Data Mining
Classification: Basic Concepts, Decision Trees, and Model Evaluation

Lecture Notes for Chapter 4

Data Mining
by
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Outline

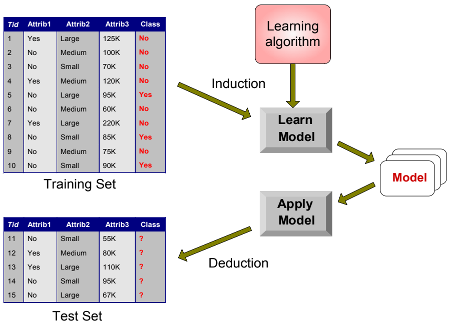
- Basic Concepts
- Decision Tree based Methods
- Model Evaluation
- Nearest Neighbor Methods
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines

4.1. Basic Concepts

Classification: Definition

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

Illustrating Classification Task



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

Training Set

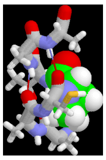
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Examples of Classification Task

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent

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



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

Classification Techniques

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

4.2. Decision Tree based Methods

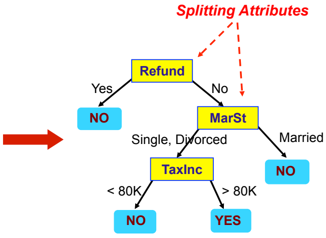
4.2.1. Basic Concepts

Example of a Decision Tree

categorical categorical continuous class

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

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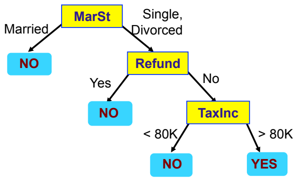
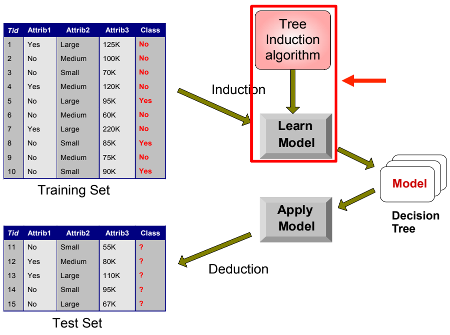
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



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

Decision Tree Classification Task



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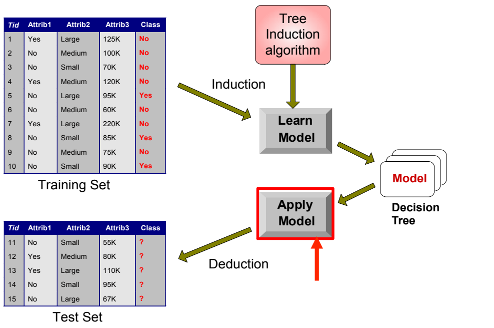
Test Set

Decision Tree Classification Task



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Training Set

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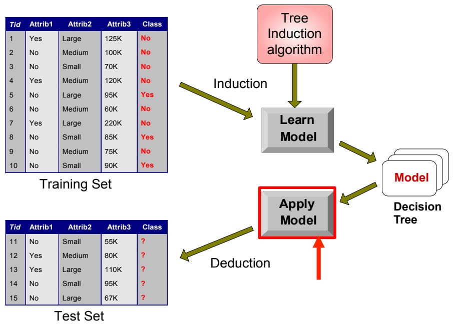
15	No	Large	67K	?

Test Set

4.2. Decision Tree based Methods

4.2.2. Decision Tree Deduction

Decision Tree Classification Task



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Training Set

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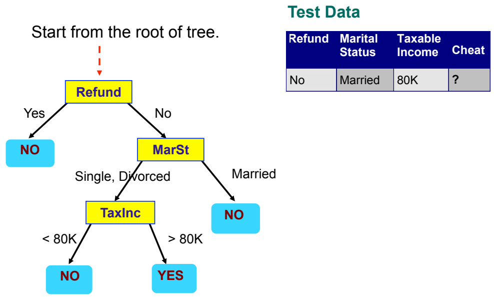
Test Set

Apply Model to Test Data

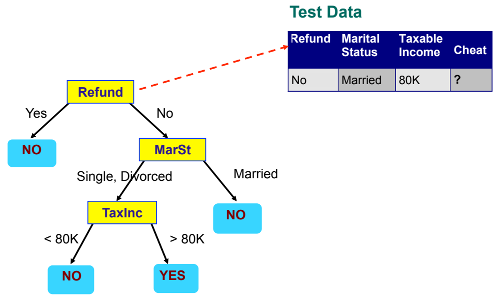


Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Start from the root of tree.

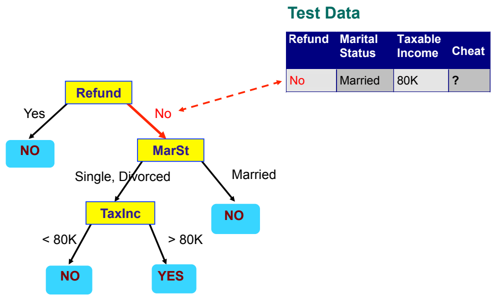
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

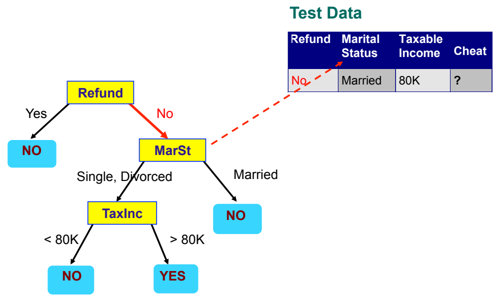
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

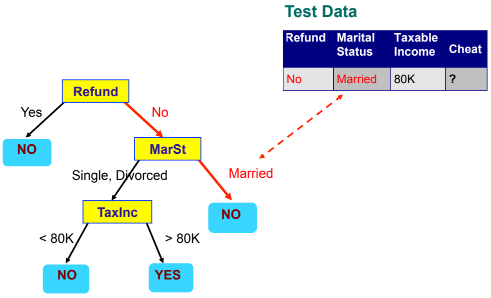
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

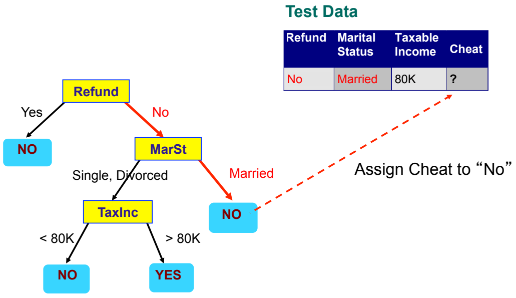
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



Test Data

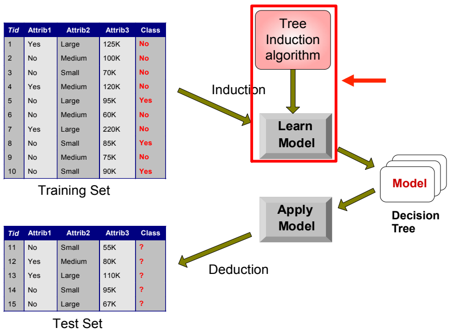
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to “No”

4.2. Decision Tree based Methods

4.2.3. Decision Tree Induction

Decision Tree Classification Task



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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 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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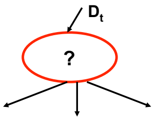

Hunt’s Algorithm

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5	No	Divorced	95K	Yes
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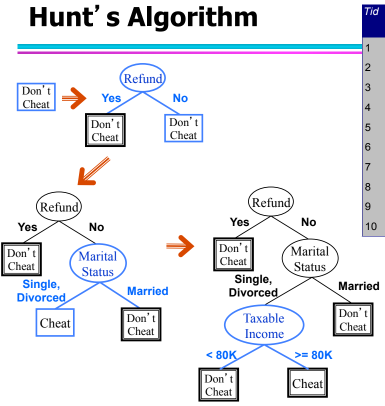

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

Tree Induction

- Greedy strategy.
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4.2. Decision Tree based Methods

4.2.3. Decision Tree Induction

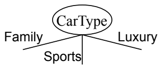
Issue 1: Specify Test Condition

How to Specify Test Condition?

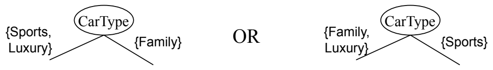
- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

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

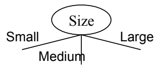


- Binary split: Divides values into two subsets. Need to find optimal partitioning.

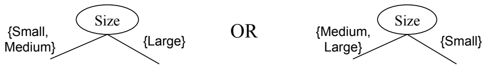


Splitting Based on Ordinal Attributes

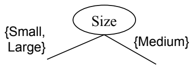
- **Multi-way split:** Use as many partitions as distinct values.



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



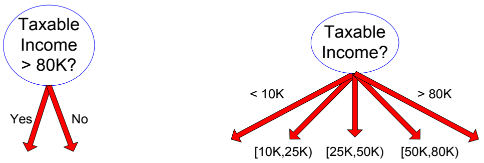
- What about this split?



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 ≥ v)
    - consider all possible splits and finds the best cut
    - can be more compute intensive

Splitting Based on Continuous Attributes



(i) Binary split

(ii) Multi-way split

4.2. Decision Tree based Methods

4.2.3. Decision Tree Induction

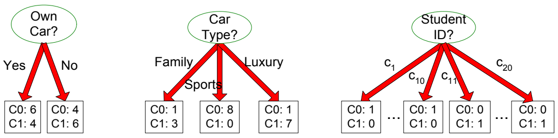
Issue 2: Determine the Best Split

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

How to determine the Best Split

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



Which test condition is the best?

How to determine the Best Split

- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

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

Measures of Node Impurity

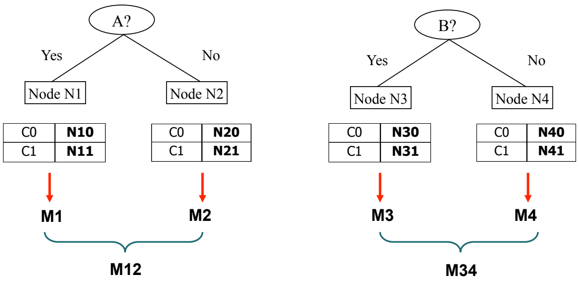
- Gini Index
- Entropy
- Misclassification error

How to Find the Best Split

Before Splitting:

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

→ **M0**



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

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

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

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

Gain = M0 – M12 vs M0 – M34

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

Measure of Impurity: GINI

- Gini Index for a given node t :

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

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

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

C1	**0**
C2	**6**
Gini=0.000	

C1	**1**
C2	**5**
Gini=0.278	

C1	**2**
C2	**4**
Gini=0.444	

C1	**3**
C2	**3**
Gini=0.500	

Examples for computing GINI

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

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

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

Gini = 1 – P(C1)^2 – P(C2)^2 = 1 – 0 – 1 = 0

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

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

Gini = 1 – (1/6)^2 – (5/6)^2 = 0.278

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

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

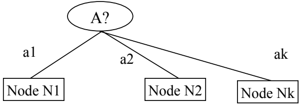
Gini = 1 – (2/6)^2 – (4/6)^2 = 0.444

Splitting Based on GINI

- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

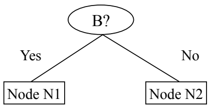
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

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



Binary Attributes: Computing GINI Index

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



	Parent
C1	**6**
C2	**6**
Gini = 0.500	

Gini(N1)
= 1 – $(5/7)^2$ – $(2/7)^2$
= 0.408

Gini(N2)
= 1 – $(1/5)^2$ – $(4/5)^2$
= 0.32

	N1	**N2**
C1	**5**	**1**
C2	**2**	**4**
Gini=0.333		

Gini(Children)
= 7/12 * 0.408 +
5/12 * 0.32
= 0.238 + 0.133
= 0.371

Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split

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

Two-way split
(find best partition of values)

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

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

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for 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! Repetition of work.

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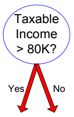


Continuous Attributes: Computing Gini Index...

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

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
Sorted Values →	60	70	75	85	90	95	100	120	125	220

Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	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	

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

Measure of Impurity: Entropy

- Entropy at a given node t:

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

(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

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

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) $\log_2$ (5/6) = 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 Entropy

- Information Gain:

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

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 Entropy

- Gain Ratio:

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

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

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

Measure of Impurity: Classification Error

- Classification error at a node t :

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

- Measures misclassification error made by a node.
  - ◆ Maximum (1 - 1/n_c) when records are equally distributed among all classes, implying least interesting information
  - ◆ Minimum (0.0) when all records belong to one class, implying most interesting information

Examples for Computing Error

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

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

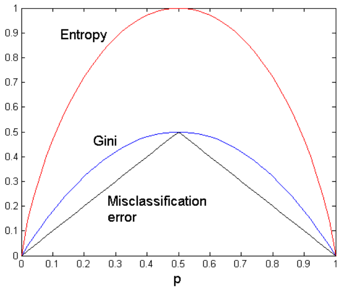
C1	**2**
C2	**4**

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

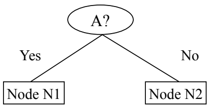
Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Comparison among Splitting Criteria

For a 2-class problem:



Misclassification Error vs Gini



	Parent
C1	**7**
C2	**3**
Gini = 0.42	
Error = 0.3	

Gini(N1)
= 1 – (3/3)^2 – (0/3)^2
= 0

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

Error(N1) = 0

Error(N2) = 3/7

	N1	**N2**
C1	**3**	**4**
C2	**0**	**3**
Gini=0.361		
Error=0.3		

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

Error(Children)

=3/10 * 0 + 7/10 * 3/7 = 0.3

Gini improves !!

4.2. Decision Tree based Methods

4.2.3. Decision Tree Induction

Issue 3: Stopping Criteria

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have the same 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

4.2. Decision Tree based Methods

4.2.4. Model Overfitting

Classification Errors

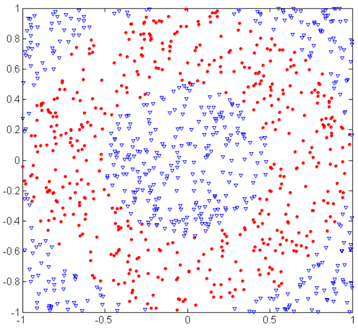
		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

- Most widely-used metric:

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

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

Underfitting and Overfitting (Example)



500 circular and 500 triangular data points.

Circular points:

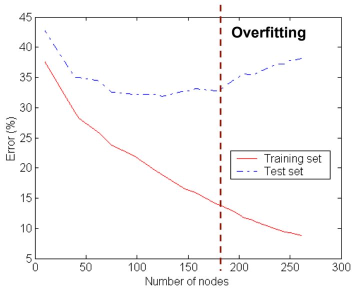
$0.5 \le \text{sqrt}(x_1^2+x_2^2) \le 1$

Triangular points:

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

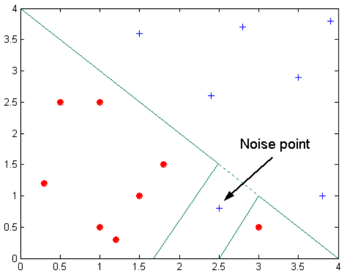
$\text{sqrt}(x_1^2+x_2^2) > 1$

Underfitting and Overfitting



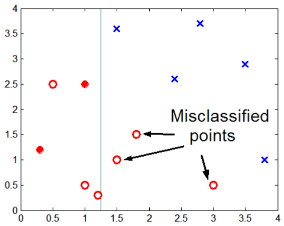
Underfitting: when model is too simple, both training and test errors are large

Overfitting 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
- Need new ways for estimating errors

4.2. Decision Tree based Methods

4.2.4. Model Overfitting

Generalization Errors

Estimating Generalization Errors

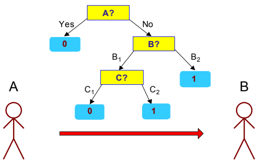
- Training errors: error on training (Σ e(t))
- Generalization errors: error on testing (Σ e’(t))
- Methods for estimating generalization errors:
  - Optimistic approach: e’(t) = e(t)
  - Pessimistic approach:
    - For each leaf node: e’(t) = (e(t)+0.5)
    - Total errors: e’(T) = e(T) + N × 0.5 (N: number of leaf nodes)
    - For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances):
      Training error = 10/1000 = 1%
      Generalization error = (10 + 30×0.5)/1000 = 2.5%
  - Reduced error pruning (REP):
    - uses validation data set to estimate generalization error

Occam’s Razor

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
- For complex models, there is a greater chance that it was fitted accidentally by errors in data
- Therefore, one should include model complexity when evaluating a model

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.

4.2. Decision Tree based Methods

4.2.4. Model Overfitting

Decision Tree Pruning

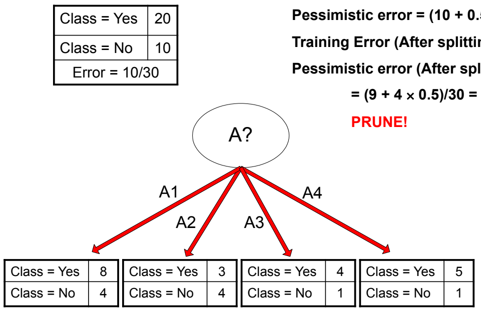
How to Address Overfitting

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

How to Address Overfitting…

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - 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	

Class = Yes	8
Class = No	4

Class = Yes	3
Class = No	4

Class = Yes	4
Class = No	1

Class = Yes	5
Class = No	1

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

PRUNE!

4.2. Decision Tree based Methods

4.2.5. Other Issues

Other Issues

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication

Data Fragmentation

- Number of instances gets smaller as you traverse down the tree
- Number of instances at the leaf nodes could be too small to make any statistically significant decision

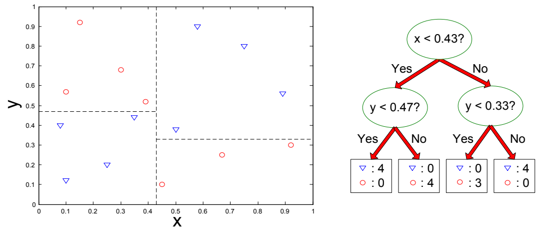
Search Strategy

- Finding an optimal decision tree is NP-hard
- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Other strategies?
  - Bottom-up
  - Bi-directional

Expressiveness

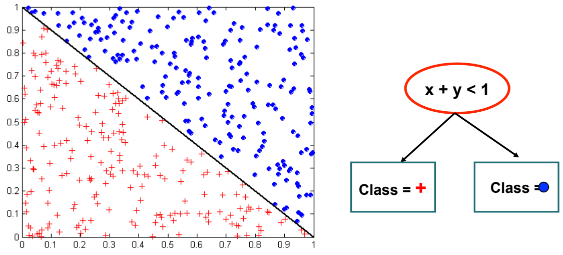
- Decision tree provides expressive representation for learning discrete-valued function
  - But they do not generalize well to certain types of Boolean functions
    - Example: parity function:
      - Class = 1 if there is an even number of Boolean attributes with truth value = True
      - Class = 0 if there is an odd number of Boolean attributes with truth value = True
    - For accurate modeling, must have a complete tree
- Not expressive enough for modeling continuous variables
  - Particularly when test condition involves only a single attribute at-a-time

Decision Boundary



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

Oblique Decision Trees



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