# Data Science - Lecture 9 Classification: Decision Trees

Dr. Faisal Kamiran

### **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**

- Greedy strategy.
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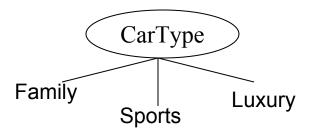
# **How to Specify Test Condition?**

- 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**

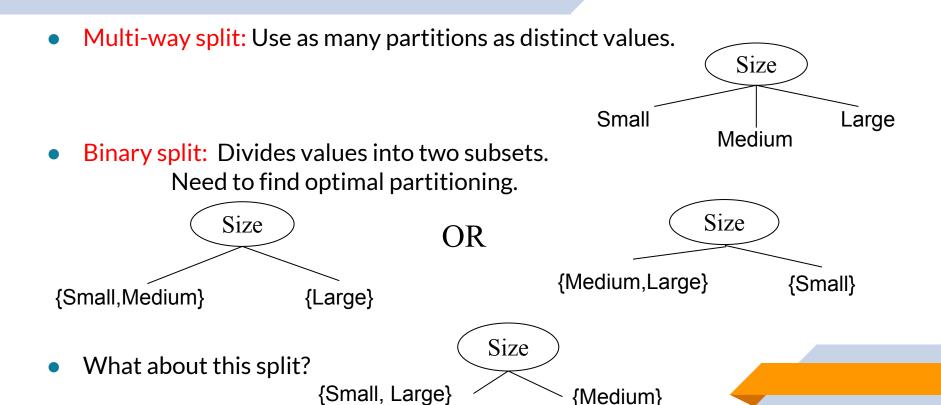
Multi-way split: Use as many partitions as distinct values.



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



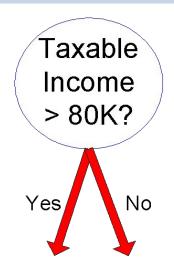
### **Splitting Based on Ordinal Attributes**



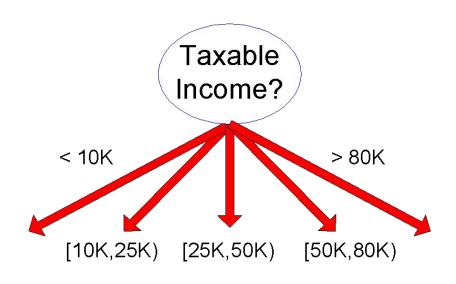
### **Splitting Based on Continuous Attributes**

- 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 ≥ v)</li>
    - 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

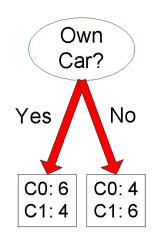
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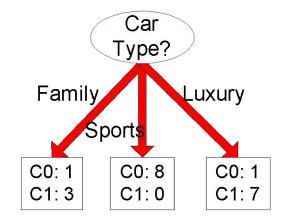
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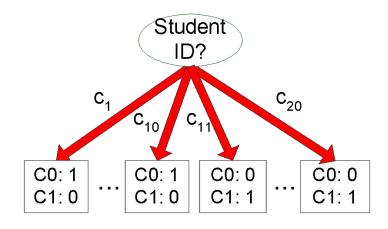
- Issues
  - Determine how to split the records
    - ◆How to specify the attribute test condition?
    - ◆ How to determine the best split?
  - Determine when to stop splitting

### 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,

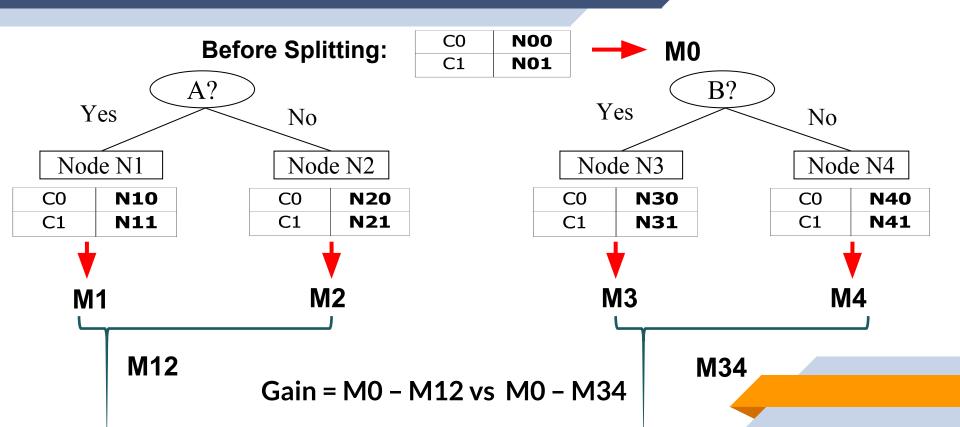
Low degree of impurity

# Measures of Node Impurity

Gini Index

- Entropy
- Misclassification error

# How to Find the Best Split



# Measure of Impurity: GINI

• Gini Index for a given node t:

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

(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	0	
C2	6	
Gini=0.000		

C1	1	
C2	5	
Gini=0.278		

C1	2	
C2	4	
Gini=0.444		

Gini=	3
C1	3

# **Examples for computing GINI**

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

C1	0
C2	6

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

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

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

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

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

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

# **Splitting Based on GINI**

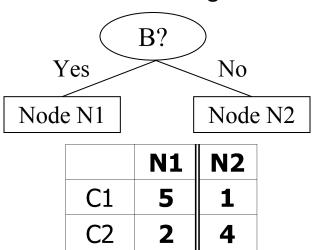
- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

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

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

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

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



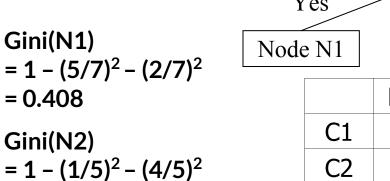
	Parent	
C1	6	
C2	6	

$$Gain(B) = 0.5$$

Splits into two partitions

= 0.32

- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for



r Partitions are sought for.				
B?				
Yes No				
Node	Node N1 Node N2			
		N1	N2	
	C1	5	1	
	C2 <b>2 4</b>			

	Parent	
C1	6	
C2	6	

$$Gain(B) = 0.5$$

Splits into two partitions

Gini(N1)

= 0.408

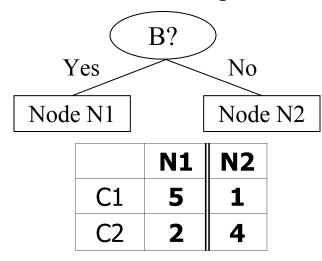
Gini(N2)

= 0.32

 $= 1 - (5/7)^2 - (2/7)^2$ 

 $= 1 - (1/5)^2 - (4/5)^2$ 

- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



Gini(Split) = 0.371

	Parent	
C1	6	
C2	6	

Gain(B) = 0.5

#### Gini(Children)

= 7/12 \* 0.408 +

5/12 \* 0.32

= 0.371

Splits into two partitions

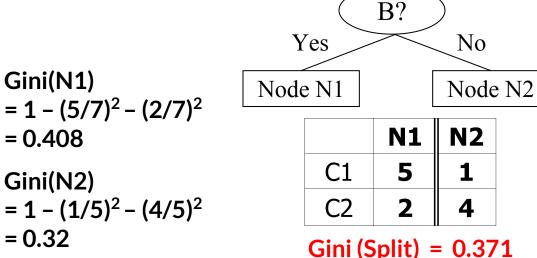
Gini(N1)

= 0.408

Gini(N2)

= 0.32

- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



	Parent	
C1	6	
C2	6	

Gain (B) = 0.5

#### Gini(Children)

$$= 0.371$$

Gain (B)=
$$0.5 - 0.371 = 0.129$$

- 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			

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

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

- 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				

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

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

- 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			

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

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

- 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				

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

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

### **Continuous Attributes: Computing Gini Index**

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

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Taxable Income > 80K?



### **Continuous Attributes: Computing Gini Index**

- Simple method to choose best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! Repetition of work.

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Taxable Income > 80K?



### 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

# Sorted Values Split Positions

ı	<u> </u>		1-2-1								·		f		f w		100			<u> </u>	C.		-
	Cheat	No			No		N	o Yes		s	Ye	S	Υe	S	N	0	N	lo	N	lo	,	No	
•		Taxable Income																					
		60			70		7	'5 85		90		)	95		100		12	120		125		220	
	<b>→</b>	55		6	65		72		80 87		7	92		9	97 1		10 1:		22 17		230		
	<b>→</b>	<b>=</b>	>	<=	>	<=	>	<b>"</b>	>	<=	>	<b>&lt;=</b>	>	<=	>	<b>=</b>	>	<=	>	<=	>	<=	>
	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		0.4	0.400 0.3		375	0.343		0.4	.417 0.400		100	<u>0.300</u> 0.3		43 0.375		0.4	0.400 0.420		20		

# Measures of Node Impurity

Gini Index

Entropy

Misclassification error

### **Entropy**

- Information is measured in bits
  - Given a probability distribution, the info required to predict an event is the distribution's *entropy*
  - Entropy gives the information required in bits (this can involve fractions of bits!)
- Formula for computing the entropy:

entropy
$$(p_1, p_2, \square, p_n) = -p_1 \log p_1 - p_2 \log p_2 \square - p_n \log p_n$$

### Entropy

Entropy at a given node t:

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

(NOTE: p(j | t) is the relative frequency of class j at node t).

- Measures homogeneity of a node.
  - igoplus Maximum (log n<sub>c</sub>) when records are equally distributed among all classes implying least information
  - Minimum (0.0) when all records belong to one class, implying most information
- Entropy based computations are similar to the GINI index computations

# **Examples for computing Entropy**

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

C1	0
C2	6

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

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

# **Examples for computing Entropy**

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

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

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

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

### **Information Gain**

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, is number of records in partition i

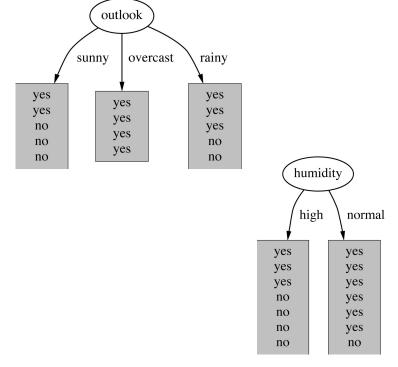
- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
- Used in ID3 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

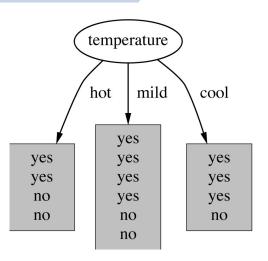
# Weather Data: Play or not Play?

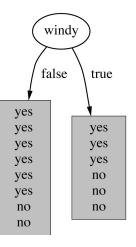
Outlook	Temperature	Humidity	Windy	Play?
sunny	hot	high	false	No
sunny	hot	high	true	No
overcast	hot	high	false	Yes
rain	mild	high	false	Yes
rain	cool	normal	false	Yes
rain	cool	normal	true	No
overcast	cool	normal	true	Yes
sunny	mild	high	false	No
sunny	cool	normal	false	Yes
rain	mild	normal	false	Yes
sunny	mild	normal	true	Yes
overcast	mild	high	true	Yes
overcast	hot	normal	false	Yes
rain	mild	high	true	No

Note:
Outlook is the
Forecast,
no relation to
Microsoft
email program

### Which attribute to select?







• "Outlook" = "Sunny": info([2,3]) = entropy(2/5,3/5) =  $-2/5\log(2/5) - 3/5\log(3/5) = 0.971$  bits

- "Outlook" = "Sunny":  $\inf([2,3]) = \exp(2/5,3/5) = -2/5\log(2/5) 3/5\log(3/5) = 0.971 \text{ bits}$
- "Outlook" = "Overcast": info([4,0]) = entropy(1,0) = -1log(1) - 0log(0) = 0 bits

- "Outlook" = "Sunny":  $\inf([2,3]) = \exp(2/5,3/5) = -2/5\log(2/5) 3/5\log(3/5) = 0.971 \text{ bits}$
- "Outlook" = "Overcast": Note: log(0) is not

$$info([4,0]) = entropy(1,0) = -1log(1) - 0log(0) = 0$$
 bits defined, but we evaluate  $0*log(0)$  as zero

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- "Outlook" = "Overcast":

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Note: log(0) is not defined, but we evaluat 0\*log(0) as zero

"Outlook" = "Rainy":

$$\inf([3,2]) = \exp(3/5,2/5) = -3/5\log(3/5) - 2/5\log(2/5) = 0.971 \text{ bits}$$

- "Outlook" = "Sunny":  $\inf([2,3]) = \exp(2/5,3/5) = -2/5\log(2/5) - 3/5\log(3/5) = 0.971 \text{ bits}$
- "Outlook" = "Overcast": Note: log(0) is not

$$\inf([4,0]) = \operatorname{entropy}(1,0) = -1\log(1) - 0\log(0) = 0 \text{ bits}$$
 defined, but we evaluate  $0*\log(0)$  as zero

- "Outlook" = "Rainy":
- $\inf([3,2]) = \operatorname{entropy}(3/5,2/5) = -3/5\log(3/5) 2/5\log(2/5) = 0.971 \text{ bits}$
- Expected information for attribute:

info([3,2],[4,0],[3,2]) = 
$$(5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$

- "Outlook" = "Sunny": info([2,3]) = entropy(2/5,3/5) =  $-2/5\log(2/5) 3/5\log(3/5) = 0.971$  bits
- "Outlook" = "Overcast":

  Note: log(0) is not defined, but we evaluate
- $\inf_{0 \text{ log(0)}} (1,0) = \text{entropy}(1,0) = -1\log(1) 0\log(0) = 0 \text{ bits}$  defined, but we obtain 0 log(0) as zero
- "Outlook" = "Rainy":
- $\inf([3,2]) = \exp(3/5,2/5) = -3/5\log(3/5) 2/5\log(2/5) = 0.971 \text{ bits}$
- Expected information for attribute:

info([3,2],[4,0],[3,2]) = 
$$(5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$
  
= 0.693 bits

## **Examples for computing Entropy**

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

C1	0
C2	6

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

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

# **Examples for computing Entropy**

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

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

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

# **Examples for computing Entropy**

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

C1	0
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Entropy = 
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$$P(C1) = 1/6$$
  $P(C2) = 5/6$ 

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

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

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

# Computing the information gain

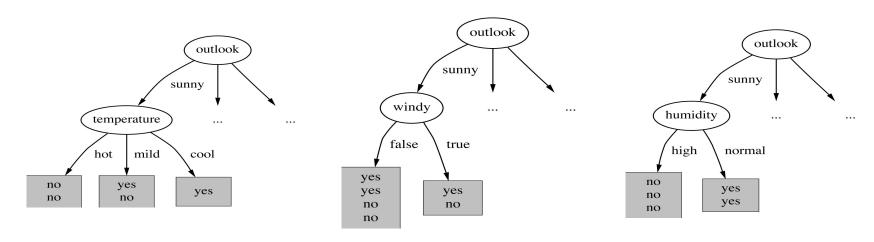
• Information gain:

```
(information before split) – (information after split)
gain("Outlook") = info([9,5]) - info([2,3],[4,0],[3,2]) = 0.940 - 0.693
= 0.247 \text{ bits}
```

Information gain for attributes from weather data:

```
gain("Outlook") = 0.247 bits
gain("Temperature") = 0.029 bits
gain("Humidity") = 0.152 bits
gain("Windy") = 0.048 bits
```

# Continuing to split

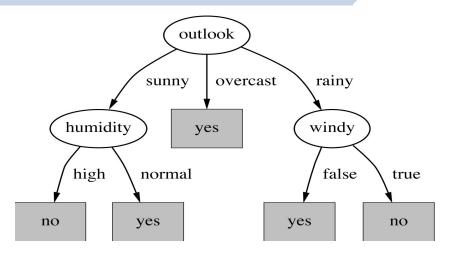


gain("Humidity") = 0.971 bits

gain("Temperature") = 0.571 bits

gain("Windy") = 0.020 bits

#### The final decision tree



- Note: not all leaves need to be pure; sometimes identical instances have different classes
  - ⇒ Splitting stops when data can't be split any further

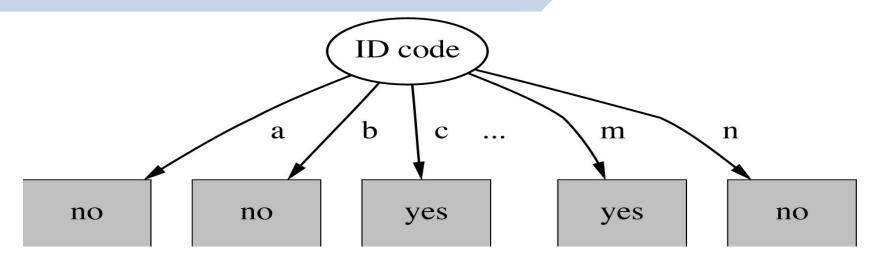
## Highly-branching attributes

- Problematic: attributes with a large number of values (extreme case: ID code)
- Subsets are more likely to be pure if there is a large number of values
  - → Information gain is biased towards choosing attributes with a large number of values
  - → This may result in overfitting (selection of an attribute that is non-optimal for prediction)

## Weather Data with ID code

ID	Outlook	Temperature	Humidity	Windy	Play?
Α	sunny	hot	high	false	No
В	sunny	hot	high	true	No
C	overcast	hot	high	false	Yes
D	rain	mild	high	false	Yes
E	rain	cool	normal	false	Yes
F	rain	cool	normal	true	No
G	overcast	cool	normal	true	Yes
Н	sunny	mild	high	false	No
I	sunny	cool	normal	false	Yes
J	rain	mild	normal	false	Yes
K	sunny	mild	normal	true	Yes
L	overcast	mild	high	true	Yes
M	overcast	hot	normal	false	Yes
N	rain	mild	high	true	No

# Split for ID Code Attribute



Entropy of split = 0 (since each leaf node is "pure", having only one case.

Information gain is maximal for ID code

#### Gain ratio

- *Gain ratio*: a modification of the information gain that reduces its bias on high-branch attributes
- Gain ratio takes number and size of branches into account when choosing an attribute
  - It corrects the information gain by taking the SplitInfo (intrinsic information) of a split into account (i.e. how much info do we need to tell which branch an instance belongs to)

## Splitting Based on INFO...

Gain Ratio:

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

Parent Node, p is split into k partitions  $n_i$  is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Designed to overcome the disadvantage of Information Gain

# Computing the gain ratio

Example: intrinsic information for ID code

info(
$$[1,1, \square, 1) = 14 \times (-1/14 \times \log 1/14) = 3.807$$
 bits

- Importance of attribute decreases as intrinsic information gets larger
- Example of gain ratio:

$$gain\_ratio("Attribute") = \frac{gain("Attribute")}{intrinsic\_info("Attribute")}$$

Example:

gain\_ratio("ID\_code") = 
$$\frac{0.940 \text{ bits}}{3.807 \text{ bits}} = 0.246$$

## Gain ratios for weather data

Outlook		Temperature	
Info:	0.693	Info:	0.911
Gain: 0.940-0.693	0.247	Gain: 0.940-0.911	0.029
Split info: info([5,4,5])	1.577	Split info: info([4,6,4])	1.362
Gain ratio: 0.247/1.577	0.156	Gain ratio: 0.029/1.362	0.021

Humidity		Windy
Info:	0.788	Info: 0.892
Gain: 0.940-0.788	0.152	Gain: 0.940-0.892 0.048
Split info: info([7,7])	1.000	Split info: info([8,6]) 0.985
Gain ratio: 0.152/1	0.152	Gain ratio: 0.048/0.985 0.049

## More on the gain ratio

- "Outlook" still comes out top
- However: "ID code" has greater gain ratio
  - Standard fix: *ad hoc* test to prevent splitting on that type of attribute
- Problem with gain ratio: it may overcompensate
  - May choose an attribute just because its intrinsic information is very low
  - Standard fix:
    - First, only consider attributes with greater than average information gain
    - Then, compare them on gain ratio

#### **Comparing Attribute Selection Measures**

- The three measures, in general, return good results but
  - Information gain:
    - biased towards multivalued attributes
  - Gain ratio:
    - Gain Ratio takes number and size of branches into account when choosing an attribute
  - Gini index:
    - biased to multivalued attributes
    - has difficulty when # of classes is large

# Measures of Node Impurity

Gini Index

- Entropy
- Misclassification error

### Splitting Criteria based on Classification Error

Classification error at a node t :

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

- Measures misclassification error made by a node.
  - Maximum (1 1/n<sub>c</sub>) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

# **Examples for Computing Error**

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

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

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

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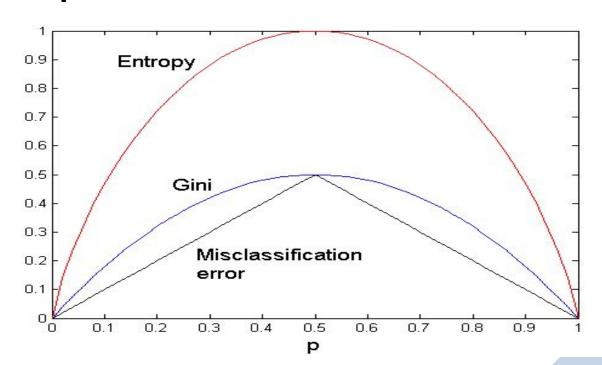
Error = 
$$1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

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

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

# Comparison among Splitting Criteria

#### For a 2-class problem:



#### **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)