CS 561/71: Decision Tree

Classification: Definition

- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*
- Find a *model* for class attribute as a function of the values of other attributes
- Goal: <u>previously unseen</u> records should be assigned a class as accurately as possible
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it
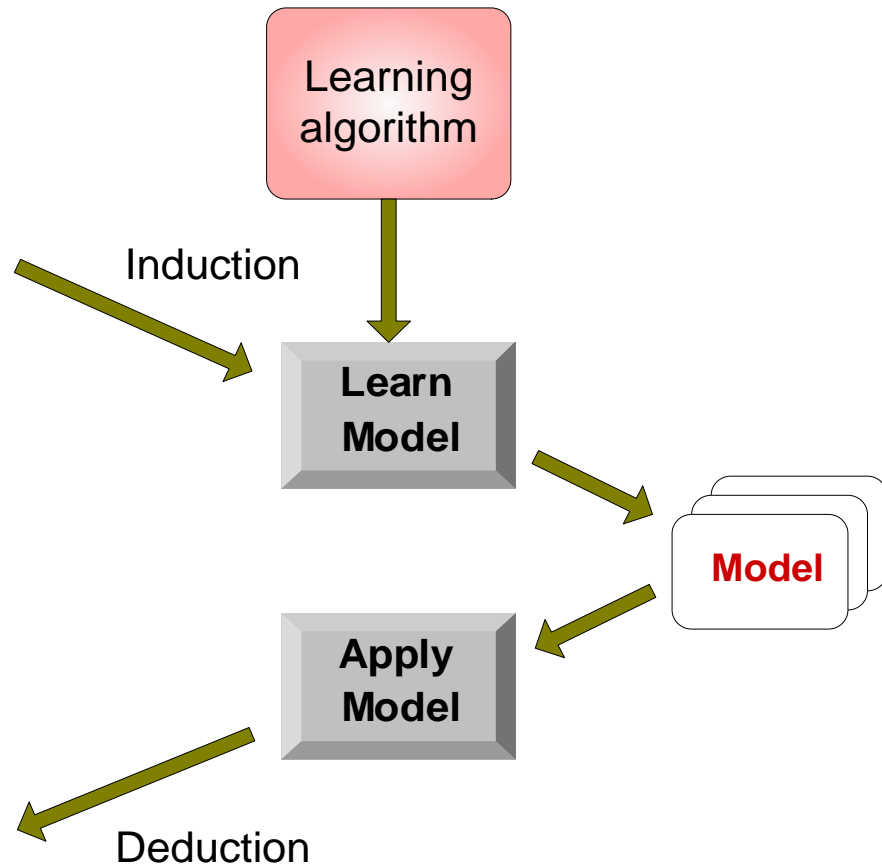
Illustrating Classification Task

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

Training Set

Learning algorithm

Induction

Learn Model

Model

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

Apply Model

Deduction

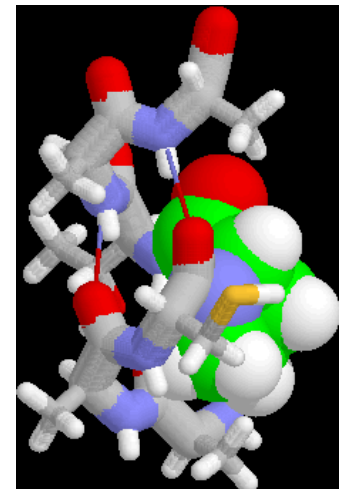# Examples of Classification Task

- Predicting tumor cells as benign or malignant

- Classifying credit card transactions as legitimate or fraudulent

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

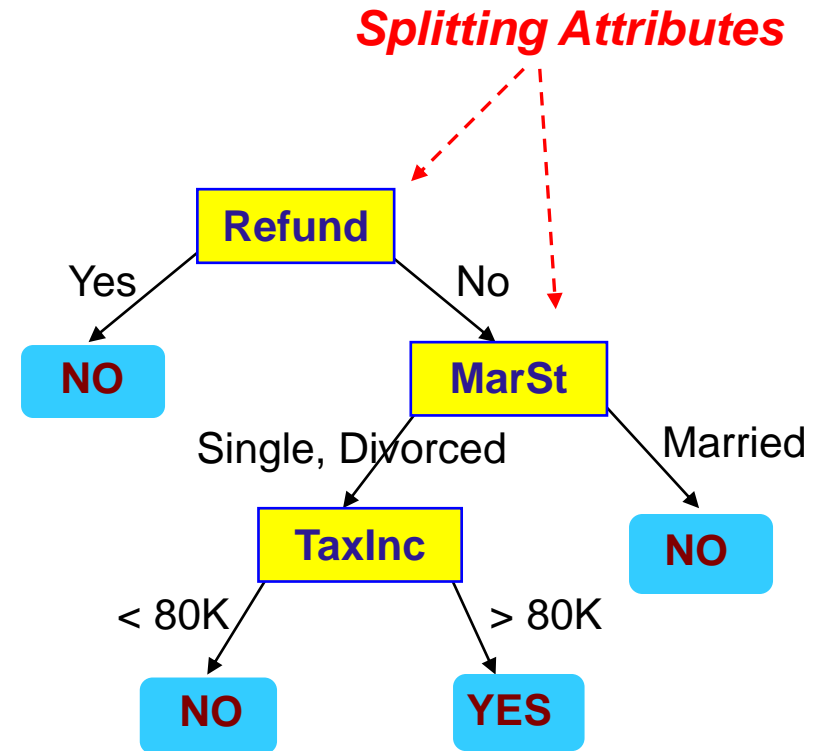- Categorizing news stories as finance, weather, entertainment, sports, etc

Example of a Decision Tree

Tid	Refund	Marital Status	Taxable Income	Cheat
	categorical	categorical	continuous	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

Splitting Attributes

```
            Refund
        Yes /      \ No
          NO        MarSt
              Single, Divorced /    \ Married
                       TaxInc         NO
                 < 80K /    \ > 80K
                    NO        YES
```

Model: Decision Tree

Another Example of Decision Tree

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

MarSt

Married → NO

Single, Divorced → Refund

Refund:
Yes → NO
No → TaxInc

TaxInc:
< 80K → NO
> 80K → 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

Induction

Tree Induction algorithm

Learn Model

Model

Decision Tree

Apply Model

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

Deduction

Apply Model to Test Data

Start from the root of tree

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Refund

Yes   No

NO

MarSt

Single, Divorced   Married

TaxInc   **NO**

< 80K   > 80K

NO   **YES**
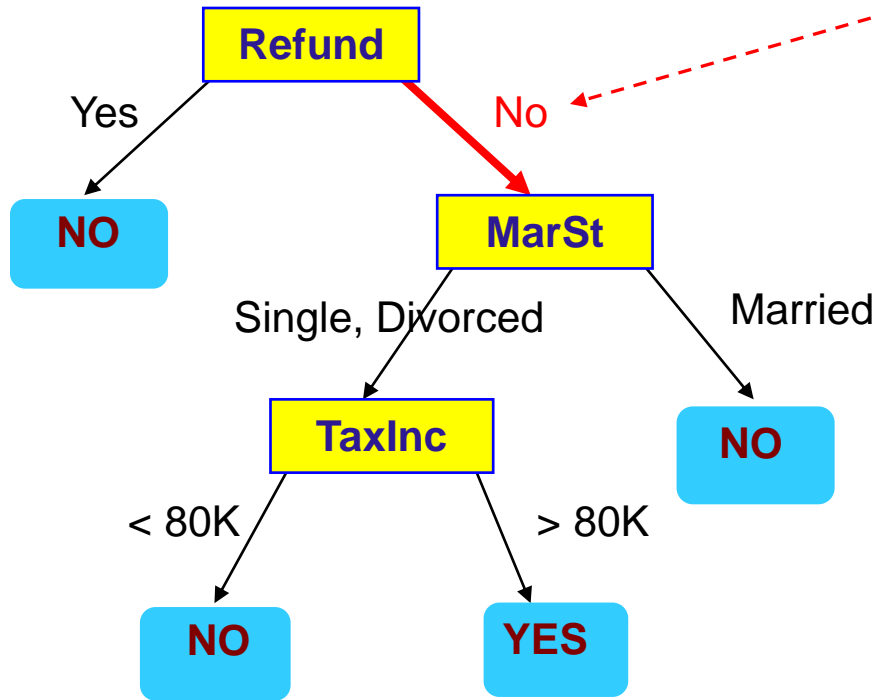
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to "No"

Decision Tree Induction

- Many Algorithms:
    - Hunt's Algorithm (*one of the earliest*)
    - CART (*Classification and Regression Tree*)
    - ID3, C4.5
    - SLIQ (*Fast scalable algorithm for large application*)
        - Can handle both numeric and categorical attributes
    - SPRINT (*scalable parallel classifier for datamining*)

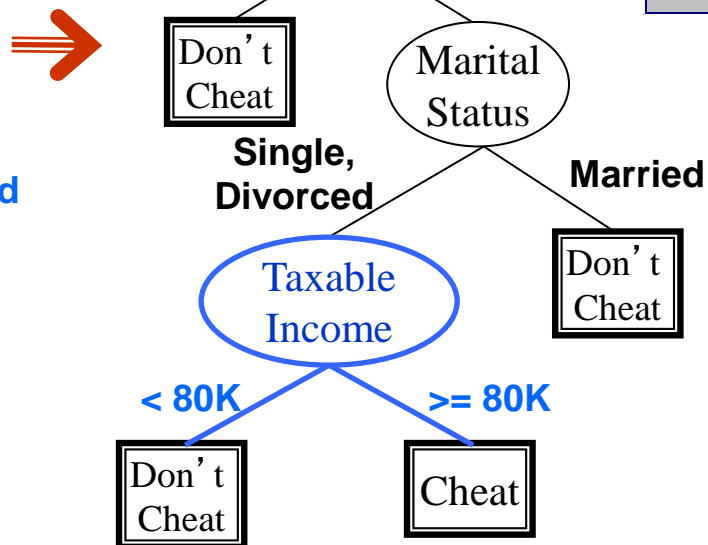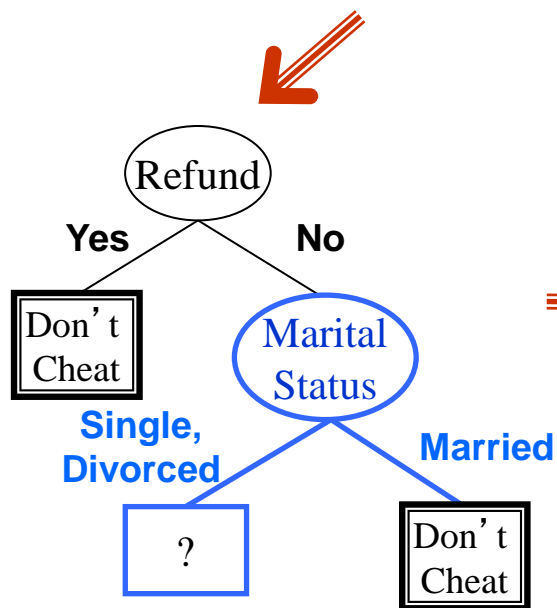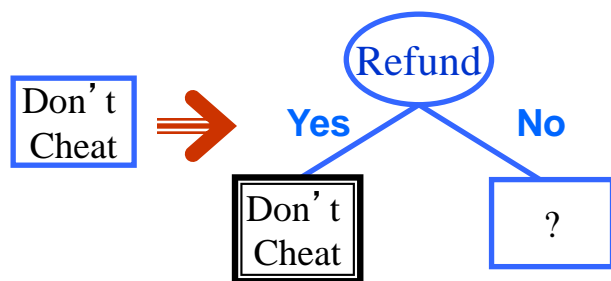# General Structure of Hunt's Algorithm

- Let D_t be the set of training records that reach a node t
- General Procedure:
  - If D_t contains records that belong the same class y_t, then t is a leaf node labeled as y_t
  - If D_t is an empty set, then t is a leaf node labeled by the default class, y_d
  - If D_t contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset

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

D_t

?

Hunt's Algorithm

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

Don't Cheat ⟹ **Refund**
- **Yes**: Don't Cheat
- **No**: ?

Refund
- **Yes**: Don't Cheat
- **No**: **Marital Status**
  - **Single, Divorced**: ?
  - **Married**: Don't Cheat

⟹

Refund
- **Yes**: Don't Cheat
- **No**: **Marital Status**
  - **Single, Divorced**: **Taxable Income**
    - **< 80K**: Don't Cheat
    - **>= 80K**: Cheat
  - **Married**: Don't Cheat

Limitations of Hunt's Algorithm

- Too stringent for use in most practical situations
  - Works only if every combination of attribute values is present in the training data, and
  - Each combination has unique class label

- Additional conditions are needed
  - Empty child node
    - None of the training records has the combination of attribute values associated with such nodes (i.e. no records associated with this node)
    - Node is a leaf node with same class label as the majority class labels of its parent node (*solution*)
  - All the records have identical attribute values (not possible to split further)
    - Class label will be same as that of the majority class of the records associated with the node

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
  - Split the records based on an attribute test that optimizes certain criterion

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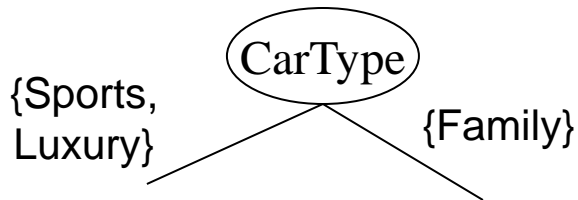 - Determine when to stop splitting

How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

- Depends on number of ways to split
  - 2-way split
  - Multi-way split
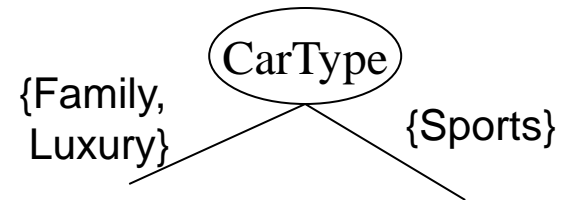
Splitting Based on Nominal Attributes

- Multi-way split: Use as many partitions as distinct values
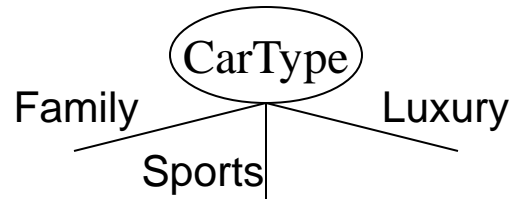
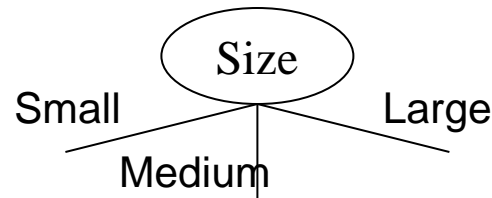- Binary split: Divides values into two subsets Need to find optimal partitioning

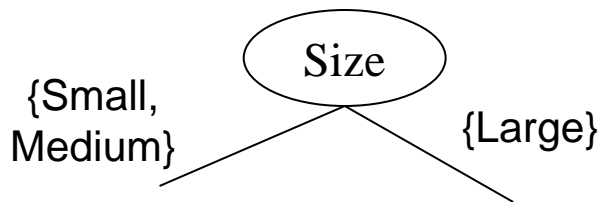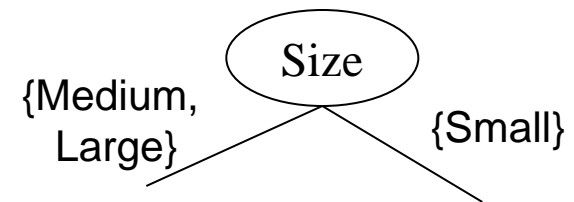# Splitting Based on Ordinal Attributes

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

Size
Small — Medium — Large

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

Size
{Small, Medium} — {Large}

OR

Size
{Medium, Large} — {Small}

☐ What about this split?

Size
{Small, Large} — {Medium}
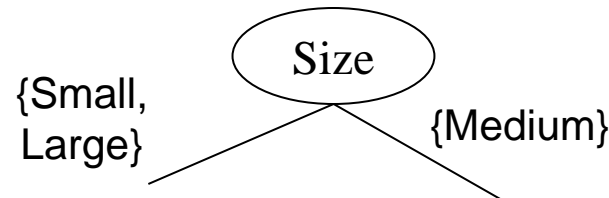
Splitting Based on Continuous Attributes

☐ Different ways of handling

- Discretization to form an ordinal categorical attribute

  ◆ Static – discretize once at the beginning

  ◆ Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering

- Binary Decision: $(A < v)$ or $(A \geq v)$

  ◆ consider all possible splits and finds the best cut

  ◆ can be more compute intensive

Splitting Based on Continuous Attributes
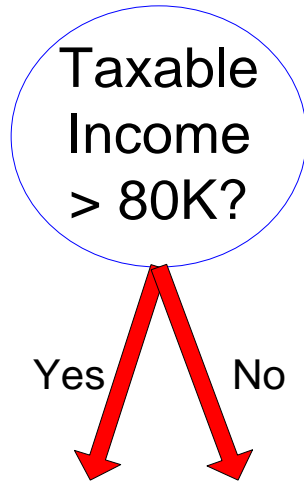
(i) Binary split
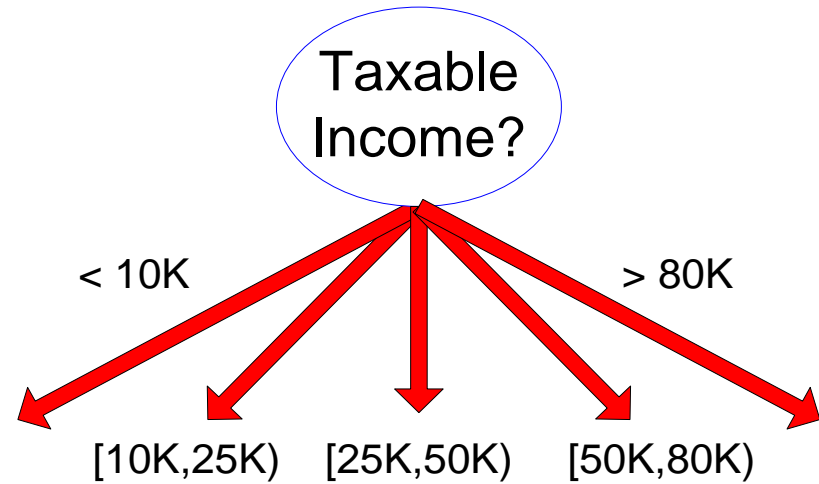
(ii) Multi-way split

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion

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

How to determine the Best Split

Before Splitting: 10 records of class 0,
10 records of class 1
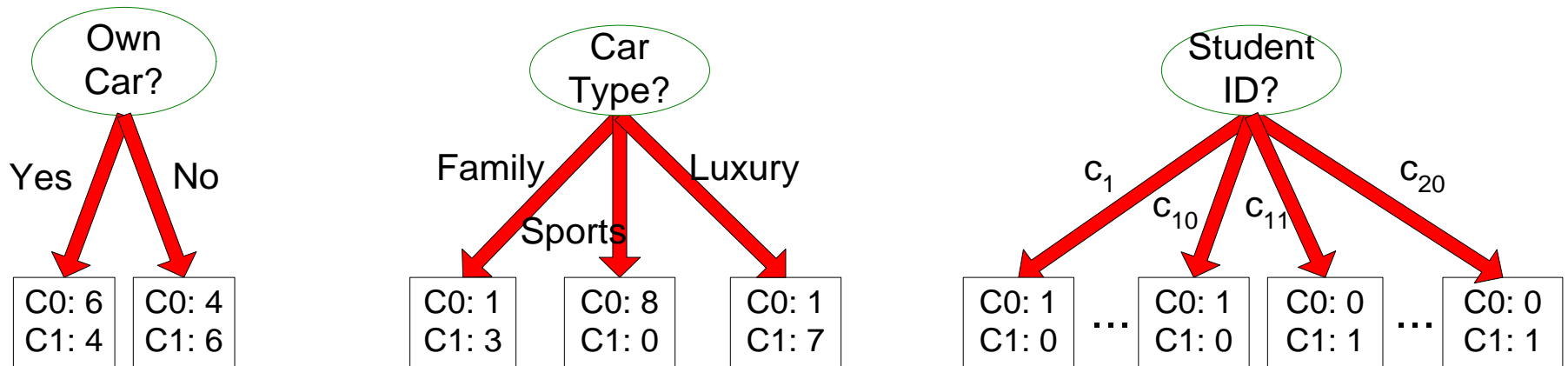
Which test condition is the best?

How to determine the Best Split

☐ Greedy approach:
 – Nodes with homogeneous class distribution are preferred

☐ Need a measure of node impurity:

| C0: 5 |
| C1: 5 |

Non-homogeneous,

High degree of impurity

| C0: 9 |
| C1: 1 |

Homogeneous,

Low degree of impurity

Measures of Node Impurity

- Gini Index

- Entropy

- Misclassification error

How to Find the Best Split?

Before Splitting:

C0	**N00**
C1	**N01**

→ **M0**

A?

Yes   No

Node N1   Node N2

C0	**N10**
C1	**N11**

C0	**N20**
C1	**N21**

M1   **M2**

M12

B?

Yes   No

Node N3   Node N4

C0	**N30**
C1	**N31**

C0	**N40**
C1	**N41**

M3   **M4**

M34

Gain = M0 – M12 vs M0 – M34

Measure of Impurity: GINI

☐ Gini Index for a given node t :

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

(NOTE: $p(j \mid t)$ 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	

C1	3
C2	3
Gini=0.500	

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

C1	1
C2	5

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

Gini = 1 – (1/6)² – (5/6)² = 0.278

C1	2
C2	4

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,

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

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

Binary Attributes: Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  - *Larger and Purer Partitions are sought for*.
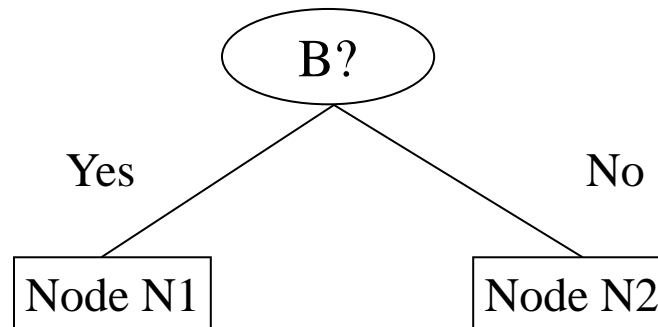
	Parent
C1	6
C2	6
Gini = 0.500	

B?

Yes   No

Node N1   Node N2

Gini(N1)
$= 1 - (5/7)^2 - (2/7)^2$
$= 0.428$

Gini(N2)
$= 1 - (1/5)^2 - (4/5)^2$
$= 0.528$

	N1	N2
C1	5	1
C2	2	4
Gini=0.469		

Gini(Children)
$= 7/12 * 0.428 +$
$\quad 5/12 * 0.528$
$= 0.469$

Categorical Attributes: Computing Gini Index

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

☐ Use the count matrix to make decisions

Multi-way split

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

Two-way split
(find best partition of values)

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

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

Continuous Attributes: Computing Gini Index

- Use binary decisions based on one value
- Several choices for splitting the 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
- Simple method to choose the best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! (Repetition of works)

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?

Yes   No

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	
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
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	

Alternative Splitting Criteria based on INFO

☐ 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

  ◆ Maximum (log n_c) when records are equally distributed among all classes implying least information

  ◆ Minimum (0.0) when all records belong to one class, implying most information

  – *Entropy based computations are similar to the GINI index computations*

Examples for computing Entropy

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

C1	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

C1	2
C2	4

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

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

Splitting Based on INFO...

- Information Gain:

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

Parent Node, p is split into k partitions;

n_i is number of records in partition i

- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)

- Used in *ID3 and C4.5*

- Disadvantage: Tends to prefer splits that result in *large number of partitions*, each being *small but pure*

Splitting Based on INFO...

☐ Gain Ratio:

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

Parent Node, p is split into k partitions

n_i is the number of records in partition i

– Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!

– Used in *C4.5*

– Designed to overcome the disadvantage of Information Gain

Splitting Criteria based on Classification Error

☐ Classification error at a node t :

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

☐ Measures misclassification error made by a node

- ◆ Maximum $(1 - 1/n_c)$ when records are equally distributed among all classes, implying least interesting information
- ◆ Minimum (0.0) when all records belong to one class, implying most interesting information

Examples for Computing Error

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

C1	**0**
C2	**6**

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

Error = 1 – max (0, 1) = 1 – 1 = 0

C1	**1**
C2	**5**

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

Error = 1 – max (1/6, 5/6) = 1 – 5/6 = 1/6

C1	**2**
C2	**4**

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

Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Misclassification Error vs Gini
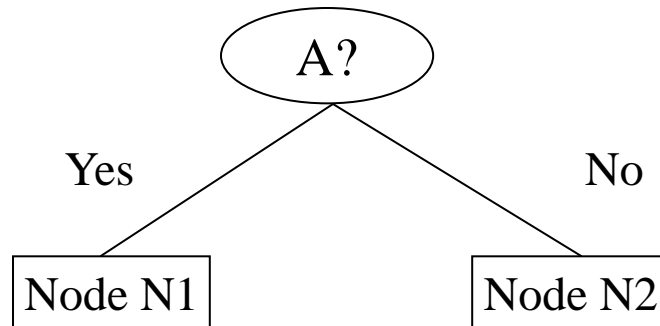
	Parent
C1	**7**
C2	**3**
Gini = 0.42	

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=0.361		

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

Gini improves !!

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*)

Practical Issues of Classification

☐ Underfitting and Overfitting

☐ Missing Values

☐ Costs of Classification

Errors

- Training errors (resubstitution error): # misclassifications in training records

- Generalization error: expected error of the model on the previously unseen records

- Good model- must have *low training error as well as low generalization error*

- Model that fits training data well *can have a poorer generalization error than a model with a higher training error*
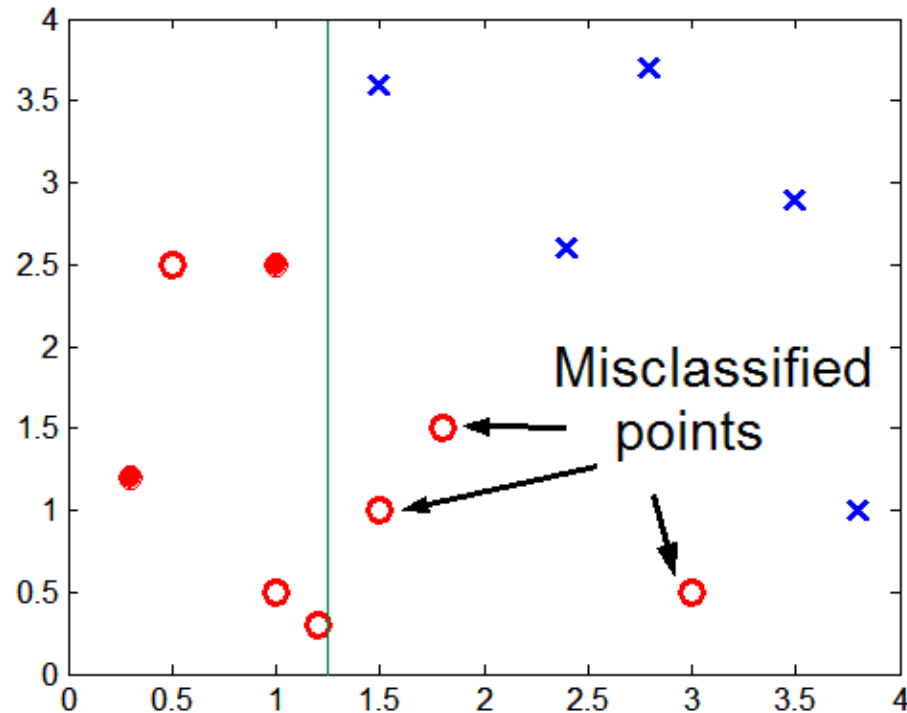
Underfitting and Overfitting
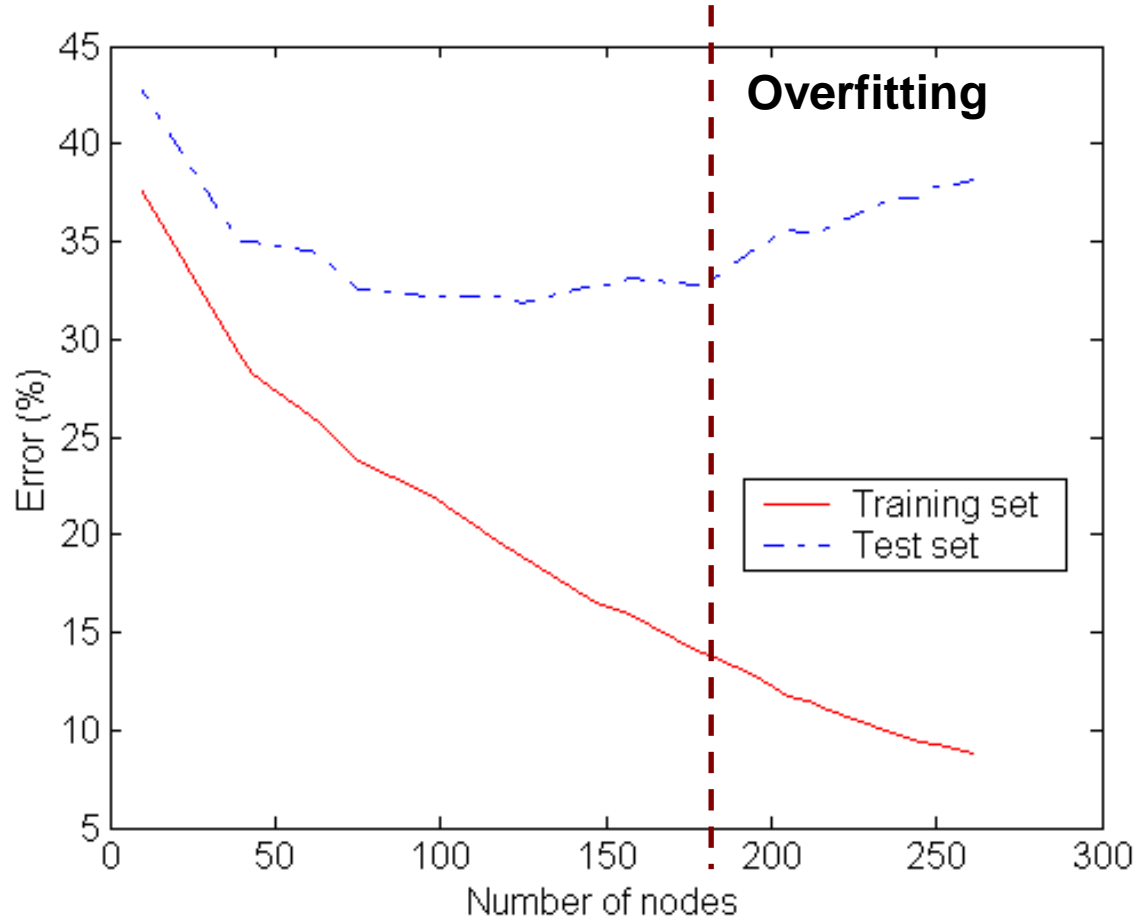
Underfitting: when model is too simple, both training and test errors are large

Overfitting due to Noise
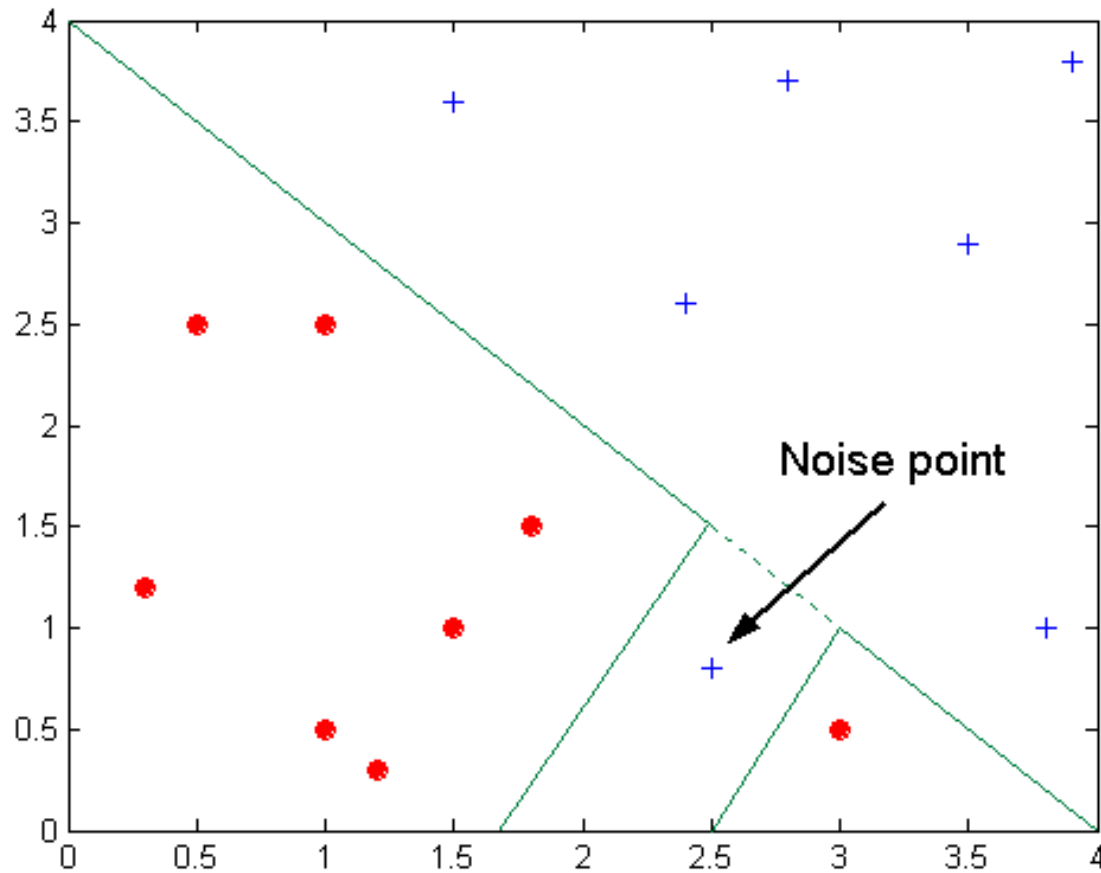
Decision boundary is distorted by noise point

Overfitting due to Insufficient Examples

Lack of data points in the lower half of the diagram makes it difficult to predict correctly the class labels of that region

- Insufficient number of training records in the region causes the decision tree to predict the test examples using other training records that are irrelevant to the classification task

Notes on Overfitting

- Overfitting results in decision trees that are more complex than necessary

- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records

- Needs new ways for estimating errors

Estimating Generalization Errors

- Re-substitution errors: error on training (Σ e(t))
- Generalization errors: error on testing (Σ e'(t))

- Methods for estimating generalization errors:
    - Optimistic approach: e'(t) = e(t)
    - Pessimistic approach:
        - For each leaf node: e'(t) = (e(t)+0.5)
        - Total errors: e'(T) = e(T) + N $\times$ 0.5 (N: number of leaf nodes)
        - For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances):
            Training error = 10/1000 = 1%

            Generalization error = (10 + 30$\times$0.5)/1000 = 2.5%
    - Reduced error pruning (REP):
   - Uses validation data set to estimate generalization error

Occam's Razor

☐ Given two models of *similar generalization errors,* one should *prefer the simpler model over the more complex model*

☐ For complex models, there is a greater chance that it was fitted accidentally by errors in data

☐ Therefore, one should include model complexity when evaluating a model

Two methods for model complexity

□ Pessimistic error estimates (*already discussed*)
  – Training error + penalty term

□ Minimum description length
  – An information theoretic approach

Minimum Description Length (MDL)
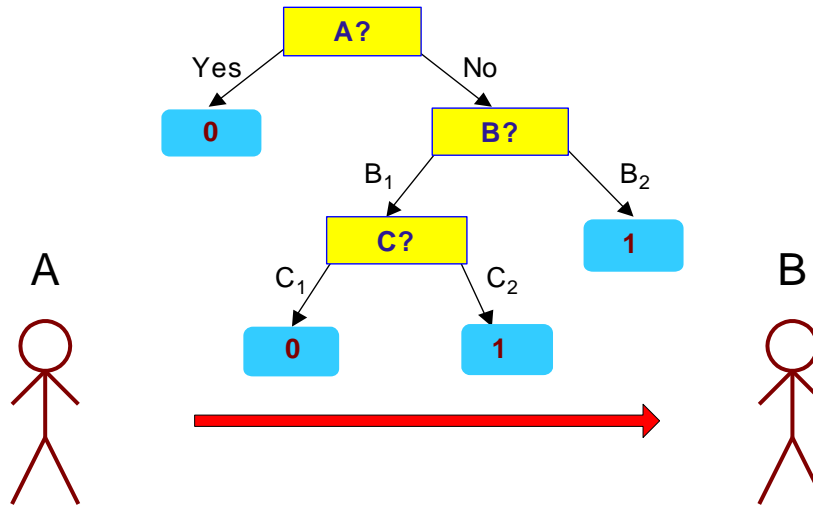
- B obtains classification of each record by requesting A to transmit
  - Cost is O(n): n-bits required to transmit message, i.e. number of records
- Alternatively, A builds a classification model that summarizes the relationships between x and y
  - For 100% accurate model, cost of transmission is equivalent to the cost of encoding the model

Minimum Description Length (MDL)

- Cost(Model, Data) = Cost(Data|Model) + Cost(Model)
  - Cost is the number of bits needed for encoding
  - Search for the least costly model

- Cost(Data|Model) encodes the misclassification errors

- Cost(Model) uses node encoding (*number of children*) plus splitting condition encoding

How to Address Overfitting?

- Pre-Pruning (Early Stopping Rule)
    - Stop the algorithm before it becomes a fully-grown tree
    - Typical stopping conditions for a node:
        - Stop if all instances belong to the same class
        - Stop if all the attribute values are the same
    - More restrictive conditions:
        - Stop if number of instances is less than some user-specified threshold
        - Stop if class distribution of instances are independent of the available features (e.g., using χ^2 test)
        - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain)

How to Address Overfitting…

☐ Post-pruning

- – Grow decision tree to its entirety
- – Trim the nodes of the decision tree in a bottom-up fashion
- – If *generalization error* improves after *trimming*, replace *sub-tree* by a *leaf node* or by the frequently occurring branch
- – Class label of leaf node is determined from *majority class* of instances in the sub-tree
- – Can use MDL for post-pruning

Example of Post-Pruning

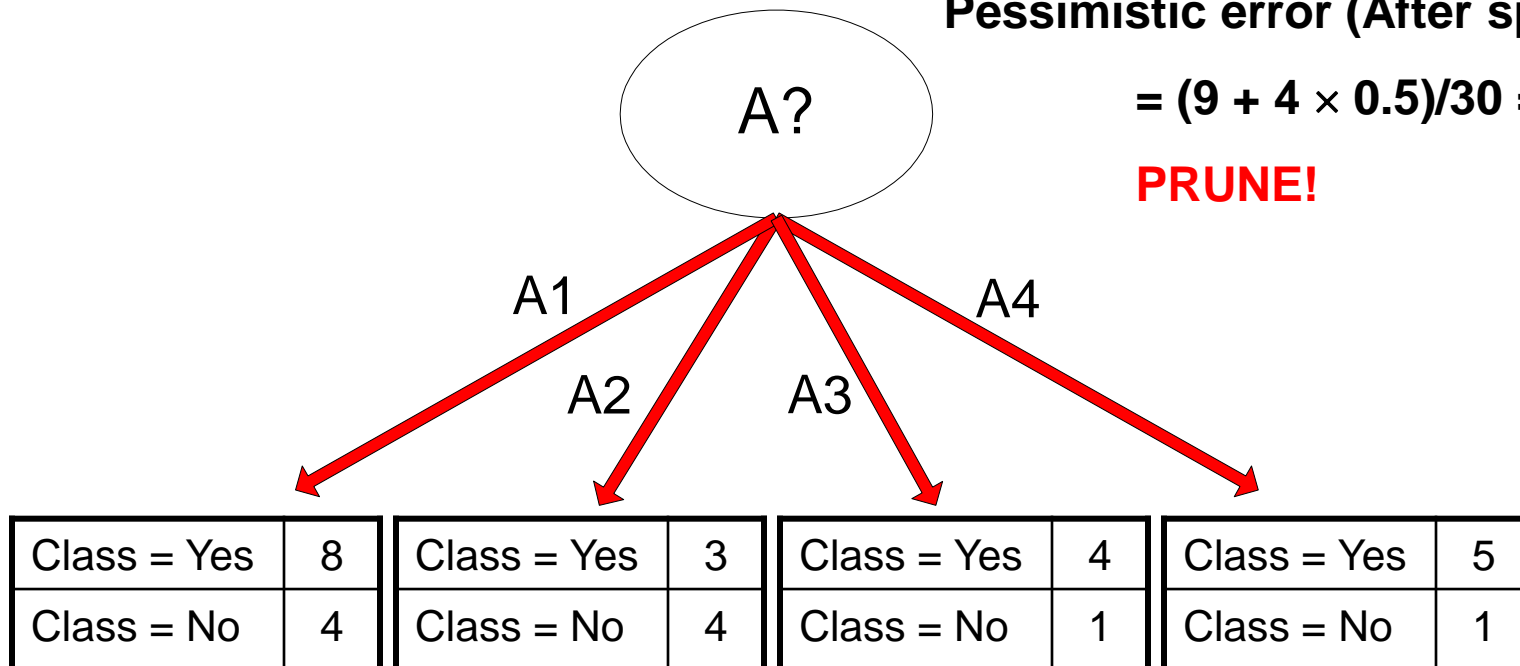| Class = Yes	20
Class = No	10
Error = 10/30	

Training Error (Before splitting) = 10/30

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

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

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

PRUNE!

A?

A1   A2   A3   A4

Class = Yes	8
Class = No	4

Class = Yes	3
Class = No	4

Class = Yes	4
Class = No	1

Class = Yes	5
Class = No	1

Examples of Post-pruning

- – Optimistic error?

    Don't prune for both cases

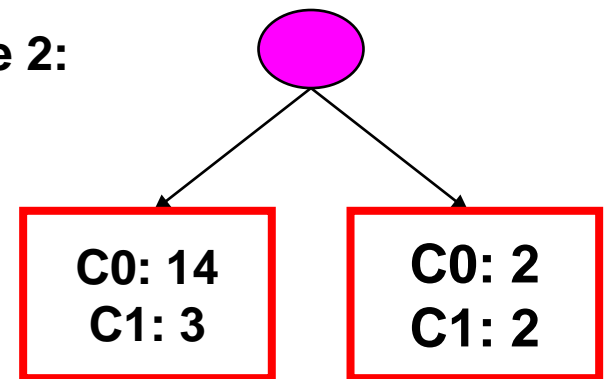- – Pessimistic error?

    Don't prune case 1, prune case 2

- – Reduced error pruning?

    Depends on validation set

Case 1:

| C0: 11 | C0: 2 |
| C1: 3 | C1: 4 |
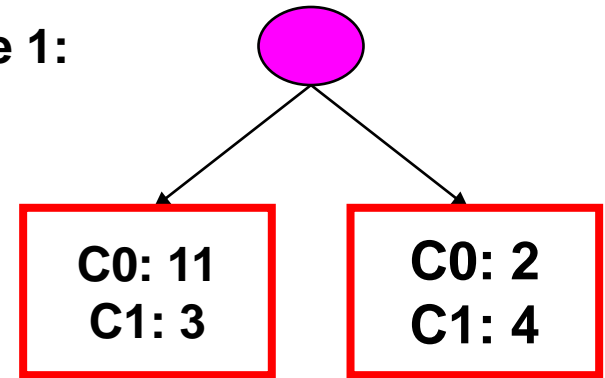
Case 2:

| C0: 14 | C0: 2 |
| C1: 3 | C1: 2 |

Handling Missing Attribute Values

- Missing values affect decision tree construction in three different ways:
  - Affects how impurity measures are computed
  - Affects how to distribute instance with missing value to child nodes
  - Affects how a test instance with missing value is classified

Computing Impurity Measure

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

Missing value

Before Splitting:

Entropy(Parent)
= -0.3 log(0.3)-(0.7)log(0.7) = 0.8813

	Class = Yes	Class = No
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

Split on Refund:

Entropy(Refund=Yes) = 0

Entropy(Refund=No)
= -(2/6)log(2/6) – (4/6)log(4/6) = 0.9183
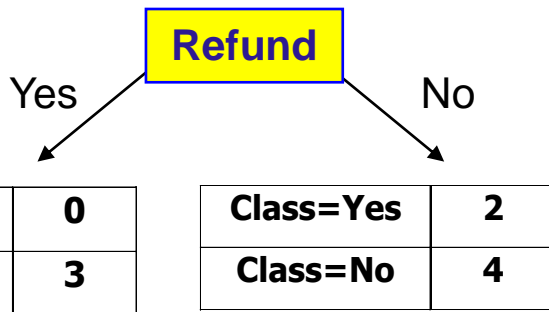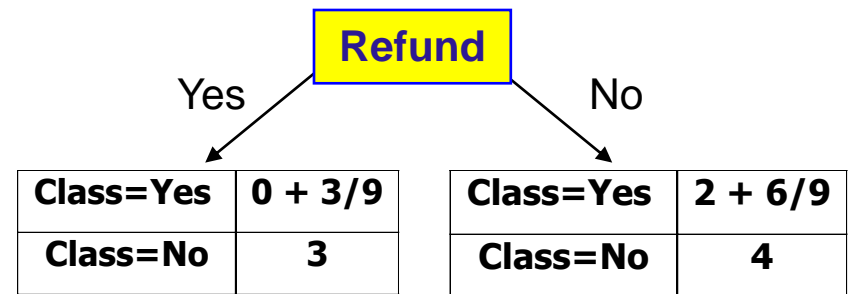
Entropy(Children)
= 0.3 (0) + 0.6 (0.9183) = 0.551

Gain = 0.9 × (0.8813 – 0.551) = 0.3303

Distribute Instances

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

Refund

Yes ← → No

Class=Yes	0
Class=No	3

Class=Yes	2
Class=No	4

Tid	Refund	Marital Status	Taxable Income	Class
10	**?**	Married	90K	**Yes**

Refund

Yes ← → No

Class=Yes	0 + 3/9
Class=No	3

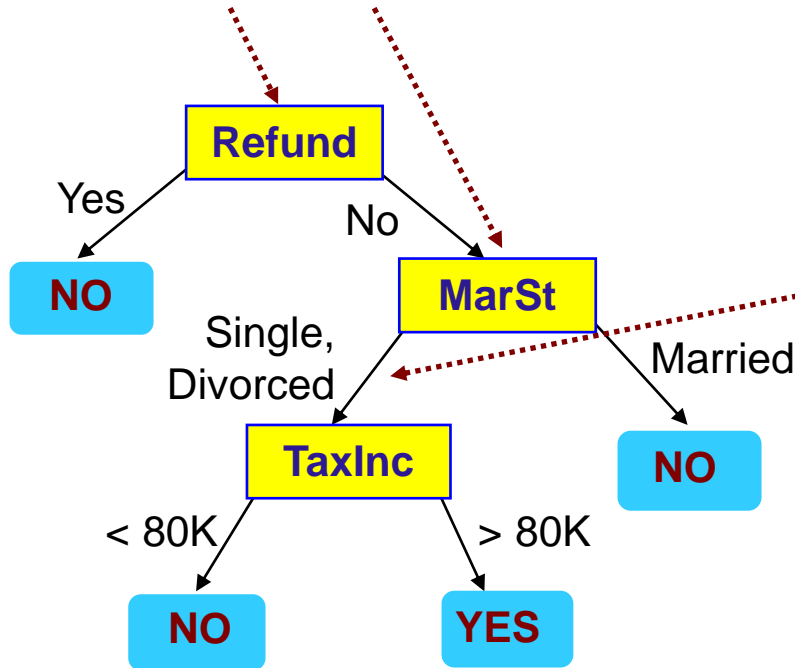| Class=Yes	2 + 6/9
Class=No	4

Probability that Refund=Yes is 3/9

Probability that Refund=No is 6/9

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

Classify Instances

New record:

Tid	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?

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

Refund

Yes / No

NO

MarSt

Single, Divorced / Married

TaxInc

NO

< 80K / > 80K

NO   **YES**

Probability that Marital Status = Married is 3.67/6.67

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

Other Issues

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication

Data Fragmentation

- Number of instances gets smaller as you traverse down the tree

- Number of instances at the leaf nodes could be too small to make any statistically significant decision

Search Strategy

□ Finding an optimal decision tree is NP-hard

□ Algorithm presented so far uses a *greedy*, *top-down*, *recursive partitioning* strategy to induce a reasonable solution

□ Other strategies?
  – Bottom-up
 – Bi-directional

Expressiveness

- Decision tree provides expressive representation for learning discrete-valued function
  - But they do not generalize well to certain types of Boolean functions
    - ◆ Example: parity function:
      - Class = 1 if there is an even number of boolean attributes with truth value = True
      - Class = 0 if there is an odd number of boolean attributes with truth value = True
    - ◆ For accurate modeling, must have a complete tree

- Not expressive enough for modeling continuous variables
  - Particularly when test condition involves only a single attribute at-a-time

Decision Boundary
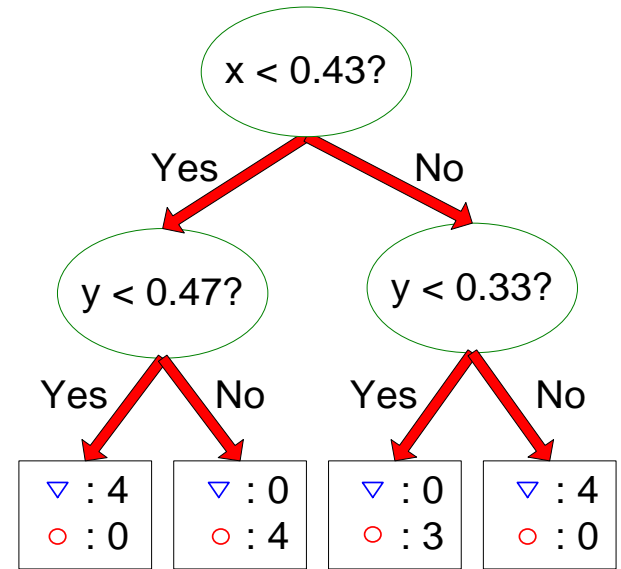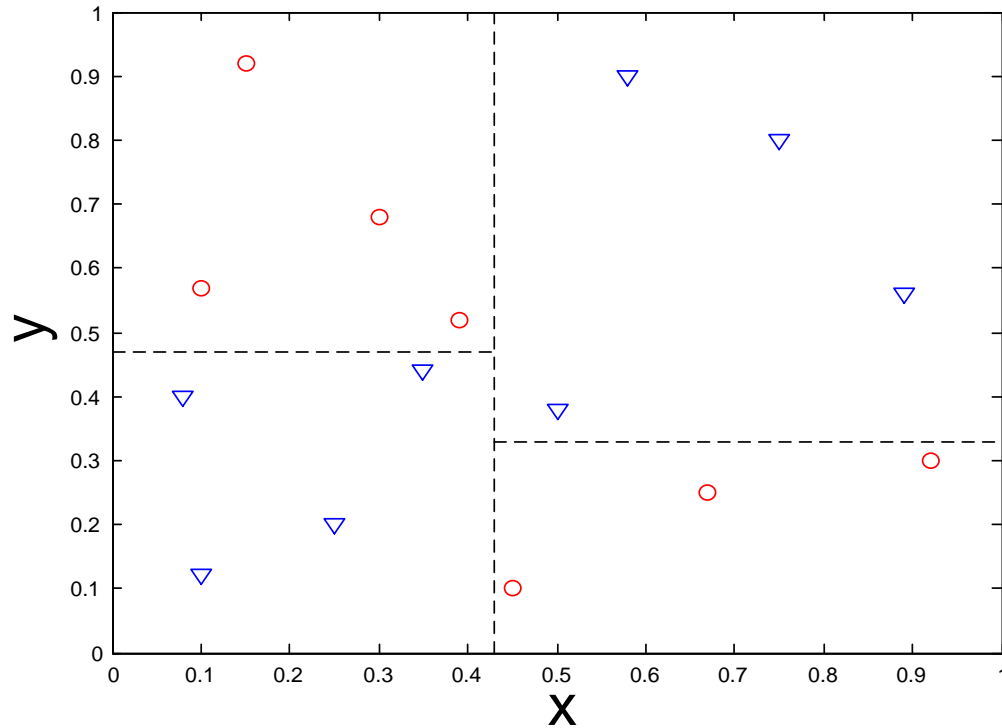
- Border line between two neighboring regions of different classes is known as decision boundary

- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

Oblique Decision Trees

$x + y < 1$

Class = **+**   Class = ●
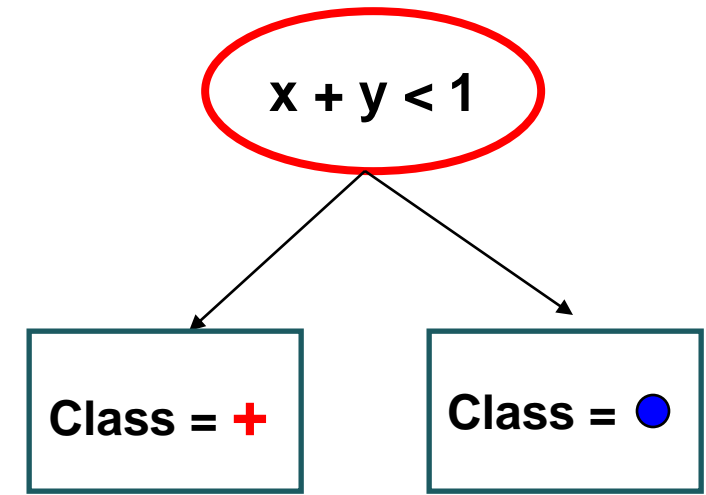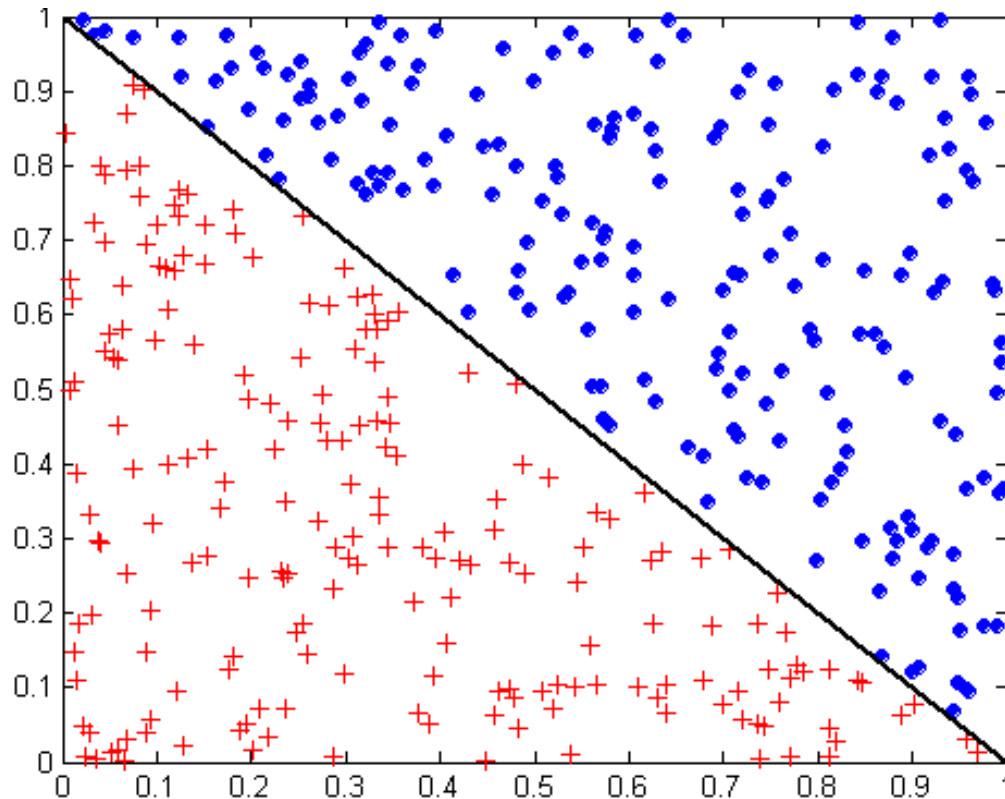
- Test condition may involve multiple attributes

- More expressive representation

- Finding optimal test condition is computationally expensive

Tree Replication
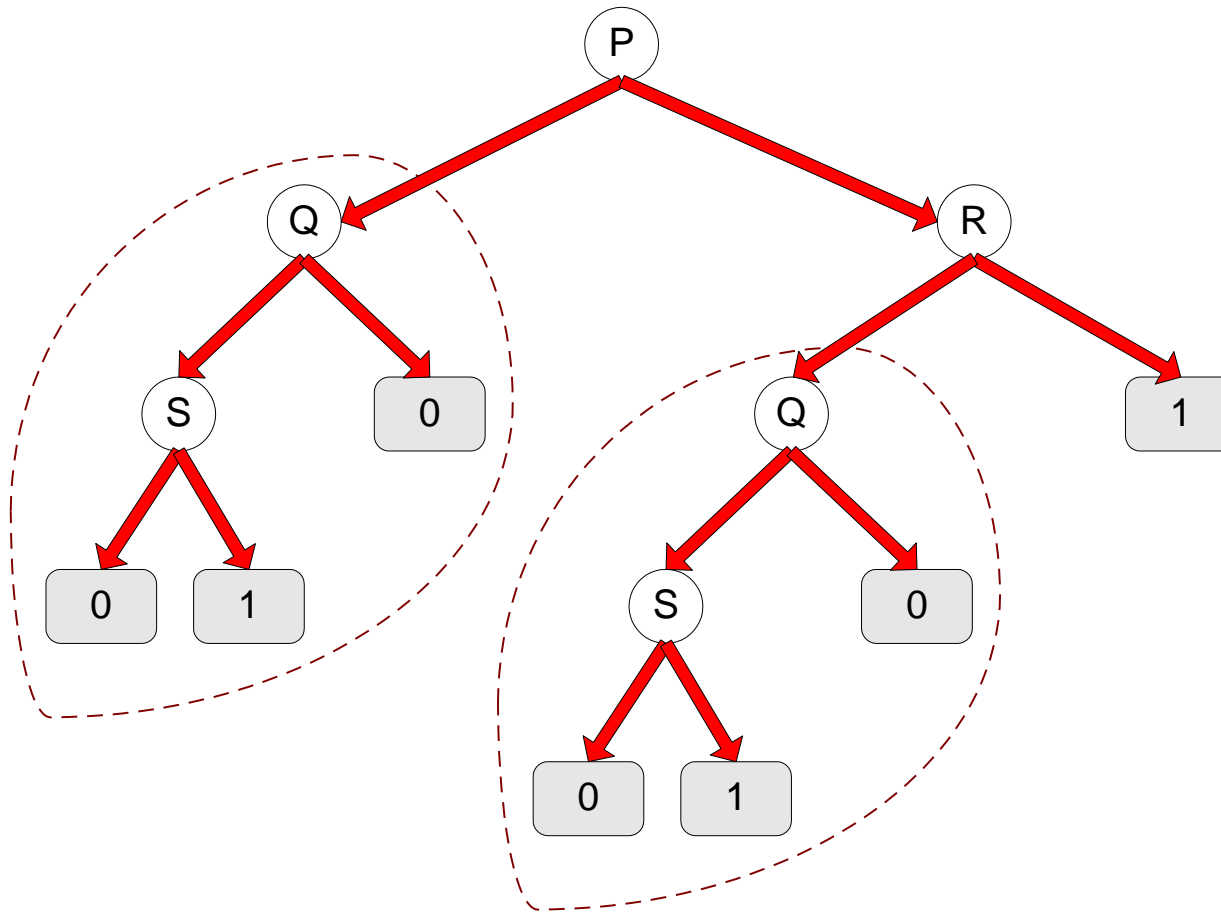
- **Same subtree appears in multiple branches**

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?

- Methods for Performance Evaluation
  - How to obtain reliable estimates?

Model Evaluation

☐ Metrics for Performance Evaluation
  – How to evaluate the performance of a model?

☐ Methods for Performance Evaluation
  – How to obtain reliable estimates?

Metrics for Performance Evaluation

☐ Focus on the predictive capability of a model
  – Rather than how fast it takes to classify or build models, scalability, etc.

☐ Confusion Matrix:

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

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation…

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

☐ Most widely-used metric:

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

Limitation of Accuracy

- Consider a 2-class problem
    - Number of Class 0 examples = 9990
    - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
    - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

		PREDICTED CLASS	
	C(i|j)	**Class=Yes**	**Class=No**
ACTUAL CLASS	**Class=Yes**	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): *Cost of misclassifying class j example as class i*

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
	C(i|j)	+	-
ACTUAL CLASS +		-1	100
ACTUAL CLASS -		1	0

Model M_1	PREDICTED CLASS		
		+	-
ACTUAL CLASS +		150	40
ACTUAL CLASS -		60	250

Accuracy = 80%

Cost = 3910

Model M_2	PREDICTED CLASS		
		+	-
ACTUAL CLASS +		250	45
ACTUAL CLASS -		5	200

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

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

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

Accuracy is proportional to cost if
1. $C(Yes|No)=C(No|Yes) = q$
2. $C(Yes|Yes)=C(No|No) = p$

$N = a + b + c + d$

$Accuracy = (a + d)/N$

$Cost = p(a + d) + q(b + c)$

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

$\quad\quad = qN - (q - p)(a + d)$

$\quad\quad = N[q - (q-p) \times Accuracy]$

Cost-Sensitive Measures

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

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

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

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

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

Model Evaluation

☐ Metrics for Performance Evaluation

   – How to evaluate the performance of a model?

☐ Methods for Performance Evaluation

   – How to obtain reliable estimates?

Methods for Performance Evaluation

☐ How to obtain a reliable estimate of performance?

☐ Performance of a model may depend on other factors besides the learning algorithm:

  – Class distribution

  – Cost of misclassification

  – Size of training and test sets

Learning Curve
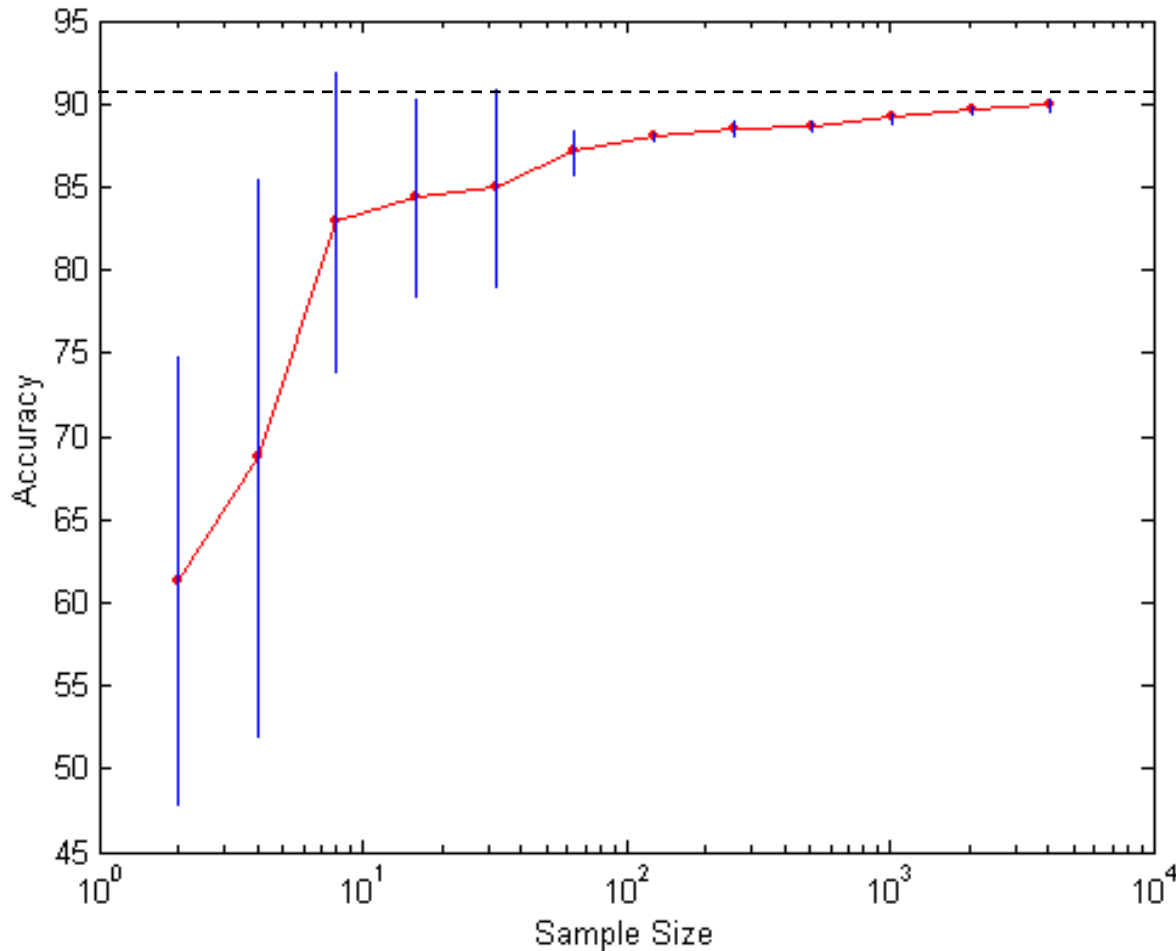
- Learning curve shows how accuracy changes with varying sample size

- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

Effect of small sample size:
- Bias in the estimate
- Variance of estimate

The *bias* of a classifier is the expected error of the classifier due to the fact that the classifier is not perfect

The *variance* of a classifier is the expected error due to the particular training set used

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
  - Less examples are available for training
  - Model depends heavily on the composition of training and test sets
    - Too small training set -larger variance
    - Too large training set- estimated accuracy not very reliable

- Random subsampling
  - Repeated holdout
  - Some instances may be used more than others for training

- **Cross validation**
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n (one record in each subset)

- **Stratified sampling**
  - Oversampling vs. Undersampling

- **Bootstrap**
  - Sampling with replacement