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

 Trees and Evaluation}

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## The classification problem

- Given a collection of records (training set )
> Each record contains a set of attribułes, 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 problem

- Example of classification

|  | Tid | Refund | Marital Status | Taxable Income | Cheat | Here, class = cheat |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | Yes | Single | 125K | No | atirioute of records. |
|  | 2 | No | Married | 100K | No |  |
| One record | 3 | No | Single | 70K | No |  |
|  | 4 | Yes | Married | 120K" | No | Goal: Try to guess value of |
|  | 5 | No | Divorced | 95K | Yes | cheat (the "class") based on the other values of that record |
|  | 6 | No | Married | 60K | No |  |
|  | 7 | Yes | Divorced | 220K | No | It's called classification |
|  | 8 | No | Single | 85K | Yes | because we try to put each |
|  | 9 | No | Married | 75K | No | record in one class/category |
|  | 10 | No | Single | 90K | Yes | ("yes", "no") |

Goal: Find function f() such that:
f (Refund, Marital Status, Taxable Income) = Cheat

## The classification problem

o Prerequisites for classification
> Must have class attribute
> Class attribute 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.


## The classification problem



## The classification problem

- 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 falso 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
o 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?

o 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, befa-sheet, or random
coil
- Categorizing news stories as finance,
weather, entertainment, sports, etc



## Classification techniques

o Decision Tree based Methods
o k-nearest neighbors

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


# General approach of existing classification techniques 

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

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


Test Set

## Performance of model?

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

|  |  | Predicłed class by model |  |
| :--- | :--- | :---: | :---: |
|  |  | Class 1 | Class 0 |
| True class it <br> belongs to | Class 1 | $\mathrm{f}_{11}$ | $\mathrm{f}_{10}$ |
|  | Class 0 | $\mathrm{f}_{01}$ | $\mathrm{f}_{00}$ |

## Performance of model?

o Metrics based on confusion matrix
> Accuracy

- Pct of correctly idenifified classes

$$
\text { Accuracy }=\frac{N C}{T}=\frac{f 11+f 00}{f 11+f 10+f 01+f 00}
$$

> Error rate

- Pct of incorrectly identified classes

$$
\text { Error rate }=\frac{N W}{T}=\frac{f 10+f 01}{f 11+f 10+f 01+f 00}
$$

## Decision Trees

## Decision Tree

- 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

|  |  |  |  | invous $d^{0^{5}}$ |
| :---: | :---: | :---: | :---: | :---: |
| 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

Splitting Attributes


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

## Decision Trees

## - Types of nodes in decision trees



## Decision Trees

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


## Decision Trees

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



## Decision Trees

- 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

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

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

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


How to apply Decision Trees to Test Data?


## How to apply Decision Trees

 to Test Data ?

# How to apply Decision Trees to Test Data ? <br> Test Data 

Refund Marita
Status Income Cheat
No,-- $\quad$ Married $80 \mathrm{~K} \quad ?$

How to apply Decision Trees to Test Data?

Test Data


Taxable Income Cheat

| No | Married | 80 K | $?$ |
| :--- | :--- | :--- | :--- |

## How to apply Decision Trees to Test Data? <br> Test Data

| Refund | Marital <br> Status | Taxable <br> Income | Cheat |
| :--- | :--- | :--- | :--- | (

Reached leaf node which contains a class.
Assign value of leaf node to cheat i.e. assign cheat to "No". Since record has been assigned to class ("No"), terminate.

## How to build Decision Trees?

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



## How to build Decision Trees?

- The problem again!

Splitting Attributes


## How to build Decision Trees?

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


## Basic approach of Hunt's

 algorithm- Let $D_{f}$ be the set of training records that reach a node $\dagger$
- General Procedure:
> If $D_{\dagger}$ contains records that belong the same class $y_{t}$, then $\dagger$ is a leaf node labeled as $y_{+}$
> If $D_{t}$ is an empty set, then $t$ is a leaf node labeled by the default class, $\mathrm{y}_{\mathrm{d}}$
> If $\mathrm{D}_{\mathrm{t}}$ 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

| 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
 each subset.

## 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

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

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


# Splitting based on Ordinal aitributes 

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

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


OR


What about this split? ${ }_{\substack{\{\text { SSmall } \\ \text { Large }\}}}$ preserve order. REMEMBER: Ordinals are about order

## Splitting based on continuous attributes

o 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: ( $\mathrm{A}<\mathrm{v}$ ) or ( $\mathrm{A} \geq \mathrm{v}$ )
consider all possible splits and finds the best cut can be more computational intensive


## Splitting based on continuous attribułes

- Examples of continuous attributes

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


## Tree Induction

- How to determine which attribute to 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

Split all records on "Own Car" attribute

Assume before spliting: 10 records of class 0, 10 records of class 1



| C0: 6 | C0: 4 |
| :--- | :--- |
| C1: 4 | C1: 6 |



Luxury


Split all records on "Student ID" attribute

Q: Which attribute (Own Car, Car Type, Student ID) is better? i.e. Which split is better? ANSWER: Car Type.

## Determine best split

o 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

## C0: 9 <br> C1: 1

Homogeneous, Low degree of impurity

## Measures of node impurity

o 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

o Gini index for a given node t

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

... where $\mathbf{p ( j |} \mid$ ) the relative frequency of class j at node $\dagger$ (Note: each node may contain records from any class)

- Observations:
> Maximum = $1-1 / n_{c}$ when records of node $\dagger$ are distributed equally among classes. Greatest impurity Minimum $=0.0$ when all records of node $\dagger$ 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

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

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

| Class 1 (C1) | 0 |
| :--- | :--- |
| Class 2 (C2) | 6 |

$P(C 1)=0 / 6=0 \quad P(C 2)=6 / 6=1$ (rel. fr/prob.)
Gini $=1-P(C 1)^{2}-P(C 2)^{2}=1-0-1=0$

| Class 1 (C1) | 1 |
| :--- | :--- |
| Class 2 (C2) | 5 |

$P(C 1)=1 / 6 \quad P(C 2)=5 / 6$
Gini $=1-(1 / 6)^{2}-(5 / 6)^{2}=0.278$

| Class 1 (C1) | 2 |
| :--- | :--- |
| Class 2 (C2) | 4 |

$P(C 1)=2 / 6 \quad P(C 2)=4 / 6$
Gini $=1-(2 / 6)^{2}-(4 / 6)^{2}=0.444$

## Gini Index

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

$$
\operatorname{Gini}_{\text {split }}=\sum_{i=1}^{k} \frac{n_{i}}{n} \operatorname{Gini}(i)
$$

... where $n_{i}=$ number of records at node $i$ and $\mathrm{n}=$ number of records at node p

## Gini Index

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

$\left.\begin{array}{l}\operatorname{Gini}(N 1)=1-(5 / 7)^{2}-(2 / 7)^{2}=0.408 \\ \operatorname{Gini}(N 2)=1-(1 / 5)^{2}-(4 / 5)^{2}=0.320\end{array}\right\}$
Gini(Split or B) $=7 / 12$ * $\operatorname{Gini}(N 1)$ $+5 / 12 * \operatorname{Gini}(N 2)=7 / 12 * 0.408$ $+5 / 12$ * $0.320=0.413$ QED


## Gini index

o Examples

| Tid | Refund | Marital <br> Status | Taxable <br> Income | Cheat |
| :--- | :--- | :--- | :--- | :--- |$|$| 1 | Yes | Single | 125 K |
| :--- | :--- | :--- | :--- |
| 2 | No | Married | 100 K |
| 3 | No | Single | 70 K |
| 4 | Yes | Married | 120 K |
| 5 | No | Divorced | No |
| 6 | No | Married | 60 K |
| 7 | Yes | Divorced | Yes |
| 8 | No | Single | 85 K |
| 9 | No | Married | No |
| 10 | No | Single | 90 K |

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


Gini(Left node) $=1-(0 / 3)^{2}-(3 / 3)^{2}=0 \quad$ Gini(Refund) $=(3 / 10) * 0+$
Gini(Right node) $\left.=1-(3 / 7)^{2}-(4 / 7)^{2}=0.489\right\rfloor(7 / 10) * 0.489=\underline{0.3423}$ QED

Gini Index - Gini gain
o Gini gain
> The difference between parent node's Gini index and Gini index of split:

$$
\text { Gini }_{\text {gain }}=\text { Gini }_{\text {Parent }}-\text { Gini }_{\text {Split }}
$$

> 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: The main idea



M12


Gain = M0 - M12 vs M0-M34 => choose attribute with biggest gain!

## Gini Index - Gini gain

o Example

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

Compute Gini gain when splitting on attribute "Refund". Cheat is class!

## Gini gain(Refund) = Gini of entire dafaset 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) $=0.42-0.3423=\underline{0.0777}$ QED

## Building Decision Trees Phase-1

- Using Gini and Gini gain to build decision trees

STEP 1: Compute Gini index for our entire dataset:
Training Data

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

Gini $=1-(2 / 6)^{2}-(4 / 6)^{2}=0.444$
STEP 2: Compute Gini index for each attribute (Split):
$\operatorname{Gini}(M)=(3 / 6)^{*} 0+(3 / 6)^{*} 0.444=0.222$
Gini $(N)=(2 / 6) * 0+(2 / 6) * 0.5+(2 / 6) * 0.5=0.333$
$\operatorname{Gini}(Q)=(2 / 6)^{*} 0.5+(2 / 6)^{*} 0.5+(2 / 6)^{*} 0=0.333$
Calculate Gini gains for each attribute:
Gini Gain $(M)=0.444-0.222=0.222$ (biggest!)
Gini Gain $(N)=0.444-0.333=0.111$
Gini $\operatorname{Gain}(Q)=0.444-0.333=0.111$
Hence, first split based on attribute $M$

## Building Decision Trees Phase-2

Root node of tree will be test on attribute M

## 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 | leaf.

We make a rule:
M1 $\rightarrow$ R2

If M has value M 1 , then $R$ is always R2. Homogeneous node! Hence no further splitting and make this a


| R1 | 2 |
| :--- | :--- |
| R2 | 1 |

1
Here, non-homogeneous node. Apply same method to split based on other attribute. Tree will grow at this branch.

## Building Decision Trees Phase-3 <br> Calculate again with the same steps.

STEP 1: Compute Gini index for our new "entire" dałaset (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:
$\operatorname{Gini}(\mathrm{N})=(1 / 3) * 0+(1 / 3) * 0+(1 / 3) * 0=0$
$\operatorname{Gini}(Q)=(1 / 3) * 0+(1 / 3) * 0+(1 / 3) * 0=0$
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 | 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 |

# 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 |  |  | CarType |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | \{Sports, Luxury\} | \{Family\} |  | \{Sports\} | \{Family, Luxury |
| C1 | 3 | 1 | C1 | 2 | 2 |
| C2 | 2 | 4 | C2 | 1 | 5 |
| Gini | 0.400 |  | Gini | 0.419 |  |

Note: for $k$ categorical values you need to check $\left(2^{\mathrm{k}}-2\right) / 2=2^{\mathrm{k}-1}-1$ 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 distinc $\dagger$ values
- Each splitting value has a count matrix associated with it
> Class counts in each of the partitions, $\mathbf{A}<\mathbf{v}$ and $\mathbf{A} \geq \mathbf{v}$
- Simple method to choose best $v$
> For each $\mathbf{v}$, scan the database to gather count matrix and compute its Gini index
Computationally Inefficient! Complexity: $O\left(n^{2}\right)$ computing

Tid Refund Marital Status

Taxable Income

| 1 | Yes | Single | 125 K | No |
| :--- | :--- | :--- | :--- | :--- |
| 2 | No | Married | 100 K | No |
| 3 | No | Single | 70 K | No |
| 4 | Yes | Married | 120 K | No |
| 5 | No | Divorced | 95 K | Yes |
| 6 | No | Married | 60 K | No |
| 7 | Yes | Divorced | 220 K | No |
| 8 | No | Single | 85 K | Yes |
| 9 | No | Married | 75 K | No |
| 10 | No | Single | 90 K | Yes |

## Gini.

Taxable
Income
$>80 \mathrm{~K}$ ?

Yes
No

Repetition of work.

# Computing Gini Index for continuous attributes 

o 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 dififer in their target (class) labels and attribute values $=>$ Set of candidate splits
> Calculate Gini Index and choose the split position that has the least gini index

| Sorted Values Split Positions | Cheat | No |  | No |  |  | No |  | Yes |  |  | Yes |  | Yes |  |  | No |  |  | No |  | No |  |  | No |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |  |  |  |  |  | xat | ble | Inc | om |  |  |  |  |  |  |  |  |  |  |
|  | $\longrightarrow$ | 60 |  | 70 |  |  | 75 |  | 85 |  | 90 |  |  | 95 |  |  | 100 |  |  | 120 |  | 125 |  |  | 220 |  |
|  | $\longrightarrow$ | 55 |  | 65 |  | 72 |  | 80 |  |  | 87 |  | 92 |  |  | 97 |  |  | 110 |  |  | 122 | 172 |  | 230 |  |
|  |  | $<=$ | > | <= | > | <= | $\geq$ | <= | , | $\geq$ | <= | > | < | = | $\geq$ | <= | $\geq$ |  | < $=$ | > | $<=$ | > | < | > | <= | $>$ |
|  | 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 |  |  | 10 |  | 75 |  | 34 |  |  | 1.7 |  | 400 |  |  | 300 |  | d. 3 | 343 |  | 375 |  | 100 |  | 420 |

# Alternative splitting criteria (besides Gini): Entropy 

o Entropy - measures information (INFO)

- Calculate Entropy for node $\dagger$ :

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

...where $p(j \mid \dagger)$ the relative frequency of class $j$ at node t. (note log = base-2 logarithm i.e. $\log _{2}$ )

- Measures homogeneity of a node Maximum $=\log n_{c}$ when all records of node equally distributed among classes
Minimum $=0.0$ when all records of node belong to one class


## Entropy

o Entropy 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.

## Entropy

o Examples: calculating the Entropy for various nodes

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

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

| Class 1 (C1) | 0 |
| :--- | :--- |
| Class 2 (C2) | 6 |

$P(C 1)=0 / 6=0 \quad P(C 2)=6 / 6=1$ (rel. fr/prob.)
Entropy $=-0 \log _{2} 0-1 \log _{2} 1=0($ note: $0 \log 0=0)$

| Class 1 (C1) | 1 |
| :--- | :--- |
| Class 2 (C2) | 5 |

$P(C 1)=1 / 6 \quad P(C 2)=5 / 6$
Entropy $=-(1 / 6) \log _{2}(1 / 6)-(5 / 6) \log _{2}(5 / 6)=$ 0.65

| Class 1 (C1) | 2 |
| :--- | :--- |
| Class 2 (C2) | 4 |

$P(C 1)=2 / 6 \quad P(C 2)=4 / 6$
Entropy $=-(2 / 6) \log _{2}(2 / 6)-(4 / 6) \log _{2}(4 / 6)=$ 0.92

## Entropy

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

$$
\text { Entropy } y_{S P L I T}=\sum_{i=1}^{k} \frac{n_{i}}{n} \operatorname{Entropy}(i)
$$

... Where $n_{i}=$ number of records at node $i$, Entropy(i) = Entropy of node/child i, $\mathrm{n}=$ number of records at node p.
Note: Compare to Gini Index of Split: Similar!

## Entropy

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

$$
\operatorname{GAIN} N_{S P L I T}=\operatorname{Entropy}(p)-\left(\sum_{i=1}^{k} \frac{n_{i}}{n} \operatorname{Entropy}(i)\right)
$$

... where $\mathrm{n}_{\mathrm{i}}$ number of records at node $\mathbf{i}, \mathrm{n}$ \# 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)
Disadvantage: Prefers splits resulting in large number of "pure" nodes/partitions (pure=low intermixing)

# Building Decision Trees Phase-1 - Using Entropy 

Training Data

| ID | $M$ | $N$ | $Q$ | $R$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $M 1$ | $N 3$ | $Q 2$ | $R 2$ |
| 2 | $M 2$ | $N 3$ | Q2 | $R 1$ |
| 3 | $M 2$ | $N 2$ | Q1 | $R 1$ |
| 4 | $M 1$ | $N 2$ | Q1 | $R 2$ |
| 5 | $M 2$ | $N 1$ | Q3 | $R 2$ |
| 6 | $M 1$ | $N 1$ | Q3 | $R 2$ |

Entropy Node = -(2/6)log2(2/6) - (4/6)log2(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) $=(3 / 6)^{*} 0+(3 / 6)^{*}[-(2 / 3) * \log 2(2 / 3)-$ $(1 / 3) * \log 2(1 / 3)]=0.4591$
$\operatorname{Entropy}(\mathrm{N})=(2 / 6)^{*} 0+(2 / 6)^{*} 1+(2 / 6)^{*} 1=0.6666$
Entropy $(Q)=(2 / 6)^{*} 1+(2 / 6)^{*} 1+(2 / 6)^{*} 0=0.6666$
Calculate Entropy gains for each attribute:
Entropy $\operatorname{Gain}(M)=0.9182-0.4591=0.4591$ (biggest!)
Entropy Gain $(\mathrm{N})=0.9182-0.6666=0.2516$
Entropy Gain $(Q)=0.9182-0.6666=0.2516$
Hence, first split based on attribute M (biggest gain)

# Building Decision Trees Phase-2 - Using Entropy 

Root node of tree will be test on attribute $M$

## Training Data

| ID | $M$ | $N$ | $Q$ | $R$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $M 1$ | $N 3$ | $Q 2$ | $R 2$ |
| 2 | $M 2$ | $N 3$ | $Q 2$ | $R 1$ |
| 3 | $M 2$ | $N 2$ | $Q 1$ | $R 1$ |
| 4 | $M 1$ | $N 2$ | $Q 1$ | $R 2$ |
| 5 | $M 2$ | $N 1$ | $Q 3$ | $R 2$ |
| 6 | $M 1$ | $N 1$ | $Q 3$ | $R 2$ |
|  |  |  |  |  |
|  |  |  |  |  |



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

# Building Decision Trees Phase-3 - Using Entropy 

Training Data

| ID | $M$ | $N$ | $Q$ | $R$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $M 1$ | $N 3$ | $Q 2$ | $R 2$ |
| 2 | $M 2$ | $N 3$ | $Q 2$ | $R 1$ |
| 3 | $M 2$ | $N 2$ | $Q 1$ | $R 1$ |
| 4 | $M 1$ | $N 2$ | Q1 | $R 2$ |
| 5 | $M 2$ | $N 1$ | Q3 | $R 2$ |
| 6 | $M 1$ | $N 1$ | Q3 | $R 2$ |

Calculate again following the same steps (leave out red rows).

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 $(\mathrm{N})=(1 / 3)^{*} 0+(1 / 3)^{*} 0+(1 / 3)^{*} 0=0$
Entropy $(Q)=(1 / 3) * 0+(1 / 3) * 0+(1 / 3) * 0=0$
Calculate Entropy gains:
Gini Gain $(\mathrm{N})=0.9182-0.0=0.9182$
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 | $M$ | $N$ | $Q$ | $R$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $M 1$ | $N 3$ | $Q 2$ | $R 2$ |
| 2 | $M 2$ | $N 3$ | $Q 2$ | $R 1$ |
| 3 | $M 2$ | $N 2$ | Q1 | $R 1$ |
| 4 | $M 1$ | $N 2$ | Q1 | $R 2$ |
| 5 | $M 2$ | $N 1$ | Q3 | $R 2$ |
| 6 | $M 1$ | $N 1$ | Q3 | $R 2$ |



## 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)

$$
\text { GainRATIO }=\frac{\text { GAIN } N_{S P L I T}}{\text { SplitINFO }} \quad \text { SplitINFO }=-\sum_{j=1}^{k} \frac{n_{i}}{n} \log \frac{n_{i}}{n}
$$

... where $n_{i}$ 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


## Entropy

- Example - Entropy split/ attribute

| Tid | Refund | Marital <br> Status | Taxable |  |
| :--- | :--- | :--- | :--- | :--- |
| Income |  |  |  |  | Cheat

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


## Entire dataset

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

Compute Entropy gain for split on "Refund" attribute. Cheat is class!
o 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 |



Calculate Entropy for parent node (entire dataset): Entropy(dataset) = -(3/10) $\log (3 / 10)-(7 / 10) \log (7 / 10)=$ $=\underline{0.8812}$

Entire dataset
Entropy(Refund) $=\underline{0.6894}$ (see previous slide)
Entropy Gain $=0.8812-0.6894=\underline{0.1918}$ QED

## Alternative splitting criteria (besides Gini): Classification error <br> - Classification error at node i

$$
\operatorname{Error}(i)=1-\max _{i}(p(i \mid t))
$$

- Measures misclassification error made by a node.

Maximum $=1-1 / n_{c}$ when records are equally distributed among all classes
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

$$
\operatorname{Error}(i)=1-\max _{i}(p(i \mid t))
$$

| Class 1 (C1) | 0 |
| :--- | :--- |
| Class 2 (C2) | 6 |

$$
\begin{aligned}
& P(C 1)=0 / 6=0 \quad P(C 2)=6 / 6=1 \text { (rel. fr/prob. }) \\
& \text { Error }=1-\max (0,1)=1-1=0
\end{aligned}
$$

| Class 1 (C1) | 1 |
| :--- | :--- |
| Class 2 (C2) | 5 |

$$
P(C 1)=1 / 6 \quad P(C 2)=5 / 6
$$

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

| Class 1 (C1) | 2 |
| :--- | :--- |
| Class 2 (C2) | 4 |

$$
\begin{aligned}
& P(C 1)=2 / 6 \quad P(C 2)=4 / 6 \\
& \text { Error }=1-\max (2 / 6,4 / 6)=1-4 / 6=1 / 3
\end{aligned}
$$

## 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 | $M$ | $N$ | $Q$ | $R$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $M 1$ | $N 3$ | $Q 2$ | $R 2$ |
| 2 | $M 2$ | $N 3$ | $Q 2$ | $R 1$ |
| 3 | $M 2$ | $N 2$ | $Q 1$ | $R 1$ |
| 4 | $M 1$ | $N 2$ | $Q 1$ | $R 2$ |
| 5 | $M 2$ | $N 1$ | $Q 3$ | $R 2$ |
| 6 | $M 1$ | $N 1$ | $Q 3$ | $R 2$ |

STEP 1: Calculate Entropy/Classification error for system

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

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
o Early termination

Note on evaluation metrics

## Evaluation metrics

Predicted class by model
Could also use Class0/Class 1

| Could also use Class0/Class 1. |  |  |
| :--- | :--- | :--- |
| True class it <br> belongs to | Positive | Negative |
|  |  |  |

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

|  |  | Predicłed class by model |  |
| :--- | :--- | :---: | :---: |
|  |  | Negative |  |
| True class it <br> belongs to | Positive | True Positive | False Positive |
|  | Negative | False Negative | True Negative |

## o 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.


## Decision Trees in $R$

## Decision Trees in $R$

- 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

## Decision Trees in $R$

## - 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)
```



```
#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
```



```
Carseats = Carseats[,-1]
```



```
# 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)
test = -train #the rest will be our testing data
# 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
# all other attributes of the Carseats dataset
tree_model = tree(High~., training_data)
```



```
plot(tree model)
# Plot does now show labels on Decision Tree. Plot tree with labels to make it easily understandable.
text(tree_model, pretty=0)
# Next, use the testing data to test the Decision tree referenced by tree_model
```


## Decision Trees in $R$

## - 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 but we will not remove it. 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$High)
# Ok, let's calculate some quality metrics of the model, in order to see how
# our model performed. We calculate accuracy and error rate of the classifier/mocel
# Calculate accuracy
modelAccuracy = sum( diag(testingDataConfusionTable)/sum(testingDataConfusionTable))
# Calculate Error rate (note could also use 1-modelAccuracy)
modelErrorRate = 1 - sum( diag(testingDataConfusionTable)/sum(testingDataConfusionTable))
# Print the result out nicely. We loooooooooove nice and clear responses.
sprintf("Model accuracy: %f, model error rate:%f", modelAccuracy,modelErrorRate )
# You can also use a different library (instead of table) for calculating the confusion matrix
library(caret) #needed for confusion matrix. Install this package (may take a while)
# Compare tree predict and attribute High from testing dataset by showing the confuction
# matrix. Look at matrix and accuracy
confusionMatrix(tree_predict, testing_data$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


## Underfitting and Overfitting

o 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

## Underfitting and Overfitting

- 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)


## Underfitting and Overfitting

- Misclassification on training set? Isn't this impossible?
> Assume now inconsistent training seł
> 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)


## Underfitting and Overfitting

o Reasons for errors on the training seł
> Training set is not a good sample
> (consistent) Noise on some attributes
> Missing attribute values
> Some class values present in small amounts

## Underfitting and Overfitting

- 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' $\dagger$ 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 dała!
- Happens when Decision Tree grows large and complex (large number of nodes)


## Underfitting and Overfitting



## 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

o Assume
> $\mathbf{e}(\mathbf{t})=$ Error on training set
$>\boldsymbol{e}^{\prime}(\mathbf{t})=$ Error on testing/unknown set (same model)

- Two approaches to estimating generalization errors

Optimistic approach
Assumes that e(t) = $e^{\prime}(t)$
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, $\mathrm{e}_{\mathrm{g}}(\mathrm{T})$

$$
e_{g}(T)=\frac{\sum_{i=1}^{k}\left[e\left(t_{i}\right)+\Omega\left(t_{i}\right)\right]}{\sum_{i=1}^{k} n\left(t_{i}\right)}=\frac{e(T)+c n_{l}}{N_{t}}
$$

... Where $\mathbf{e}(\mathrm{T})=$ generalization error of decision tree, $N_{\dagger}=$ number of records in training set, $n_{I}=$ number of leaves in decision tree and $c=$ penalty (usually 0.5)

## Estimating generalization errors

- Example


Estimated pessimistic error for decision tree:
$\mathrm{e}_{\mathrm{g}}(\mathrm{T})=\left(3+0.5^{*} 2\right) / 12=0.333$
(Note: if there were 3 "children"/nodes (same \#records and error): $\left(3+0.5^{*} 3\right) / 12=\underline{0.375}$ (increased penalty for complexity)

## Addressing Overfitting

o 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
o 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
> Grow decision tree to its entirety from the training seł
> 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

| Class $=$ Yes | 20 |
| :---: | :---: |
| Class $=$ No | 10 |
| Error $=10 / 30$ |  |

Assume fully grown tree from training set
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 THIS NODE! Replace with leaf node "Yes" (majority in subtree)

| Class $=$ Yes | 8 | Class $=$ Yes | 3 | Class $=$ Yes | 4 | Class $=$ Yes | 5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Class $=$ No | 4 | Class $=$ No | 4 | Class $=$ No | 1 | Class $=$ No | 1 |

## 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 ał least one record
- Is in general cheaper


## Missing values

## Handling missing values

o 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 

## Before Splitting:

$$
\begin{aligned}
& \text { Entropy(Parent) } \\
& =-0.3 \log (0.3)-(0.7) \log (0.7)=0.8813
\end{aligned}
$$

| Tid | Refund | Marital <br> Status | Taxable <br> Income | Class |
| :--- | :--- | :--- | :--- | :--- |
| 1 | Yes | Single | 125 K | No |
| 2 | No | Married | 100 K | No |
| 3 | No | Single | 70 K | No |
| 4 | Yes | Married | 120 K | No |
| 5 | No | Divorced | 95 K | Yes |
| 6 | No | Married | 60 K | No |
| 7 | Yes | Divorced | 220 K | No |
| 8 | No | Single | 85 K | Yes |
| 9 | No | Married | 75 K | No |
| 10 | $?$ | Single | 90 K | Yes |


|  | Class=Yes | Class=No |
| :--- | :---: | :---: |
| Refund=Yes | 0 | 3 |
| Refund=No | 2 | 4 |
| Refund=? | 1 | 0 |

## Split on Refund:

Entropy(Refund=Yes) $=0$
Entropy(Refund=No) =
$=-(2 / 6) \log (2 / 6)-(4 / 6) \log (4 / 6)=0.9183$
Entropy(Children)

$$
\text { Probability of this }=0.3(0)+0.6(0.9183)=0.551
$$

Missing value
Entropy Gain $=0.9$ * $(0.8813-0.551)=0.3303$

# Missing values - How to distribute instances 

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

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

Probability that Refund=Yes is 3/9
Probability that Refund=No is 6/9
Assign record with unknown Refund to the left child with weight $=3 / 9$ and to the right child with weight $=6 / 9$


## Missing values - Classifying unknown records

New/unknown record:


|  | Married | Single | Divorced | Total |
| :--- | :---: | :---: | :---: | :---: |
| Class=No | 3 | 1 | 0 | 4 |
| Class=Yes | $6 / 9$ | 1 | 1 | 2.67 |
| Total | 3.67 | 2 | 1 | 6.67 |

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

## Summary

## 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 festing and unknown data
Decision Trees have also problems though Most important one is Overfitting

Appendices

## Appendix A: Gini index of

## node

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

Assume $m$ classes, with $i \in\{1,2,3, \ldots, m\}$ 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 to NOT belong to class 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 $\mathbf{P}(\mathbf{i})=\mathrm{f}_{\mathrm{i}}\left(1-\mathrm{f}_{\mathrm{i}}\right)$
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 fotal probability of error will hence be:

$$
\begin{aligned}
& P(1 \text { OR } 2 \text { OR } 3 \text { OR } \ldots \text { OR } m)=P(1)+P(2)+P(3)+\ldots+P(m)= \\
& =\sum_{i=1}^{m} f_{i}\left(1-f_{i}\right)=\sum_{i=1}^{m}\left(f_{i}-f_{i}^{2}\right)=\sum_{i=1}^{m} f_{i}-\sum_{i=1}^{m} f_{i}^{2}=1-\sum_{i=1}^{m} f_{i}^{2}
\end{aligned}
$$

## Appendix B: Bibliography

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