Classification

Decision Trees

Huiping Cao

Examples of a Decision Tree

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

Refund: categorical

Marital Status: categorical

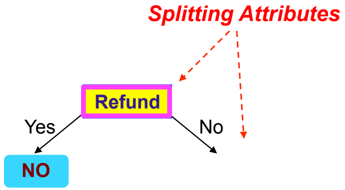
Taxable Income: continuous

Cheat: class

Examples of a Decision Tree (cont.)

	categorical	categorical	continuous	class
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**

Training Data



Model: Decision Tree

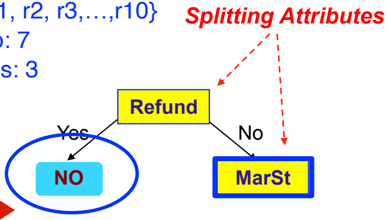
Examples of a Decision Tree (cont.)

categorical · categorical · continuous · class

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

Training Data

Dt1={r1, r2, r3,…,r10}
C0=No: 7
C1=Yes: 3



Model: Decision Tree

Examples of a Decision Tree (cont.)

categorical categorical continuous class

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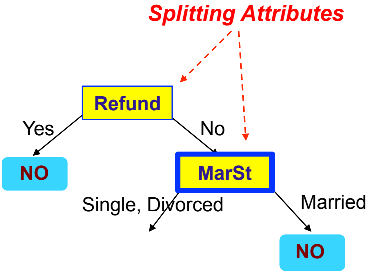
2	No	Married	100K	No
3	No	Single	70K	No
~~4~~	~~Yes~~	~~Married~~	~~120K~~	~~No~~
5	No	Divorced	95K	Yes
6	No	Married	60K	No
~~7~~	~~Yes~~	~~Divorced~~	~~220K~~	~~No~~
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Examples of a Decision Tree (cont.)

categorical categorical continuous class

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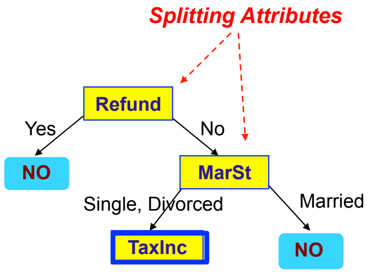
3	No	Single	70K	No
~~4~~	~~Yes~~	~~Married~~	~~120K~~	~~No~~
5	No	Divorced	95K	Yes
~~6~~	~~No~~	~~Married~~	~~60K~~	~~No~~
~~7~~	~~Yes~~	~~Divorced~~	~~220K~~	~~No~~
8	No	Single	85K	Yes
~~9~~	~~No~~	~~Married~~	~~75K~~	~~No~~
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Examples of a Decision Tree (cont.)

categorical categorical continuous class

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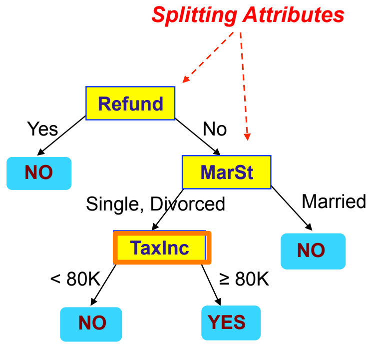
5	No	Divorced	95K	Yes
~~6~~	~~No~~	~~Married~~	~~60K~~	~~No~~
~~7~~	~~Yes~~	~~Divorced~~	~~220K~~	~~No~~
8	No	Single	85K	Yes
~~9~~	~~No~~	~~Married~~	~~75K~~	~~No~~
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Examples of a Decision Tree (cont.)

categorical categorical continuous class

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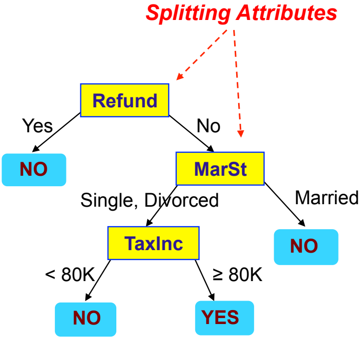
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Examples of a Decision Tree (cont.)

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
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3	No	Single	70K	No
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5	No	Divorced	95K	Yes
6	No	Married	60K	No
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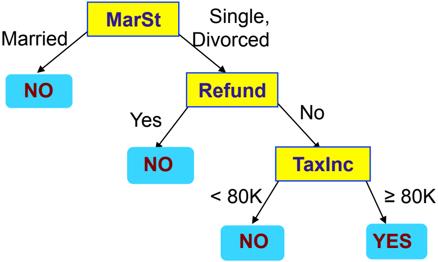
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

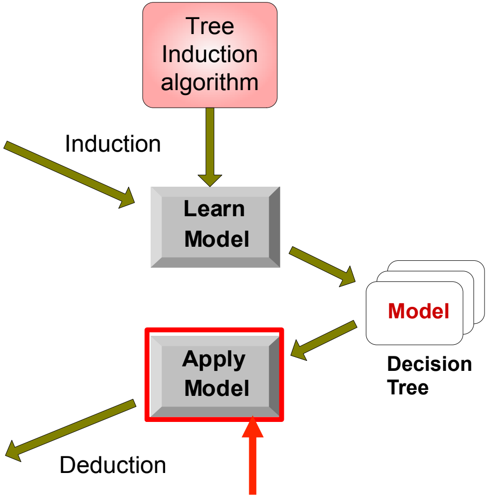


There could be more than one tree that fits the same data!

Decision Tree Classification Task

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

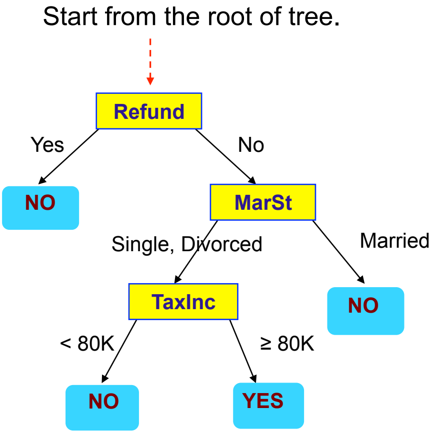
Training Set



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

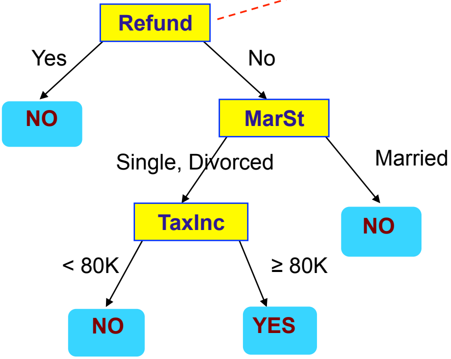
Example: Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Example: Apply Model to Test Data (cont.)



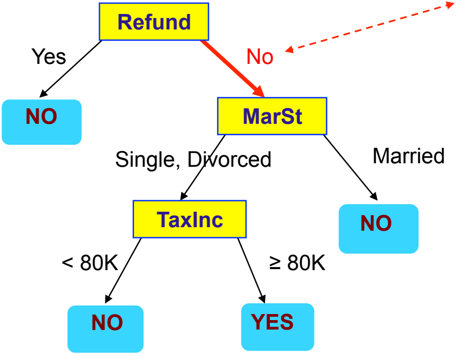
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Example: Apply Model to Test Data (cont.)

Test Data

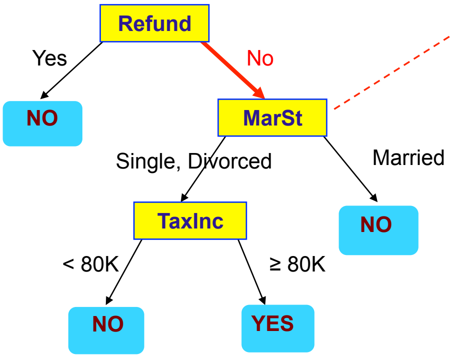
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Example: Apply Model to Test Data (cont.)

Test Data

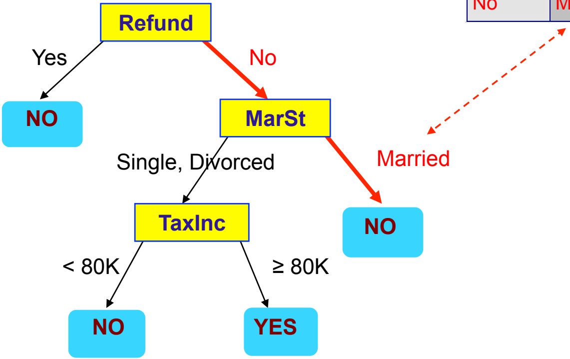
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



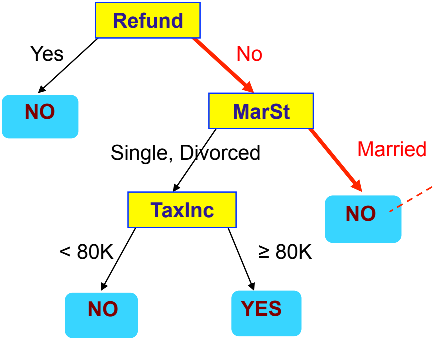
Example: Apply Model to Test Data (cont.)

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Example: Apply Model to Test Data (cont.)



Test Data

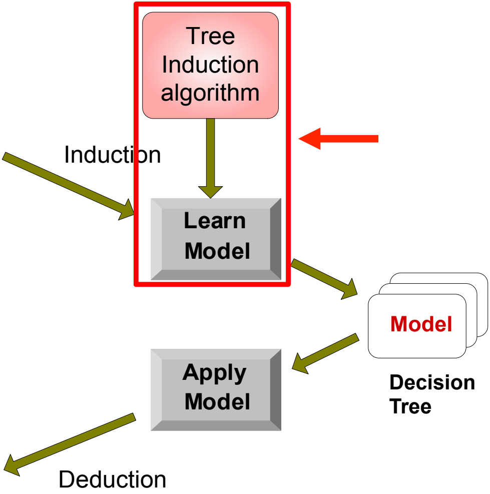
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to "No"

Decision Tree 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

Decision Tree Induction

- How many trees? Exponential in the number of attributes
- Many Algorithms: reasonably accurate, suboptimal, reasonable amount of time
    - Hunt's Algorithm (basis of many others)
    - CART (Classification and Regression Trees), a book by Breiman et al.
    - ID3, C4.5 by Quinlan

Hunt's algorithm

- Let D_t be the set of training records that reach a node t
- $y = \{y_1, y_2, \cdots, y_c\}$ are class labels
- 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

Decision Tree Induction Algorithms – Design Issues

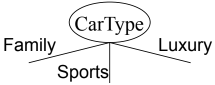
- How should the training records be split?
  - How to specify the attribute test condition?
  - How to determine the best split?
  - Greedy strategy: split the records based on an attribute test that optimizes certain criterion
- When to stop splitting
  - Naive: (1) all the records have identical attribute values; or (2) all the records belong to the same class
  - Is there any better way? Early stop?

Specify the Attribute 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

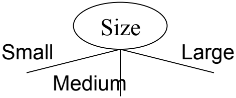
- Multi-way split: Use as many partitions as distinct values



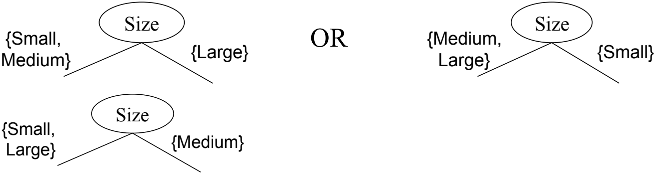
- Binary split: Divides values into two subsets. Need to find optimal partitioning.

Splitting Based on Ordinal Attributes

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



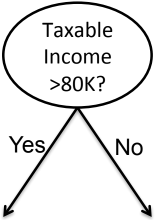
- Binary split: Divides values into two subsets. Need to find optimal partitioning and preserve the order among attribute values.



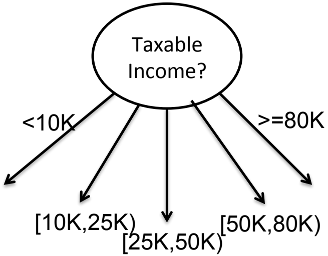
Splitting Based on Continuous Attributes

- 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 find the best cut
    - Can be more compute intensive

Splitting Based on Continuous Attributes – Example



(i) Binary split

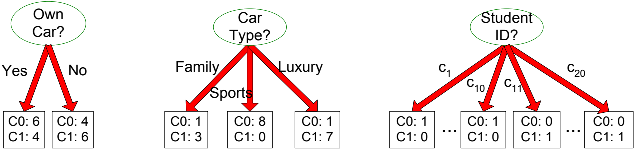


(ii) Multi-way split

Determine the best split

Before Splitting:

- 10 records of class 0
- 10 records of class 1



Which test condition is the best?

Determine the Best Split – Node Impurity

- Splitting criterion
  - Splitting attribute
  - Splitting point or splitting subset
  - Ideally, the resulting partitions at each branch are as "pure" as possible.
- Need a measure of node impurity
  - The smaller the degree of impurity, the more skewed the class distribution. The BETTER.
  - Node with class distribution (0,1) has zero impurity.
  - Node with class distribution (0.5,0.5) has highest impurity.

Measures of Node Impurity

- Gini Index

$$Gini(t) = 1 - \sum_{i=0}^{c-1}[p(i|t)]^2$$

  $p(i|t)$: the probability that an instance t in D_t belongs to class C_i, estimated by $\frac{n_i}{|D_t|}$, where n_i is the number of instances with class label C_i.

- Entropy

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

  Log uses base 2: information is encoded in bits.

- Classification error

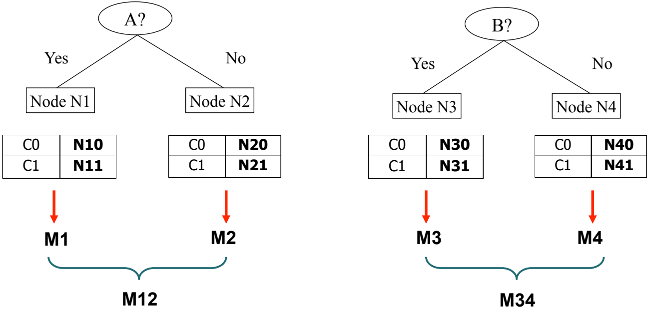
$$Classification\ error(t) = 1 - max_i[p(i|t)]$$

Determine the Best Split– Information Gain

Before splitting:

C0	N00
C1	N01

$M0 = I(N)$



- Gain: $\Delta = I(parent) - \sum_{j=1}^{k} \frac{N(v_j)}{N} I(v_j)$
- $Gain = M0 - M12 \ vs \ \ M0 - M34$

Measures of Node Impurity – Gini

$$Gini(t) = 1 - \sum_{i=0}^{c-1} [p(i|t)]^2$$

$p(i|t)$: the relative frequency of class i at node t.

- Maximum? $(1 - \frac{1}{n_c})$ 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
- First used in CART, which allows only binary splitting

Measures of Node Impurity – Gini

C1	0
C2	6

C1	1
C2	5

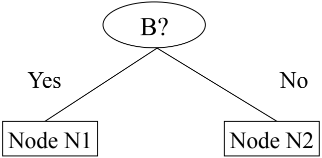
C1	2
C2	4

C1	3
C2	3

Gini?

- $1 - (\frac{0}{6})^2 - (\frac{6}{6})^2 = 0$
- $1 - (\frac{1}{6})^2 - (\frac{5}{6})^2 = \frac{10}{36} = 0.278$
- $1 - (\frac{2}{6})^2 - (\frac{4}{6})^2 = \frac{16}{36} = 0.444$
- 0.5

Binary Attributes: Computing Gini Index



	Parent	N1	N2
C1	6	5	1
C2	6	2	4

- $Gini(Parent) = 0.5$
- $Gini(N1) = 1 - (5/7)^2 - (2/7)^2$
- $Gini(N2) = 1 - (1/5)^2 - (4/5)^2$
- $Gini(Children) = 7/12 * Gini(N1) + 5/12 * Gini(N2)$
- $Gain = Gini(Parent) - Gini(Children)$

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	

Calculation example?

Categorical Attributes: Computing Gini Index

- Gini(family) = 1-(1/25)-(16/25)=(8/25)
- Gini(sports) = 1-(4/9)-(1/9)=(4/9)
- Gini(luxury) = 1/2
- Gini(all) = (5/10)*(8/25)+(3/10)*(4/9)+(2/10)*(1/2) =(4/25)+(2/15)+(1/10) = (24+20+15)/150 = 59/150 = 0.393

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.

Continuous Attributes: Computing Gini Index

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

Continuous Attributes: Computing Gini Index

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

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
Taxable 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	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		*0.300*		0.343		0.375		0.400		0.420	

Entropy

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

- 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

Examples for Computing Entropy

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

C1	0
C2	6

C1	1
C2	5

C1	2
C2	4

C1	3
C2	3

Entropy?

- $-0log0 - 1log1 = 0$ (prob. is 0 means it does not happen, let $0log0 = 0$)
- $-\frac{1}{6}log(\frac{1}{6}) - \frac{5}{6}log(\frac{5}{6}) = 0.65$
- $-\frac{2}{6}log(\frac{2}{6}) - \frac{4}{6}log(\frac{4}{6}) = 0.92$

Splitting Based on Information Gain

$$Information\ Gain = Entropy(p) - \sum_{j=1}^{k} \frac{N(v_j)}{N} Entropy(v_j)$$

- Used in ID3
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.
- Consider partition on ID? $Entropy(children) = 0$

Splitting Based on Gain Ratio

$$Gain\ Ratio = \frac{Information\ Gain}{Split\ Info}$$

$$Split\ Info = \sum_{j=1}^{k} \left(\frac{n_j}{n} log\left(\frac{n_j}{n}\right)\right)$$

- Parent node p is split into k partitions
- n_j is the number of records in partition j
- Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5, successor of ID3
- Designed to overcome the disadvantage of Information Gain

Classification Error

$$Error(t) = 1 - max_i p(i|t)$$

- 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 Classification Error

$$Error(t) = 1 - max_i p(i|t)$$

C1	0
C2	6

C1	1
C2	5

C1	2
C2	4

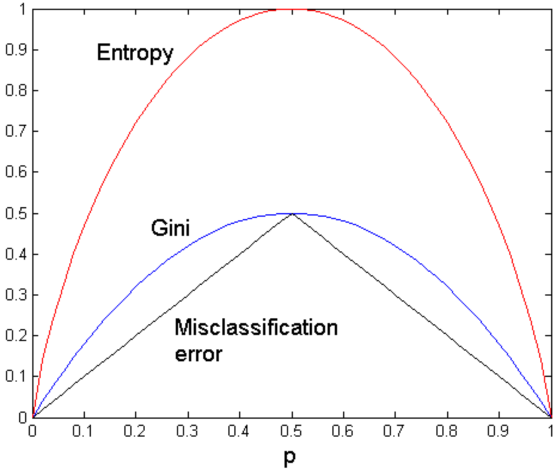
C1	3
C2	3

Classification Error?

- $1 - max(0, 1) = 0$
- $1 - max(1/6, 5/6) = 1 - 5/6 = 1/6$
- $1 - max(2/6, 4/6) = 1 - 4/6 = 1/3$
- 0.5

Comparison among Splitting Criteria

For a 2-class problem:



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: use threshold

Examples

- ID3: Use Entropy, Information gain
- C4.5: Use Entropy, Normalized Information Gain (Gain Ratio)
  Download the software from:
  `http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz`
- CART: Uses Gini Index, only binary splits

Which measure is the best?

- Time complexity of DT induction increases exponentially with tree height $\rightarrow$ shallower trees
- Shallow trees tend to have a large number of leaves and higher error rates

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.
- Download the software from:
  `http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz`

DT Example (1)

RID	age	income	student	credit_rating	buys_computer
1	$<= 30$	high	no	fair	no
2	$<= 30$	high	no	excellent	no
3	$31 \cdots 40$	high	no	fair	yes
4	> 40	medium	no	fair	yes
5	> 40	low	yes	fair	yes
6	> 40	low	yes	excellent	no
7	$31 \cdots 40$	low	yes	excellent	yes
8	$<= 30$	medium	no	fair	no
9	$<= 30$	low	yes	fair	yes
10	> 40	medium	yes	fair	yes
11	$<= 30$	medium	yes	excellent	yes
12	$31 \cdots 40$	medium	no	excellent	yes
13	$31 \cdots 40$	high	yes	fair	yes
14	> 40	medium	no	excellent	no

Class label attribute: *buys_computer*
Preprocess *age* attribute:

- $<= 30$: young
- $31 \cdots 40$: middle_aged
- > 40: senior

DT Example (2)

RID	age	income	student	credit_rating	buys_computer
1	young	high	no	fair	no
2	young	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	young	medium	no	fair	no
9	young	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	young	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

DT Example (3) – Information gain based on Gini Index

Number of classes:

- C_1: for *yes*, 9
- C_2: for *no*, 5

$Gini(D) = 1 - (\frac{9}{14})^2 - (\frac{5}{14})^2 = 0.459$

Consider using attribute *income* as splitting attribute:

- D_1: *income* is {low, medium}
  $Gini(D_1) = 1 - (\frac{6}{10})^2 - (\frac{4}{10})^2 = \frac{48}{100}$
- D_2: *income* is {high}
  $Gini(D_2) = 1 - (\frac{2}{4})^2 - (\frac{2}{4})^2 = \frac{1}{2}$
- $Gini(children) = \frac{10}{14} * \frac{48}{100} + \frac{4}{14} * \frac{1}{2} = \frac{12}{35} + \frac{1}{7} = \frac{17}{35} = 0.486$
- $Gain = Gini(D) - Gini(children) = -0.027$

DT Example (4) – Information gain based on Entropy

$$Entropy(D) = -\frac{9}{14}log_2(\frac{9}{14}) - \frac{5}{14}log_2(\frac{5}{14}) = 0.94$$

Compute the expected entropy for *each* attribute.
Start with attribute *age*.
Consider multi-split (i.e., 3-split). D_{young}: 2 yes, 3 no;

$$Avg\ Entropy = 0.694$$

Calculation?

$$Gain(age) = 0.94 - 0.694 = 0.246$$

Compute gain for other attributes: Gain(income) = 0.029, Gain(student), etc.

DT Example (5) – Gain ratio

Consider attribute *income*.

- low: 4
- medium: 6
- high: 4

$$Split\ Info(D) = -\frac{4}{14}log_2(\frac{4}{14}) - \frac{6}{14}log_2(\frac{6}{14}) - \frac{4}{14}log_2(\frac{4}{14}) = 0.926$$

$$Gain\ ratio(income) = \frac{0.029}{0.926} = 0.031$$

Building a decision tree - Python example

Building a decision tree does not need to standardize the attribute values.

```
from sklearn import tree
from sklearn.tree import DecisionTreeClassifier

tree_model = DecisionTreeClassifier(criterion='gini',
                                    max_depth=4,
                                    random_state=1)
tree_model.fit(X_train, y_train)

tree.plot_tree(tree_model)
plt.show()
```

Prediction - Python example

- `predict(self,X,check_input=True)`
  Predict class (or regression value) for X.
- `predict_proba(self,X,check_input=True)`
  Predict class probabilities of the input samples X.

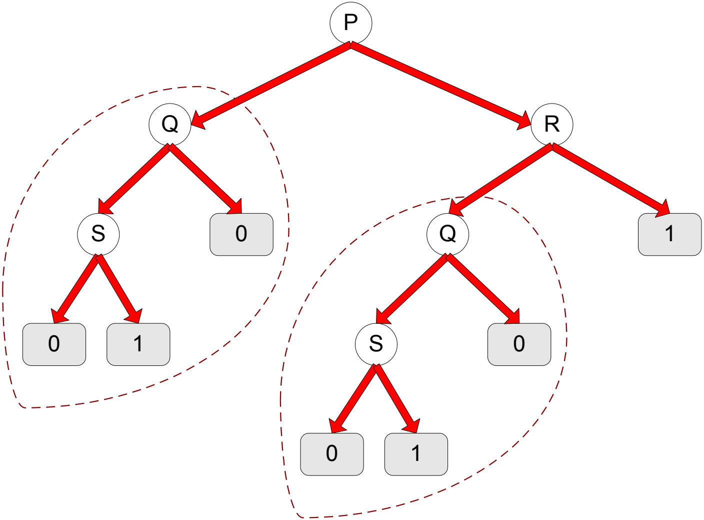
Decision Tree Based Classification – Advantages

- 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

Decision Boundary

- Decision boundary: border line between two neighboring regions of different classes
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time.
- **Oblique decision tree**
  - Test condition may involve multiple attributes $x + y < 1$
  - More expressive representation
  - Finding optimal test condition is computationally expensive
- **Constructive induction**
  - Purpose: partition the data into homogeneous, non-rectangular regions.
  - Composite attribute

Tree Replication



References

- Chapter 3: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar
- DecisionTreeClassifier: `https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html`