DATA MINING
LECTURE 10

Classification

Basic Concepts

Decision Trees

Catching tax-evasion

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

Tax-return data for year 2011

A new tax return for 2012
Is this a cheating tax return?

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

An instance of the classification problem: learn a method for discriminating between records of different classes (cheaters vs non-cheaters)

What is classification?

$x \rightarrow \boxed{f} \rightarrow y$ $y = \{ \text{yes}, \text{No} \}$

- **Classification** is the task of ***learning a target function*** **f** that maps attribute set **x** to one of the predefined class labels **y**

$x = \{ \text{Refund}, \text{Marital Status}, \text{TI} \}$

	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**

One of the attributes is the class attribute
In this case: Cheat

Two class labels (or classes): Yes (1), No (0)

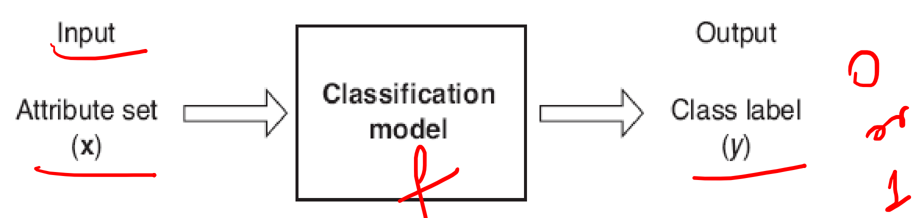


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

Why classification?

- The target function f is known as a classification model
- Descriptive modeling: Explanatory tool to distinguish between objects of different classes (e.g., understand why people cheat on their taxes)
- Predictive modeling: Predict a class of a previously unseen record

Examples of Classification Tasks

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent
- Categorizing news stories as finance, weather, entertainment, sports, etc
- Identifying spam email, spam web pages, adult content
- Understanding if a web query has commercial intent or not

General approach to classification

training

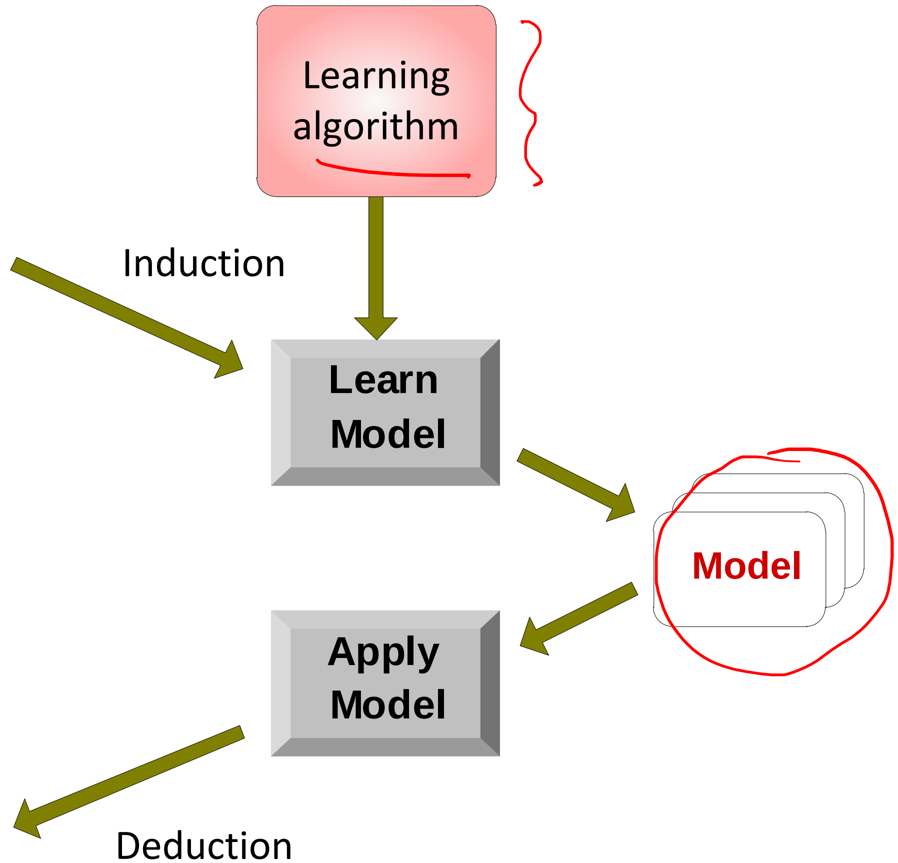
test

- Training set consists of records with known class labels
- Training set is used to build a classification model
- A labeled test set of previously unseen data records is used to evaluate the quality of the model.
- The classification model is applied to new records with unknown class labels

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



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

Evaluation of classification models

Total no. of +ve records..

FN → are the no. of +ve records missed by the model to predict correctly.

TP → are the no. of +ve records correctly predicted by the model

True +ve

- Counts of test records that are correctly (or incorrectly) predicted by the classification model
- **Confusion matrix**

1 - +ve
0 - -ve

Actual Class

Predicted Class

Actual Class	Predicted Class: Class = 1	Predicted Class: Class = 0
Class = 1	f_{11} TP	f_{10} FN
Class = 0	f_{01} FP	f_{00} TN

Precision

Recall

F1 score

predicted class

$$\text{Accuracy} = \frac{\#\,\text{correct predictions}}{\text{total}\,\#\,\text{of predictions}} = \frac{f_{11} + f_{00}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

$$\text{Error rate} = \frac{\#\,\text{wrong predictions}}{\text{total}\,\#\,\text{of predictions}} = \frac{f_{10} + f_{01}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

P = TP + FP / TP + FP + FN + TN

R = TP + FN

F1 = 2 * P * R / P + R

Classification Techniques

- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines

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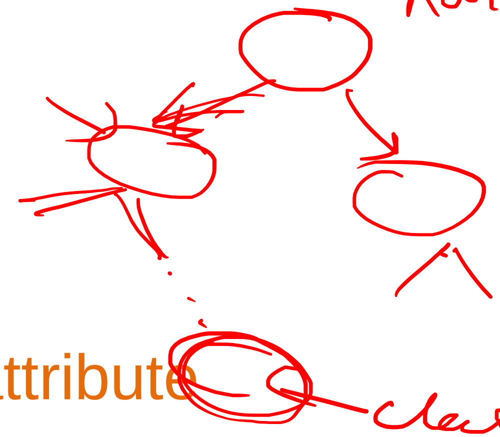
Decision Trees



- Decision tree
  - A flow-chart-like tree structure
  - Internal node denotes a test on an attribute
  - Branch represents an outcome of the test
  - Leaf nodes represent class labels or class distribution

Root node →

Internal nodes

Leaf or terminal nodes

Example of a Decision Tree

categorical categorical continuous class

yes No

Single married Divorced

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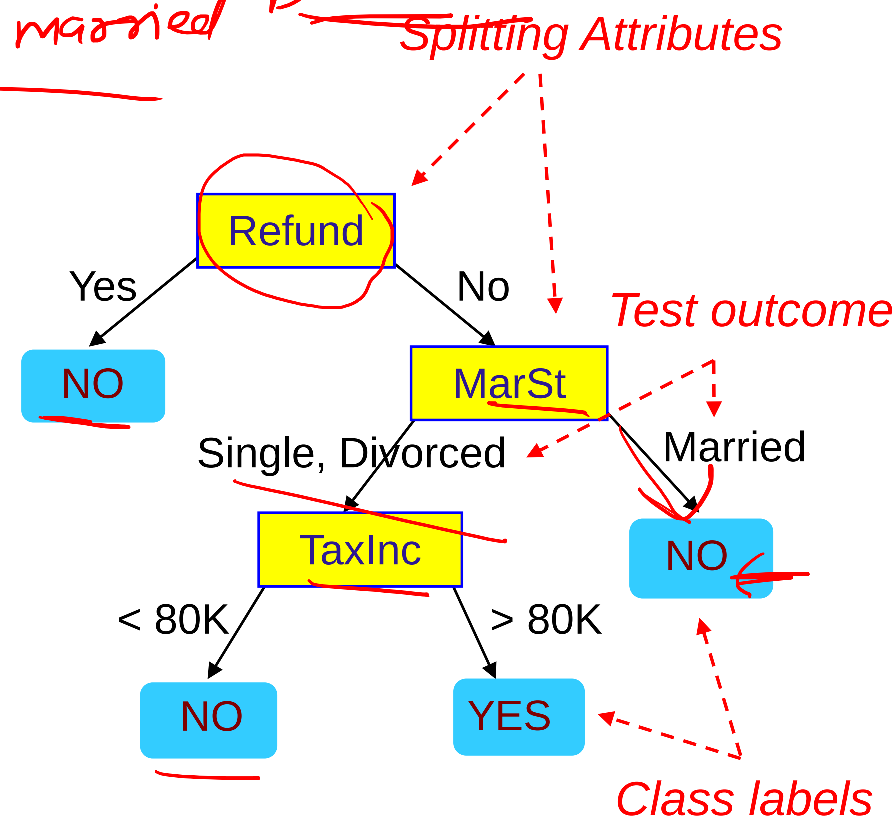
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Another Example of Decision Tree

	categorical	categorical	continuous	class
Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
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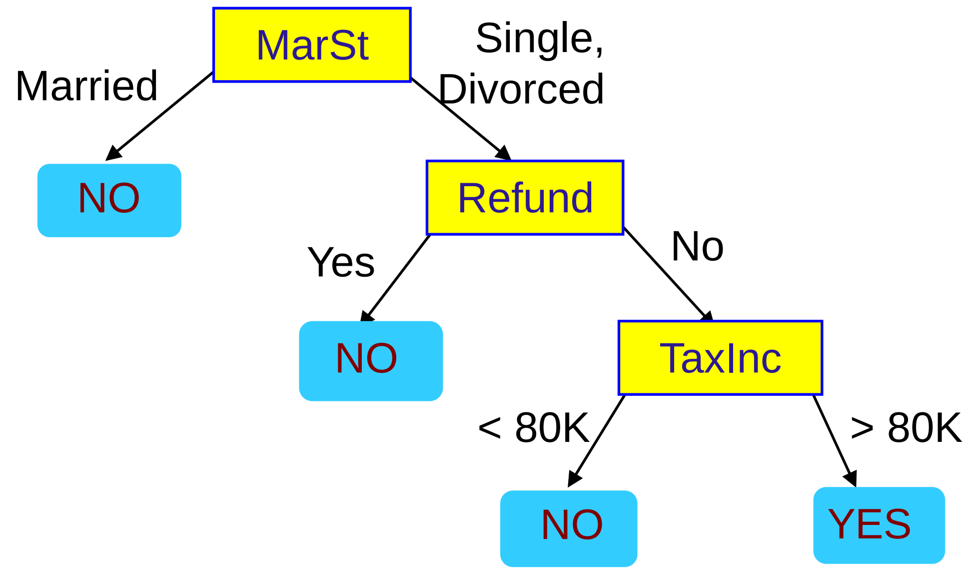
10	No	Single	90K	**Yes**

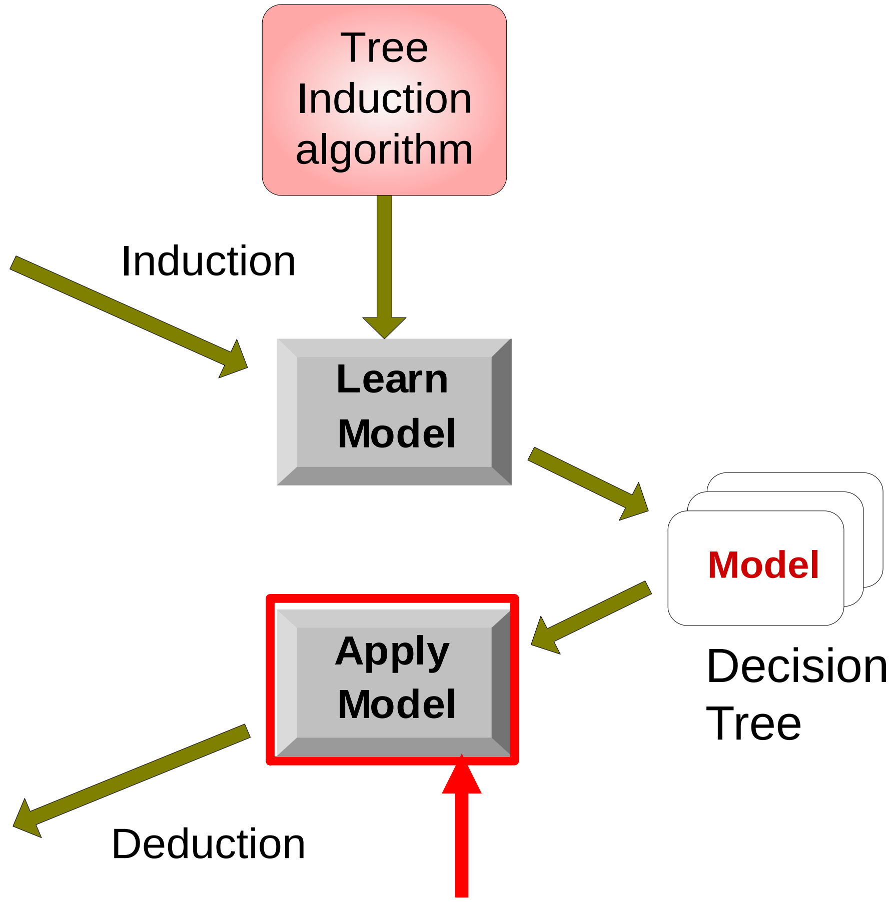


There could be more than one tree that fits the same data!

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	?
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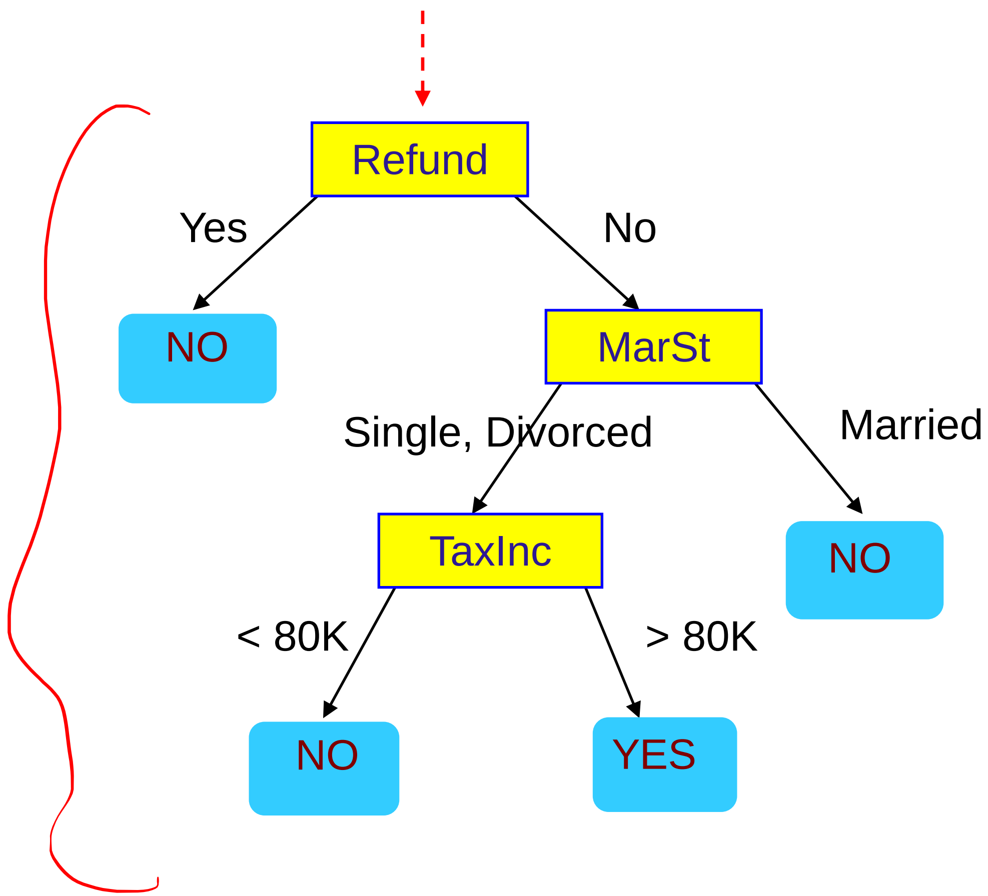
15	No	Large	67K	?

Test Set

Apply Model to Test Data

Start from the root of tree.



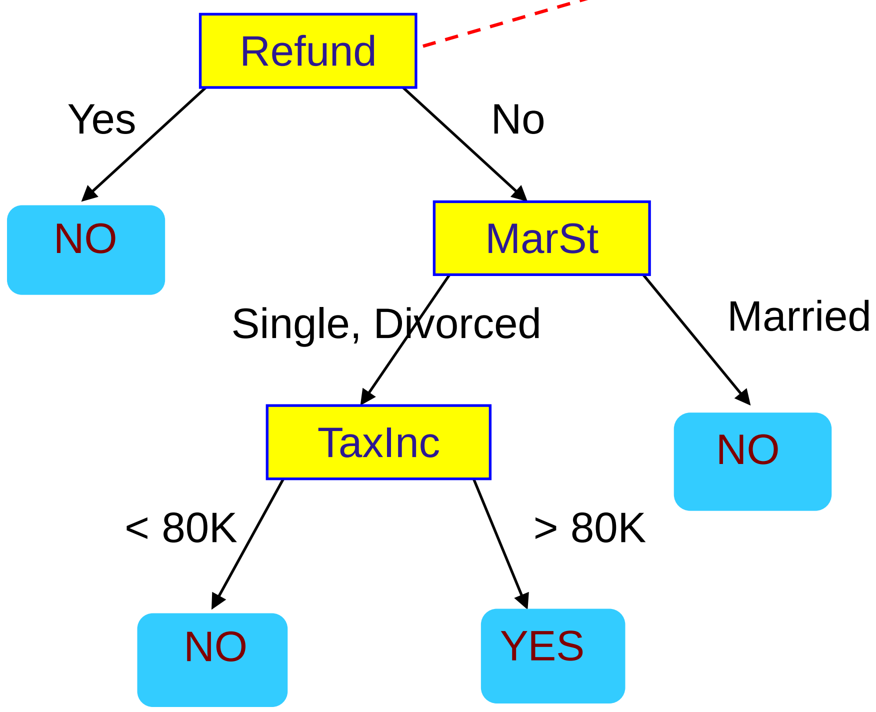
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

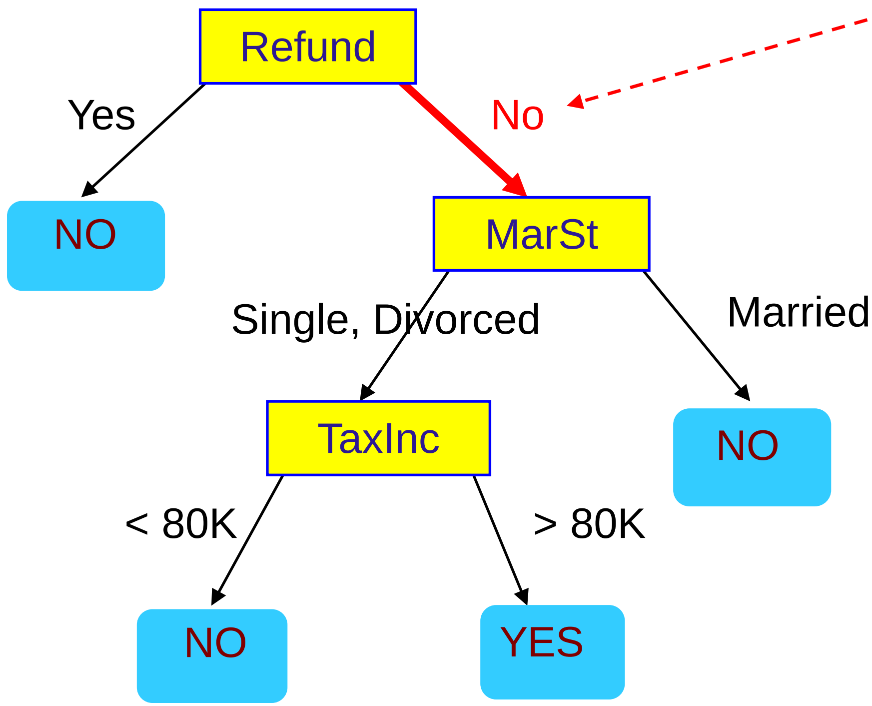
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data



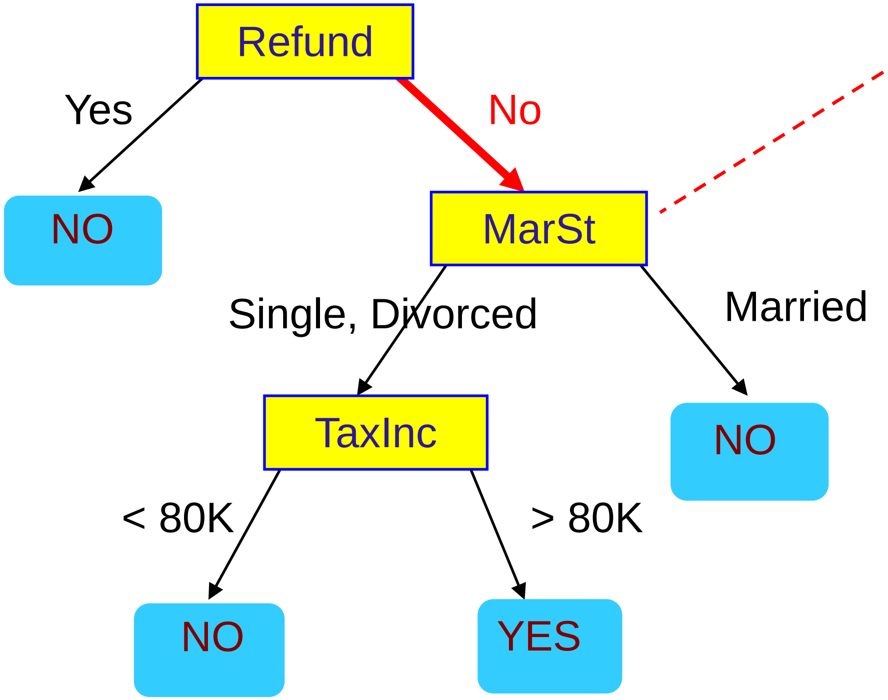
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

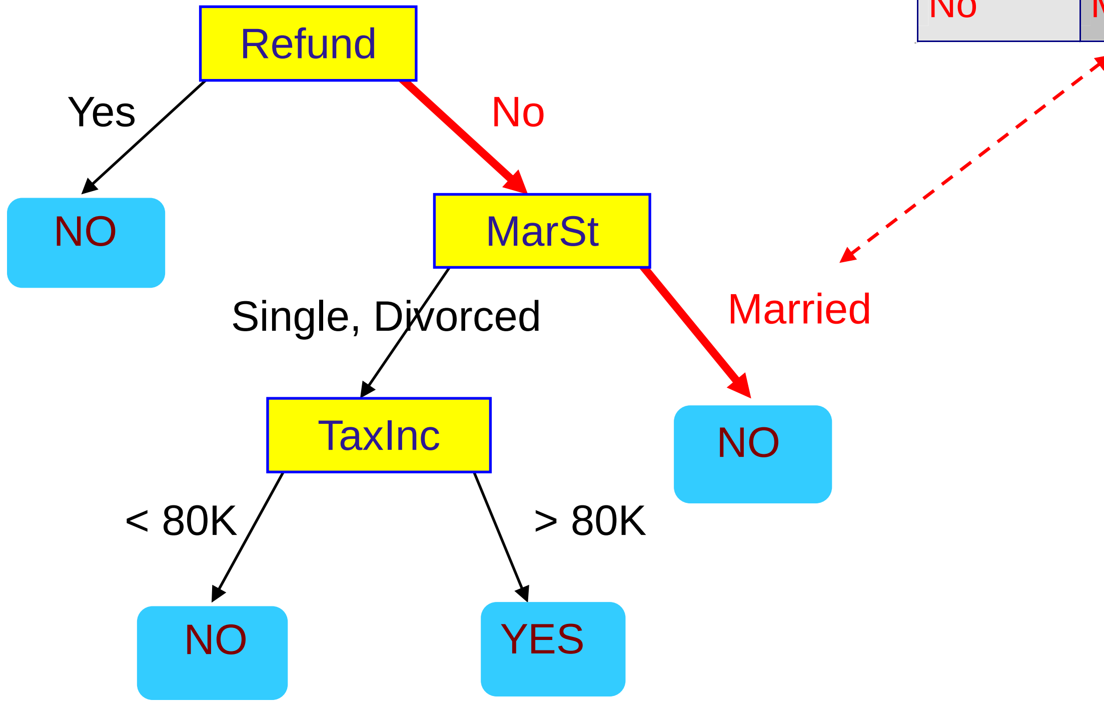
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

Test Data

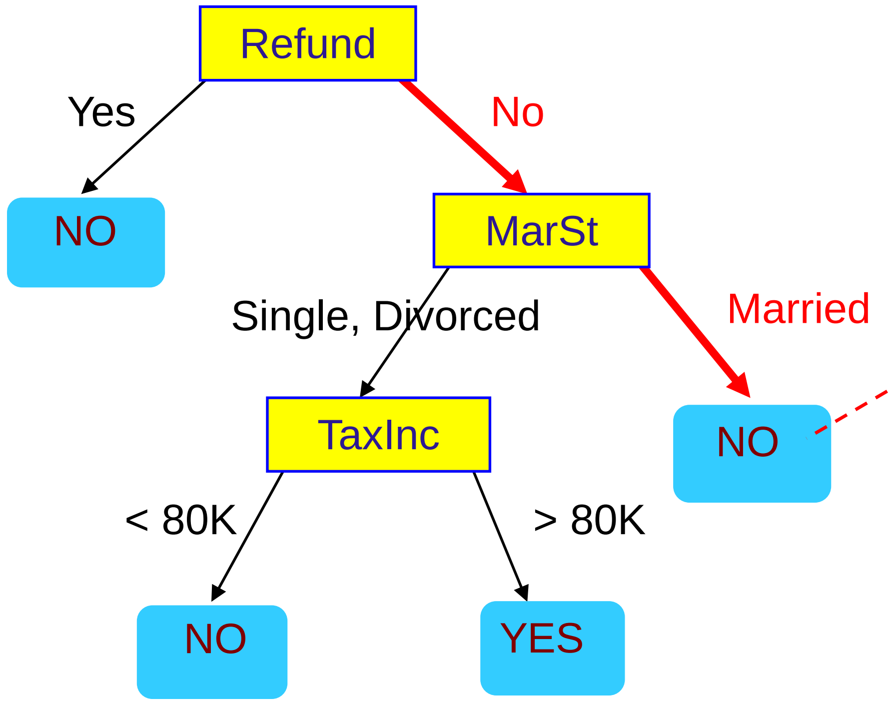
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	**?**



Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to “No”

Decision Tree Classification Task

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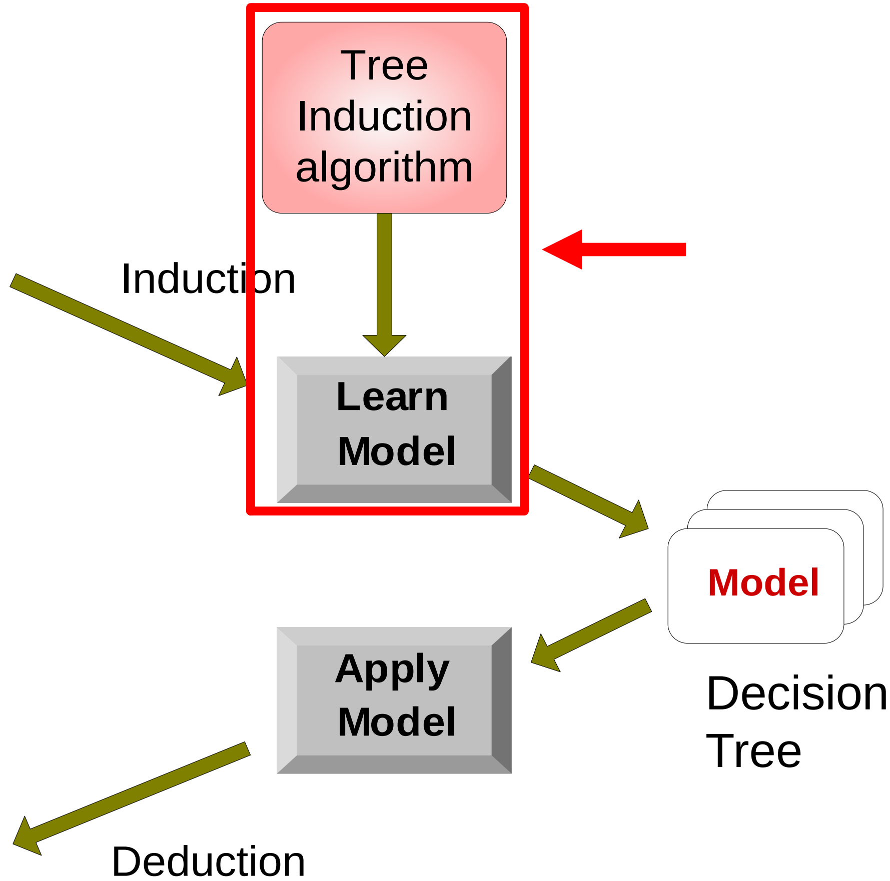
Training Set



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Test Set

Tree Induction

- Finding the best decision tree is NP-hard

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

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

Refund → node t

D → Dataset (table), D_t → column 1 D_{Refund} → column 1

General Structure of Hunt's Algorithm

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

$D_t \rightarrow D_{Refund}$.

- 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 with the same attribute values, then t is a leaf node labeled with the majority class 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.

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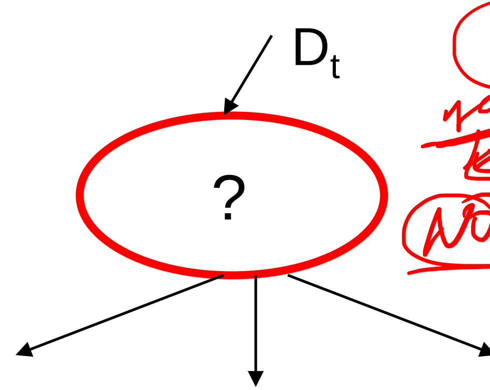
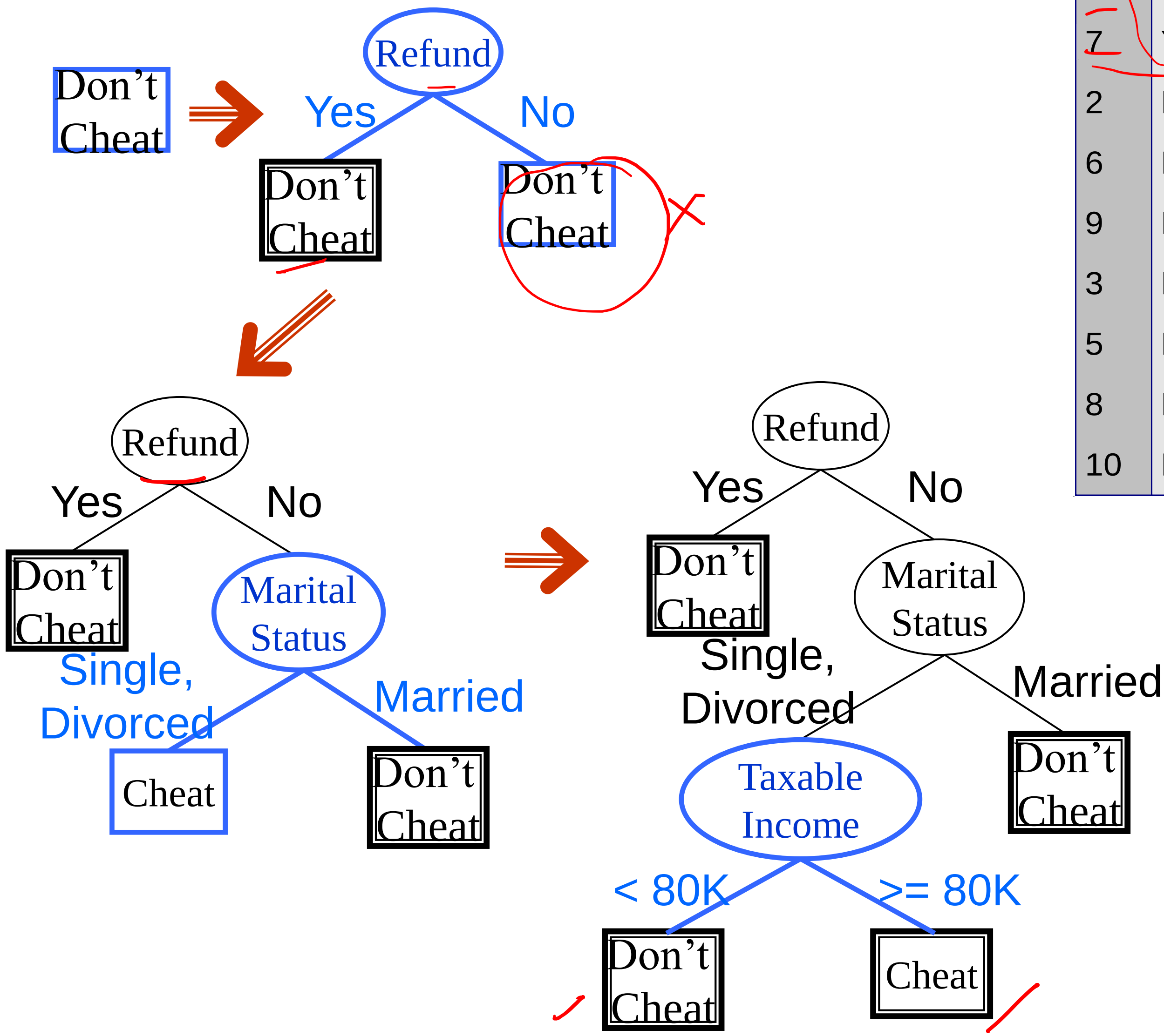


Refund

yes   no

NO

Hunt's Algorithm



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5	No	Divorced	95K	Yes
8	No	Single	85K	Yes
10	No	Single	90K	Yes

Constructing decision-trees (pseudocode)

GenDecTree(Sample **S**, Features **F**)

1. **If stopping_condition(S,F)** = true **then**
   a. **leaf = createNode()**
   b. **leaf.label= Classify(S)**
   c. **return leaf**
2. **root = createNode()**
3. **root.test_condition = findBestSplit(S,F)**
4. **V = {v| v a** possible outcome of **root.test_condition}**
5. **for** ***each*** value **vєV**:
   a. **S_v: = {s | root.test_condition(s)** = **v** and **s є S}**;
   b. **child = GenDecTree(S_v ,F**) ;
   c. Add **child** as a descent of **root** and label the edge **(root→child) as v**
6. **return root**

Tree Induction

- Issues
  - How to **Classify** a leaf node
    - Assign the majority class
    - If leaf is empty, assign the default class – the class that has the highest popularity.
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

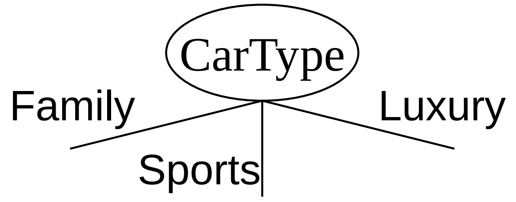
How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

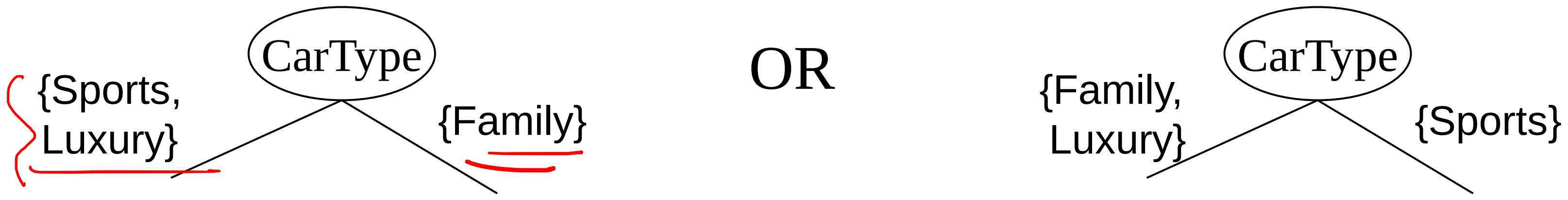
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

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

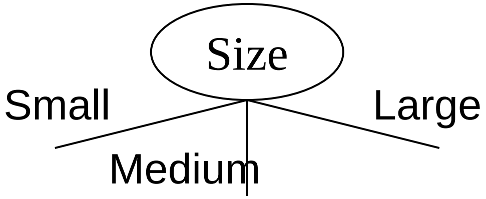


- Binary split: Divides values into two subsets. Need to find optimal partitioning.

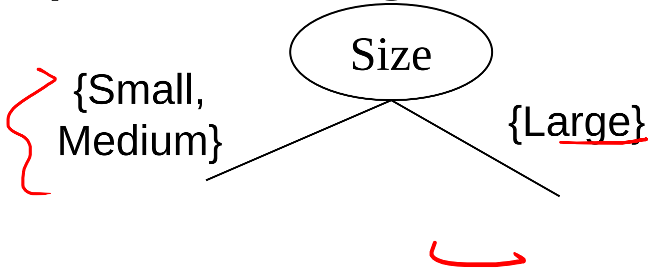


Splitting Based on Ordinal Attributes

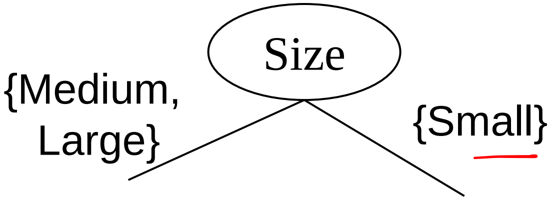
- Multi-way split: Use as many partitions as distinct values.



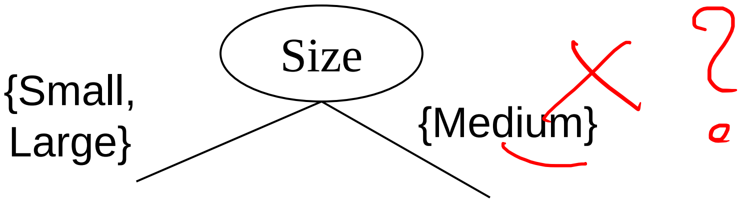
- Binary split: Divides values into two subsets – respects the order. Need to find optimal partitioning.



OR



- What about this split?



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

Annual Income

> 80K

yes

No

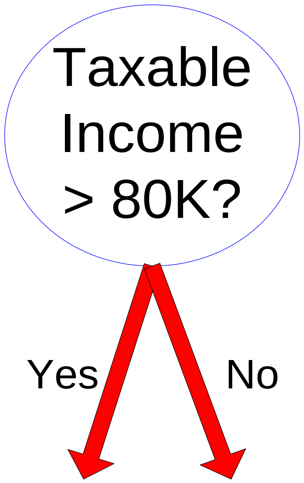
Annual Income

<10K

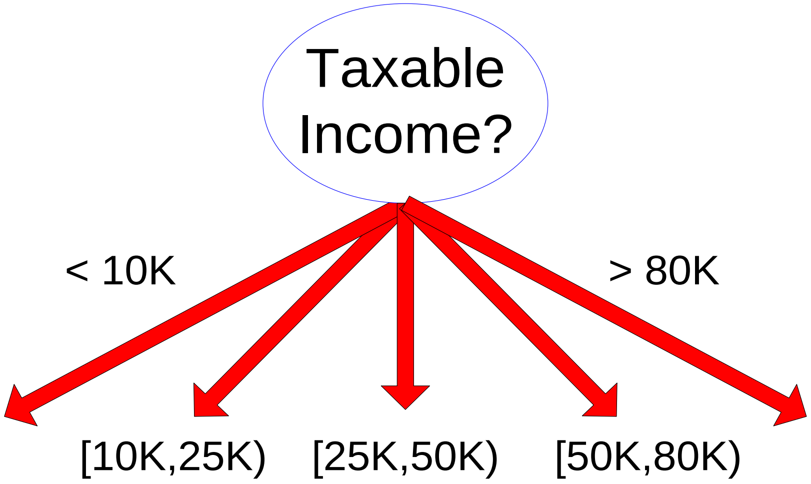
> 80K

{10, 25} {25, 50} {50, 80}

Splitting Based on Continuous Attributes



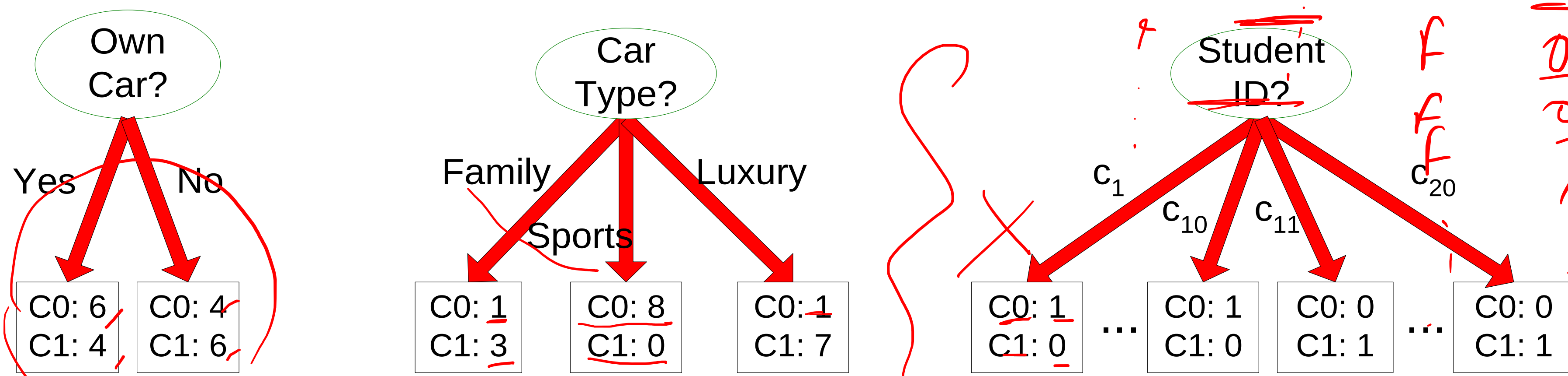
(i) Binary split



(ii) Multi-way split

How to determine the Best Split

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



Which test condition is the best?

C0 : 10
C1 : 0

C0 : 0
C1 : 10

StId	OwnCar	Cartype	labels
1	Yes	Family	
2	yes	S	0
3	NO	L	1
4		F	0
		F	0
		F	1

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

C0: 10
C1: 0

- Ideas?

Measuring Node Impurity

- p(i|t): fraction of records associated with node **t** belonging to class **i**

yes/No

Refund

$$\text{Entropy}(t) = -\sum_{i=1}^{c} p(i\,|\,t)\log p(i\,|\,t)$$

$0 \log 0 = 0 p(0|t) = 0$

- Used in ID3 and C4.5

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

- Used in CART, SLIQ, SPRINT.

$$\text{Classification error}(t) = 1 - \max_i \left[p(i\,|\,t)\right]$$

Gain

I(.) is the impurity measure of the given node
N is the total no. of records at the parent node | K is the no. of att. values

- ***Gain of an attribute split:*** compare the impurity of the parent node with the average impurity of the child nodes

$$\Delta = I(parent) - \sum_{j=1}^{k} \frac{N(v_j)}{N} I(v_j)$$

→ no. of records associated with the child node v_j

- Maximizing the gain ⇔ Minimizing the weighted average impurity measure of children nodes
- If **I() = Entropy(),** then Δ_{info} is called **information gain**

Example

$$\begin{array}{ll} C1 & 3 \\ C2 & 3 \end{array}$$

$Gini = 1 - (3/6)^2 - (3/6)^2 = 0.5$

$Entropy = -3/6 \log(3/6) - (3/6) \log(3/6)$

$Error = 1 - \max\{3/6 \;\; 3/6\} = 0.5 = 1$

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

$1 - \sum_{i=1}^{c} P(i)^2$

Entropy = – 0 log 0 – 1 log 1 = – 0 – 0 = 0

Error = 1 – max (0, 1) = 1 – 1 = 0

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

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

Gini = 1 – (1/6)^2 – (5/6)^2 = 0.278

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

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

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

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

Gini = 1 – (2/6)^2 – (4/6)^2 = 0.444

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

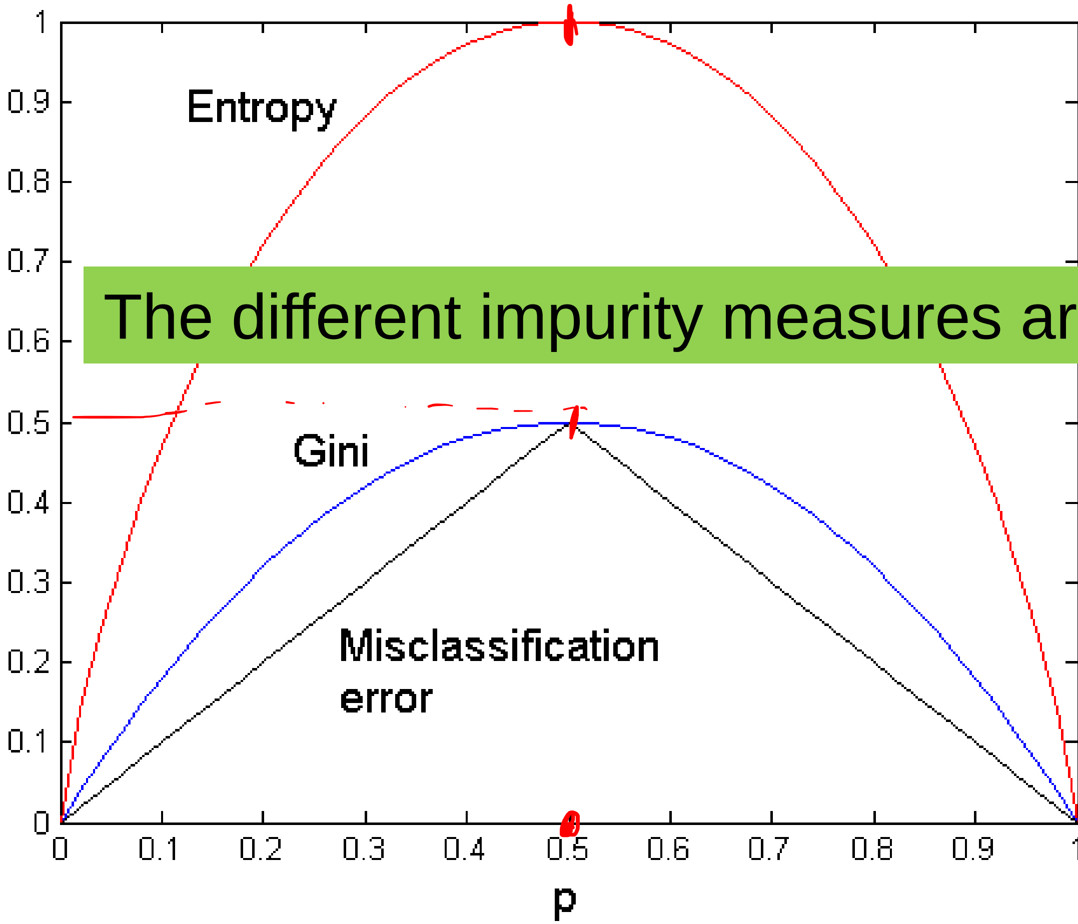
Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Impurity measures

- All of the impurity measures take value zero (minimum) for the case of a pure node where a single value has probability 1
- All of the impurity measures take maximum value when the class distribution in a node is uniform.

Comparison among Splitting Criteria

For a 2-class problem:



The different impurity measures are consistent

C0 = 3

C1 = 3

0.5

Categorical Attributes

- For binary values split in two
- For multivalued attributes, 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

10 → 7 → 3 → 1

- Use Binary Decisions based on one value
- 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
- Exhaustive method to choose best v
  - For each v, scan the database to gather count matrix and compute the impurity index
  - Computationally Inefficient! Repetition of work.

R
yes NO
MS

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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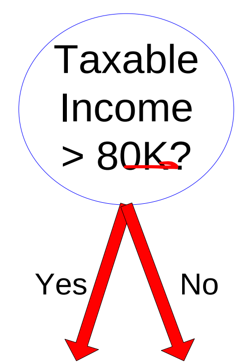
9	No	Married	75K	No
10	No	Single	90K	Yes



< 55
yes 0
No 0

≥ 55
yes - 3
No - 7

Continuous Attributes

$Gini(<=55) = 1 - (0+0) = 1$

$Gini(>55) = 1 - (3/10)^2 - (7/10)^2 = 0.42$

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

$Gini = 0/10 \times 1 + 10/10 \times 0.420$

$= 0 + 0.420 = 0.420$

$P\left(\frac{\text{yes+No}}{\text{total no. of records}}\right) \times Gini(<=55) + \_\_ \times Gini(>55) =$

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	

Splitting based on impurity

- Impurity measures favor attributes with large number of values

- A test condition with large number of outcomes may not be desirable
  - # of records in each partition is too small to make predictions

Splitting based on INFO

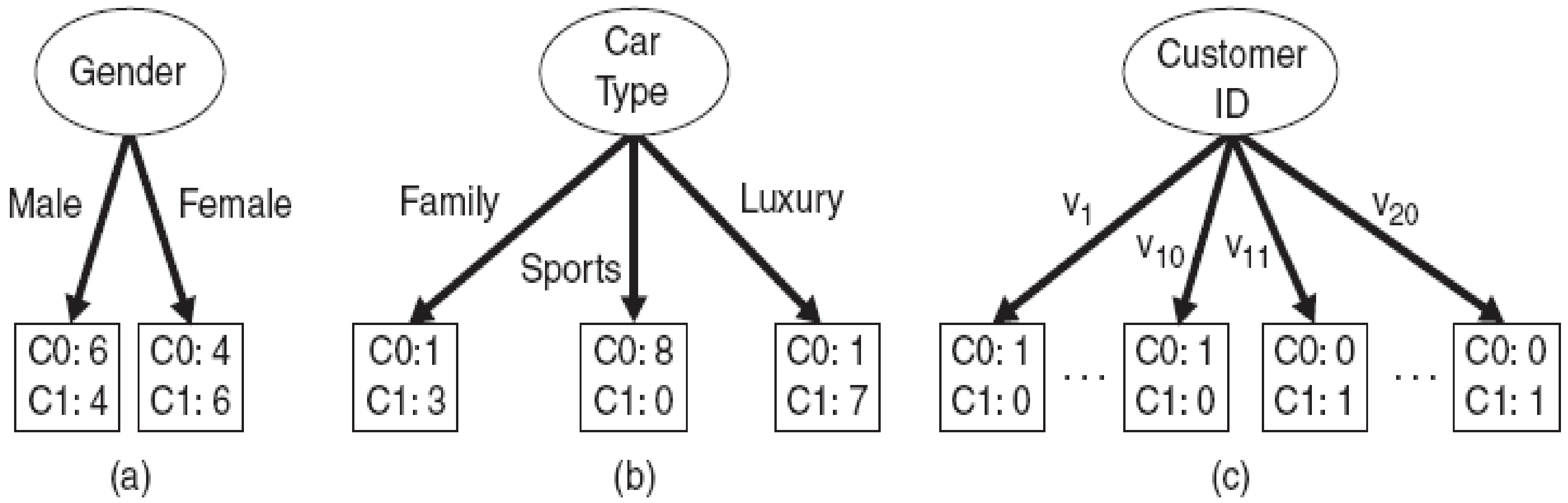


Figure 4.12. Multiway versus binary splits.

Gain Ratio

- Splitting using information gain

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

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 impurity

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)

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

Example: C4.5

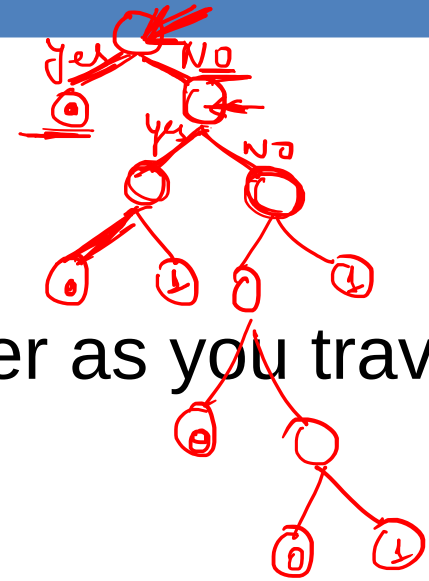
- Simple depth-first construction.
- Uses Information Gain
- Sorts Continuous Attributes at each node.
- Needs entire data to fit in memory.
- Unsuitable for Large Datasets.
  - Needs out-of-core sorting.

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

Other Issues

- Data Fragmentation
- Expressiveness

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

condition

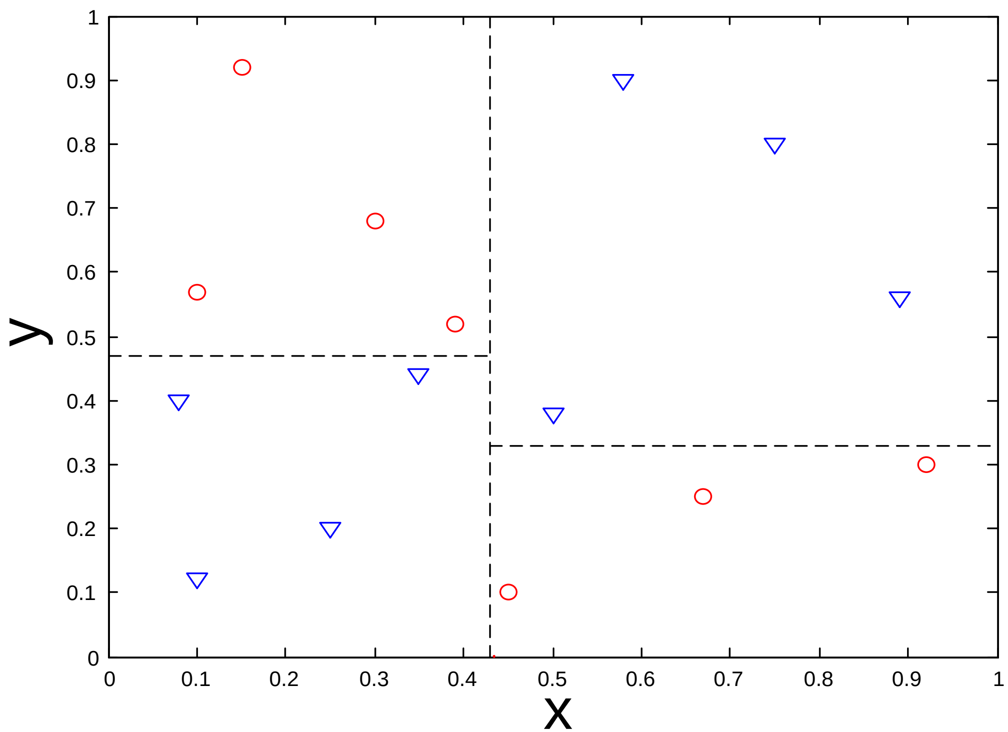
- You can introduce a lower bound on the number of items per leaf node in the stopping criterion.

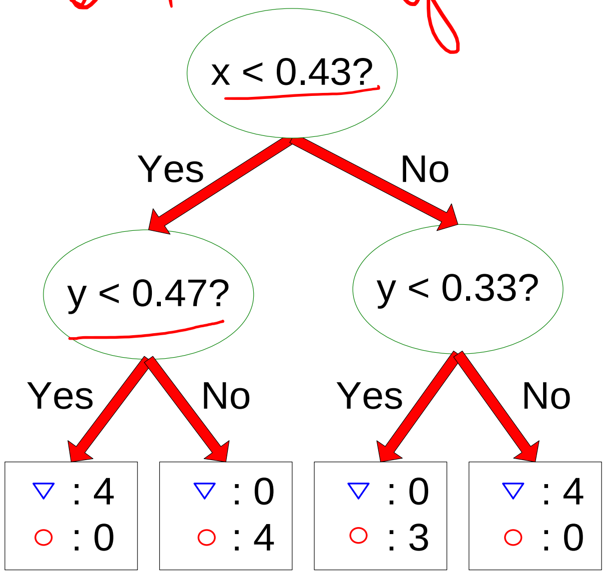
Expressiveness

- A classifier defines a function that discriminates between two (or more) classes.
- The expressiveness of a classifier is the class of functions that it can model, and the kind of data that it can separate
  - When we have discrete (or binary) values, we are interested in the class of boolean functions that can be modeled
  - If the data-points are real vectors we talk about the decision boundary that the classifier can model

Decision Boundary

limit your expressiveness of your model





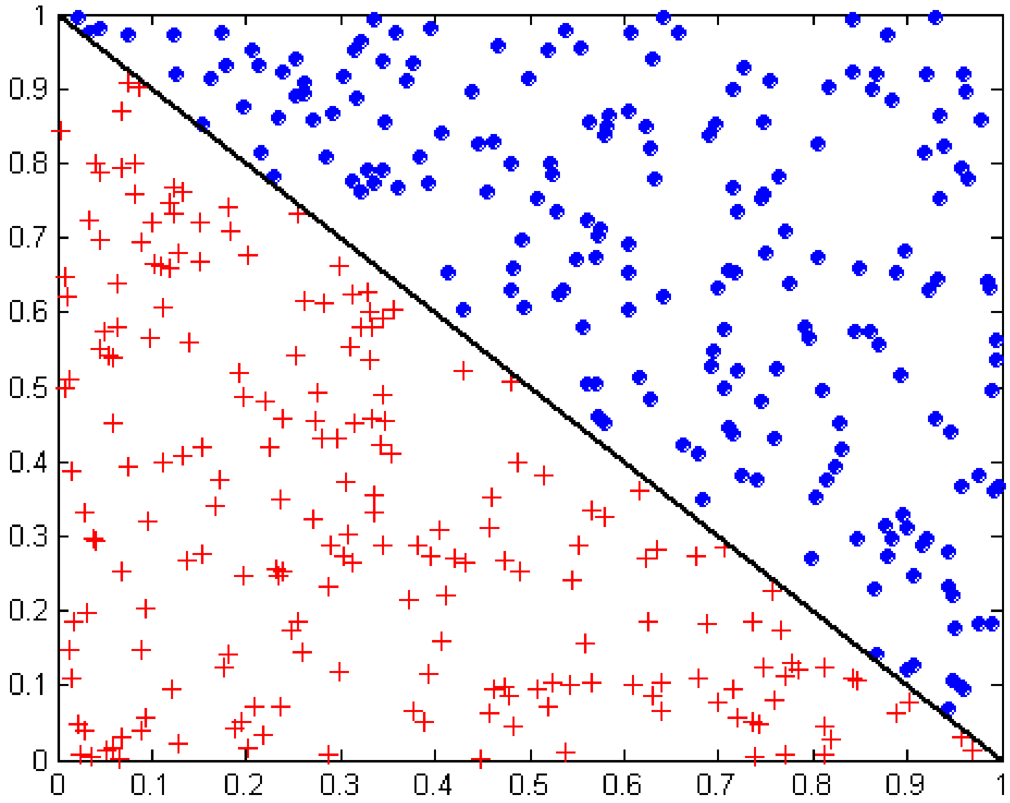
- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

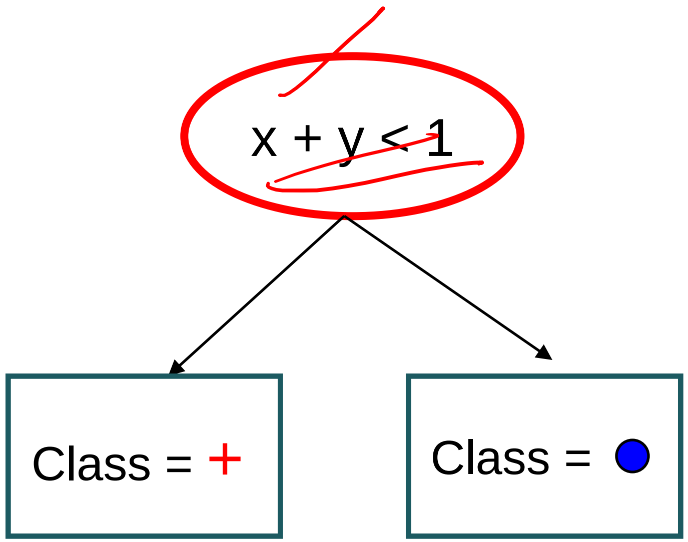
Expressiveness

- 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

- Less expressive for modeling continuous variables
  - Particularly when test condition involves only a single attribute at-a-time

Oblique Decision Trees



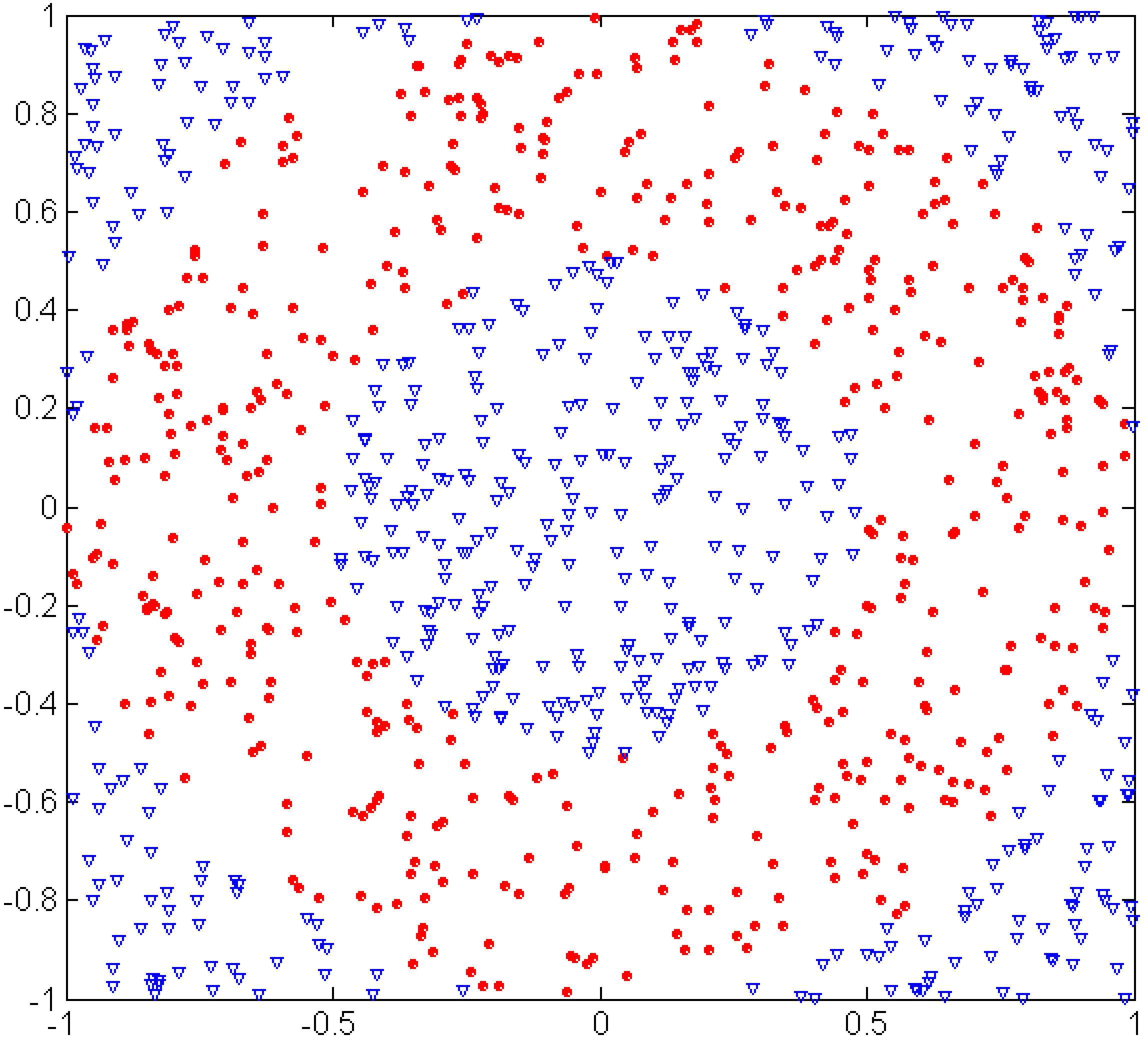


- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive

Practical Issues of Classification

- Underfitting and Overfitting
- Evaluation

Underfitting and Overfitting (Example)



500 circular and 500 triangular data points.

Circular points:

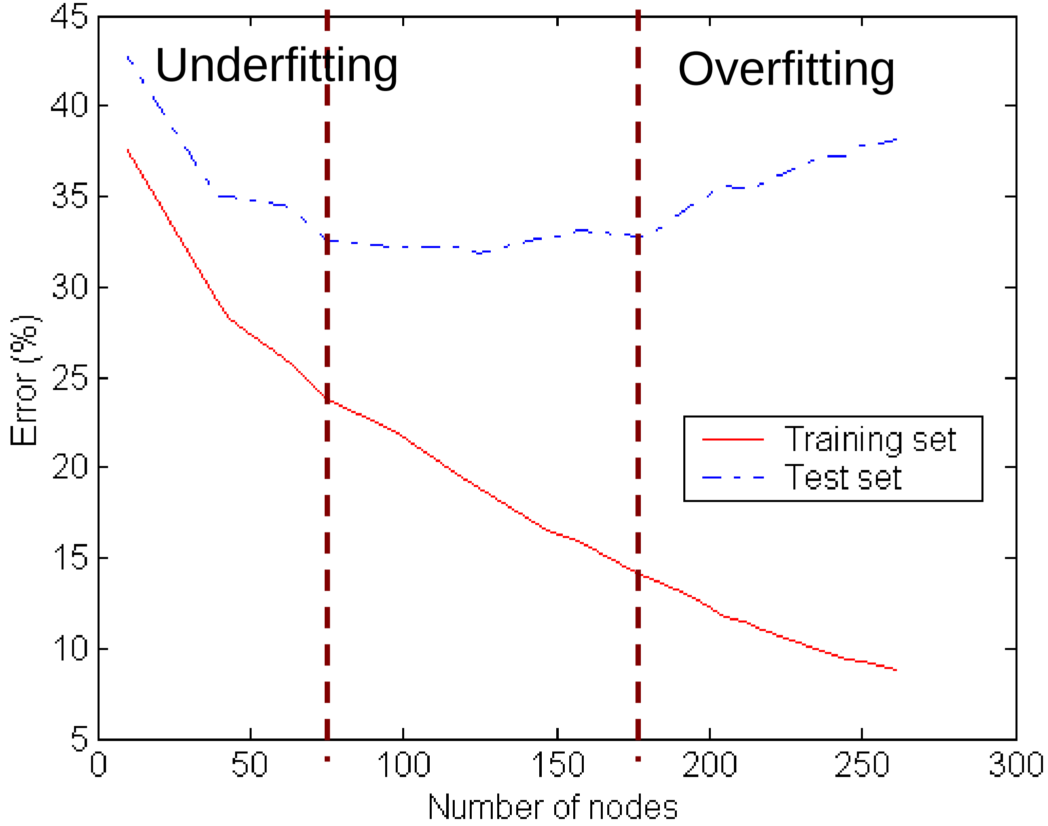
$0.5 \leq \mathrm{sqrt}(x_1^2+x_2^2) \leq 1$

Triangular points:

$\mathrm{sqrt}(x_1^2+x_2^2) > 0.5$ or

$\mathrm{sqrt}(x_1^2+x_2^2) < 1$

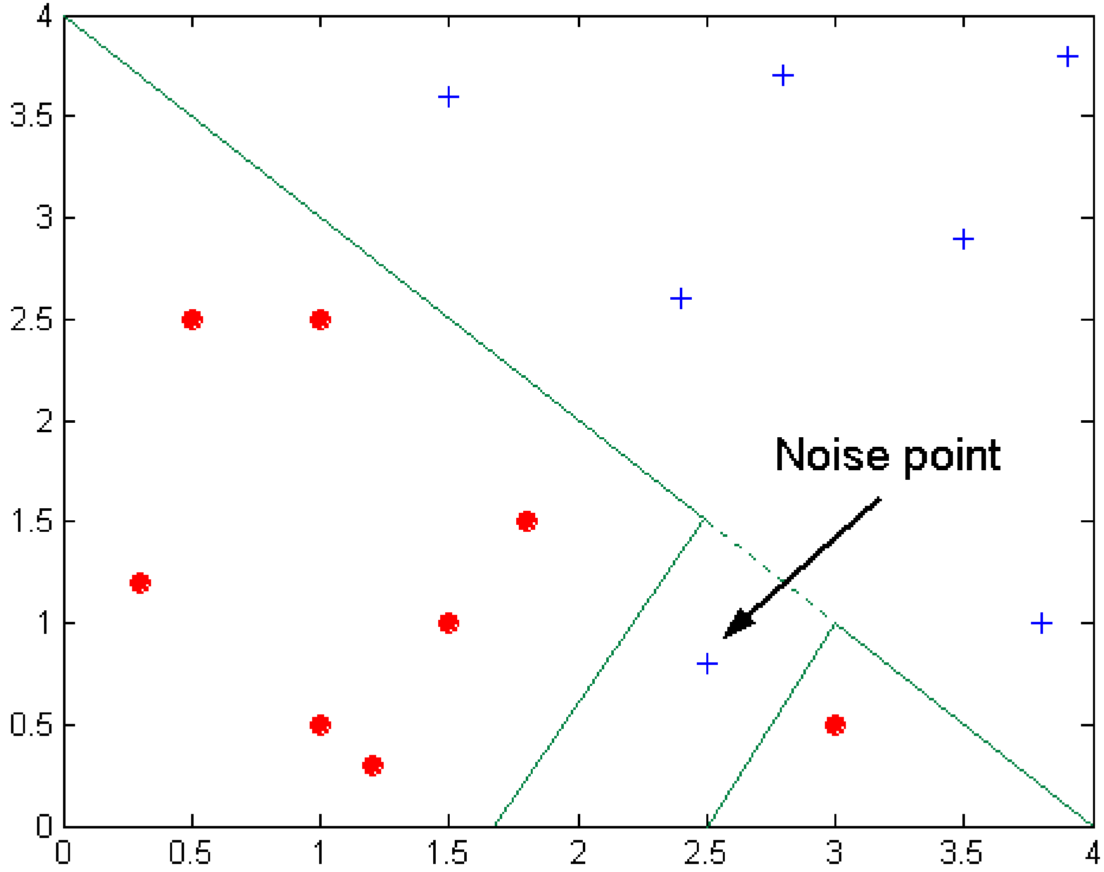
Underfitting and Overfitting



Underfitting: when model is too simple, both training and test errors are large

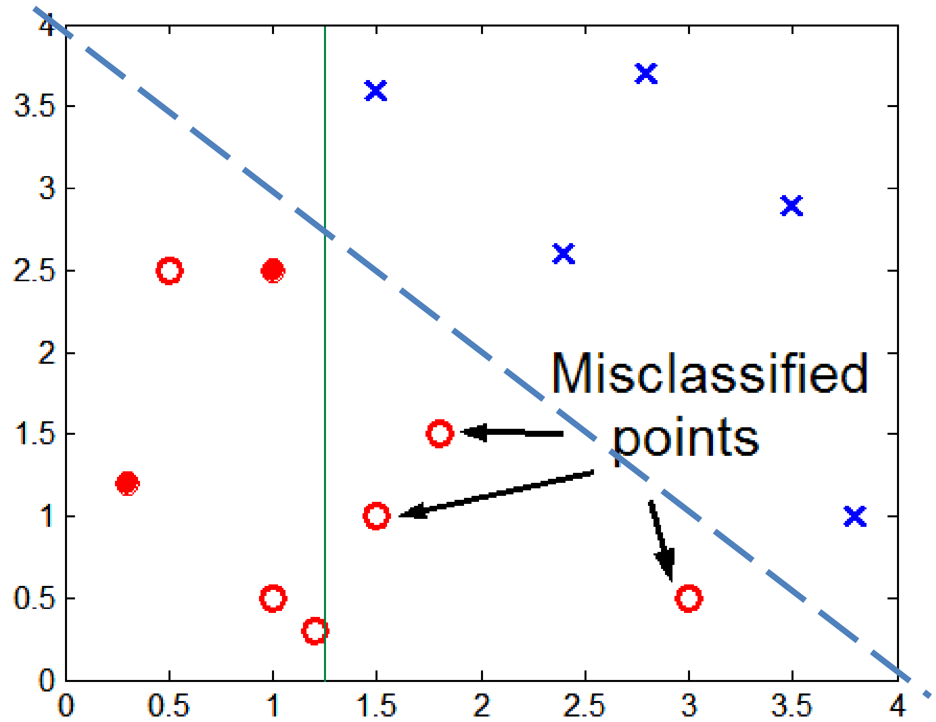
Overfitting: when model is too complex it models the details of the training set and fails on the test set

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

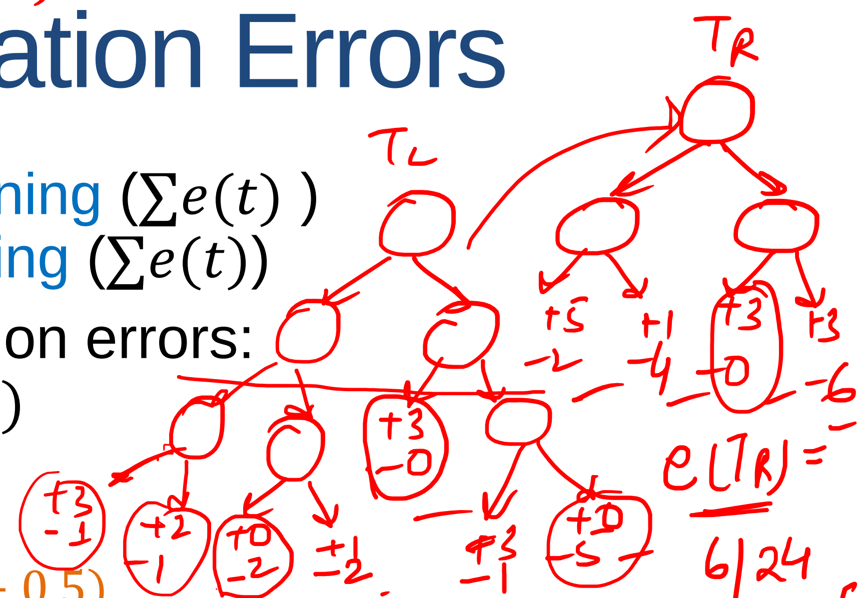
- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records
  - The model does not generalize well

- Need new ways for estimating errors

Estimating Generalization Errors

$\Omega(t) = 0.5$; $\Omega(t) = 1$

- Re-substitution errors: error on training ($\sum e(t)$)
- Generalization errors: error on testing ($\sum e(t)$)
- 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)
      - Penalize large trees
    - For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances)
      - Training error = 10/1000 = 1 %
      - Generalization error = (10 + 30×0.5)/1000 = 2.5%
  - Using validation set:
    - Split data into training, validation, test
    - Use validation dataset to estimate generalization error
    - Drawback: less data for training.



$e(T_R) = 6/24 = 0.25$

$e(T_L) = 4/24 = 0.167$

100

80 : 20

Tr Te

80 : 20

Tr Val

$e_g(T_L) = \frac{4}{24} = 0.458$

$e_g(T_L) = \frac{4 + 7 \times 0.5}{24} = 0.3125$

$e_g(T_R) = 10 = 0.417$

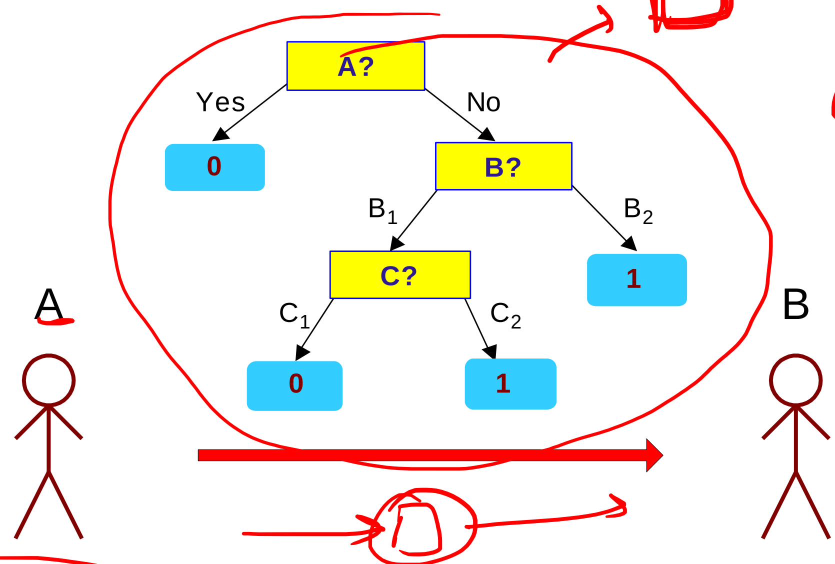
$e_g(T_R) = \frac{6 + 4 \times 0.5}{24} = 0.333$

Occam's Razor (principle of parsimony)

- 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

Minimum Description Length (MDL)

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



$\theta(n)$

X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- Cost(Model,Data) = Cost(Data|Model) + Cost(Model)
  - Search for the least costly model.

less complex models

- Cost(Data|Model) encodes the misclassification errors.
- Cost(Model) encodes the decision tree
  - 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

stop

+3
- 0

No

  - 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.
  - 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

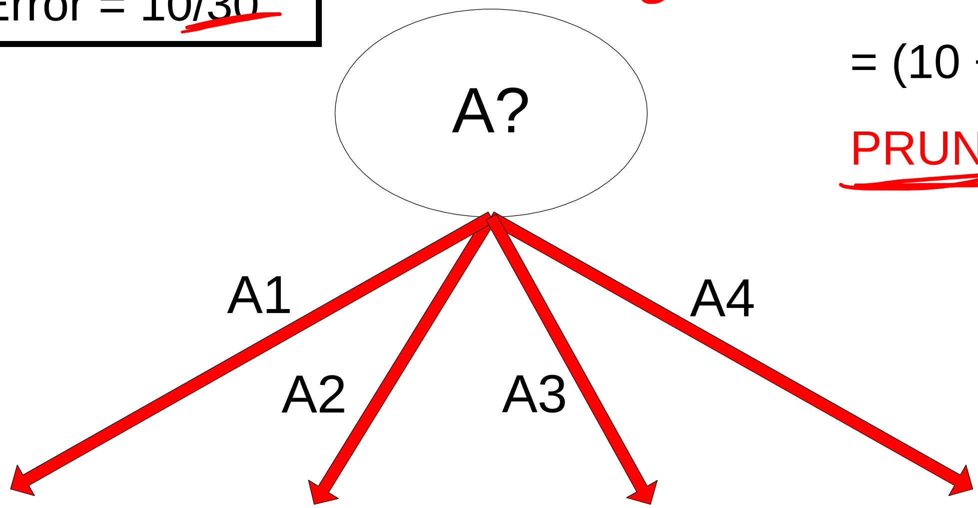
Training Error (After splitting) = 9/30 10/30

Pessimistic error (After splitting)

$= (10 + 4 \times 0.5)/30 = 11/30$

PRUNE!

10.5 → 11



Class = Yes	8
Class = No	4

Class = Yes	3
Class = No	4

Class = Yes	4
Class = No	1

Class = Yes	5
Class = No	1

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 Model Comparison
  - How to compare the relative performance among competing models?

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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	
		Class=Yes	Class=No
ACTUAL CLASS	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	
		Class=Yes	Class=No
ACTUAL CLASS	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 ← lower weight w_1
  - Number of Class 1 examples = 10 ← higher weight w_2

- 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	
ACTUAL CLASS		
C(i|j)	**Class=Yes** a	**Class=No** b
Class=Yes	C(Yes|Yes) P(yes|yes)	C(No|Yes) P(No|yes)
Class=No	C(Yes|No) c P(yes|No)	C(No|No) d P(No|No)

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

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

3

Computing Cost of Classification

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

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

Accuracy = 80%

Cost = 3910

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

$N = a + b + c + d$

$\text{Accuracy} = (a + d)/N$

$$\begin{aligned}\text{Cost} &= p\,(a + d) + q\,(b + c) \\ &= p\,(a + d) + q\,(N - a - d) \\ &= q\,N - (q - p)(a + d) \\ &= N\,[q - (q-p) \times \text{Accuracy}]\end{aligned}$$

Precision-Recall

rate of true records out the total +ve records detected by the model

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

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

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

total ~~true~~ actually +ve records

$$\text{F-measure (F)} = \frac{1}{\left(\frac{1/r + 1/p}{2}\right)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c} = \frac{2TP}{2TP+FP+FN}$$

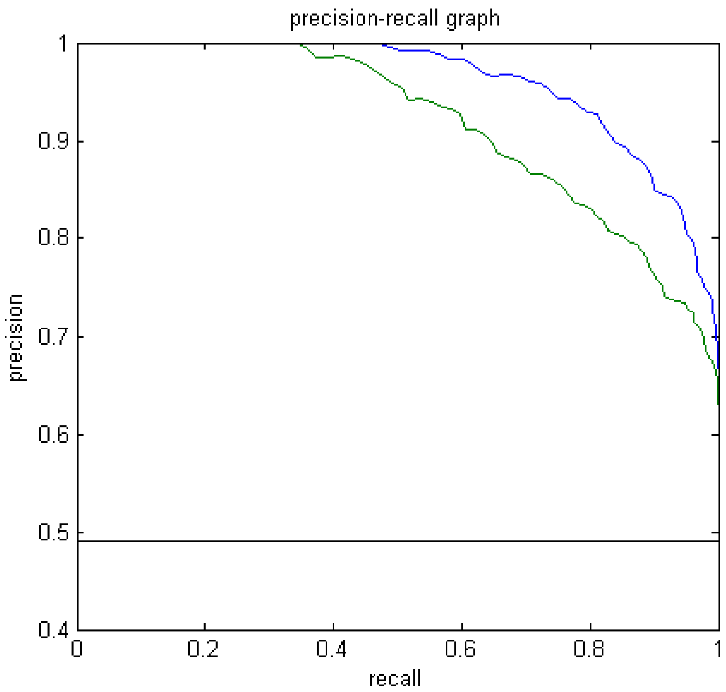
F1

$$\boxed{\frac{2 \times P \times R}{P+R}}$$

- 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)

Precision-Recall plot

- Usually for parameterized models, it controls the precision/recall tradeoff



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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

Methods of Estimation

- Holdout
  - Reserve **2/3** for training and **1/3** for testing
- Random subsampling
  - One sample may be biased -- Repeated holdout
- 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**
  - Guarantees that each record is used the same number of times for training and testing
- Bootstrap
  - Sampling with replacement
  - ~63% of records used for training, ~27% for testing

70 | 30

100

70 → 30

10 | 70 | 20

20 | 70 | 10

10 10 10 10 10

1 | 2 | 3 | 4 | 5

5 -

Dealing with class Imbalance

- If the class we are interested in is very rare, then the classifier will ignore it.
  - The class imbalance problem

10 +ve

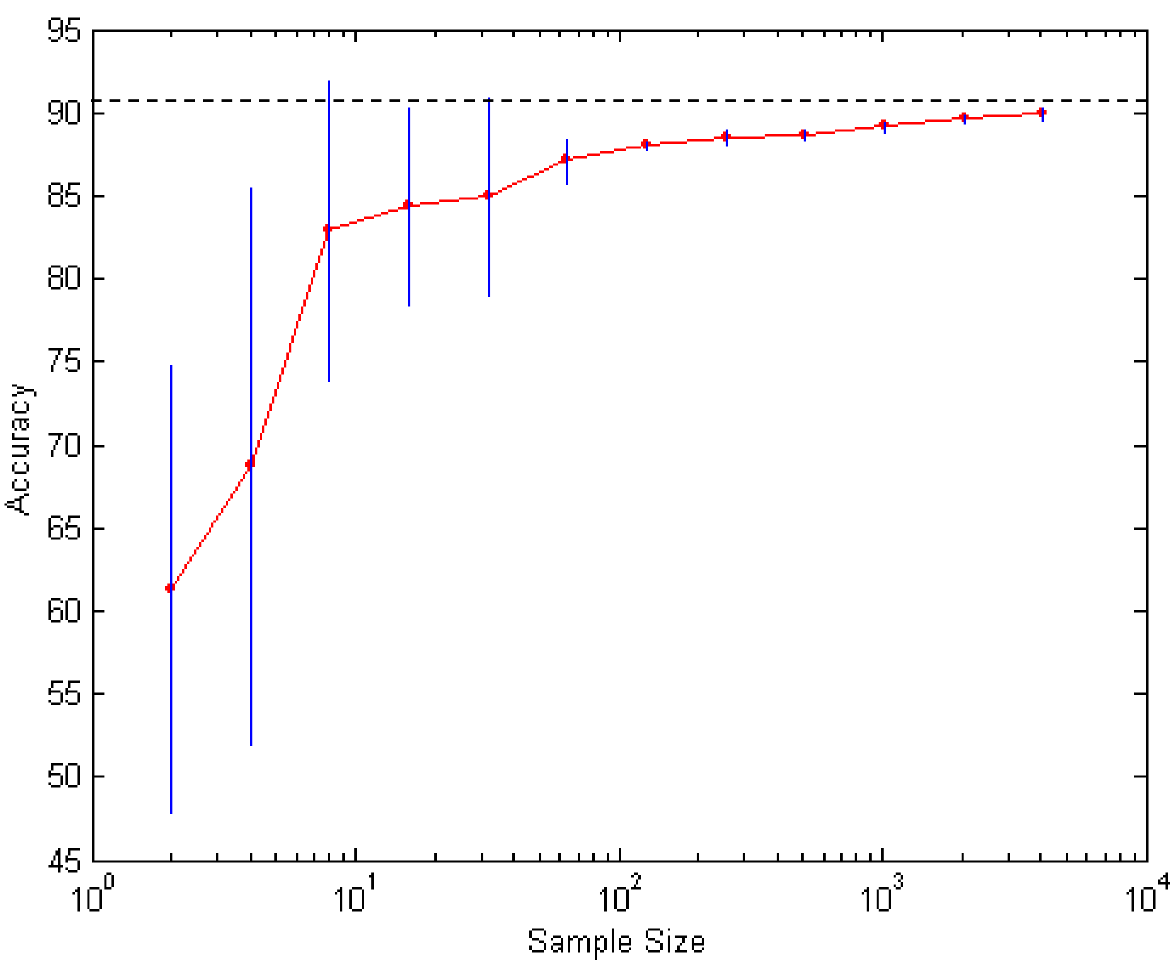
90 +ve

10 -ve

80 -ve

- Solution
  - We can modify the optimization criterion by using a cost sensitive metric
  - We can balance the class distribution
    - Sample from the larger class so that the size of the two classes is the same
    - Replicate the data of the class of interest so that the classes are balanced
      - Over-fitting issues

Learning Curve



- Learning curve shows how accuracy changes with varying sample size

- Requires a sampling schedule for creating learning curve

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

Model Evaluation

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ROC (Receiver Operating Characteristic)

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- **ROC** curve plots **TPR** (on the **y**-axis) against **FPR** (on the **x**-axis)

$$TPR = \frac{TP}{TP + FN} = \text{Recall}$$

Fraction of positive instances predicted correctly

$$FPR = \frac{FP}{FP + TN}$$

Fraction of negative instances predicted incorrectly

	PREDICTED CLASS		
Actual		Yes	No
	Yes	a (TP)	b (FN)
	No	c (FP)	d (TN)

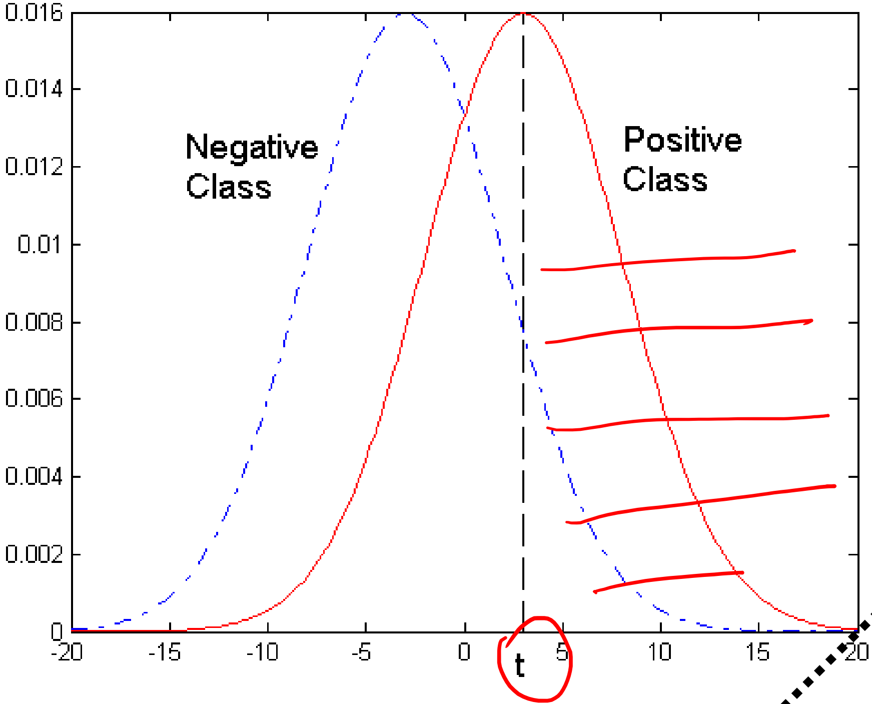
ROC (Receiver Operating Characteristic)

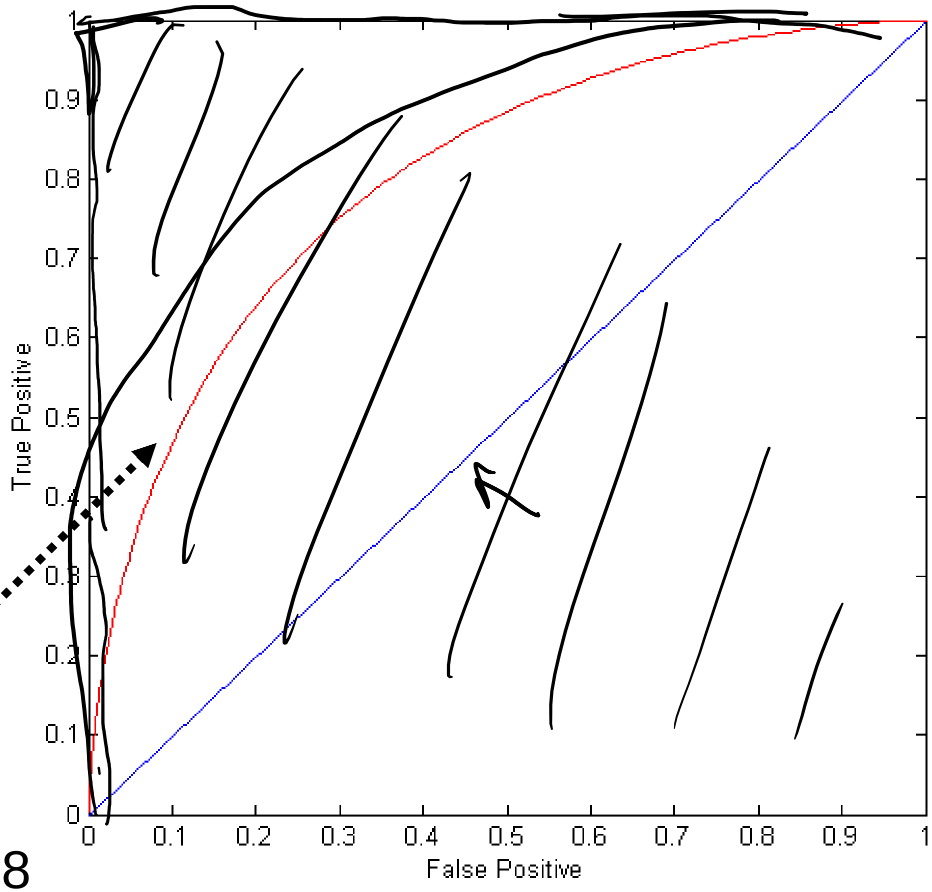
- Performance of a classifier represented as a point on the **ROC** curve
- Changing some parameter of the algorithm, sample distribution or cost matrix changes the location of the point

ROC Curve

- **1**-dimensional data set containing **2** classes (***positive*** and ***negative***)

- any points located at **x > t** is classified as ***positive***





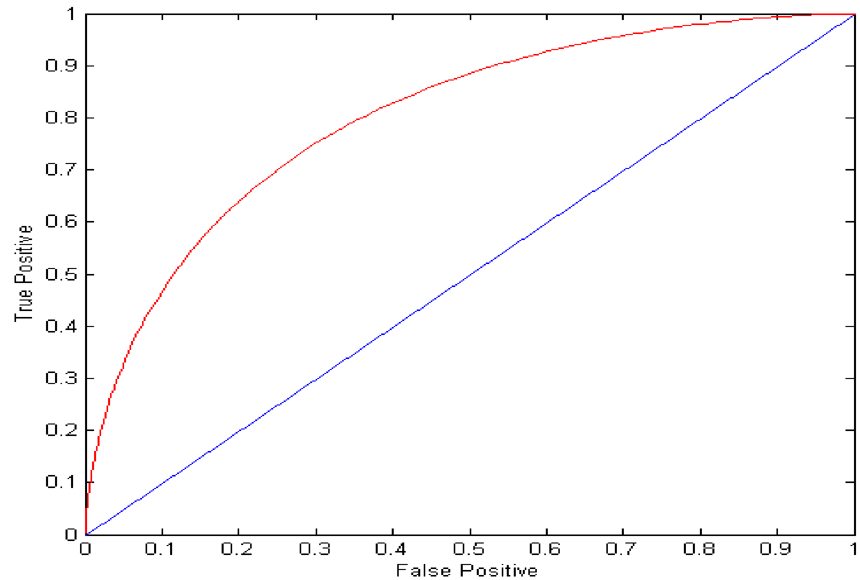
At threshold **t**:

TP=0.5, FN=0.5, FP=0.12, FN=0.88

ROC Curve

(TP,FP):

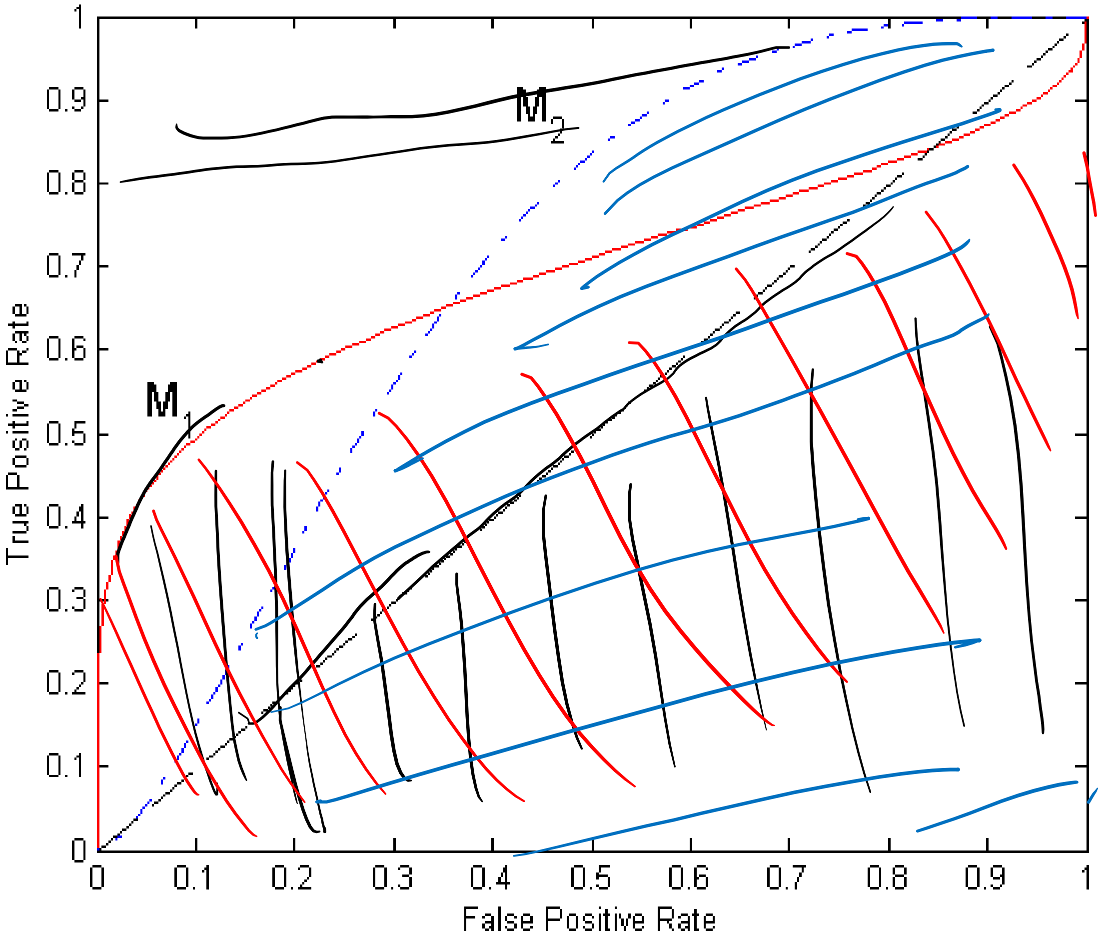
- (0,0): declare everything
  to be negative class
- (1,1): declare everything
  to be positive class
- (1,0): ideal



- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - prediction is opposite of the true class

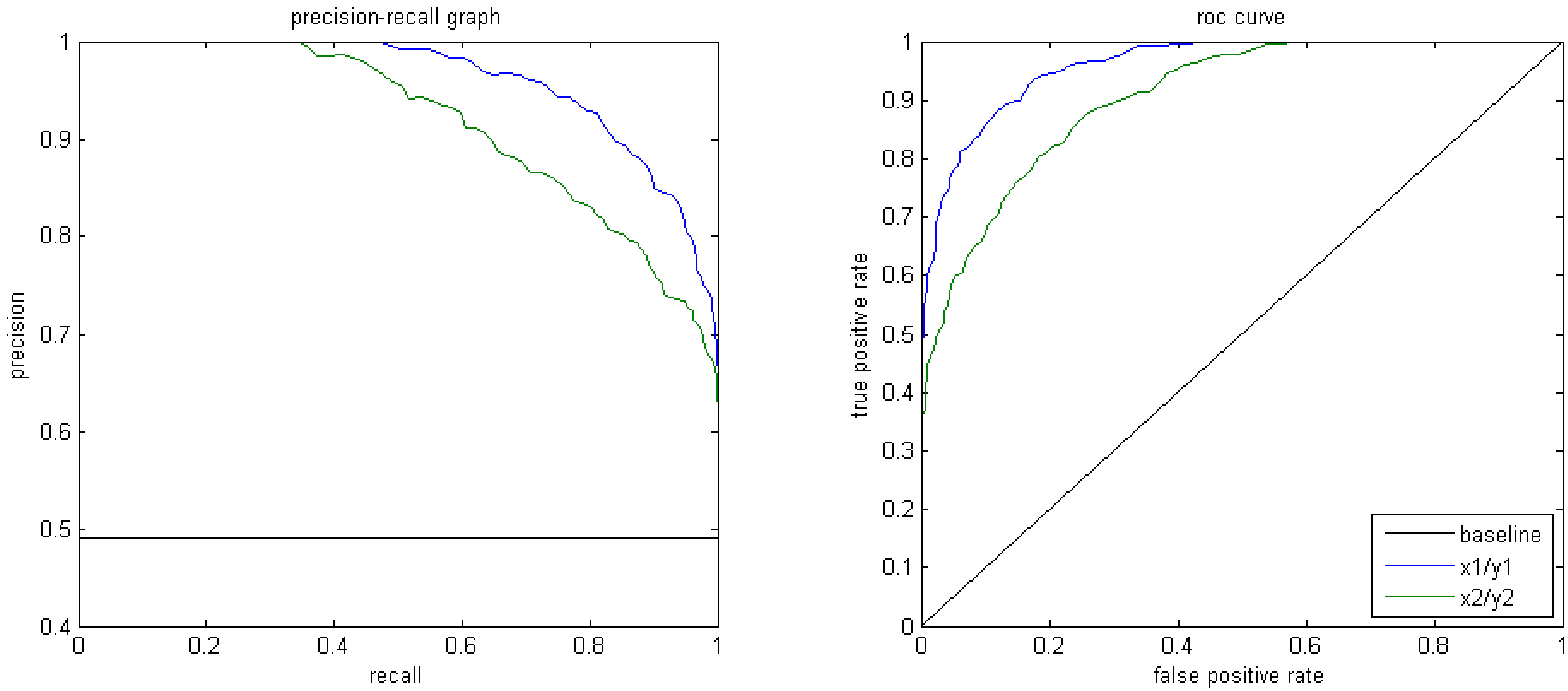
	PREDICTED CLASS		
		Yes	No
Actual	Yes	a (TP)	b (FN)
	No	c (FP)	d (TN)

Using ROC for Model Comparison



- No model consistently outperform the other
  - M_1 is better for small FPR
  - M_2 is better for large FPR
- Area Under the ROC curve (AUC)
  - Ideal: Area = 1
  - Random guess:
    - Area = 0.5

ROC curve vs Precision-Recall curve



Area Under the Curve (AUC) as a single number for evaluation