Classification: Decision Tree

CSE 4334 / 5334 Data Mining
Spring 2019

Won Hwa Kim

(Slides courtesy of Pang-Ning Tan, Michael Steinbach and Vipin Kumar, and Jiawei Han, Micheline Kamber and Jian Pei)

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.

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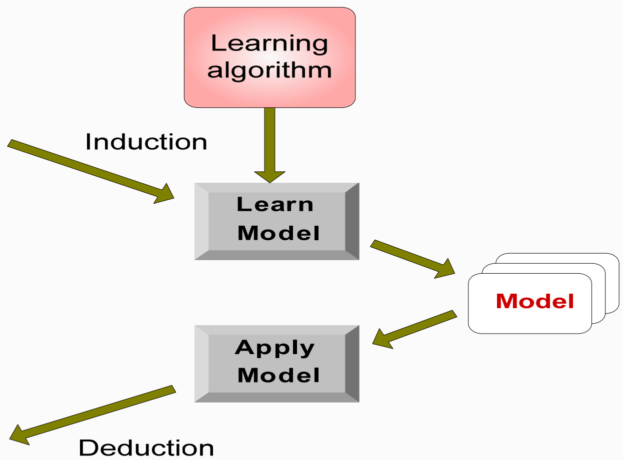
Illustrating Classification Task

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

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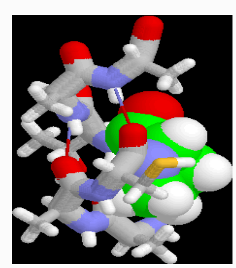
Examples of Classification Task

- 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



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Classification vs. Prediction

Classification

- Predicts categorical class labels
- Most suited for nominal attributes
- Less effective for ordinal attributes

Prediction

- models continuous-valued functions or ordinal attributes, i.e., predicts unknown or missing values
- E.g., Linear regression

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Supervised vs. Unsupervised Learning

Supervised learning (e.g., classification)

- Supervision: The training data (observations, measurements, etc.) are accompanied by labels indicating the class of the observations
- New data is classified based on the training set

Unsupervised learning (e.g., clustering)

- The class labels of training data is unknown
- Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

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Classification Techniques

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

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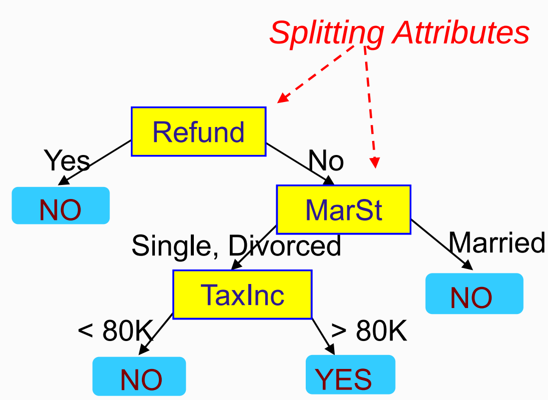
Example of a Decision Tree

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

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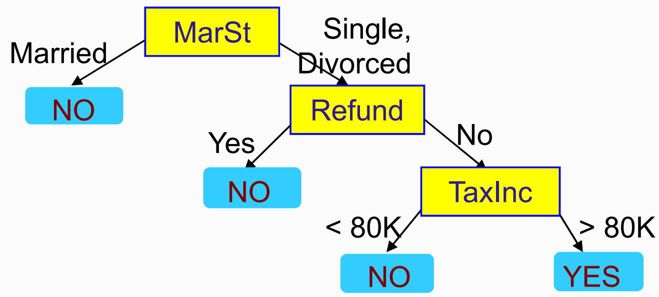
Another Example of Decision Tree

categorical categorical continuous class

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



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

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Decision Tree Classification Task

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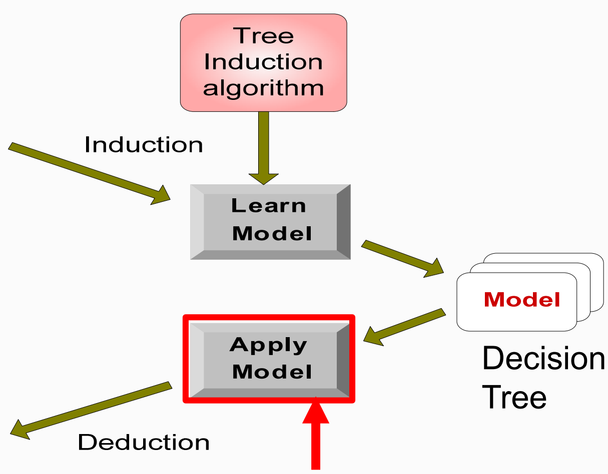
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Set

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

Test Set



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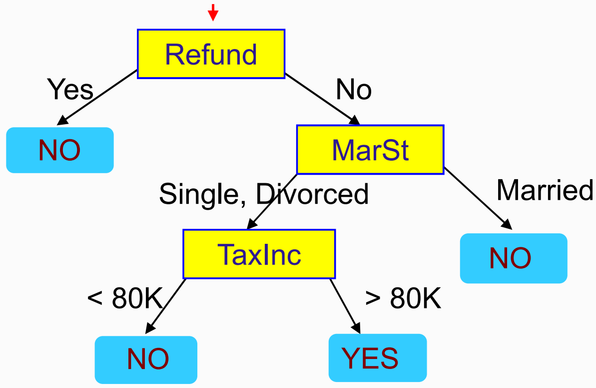
Apply Model to Test Data

Start from the root of tree.



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

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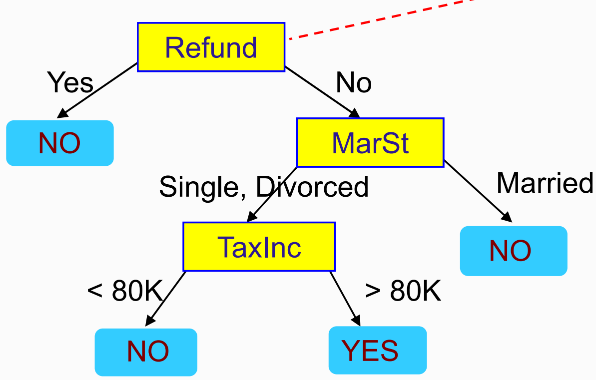
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

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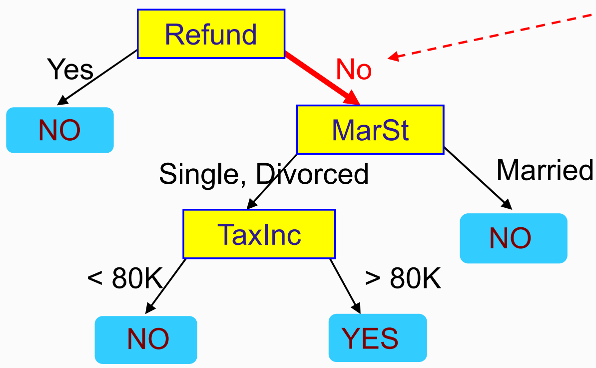
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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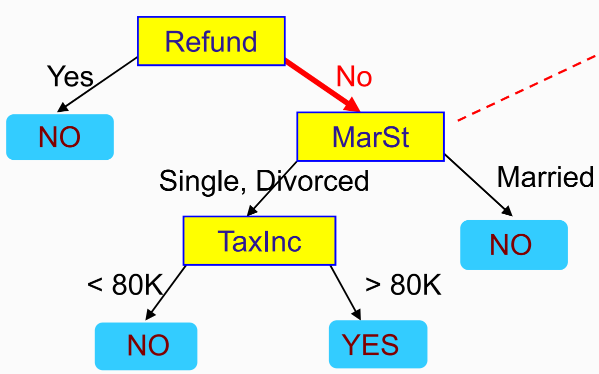
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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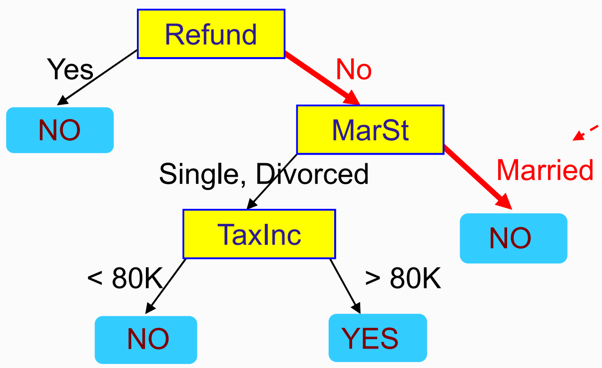
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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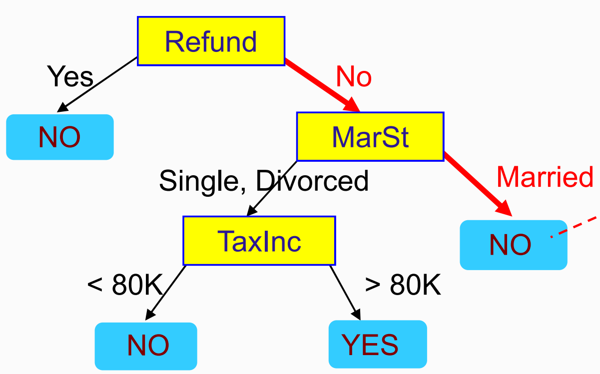
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to "No"

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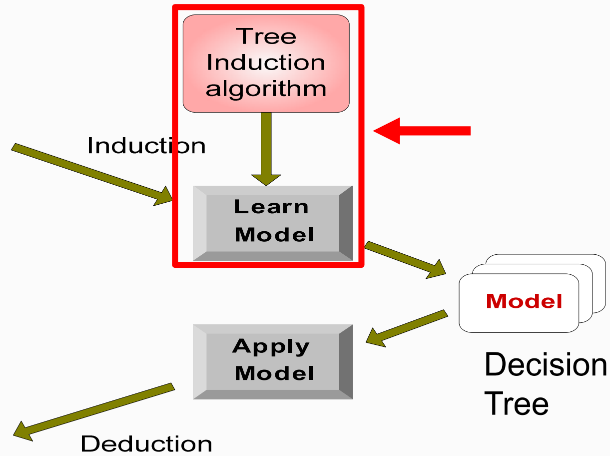
Training Set

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

Test Set



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Decision Tree Induction

Large search space

- Exponential size, with respect to the set of attributes
- Finding the optimal decision tree is computationally infeasible

Efficient algorithm for accurate suboptimal decision tree

- Greedy strategy
- Grow the tree by making locally optimally decisions in selecting the attributes

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Decision Tree Induction

Many Algorithms:

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

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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 majority class among the records of Dt's parent node.
  - If D_t contains records that have identical values on all attributes but the class attribute, then t is a leaf node labeled by the majority class among D_t's records.
  - If none of the above conditions is satisfied, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

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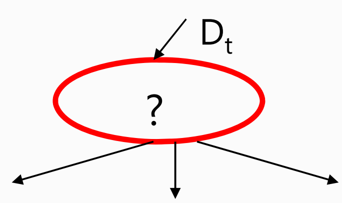

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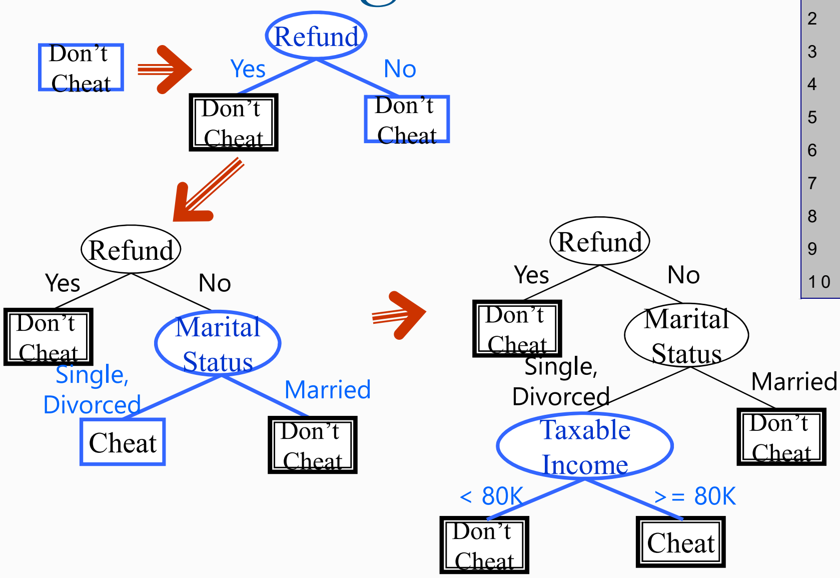
Hunt's Algorithm



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6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

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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

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How to Specify Test Condition?

Depends on attribute types

- Categorical vs. Numeric
  - Categorical attributes: Nominal, Ordinal
  - Numeric attributes: Interval, Ratio
- Discrete vs. Continuous

Depends on number of ways to split

- 2-way split
- Multi-way split

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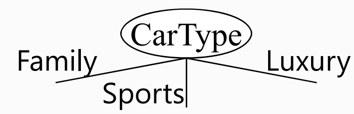
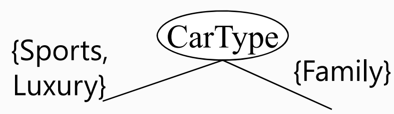
Splitting Based on Nominal Attributes

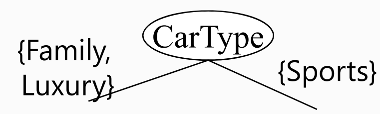
Multi-way split: Use as many partitions as distinct values.



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



OR



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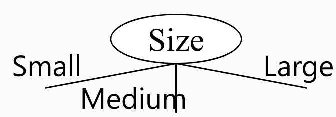
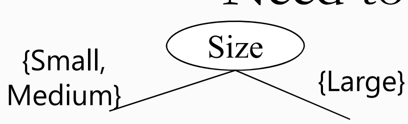
Splitting Based on Ordinal Attributes

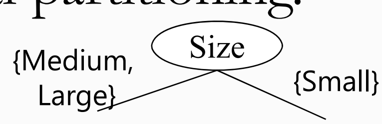
Multi-way split: Use as many partitions as distinct values.



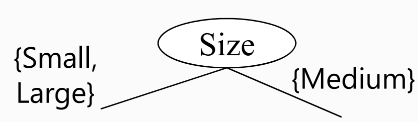
Binary split: Divides values into two subsets. Need to find optimal partitioning.



OR



What about this split?



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Splitting Based on Continuous Attributes

Different ways of handling

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

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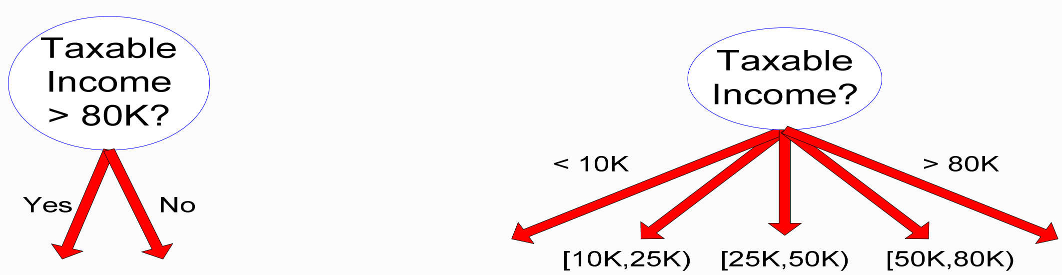
Splitting Based on Continuous Attributes



(i) Binary split (ii) Multi-way split

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Tree Induction

Greedy strategy.

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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

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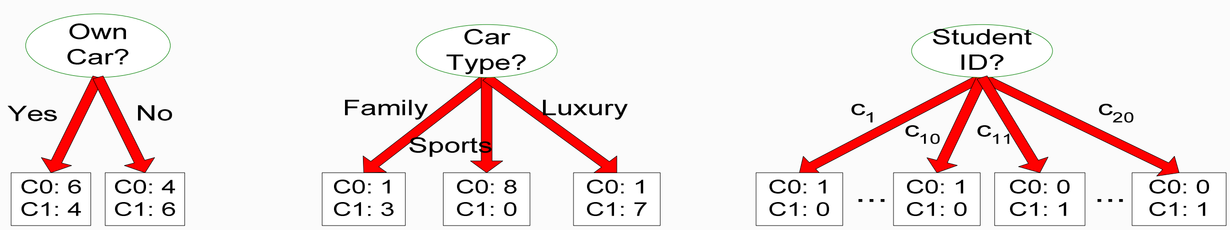
How to determine the Best Split

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



Which test condition is the best?

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How to determine the Best Split

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

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

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Measures of Node Impurity

Gini Index

Entropy

Misclassification error

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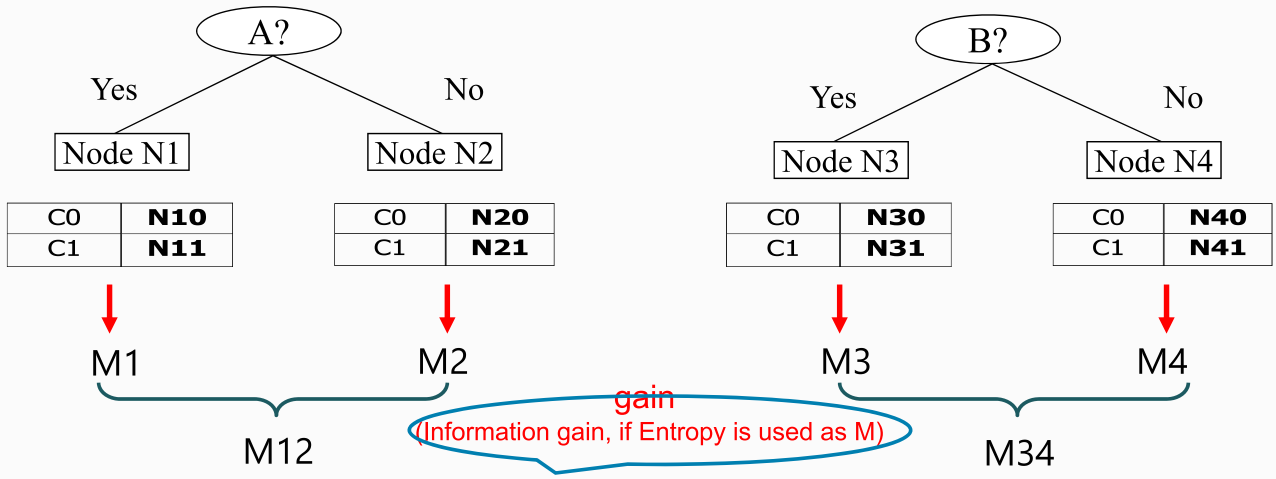
How to Find the Best Split

Before Splitting:

C0	N00
C1	N01

→ M0



Gain = M0 – M12 vs M0 – M34

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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	

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Examples for computing GINI

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

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

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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.

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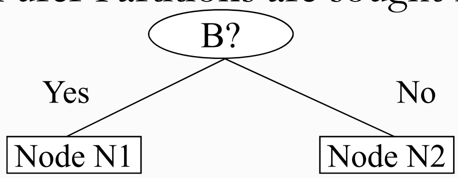
Binary Attributes: Computing GINI Index

- 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=0.371		

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

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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	

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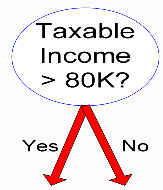
Continuous Attributes: Computing Gini Index

- 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.

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



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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	

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Alternative Splitting Criteria based on INFO

Entropy at a given node t:

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

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

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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) $\log_2$ (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

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Why is that 0 log 0 = 0 ?

$$\lim_{x\to 0} x\, log_2(x) = \lim_{x\to 0} \frac{\frac{ln(x)}{ln(2)}}{x^{-1}} = \lim_{x\to 0} \frac{\frac{x^{-1}}{ln(2)}}{-x^{-2}} = \lim_{x\to 0} \frac{-x}{ln(2)} = 0$$

L'Hospital's Rule (Wikipedia)

If

$\lim_{x\to c} f(x) = \lim_{x\to c} g(x) = 0$ or $\pm\infty$, and

$\lim_{x\to c} \frac{f'(x)}{g'(x)}$ exists, and

$g'(x) \neq 0$ for all x in I with $x \neq c$,

then

$$\lim_{x\to c} \frac{f(x)}{g(x)} = \lim_{x\to c} \frac{f'(x)}{g'(x)}.$$

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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.

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Splitting Based on INFO...

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
- Designed to overcome the disadvantage of Information Gain

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Splitting Criteria based on Classification Error

Classification error at a node t :

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

Measures misclassification error made by a node.

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

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Examples for Computing Error

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

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

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

Error = 1 – max (0, 1) = 1 – 1 = 0

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

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

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

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

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

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

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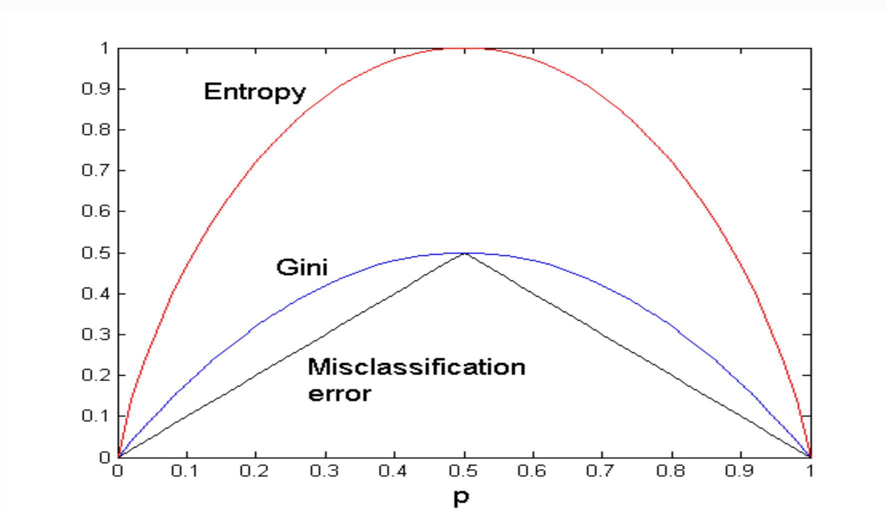
Comparison among Splitting Criteria

For a 2-class problem:



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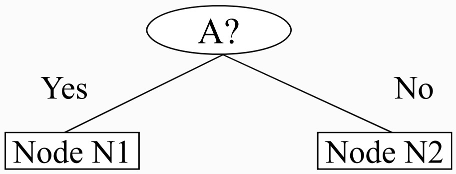
Misclassification Error vs Gini



	Parent
C1	7
C2	3
Gini = 0.42	

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

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

	N1	N2
C1	3	4
C2	0	3
Gini=0.342		

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

Gini improves !!

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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

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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
  - What to do? majority voting
- Early termination, e.g., when the information gain is below a threshold.

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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

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Example: C4.5

Simple depth-first construction.

Uses Information Gain

Sorts Continuous Attributes at each node.

Needs entire data to fit in memory.

Unsuitable for Large Datasets.

- Needs out-of-core sorting.

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

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