Classification

Part 1

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Overview

- Introduction to classification
- Different techniques for classification
- Decision Tree Classifiers
  - How decision tree works?
  - How to build a decision tree?
  - Methods for splitting
  - Measures for selecting the best split
  - Practical Challenges in Classification
  - Handling over-fitting
  - Handling missing attribute values
  - Other issues

Classification : Definition

- Given a set of records (called the *training set*)
  - Each record contains a set of *attributes*
  - One of the attributes is the *class*
- Find a *model* for the class attribute as a function of the values of other attributes
- *Goal*: Previously *unseen* records should be assigned to a class as accurately as possible
  - Usually, the given data set is divided into training and test set, with training set used to build the model and *test set* used to validate it. The accuracy of the model is determined on the test set.

Classification Model

- In general a classification model can be used for the following purposes:
  - It can serve as a explanatory tool for distinguishing objects of different classes. This is the *descriptive* element of the classification model
  - It can be used to predict the class labels of new records. This is the *predictive* element of the classification model

General Approach

- To build a classification model, the labeled data set is initially partitioned in to two disjoint sets, known as *training set* and *test set*, respectively
- Next, a *classification technique* is applied to the training set to induce a *classification model*
- Each classification technique applies a *learning algorithm*

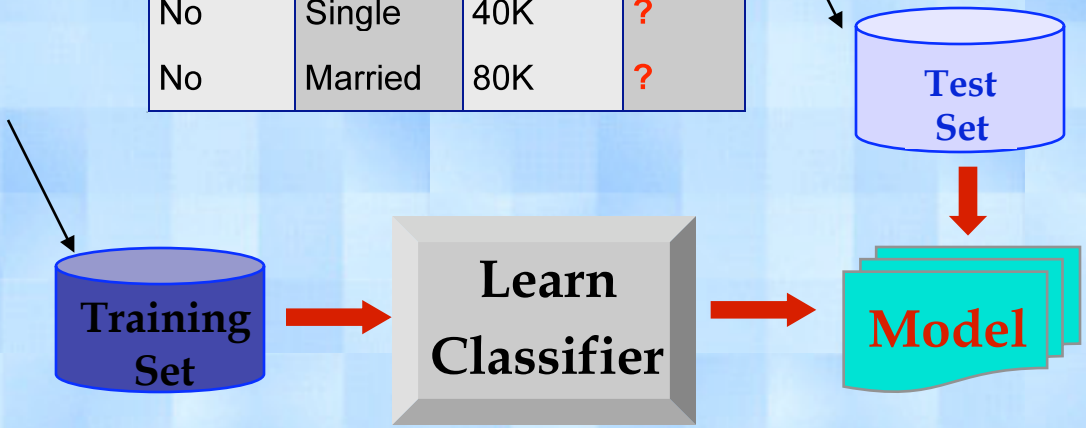
General Approach

- The goal of a learning algorithm is to build a model that has good *generalization capability*
  - That is it must not only fit the training set well but can also predict correctly the class labels of many previously unseen records
- To evaluate how well the induced model performs on records it has not seen earlier, we can apply it to the test set

General Approach

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

Refund	Marital Status	Taxable Income	Cheat
No	Single	75K	?
Yes	Married	50K	?
No	Married	150K	?
Yes	Divorced	90K	?
No	Single	40K	?
No	Married	80K	?

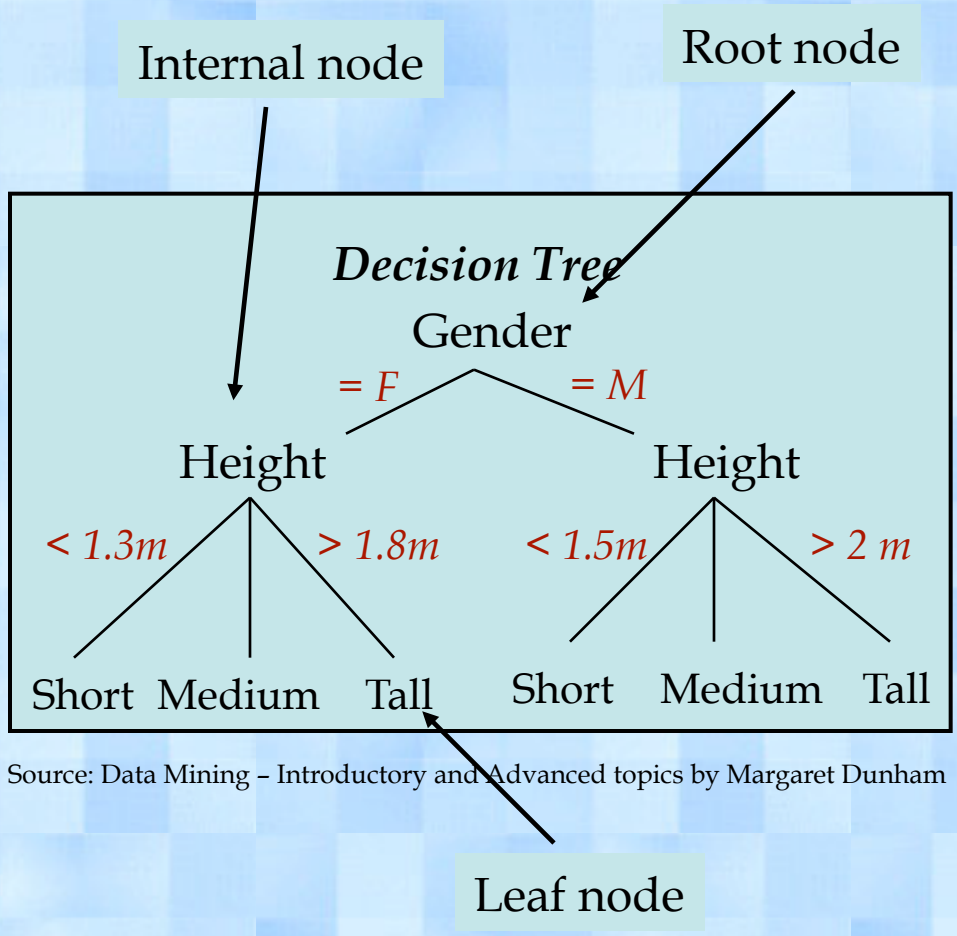


Classification Techniques

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

Decision Tree Based Classification

- A decision tree is a hierarchical structure of nodes and directed edges. There are three types of nodes in a decision tree:
  - A *root node*, which has no incoming edges and zero or more outgoing edges
  - *Internal nodes*, each of which have exactly one incoming edge and two or more outgoing edges
  - *Leaf nodes*, each of which have exactly one incoming edge and no outgoing edges. Each leaf node also has a class label attached to it



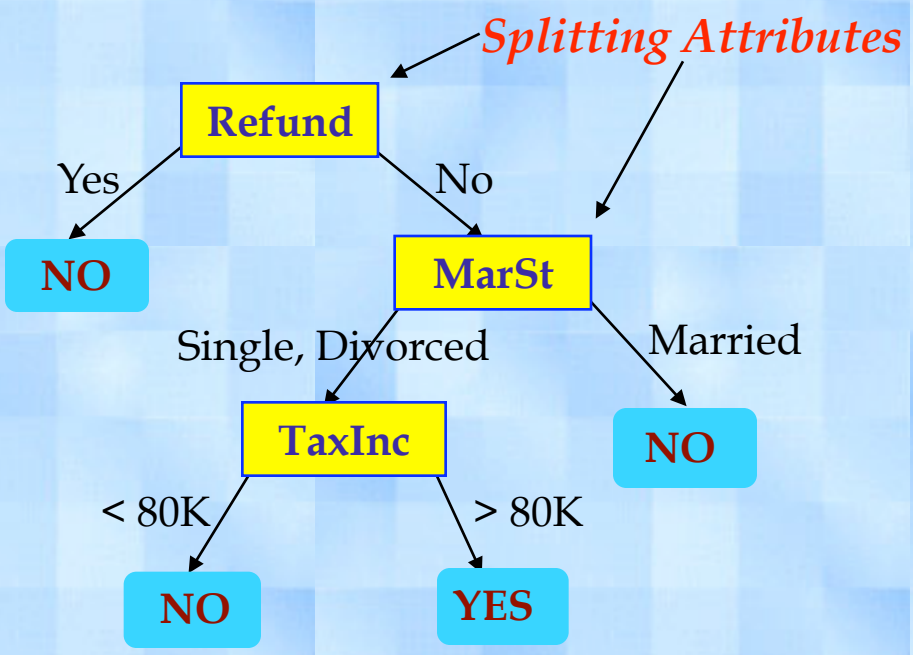
Source: Data Mining – Introductory and Advanced topics by Margaret Dunham

Decision Tree Based Classification

- One of the most widely used classification technique
- Highly expressive in terms of capturing relationships among discrete variables
- Relatively inexpensive to construct and extremely fast at classifying new records
- Easy to interpret
- Can effectively handle both missing values and noisy data
- Comparable or better accuracy than other techniques in many applications

Example Decision Tree

Tid	Refund (categorical)	Marital Status (categorical)	Taxable Income (continuous)	Cheat (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



The splitting attribute at a node is determined based on the GINI index

Another Example of Decision Tree

Tid	Refund (categorical)	Marital Status (categorical)	Taxable Income (continuous)	Cheat (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
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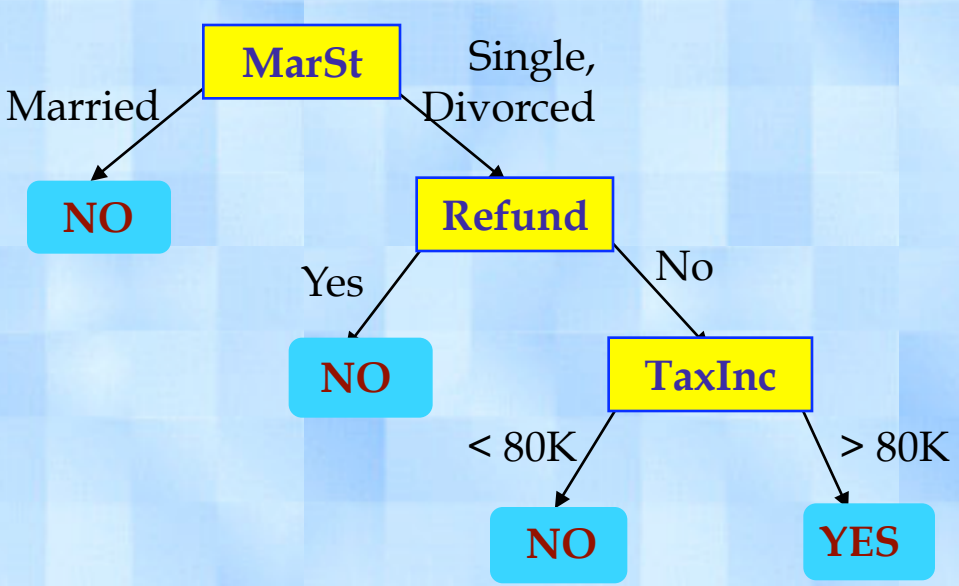


There could be more than one tree that fits the same data!

Decision Tree Algorithms

- Many algorithms
  - Hunt's algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ, SPRINT
- General Structure
  - Tree induction
  - Tree pruning

Hunt's Algorithm

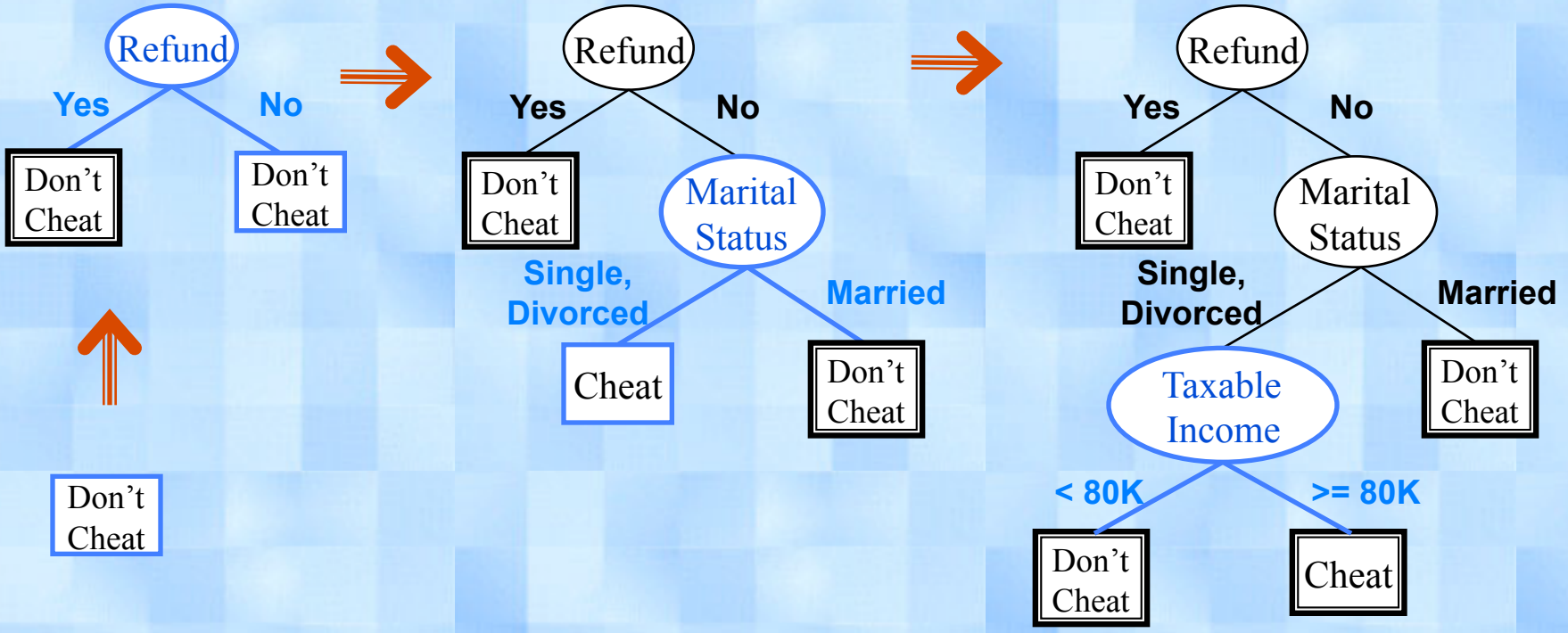
- Most of the decision tree induction algorithms are based on original ideas proposed in Hunt's Algorithm
- Let D_t be the training set and y be the set of class labels $\{y_1, y_2, \ldots, y_c\}$
  - If D_t contains records that belong to the same class, y_k, then its decision tree consists of leaf node labeled as y_k
  - If D_t is an empty set, then its decision tree is a leaf node whose class label is determined from other information such as the majority class of the records

Hunt's Algorithm

- If D_t contains records that belong to several classes, then a *test condition*, based on one of the attributes of D_t, is applied to split the data in to more homogenous subsets
  - The test condition is associated with the root node of the decision tree for D_t. D_t is then partitioned into smaller subsets, with one subset for each outcome of the test condition. The outcomes are indicated by the outgoing links from the root node. This method is then recursively applied to each subset created by the test condition

Example of Hunt's Algorithm

- Attributes: Refund (Yes, No), Marital Status (Single, Divorced, Married), Taxable Income (continuous)
- Class: Cheat, Don't Cheat

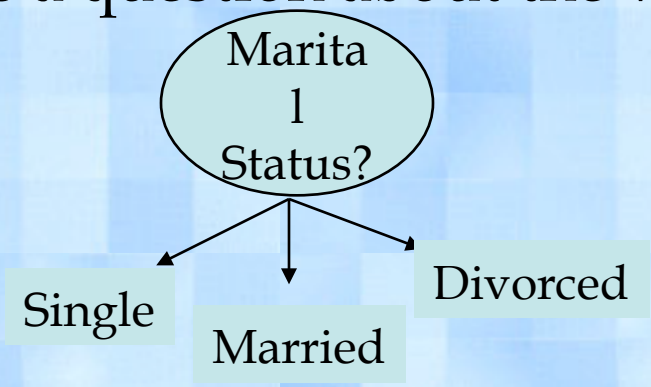


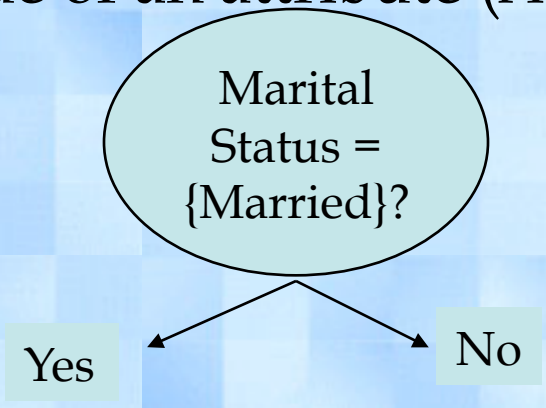
Tree Induction

- Determine how to split the records
  - Use greedy heuristics to make a series of locally optimum decision about which attribute to use for partitioning the data
  - At each step of the greedy algorithm, a test condition is applied to split the data in to subsets with a more homogenous class distribution
    - How to specify test condition for each attribute
    - How to determine the best split
- Determine when to stop splitting
  - A stopping condition is needed to terminate tree growing process. Stop expanding a node
    - if all the instances belong to the same class
    - if all the instances have similar attribute values

Methods For Splitting

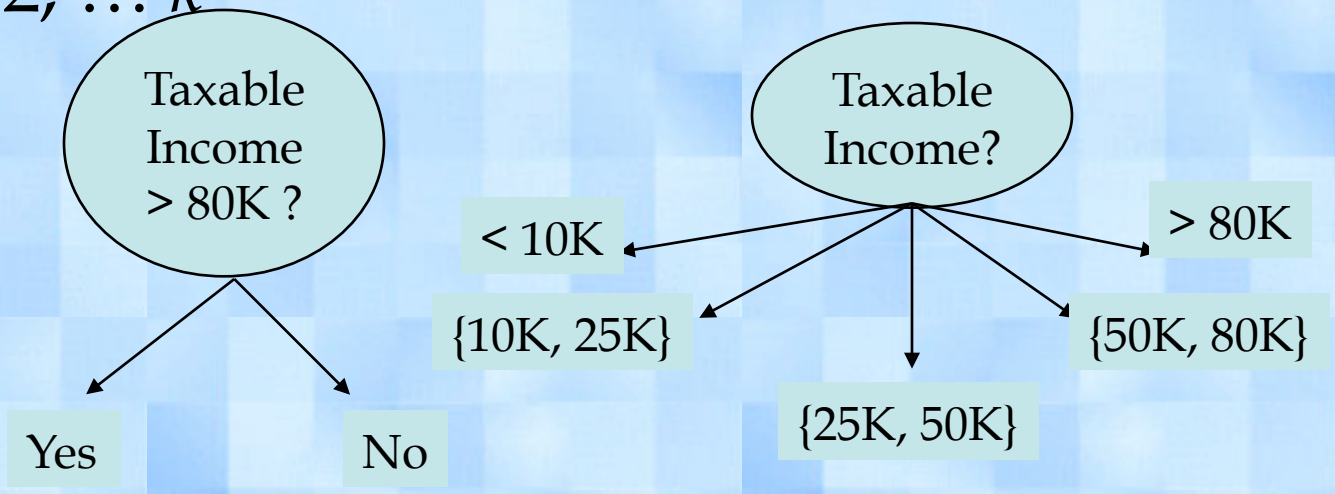
- A key step towards building a decision tree is to find an appropriate test condition for splitting data
- Categorical attributes
  - The test condition can be expressed as an attribute-value pair ($A = v$?), whose outcomes are Yes / No, or as a question about the value of an attribute (A?)





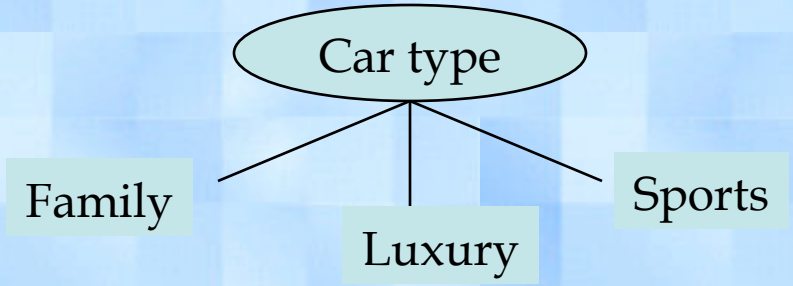
Methods For Splitting

- Continuous attributes
  - The test condition can be expressed in terms of a binary decision ($A < v$?) or ($A >= v$?), whose outcomes are Yes / No, or as a range query whose outcomes are $v_i <= A <= v_{i+1}$, for $i = 1, 2, \ldots k$

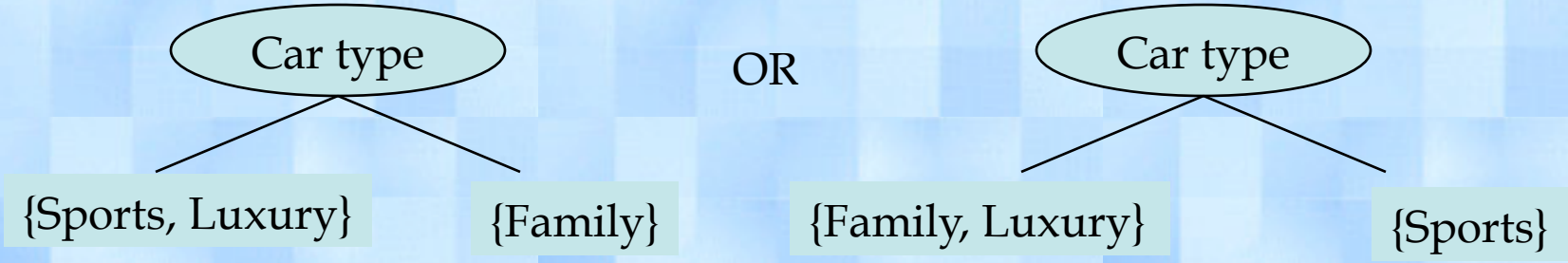


Splitting Based on Nominal Attributes

- Each partition has subset of values signifying it
- Multi-way split: Use as many partitions as distinct values

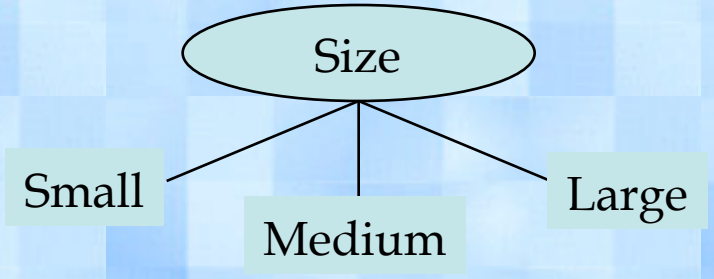


- Binary split: Divides values in to two subsets. Need to find optimal partitioning

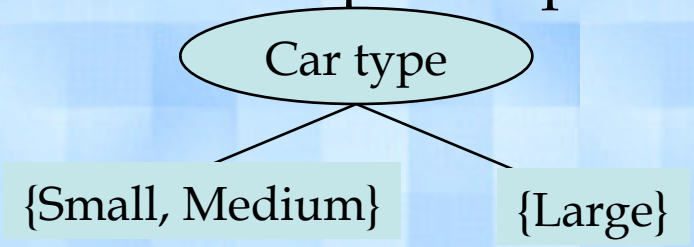


Splitting Based on Ordinal Attributes

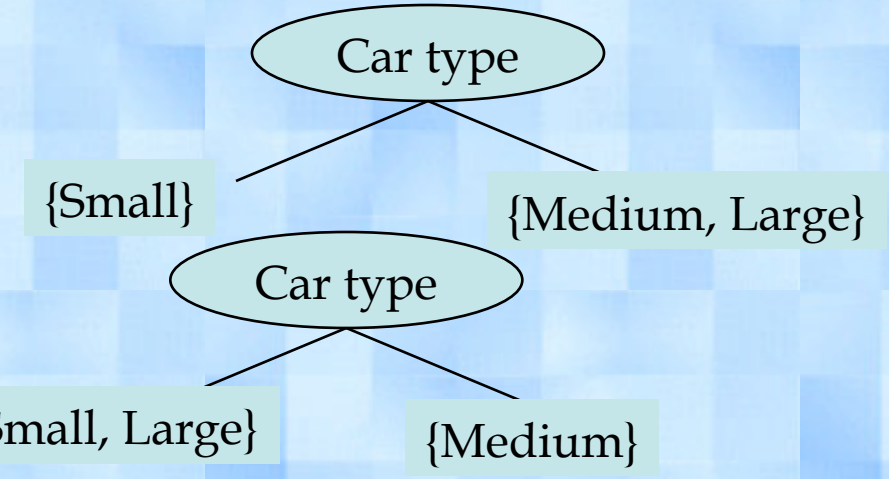
- Each partition has subset of values signifying it
- Multi-way split: Use as many partitions as distinct values



- Binary split: Divide values in to two subsets. Need to find optimal partitioning



OR



- What about this split?

Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization: to form an ordinal category attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing or clustering
  - Binary Decision: ($A < v$) or ($A >= v$)
    - Consider all possible splits and finds the best cut
    - Can be more compute intensive

Splitting Criterion

- There are many test conditions one could apply to partition a collection of records in to smaller subsets
- Various measures are available to determine which test condition provides the best split
  - Gini Index
  - Entropy / Information Gain
  - Classification Error

Splitting Criterion : 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)

  - Measures impurity of 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 of 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.
- Splitting Criterion: Minimize Gini Index of the Split.
- When a node p is split into k partitions (children), the quality of split is computed as,

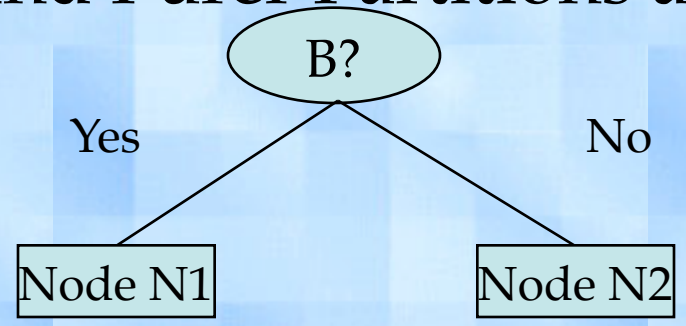
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

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	

	N1	N2
C1	0	6
C2	6	0
Gini=0.000		

	N1	N2
C1	5	1
C2	1	5
Gini=0.278		

	N1	N2
C1	4	2
C2	3	3
Gini=0.486		

	N1	N2
C1	3	3
C2	3	3
Gini=0.500		

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	

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

- 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		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 Criterion : INFO

- Entropy at a given node *t*:

$$Entropy(t) = -\sum_j p(j \mid t) \log p(j \mid t)$$

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

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

C1	0
C2	6

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

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

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 Criterion : 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 of Computing Classification 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

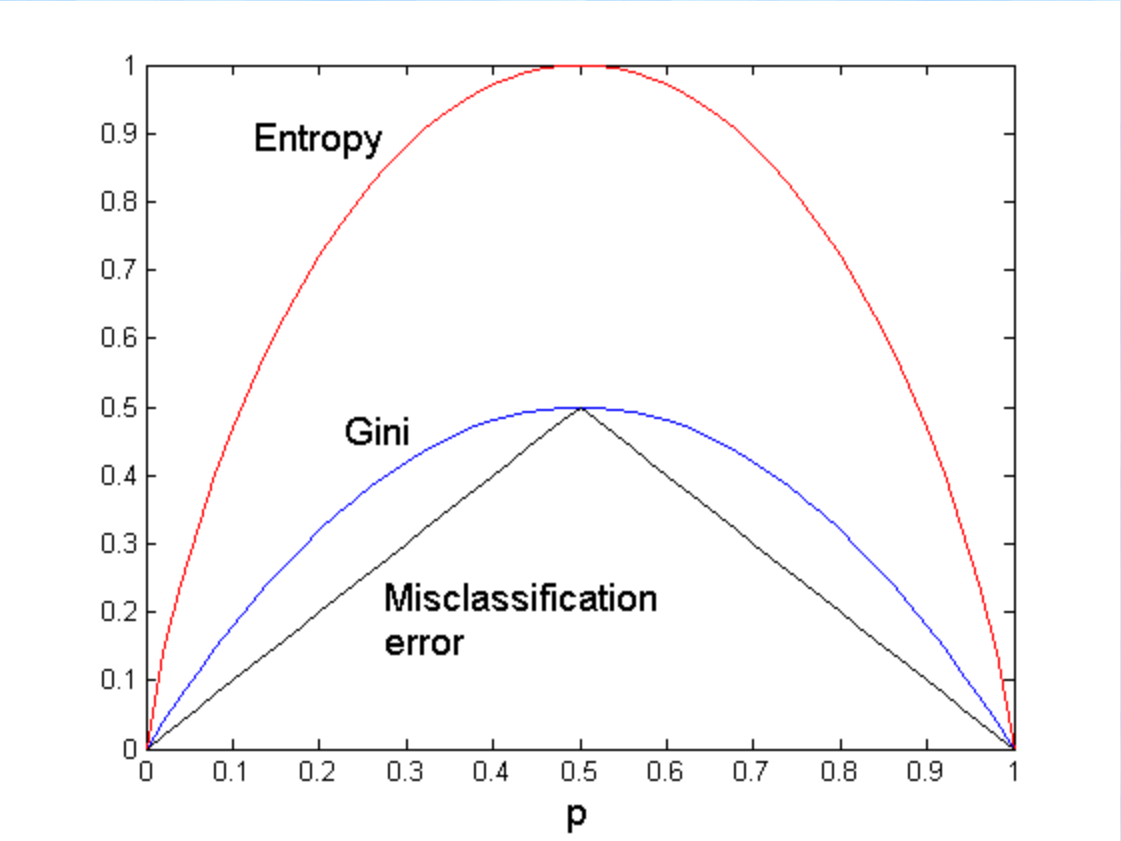
C1	2
C2	4

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

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

Comparison Among Splitting Criteria

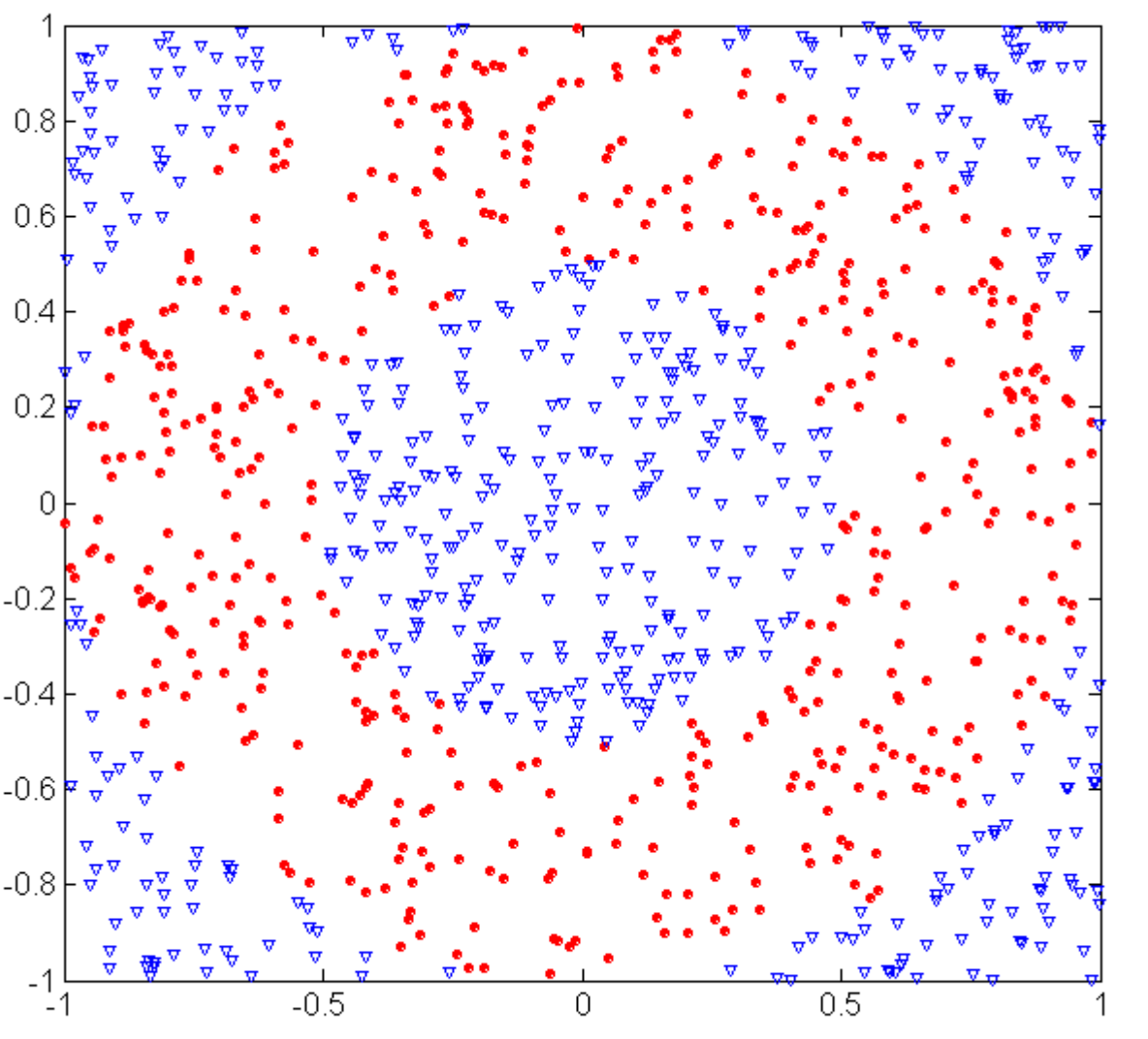
- For a 2-class problem:



Practical Challenges in Classification

- Over-fitting
  - Model performs well on training set, but poorly on test set
- Missing Values
- Data Heterogeneity
- Costs
  - Costs for measuring attributes
  - Costs for misclassification

Example of over-fitting



500 circular and 500 triangular data points.

Circular points:

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

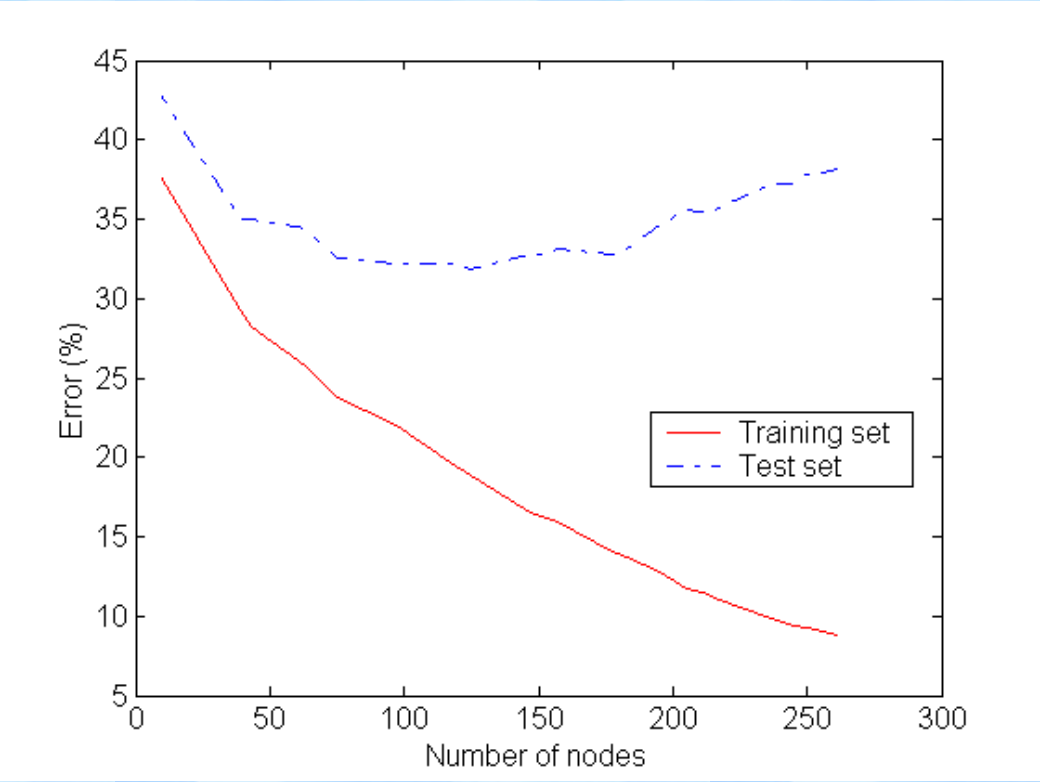
Triangular points:

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

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

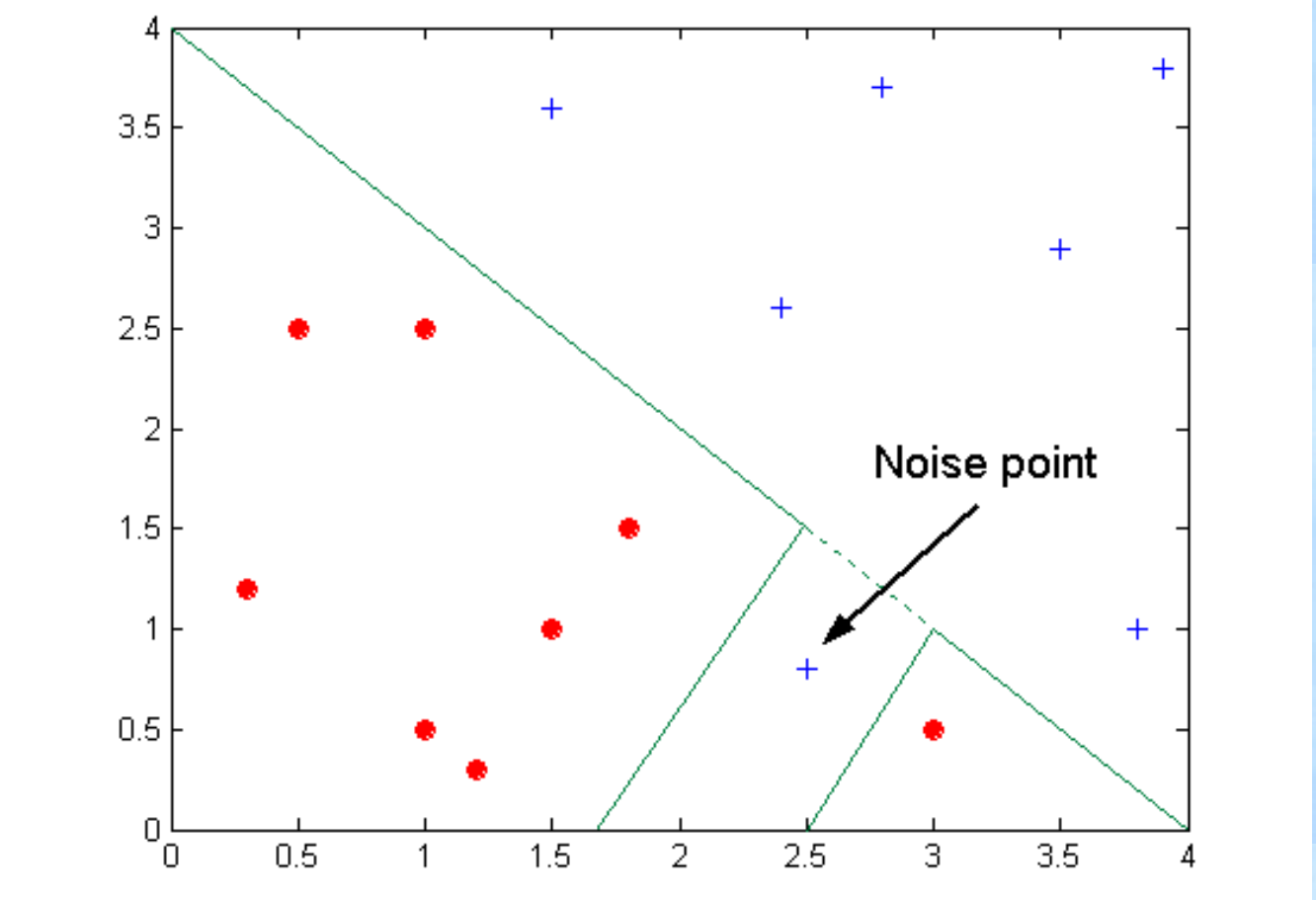
Over-fitting

- If the model is too simple, it may not fit the training and test sets well. If the model is too complex, over- fitting may occur and reduce its ability to generalize beyond training instances



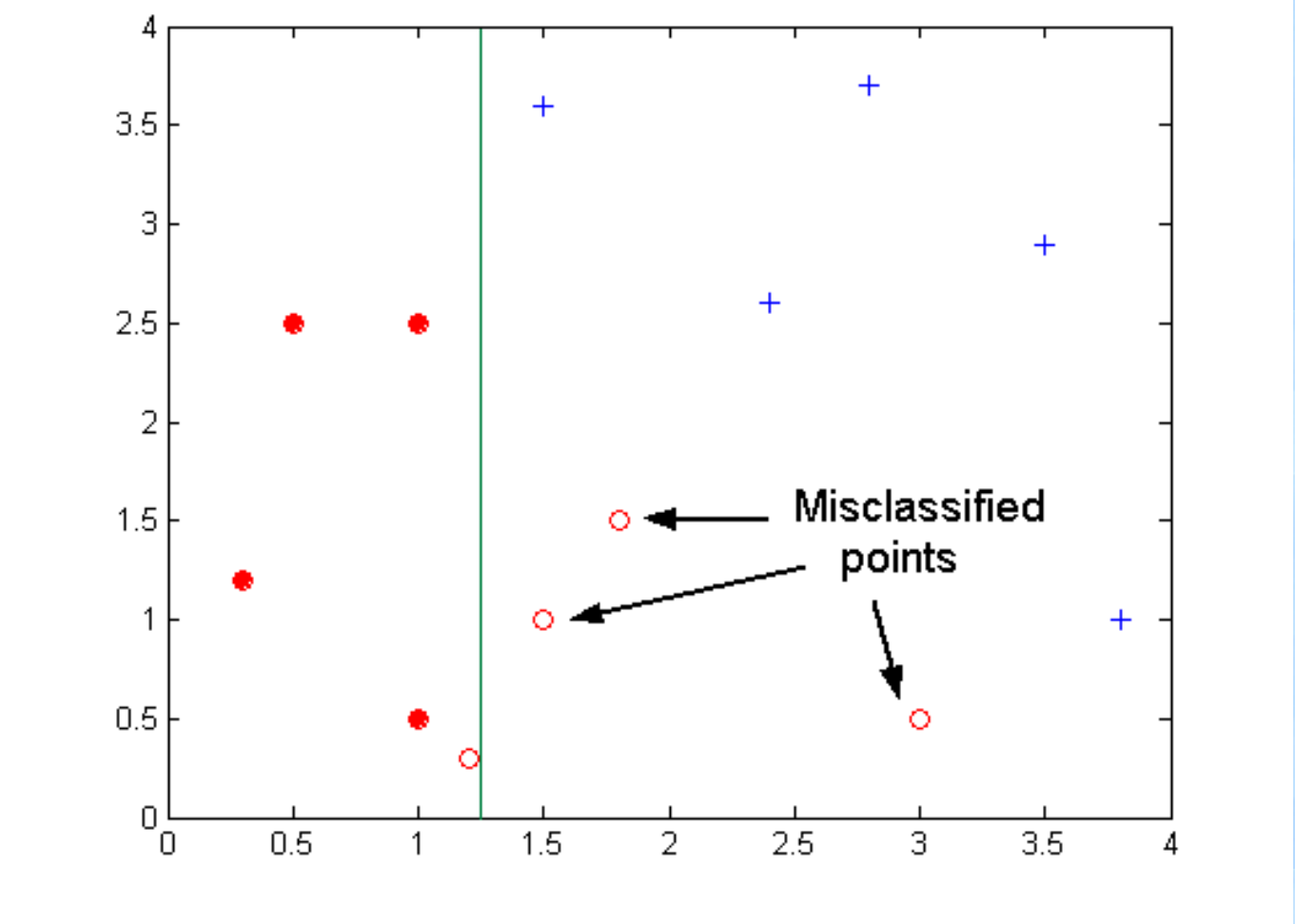
Training Set and Test Set errors for decision trees at different model complexity

Over-fitting due to noise



Decision boundary is distorted by noise point

Over-fitting Due to Insufficient Training



Insufficient number of training points may cause the decision boundary to change

Estimating Generalization Error

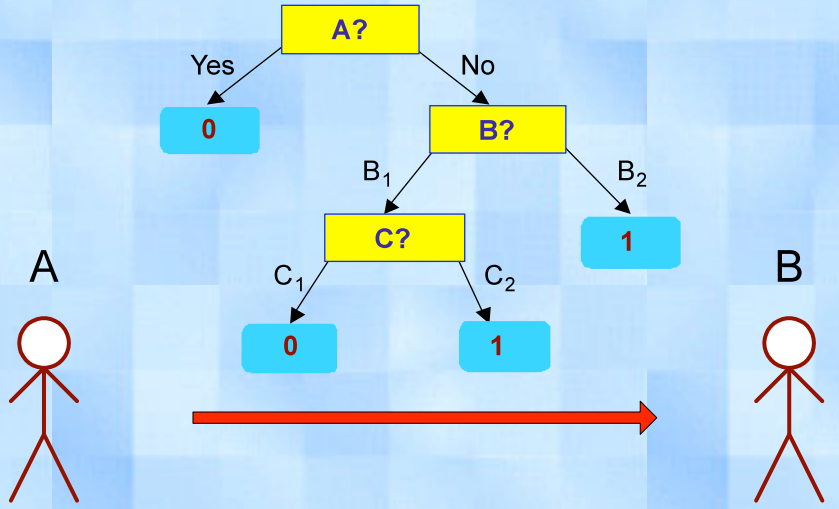
- *Re-substitution errors*: error on training ($\Sigma\, e(t)$)
- *Generalization errors*: error on testing ($\Sigma\, e'(t)$)
- Method for estimating generalization errors:
  - *Optimistic approach*: $e'(t) = e(t)$
  - *Pessimistic approach*:
    - For each leaf node: $e'(t) = (e(t)+0.5)$
    - Total errors: $e'(T) = e(T) + N/2$ (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 + 30×0.5)/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 the data
- Therefore, one should include model complexity when evaluating a model

Minimum Description Length (MDL) Based Tree Pruning

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- 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 Over-fitting

- 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 Over-fitting

- 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

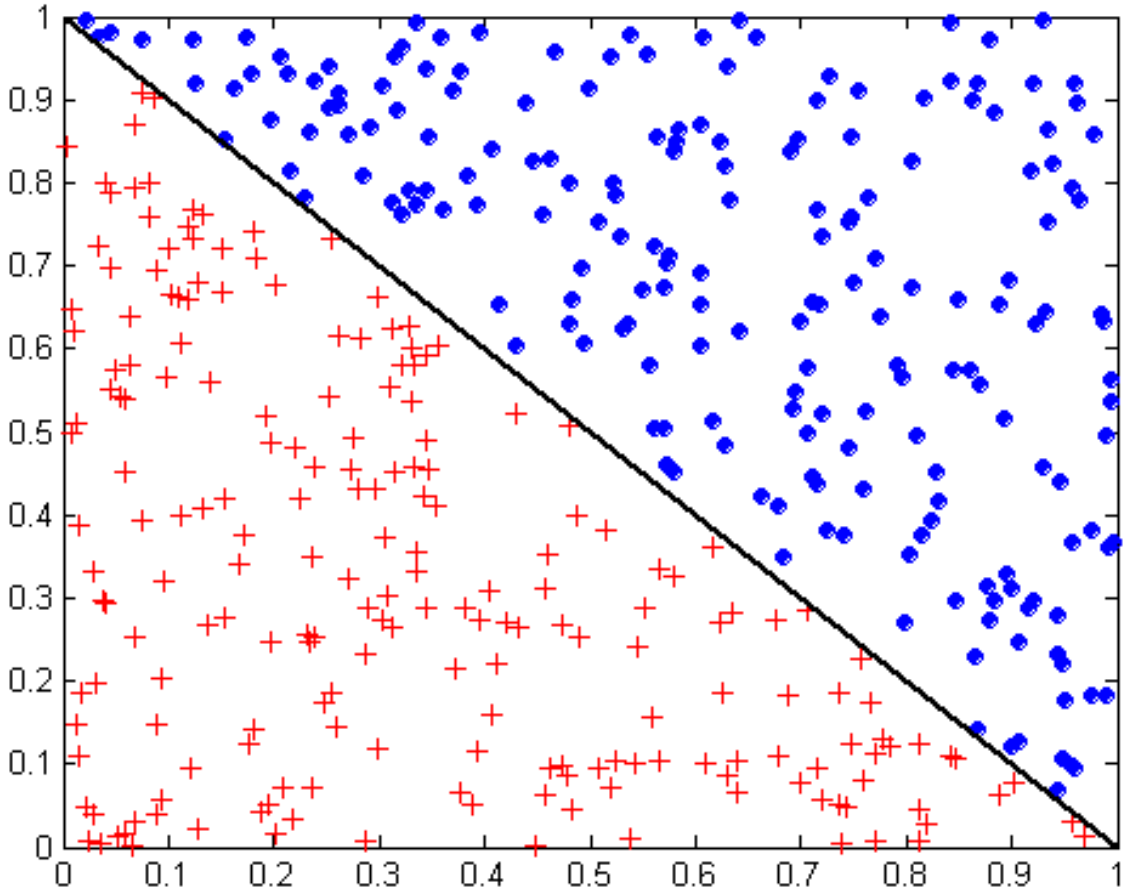
Handling Missing Attribute Values

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

Other Issues

- Data Fragmentation
  - Number of records get smaller as you traverse down the tree
  - Number of records at the leaf nodes could be too small to make any statistically significant decision
- Difficult to interpret large-sized trees
  - Tree could be large because of using a single attribute in the test condition
  - Oblique decision trees
- Tree Replication
  - Subtree may appear at different parts of a decision tree
  - Constructive induction: create new attributes by combining existing attributes

Oblique Decision Trees



Tree Replication Problem