Data Mining
Classification: Basic Concepts and Techniques

Lecture Notes for Chapter 3

Introduction to Data Mining, 2nd Edition

by

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Classification: Definition

- Given a collection of records (**training set**)
  - Each record is by characterized by a tuple $(\boldsymbol{x},y)$, where $\boldsymbol{x}$ is the **attribute set** and y is the **class label**
    - $\boldsymbol{x}$: attribute, predictor, independent variable, input
    - y: class, response, dependent variable, output
- **Task**: Learn a **model** that maps each attribute set $\boldsymbol{x}$ into one of the predefined class labels y
- **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.

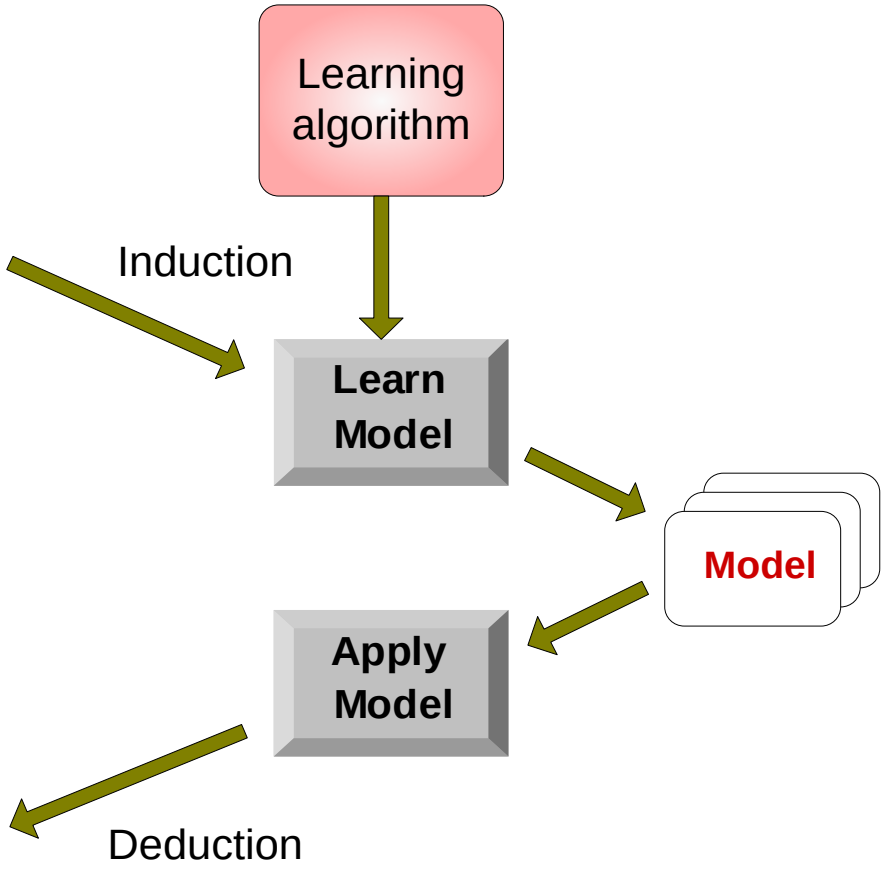
Supervised learning

- Cluster analysis and association rules are not concerned with a specific target attribute.
- **Supervised learning** refers to problems where the value of a target attribute should be predicted based on the values of other attributes.
- Problems with a categorical target attribute are called **classification**, problems with a numerical target attribute are called **regression**.

General Approach for Building Classification Model

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

Examples of Classification Task

Task	Attribute set, $\boldsymbol{x}$	Class label, y
Categorizing email messages	Features extracted from email message header and content	spam or non-spam
Identifying tumor cells	Features extracted from MRI scans	malignant or benign cells
Cataloging galaxies	Features extracted from telescope images	Elliptical, spiral, or irregular-shaped galaxies

Classification Techniques

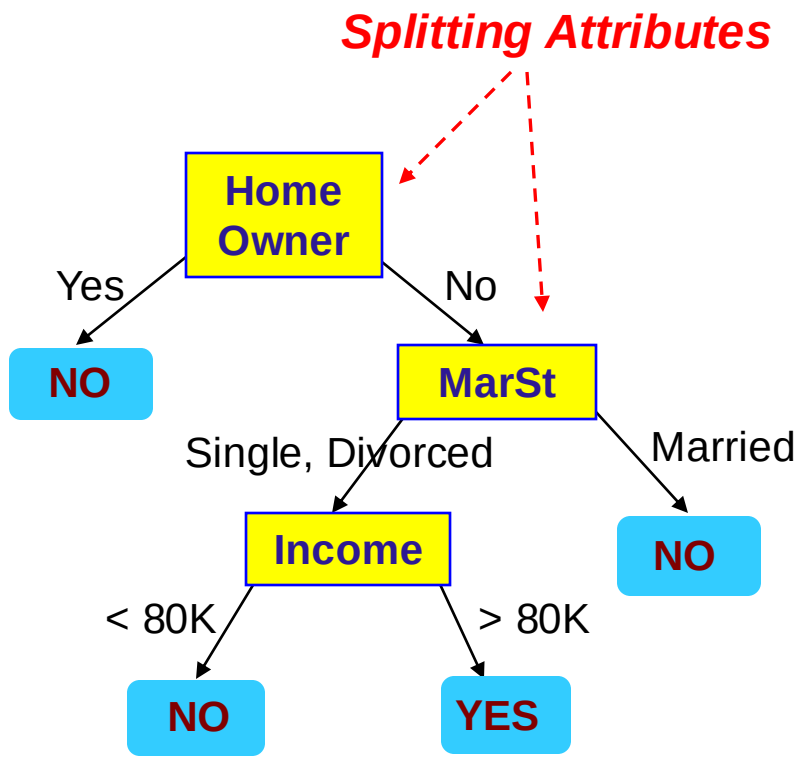
- Base Classifiers
  - Decision Tree based Methods
  - Rule-based Methods
  - Nearest-neighbor
  - Neural Networks
  - Deep Learning
  - Naïve Bayes and Bayesian Belief Networks
  - Support Vector Machines
- Ensemble Classifiers
  - Boosting, Bagging, Random Forests

Example of a Decision Tree

Consider the problem of predicting whether a loan borrower will repay the loan or default on the loan payments.

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
	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



Model: Decision Tree

Another Example of Decision Tree

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
		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
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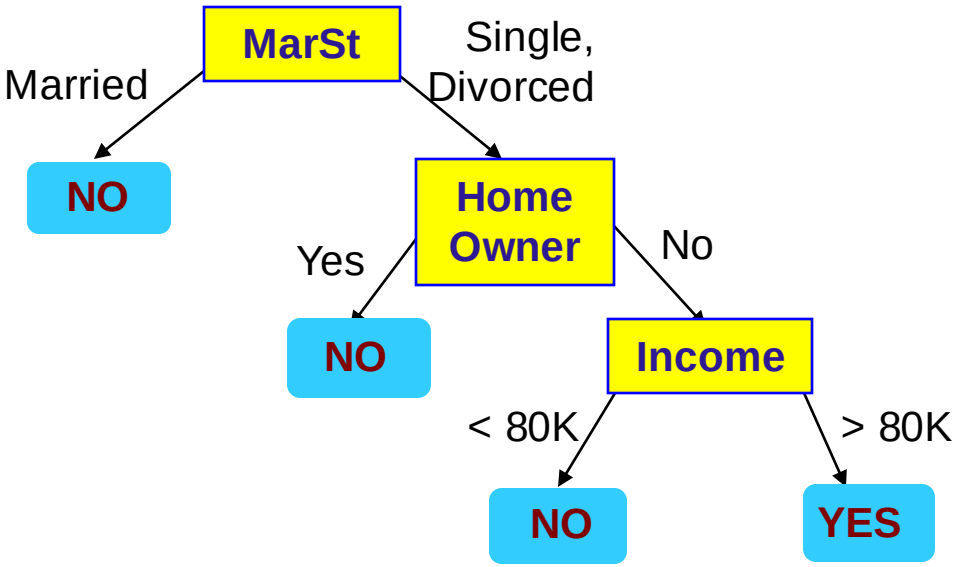
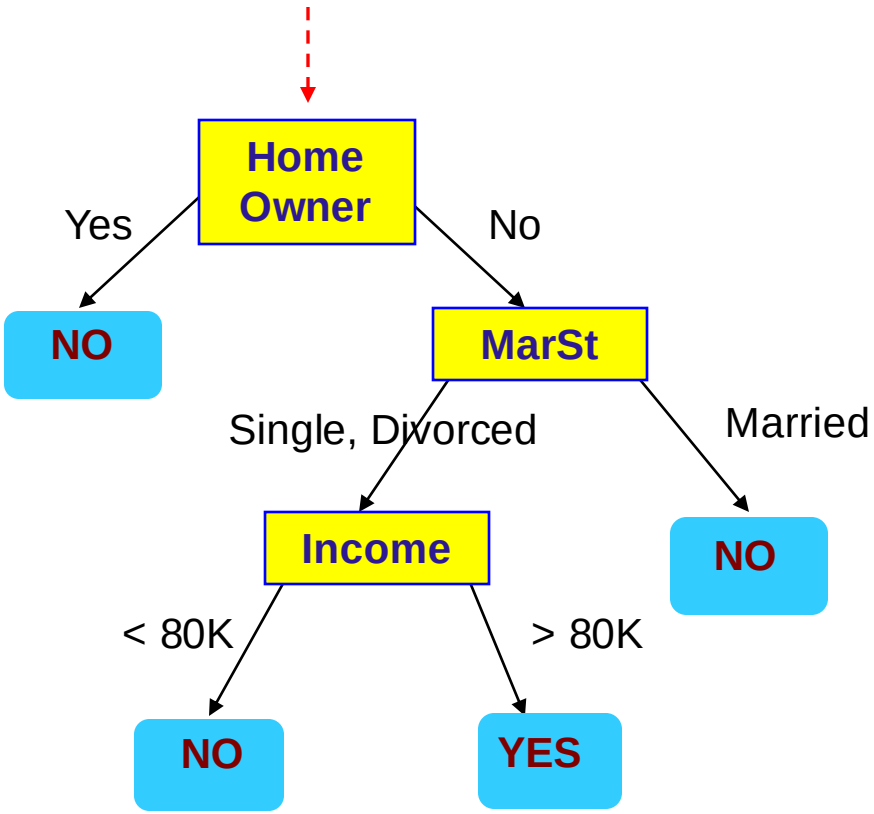
10	No	Single	90K	Yes



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

Apply Model to Test Data

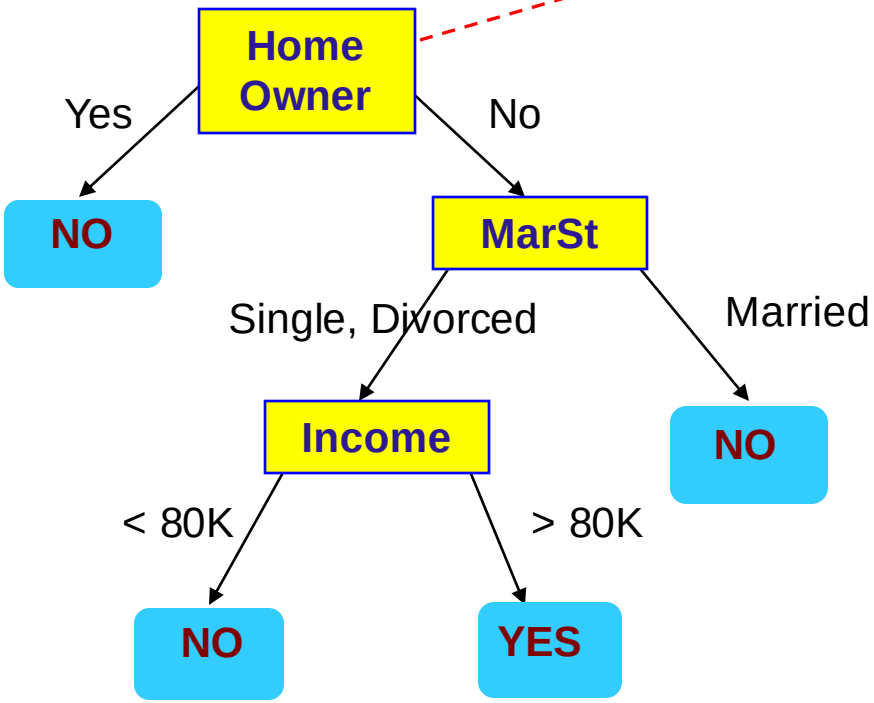
Start from the root of tree.



Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?

Apply Model to Test Data



Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
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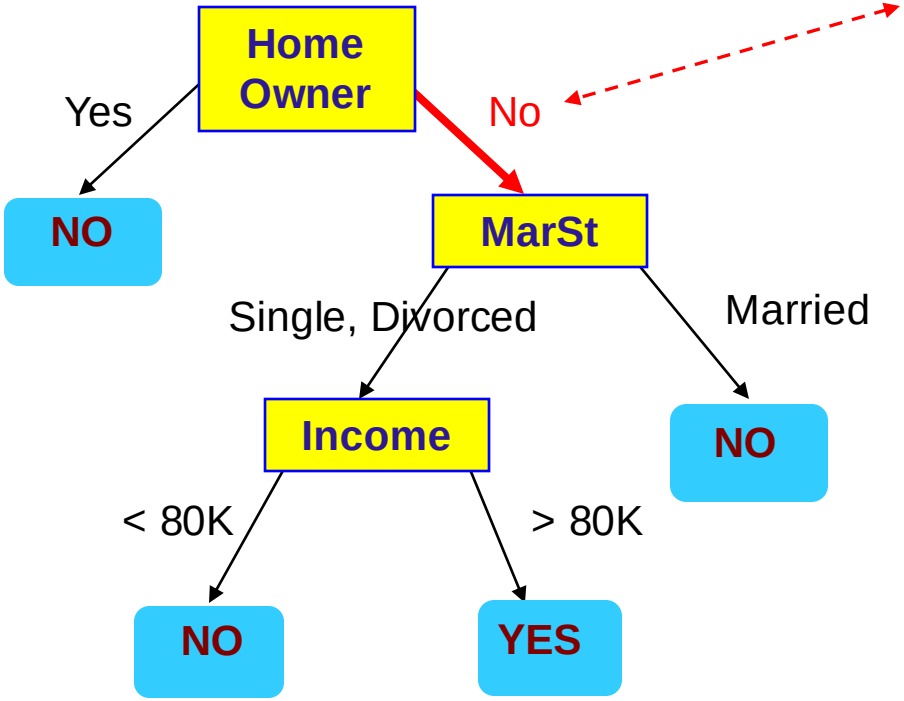
Apply Model to Test Data



Test Data

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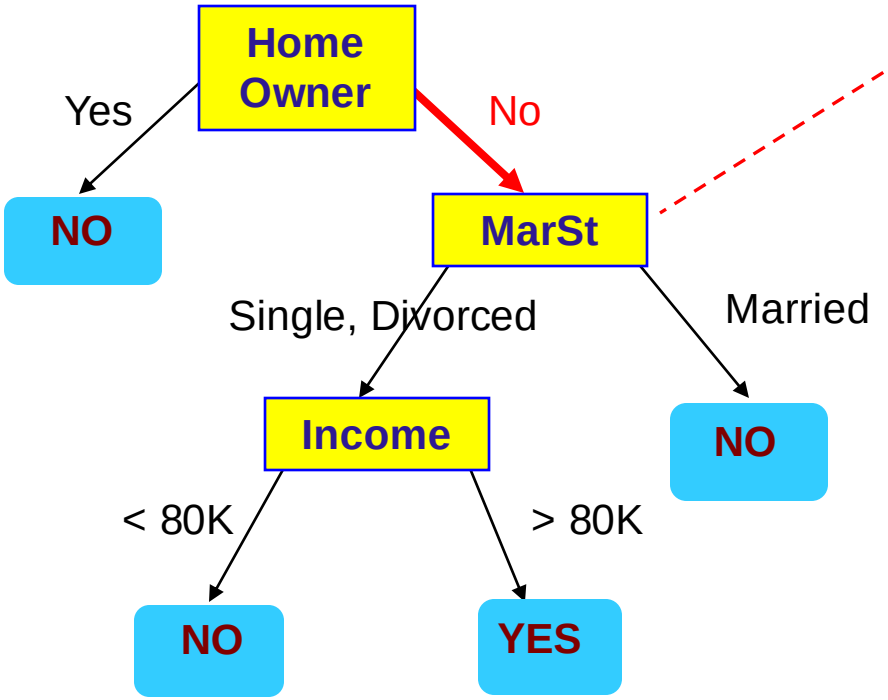

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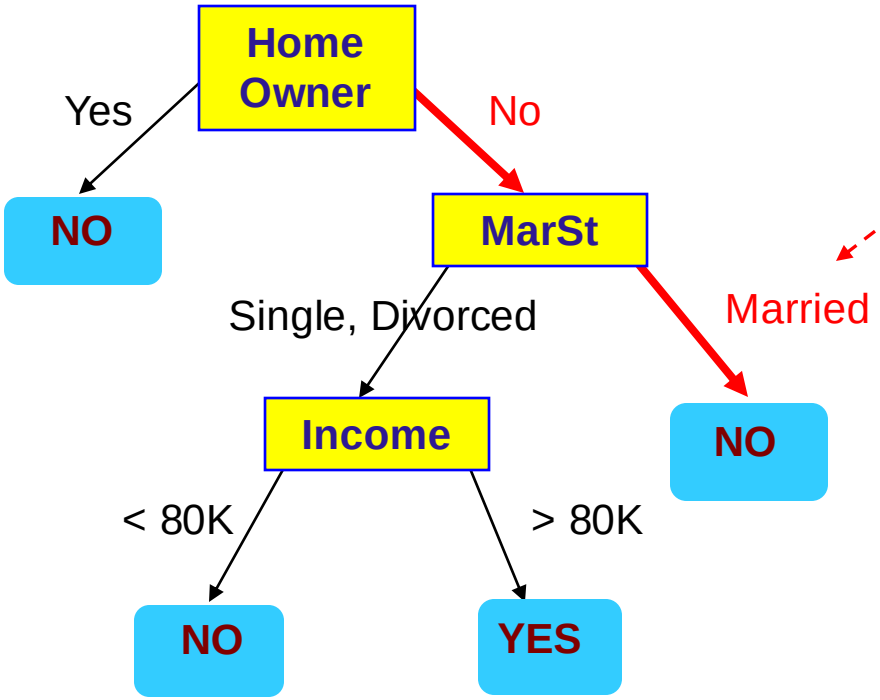

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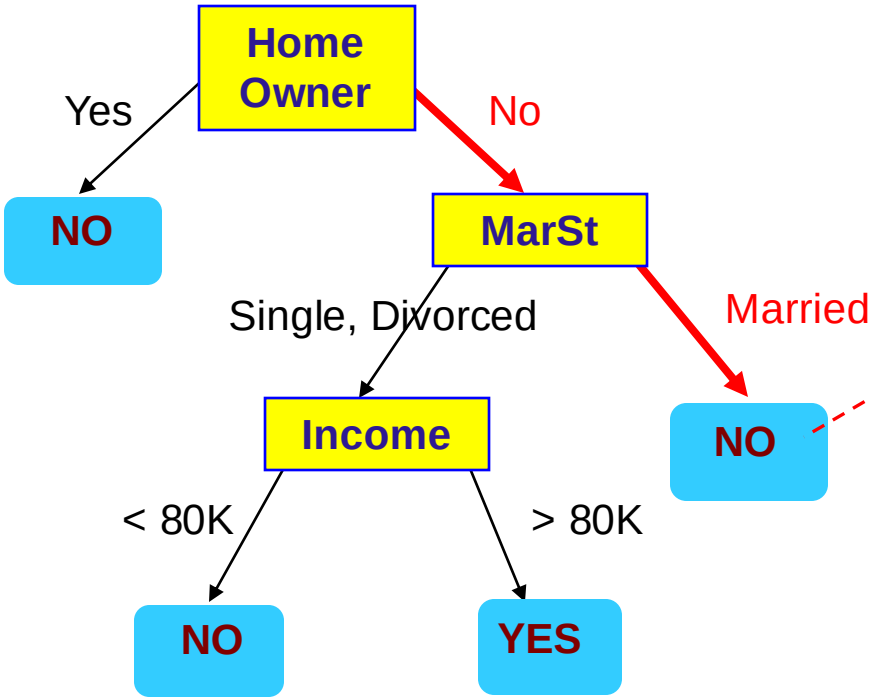

Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?

Assign Defaulted to "No"

Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
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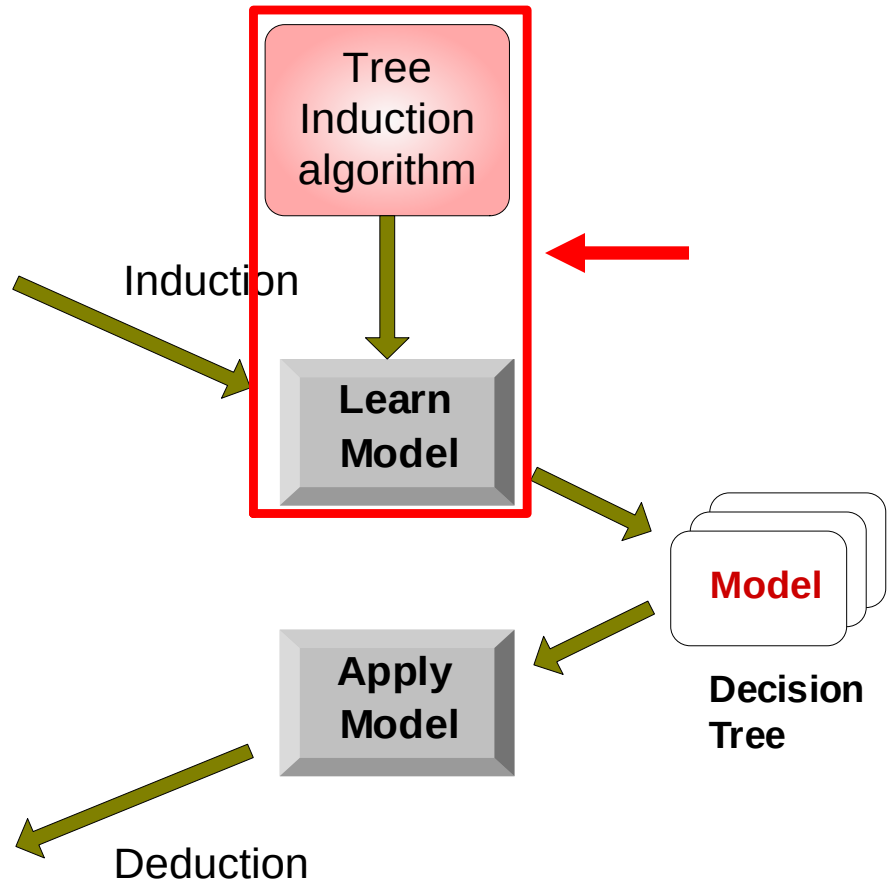
Training Set



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Test Set

Decision Tree Induction

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

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 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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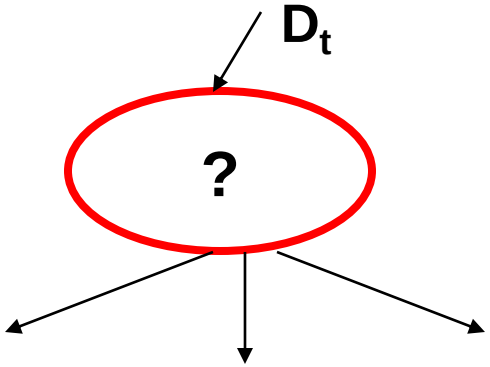

Hunt's Algorithm

Defaulted = No

(7,3)

(a)

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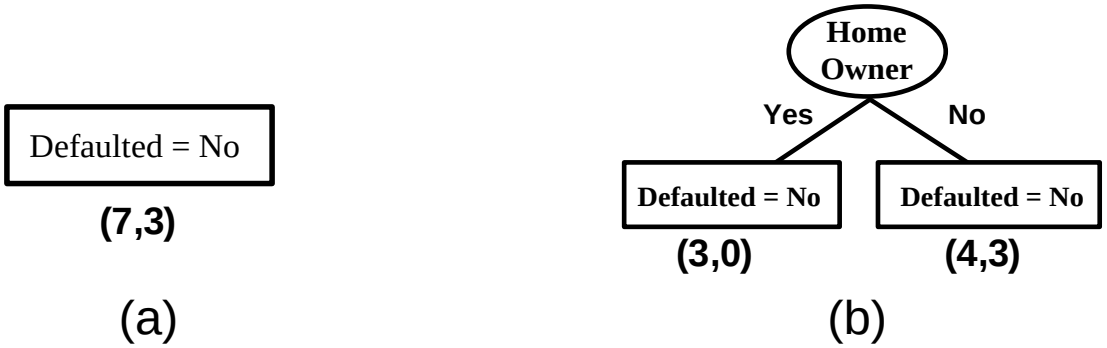
Hunt's Algorithm



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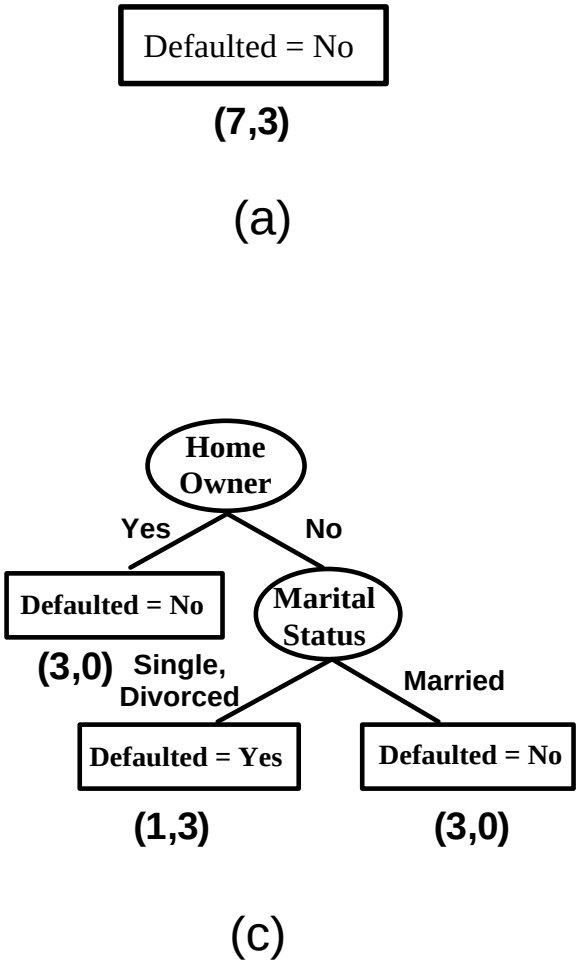
Hunt's Algorithm



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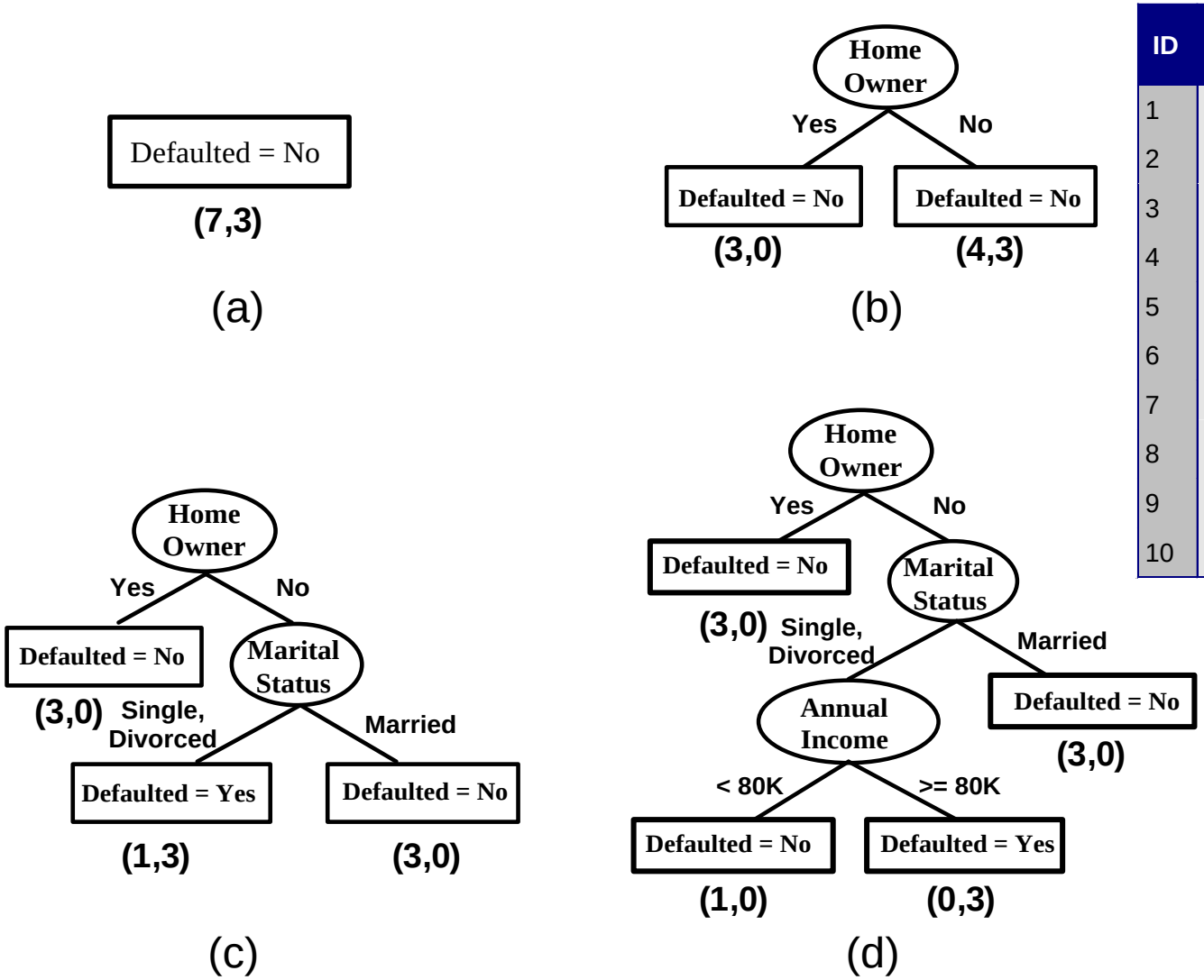
Hunt's Algorithm



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Design Issues of Decision Tree Induction

- **Greedy strategy:**
  - the number of possible decision trees can be very large, many decision tree algorithms employ a heuristic-based approach to guide their search in the vast hypothesis space.
  - **Split the records based on an attribute test that optimizes certain criterion.**

Tree Induction

- **How should training records be split?**
  - Method for specifying test condition
    - depending on attribute types
  - Measure for evaluating the goodness of a test condition
- **How should the splitting procedure stop?**
  - Stop splitting if all the records belong to the same class or have identical attribute values
  - Early termination

How to specify the attribute test condition?

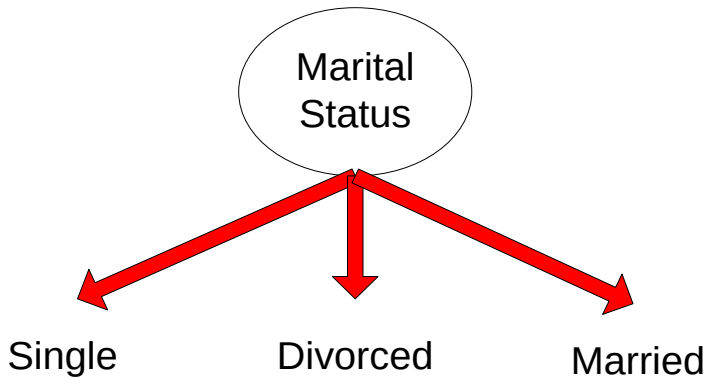
Methods for Expressing Test Conditions

- Depends on attribute types
  - Binary
  - Nominal
  - Ordinal
  - Continuous

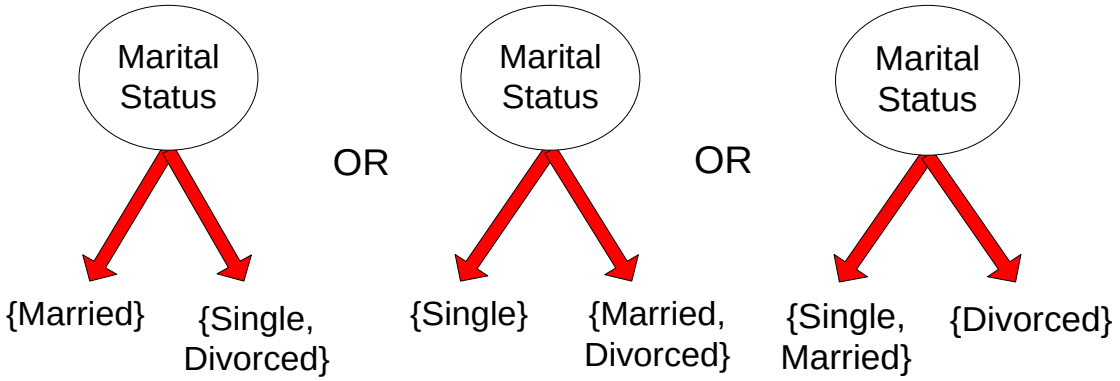
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Test Condition for Nominal Attributes

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

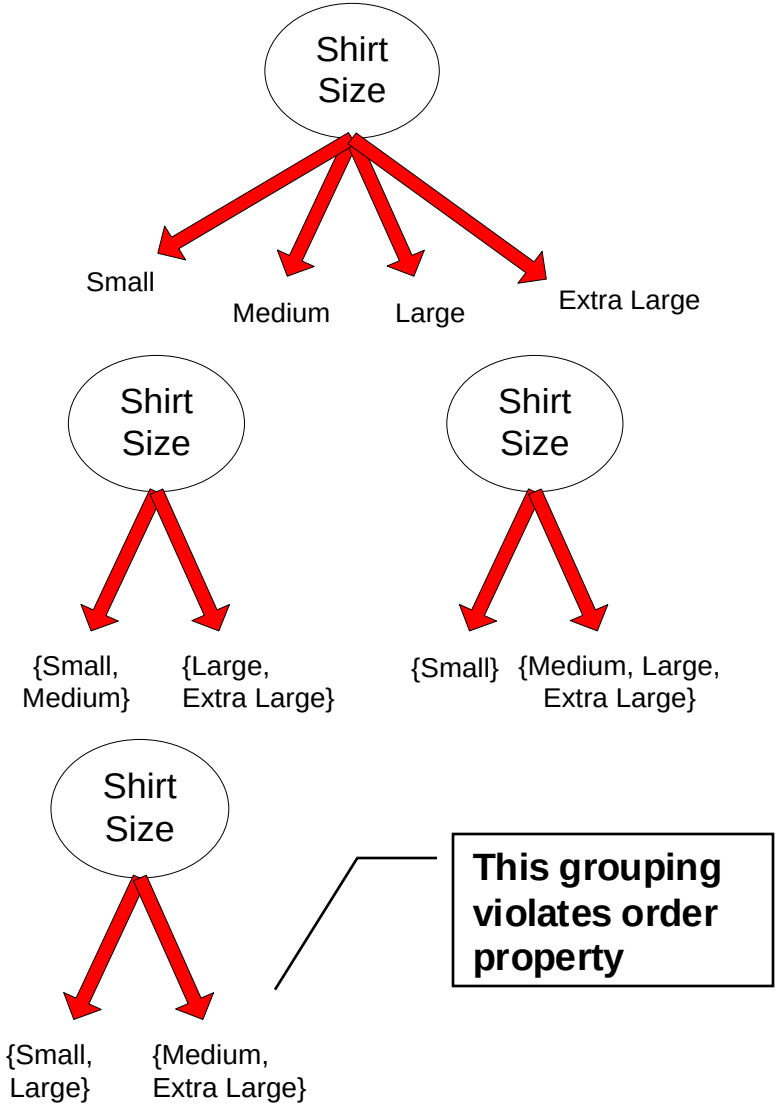


- Binary split:
  - Divides values into two subsets

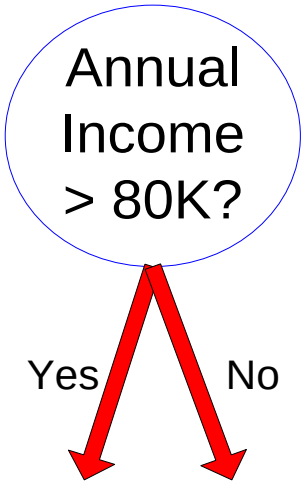


Test Condition for Ordinal Attributes

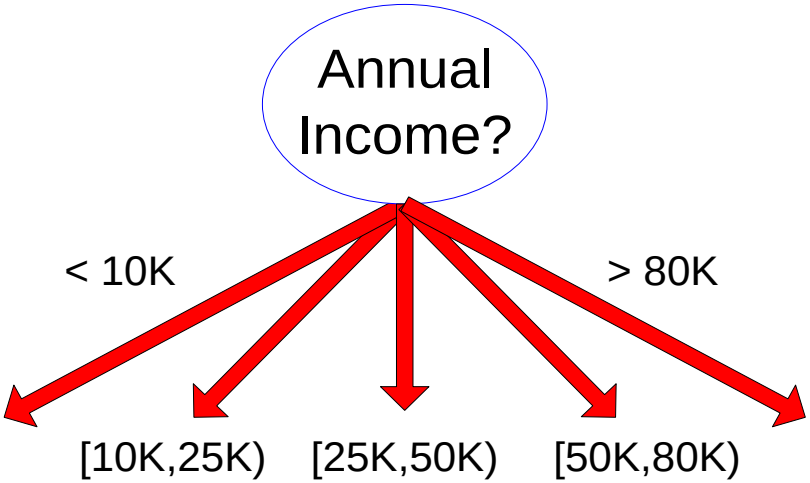
- Multi-way split:
  - Use as many partitions as distinct values
- Binary split:
  - Divides values into two subsets
  - Preserve order property among attribute values



Test Condition for Continuous Attributes



(i) Binary split



(ii) Multi-way split

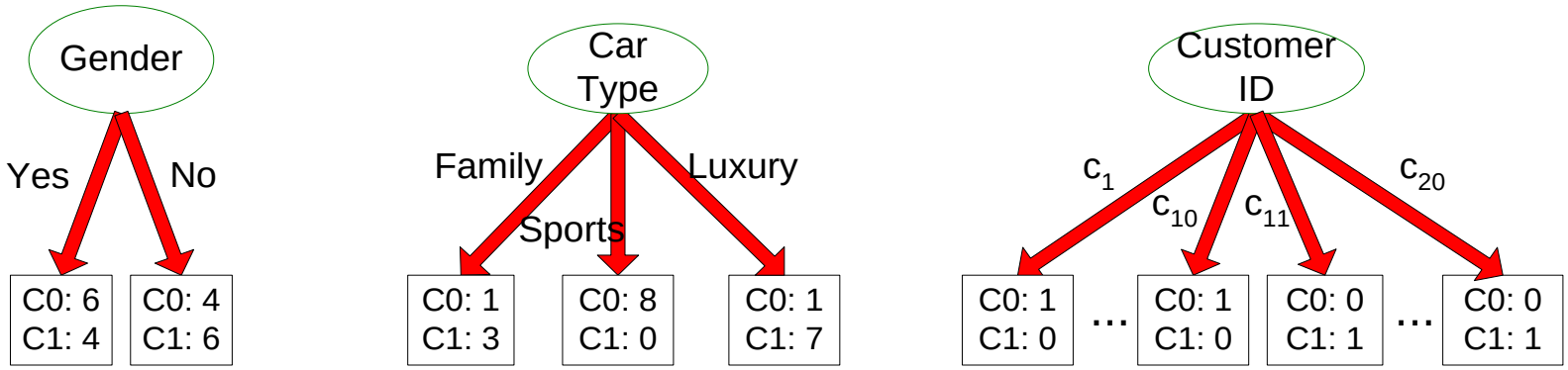
Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
    - Static – discretize once at the beginning
    - Dynamic – repeat at each node
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - consider all possible splits and finds the best cut
    - can be more compute intensive

How to determine the Best Split

Customer Id	Gender	Car Type	Shirt Size	Class
1	M	Family	Small	C0
2	M	Sports	Medium	C0
3	M	Sports	Medium	C0
4	M	Sports	Large	C0
5	M	Sports	Extra Large	C0
6	M	Sports	Extra Large	C0
7	F	Sports	Small	C0
8	F	Sports	Small	C0
9	F	Sports	Medium	C0
10	F	Luxury	Large	C0
11	M	Family	Large	C1
12	M	Family	Extra Large	C1
13	M	Family	Medium	C1
14	M	Luxury	Extra Large	C1
15	F	Luxury	Small	C1
16	F	Luxury	Small	C1
17	F	Luxury	Medium	C1
18	F	Luxury	Medium	C1
19	F	Luxury	Medium	C1
20	F	Luxury	Large	C1

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



Which test condition is the best?

Tree Induction

How to determine the best split?

How to determine the Best Split

- Greedy approach:
  - Nodes with purer / homogeneous class distribution are preferred

- Need a measure of node impurity:

C0: 5 C1: 5	C0: 9 C1: 1
High degree of impurity, **Non-homogeneous**	**Low degree of impurity,** **Homogeneous**

Measures of Node Impurity

- Gini Index

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

- Entropy

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

- Misclassification error

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

Finding the Best Split

1. Compute impurity measure (P) before splitting
2. Compute impurity measure (M) after splitting
   - Compute impurity measure of each child node
   - M is the **weighted impurity** of children
3. Choose the attribute test condition that produces the highest gain

$$\textbf{Gain} = \textbf{P} - \textbf{M}$$

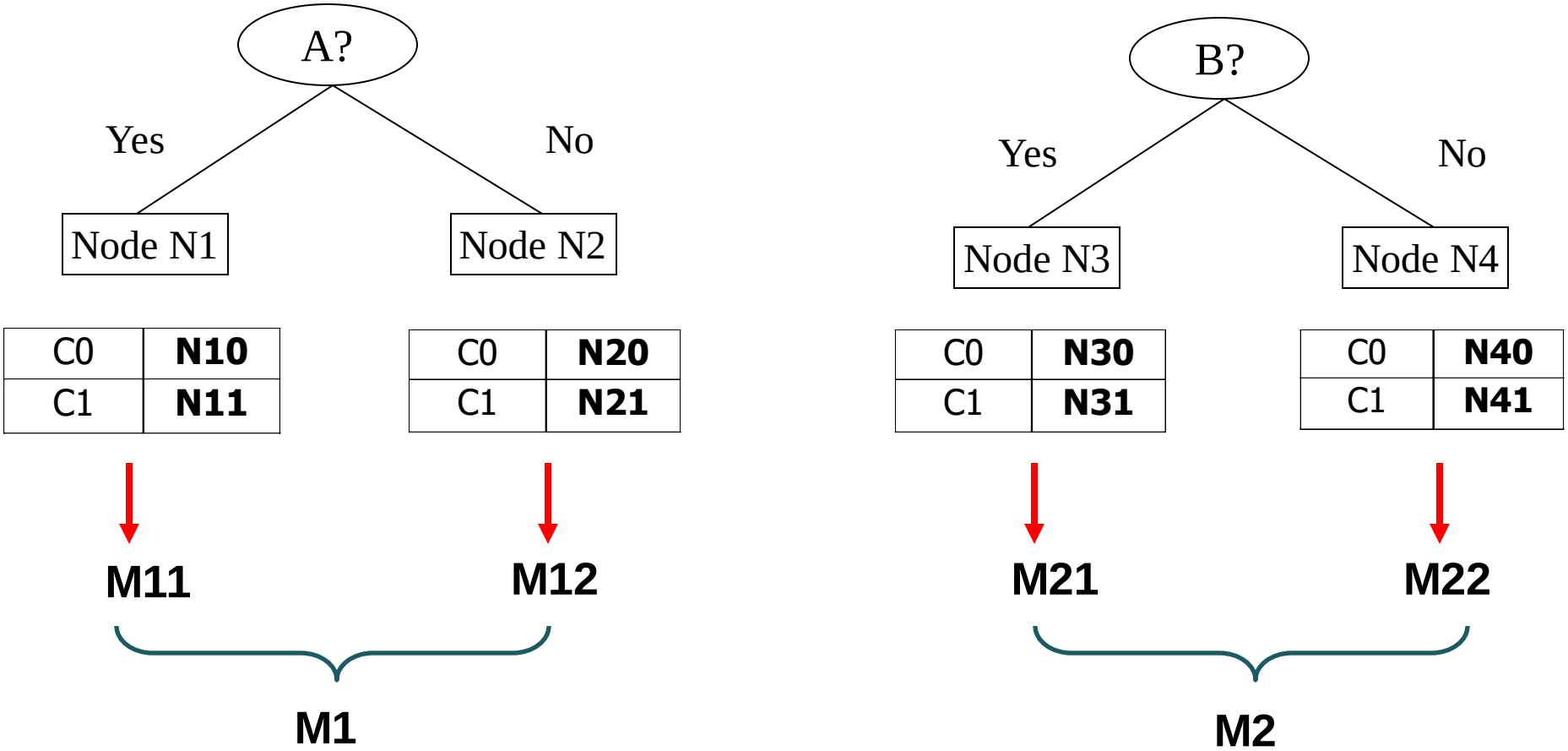
or equivalently, lowest impurity measure after splitting (M)

Finding the Best Split

Before Splitting:

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

→ **P**



Gain = P – M1 vs P – M2

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**

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).

- For 2-class problem (p, 1 – p):
  - GINI = $1 - p^2 - (1 - p)^2 = 2p\,(1-p)$

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	

Computing Gini Index of a Single Node

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

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

Gini Index for a Collection of Nodes

- When a node p is split into k partitions (children)

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

where, n_i = number of records at child i,

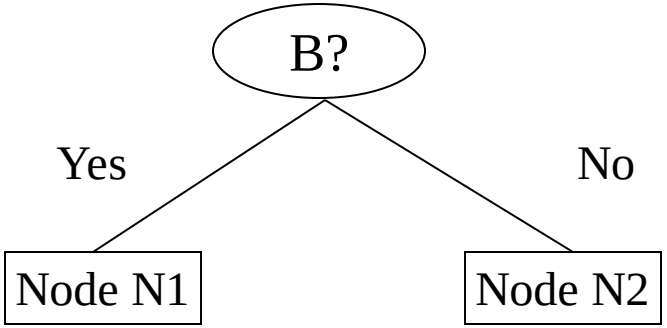
n = number of records at parent node p.

- Choose the attribute that minimizes weighted average Gini index of the children

- Gini index is used in decision tree algorithms such as CART, SLIQ, SPRINT

Binary Attributes: Computing GINI Index

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



	Parent
C1	**7**
C2	**5**
Gini = 0.486	

Gini(N1)
= 1 – $(5/6)^2$ – $(1/6)^2$
= 0.278

Gini(N2)
= 1 – $(2/6)^2$ – $(4/6)^2$
= 0.444

	N1	N2
C1	**5**	**2**
C2	**1**	**4**
Gini=0.361		

Weighted Gini of N1 N2
= 6/12 * 0.278 +
6/12 * 0.444
= 0.361

Gain = 0.486 – 0.361 = 0.125

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	8	1
C2	3	0	7
Gini	0.163		

Two-way split
(find best partition of values)

	CarType	
	{Sports, Luxury}	{Family}
C1	9	1
C2	7	3
Gini	0.468	

	CarType	
	{Sports}	{Family, Luxury}
C1	8	2
C2	0	10
Gini	0.167	

Which of these is the best?

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible **splitting values** = Number of **distinct values**
- Each splitting value has a **count matrix** associated with it
  - Class counts in each of the partitions, A < v and A ≥ v
- Simple method to choose best v
  - For each v, scan the database to gather count matrix and **compute its Gini index**
  - Computationally Inefficient! ($O(N^2)$) Repetition of work.

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9	No	Married	75K	No
10	No	Single	90K	Yes

Annual Income ?

	≤ 80	> 80
Defaulted Yes	0	3
Defaulted No	3	4

Continuous Attributes: Computing Gini Index…

- For efficient computation O(NlogN): 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
	Annual Income									
Sorted Values →	60	70	75	85	90	95	100	120	125	220

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			
	Annual 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	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>

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
	Annual 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														
No							3	4														
Gini							0.343															

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	
	Annual 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	

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	
	Annual 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	

Measure of Impurity: Entropy

- 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).

- 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 quite similar to the GINI index computations

Computing Entropy of a Single Node

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

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

Computing Information Gain After Splitting

- Information Gain:

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

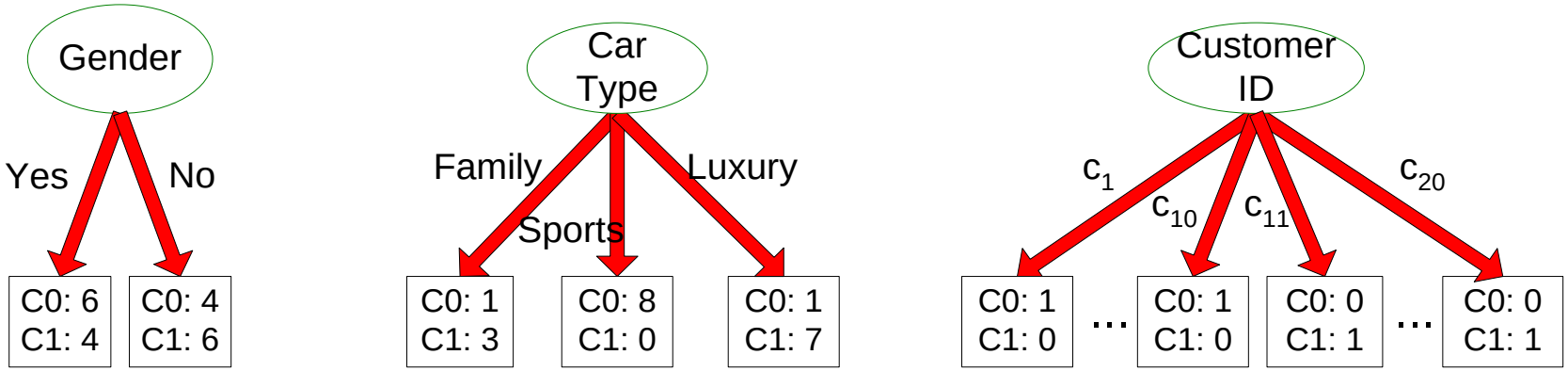
Parent Node, p is split into k partitions;

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 the ID3 and C4.5 decision tree algorithms
  - **Disadvantage**: Tends to prefer splits that result in large number of partitions, each being small but pure.

Problem with large number of partitions

- Node impurity measures tend to prefer splits that result in large number of partitions, each being small but pure



  - Customer ID has **highest information gain** because entropy for all the children is zero
  - **Can we use such a test condition on new test instances?**

Solution

- A **low impurity value alone is insufficient** to find a good attribute test condition for a node
- **Solution**: Consider the **number of children** produced by the splitting attribute in the identification of the best split
- High number of child nodes implies more complexity

- **Method 1**: Generate only binary decision trees
  - This strategy is employed by decision tree classifiers such as CART
- **Method 2**: Modify the splitting criterion to take into account the number of partitions produced by the attribute

Gain Ratio

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO}$$

$$SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions

n_i is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO).
  - **Higher entropy partitioning (large number of small partitions) is penalized!**
- Used in C4.5 algorithm
- Designed to overcome the disadvantage of Information Gain

Gain Ratio

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO}$$

$$SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions

n_i is the number of records in partition i

	CarType		
	Family	Sports	Luxury
C1	1	8	1
C2	3	0	7
Gini	0.163		

SplitINFO = 1.52

	CarType	
	{Sports, Luxury}	{Family}
C1	9	1
C2	7	3
Gini	0.468	

SplitINFO = 0.72

	CarType	
	{Sports}	{Family, Luxury}
C1	8	2
C2	0	10
Gini	0.167	

SplitINFO = 0.97

Measure of Impurity: Classification Error

- Classification error at a node t :

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

  - Maximum (1 - 1/n_c) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0) when all records belong to one class, implying most interesting information

Computing Error of a Single Node

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

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

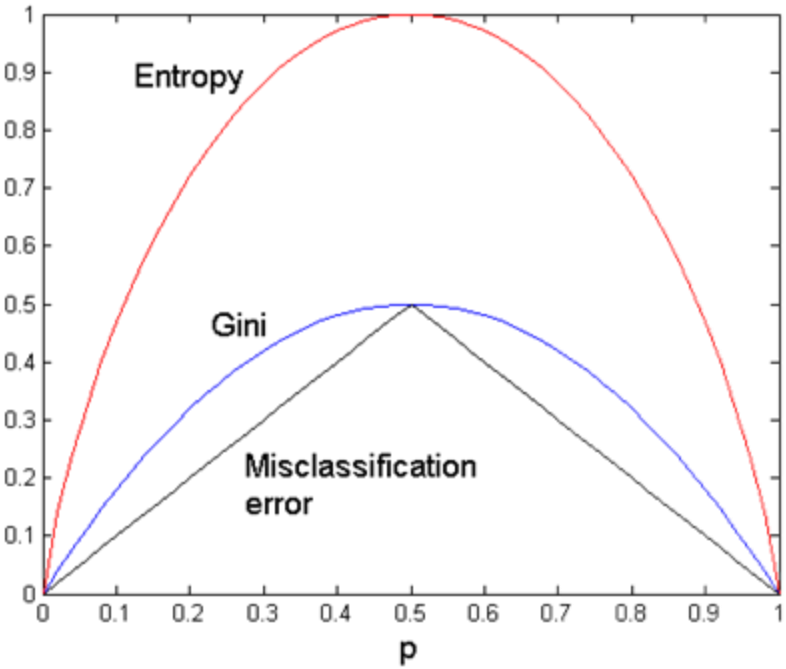
C1	**2**
C2	**4**

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

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

Comparison among Impurity Measures

For a 2-class problem:

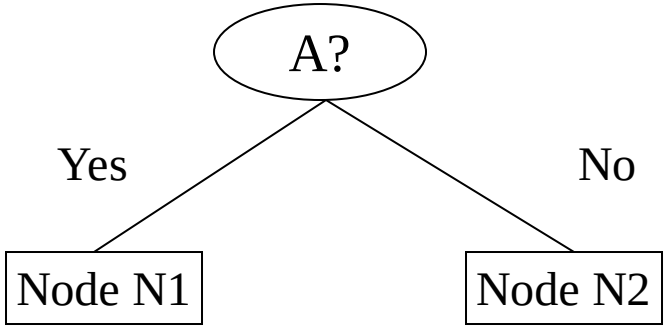


Consistency among the impurity mesures

- if a node N1 has lower entropy than node N2, then the Gini index and error rate of N1 will also be lower than that of N2

The attribute chosen as splitting criterion by the impurity measures can still be different!

Misclassification Error vs Gini Index



	Parent
C1	7
C2	3
Gini = 0.42	

Gini(N1)
= 1 – $(3/3)^2$ – $(0/3)^2$
= 0

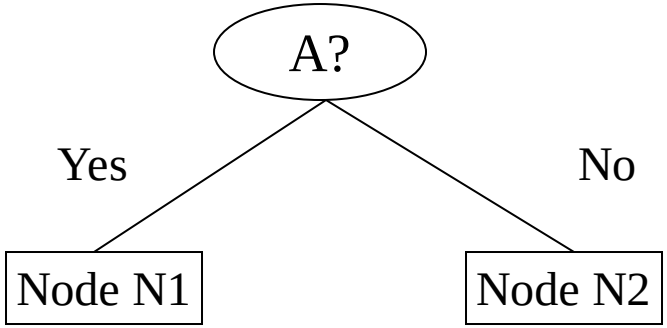
Gini(N2)
= 1 – $(4/7)^2$ – $(3/7)^2$
= 0.489

	N1	N2
C1	3	4
C2	0	3
Gini=0.342		

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

Gini improves but error remains the same!!

Misclassification Error vs Gini Index



	Parent
C1	**7**
C2	**3**
Gini = 0.42	

	N1	N2
C1	**3**	**4**
C2	**0**	**3**
Gini=0.342		

	N1	N2
C1	**3**	**4**
C2	**1**	**2**
Gini=0.416		

Misclassification error for all three cases = 0.3 !

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)

Advantages of Decision Tree

- Easy to interpret for small-sized trees
- Accuracy is comparable to other classification techniques for many simple data sets
- Robust to noise (especially when methods to avoid overfitting are employed)
- **Can easily handle redundant or irrelevant attributes**
- Inexpensive to construct
- Extremely fast at classifying unknown record
- Handle Missing Values

Irrelevant Attributes

- **Irrelevant** attributes are poorly associated with the target class labels, so they have little or no gain in purity
- In case of a **large number** of irrelevant attributes, some of them may be accidentally chosen during the tree-growing process
- Feature selection techniques can help to eliminate the irrelevant attributes during preprocessing

Redundant Attributes

- Decision trees can handle the presence of redundant attributes
- An attribute is **redundant** if it is strongly **correlated** with another attribute in the data
- Since redundant attributes show **similar gains** in purity if they are selected for splitting, **only one** of them will be selected as an attribute test condition in the decision tree algorithm.

Advantages of Decision Tree

- Easy to interpret for small-sized trees
- Accuracy is comparable to other classification techniques for many simple data sets
- Robust to noise (especially when methods to avoid overfitting are employed)
- Can easily handle redundant or irrelevant attributes
- **Inexpensive to construct**
- **Extremely fast at classifying unknown record**
- Handle Missing Values

Computational Complexity

- Finding an optimal decision tree is NP-hard
- Hunt's Algorithm uses a greedy, top-down, recursive partitioning strategy for growing a decision tree
- Such techniques quickly construct a reasonably good decision tree even when the training set size is very large.
- **Construction DT Complexity**: O(M N log N) where M=n. attributes, N=n. instances
- Once a decision tree has been built, **classifying** a test record is **extremely fast**, with a worst-case complexity of O(w), where w is the **maximum depth of the tree.**

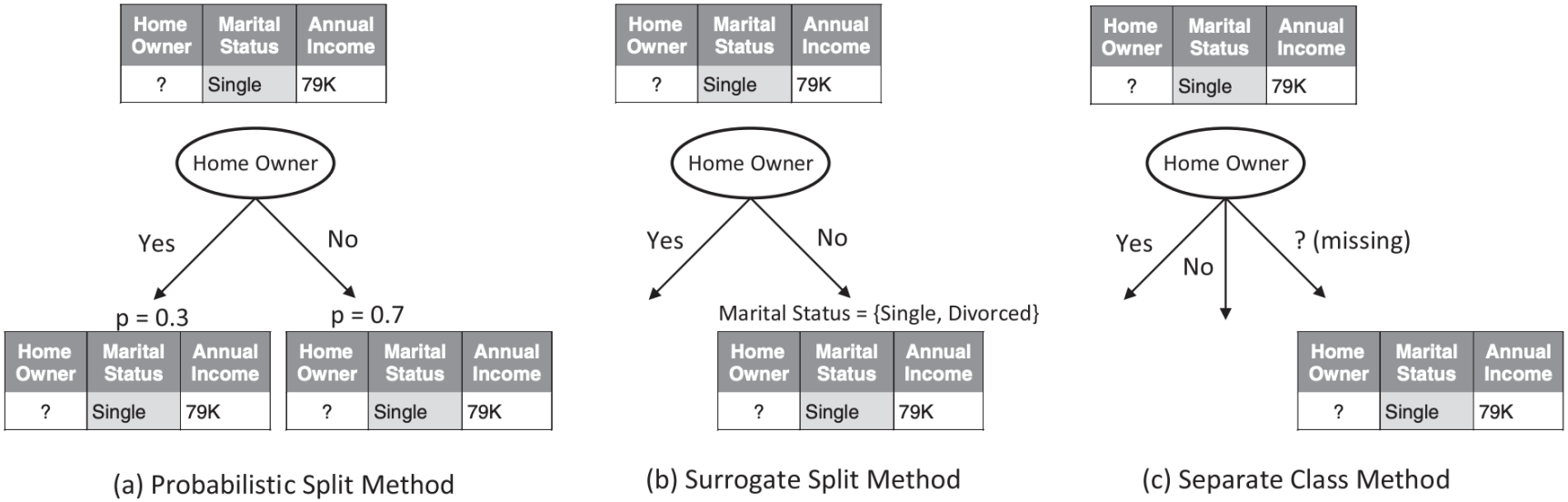
Advantages of Decision Tree

- Easy to interpret for small-sized trees
- Accuracy is comparable to other classification techniques for many simple data sets
- Robust to noise (especially when methods to avoid overfitting are employed)
- Can easily handle redundant or irrelevant attributes
- Inexpensive to construct
- Extremely fast at classifying unknown record
- **Handle Missing Values**

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

Handling missing values in training



(a) Probabilistic Split Method

(b) Surrogate Split Method

(c) Separate Class Method

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

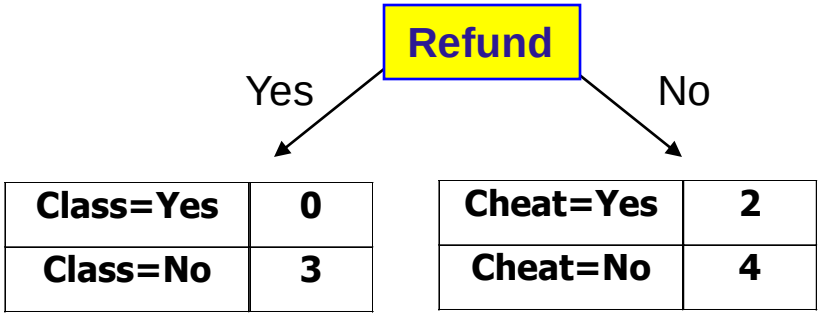
Entropy(Refund=No)
= -(2/6)log(2/6) – (4/6)log(4/6) = 0.9183

Entropy(Children)
= 0.3 (0) + 0.6 (0.9183) = 0.551

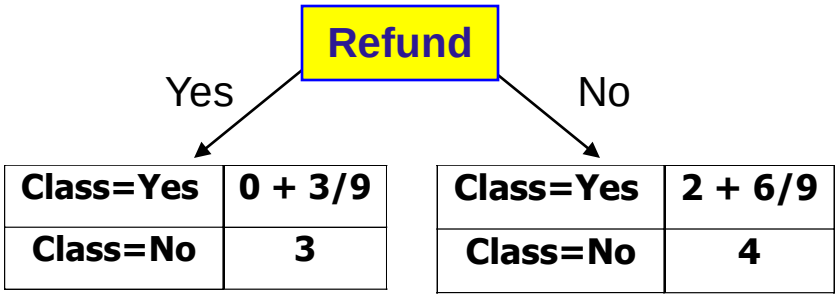
Gain = 0.8813 – 0.551 = 0.3303

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



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



Probability that Refund=Yes is 3/9

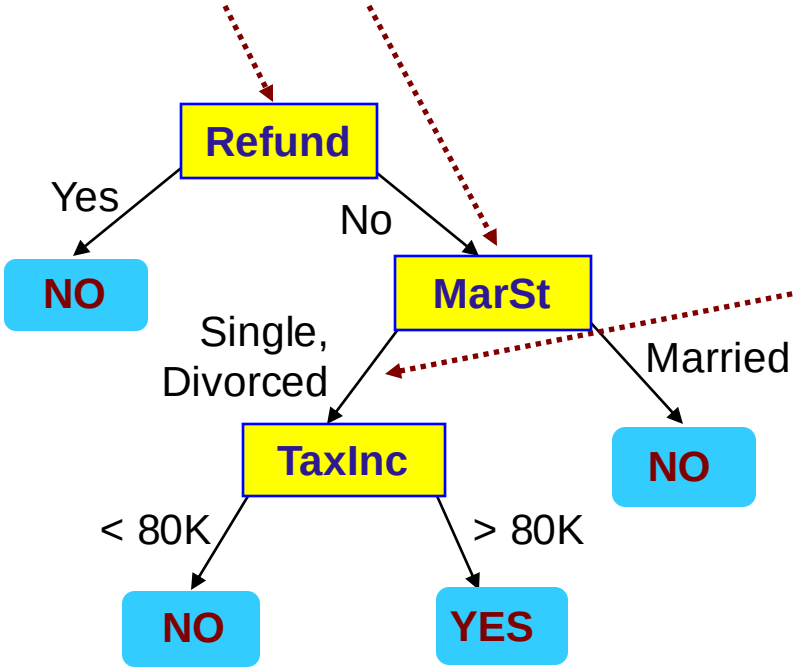
Probability that Refund=No is 6/9

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

Probabilistic split method (C4.5)

Probability that Marital Status = Married is 3.67/6.67

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

Algorithms: ID3, C4.5, C5.0, CART

- **ID3** uses the Hunt's algorithm with information gain criterion and gain ratio

- **C4.5** improves **ID3**
  - Needs entire data to fit in memory
  - Handles missing attributes and continuous attributes
  - Performs tree post-pruning
  - **C5.0** is the current commercial successor of ***C4.5***
  - Unsuitable for Large Datasets

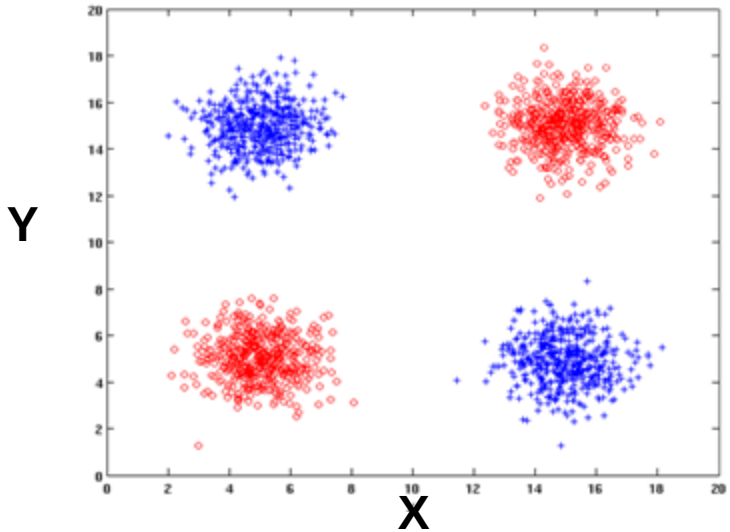
- **CART** builds multivariate decision (binary) trees

Disadvantages

- Space of possible decision trees is exponentially large.
- Greedy approaches are often unable to find the best tree.
- Does not take into account **interactions** between attributes
- Each decision boundary involves **only a single attribute**

Handling interactions

Interacting attributes: able to distinguish between classes when used together, but individually they provide little or no information.



+ : 1000 instances

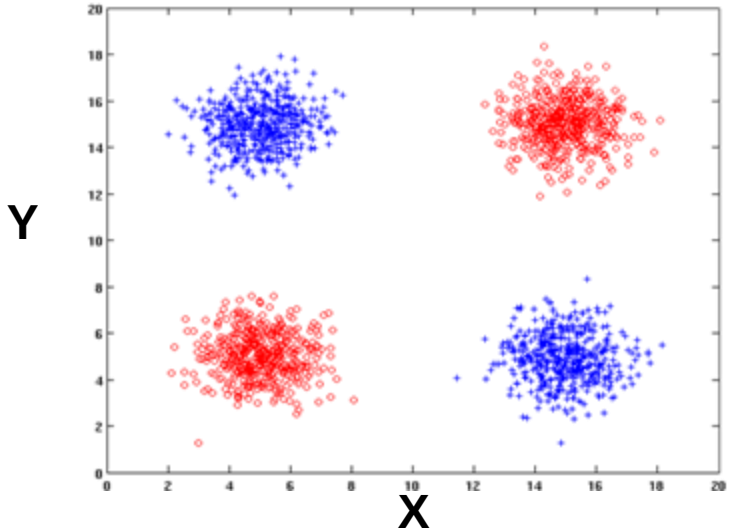
o : 1000 instances

Test Condition:
X ≤ 10 and Y ≤ 10

Entropy (X) : 0.99
Entropy (Y) : 0.99

No reduction in the impurity measure when used individually

Handling interactions



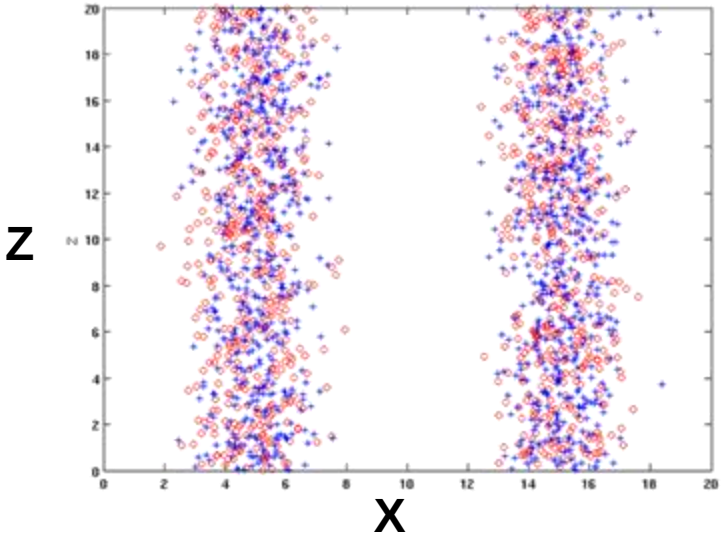
+ : 1000 instances

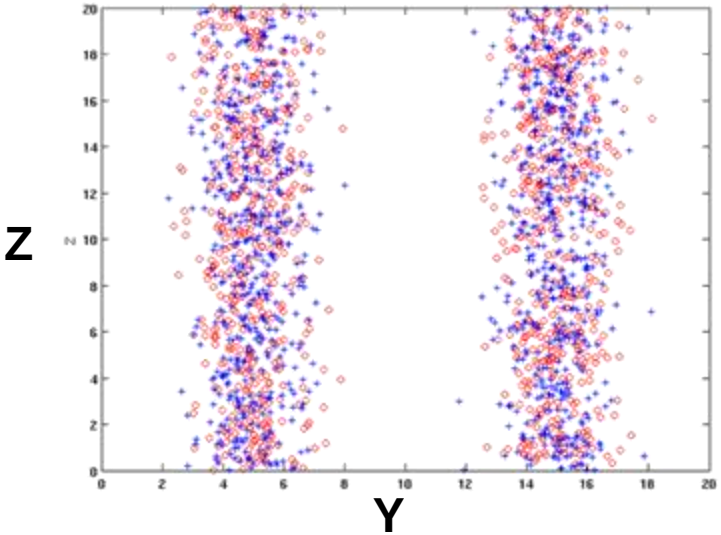
o : 1000 instances

Adding Z as a noisy attribute generated from a uniform distribution

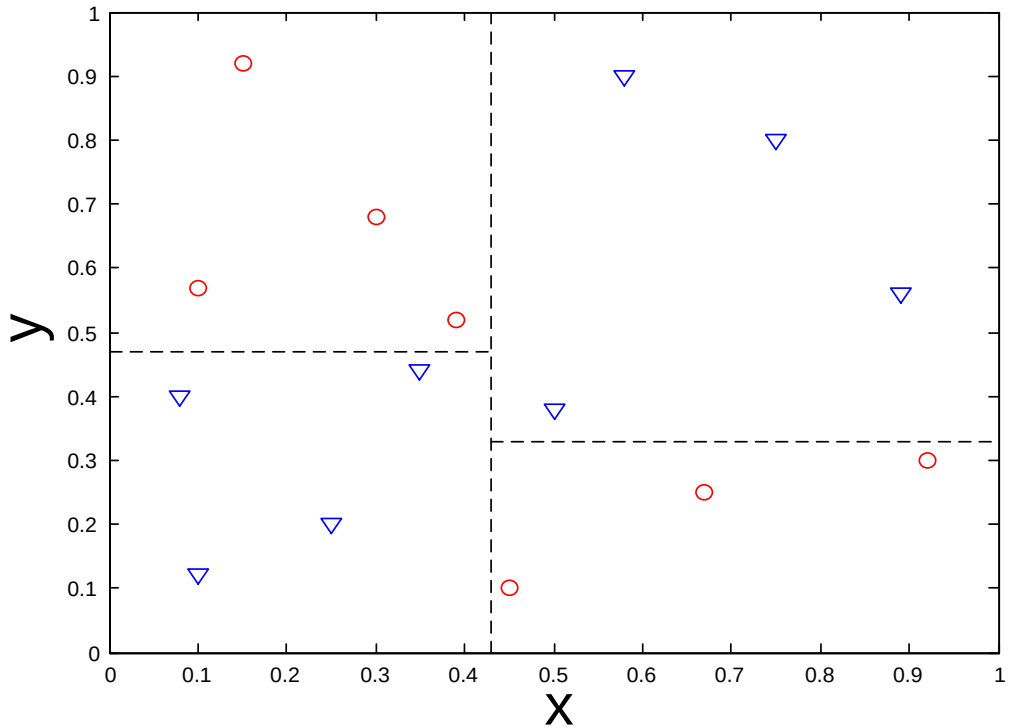
Entropy (X) : 0.99
Entropy (Y) : 0.99
Entropy (Z) : 0.98

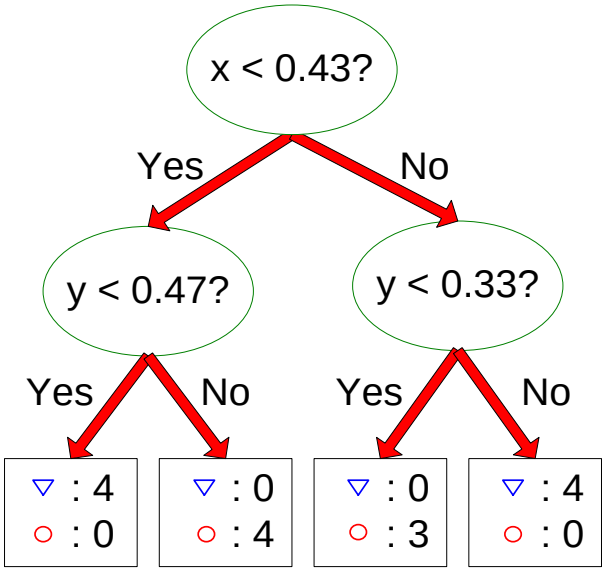
Attribute Z will be chosen for splitting!





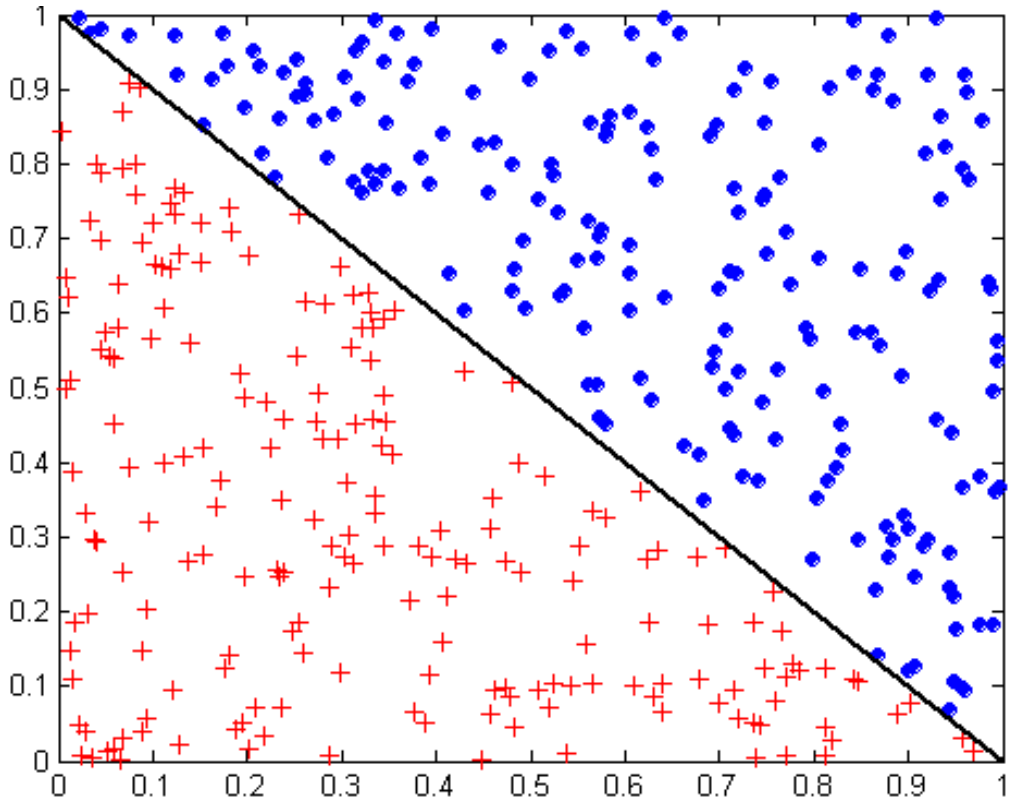
Decision Boundary

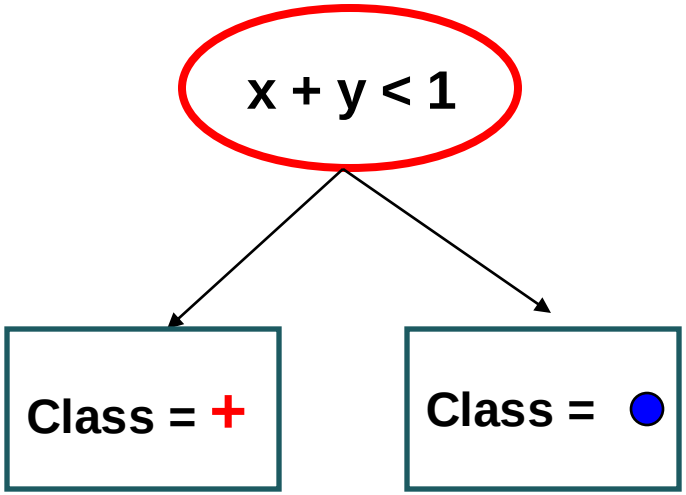




- Border line between two neighboring regions of different classes is known as **decision boundary**
- Decision boundary is **parallel to axes** because test condition involves a single attribute at-a-time

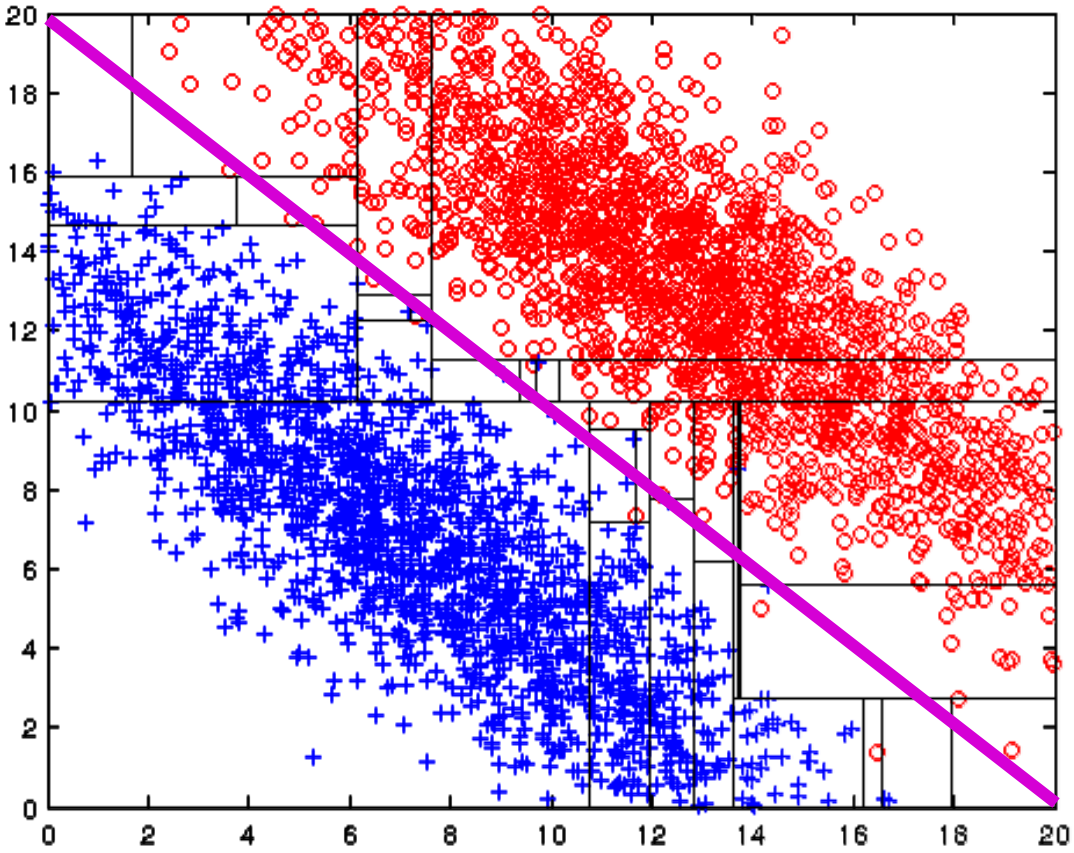
Oblique Decision Trees





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

Limitations of single attribute-based decision boundaries



Both positive (+) and negative (o) classes generated from skewed Gaussians with centers at (8,8) and (12,12) respectively.

Test Condition

$x + y < 20$

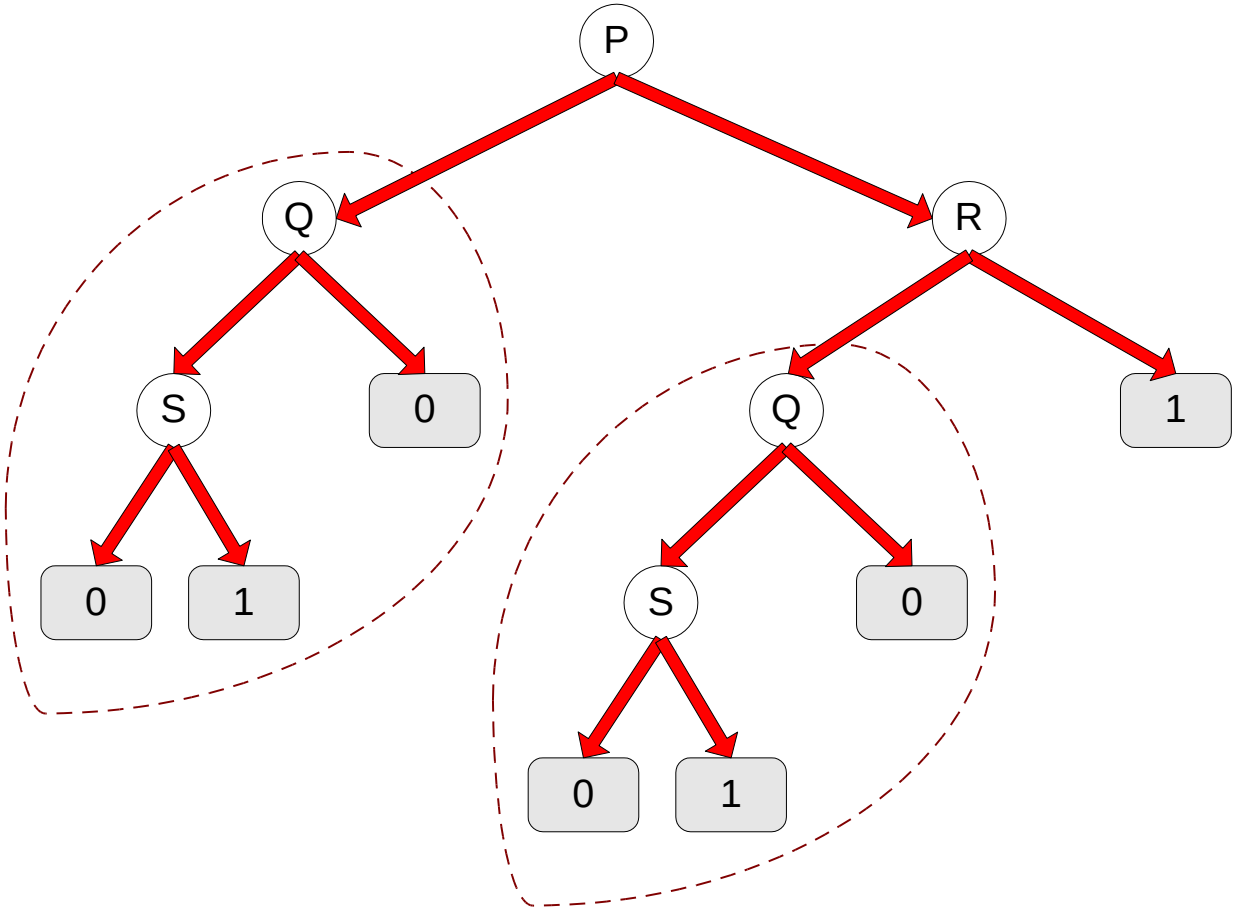
Other Issues

- Data Fragmentation
- 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**

Tree Replication



Same subtree appears in multiple branches

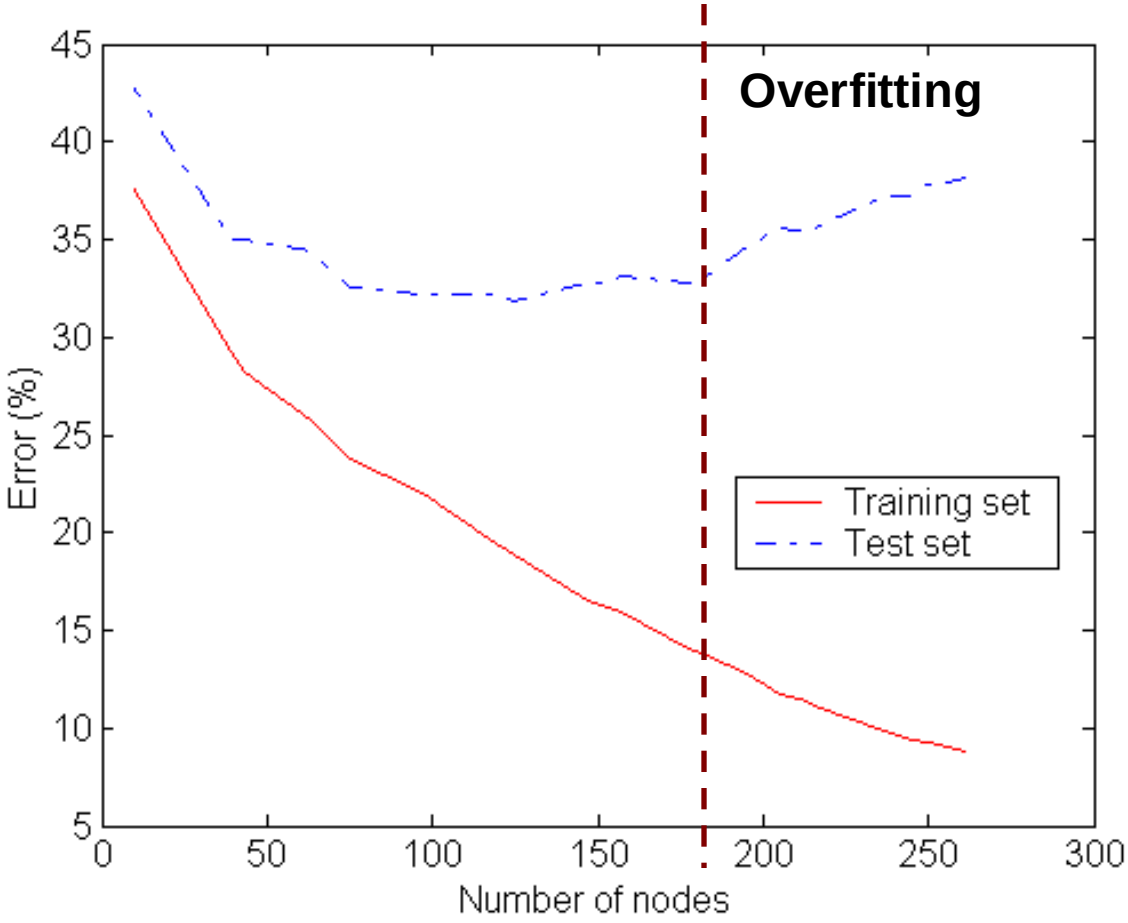
Practical Issues of Classification

- Underfitting and Overfitting
- Costs of Classification

Classification Errors

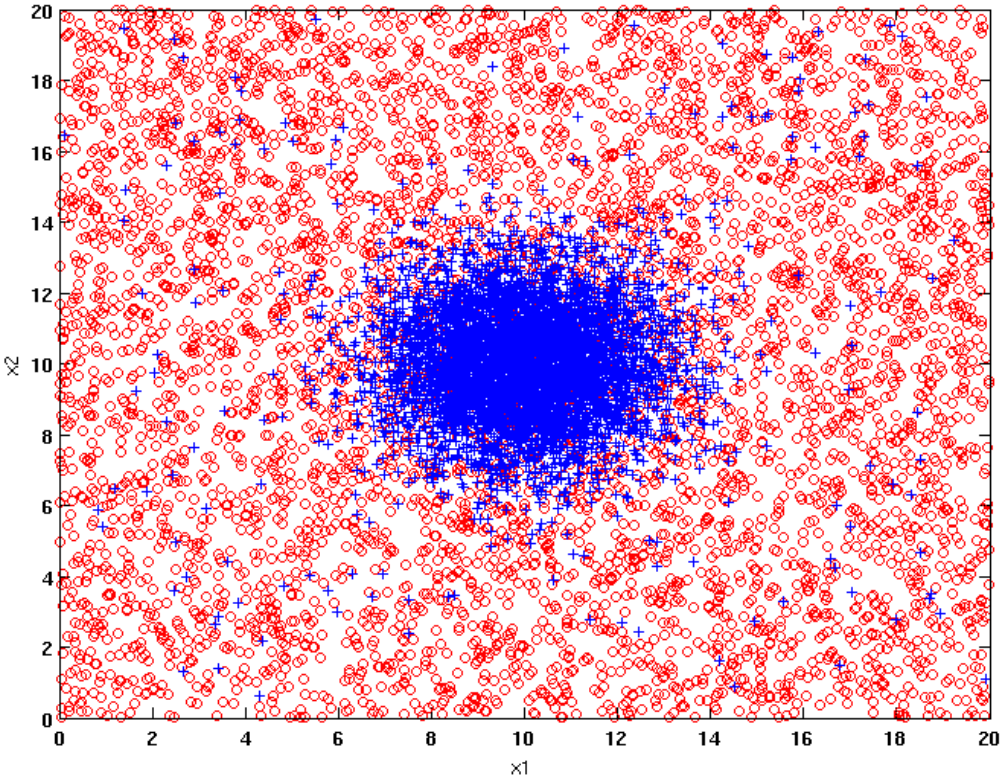
- Training errors (apparent errors)
  - Errors committed on the training set
- Test errors
  - Errors committed on the test set
- Generalization errors
  - Expected error of a model over random selection of records from same distribution

Underfitting and Overfitting



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

Example Data Set



Two class problem:

+ : 5200 instances

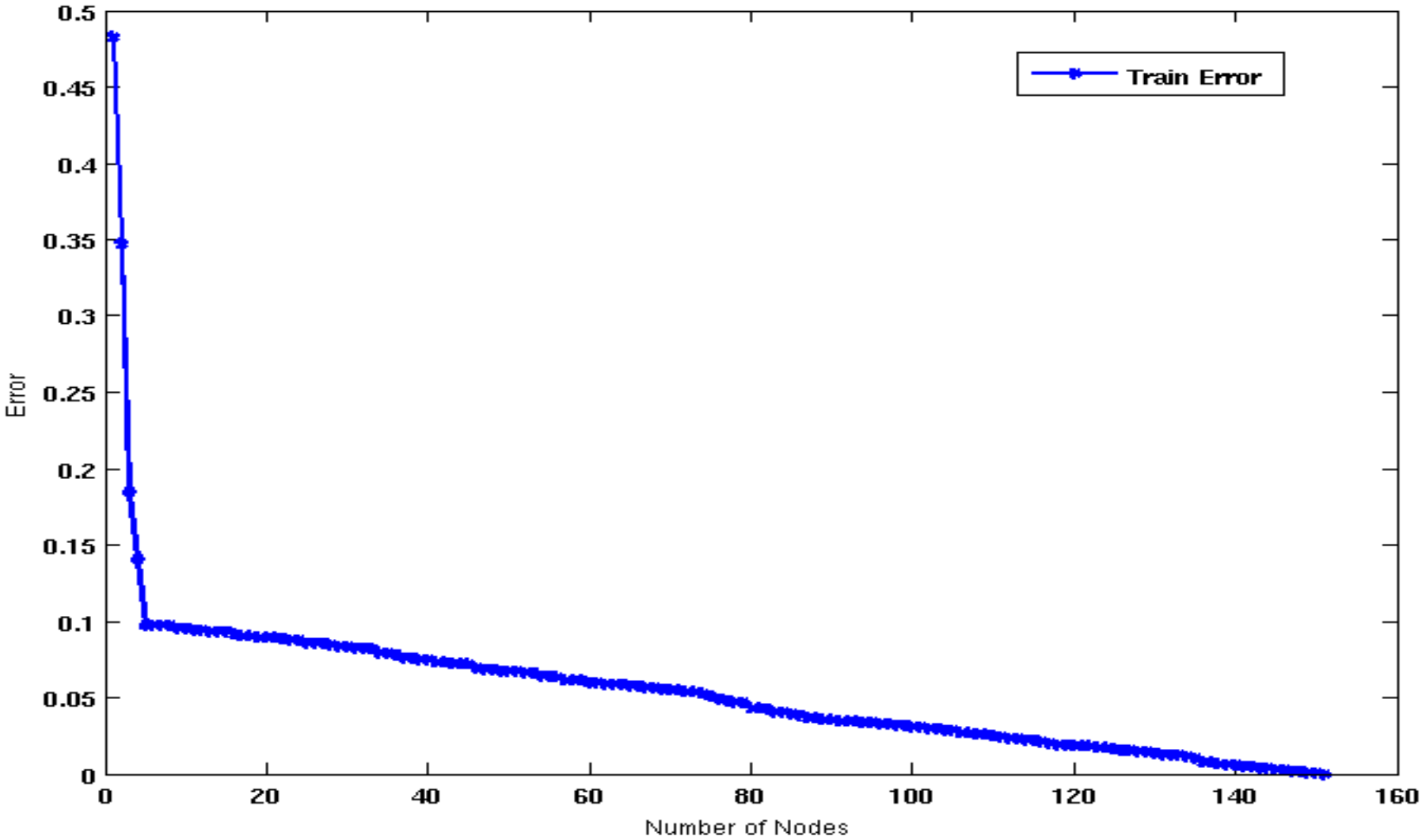
- **5000 instances generated from a Gaussian centered at (10,10)**
- **200 noisy instances added**

o : 5200 instances

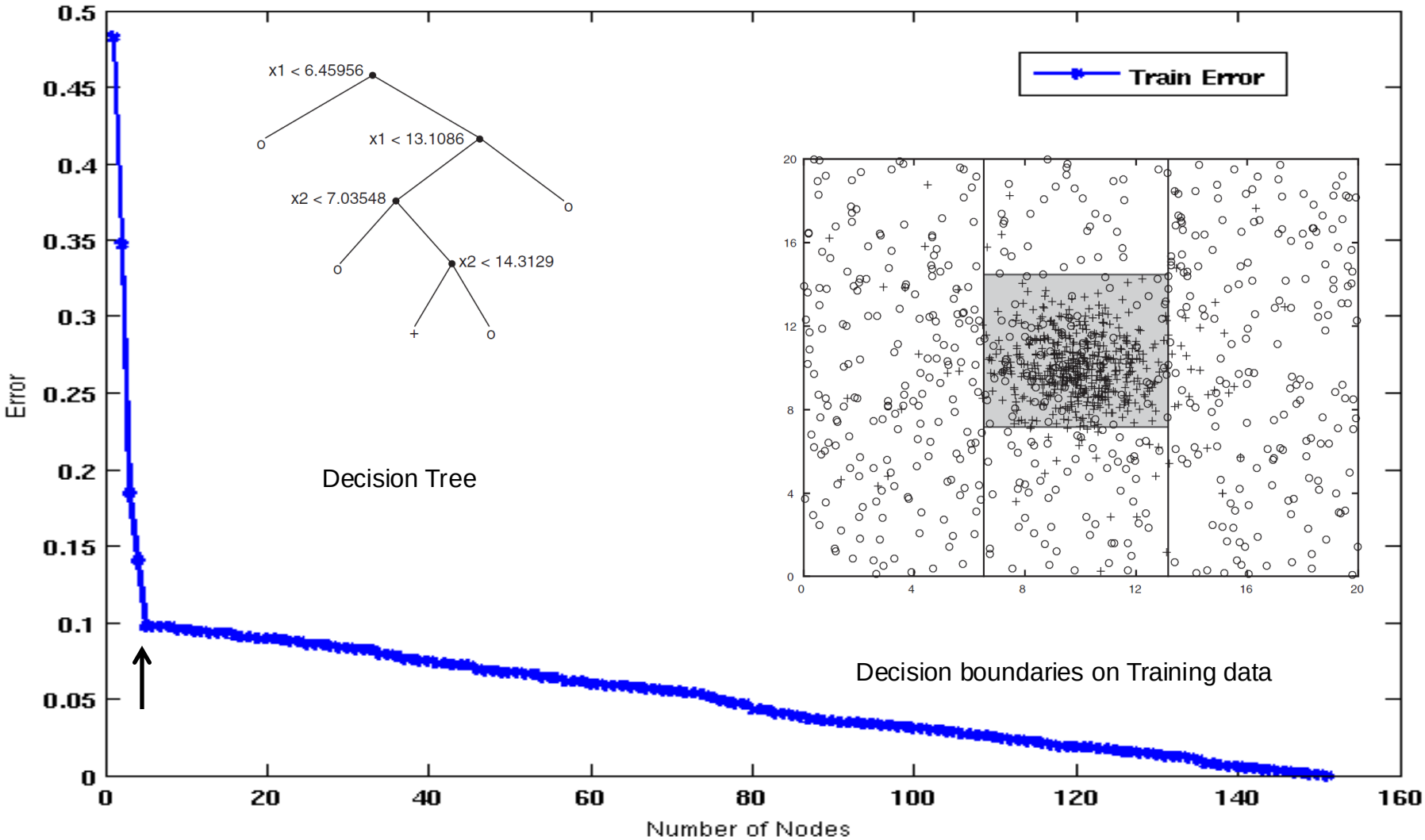
- **Generated from a uniform distribution**

10 % of the data used for training and 90% of the data used for testing

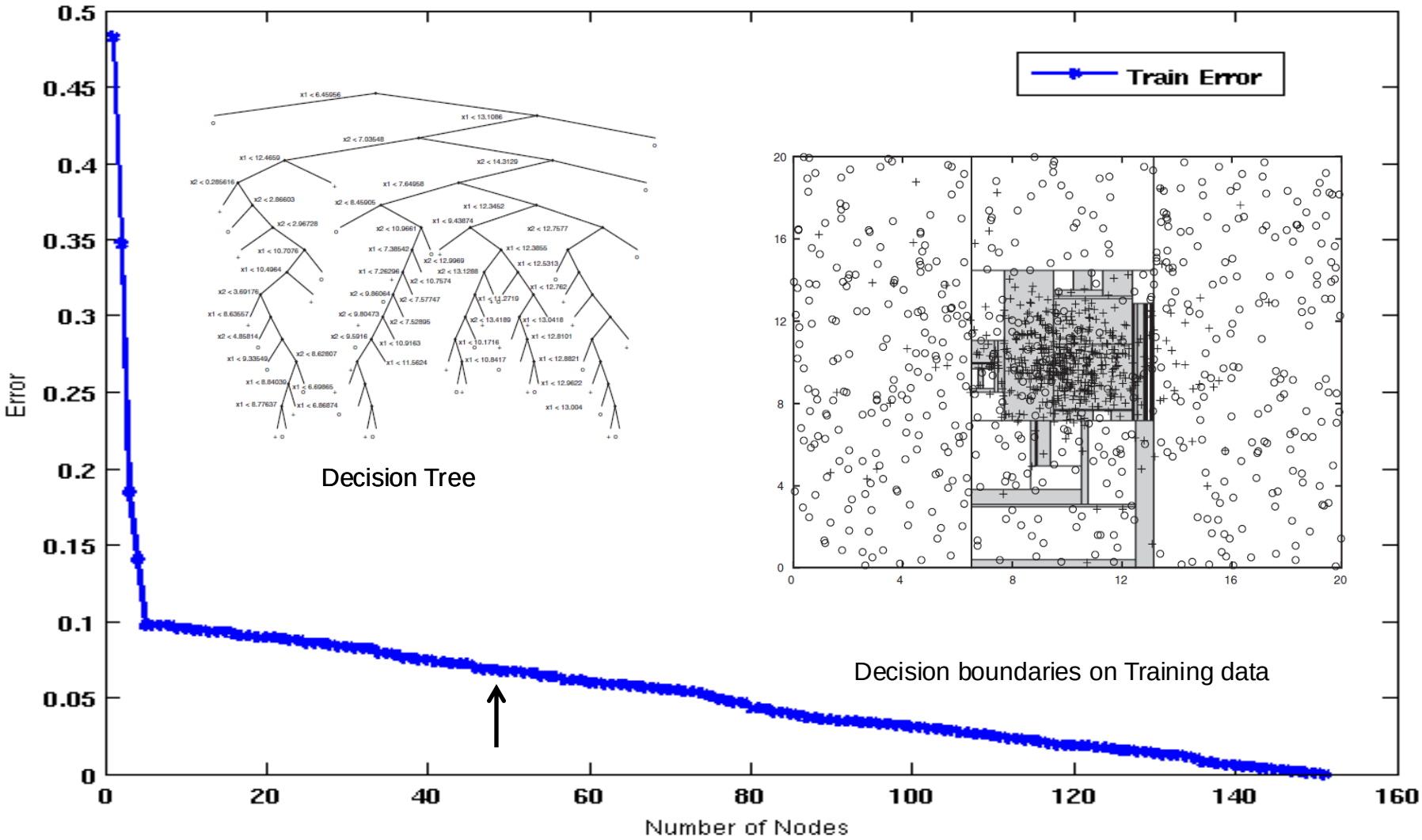
Increasing number of nodes in Decision Trees



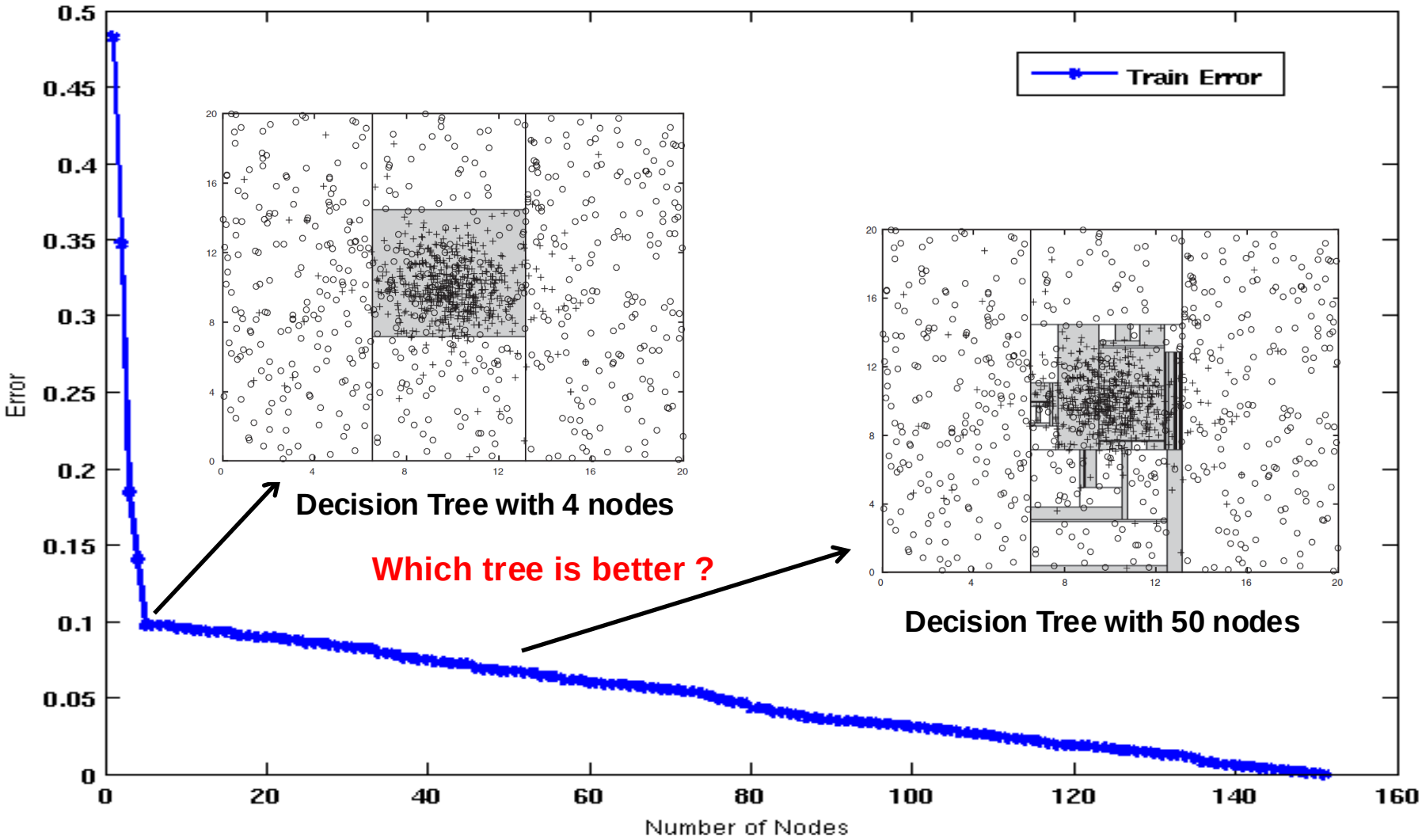
Decision Tree with 4 nodes



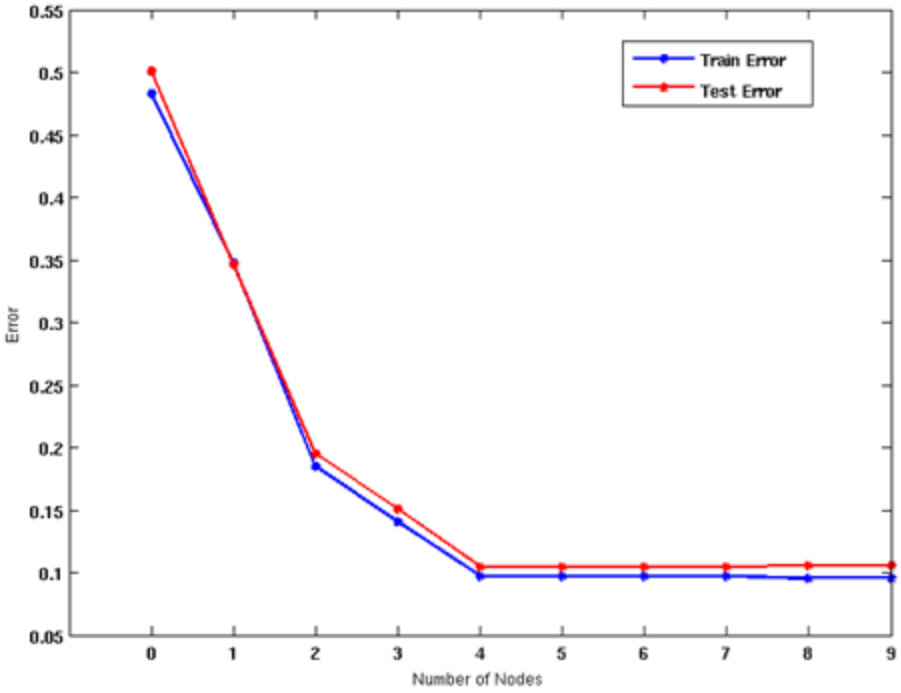
Decision Tree with 50 nodes

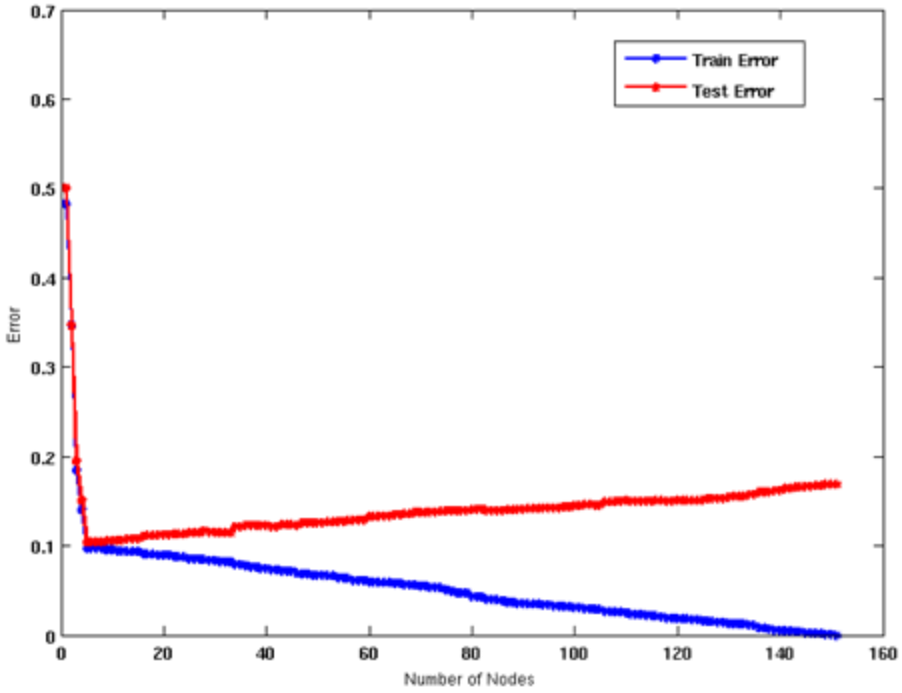


Which tree is better?



Model Overfitting

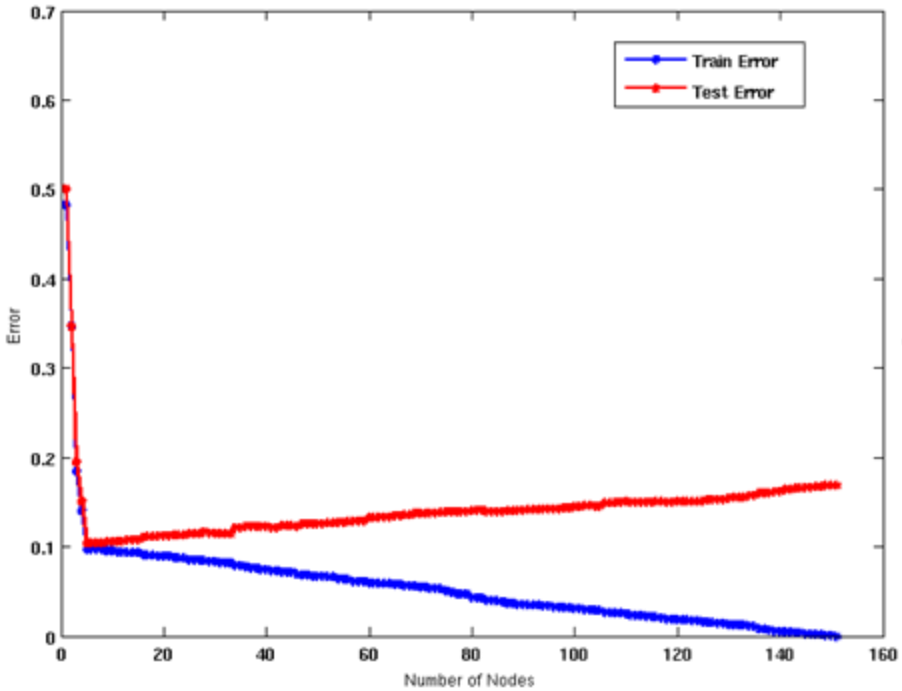


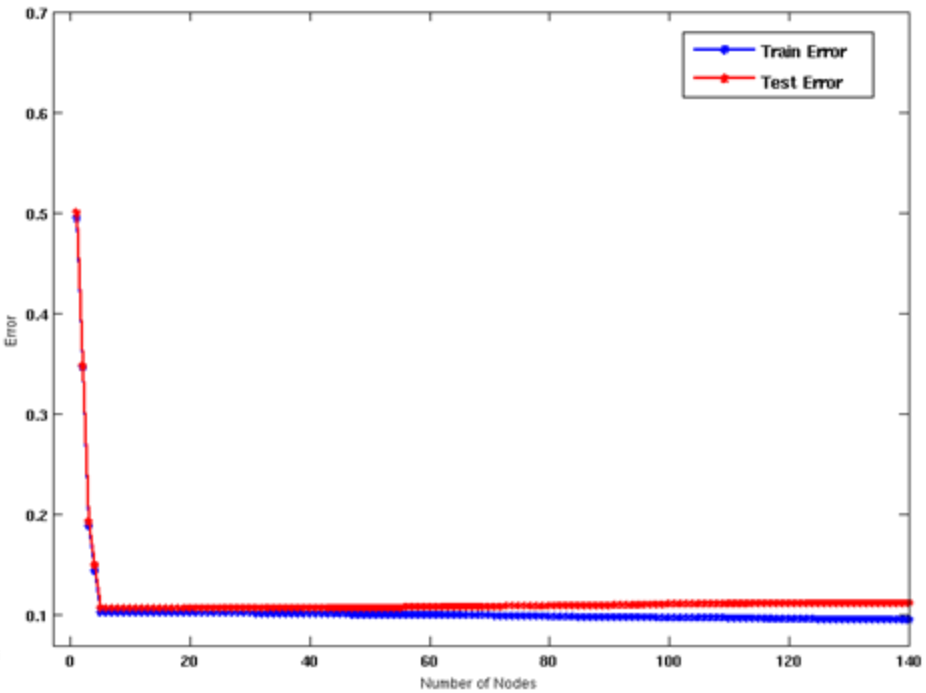


Underfitting: when model is too simple, both training and test errors are large

Overfitting: when model is too complex, training error is small but test error is large

Model Overfitting

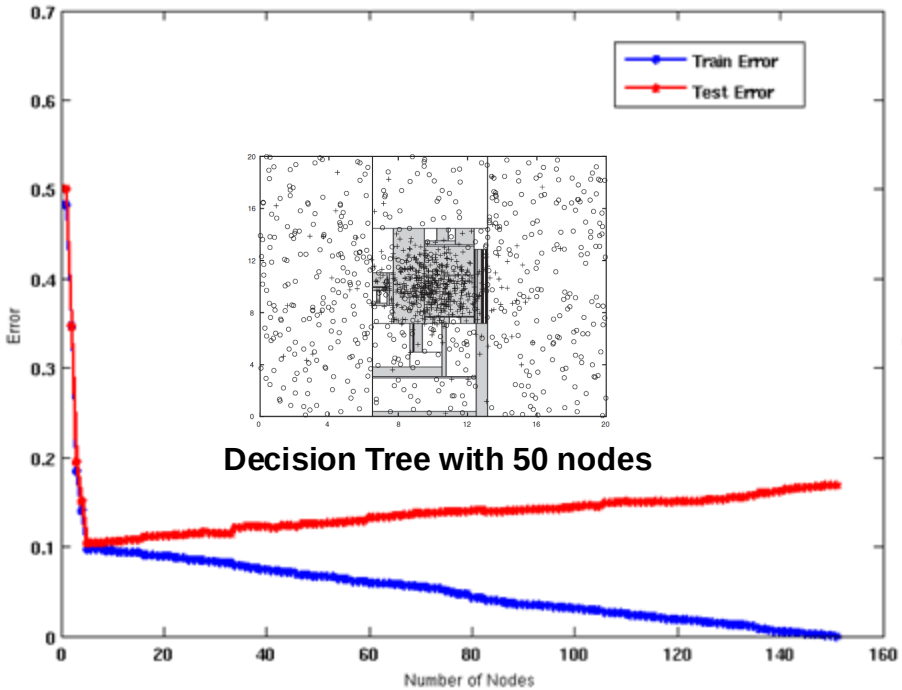


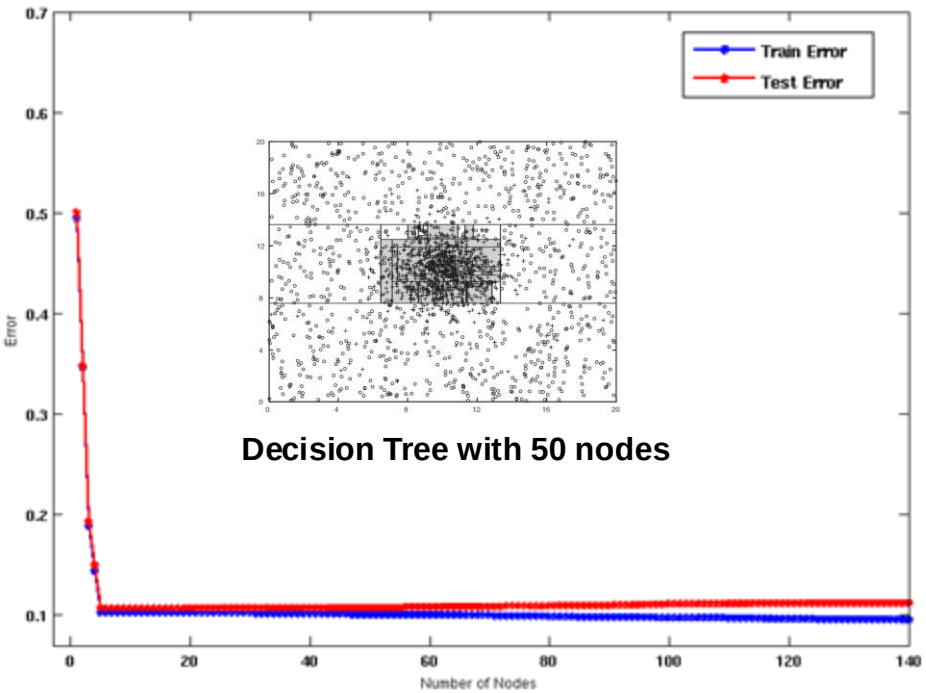


Using twice the number of data instances

- If training data is under-representative, testing errors increase and training errors decrease on increasing number of nodes
- Increasing the size of training data reduces the difference between training and testing errors at a given number of nodes

Model Overfitting

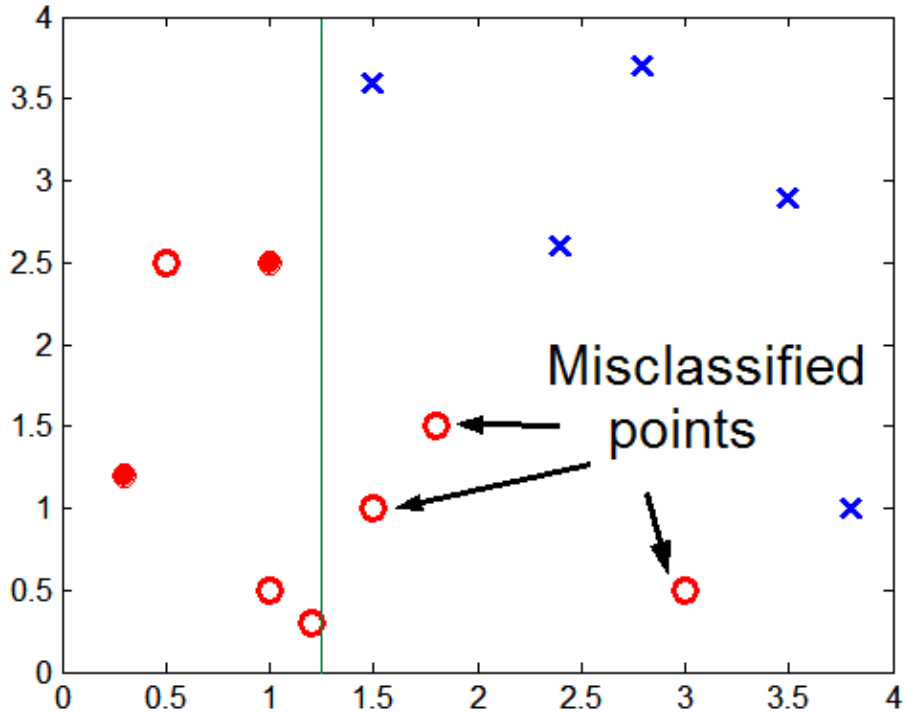




Using twice the number of data instances

- If training data is under-representative, testing errors increase and training errors decrease on increasing number of nodes
- Increasing the size of training data reduces the difference between training and testing errors at a given number of nodes

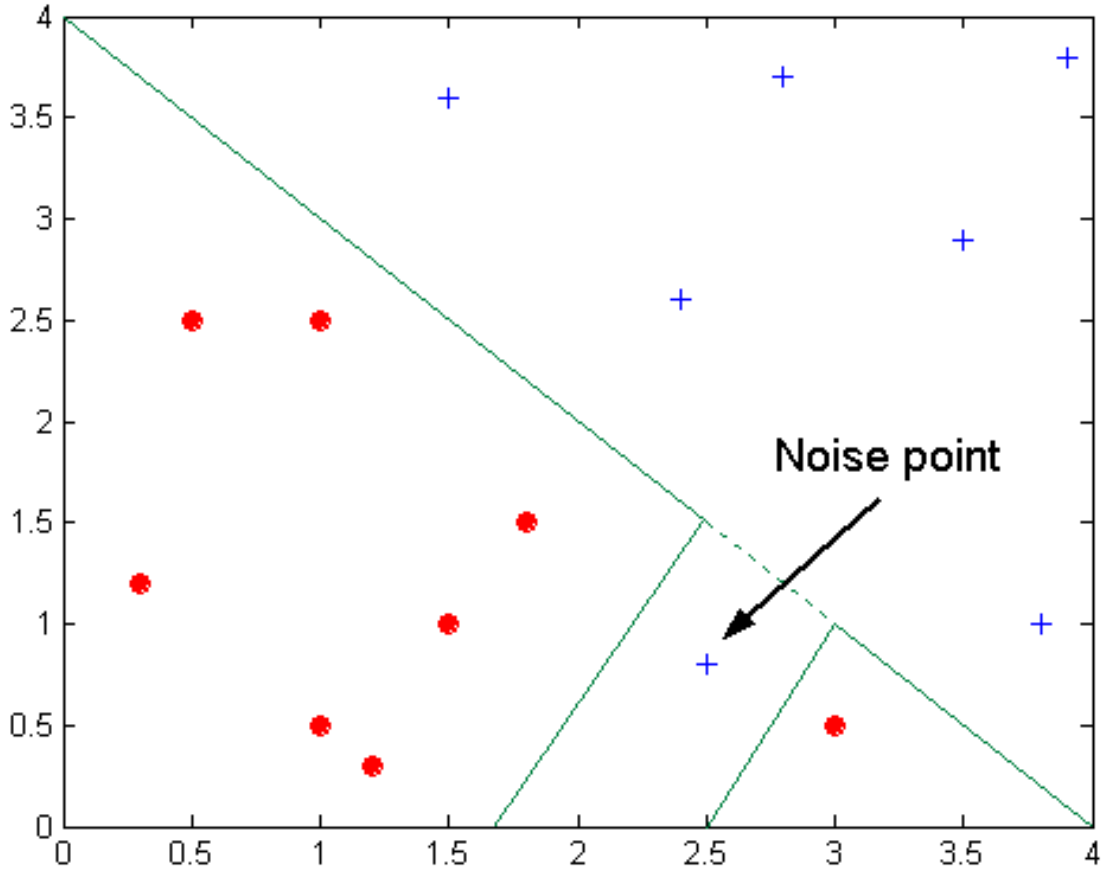
Overfitting due to Insufficient Examples



- 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**

Overfitting due to Noise



Decision boundary is distorted by noise point

Notes on Overfitting

- Overfitting results in decision trees that <u>are more complex</u> than necessary
- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records
- Need new ways for estimating errors

Model Selection

- Performed during model building
- Purpose is to ensure that model is not overly complex (to avoid overfitting)
- Need to estimate generalization error
  - Using Validation Set
  - Incorporating Model Complexity
  - Estimating Statistical Bounds

Model Selection Using Validation Set

- Divide <u>training</u> data into two parts:
  - Training set:
    - use for model building
  - Validation set:
    - use for estimating generalization error
    - Note: validation set is not the same as test set

- Drawback:
  - Less data available for training

Model Selection Incorporating Model Complexity

- Rationale: Occam's Razor
  - Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
  - A complex model has a greater chance of being fitted accidentally by errors in data
  - Therefore, one should include model complexity when evaluating a model

Gen. Error(Model) = Train. Error(Model, Train. Data) + α x Complexity(Model)

Estimating Generalization Errors

- Re-substitution errors: error on training (Σ err(t))
- Generalization errors: error on testing (Σ err$'$(t))
- Methods for estimating generalization errors:
  - Pessimistic approach
  - Optimistic approach
  - Reduced error pruning (REP): uses validation data set to estimate generalization error

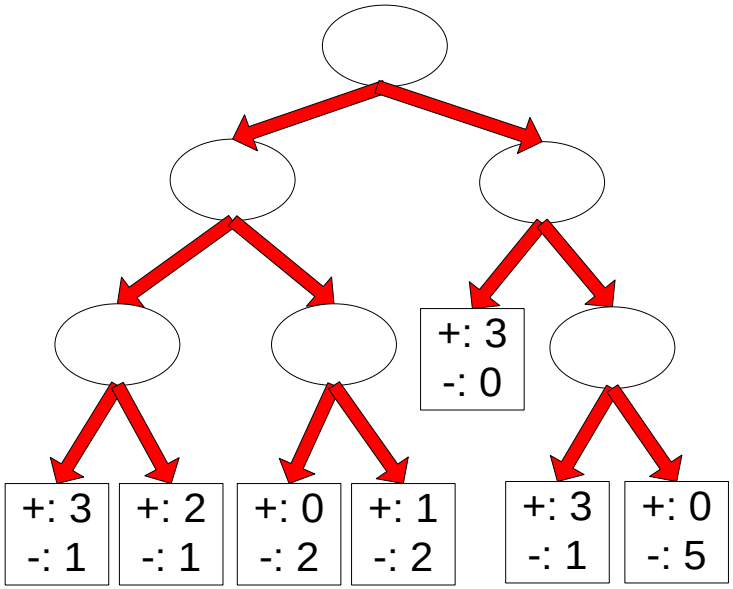
Estimating the Complexity of Decision Trees

Pessimistic Error Estimate of decision tree T with k leaf nodes:

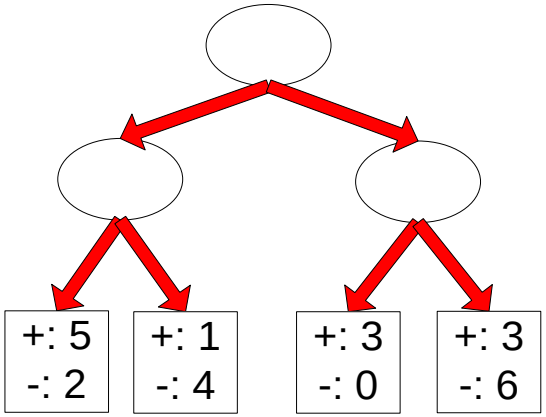
$$err_{gen}(T) = err(T) + \Omega \times \frac{k}{N_{train}},$$

- err(T): error rate on all training records
- Ω: Relative cost of adding a leaf node
- k: number of leaf nodes
- N_{train}: total number of training records

Estimating the Complexity of Decision Trees: Example



Decision Tree, T_L



Decision Tree, T_R

$e(T_L) = 4/24$

$e(T_R) = 6/24$

$\Omega = 1$

$e_{gen}(T_L) = 4/24 + 1*7/24 = 11/24 = 0.458$

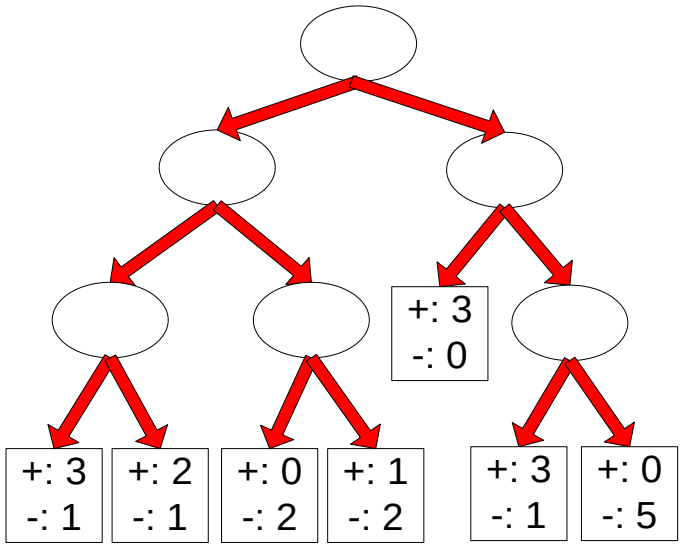
$e_{gen}(T_R) = 6/24 + 1*4/24 = 10/24 = 0.417$

$$err_{gen}(T) = err(T) + \Omega \times \frac{k}{N_{train}},$$

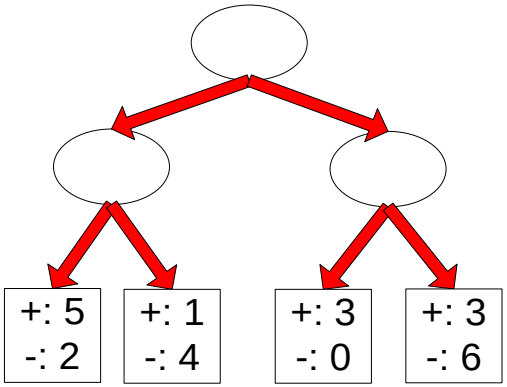
Estimating the Complexity of Decision Trees

Re-substitution Estimate:

- Using training error as an **optimistic** estimate of generalization error
- Referred to as optimistic error estimate



Decision Tree, T_L



Decision Tree, T_R

$e(T_L) = 4/24$

$e(T_R) = 6/24$

Occam's Razor

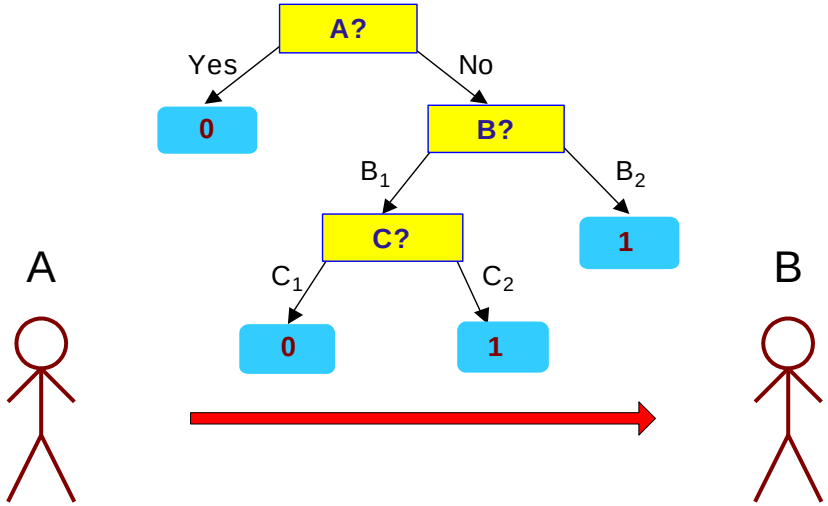
- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model

- 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

Minimum Description Length (MDL)

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



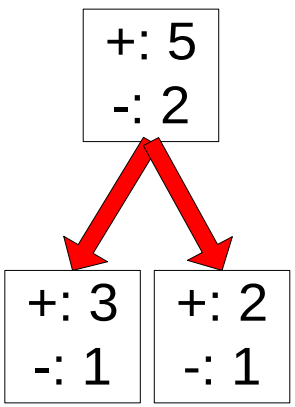
X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- 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.

Estimating Statistical Bounds

Apply a **statistical correction** to the training error rate of the model that is indicative of its model complexity.

- Need **probability distribution of training error**: available or assumed.
- The number of errors committed by a leaf node in a decision tree can be assumed to follow a **binomial distribution.**



Before splitting: e = 2/7, e'(7, 2/7, 0.25) = 0.503

e'(T) = 7 × 0.503 = 3.521

After splitting:

$e(T_L)$ = 1/4, e'(4, 1/4, 0.25) = 0.537

$e(T_R)$ = 1/3, e'(3, 1/3, 0.25) = 0.650

e'(T) = 4 × 0.537 + 3 × 0.650 = 4.098

$$e'(N,e,\alpha) = \frac{e + \frac{z_{\alpha/2}^2}{2N} + z_{\alpha/2}\sqrt{\frac{e(1-e)}{N} + \frac{z_{\alpha/2}^2}{4N^2}}}{1 + \frac{z_{\alpha/2}^2}{N}}$$

Therefore, do not split

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 expanding the current node does not improve impurity measures (e.g., Gini or information gain).
    - Stop if estimated generalization error falls below certain threshold

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	

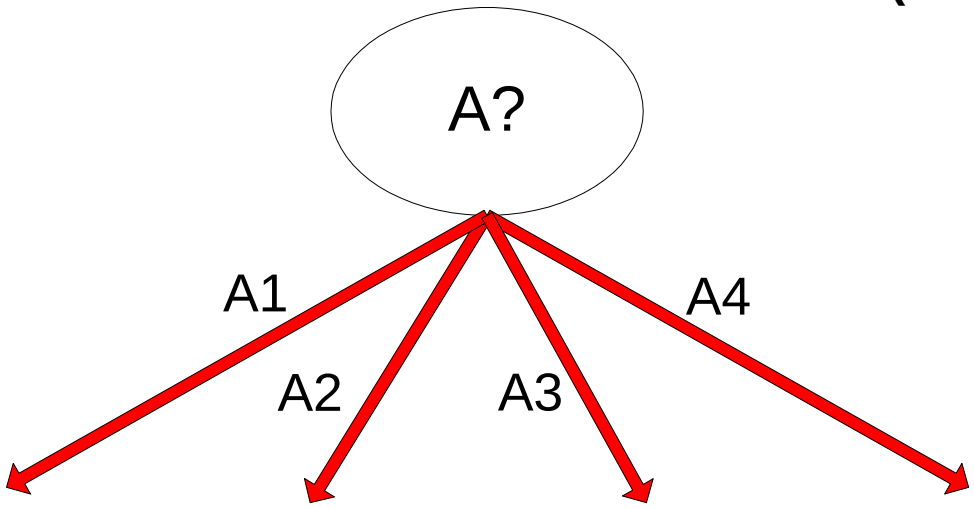
Training Error (Before splitting) = 10/30

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

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

= (9 + 4 × 0.5)/30 = 11/30



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

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		
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	
		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
  - 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		
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	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		
ACTUAL CLASS	C(i|j)	+	-
	+	-1	100
	-	1	0

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

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

Accuracy = 80%

Cost = 3910

Accuracy = 90%

Cost = 4255

Cost-Sensitive Measures

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

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

$$\text{F-measure (F)} = \frac{2rp}{r + p} = \frac{2TP}{2TP + FN + FP}$$

- 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)

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

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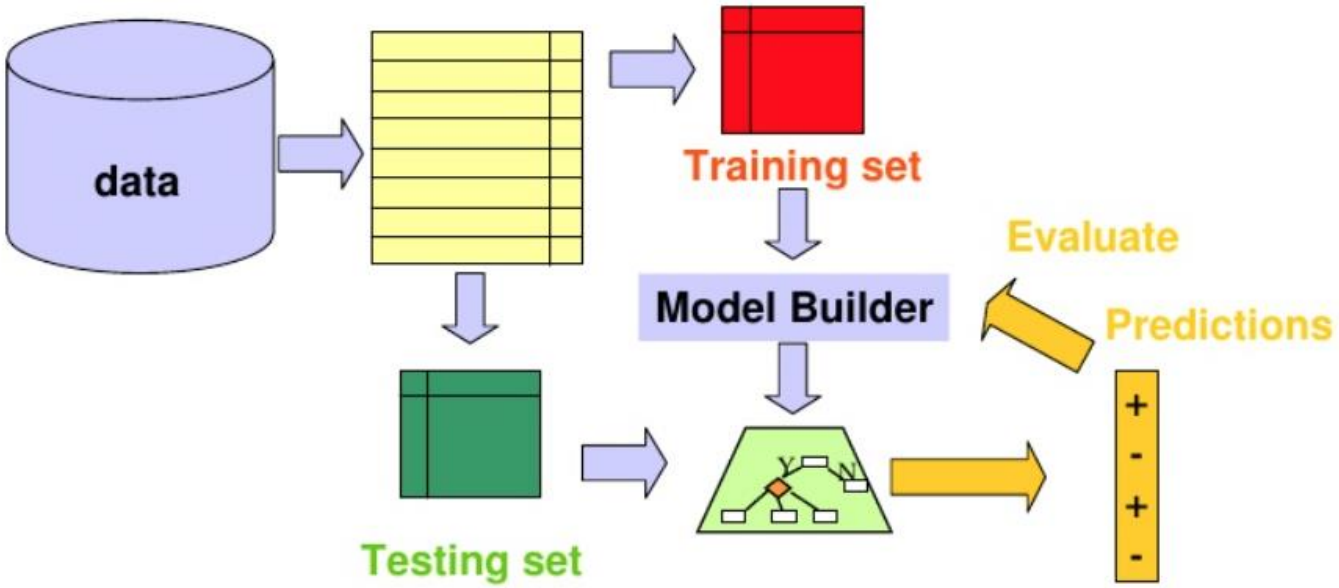
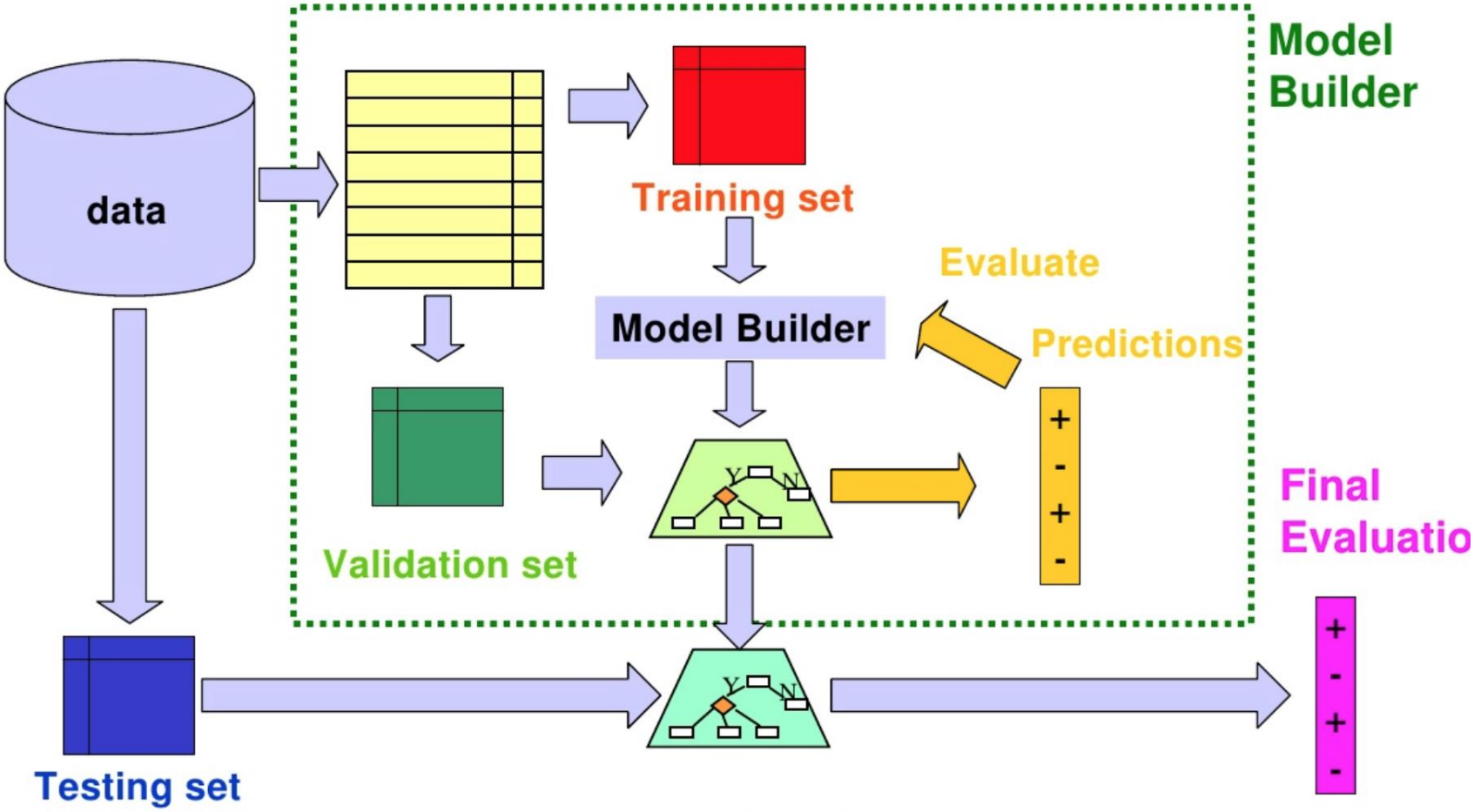
Methods for evaluation



Parameter Tuning

- It is important that the test data is not used in any way to create the classifier
- Some learning schemes operate in two stages:
  - **Stage 1**: builds the basic structure
  - **Stage 2**: optimizes parameter settings
  - **The test data can't be used for parameter tuning!**
  - Proper procedure uses three sets:
    - training data,
    - validation data,
    - test data
  - **Validation data is used to optimize parameters**
- Once evaluation is complete, all the data can be used to build the final classifier
- Generally, the larger the training data the better the classifier
- The larger the test data the more accurate the error estimate

Evaluation: training, validation, test

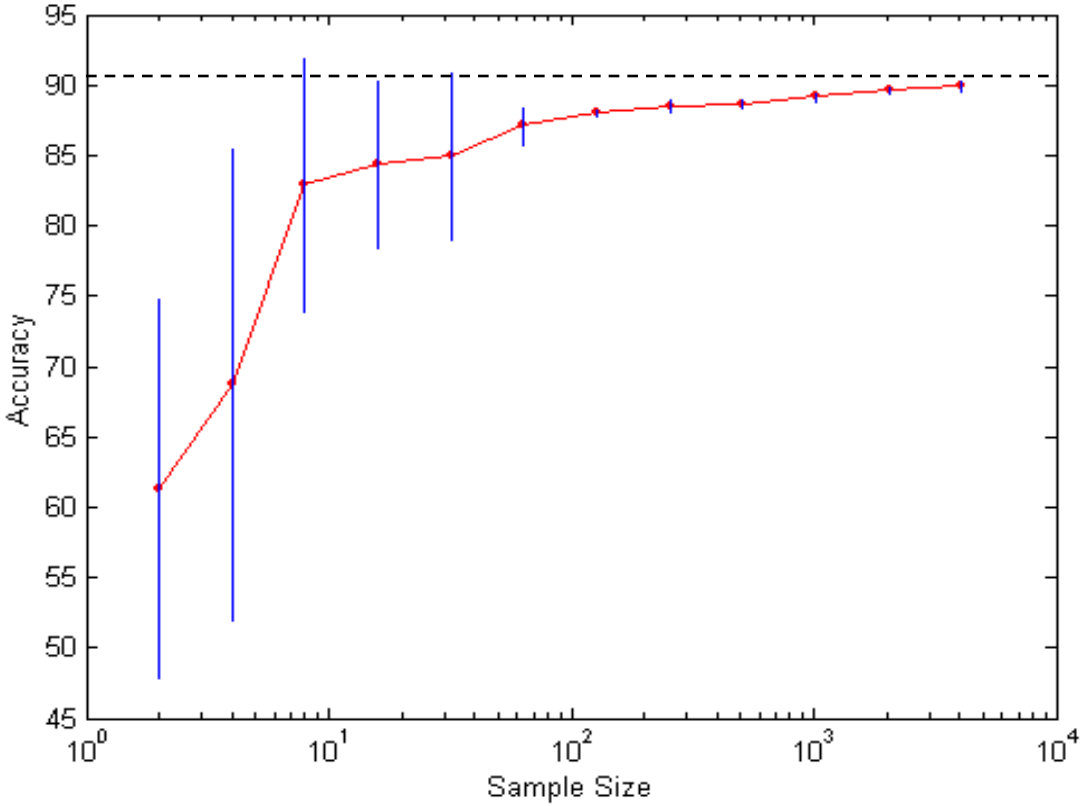


Methods for Performance Evaluation

- 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

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

1. **How much a classification model benefits from adding more training data?**
2. **Does the model suffer from a variance error or a bias error?**

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - 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
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

Small & Unbalanced Data

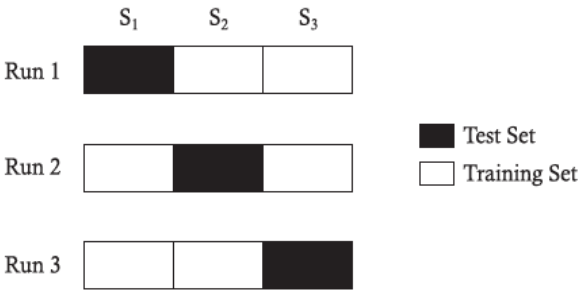
- The holdout method reserves a certain amount for **testing** and uses the remainder for **training**
- Usually, **one third for testing**, the rest for training
- For small or “unbalanced” datasets, **samples might not be representative**
  - For instance, few or none instances of some classes
- Stratified sample
  - **Balancing the data**
  - Make sure that each class is represented with approximately equal proportions in both subsets

Repeated holdout method

- Holdout estimate can be made more reliable by **repeating the process with different subsamples**
  - In each iteration, a certain proportion is **randomly selected for training** (possibly with stratification)
  - The error rates on the different iterations are **averaged** to yield an overall error rate
- This is called the **repeated holdout method**
- Still not optimum: the different test sets overlap

Cross-validation

- Avoids overlapping test sets
  - **First step:** data is split into k subsets of equal size
  - **Second step:** each subset in turn is used for testing and the remainder for training
- This is called **k-fold cross-validation**



- Often the subsets are stratified before cross-validation is performed
- The **error estimates** are **averaged** to yield an overall error estimate
- **Even better:** repeated stratified cross-validation
  E.g. ten-fold cross-validation is repeated ten times and results are averaged (reduces the variance)

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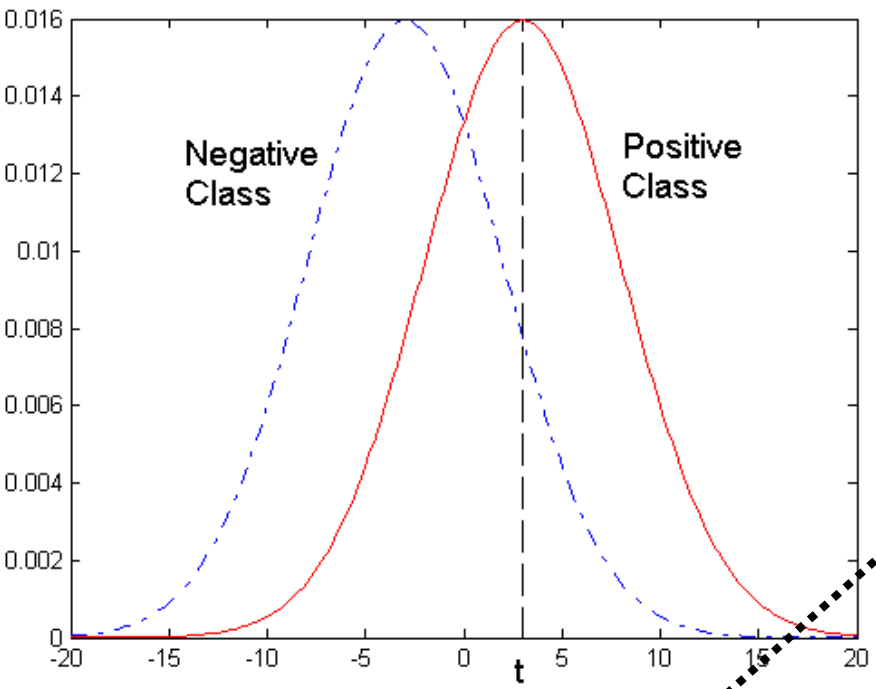
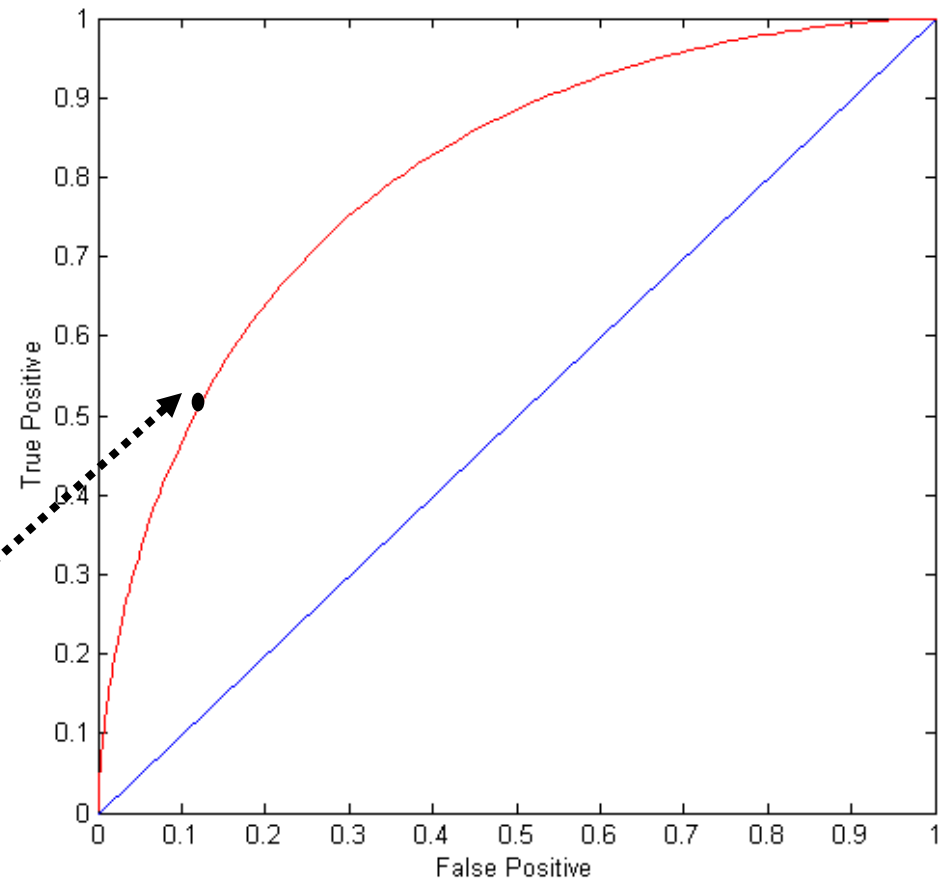
ROC (Receiver Operating Characteristic)

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- **Performance of each classifier represented as a point on the ROC curve**
  - changing the threshold of 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:

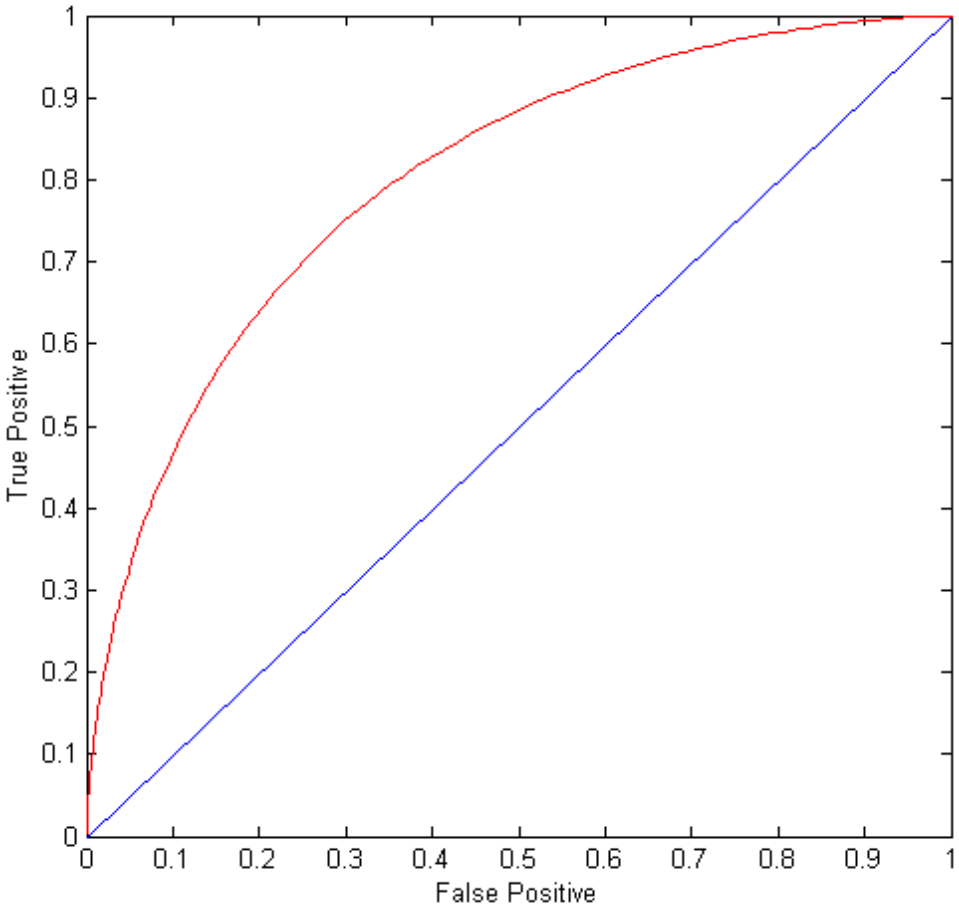
TP=0.5, FN=0.5, FP=0.12, FN=0.88

ROC Curve

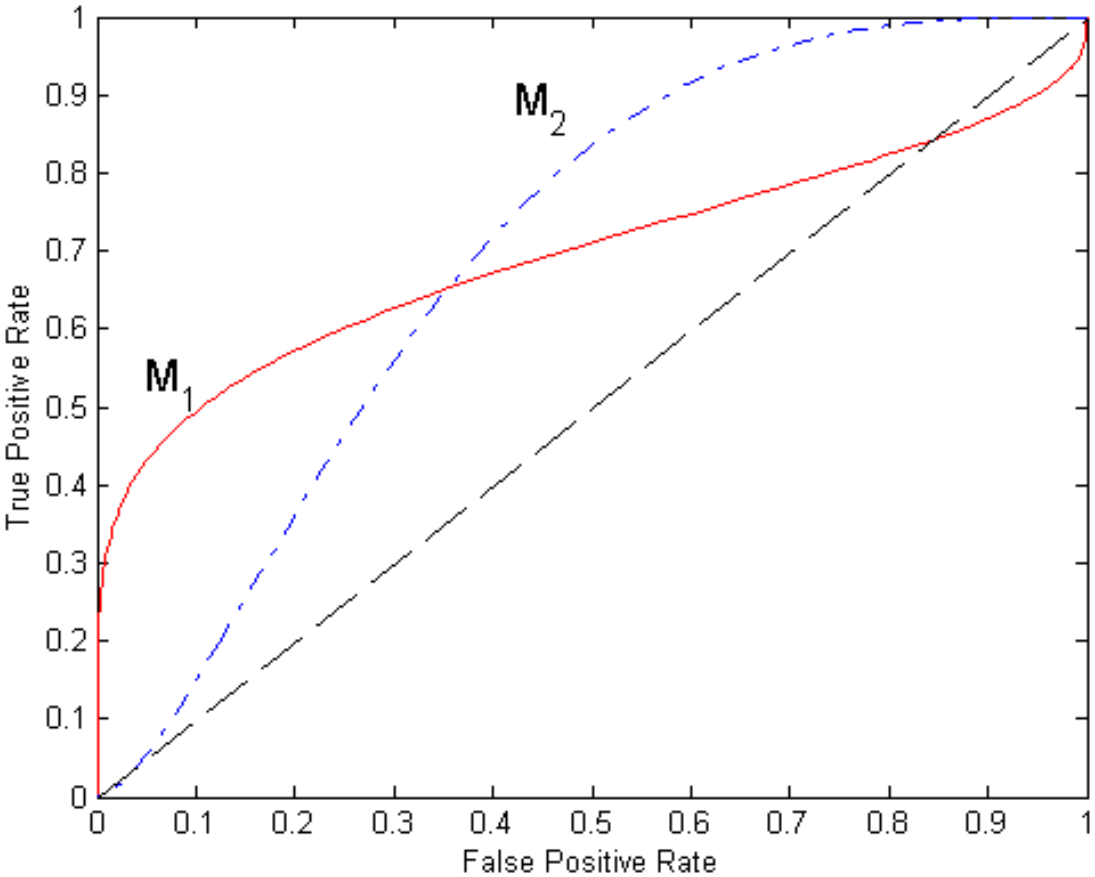
(TP,FP):

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

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



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
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

How to Construct an ROC curve

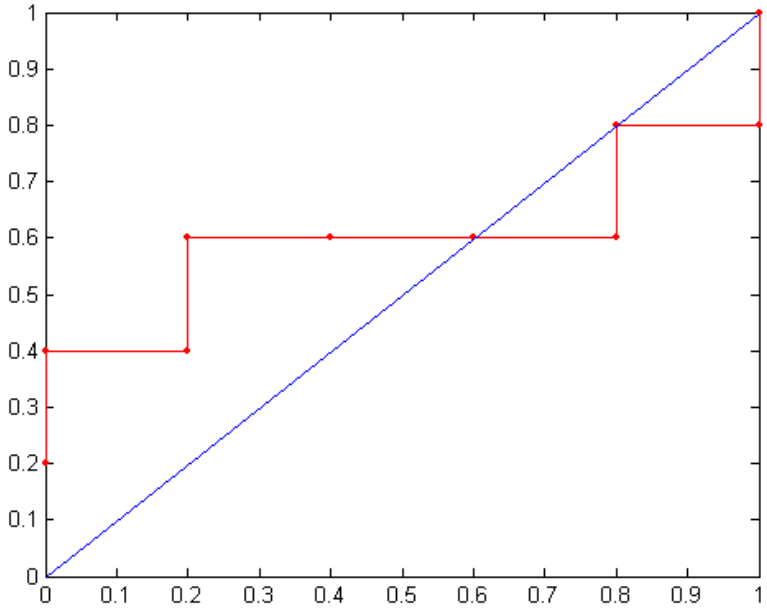
Instance	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

How to construct an ROC curve

	Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=		0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
	TP	5	4	4	3	3	3	3	2	2	1	0
	FP	5	5	4	4	3	2	1	1	0	0	0
	TN	0	0	1	1	2	3	4	4	5	5	5
	FN	0	1	1	2	2	2	2	3	3	4	5
→	TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
→	FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve:



Inst.	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

Test of Significance

- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances

- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in performance measure be explained as a result of **random fluctuations** in the test set?

Confidence Interval for Accuracy

- Prediction can be regarded as a Bernoulli trial (binomial random experiment)
  - A Bernoulli trial has 2 possible outcomes
  - Possible outcomes for prediction: correct or wrong
  - Probability of success is constant
  - Collection of Bernoulli trials has a Binomial distribution:
    - $x \sim Bin(N, p)$ **x:** # of correct predictions, **N** trials, **p** constant prob.
    - e.g: Toss a fair coin 50 times, how many heads would turn up?
      Expected number of heads = $N \times p = 50 \times 0.5 = 25$

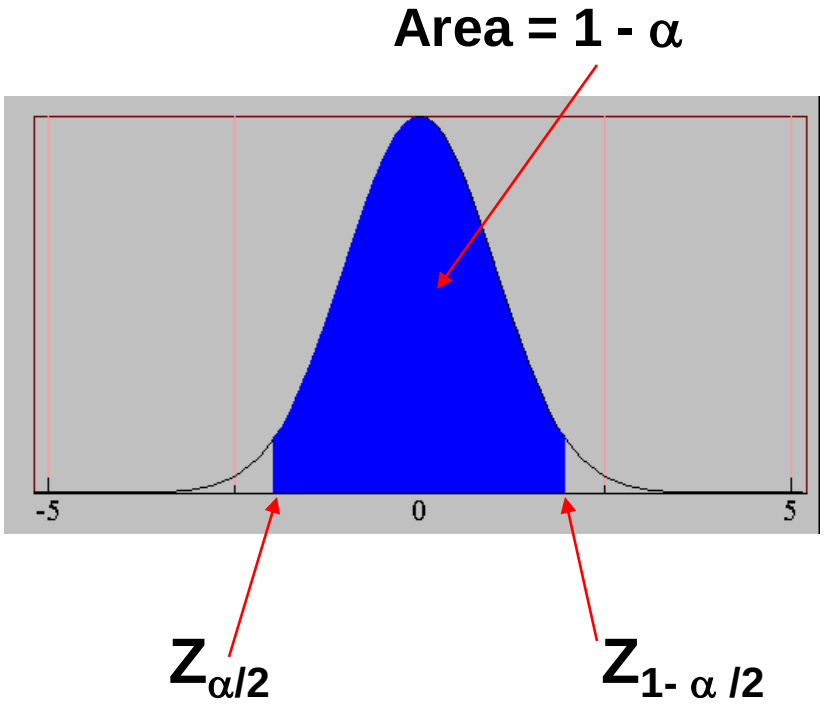
Given x (# of correct predictions) or equivalently, acc=x/N, and N (# of test instances)

Can we predict p (true accuracy of model)?

Confidence Interval for Accuracy

- For large test sets (N > 30),
  - acc has a normal distribution with mean p and variance p(1-p)/N
  - the confidence interval for acc can be derived as follows:

$$P(Z_{\alpha/2} < \frac{acc - p}{\sqrt{p(1-p)/N}} < Z_{1-\alpha/2}) = 1 - \alpha$$



- Confidence Interval for p:

$$p = \frac{2 \times N \times acc + Z^2_{\alpha/2} \pm \sqrt{Z^2_{\alpha/2} + 4 \times N \times acc - 4 \times N \times acc^2}}{2(N + Z^2_{\alpha/2})}$$

Confidence Interval for Accuracy

- Consider a model that produces an accuracy of 80% when evaluated on 100 test instances:
  - N=100, acc = 0.8
  - Let $1-\alpha = 0.95$ (95% confidence)
  - **Which is the confidence interval?**
  - From probability table, $Z_{\alpha/2}=1.96$

N	50	100	500	1000	5000
p(lower)	0.670	0.711	0.763	0.774	0.789
p(upper)	0.888	0.866	0.833	0.824	0.811

$1-\alpha$	Z
0.99	2.58
0.98	2.33
0.95	1.96
0.90	1.65

Comparing Performance of 2 Models

- Given two models, say M1 and M2, which is better?
  - M1 is tested on D1 (size=n1), found error rate = e_1
  - M2 is tested on D2 (size=n2), found error rate = e_2
  - Assume D1 and D2 are independent
  - If n1 and n2 are sufficiently large, then

$$e_1 \sim N(\mu_1, \sigma_1)$$
$$e_2 \sim N(\mu_2, \sigma_2)$$

  - Approximate variance of error rates: $\hat{\sigma}_i = \frac{e_i(1-e_i)}{n_i}$

Comparing Performance of 2 Models

- To test if performance difference is statistically significant: $d = e_1 - e_2$
  - $d \sim N(d_t, \sigma_t)$ where d_t is the true difference
  - Since D1 and D2 are independent, their variance adds up:

$$s_t^2 = s_1^2 + s_2^2 \approx \hat{s}_1^2 + \hat{s}_2^2$$

$$= \frac{e1(1-e1)}{n1} + \frac{e2(1-e2)}{n2}$$

  - It can be shown at $(1-\alpha)$ confidence level,

$$d_t = d \pm Z_{\alpha/2} \hat{\sigma}_t$$

An Illustrative Example

- Given: M1: n1 = 30, e1 = 0.15
  M2: n2 = 5000, e2 = 0.25

- d = |e2 – e1| = 0.1 (2-sided test to check: dt = 0 or dt <> 0)

$$\hat{s}_d^2 = \frac{0.15(1-0.15)}{30} + \frac{0.25(1-0.25)}{5000} = 0.0043$$

- At 95% confidence level, $Z_{\alpha/2}$=1.96

$$d_t = 0.100 \pm 1.96 \times \sqrt{0.0043} = 0.100 \pm 0.128$$

=> Interval contains 0 => difference may not be statistically significant