Data Mining
Classification: Basic Concepts and Techniques

Lecture Notes for Chapter 3

Introduction to Data Mining

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

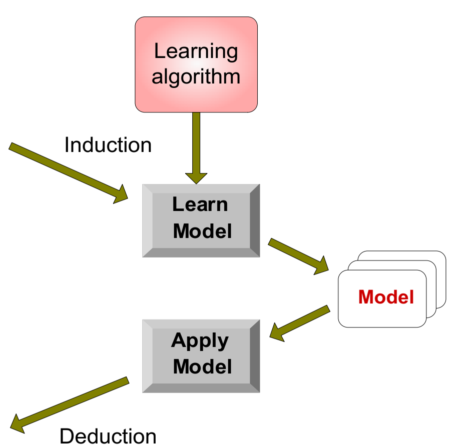
Examples of Classification Task

Task	Attribute set, 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

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

Classification Techniques

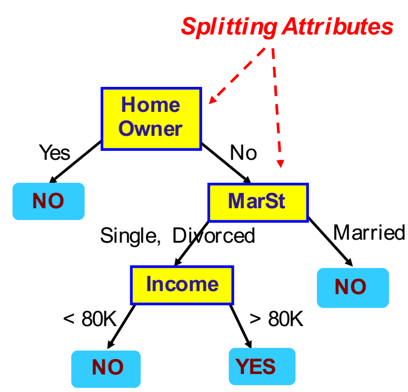
- Base Classifiers
  - Decision Tree based Methods
  - Rule-based Methods
  - Nearest-neighbor
  - Neural Networks
  - Naïve Bayes and Bayesian Belief Networks
  - Support Vector Machines
- Ensemble Classifiers
  - Boosting, Bagging, Random Forests

Example of a Decision Tree

categorical categorical continuous class

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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

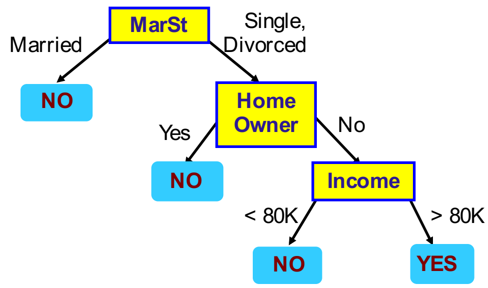


Model: Decision Tree

Another Example of Decision Tree

categorical categorical continuous class

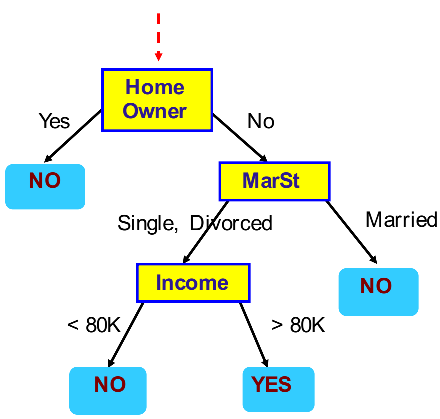
ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



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

Apply Model to Test Data

Start from the root of tree.



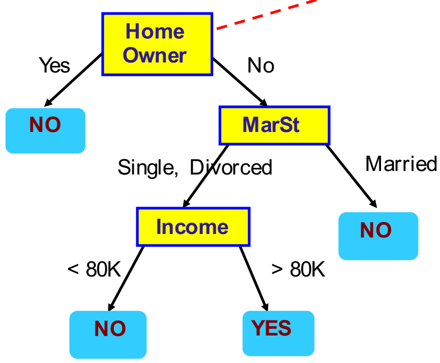
Test Data

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

Apply Model to Test Data

Test Data

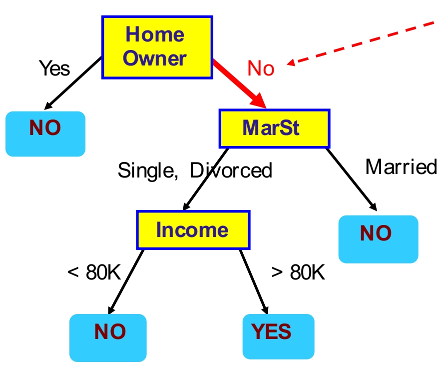
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

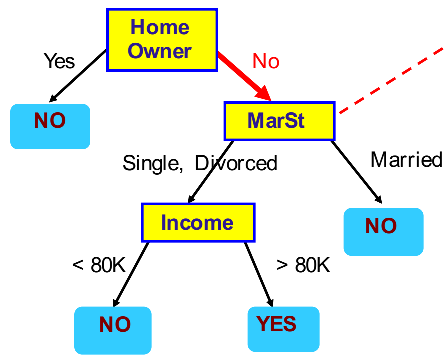
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

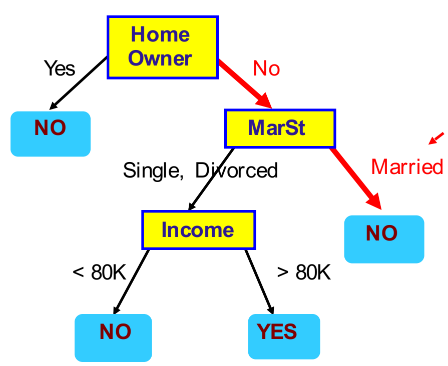
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

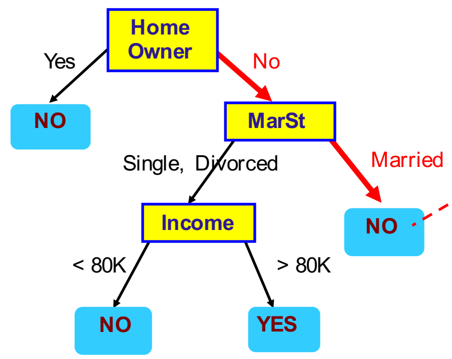
Home Owner	Marital Status	Annual Income	Defaulted Borrower
No	Married	80K	?



Apply Model to Test Data

Test Data

Home Owner	Marital Status	Annual Income	Defaulted Borrower
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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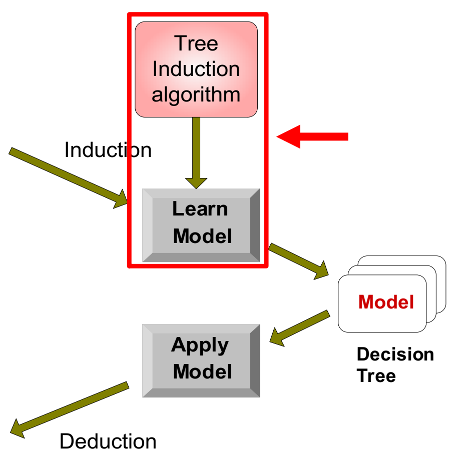
Test Set



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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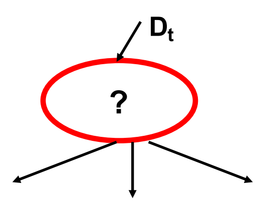
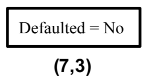


Hunt’s Algorithm



(a)

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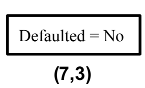
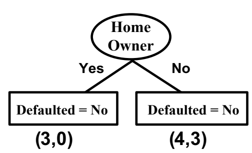
Hunt’s Algorithm



(a)



(b)

ID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
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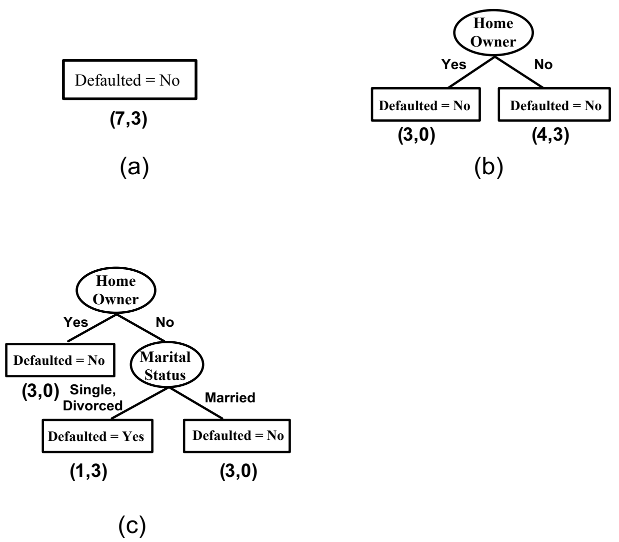
Hunt's Algorithm



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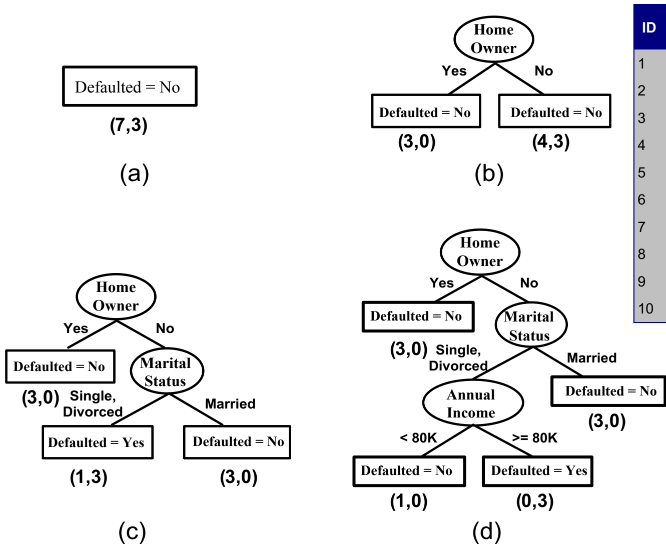
Hunt's Algorithm



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Design Issues of Decision 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

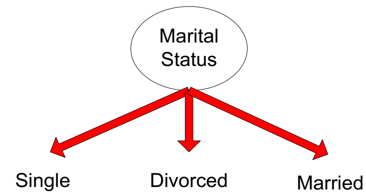
Methods for Expressing Test Conditions

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

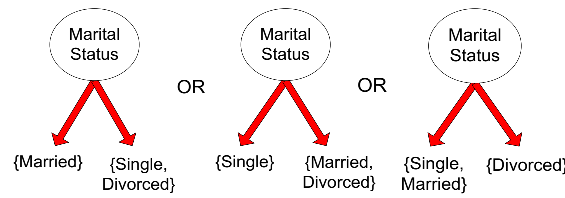
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Test Condition for Nominal Attributes

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

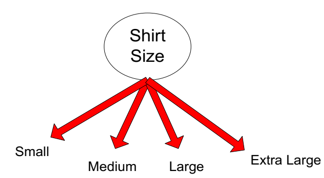


- Binary split:
  - Divides values into two subsets

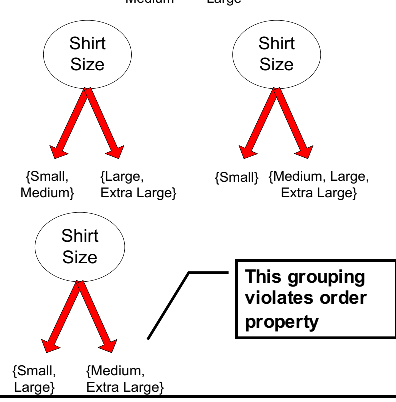


Test Condition for Ordinal Attributes

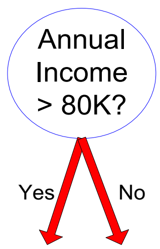
- Multi-way split:
  - Use as many partitions as distinct values



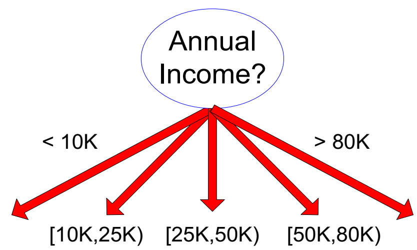
- Binary split:
  - Divides values into two subsets
  - Preserve order property among attribute values



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

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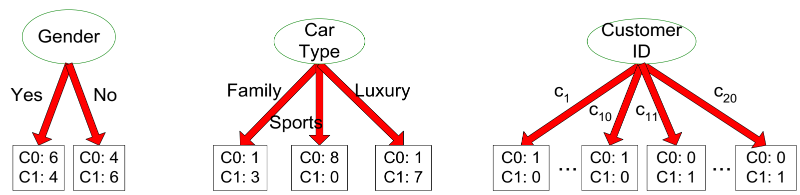
How to determine the Best Split

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?

How to determine the Best Split

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

C0: 5
C1: 5

High degree of impurity

C0: 9
C1: 1

Low degree of impurity

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

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

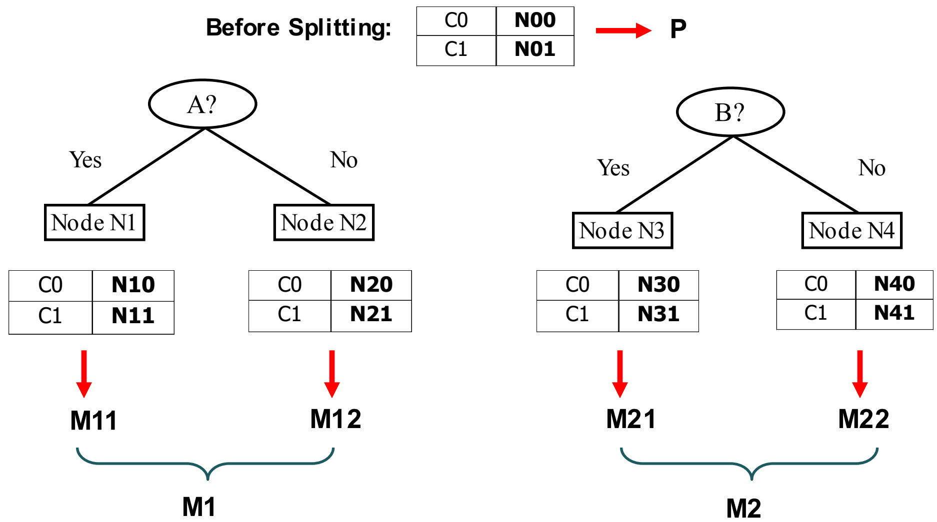
Finding the Best Split

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

   Gain = P – M

   or equivalently, lowest impurity measure after splitting (M)

Finding the Best Split



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

Computing 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,

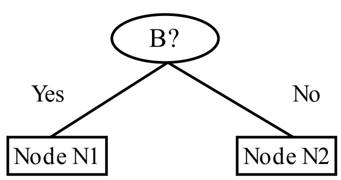
n = number of records at parent node p.

- 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! Repetition of work.

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8	No	Single	85K	Yes
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: 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
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	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...

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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,
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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	1	2												
No							3	4	3	4												
Gini							0.343		0.417													

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

Sorted Values →

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
Annual Income										
	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:

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

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

- 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

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

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:

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

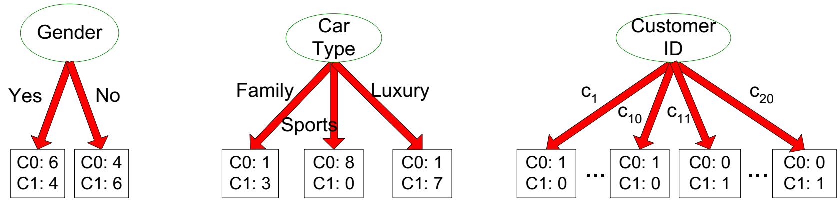
Parent Node, p is split into k partitions;
n_i is number of records in partition i

  – Choose the split that achieves most reduction (maximizes GAIN)

  – Used in the ID3 and C4.5 decision tree algorithms

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

Gain Ratio

- Gain Ratio:

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

Parent Node, p is split into k partitions

n_i is the number of records in partition i

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

Gain Ratio

- Gain Ratio:

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

Parent Node, p is split into k partitions

n_i is the number of records in partition i

	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

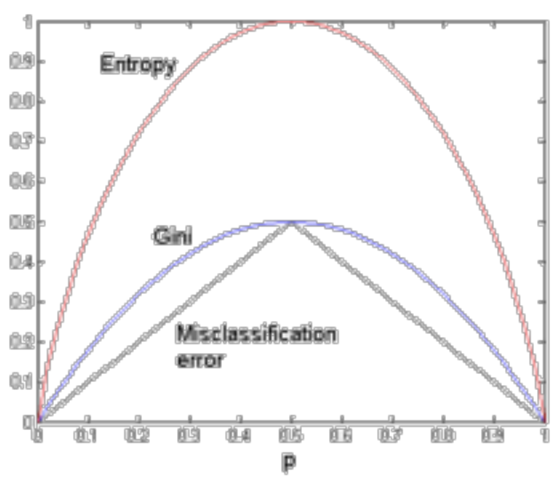
C1	**2**
C2	**4**

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

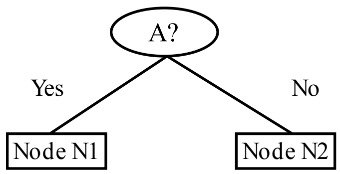
Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Comparison among Impurity Measures

For a 2-class problem:



Misclassification Error vs Gini Index



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

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

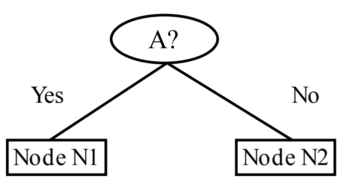
Gini(N2)
= 1 – $(4/7)^2$ – $(3/7)^2$
= 0.489

	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		

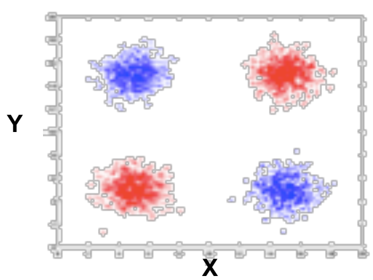
	N1	N2
C1	**3**	**4**
C2	**1**	**2**
Gini=0.416		

Misclassification error for all three cases = 0.3 !

Decision Tree Based Classification

- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Robust to noise (especially when methods to avoid overfitting are employed)
  - Can easily handle redundant or irrelevant attributes (unless the attributes are interacting)
- 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

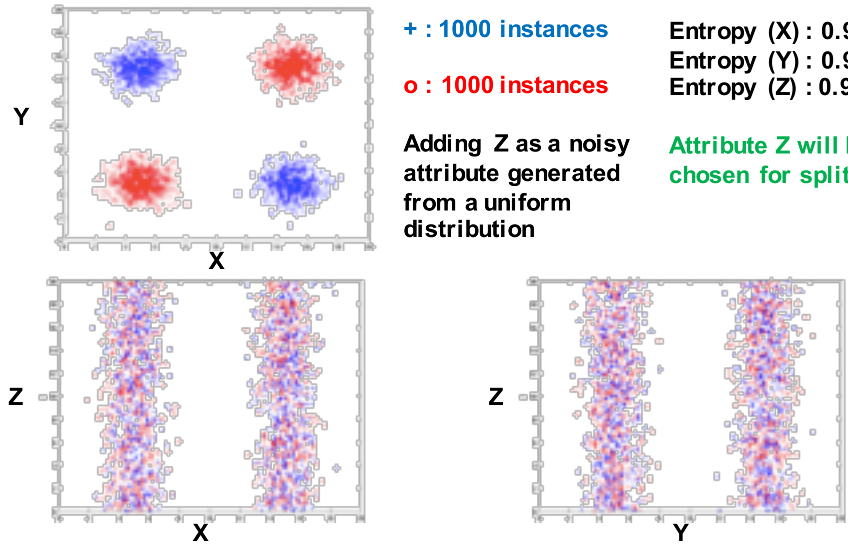


+ : 1000 instances

o : 1000 instances

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

Handling interactions



+ : 1000 instances

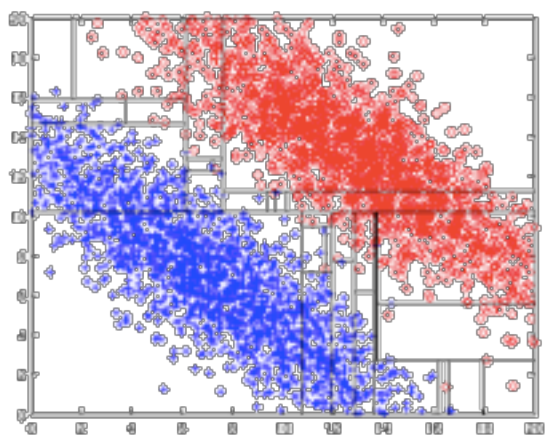
o : 1000 instances

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!

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.