### Managing Big Data Basic Classification: Concepts, Decision Trees and Evaluation

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Given a collection of records (training set)

- > Each record contains a set of **attributes**, one of the attributes is (always) 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.

# The classification problemExample of classification



Goal: Find function f() such that: f (Refund Marital Status Taxable

f (Refund, Marital Status, Taxable Income) = Cheat

### Prerequisites for classification

- > Must have class attribute
- > <u>Class attribute</u> MUST BE discrete
  - I.e. set of values of class attribute countable, fixed and known beforehand.
- Other attributes of records (except class attribute) can be anything: discrete and/or continuous.



#### NOTE:

When class is a continuous attribute, then such tasks are called regression (which you probably know but we won't deal with this). **Basic difference between** classification and regression.

Again, here we're interested only in situations where class is a discrete attribute (=classification).

"Class" also mentioned as: categories, category labels, labels.

 Formal definition of the classification problem

> "Classification is the task of learning a target-function f, that maps each attribute set x to one of the predefined class labels y."

 Target-function f also known as classification model or simply model.

### Usefulness?

### Descriptive modeling

- Used as an explanatory tool for distinguishing objects in different categories
  - E.g. for biologists to explain how a mammal, bird, fish is defined based on some characteristics

### • Predictive modeling

- Used as a tool to predict the label of a class of unknown objects
  - E.g. predict whether or not customers will be defaulting on loans or not

# When does classification perform best?

### Best

> When class attribute is binary (i.e. only has only two distinct values) or is nominal

### Not so good

- When class attribute is ordinal (=values can be ordered e.g. Small, Medium, Large, XLarge)
  - Classification does not take into consideration the ordering that ordinals imply – be careful
- When class attribute resembles hierarchy (category/subcategory)
- Our focus: class attribute is binary or nominal

## Real application domains?

- 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
- k-nearest neighbors
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines (SVD)

## General approach of existing classification techniques

In <u>training set</u>: class of each record already known and correct and this creates the model!

In <u>testing set</u>: class of each record unknown and the goal is to find it by applying the model.



## Performance of model?

- The goal is to find a model that assigns to each record the correct class
- However, errors may occur
  - What is an "Error"? Model puts record in class j when it in reality, it belongs to class k.
- Confusion matrix tells us the performance

		Predicted class by model		
		Class 1	Class 0	
True class it belongs to	Class 1	f <sub>11</sub>	f <sub>10</sub>	
	Class 0	f <sub>01</sub>	f <sub>oo</sub>	

**Confusion matrix:** f11 tells us the number of class 1 items that have been put by algorithm in class 1. In general: fij = number of items in class i predicted by model as class j.

### Performance of model?

- Metrics based on confusion matrix
  - > Accuracy
    - Pct of correctly identified classes

Accuracy =  $\frac{NC}{T} = \frac{f11 + f00}{f11 + f10 + f01 + f00}$ 

- > Error rate
  - Pct of incorrectly identified classes

Error rate =  $\frac{NW}{T} = \frac{f10 + f01}{f11 + f10 + f01 + f00}$ 

### What is a decision tree?

- A hierarchical structure, with nodes and edges, which recursively partitions the data (records) into classes, by examining the values of its attributes.
- Build classification of regression models in the form of a tree (hierarchical structure)
- > Decision trees are models
  - Built by the training set to determine the structure
  - Used by the testing set to assign records into a class
- The basic idea: perform a series of steps/comparisons in order to reach a conclusion (=i.e. class). The decision tree tells you which comparisons to make.

## Decision Tree: example



Training Data

### Model: Decision Tree

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

# Decision Trees Types of nodes in decision trees



 In decision trees, each leaf/terminal node is assigned a class label (i.e. one value of the class attribute)



### Non-terminal nodes (i.e. root and internal nodes) contain test conditions on the record's attributes.



### Edges have labels, indicating the values of the test condition



### Using Decision Trees

- Decision trees (=the model) are built by using the training data
  - > Where the class is already known and correct
- Decision trees (=the model) are used by testing and unknown sets to classify the data

### Using Decision Trees



## How to apply Decision Trees to Test Data ?

## Start from the root of tree and apply conditions to record of test data.



#### Test Data









## How to apply Decision Trees to Test Data ? Test Data



## How to apply Decision Trees to Test Data ?



## How to build Decision Trees?





## How to build Decision Trees?

- Building Decision Tree based on training set using Tree Induction
- Many Algorithms :
  - > Hunt's algorithm (one of the earliest)
  - > CART
  - > ID3, C4.5
  - > SLIQ, SPRINT

# Basic approach of Hunt's algorithm

- Let D<sub>t</sub> be the set of training records that reach a node t
- General Procedure:
  - If D<sub>t</sub> contains records that belong the same class y<sub>t</sub>, then t is a leaf node labeled as y<sub>t</sub>
  - If D<sub>t</sub> is an empty set, then t is a leaf node labeled by the default class, y<sub>d</sub>
  - If D<sub>t</sub> contains records that belong to more than one class (note: this is the training set and we know the class), use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

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



### Hunt's algorithm: example



### Tree Induction

- Greedy strategy (greedy algorithms)
  - Split the records of the training set based on an attribute that optimizes \*now\* a certain criterion
- Some serious issues though
  - > How to split the records?
    - How to specify attribute test condition for nonterminal nodes?
    - Which attribute to select, i.e. how to determine best split?
  - > When to stop splitting?

## How to specify test condition?

- Depends on attribute types of records.
   Can be:
  - > 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. E.g.



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


# 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.



# Splitting based on continuous attributes

O Different ways of handling

- Discretization to form an <u>ordinal categorical</u> <u>attribute</u>
  - 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  $(A \ge v)$ 
  - consider all possible splits and finds the best cut
  - can be more computational intensive

# Splitting based on continuous attributes

Examples of continuous attributes



### Tree Induction

It is the select for split i.e. determine best split?

- Is it possible to somehow measure the "goodness"/quality of a split based on some attribute?
  - If yes, select the split with the best quality
  - (Answer: YES, there are measures.)

# Determine best split Intuitive observations in order to come up with a measure



**This means:** If splitting based on attribute "Own car", then out of all records with value "Yes" in "Own Car", 6 belong in class 0 and 4 in class 1. Q: Which attribute (Own Car, Car Type, Student ID) is better? i.e. Which split is better? ANSWER: Car Type.

# Determine best split

- All algorithms have greedy and divide and conquer approach:
  - Nodes with homogeneous class distribution are preferred
    - Homogeneous? Low impurity, low intermixing of records belonging to different classes, records to belong mostly to one class
- Need a measure of node impurity:

### Split records on attribute A

Non-homogeneous, High degree of impurity Split (same) records on attribute B



Homogeneous, Low degree of impurity

# Measures of node impurity

### Three measures of node impurity

- > Gini index
- > Entropy
- > Misclassification error
- Different algorithms use different node impurity measures. E.g.
  - > ID3, C4.5 uses Entropy
  - > Hunt, CART, SLIQ, SPRINT uses Gini index

### Gini Index

### Gini index for a given node t

$$Gini(t) = 1 - \sum_{j} [p(j|t)]^2$$

...where p(j t) the relative frequency of class j at node t (Note: each node may contain records from any class)

### • Observations:

- Maximum = 1 1/n<sub>c</sub> when records of node t are distributed equally among classes. Greatest impurity
- Minimum = 0.0 when all records of node t belong to only one class. Smallest (no) impurity.
- > Lower values are better/preferred!
- Understanding Gini index? Measures how often (=probability) a randomly chosen record would be placed in the incorrect class.

Gini index

### • Examples: calculating the Gini index for various nodes $Gini(t) = 1 - \sum [p(j|t)]^2$

A node with: 0 rec in class 0, 6 rec in class 1

Class 1 (C1)	0
Class 2 (C2)	6

Class 1 (C1)	1
Class 2 (C2)	5

Class 1 (C1)	2
Class 2 (C2)	4

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1 (rel. fr/prob.) Gini = 1 -  $P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$ 

P(C1) = 1/6 P(C2) = 5/6Gini = 1 - (1/6)<sup>2</sup> - (5/6)<sup>2</sup> = 0.278

P(C1) = 2/6 P(C2) = 4/6Gini = 1 - (2/6)<sup>2</sup> - (4/6)<sup>2</sup> = 0.444

### Gini Index

- Calculate <u>Gini Index for splits</u> (also referred to as "Gini Index of attribute")
- Assume a node p is split (based on attribute) into k partitions ("children") then Gini Index of split:

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

...where n<sub>i</sub> = number of records at node i and **n** = number of records at node p

# Gini Index

• Example: assume binary split. What is the Gini index of this split?



Gini(N1) =  $1 - (5/7)^2 - (2/7)^2 = 0.408^2$ Gini(N2) =  $1 - (1/5)^2 - (4/5)^2 = 0.320^2$ 

Gini(Split or B) = 7/12 \* Gini(N1) + 5/12 \* Gini(N2) = 7/12 \* 0.408 + 5/12 \* 0.320 = <u>0.413 QED</u> Gini index

### • Examples

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

Compute Gini index for "Refund" attribute (i.e. compute Gini index of split based on "Refund"). <u>Cheat is class!</u> If we split based on "Refund" we get:



Gini(Left node) =  $1 - (0/3)^2 - (3/3)^2 = 0$ Gini(Right node) =  $1 - (3/7)^2 - (4/7)^2 = 0.489$ Gini(Right node) =  $1 - (3/7)^2 - (4/7)^2 = 0.489$ Gini(Right node) = 0.3423 QED

### Gini Index – Gini gain

### • Gini gain

The difference between parent node's Gini index and Gini index of split:

Gini<sub>gain</sub> = Gini<sub>Parent</sub> - Gini<sub>Split</sub>

- > Measures how Gini index improves
- > Goal: maximize gain, i.e. this difference, which determines which attribute to select for splitting in this step.
- Important: Used in algorithms to select attributes and build decision trees.



# Gini Index – Gini gain

### • Example

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

Compute Gini gain when splitting on attribute "Refund". <u>Cheat is class!</u>

Gini gain(Refund) = Gini of entire dataset – Gini(Refund)

We have already calculated Gini of attribute "Refund" (=0.3423).

Gini of our entire data set is also called "Gini of overall collection of training examples" or "Gini of system":

Gini(training set) =  $1 - (3/10)^2 - (7/10)^2 = 0.42$ 

Gini gain(Refund) = 0.42 – 0.3423 = 0.0777 QED

# Building Decision Trees Phase-1 Using Gini and Gini gain to build decision trees

Training Data

ID	M	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2

dataset:

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

**STEP 2:** Compute Gini index for each attribute (Split): Gini(M) = (3/6)\*0 + (3/6)\*0.444 = 0.222Gini(N) = (2/6)\*0 + (2/6)\*0.5 + (2/6)\*0.5 = 0.333Gini(Q) = (2/6)\*0.5 + (2/6)\*0.5 + (2/6)\*0 = 0.333

**STEP 3:** Calculate Gini gains for each attribute: **Gini Gain(M) = 0.444 - 0.222 = 0.222 (biggest!)** Gini Gain(N) = 0.444 - 0.333 = 0.111Gini Gain(Q) = 0.444 - 0.333 = 0.111

Hence, first split based on attribute M

# Building Decision Trees Phase-2

### Training Data

ID	Μ	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2



 $M1 \rightarrow R2$ 

Here, non-homogeneous node. Apply same method to split based on other attribute. Tree will grow at this branch.

# Building Decision Trees

Phase-3

### Training Data

ID	Μ	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2

### Calculate again with the same steps.

**STEP 1:** Compute Gini index for our **new "entire" dataset** (leave out red-ish rows. These have already been classified):

#### Gini = $1 - (2/3)^2 - (1/3)^2 = 0.444$

STEP 2: Compute Gini index for each attribute: Gini(N) = (1/3)\*0 + (1/3)\*0+(1/3)\*0 = 0Gini(Q) = (1/3)\*0 + (1/3)\*0 + (1/3)\*0 = 0

**STEP 3:** Calculate Gini gains: Gini Gain(N) = 0.444 – 0.0 = **0.444** Gini Gain(Q) = 0.444 – 0.0 = **0.444** 

Equal Gini gains. Hence, both are equally good. choose one of N, Q. Assume we choose N (can also choose Q).

# Building Decision Trees Phase-4

### Training Data

ID	Μ	Ν	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2



# Computing Gini Index for categorical attributes

- 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					
Gini(CarType)						

Two-way split (find best partition of values)

	CarType			CarT	уре
	{Sports, Luxury}	{Family}		{Sports}	{Family, Luxury}
C1	3	1	C1	2	2
C2	2	4	C2	1	5
Gini	0.400		Gini	0.4	19

Note: for k categorical values you need to check  $(2^{k} - 2)/2 = 2^{k-1} - 1$  partitions

# Computing Gini Index for **continuous** attributes

- 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  $A \ge v$

Simple method to choose best v

- For each v, scan the database to gather count matrix and compute its Gini index
- Computationally Inefficient! Complexity: O(n<sup>2</sup>) computing Gini.
  - 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



# Computing Gini Index for **continuous** attributes

- How to improve speed?
- For efficient computation: for each attribute,
  - Sort the attribute on values. Complexity O(nlogn) =>better!
  - Linearly scan these values, each time updating the count matrix and computing Gini index. Some optimization tricks:
    - Choose split points at midpoint between values
    - Identify adjacent examples that differ in their target (class) labels and attribute values => Set of <u>candidate splits</u>

Calculate Gini Index and choose the split position that has the least gini index

	Cheat		No		Nc	)	N	0	Ye	S	Ye	S	Ye	es	N	lo	N	lo	N	lo		No	
			Taxable Income																				
Sorted Values		(	60		70	)	7	5	85	5	9(	)	9	5	1(	00	12	20	1:	25		220	
Split Positions		5	5	6	5	7	2	8	0	8	57	9	2	9	7	11	0	12	22	17	2	23	0
		<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
	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	0.4	20	0.4	00	0.3	<b>575</b>	0.3	43	0.4	117	0.4	100	<u>0.3</u>	<u>800</u>	0.3	43	0.3	875	0.4	00	0.4	20

Alternative splitting criteria (besides Gini): **Entropy** 

Entropy – measures information (INFO)
 Calculate Entropy for node t :

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

...where p(j | t) the relative frequency of class j at node t. (note  $log = base-2 logarithm i.e. log_2$ )

Measures homogeneity of a node

- Maximum = log n<sub>c</sub> when all records of node equally distributed among classes
- Minimum = 0.0 when all records of node belong to one class

### Intropy measures information in a node

- Yes, you can measure amount of information!
- Intuitively: when all records of node belong to one class, implies most information. Wen records of node belong to different classes, least information
- > Try to maximize amount of information gain
- Entropy based computations similar to Gini Index computations.

### • Examples: calculating the Entropy for various nodes Entropy(t) = $-\sum p(j|t)\log p(j|t)$

A node with: 0 rec in class 0, 6 rec in class 1

Class 1 (C1)	0
Class 2 (C2)	6

Class 1 (C1)	1
Class 2 (C2)	5

Class 1 (C1)	2
Class 2 (C2)	4

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1 (rel. fr/prob.) Entropy =  $-0\log_2 0 - 1\log_2 1 = 0$  (note:  $0\log_0 = 0$ )

 $P(C1) = 1/6 \qquad P(C2) = 5/6$ Entropy = - (1/6)log<sub>2</sub> (1/6) - (5/6)log<sub>2</sub> (5/6) = 0.65  $P(C1) = 2/6 \qquad P(C2) = 4/6$ Entropy = -(2/6)log<sub>2</sub> (2/6) - (4/6)log<sub>2</sub> (4/6) = 0.92

### Entropy of split

> Assume node p is split into k children, then Entropy of split (or Entropy of attribute):

$$Entropy_{SPLIT} = \sum_{i=1}^{k} \frac{n_i}{n} Entropy(i)$$

...where n<sub>i</sub> = number of records at node i, Entropy(i) = Entropy of node/child i, n = number of records at node p. Note: Compare to Gini Index of Split: Similar!

Information gain

Measuring the gain of information when splitting on an attribute. Assume parent node p split into k partitions (children):

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

...where **n**<sub>i</sub> number of records at node **i**, **n** # of records at parent and **Entropy(i)** entropy of child i (note similar to Gini)

- Measures reduction in entropy because of split. Choose split that achieves most reduction (maximizes GAIN)
- <u>Disadvantage</u>: Prefers splits resulting in large number of "pure" nodes/partitions (pure=low intermixing)

# Building Decision Trees Phase-1 – **Using Entropy**

### Training Data

ID	Μ	Ν	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Ql	R1
4	M1	N2	Ql	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2

**<u>STEP 1:</u>** Compute Entropy for our entire training data (Entropy of node):

Entropy Node =  $-(2/6)\log_2(2/6) - (4/6)\log_2(4/6) = 0.9182$ 

**STEP 2:** Compute Entropy for each attribute of node i.e. split node based on each attribute (split – use formula on slide 62): Entropy(M) = (3/6)\*0 + (3/6)\*[-(2/3)\*log2(2/3) - (1/3)\*log2(1/3)] = 0.4591Entropy(N) = (2/6)\*0 + (2/6)\*1 + (2/6)\*1 = 0.6666Entropy(Q) = (2/6)\*1 + (2/6)\*1 + (2/6)\*0 = 0.6666

**STEP 3:** Calculate Entropy gains for each attribute: **Entropy Gain(M) = 0.9182 - 0.4591 = 0.4591 (biggest!)** Entropy Gain(N) = 0.9182 - 0.6666 = 0.2516Entropy Gain(Q) = 0.9182 - 0.6666 = 0.2516

Hence, first split based on attribute M (biggest gain)

# Building Decision Trees Phase-2 – **Using Entropy**

leaf.

 $M1 \rightarrow R2$ 

We make a rule:

### Training Data

ID	Μ	Ν	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2



Here, non-homogeneous node. Apply same method to split based on other attribute. Tree will grow at this branch.

Root node of tree will be

# Building Decision Trees Phase-3 – **Using Entropy**

### Training Data

ID	Μ	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2

#### <u>Calculate again following the same steps (leave out red</u> <u>rows).</u>

**STEP 1:** Compute Entropy for our **new "entire" node/dataset** (leave out red-ish rows. These have already been classified):

Entropy node =  $-(2/3)\log_2(2/3) - (1/3)\log_2(1/3) = 0.9182$ 

**STEP 2:** Compute Entropy for each attribute (use formula on slide 62): Entropy(N) = (1/3)\*0 + (1/3)\*0+(1/3)\*0 = 0Entropy(Q) = (1/3)\*0 + (1/3)\*0 = 0

**STEP 3:** Calculate Entropy gains: Gini Gain(N) = 0.9182 – 0.0 = **0.9182** Gini Gain(Q) = 0.9182 – 0.0 = **0.9182** 

Equal Entropy gains. Hence, both attributes are equally good. Choose one of N, Q. Assume we choose N (can also choose Q).

# Building Decision Trees Phase-4 – **Using Entropy**

Training Data

ID	Μ	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2



# Entropy – Gain ratio

### Gain ratio

- alternative way instead of information gain to solve information gain problems.
- Assume node p is split into k partitions (children)

 $GainRATIO = \frac{GAIN_{SPLIT}}{SplitINFO} \qquad SplitINFO = -\sum_{j=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$ 

### ... where n<sub>i</sub> is number of records in partition i

 Adjust information gain by the entropy of the partition. Large number of small partitions is penalized (i.e. higher entropy partitions)

Overcomes disadvantages of Information gain
 Used in C4.5

#### Example – Entropy split/ attribute

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

<u>Compute Entropy for "Refund"</u> attribute (i.e. compute Entropy of split based on "Refund"). <u>Cheat is class!</u> If we split based on "Refund" we get:



Entire dataset

Entropy(Refund="yes") =  $-(3/3)\log(3/3) - (0/3)\log(0/3) = 0$ Entropy(Refund="no") =  $-(3/7)\log(3/7) - (4/7)\log(4/7) = 0.9852$  Entropy(Refund) = (3/10) \* 0 + (7/10) \* 0.9852 = <u>0.6894</u> QED

#### Compute **Entropy gain** for split on "Refund" attribute. <u>Cheat is class!</u>

3

Cheat=

### Example – Entropy Gain

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	

Entropy

Entire dataset



Calculate Entropy for parent node (entire dataset): Entropy(dataset) = -(3/10)log(3/10) – (7/10)log(7/10)= = <u>0.8812</u>

Entropy(Refund) = 0.6894 (see previous slide)

Entropy Gain = 0.8812 - 0.6894 = 0.1918 QED

Alternative splitting criteria (besides Gini): Classification error

Classification error at node i

 $Error(i) = 1 - max_i(p(i|t))$ 

 Measures misclassification error made by a node.

 Maximum = 1-1/n<sub>c</sub> when records are equally distributed among all classes

Minimum = 0.0, when all records belong to one class

# Classification error

### Examples: calculating the Classification error for various nodes

A node with: 0 rec in class 0, 6 rec in class 1

Class 1 (C1)	0
Class 2 (C2)	6

Class 1 (C1)	1
Class 2 (C2)	5

Class 1 (C1)	2
Class 2 (C2)	4

 $\overline{Error(i)} = 1 - max_i(p(i|t))$ 

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1 (rel. fr/prob.) Error = 1 - max(0, 1) = 1-1 = 0

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

Error =  $1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$ 

P(C1) = 2/6 P(C2) = 4/6Error = 1 - max(2/6, 4/6) = 1 - 4/6 = 1/3
### **Building Decision Trees**

#### Using criteria Entropy and Classification error to build Decision Trees in the same way the Gini index is used

#### Training Data

ID	Μ	N	Q	R
1	M1	N3	Q2	R2
2	M2	N3	Q2	R1
3	M2	N2	Q1	R1
4	M1	N2	Q1	R2
5	M2	N1	Q3	R2
6	M1	N1	Q3	R2

**STEP 1:** Calculate Entropy/Classification error for system

**STEP 2:** For each attribute compute Entropy/Classification error (Entropy split/attribute etc)

**STEP 3:** Calculate gains. Choose attribute with biggest gain and make it node....

... etc ...

## Comparing splitting criteria

#### • For a **2-class problem** (Q: why 2-class?)



# Stopping criteria for Tree induction

- Stop expanding when training set is empty
- 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

## Note on evaluation metrics

## **Evaluation** metrics



- Accuracy
  - Correctly identified categories (all)
- Precision
  - Proportion of positive class identification was correct = TP / (TP + FP) i.e.

Recall

- Recall
  - Proportion of actual positives was correct = TP / (TP + FN) i.e. how much of actual positive were identified.
- F-measure (0 to 1) the greater the better.
  - Single number for Precision and Recall: F-measure = (2\*Precision\*Recall)/(Precision + Recall) i.e. harmonic mean!

Important: Above is a 2 class problem. Yet, can generalize Accuracy/Precision/Recall to problems with more than 2 classes.

## **Evaluation metrics**

		Predicted class by model		
		Positive	Negative	
True class it	Positive	True Positive	False Positive	
belongs to	Negative	False Negative	True Negative	

#### • When to use Precision, Recall, F-measure?

- > When your classification dataset is imbalanced
  - When the distribution of rows in known classes is biased or skewed in the training set!
    - More clearly: don't have the same amount of obs in each class in your training set. Severe
- > Type of research
  - E.g. In medicine, false negative much more important than say false positive. Hence, Recall much more important. For YT recommendations, Precision better.
- If balanced, accuracy is fine.

 In R, two ways of building and using Decision Trees

#### > Using the rpart package

- Recursive partitioning for classification
- Documentation
  - See: https://cran.r-project.org/web/packages/rpart/rpart.pdf
- > Using the tree package
  - Example in R presented in next slides
    - Code in next slide(s) uses Carseats dataset of package ISLR, a simulated dataset containing sales of child car seats at 400 different stores

#### Building/training a decision tree in R (tree library)

#includes the Carseats dataset, a simulated dataset containing sales of child car seats at 400 different stores library(ISLR) #library for Classification and Regression Trees library(tree) #Add Carseats dataset to R's path making thus Carseats dataset available to R attach (Carseats) #Take a quick look at the data (peek at data) head(Carseats) # The aim of this example is to predict the value for the Sales attribute in the Carseats dataset (i.e. class=Sales). However, # Sales attribute is continuous hence we have to transform it into a discrete (=categorical) variable. #take a look at the values of attribute Sales in the Carseats dataset range(Sales) #Sales is a continuous attribute ranging from 0.00 up until 16.27. We make an assumption and say that if Sales >= 8 then Sales is High, #otherwise not. High = ifelse(Sales>=8, "Yes", "No") # Now High is a list containing Yes/No values, one for each record in dataset # We must now attach High to the Carseats dataset, increasing its dimension by 1. Carseats = data.frame(Carseats, High) # The Sales attribute is no longer needed, since we have transformed it into a discrete value as specified by High. Sales # is the first attribute of the Carseats dataset, so get rid of it (i.e. remove it from the Carseats dataset). Dimension reduces by 1 Carseats = Carseats[,-1] # We have made our class attribute a distinct value. Now, select randomly some records from Carseats in order to create the training # dataset set.seed(2) # initialize random number generator. Note: if you keep 2, the same records will always be selected # Create training set. Get 200 random numbers from 1 to 400. train = sample( 1:nrow(Carseats), nrow(Carseats)/2) # Train contains the indexes of the records in Carseats that will be included into the training set. Create the actual dataset training data = Carseats[train,] # Create the decision tree using the training data. We want to predict High based on tree model = tree(High~., training data) # Decision tree built. Variable tree model holds now our Decision tree as it has been created from the training set. Now visualize it plot(tree model) text(tree model, pretty=0)

#### Using Decision tree to classify testing data in R (tree library)

#...continued from previous slide ...

# Now that we have built/trained our decision tree, apply it on the testing dataset

# First, select records from Carseats that will comprise our testing dataset. Note: # the testing dataset has the High attribute <u>but we will not remove it</u>. This is # because we will need this to calculate accuracy and error rate. In addition, the # tree library will ignore this attribute anyway.

testing\_data = Carseats[test,]

# Peek at testing data

head(testing data)

# Predict the class attribute (High) for the testing dataset. Apply testing dataset tree predict = predict(tree model, testing data, type="class")

# Prediction done. Now tree\_predict is a one dimensional data structure (separate # from testing dataset) that holds one value "Yes"/"No" for each record in testing # set. I.e. the first value in tree\_predict corresponds to the first record in # testing set.

# Now, try to evaluate how well our testing data was classified by calculating the # Confusion Matrix. There are two ways to do this:

# Using the 'table' command, which

# compares tree\_predict and attribute High from testing dataset like this: testingDataConfusionTable = table(tree\_predict, testing\_data\$High)

# Ok, let's calculate some quality metrics of the model, in order to see how # our model performed. We calculate accuracy and error rate of the classifier/mocel

# Calculate accuracy
modelAccuracy = sum( diag(testingDataConfusionTable)/sum(testingDataConfusionTable))

# Calculate Error rate (note could also use 1-modelAccuracy)
modelErrorRate = 1 - sum( diag(testingDataConfusionTable)/sum(testingDataConfusionTable))

# Print the result out nicely. We looooooooove nice and clear responses.
sprintf("Model accuracy: %f, model error rate:%f", modelAccuracy,modelErrorRate )

# You can also use a different library (instead of table) for calculating the confusion matrix library(caret) #needed for confusion matrix. Install this package (may take a while) # Compare tree\_predict and attribute High from testing dataset by showing the confuction # matrix. Look at matrix and accuracy confusionMatrix(tree predict, testing data\$High)

## **Evaluation**

Practical issues of classification

- Important aspects of classification using Decision Trees
  - > Underfitting and Overfitting
  - > How to cope with missing values?
  - > Cost of classification

- There are two types of errors when dealing with decision trees
  - Training errors (aka resubstitution errors aka apparent error)
    - Number of misclassifications of records in the training set
  - > Generalization errors
    - Expected errors of misclassifications when model is applied on unknown records (or the testing set)
- How to measure misclassification? (see confusion matrix)
  - > Absolute number of records wrongly classified
  - Pct of records wrongly classified

- Misclassification on training set? Isn't this impossible?
  - > Given consistent training set, will algorithms produce zero error on training set?
  - > Considering termination conditions:
    - Training set empty: zero error
    - All records have the same class: zero error
    - No attributes left to split: impossible (consistent training set)
    - No attribute with positive information gain: possible bur unusual
  - So, in general, under such circumstance it is impossible (occasional possible)

- Misclassification on training set? Isn't this impossible?
  - > Assume now inconsistent training set
  - > Consider termination conditions
    - Training set empty: zero error
    - All instances have the same class: zero error
    - No attributes left to split on: inconsistent class.
       Choosing most common class minimizes error
    - No attribute has positive information gain: possible but unusual
  - So, in such situations, it is possible. You have a minimum error on the classification of the training set (training error)

Reasons for errors on the training set

- > Training set is not a good sample
- > (consistent) Noise on some attributes
- > Missing attribute values
- > Some class values present in small amounts

- Are training errors and generalization errors –for a particular model-related?
- Is the following true?
  - \* "Assume two models (also called Hypothesis) A and B over the same training set. If training\_error(A) < training\_error(B) then Generalization\_error(A) < Generalization\_error(B)" ?
    - No. That's WRONG!

### Underfitting

#### • Underfitting

- > When both training errors and generalization errors are large.
  - Happens when Decision Tree is too simple (i.e. small number of nodes)
  - When Decision tree has few nodes, it can't deduce the structure/relationships of attributes
    - Some data will not fit. Hence errors.

## Overfitting

#### Overfitting

- > When training error is very small but generalization errors are large
  - Happens when the Decision Tree adapts too well on the training data. I.e. perfectly fits training data and hence works only for training data !
  - Happens when Decision Tree grows large and complex (large number of nodes)



#### Notes on overfitting

 Overfitting results in decision trees that are more complex than necessary

- > Complex? => More nodes
- 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

 Important step to improve complex decision trees

# Estimating generalization errors

#### Assume

- > e(t) = Error on training set
- > e'(t) = Error on testing/unknown set (same model)
- Two approaches to estimating generalization errors
  - > Optimistic approach
    - Assumes that e(t) = e'(t)
    - As discussed, rather not good estimation
      - Especially for complex decision trees due to overfitting

# Estimating generalization errors

 Two approaches to estimating generalization errors (cont.)

#### > Pessimistic approach

- The idea: give complex decision trees a penalty and calculate a pessimistic/increased error due to this complexity
  - Affects leaves of tree

Pessimistic error for a decision tree (or subtree!) T, e<sub>a</sub>(T)

$$e_g(T) = \frac{\sum_{i=1}^{k} [e(t_i) + \Omega(t_i)]}{\sum_{i=1}^{k} n(t_i)} = \frac{e(T) + cn_l}{N_t}$$

...where e(T) = generalization error of decision tree,  $N_t$  = number of records in training set,  $n_t$  = number of leaves in decision tree and c = penalty (usually 0.5)



Estimated pessimistic error for decision tree:  $e_g(T) = (3+0.5*2) / 12 = 0.333$ (Note: if there were 3 "children"/nodes (same #records and error): (3+0.5\*3)/12 = 0.375 (increased penalty for complexity)

## Addressing Overfitting

#### Tree pruning

- Pruning? Get rid/remove of some sections of the decision tree
- Reduces the complexity of the tree (due to removal of nodes)
- > That way improves accuracy and addresses overfitting
- Two approaches to pruning
  - > Pre-pruning
  - > Post-pruning

#### How to address Overfitting

#### Pre-Pruning (Early Stopping Rule)

- Stop the algorithm before it becomes a fully-grown tree during the training phase
- > 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
  - Apply  $\chi^2$  test to check if class distribution of instances are independent of the available features. If so, stop
  - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

### How to address Overfitting

#### Post-pruning

- Srow decision tree to its entirety from the training set
- 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
   Use of pessimistic error
- Class label of leaf node is determined from majority class of instances in the sub-tree
- Can use other methods e.g. MDL for postpruning

## **Example of Post-Pruning**



# Estimating generalization errors

#### What does penalty of 0.5 mean?

 Means that for binary split, a node should always be grown along children if classification improves at least one record

Is in general cheaper

## **Missing values**

#### Handling missing 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

#### Missing values – computing impurity measure – Entropy Gain

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	<b>C</b>
6	No	Married	60K	No	
7	Yes	Divorced	220K	No	
8	No	Single	85K	Yes	
9	No	Married	75K	No	
10	?	Single	90K	Yes	
Probability of this – gain					E

#### $\frac{\text{Before Splitting:}}{\text{Entropy(Parent)}}$ = -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

#### <u>Split on Refund:</u>

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

Entropy Gain = 0.9 \* (0.8813 – 0.551) = 0.3303

# Missing values – How to distribute instances

	Tid	Refund	Marital Status	Taxable Income	Cla	SS		
	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	5		
	6	No	Married	60K	No			
	7	Yes	Divorced	220K	No			
	8	No	Single	85K	Yes	5		
	9	No	Married	75K	No			
RefundYesNo								
Class=Yes		Yes	0	Class=Y	es		2	
Class=No		No	3	Class=N	10		4	



# Missing values – Classifying unknown records





## Summary

- Classification is the problem of predicting the value of a categorical attribute (called the class) from a set of categorical/discrete/continuous attributes
- Decision Trees are one form of solving this problem
  - > Easy to understand
  - > Easy to implement
  - > Easy to use
  - Computationally cheap
- Decision Trees are created (grown) from training sets, where the class is known and applied to testing and unknown data
- Decision Trees have also problems though
  - Most important one is Overfitting
## Appendices

## Appendix A: Gini index of node

## Proof of the "Gini Index of node" formula:

Assume **m classes**, with  $i \in \{1, 2, 3, ..., m\}$  denoting the class and  $f_i$  the fraction of items of a node labelled as belonging to class i . Assume now a randomly selected record labelled as belonging to class i. The probability of this random record <u>to NOT belong to class i</u> is  $(1-f_i)$ . Since all records are **not drawn with equal probability**, the probability of selecting an item labelled as belonging to class i is  $f_i$ . Hence, drawing a random record with label i, and the selected record not belonging to class i has probability  $P(i) = f_i(1-f_i)$ where P(i) means the probability of selecting record labelled as belonging to i, and record does not belong to class I (i.e. is error) The total probability of error will hence be:

 $P(1 \text{ } OR 2 \text{ } OR 3 \text{ } OR \dots \text{ } OR m) = P(1) + P(2) + P(3) + \dots + P(m) =$ 

$$=\sum_{i=1}^{m} f_i(1-f_i) = \sum_{i=1}^{m} (f_i - f_i^2) = \sum_{i=1}^{m} f_i - \sum_{i=1}^{m} f_i^2 = 1 - \sum_{i=1}^{m} f_i^2$$

## Appendix B: Bibliography

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