Classification: Basic Concepts and Techniques

Lecture Notes for Chapter 3

Principles of Data Mining
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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
 - \bullet x: attribute, predictor, independent variable, input
 - \bullet y: class, response, dependent variable, output

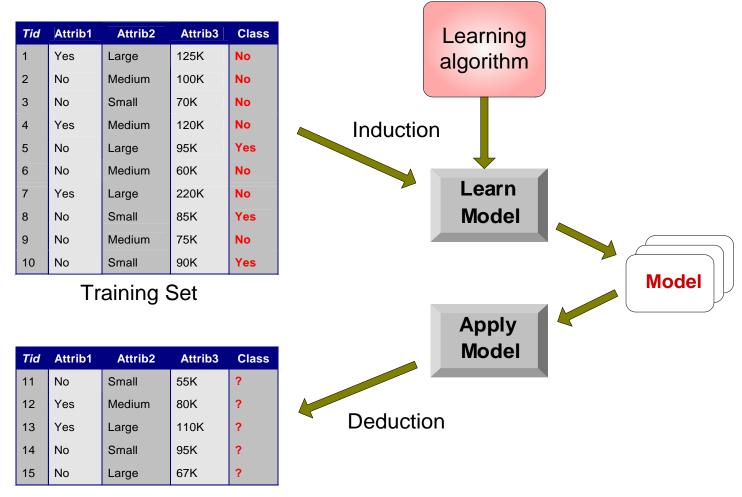
Task:

— Learn a model that maps each attribute set \boldsymbol{x} into one of the predefined class labels \boldsymbol{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

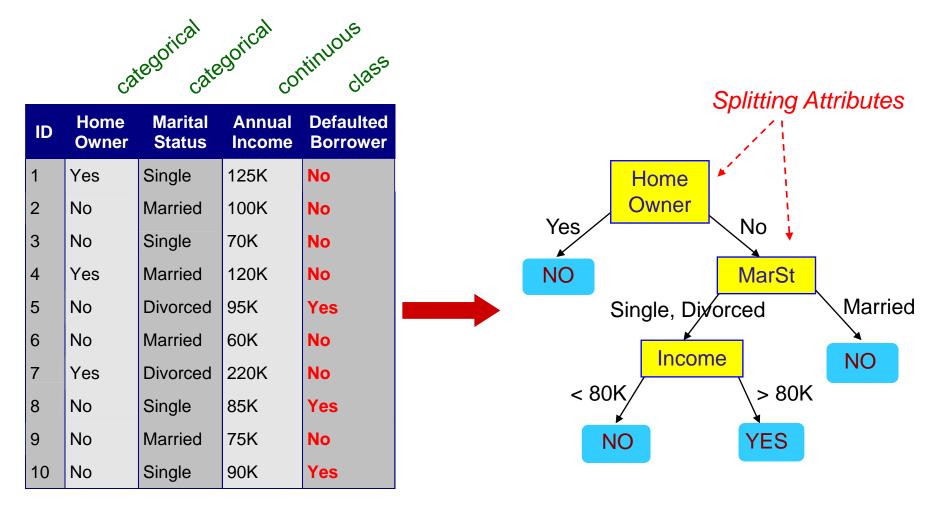


Test Set

Classification Techniques

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

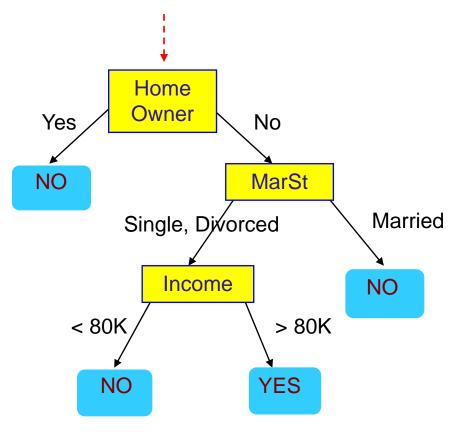
Example of a Decision Tree



Training Data

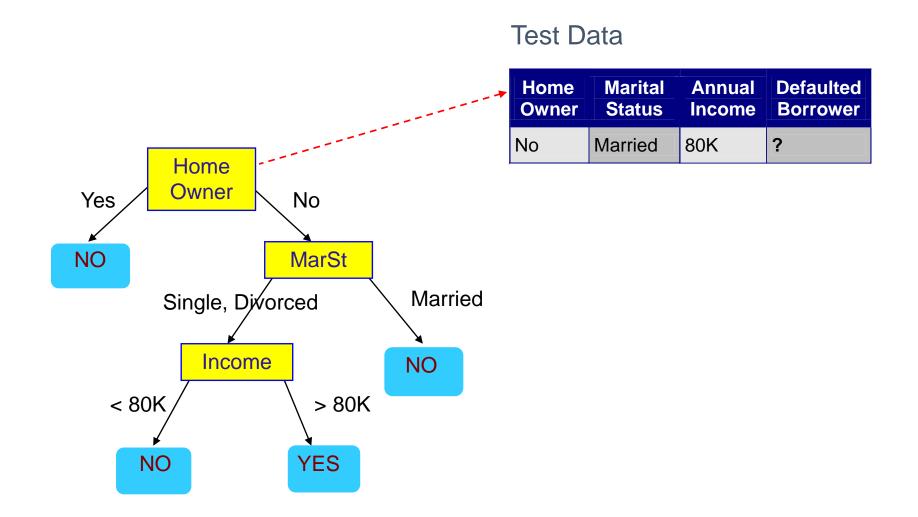
Model: Decision Tree

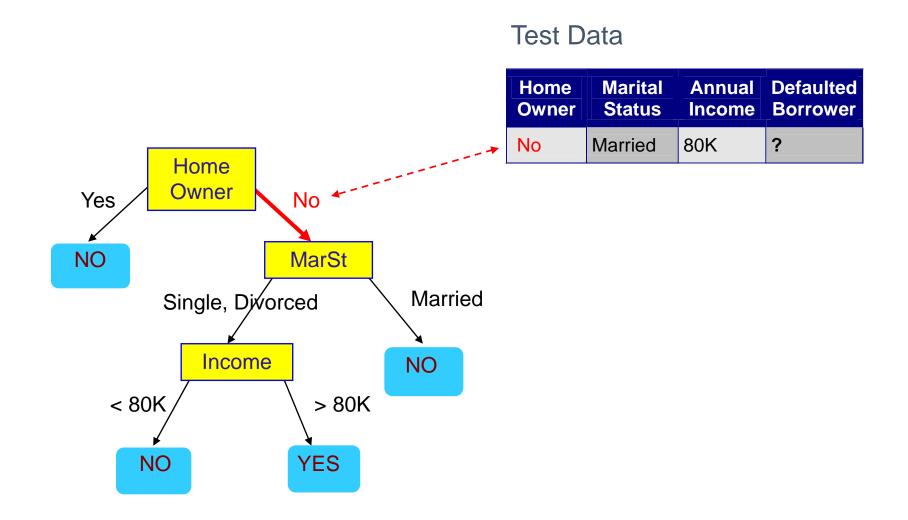
Start from the root of tree.

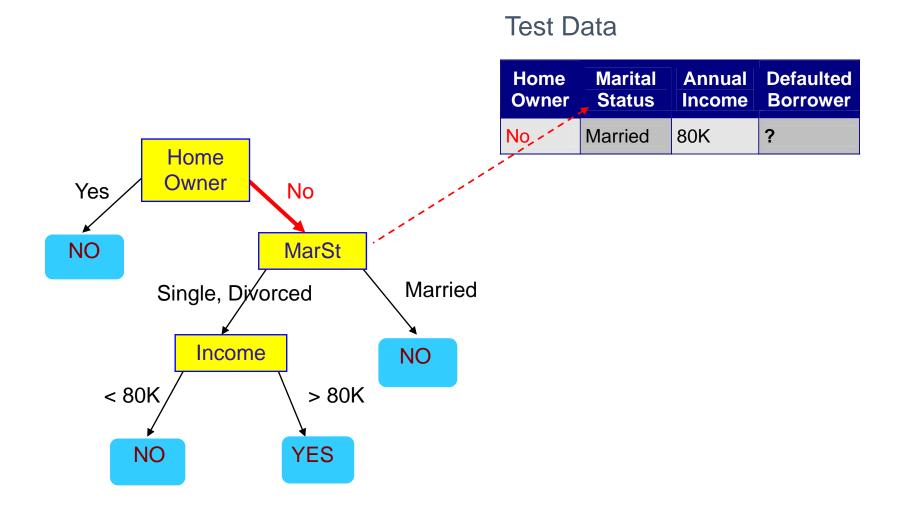


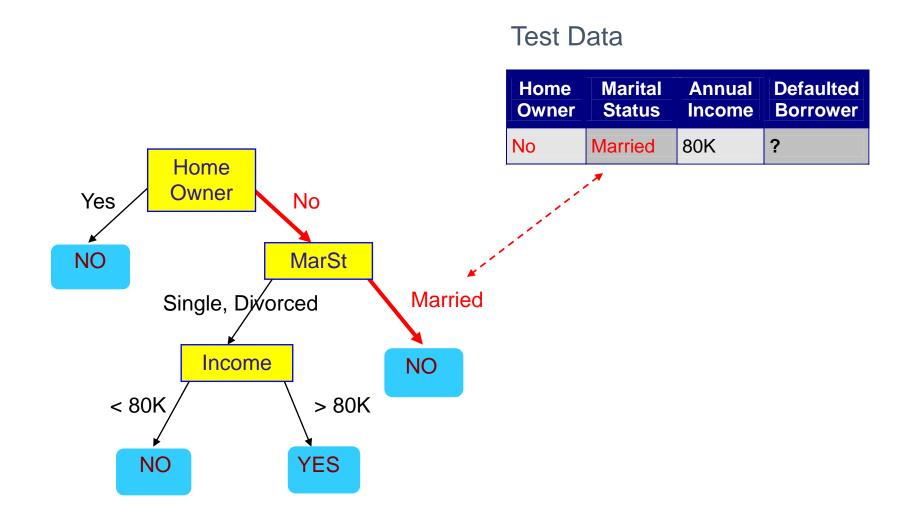
Test Data

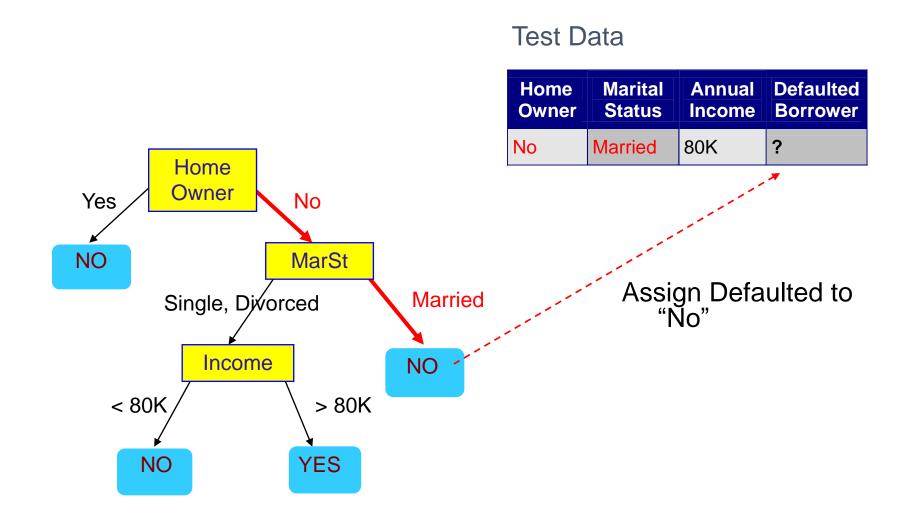
Home Owner			Defaulted Borrower
No	Married	80K	?







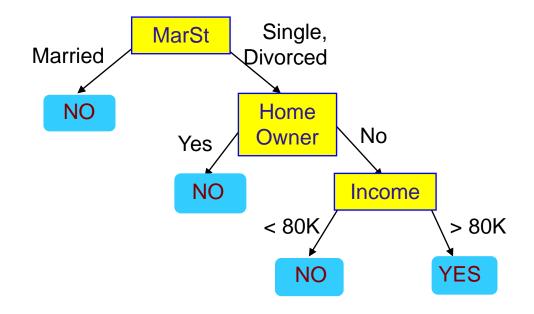




Another Example of Decision Tree

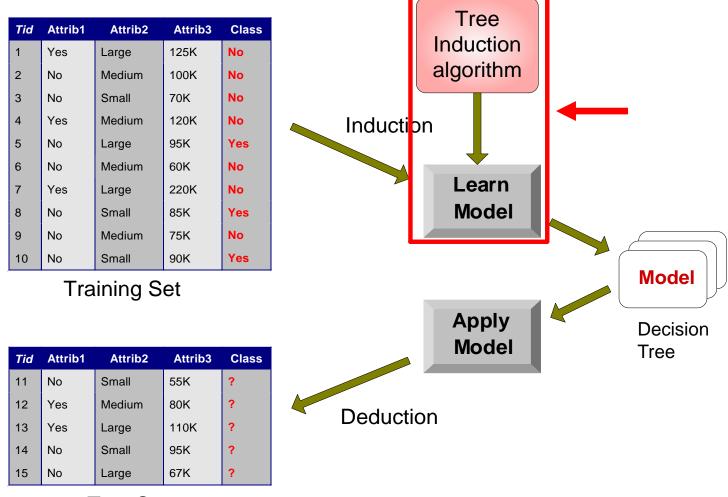
categorical continuous

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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



Test Set

Decision Tree Induction

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

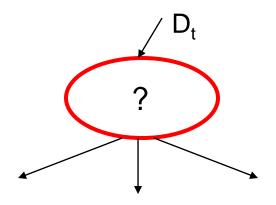
General Structure of Hunt's Algorithm

Let D_t be the set of training records that reach a node t

General Procedure:

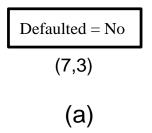
- If D_t contains records that belong the same class y_t, then t is a leaf node labeled as y_t
- If D_t contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

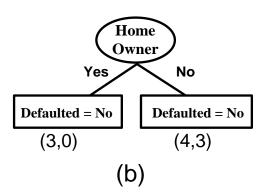
ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
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3	No	Single	70K	No
4	Yes	Married	120K	No
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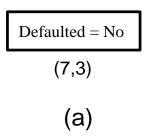
Defaulted = No
(7,3)
(a)

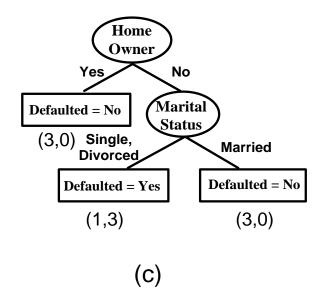
ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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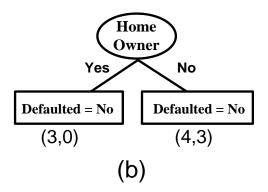




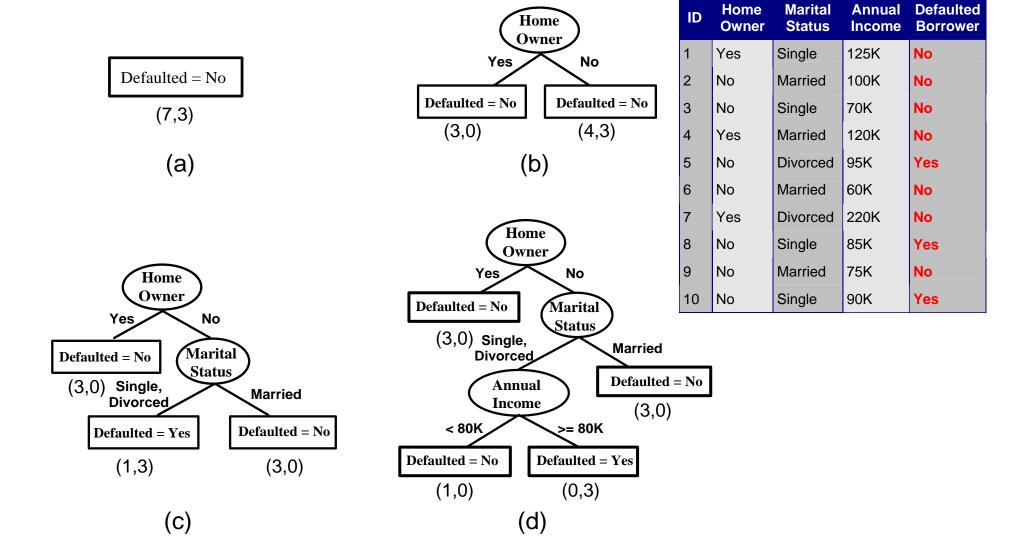
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10	No	Single	90K	Yes



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

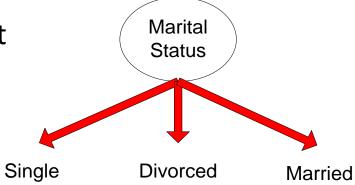
Depends on number of ways to split

- 2-way split
- Multi-way split

Test Condition for Nominal Attributes

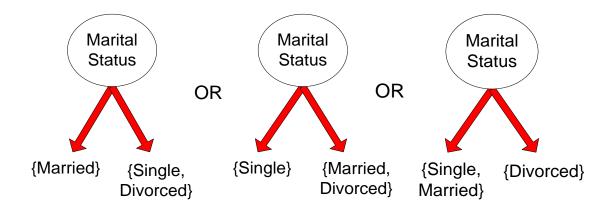
☐ Multi-way split:

Use as many partitions as distinct values.



☐ Binary split:

Divides values into two subsets



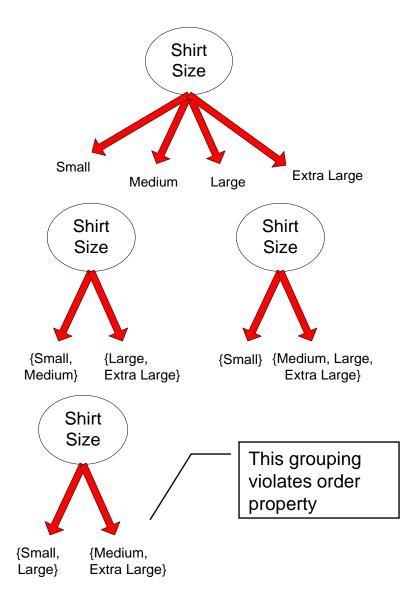
Test Condition for Ordinal Attributes

Multi-way split:

Use as many partitions as distinct values

l Binary split:

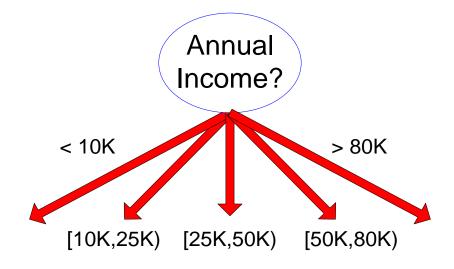
- Divides values into two subsets
- Preserve order property among attribute values



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

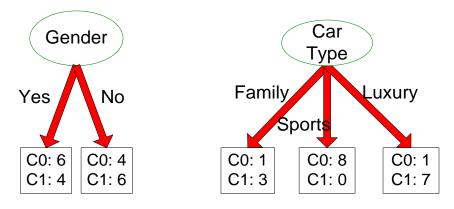
Ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.

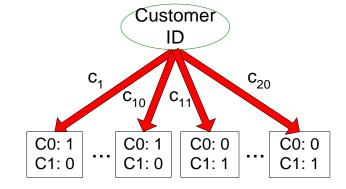
- Static discretize once at the beginning
- Dynamic repeat at each node
- Binary Decision: (A < v) or $(A \ge v)$
 - consider all possible splits and finds the best cut
 - can be more compute intensive

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	\mathbf{M}	Sports	Medium	C0
4	\mathbf{M}	Sports	Large	C0
5	\mathbf{M}	Sports	Extra Large	C0
6	M	Sports	Extra Large	C0
7	\mathbf{F}	Sports	Small	C0
8	F	Sports	Small	C0
9	\mathbf{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	\mathbf{F}	Luxury	Medium	C1
18	\mathbf{F}	Luxury	Medium	C1
19	\mathbf{F}	Luxury	Medium	C1
20	F	Luxury	Large	C1





Which test condition is the best?

How to determine the Best Split

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

C0: 5

C1: 5

C0: 9

C1: 1

High degree of impurity

Low degree of impurity

Measures of Node Impurity

Gini Index =
$$1 - \sum_{i=0}^{c-1} p_i(t)^2$$
 Where $p_i(t)$ is the frequence of class i at node t , and c is the total number of classes

Where $p_i(t)$ is the frequency the total number of classes

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

I Misclassification error

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

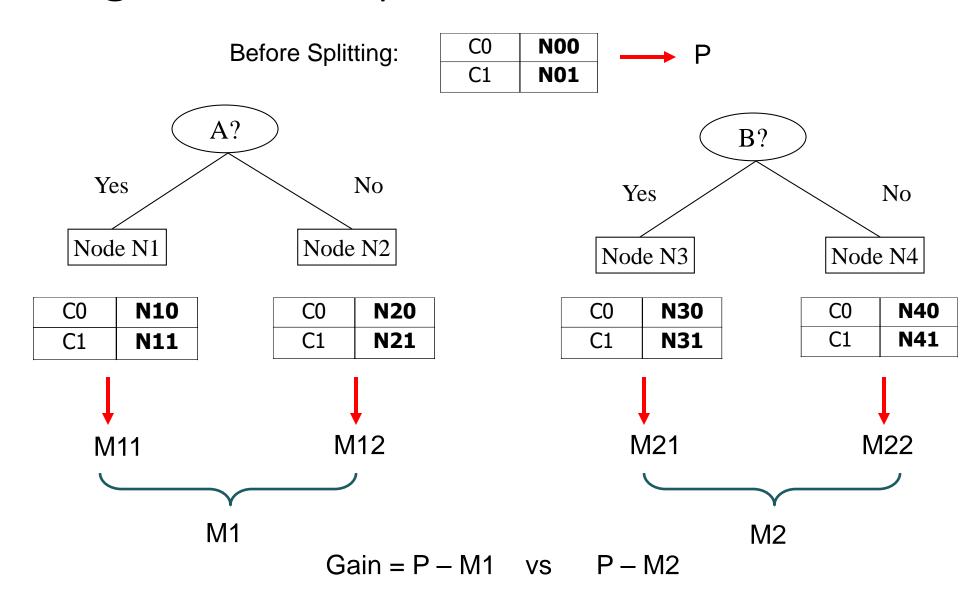
Finding the Best Split

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

$$Gain = P - M$$

or equivalently, lowest impurity measure after splitting (M)

Finding the Best Split



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	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

$$P(C1) = 0/6 = 0$$
 $P(C2) = 6/6 = 1$
 $Gini = 1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$

C1	1
C2	5

P(C1) =
$$1/6$$
 P(C2) = $5/6$
Gini = $1 - (1/6)^2 - (5/6)^2 = 0.278$

$$P(C1) = 2/6$$
 $P(C2) = 4/6$
 $Gini = 1 - (2/6)^2 - (4/6)^2 = 0.444$

Computing Gini Index for a Collection of Nodes

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

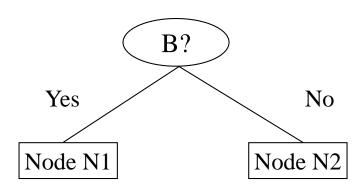
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

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

- I Choose the attribute that minimizes weighted average Gini index of the children
- I Gini index is used in decision tree algorithms such as CART, SLIQ, SPRINT

Binary Attributes: Computing GINI Index

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



	Parent	
C1	7	
C2	5	
Gini = 0.486		

Gini(N1)

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

$$= 0.278$$

Gini(N2)

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

= 0.444

	N1	N2
C1	5	2
C2	1	4
Gini=0.361		

Weighted Gini of N1 N2

$$= 6/12 * 0.278 +$$

$$= 0.361$$

Gain =
$$0.486 - 0.361 = 0.125$$

Categorical Attributes: Computing Gini Index

- I For each distinct value, gather counts for each class in the dataset
- I 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						

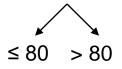
	CarType						
	{Sports}	{Family, Luxury}					
C1	8	2					
C2	0	10					
Gini	0.167						

Which of these is the best?

- I Use Binary Decisions based on one value
- I Several Choices for the splitting value
 - Number of possible splitting values
 - = Number of distinct values
- I Each splitting value has a count matrix associated with it
 - Class counts in each of the partitions, A≤ v and A > v
- I 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.

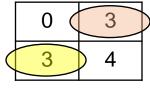
ID	Home Owner	Marital Status	Annual Income	Defaulted
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes





Defaulted Yes

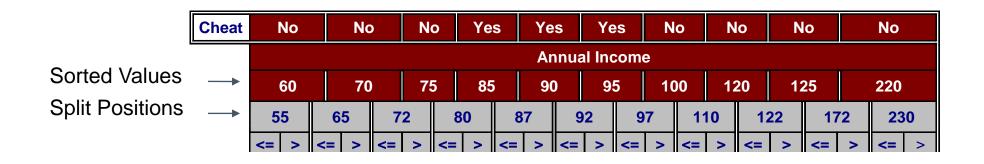
Defaulted No



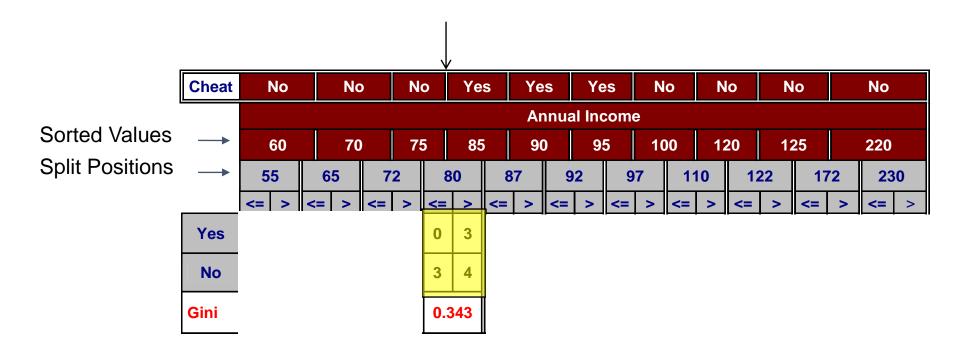
- I For efficient computation: for each attribute,
 - Sort the attribute on values
 - Linearly scan these values, each time updating the count matrix and computing gini index
 - Choose the split position that has the least gini index

	Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
•		Annual Income									
Sorted Values	\rightarrow	60	70	75	85	90	95	100	120	125	220

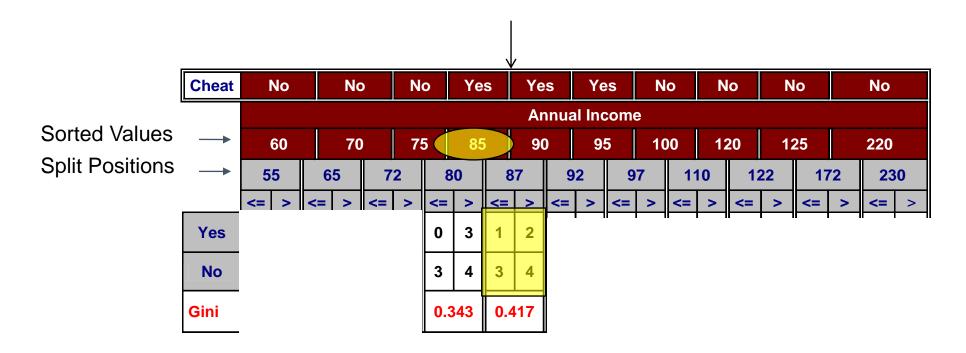
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	Cheat		No		No)	N	0	Ye	s	Ye	s	Υe	es	N	0	N	lo	N	lo		No	
Sorted Values											Ar	nnua	ıl Inc	come	•								
			60		70)	7	5	85	,	90)	9	5	10	00	12	20	12	25		220	
Split Positions	→	5	5	6	5	7	2	8	0	8	7	9	2	9	7	11	10	12	22	17	72	23	0
		"	^	<=	>	<=	>	\=	^	<=	>	<=	^	\=	>	\=	>	"	>	\=	>	<=	>
	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	75	0.3	43	0.4	117	0.4	100	<u>0.3</u>	<u>800</u>	0.3	43	0.3	75	0.4	100	0.4	20

Measure of Impurity: Entropy

I Entropy at a given node *t*

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

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

- igoplus 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

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

C1	0
C2	6

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

C1	1
C2	5

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

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

Computing Information Gain After Splitting

Information Gain:

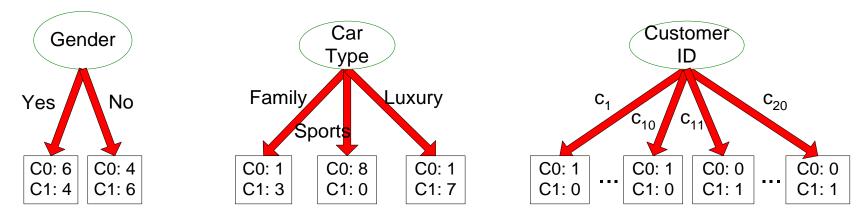
$$Gain_{split} = Entropy(p) - \sum_{i=1}^{k} \frac{n_i}{n} Entropy(i)$$

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

I Gain Ratio:

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

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

I Gain Ratio:

$$Gain Ratio = \frac{Gain_{split}}{Split Info} \qquad Split Info = \sum_{i=1}^{k} \frac{n_i}{n} log_2 \frac{n_i}{n}$$

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									

$$SplitINFO = 1.52$$

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

$$SplitINFO = 0.72$$

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

$$SplitINFO = 0.97$$

Measure of Impurity: Classification Error

I 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

$$Error(t) = 1 - \max_{i}[p_i(t)]$$

C1	0
C2	6

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

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

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

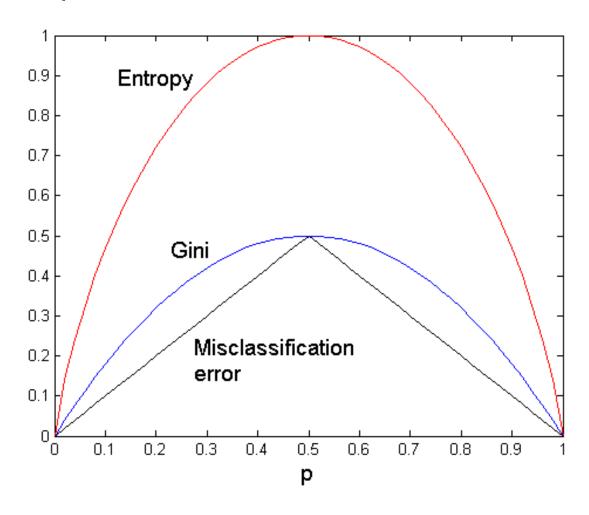
Error =
$$1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

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

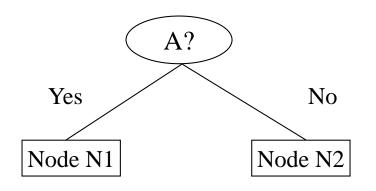
Error =
$$1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$$

Comparison among Impurity Measures

For a 2-class problem:



Misclassification Error vs Gini Index



	Parent	
C1	7	
C2	3	
Gini = 0.42		

Gini(N1)
=
$$1 - (3/3)^2 - (0/3)^2$$

= 0

Gini(N2)
=
$$1 - (4/7)^2 - (3/7)^2$$

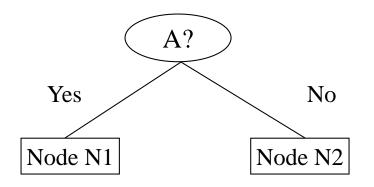
= 0.489

	N1	N2
C1	3	4
C2	0	3
Gini=0.342		

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

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

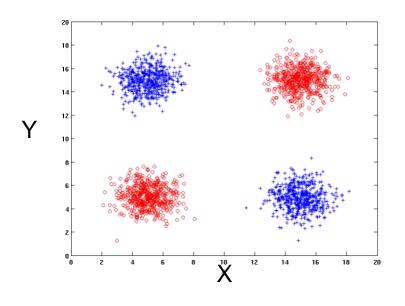
Advantages:

- 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:

- Space of possible decision trees is exponentially large. Greedy approaches are often unable to find the best tree.
- Does not take into account interactions between attributes
- Each decision boundary involves only a single attribute

Handling interactions



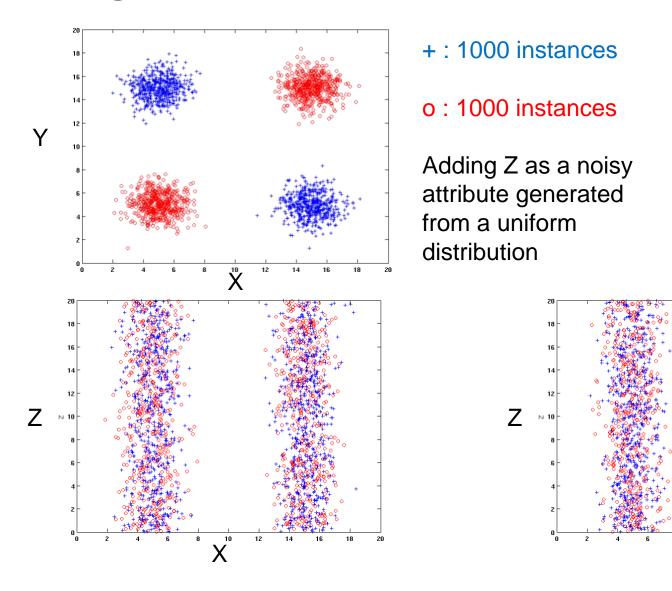
+: 1000 instances

o: 1000 instances

Entropy (X): 0.99

Entropy (Y): 0.99

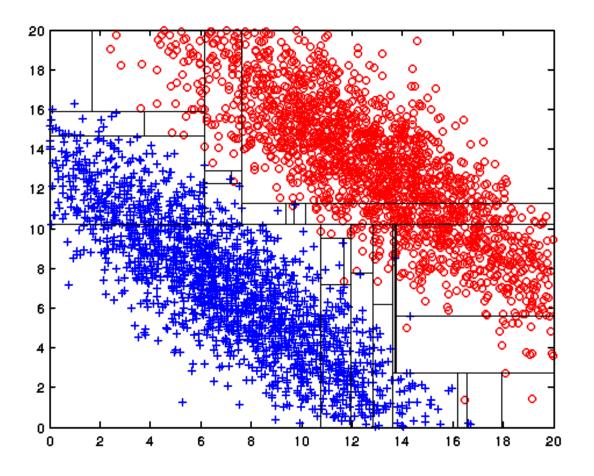
Handling interactions



Entropy (X): 0.99 Entropy (Y): 0.99 Entropy (Z): 0.98

Attribute Z will be chosen for splitting!

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.