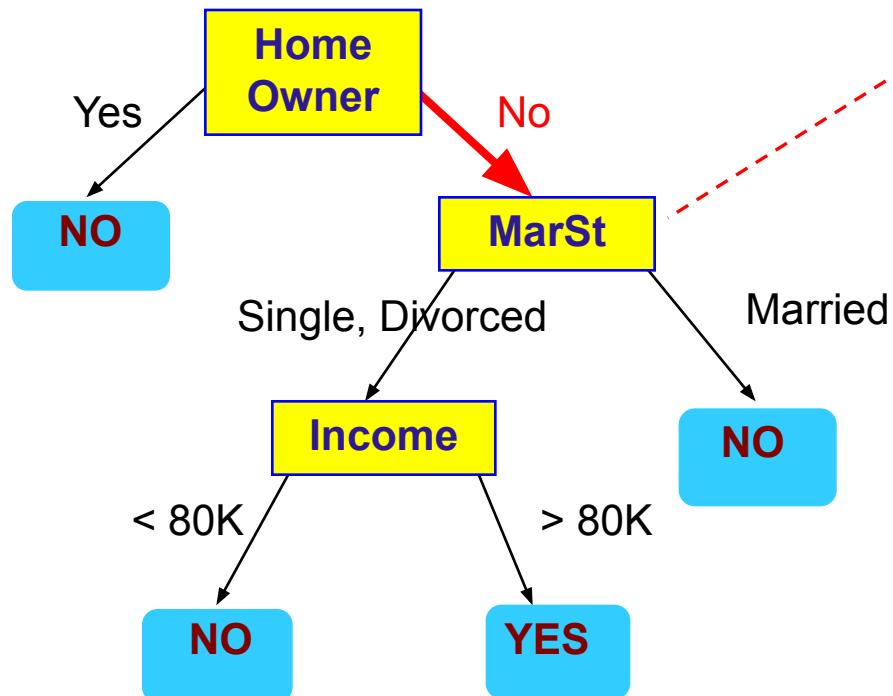
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

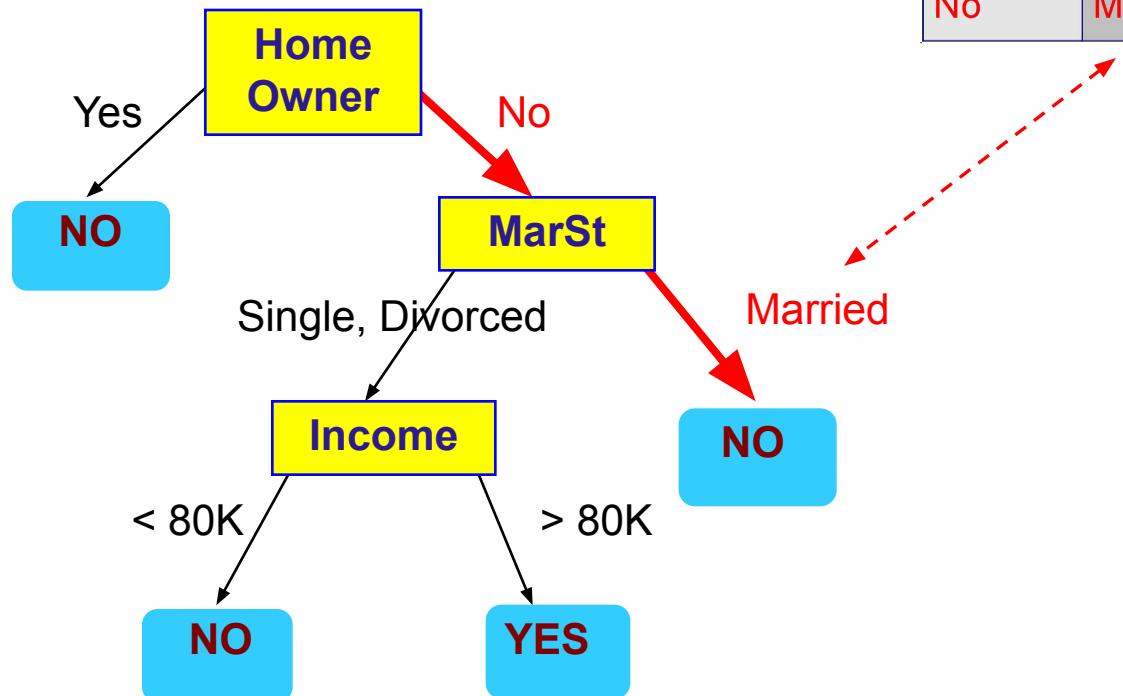
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

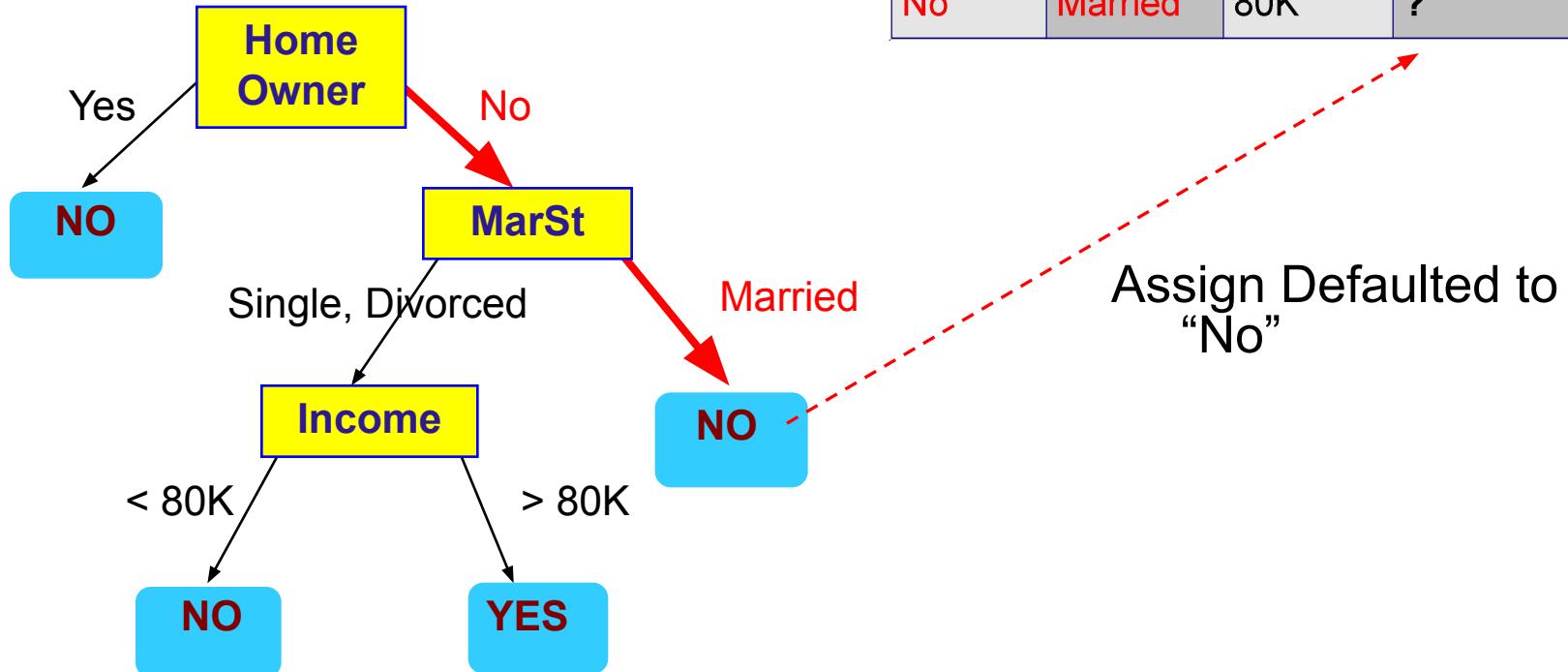
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



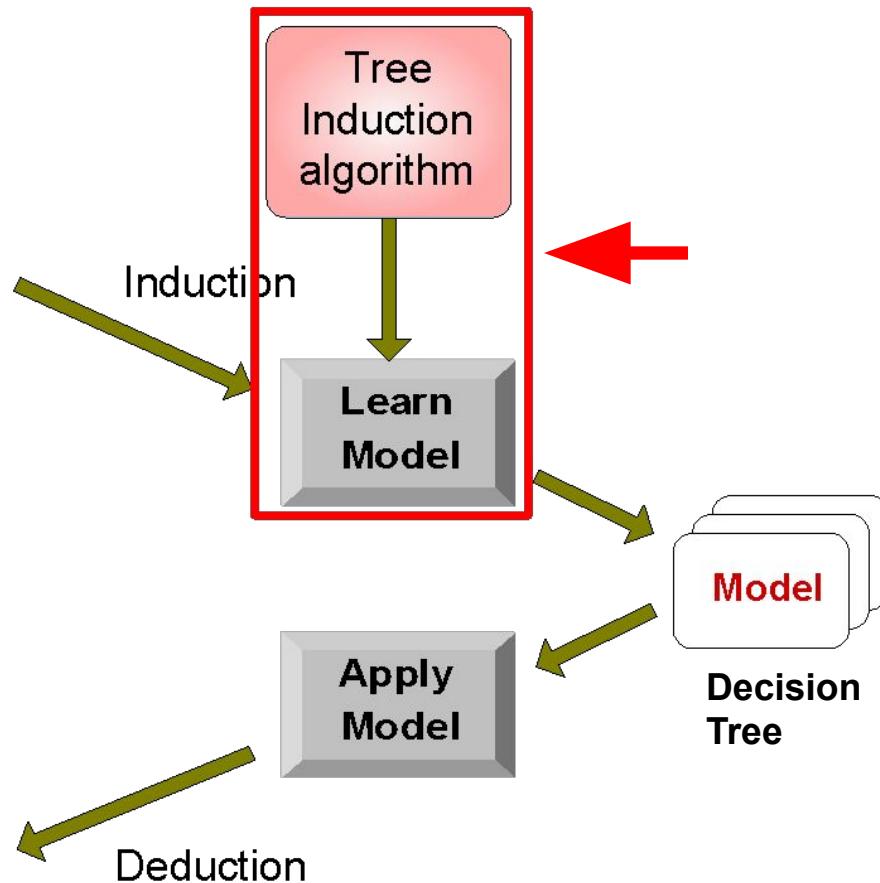
Decision Tree Classification Task

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Test Set



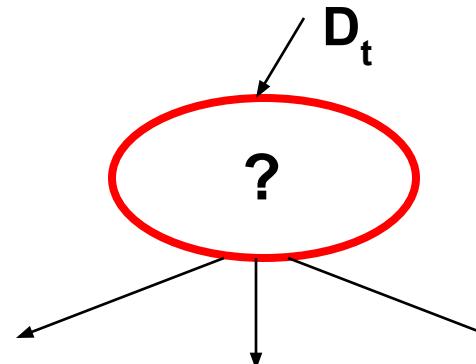
Decision Tree Induction

- 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 to the same class y_t , then t is a leaf node labeled as y_t
 - 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.

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8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Hunt's Algorithm

Defaulted = No

(7,3)

(a)

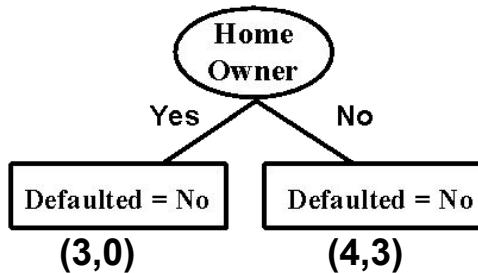
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10	No	Single	90K	Yes

Hunt's Algorithm

Defaulted = No

(7,3)

(a)



(b)

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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9	No	Married	75K	No
10	No	Single	90K	Yes

Hunt's Algorithm

Defaulted = No

(7,3)

(a)

Home Owner

Yes

Defaulted = No

(3,0)

No

Defaulted = No

(4,3)

(b)

Home Owner

Yes

Defaulted = No

(3,0) Single,
Divorced

No

Marital Status

Married

Defaulted = Yes

(1,3)

Defaulted = No

(3,0)

(c)

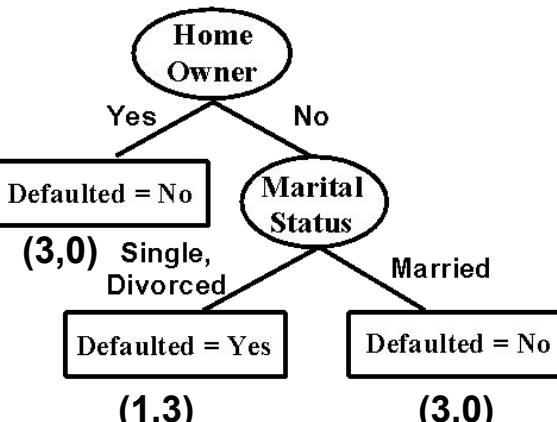
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Hunt's Algorithm

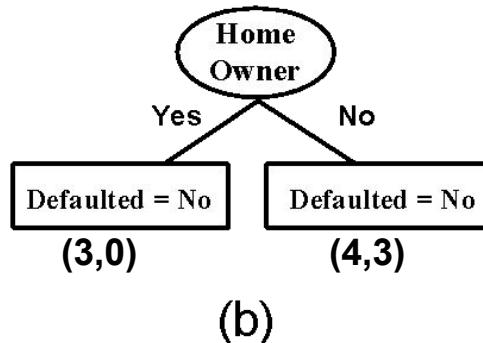
Defaulted = No

(7,3)

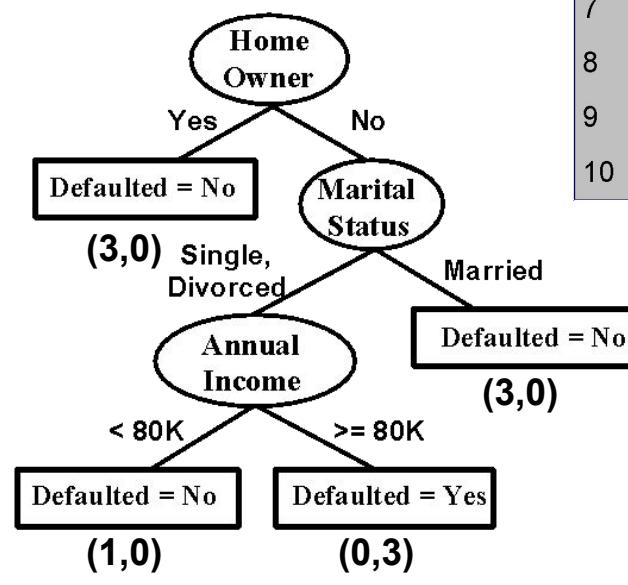
(a)



(c)



(b)



(d)

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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7	Yes	Divorced	220K	No
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10	No	Single	90K	Yes

Design Issues of Decision Tree Induction

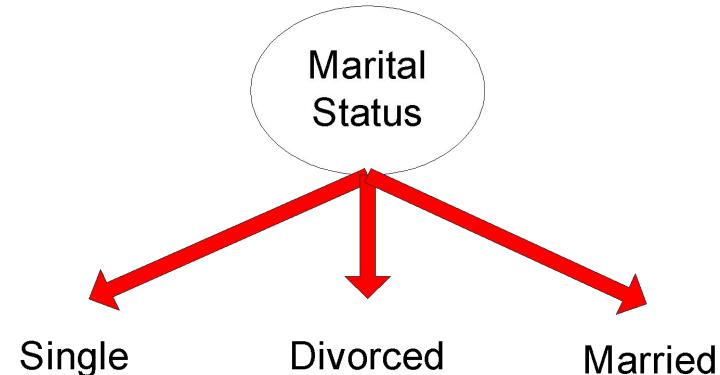
- How should training records be split?
 - Method for specifying test condition
 - ◆ depending on attribute types
 - Measure for evaluating the goodness of a test condition
- How should the splitting procedure stop?
 - Stop splitting if all the records belong to the same class or have identical attribute values
 - Early termination

Methods for Expressing Test Conditions

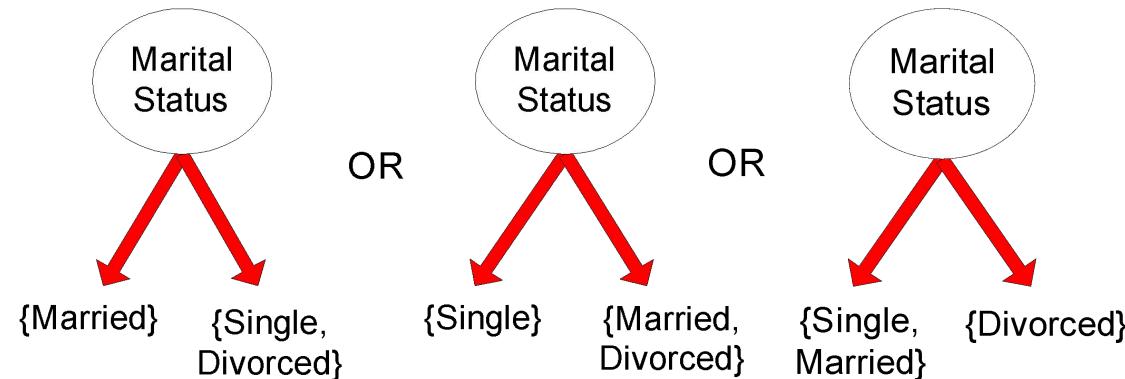
- Depends on attribute types
 - Binary
 - Nominal
 - Ordinal
 - Continuous
- Depends on number of ways to split
 - 2-way split
 - Multi-way split

Test Condition for Nominal Attributes

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

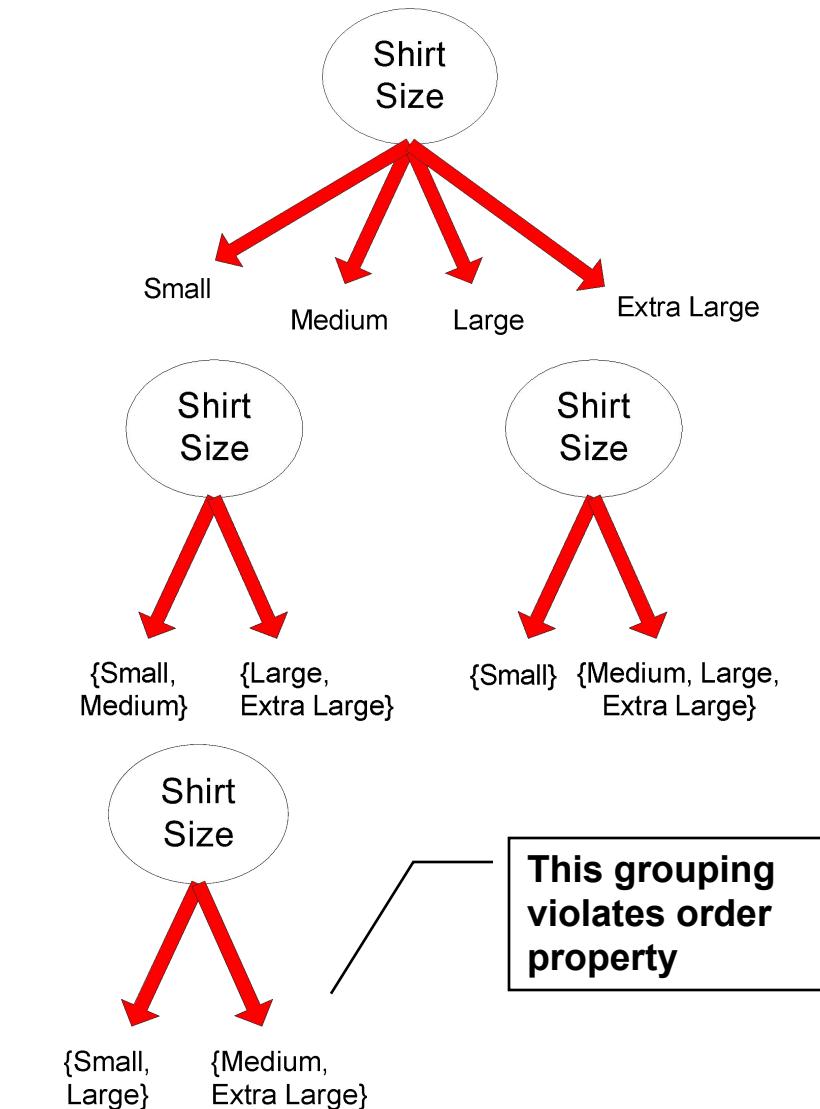


- Binary split:
 - Divides values into two subsets

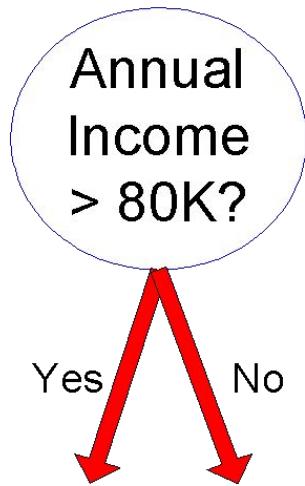


Test Condition for Ordinal Attributes

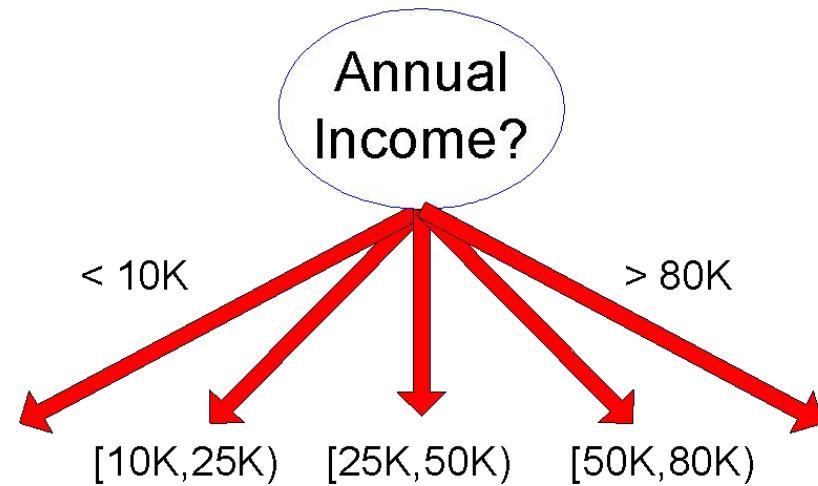
- Multi-way split:
 - Use as many partitions as distinct values
- Binary split:
 - Divides values into two subsets
 - Preserve order property among attribute values



Test Condition for Continuous Attributes



(i) Binary split



(ii) Multi-way split

Splitting Based on Continuous Attributes

- Different ways of handling
 - **Discretization** to form an ordinal categorical attribute

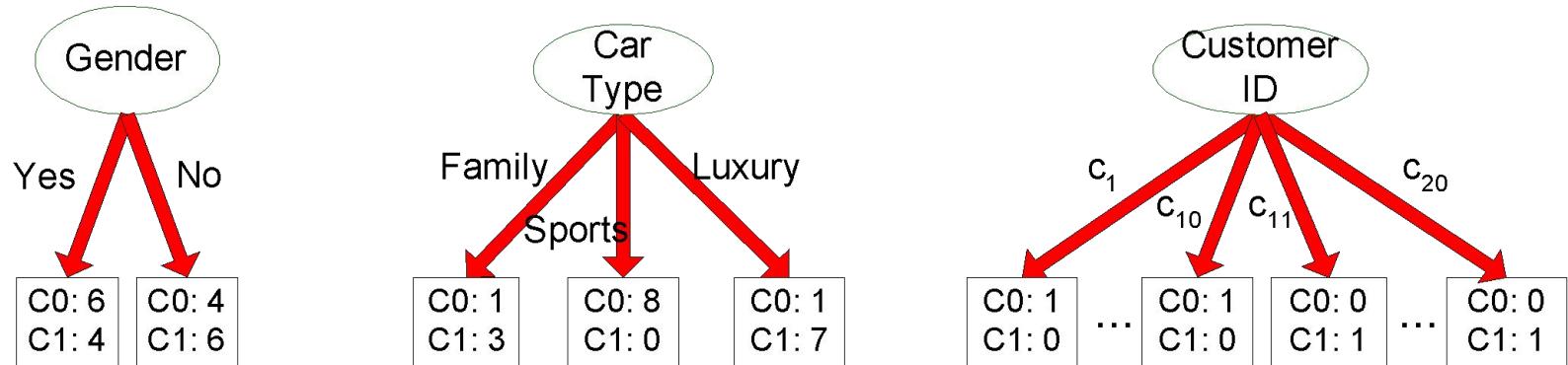
Ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.

 - ◆ Static – discretize once at the beginning
 - ◆ Dynamic – repeat at each node
 - **Binary Decision:** $(A < v)$ or $(A \geq v)$
 - ◆ consider all possible splits and finds the best cut
 - ◆ can be more compute intensive

How to determine the Best Split

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

Customer Id	Gender	Car Type	Shirt Size	Class
1	M	Family	Small	C0
2	M	Sports	Medium	C0
3	M	Sports	Medium	C0
4	M	Sports	Large	C0
5	M	Sports	Extra Large	C0
6	M	Sports	Extra Large	C0
7	F	Sports	Small	C0
8	F	Sports	Small	C0
9	F	Sports	Medium	C0
10	F	Luxury	Large	C0
11	M	Family	Large	C1
12	M	Family	Extra Large	C1
13	M	Family	Medium	C1
14	M	Luxury	Extra Large	C1
15	F	Luxury	Small	C1
16	F	Luxury	Small	C1
17	F	Luxury	Medium	C1
18	F	Luxury	Medium	C1
19	F	Luxury	Medium	C1
20	F	Luxury	Large	C1



Which test condition is the best?

How to determine the Best Split

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

C0: 5
C1: 5

High degree of impurity

C0: 9
C1: 1

Low degree of impurity

Measures of Node Impurity

- Gini Index

$$Gini\ Index = 1 - \sum_{i=0}^{c-1} p_i(t)^2$$

Where $p_i(t)$ is the frequency of class i at node t , and c is the total number of classes

- Entropy

$$Entropy = - \sum_{i=0}^{c-1} p_i(t) \log_2 p_i(t)$$

- Misclassification error

$$Classification\ error = 1 - \max[p_i(t)]$$

Finding the Best Split

1. Compute impurity measure (P) before splitting
2. Compute impurity measure (M) after splitting
 - Compute impurity measure of each child node
 - M is the weighted impurity of child nodes
3. Choose the attribute test condition that produces the highest gain

$$\text{Gain} = P - M$$

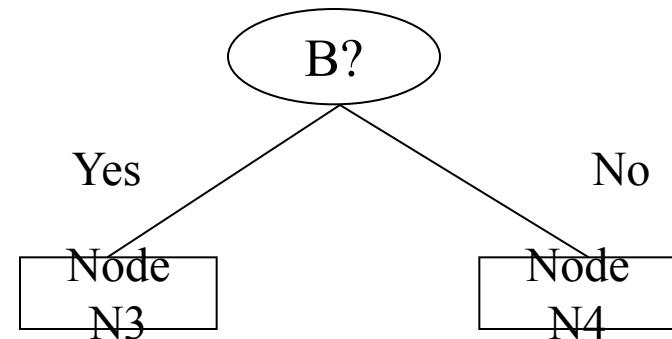
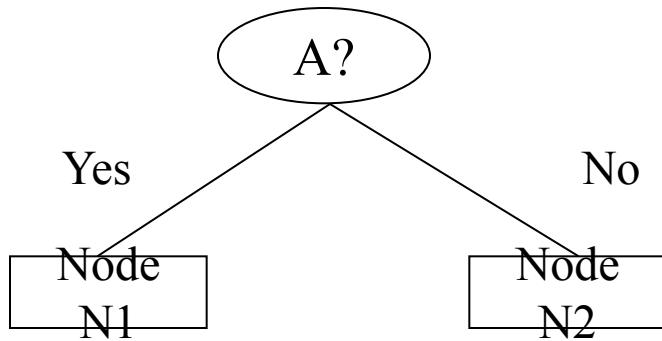
or equivalently, lowest impurity measure after splitting (M)

Finding the Best Split

Before Splitting:

C0	N00
C1	N01

→ P



C0	N10
C1	N11

C0	N20
C1	N21

C0	N30
C1	N31

C0	N40
C1	N41

M11

M12

M21

M22

M1

M2

$$\text{Gain} = P - M1 \quad \text{vs} \quad P - M2$$

Measure of Impurity: GINI

- ## • Gini Index for a given node t

$$Gini\ Index = 1 - \sum_{i=0}^{c-1} p_i(t)^2$$

Where $p_i(t)$ is the frequency of class i at node t , and c is the total number of classes

- Maximum of $1 - 1/c$ when records are equally distributed among all classes, implying the least beneficial situation for classification
 - Minimum of 0 when all records belong to one class, implying the most beneficial situation for classification

Measure of Impurity: GINI

- Gini Index for a given node t :

$$Gini\ Index = 1 - \sum_{i=0}^{c-1} p_i(t)^2$$

- For 2-class problem ($p, 1 - p$):
 - ◆ $GINI = 1 - p^2 - (1 - p)^2 = 2p(1-p)$

C1	0
C2	6
Gini=0.000	

C1	1
C2	5
Gini=0.278	

C1	2
C2	4
Gini=0.444	

C1	3
C2	3
Gini=0.500	

Computing Gini Index of a Single Node

$$Gini\ Index = 1 - \sum_{i=0}^{c-1} p_i(t)^2$$

C1	0
C2	6

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

$$\text{Gini} = 1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$$

C1	1
C2	5

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

$$\text{Gini} = 1 - (1/6)^2 - (5/6)^2 = 0.278$$

C1	2
C2	4

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

$$\text{Gini} = 1 - (2/6)^2 - (4/6)^2 = 0.444$$

Computing Gini Index for a Collection of Nodes

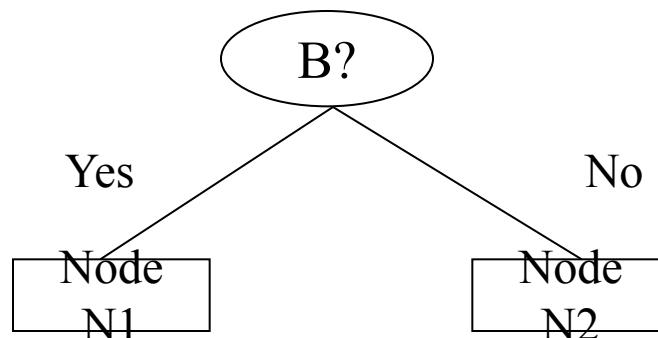
- When a node p is split into k partitions (children)

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

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

Binary Attributes: Computing GINI Index

- Splits into two partitions (child nodes)
- Effect of Weighing partitions:
 - Larger and purer partitions are sought



Gini(N1)

$$\begin{aligned} &= 1 - (5/6)^2 - (1/6)^2 \\ &= 0.278 \end{aligned}$$

Gini(N2)

$$\begin{aligned} &= 1 - (2/6)^2 - (4/6)^2 \\ &= 0.444 \end{aligned}$$

	N1	N2
C1	5	2
C2	1	4
Gini=0.361		

	Parent
C1	7
C2	5
Gini = 0.486	

Weighted Gini of N1 N2

$$\begin{aligned} &= 6/12 * 0.278 + \\ &\quad 6/12 * 0.444 \\ &= 0.361 \end{aligned}$$

$$\text{Gain} = 0.486 - 0.361 = 0.125$$

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	8	1
C2	3	0	7
Gini	0.163		

Two-way split

(find best partition of values)

CarType			
	{Sports, Luxury}	{Family}	
C1	9	1	
C2	7	3	
Gini	0.468		

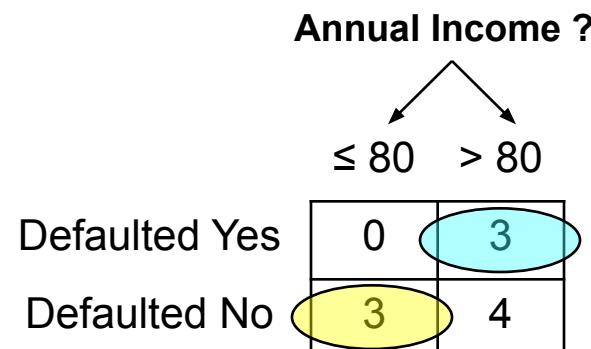
CarType			
	{Sports}	{Family, Luxury}	
C1	8	2	
C2	0	10	
Gini	0.167		

Which of these is the best?

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, $A \leq v$ and $A > v$
- 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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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	
Annual Income											
Sorted Values	→	60	70	75	85	90	95	100	120	125	220

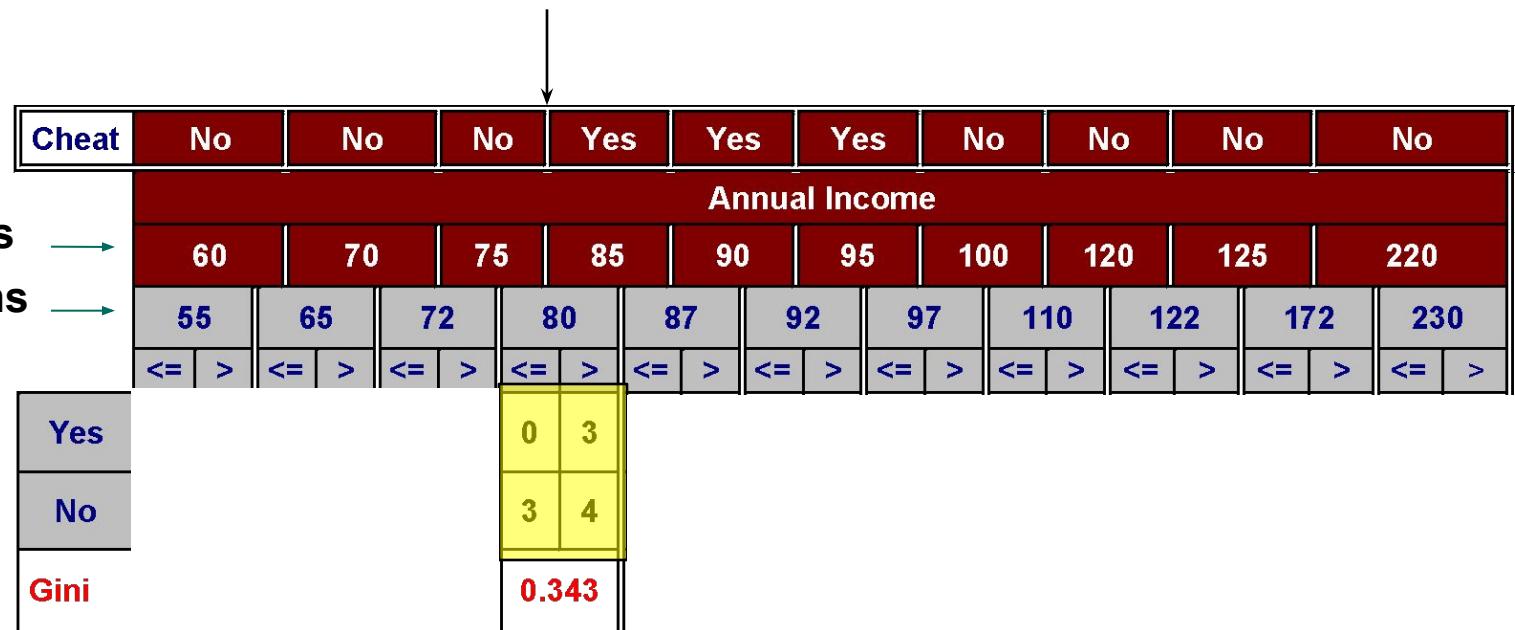
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Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No	
Annual Income											
Sorted Values	60	70	75	85	90	95	100	120	125	220	
Split Positions	55	65	72	80	87	92	97	110	122	172	230
	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	

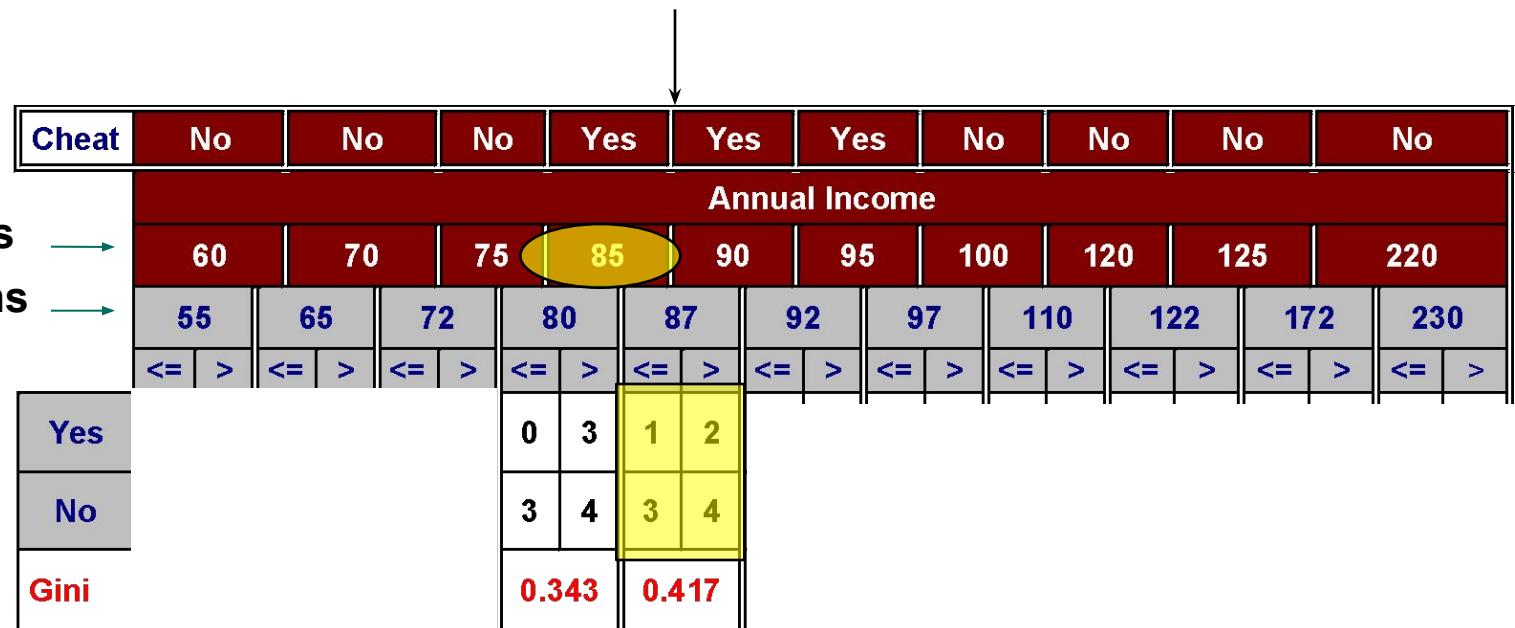
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Annual Income											
Sorted Values →	60	70	75	85	90	95	100	120	125	220	
Split Positions →	55	65	72	80	87	92	97	110	122	172	230
	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	
Yes	0 3	0 3	0 3	0 3	1 2	2 1	3 0	3 0	3 0	3 0	
No	0 7	1 6	2 5	3 4	3 4	3 4	3 4	4 3	5 2	6 1	
Gini	0.420	0.400	0.375	0.343	0.417	0.400	0.300	0.343	0.375	0.400	

Measure of Impurity: Entropy

- Entropy at a given node t

$$\text{Entropy} = - \sum_{i=0}^{c-1} p_i(t) \log_2 p_i(t)$$

Where $p_i(t)$ is the frequency of class i at node t , and c is the total number of classes

- ◆ Maximum of $\log_2 c$ when records are equally distributed among all classes, implying the least beneficial situation for classification
 - ◆ Minimum of 0 when all records belong to one class, implying most beneficial situation for classification
-
- Entropy based computations are quite similar to the GINI index computations

Computing Entropy of a Single Node

$$\text{Entropy} = - \sum_{i=0}^{c-1} p_i(t) \log_2 p_i(t)$$

C1	0
C2	6

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

$$\text{Entropy} = -0 \log 0 - 1 \log 1 = -0 - 0 = 0$$

C1	1
C2	5

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

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

C1	2
C2	4

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

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

Computing Information Gain After Splitting

Information Gain:

$$Gain_{split} = Entropy(p) - \sum_{i=1}^k \frac{n_i}{n} Entropy(i)$$

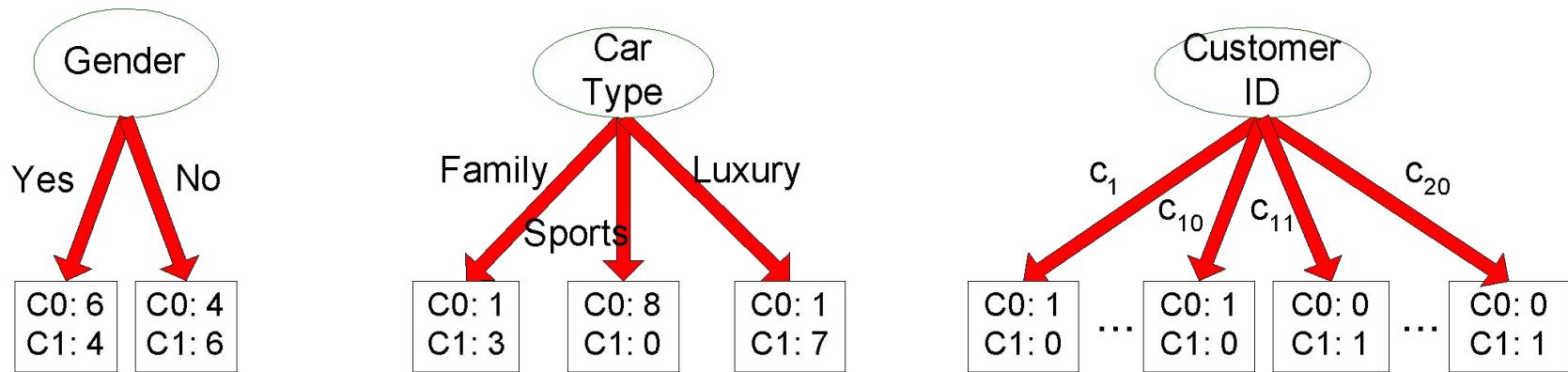
Parent Node, p is split into k partitions (children)

n_i is number of records in child node i

- Choose the split that achieves most reduction (maximizes GAIN)
- Used in the ID3 and C4.5 decision tree algorithms
- Information gain is the mutual information between the class variable and the splitting variable

Problem with large number of partitions

- Node impurity measures tend to prefer splits that result in large number of partitions, each being small but pure



- Customer ID has highest information gain because entropy for all the children is zero

Gain Ratio

- Gain Ratio:

$$\text{Gain Ratio} = \frac{\text{Gain}_{\text{split}}}{\text{Split Info}}$$
$$\text{Split Info} = - \sum_{i=1}^k \frac{n_i}{n} \log_2 \frac{n_i}{n}$$

Parent Node, p is split into k partitions (children)

n_i is number of records in child node i

- Adjusts Information Gain by the entropy of the partitioning (*Split Info*).
 - ◆ Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5 algorithm
- Designed to overcome the disadvantage of Information Gain

Gain Ratio

- Gain Ratio:

$$Gain\ Ratio = \frac{Gain_{split}}{Split\ Info}$$

$$Split\ Info = \sum_{i=1}^k \frac{n_i}{n} \log_2 \frac{n_i}{n}$$

Parent Node, p is split into k partitions (children)

n_i is number of records in child node i

CarType			
	Family	Sports	Luxury
C1	1	8	1
C2	3	0	7
Gini	0.163		

$$\text{SplitINFO} = 1.52$$

CarType		
	{Sports, Luxury}	{Family}
C1	9	1
C2	7	3
Gini	0.468	

$$\text{SplitINFO} = 0.72$$

CarType		
	{Sports}	{Family, Luxury}
C1	8	2
C2	0	10
Gini	0.167	

$$\text{SplitINFO} = 0.97$$

Measure of Impurity: Classification Error

- Classification error at a node t

$$Error(t) = 1 - \max_i[p_i(t)]$$

- Maximum of $1 - 1/c$ when records are equally distributed among all classes, implying the least interesting situation
- Minimum of 0 when all records belong to one class, implying the most interesting situation

Computing Error of a Single Node

$$\text{Error}(t) = 1 - \max_i[p_i(t)]$$

C1	0
C2	6

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

$$\text{Error} = 1 - \max(0, 1) = 1 - 1 = 0$$

C1	1
C2	5

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

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

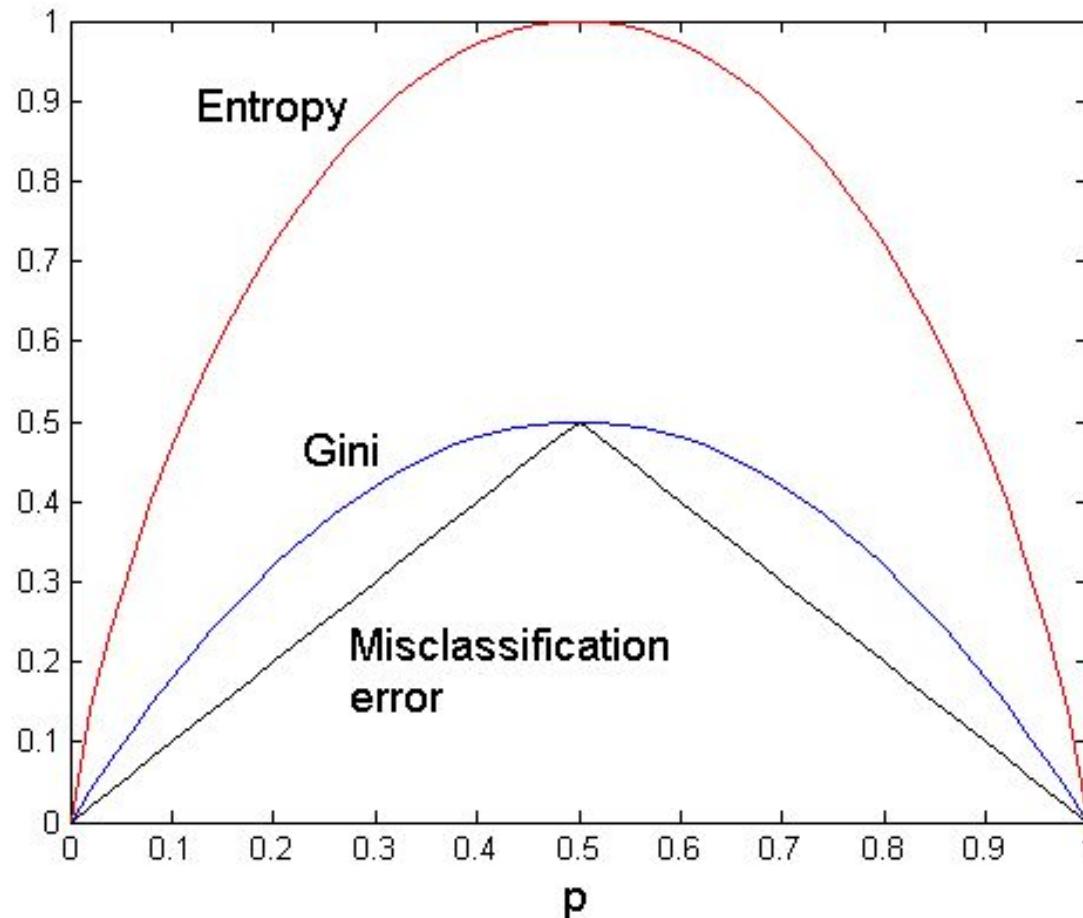
C1	2
C2	4

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

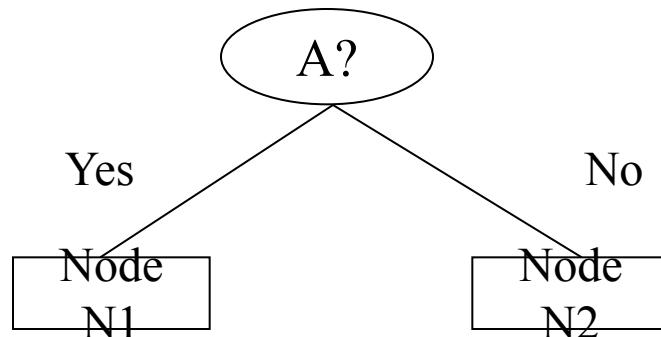
$$\text{Error} = 1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$$

Comparison among Impurity Measures

For a 2-class problem:



Misclassification Error vs Gini Index



	Parent
C1	7
C2	3
Gini = 0.42	

Gini(N1)

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

Gini(N2)

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

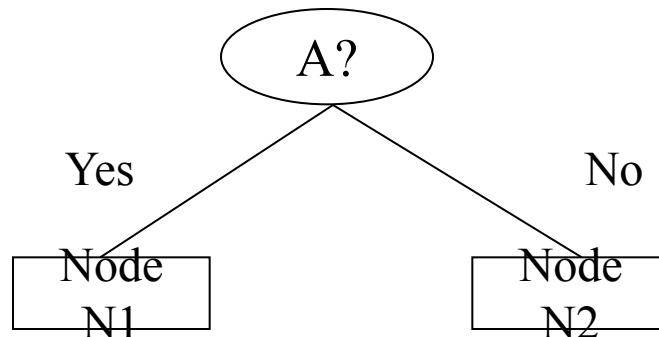
	N1	N2
C1	3	4
C2	0	3
Gini=0.342		

Gini(Children)

$$\begin{aligned} &= 3/10 * 0 \\ &+ 7/10 * 0.489 \\ &= 0.342 \end{aligned}$$

**Gini improves but
error remains the
same!!**

Misclassification Error vs Gini Index



	Parent
C1	7
C2	3
Gini = 0.42	

	N1	N2
C1	3	4
C2	0	3
Gini=0.342		

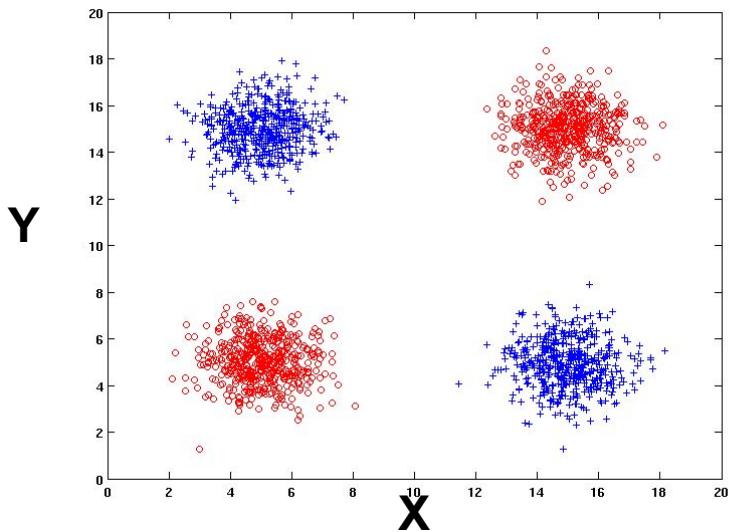
	N1	N2
C1	3	4
C2	1	2
Gini=0.416		

Misclassification error for all three cases = 0.3 !

Decision Tree Based Classification

- Advantages:
 - Relatively inexpensive to construct
 - Extremely fast at classifying unknown records
 - Easy to interpret for small-sized trees
 - Robust to noise (especially when methods to avoid overfitting are employed)
 - Can easily handle redundant or irrelevant attributes (unless the attributes are interacting)
- Disadvantages:
 - Due to the greedy nature of splitting criterion, interacting attributes (that can distinguish between classes together but not individually) may be passed over in favor of other attributes that are less discriminating.
 - Each decision boundary involves only a single attribute

Handling interactions



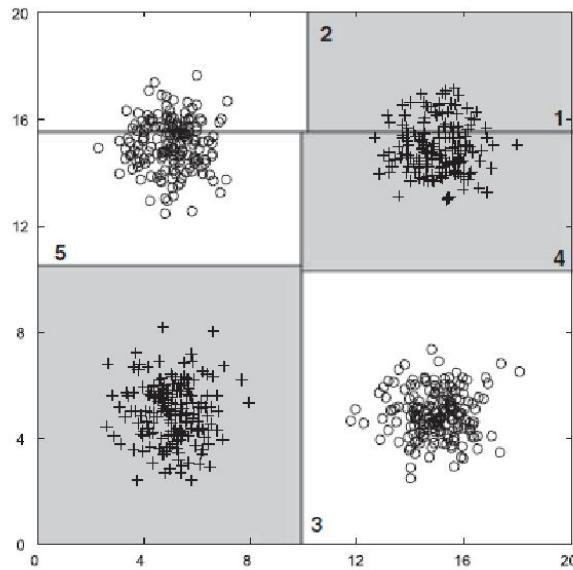
+ : 1000 instances

o : 1000 instances

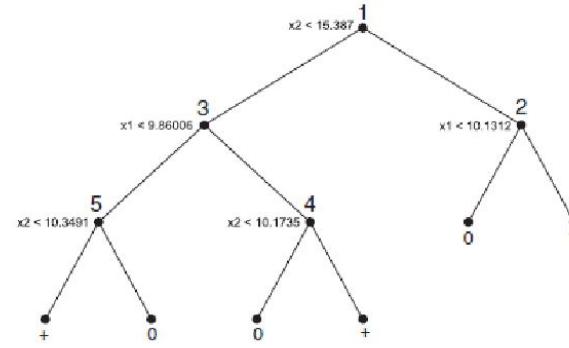
Entropy (X) : 0.99

Entropy (Y) : 0.99

Handling interactions



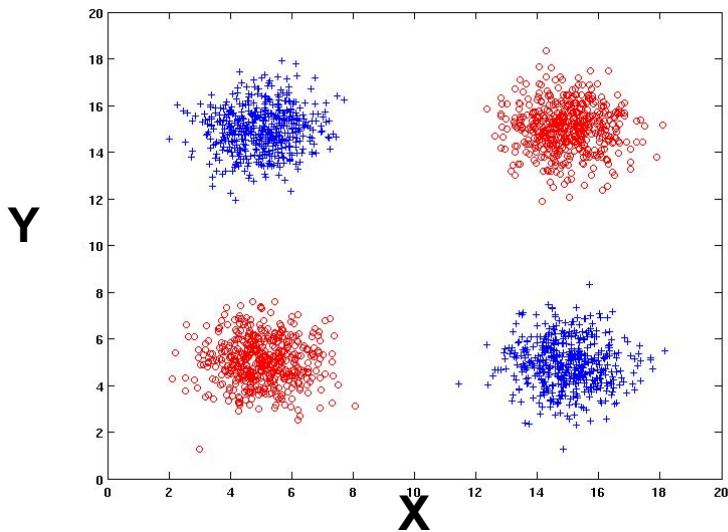
(a) Decision boundary for tree with 6 leaf nodes.



(b) Decision tree with 6 leaf nodes.

Figure 3.28. Decision tree with 6 leaf nodes using X and Y as attributes. Splits have been numbered from 1 to 5 in order of other occurrence in the tree.

Handling interactions given irrelevant attributes



+ : 1000 instances

o : 1000 instances

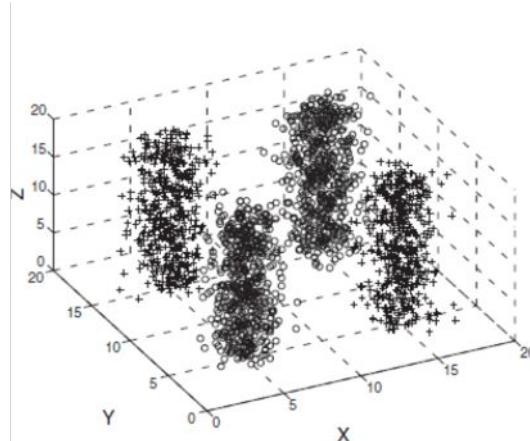
Adding Z as a noisy attribute generated from a uniform distribution

Entropy (X) : 0.99

Entropy (Y) : 0.99

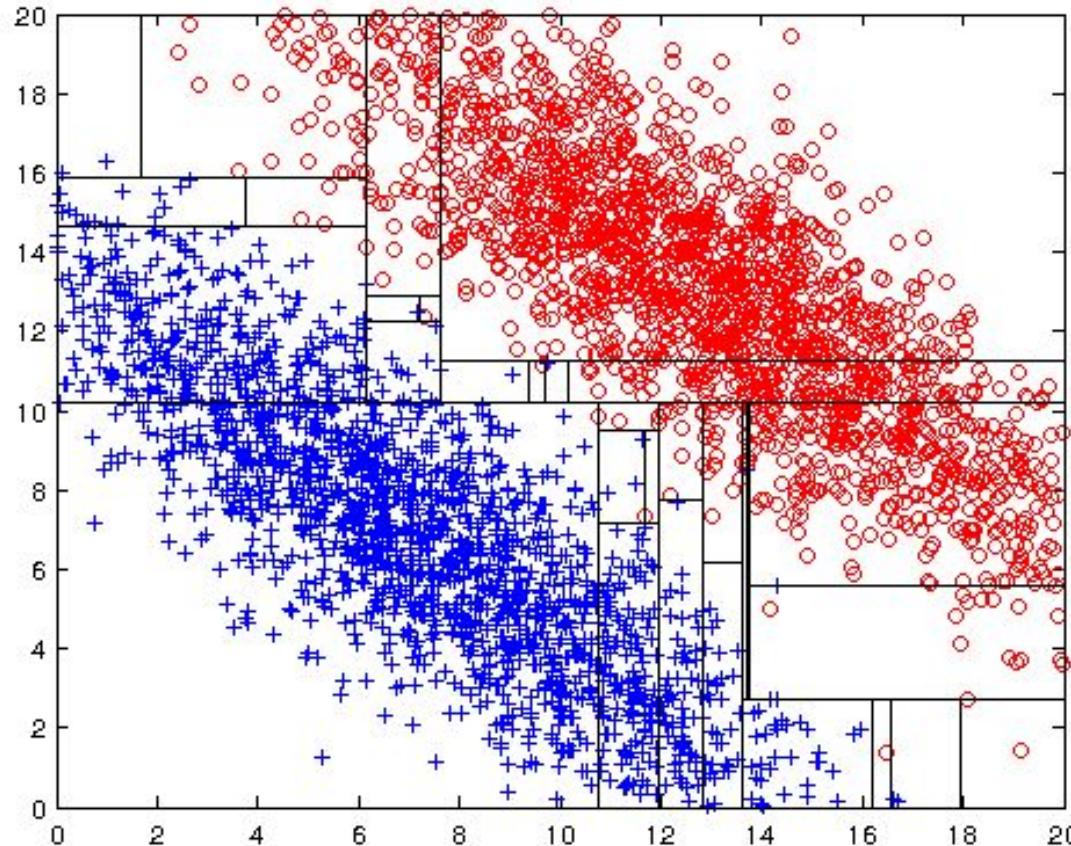
Entropy (Z) : 0.98

Attribute Z will be chosen for splitting!



(a) Three-dimensional data with attributes X , Y , and Z .

Limitations of single attribute-based decision boundaries



Both positive (+) and negative (o) classes generated from skewed Gaussians with centers at (8,8) and (12,12) respectively.