

“Tree” Predictive Models

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Revision

What classifiers have we learned?

- kNN (class), wkNN (kkn): numeric inputs only, curse of dimensionality
- Logistic Regression (`glm(family=binomial)`), Multinomial LR/Softmax Regression (`nnet`), LDA (MASS): limited to linear separable data
- Naive Bayes (`naivebayes`): can't handle numeric input well
- ANN (`neuralnet`, `ANN2`): difficult to decide how many hidden layers, see

<https://stackoverflow.com/questions/35520587/>

how-to-determine-the-number-of-layers-and-nodes-of-a-neural-network

Revision (cont)

What regressors have we learned?

- Linear Model (lm): limited to linear data
- kNN (FNN), wkNN (kkn): numeric inputs only, curse of dimensionality

Outline

- 1 Theory and Terminologies
- 2 Impurity Measures
- 3 Implementations
- 4 Practical Considerations

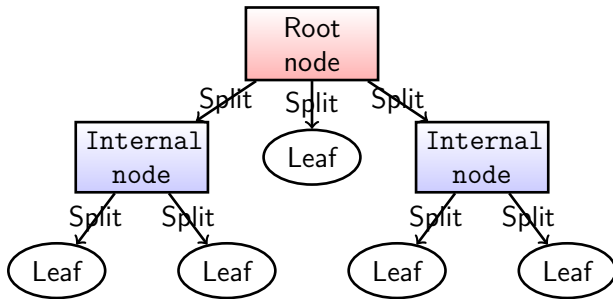
Theory / Terminologies

A *decision tree* algorithm is a non-parametric method for classification (and regression). It can handle categorical features and extra the predicate logic from features.

The assumption of decision tree is “the data must be clean and logical”. Based on this assumption, the algorithm uses **information theory** to compress the data table into a “decision tree”.

Theory / Terminologies (cont)

According to https://en.wikipedia.org/wiki/Decision_tree, a decision tree is a “flowchart”-like structure in which each *internal node* (the decision node) represents a “test” on a “predictor” or an “attribute”, each branch represents the outcome of the test, and each **leaf node** represents a class label (decision taken after computing all attributes).



Theory / Terminologies (cont)

Decision trees have several nice advantages over kNN (as a non-parametric model):

- 1 once the tree is constructed, the training data does not need to be stored. Instead, we can simply store how many points of each label ended up in each leaf — typically these are pure so we just have to store the label of all points;
- 2 decision trees are very fast during test time, as test inputs simply need to traverse down the tree to a leaf (label);
- 3 decision trees require no metric because the splits are based on feature thresholds and not distances.

Theory / Terminologies (cont)

The goal in building a decision tree is to make sure it is “maximally compact” and “only has pure leaves”.

A **consistent tree** is possible if no two input vectors have identical features but different labels.

Consider the data table with K classes:

$$S = \{(x_1, y_1), \dots, (x_n, y_n)\}, y_i \in \{1, \dots, K\}.$$

Example

Example 1: Consider the truth table we learned in Discrete Maths:

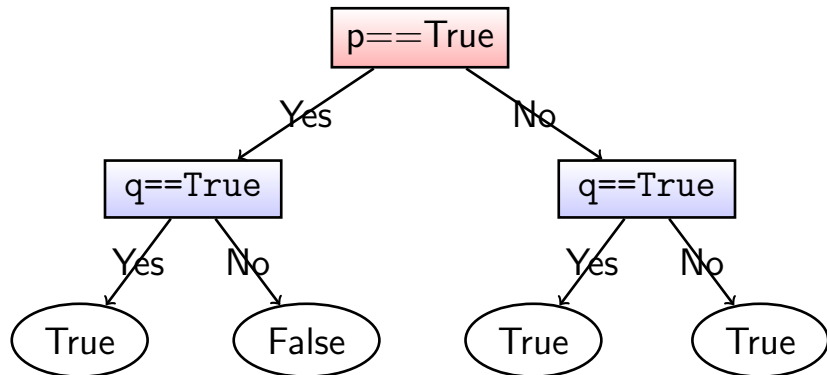
p	q	$p \rightarrow q$
T	T	T
T	F	F
F	T	T
F	F	T

where p are q are propositions.

The decision tree from this table will be **consistent** because no repeated inputs with different outputs.

Example (cont)

Just encode all entries into a decision tree:



Problem with Brute-force: $p = 10$, each column 3 classes
→ $3^{10} = 59049$ leaves!

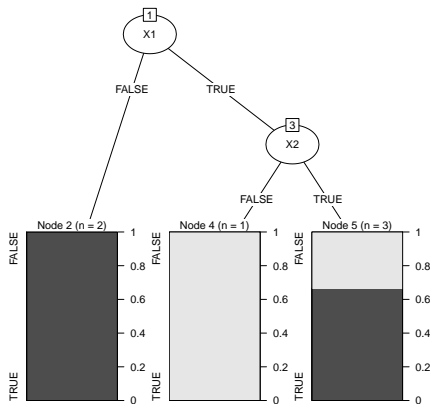
Example (cont)

Example 2: An Inconsistent Table:

Table

X_1	X_2	Y
T	T	T
T	T	F
T	T	T
T	F	F
F	T	T
F	F	T

The ID3 tree of this table is shown below.



Tree Construction

Brute-force tree construction do not give us “economical” decision tree!

Smart “splitting” of the data S should be used! The most popular way of splitting a data is to “split” based on a selected predictor (depending on whether it is categorical or numerical). The **splitting criteria** differ as follows:

predictors	qualitative (categorical)	quantitative (numerical)
splits	disjoint subsets of the predictor categories	disjoint ranges of the predictors value

Tree Construction (cont)

For the qualitative predictors, there are two types of splitting criteria:

- 1 *Binary split*: Divides values into two subsets.
- 2 *Multi-way split / L-way split*: Use as many partitions as distinct values.

For the splitting, we know what we don't want to have a uniform distribution: $p_1 = p_2 = \dots = p_K = \frac{1}{K}$. This is the worst case since each leaf is equally likely because the prediction is going to be a random guessing.

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“Impurity” Measures

“Impurity” measures are used to choose the “best” predictor to perform “splitting” for the “decision-tree construction algorithm”. The “impurity” measures generally measure the homogeneity of the target variable within the subsets. We introduce them following https://en.wikipedia.org/wiki/Decision_tree_learning:

- Gini Impurity Index (default in ‘rpart’)
- Entropy and Information Gain
- Variance Reduction (?)
- Deviance (using in ‘tree’)
- Gain Ratio

Gini Impurity (Index)

Gini impurity is used by the *CART* (*classification and regression tree*) algorithm for classification trees. It is defined as a measure of total variance across the K classes:

$$G(S) = \sum_{j=1}^K p_j(1 - p_j) = 1 - \sum_{j=1}^K p_j^2, \quad p_j = \frac{|S_j|}{|S|} \quad (1)$$

where p_j is the proportion of observations in S that belong to class j and $S_j = \{(x, y) \in S : y = j\} \subseteq S$ (all inputs with labels j) such that $S_i \cap S_k = \emptyset$ when $i \neq k$ and $S = S_1 \cup \dots \cup S_K$.

Gini Impurity (cont)

Gini impurity will be maximised when observations are heterogeneous, i.e. **impure**. For example, when all classes are **uniformly distributed**, i.e.

$p_1 = \dots = p_K = \frac{1}{K}$, then

$$G(S) = 1 - \sum_{k=1}^K \frac{1}{K^2} = 1 - \frac{1}{K}.$$

Gini impurity will be minimised when observations are homogeneous, i.e. **pure**. For example, when one class is having all the observations or is empty, then

$$G(S) = 1 - 1 = 0.$$

Gini Impurity (cont)

The *Gini impurity of a tree* is defined as

$$G^T(\underbrace{\{S_1, \dots, S_L\}}_{S^A}) = \sum_{i=1}^L \frac{|S_i|}{|S|} G^T(S_i). \quad (2)$$

In the splitting of a decision tree, we want a branch with more “pure” nodes, so the predictor with the **lowest** Gini impurity is selected as the splitting predictor and the tree algorithm is repeated for the subsequent nodes.

Gini Impurity (cont)

Example 3: (Tennis / Golf Example) [Mit97, §3.4.2].

Day	Outlook	Temperature	Humidity	Wind	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Compute the **Gini impurity** of each feature (excluding Day) with respect to the output “Play”.

Gini Impurity (cont)

Example 3: (cont)

Let S_{Weak} and S_{Strong} be the split of Wind is “Weak” and “Strong” respectively, $S^{Wind} = \{S_{Weak}, S_{Strong}\}$,

$S_{Weak,Yes} = S_{Weak} \cap \{Play = Yes\}$, ..., and

$S_{Strong,No} = S_{Strong} \cap \{Play = No\}$, etc.

$$\mathbb{P}(S_{Weak}) = \frac{8}{14}; \quad \mathbb{P}(S_{Strong}) = \frac{6}{14}$$

$$\mathbb{P}(S_{Weak,Yes}) = \frac{6}{8}; \quad \mathbb{P}(S_{Weak,No}) = \frac{2}{8} \Rightarrow G(S_{Weak}) = 1 - \left(\frac{6}{8}\right)^2 - \left(\frac{2}{8}\right)^2 = 0.375$$

$$\mathbb{P}(S_{Strong,Yes}) = \frac{3}{6}; \quad \mathbb{P}(S_{Strong,No}) = \frac{3}{6} \Rightarrow G(S_{Strong}) = 1 - \left(\frac{3}{6}\right)^2 - \left(\frac{3}{6}\right)^2 = 0.5$$

$$G(S^{Wind}) = \frac{8}{14}(0.375) + \frac{6}{14}(0.5) = 0.4286$$

Gini Impurity (cont)

Example 3: (cont) Gini impurity of Humidity:

- $\mathbb{P}(S_{High}) = \frac{7}{14}; \quad \mathbb{P}(S_{Normal}) = \frac{7}{14}$
- $\mathbb{P}(S_{High,Yes}) = \frac{3}{7}; \quad \mathbb{P}(S_{High,No}) = \frac{4}{7} \Rightarrow$
 $G(S_{High}) = 1 - \left(\frac{3}{7}\right)^2 - \left(\frac{4}{7}\right)^2 = 0.4898$
- $\mathbb{P}(S_{Normal,Yes}) = \frac{6}{7}; \quad \mathbb{P}(S_{Normal,No}) = \frac{1}{7} \Rightarrow$
 $G(S_{Normal}) = 1 - \left(\frac{6}{7}\right)^2 - \left(\frac{1}{7}\right)^2 = 0.2449$
- $G(S^{Humidity}) = \frac{7}{14}(0.4898) + \frac{7}{14}(0.2449) = 0.3674$

Gini Impurity (cont)

Example 3: (cont)

Try and see if you can find

$$G(S^{Temperature}) = 0.4405$$

$$G(S^{Outlook}) = 0.3429$$

Entropy and Information Gain

Information gain is used by the ID3, C4.5 and C5.0 tree-generation algorithms. Information gain is based on the concept of Entropy and information content from information theory [CT06]:

$$H(S) = - \sum_{j=1}^K p_j \log_2 p_j \quad (3)$$

where p_j is the proportion of observations in S that belong to class $j \in \{1, \dots, K\}$ and S a collection with K number of classes.

Entropy and Information Gain (cont)

The entropy over tree ($Values(A) = \{1, \dots, L\}$) is

$$H^T(\underbrace{\{S_1, \dots, S_L\}}_{S^A}) = \sum_{i \in Values(A)} \frac{|S_i|}{|S|} H(S_i). \quad (4)$$

The *information gain* (IG) measures how well a given predictor separates the training data S according to their response variable classification:

$$IG(S^A) = H(S) - H^T(S^A) \quad (5)$$

where S_i is the subset of S for which predictor A is belonging to class i .

Features that perfectly partition should give **maximal information gain** or **minimal entropy**.

Entropy and Information Gain (cont)

Example 4: Consider the tennis data from **Example 3**. Compute the **information gain** of all features (note: Day is not a feature).

The **overall entropy (of the target output) before splitting**:

$$H(S) = -\left(\frac{9}{14} \log_2 \frac{9}{14} + \frac{5}{14} \log_2 \frac{5}{14}\right) = \underline{0.9403}$$

Entropy and Information Gain (cont)

Example 4: (cont)

The entropy and information gain **after splitting on Wind** are

- $\mathbb{P}(S_{Weak, Yes}) = \frac{6}{8}; \quad \mathbb{P}(S_{Weak, No}) = \frac{2}{8} \Rightarrow$
 $H(S_{Weak}) = -\left(\frac{6}{8} \log_2 \frac{6}{8} + \frac{2}{8} \log_2 \frac{2}{8}\right) = 0.8113$
- $\mathbb{P}(S_{Strong, Yes}) = \frac{3}{6}; \quad \mathbb{P}(S_{Strong, No}) = \frac{3}{6} \Rightarrow$
 $H(S_{Strong}) = -\left(\frac{3}{6} \log_2 \frac{3}{6} + \frac{3}{6} \log_2 \frac{3}{6}\right) = 1$
- $H(S^{Wind}) = \frac{8}{14}H(S_{Weak}) + \frac{6}{14}H(S_{Strong}) = 0.8922$
 $IG(S^{Wind}) = H(S) - H(S^{Wind}) = 0.9403 - 0.8922 = 0.0481$

Entropy and Information Gain (cont)

Example 4: (cont)

The information gain **after splitting on** Humidity:

- $\mathbb{P}(S_{High}, Yes) = \frac{3}{7}, \quad \mathbb{P}(S_{High}, No) = \frac{4}{7}$
 $\Rightarrow H(S_{High}) = 0.9852$
- $\mathbb{P}(S_{Normal}, Yes) = \frac{6}{7}, \quad \mathbb{P}(S_{Normal}, No) = \frac{1}{7}$
 $\Rightarrow H(S_{Normal}) = 0.5917$
- $H(S^{Humidity}) = \frac{7}{14}H(S_{High}) + \frac{7}{14}H(S_{Normal}) = 0.7885$
 $IG(S^{Humidity}) = 0.9403 - 0.7885 \approx 0.1518$

Gini Impurity (cont)

Example 4: (cont)

Try and see if you can find

$$H(S^{Temperature}) = 0.9111$$

$$IG(S^{Temperature}) = 0.0292$$

$$H(S^{Outlook}) = 0.6936$$

$$IG(S^{Outlook}) = 0.2467$$

Entropy and Information Gain (cont)

A simple R implementation is listed below.

```
entropy = function(S) {
  counts = table(S)
  p = counts/sum(counts)
  return(-sum(ifelse(p==0,0,p*log2(p))))
}

# A = split_attribute_name, R = target / response name
info_gain = function(d.f,A,R="target") {
  HS = entropy(d.f[R])
  counts = table(unlist(d.f[A]))
  p = counts/sum(counts)
  HSi = unlist(lapply(split(d.f, d.f[A]), function(s) {
    entropy(s[R]) })))
  return(HS - sum(p*HSi))
}

d.f = read.csv('playtennis.csv')
print(entropy(d.f$playtennis))
print(info_gain(d.f, 'wind', 'playtennis'))
```

Entropy and Information Gain (cont)

A simple Python implementation is listed below.

```
import numpy as np, pandas as pd

def entropy(S):
    _, counts = np.unique(S, return_counts=True)
    p = counts/np.sum(counts)
    return -sum(p[i]*np.log2(p[i]) for i in range(len(p))
                if p[i]!=0.0)

# A = split_attribute_name, T = target / response name
def info_gain(df,A,T="target"):
    HS = entropy(df[T])
    valsA, counts = np.unique(df[A].tolist(), return_counts=True)
    p = counts/np.sum(counts)
    HSi = [entropy(df.where(df[A]==i).dropna()[T]) for i in valsA]
    return HS - sum(p*np.array(HSi))

df = pd.read_csv('playtennis.csv')
print(entropy(df['playtennis']))
print(info_gain(df, 'wind', 'playtennis'))
```

Variance Reduction

Variance reduction [BFSO84] is often employed in cases where the target variable is continuous (regression tree): The variance reduction of a node N is defined as the total reduction of the variance of the target variable x due to the split at this node:

$$I_V(N) = \frac{1}{|S|^2} \sum_{i \in S} \sum_{j \in S} \frac{1}{2} (x_i - x_j)^2 - \left(\frac{1}{|S_t|^2} \sum_{i \in S_t} \sum_{j \in S_t} \frac{1}{2} (x_i - x_j)^2 + \frac{1}{|S_f|^2} \sum_{i \in S_f} \sum_{j \in S_f} \frac{1}{2} (x_i - x_j)^2 \right)$$

where S , S_t , and S_f are the set of presplit sample indices, set of sample indices for which the split test is true, and set of sample indices for which the split test is false, respectively.

Gain Ratio

There is a natural bias in information gain measure that **favours** predictors with large number of values. For example, use Day as a predictor to calculate the information gain of “tennis” data table.

- For $i = 1, 2, 6, 8, 14$, $\mathbb{P}(S_{D_i, \text{Yes}}) = 0$, $\mathbb{P}(S_{D_i, \text{No}}) = 1$
 $\Rightarrow H(S_{D_i}) = -(0 \times \log_2 0 + 1 \times \log_2 1) = 0$
- For $i = 3, 4, 5, 7, 9, 10, 11, 12, 13$, $\mathbb{P}(S_{D_i, \text{Yes}}) = 1$,
 $\mathbb{P}(S_{D_i, \text{No}}) = 0$
 $\Rightarrow H(S_{D_i}) = -(1 \times \log_2 1 + 0 \times \log_2 0) = 0$
- $IG(S^{\text{Day}}) = 0.9403 - \frac{1}{14} \times 0 - \dots - \frac{1}{14} \times 0 = 0.9403$.

Gain Ratio (cont)

If “Day” is an attribute, it will win out as the root but it is useless in prediction just like a person’s id number is useless in identifying the performance of a person.

Gain ratio is a modification of information gain that **reduces its bias** on highly branching predictors.

The *intrinsic information* of A , is the entropy of the “splitting factor”:

$$H(A) = - \sum_{i=1}^K \frac{|A_i|}{|A|} \log_2 \frac{|A_i|}{|A|}. \quad (6)$$

Gain Ratio (cont)

The gain ratio, $R(S^A)$ is defined as

$$R(S^A) = \frac{IG(S^A)}{H(A)} \quad (7)$$

where $IG(S^A)$ is the information gain (5).

The predictor with the maximum gain ratio is selected as the splitting predictor and the algorithm is similar to the information gain.

Gain Ratio (cont)

Example 5: (Final Exam Jan 2019, Q2(b))

Gain ratio is a modification of information gain. Discuss on why and how the modification is done on information gain. (2 marks)

Solution: Gain ratio is a modification of information gain that **reduces its bias on highly branching predictors**. It takes into account the number and size of branches when choosing a predictor. This is done by normalising information gain by the intrinsic information of a split, which is defined as the information need to determine the branch to which an observation belongs.

Gain Ratio (cont)

Example 6: Compute the **gain ratio** of the output “Play” against other features (excluding Day).

Solution: The gain ratio of Wind:

- $H(S) = 0.9403$
- $IG(S^{Wind}) = 0.0481$
- $H(Wind) = -(\frac{8}{14} \log_2 \frac{8}{14} + \frac{6}{14} \log_2 \frac{6}{14}) = 0.9852$
- $R(S^{Wind}) = \frac{IG(S^{Wind})}{H(Wind)} = 0.0488$

Gain Ratio (cont)

Example 6: (cont)

The calculation of gain ratio of Humidity:

- $IG(S^{Humidity}) = 0.9403 - \frac{7}{14} \times 0.9852 - \frac{7}{14} \times 0.5917 = 0.1519$
- $H(Humidity) = -(\frac{7}{14} \log_2 \frac{7}{14} + \frac{7}{14} \log_2 \frac{7}{14}) = 1$
- $R(S^{Humidity}) = 0.1519$

Try to use the steps above to check that

$$R(S^{Temperature}) = 0.0188$$

$$R(S^{Outlook}) = 0.1564.$$

Gain Ratio (cont)

Example 7: (Final Exam Jan 2019, Q2(a))

State definition for the following terms:

- (i) Entropy (1 mark)
- (ii) Information gain (1 mark)
- (iii) Intrinsic information (1 mark)
- (iv) Gain ratio (1 mark)
- (v) Gini impurity (1 mark)

Gain Ratio (cont)

Example 7: (cont)

Solution:

- (i) Entropy characterises the impurity in a collection of data.
- (ii) Information gain measures how well a given split separates the data according to their response variable classification.
- (iii) Intrinsic information represents the potential information generated by splitting the data into different partitions.
- (iv) Gain ratio is the normalisation of information gain by intrinsic information.
- (v) Gini impurity measures total variance across the classes.

Gain Ratio (cont)

Example 8: (SRM-02-18, Q9)

A classification tree is being constructed to predict if an insurance policy will lapse. A random sample of 100 policies contains 30 that lapsed. Consider two splits:

Split 1: One node has 20 observations with 12 lapses and one node has 80 observations with 18 lapses.

Split 2: One node has 10 observations with 8 lapses and one node has 90 observations with 22 lapses.

Gain Ratio (cont)

Example 8: (cont)

The total Gini impurity after a split is the weighted average of the Gini impurity at each node, with the weights proportional to the number of observations in each node.

The total entropy after a split is the weighted average of the entropy at each node, with the weights proportional to the number of observations in each node.

Gain Ratio (cont)

Example 8: (cont)

Determine which of the following statements is/are true?

- I. Split 1 is preferred based on the total Gini impurity.
 - II. Split 1 is preferred based on the total entropy.
 - III. Split 1 is preferred based on having fewer classification errors.
-
- (A) I only
 - (B) II only
 - (C) III only
 - (D) I, II, and III
 - (E) The correct answer is not given by (A), (B), (C), or (D).

Gain Ratio (cont)

Example 8: (cont)

Solution:

$$\begin{aligned}\text{Gini}(\text{Split 1}) &= \frac{20}{100} \left[1 - \left(\frac{12}{20} \right)^2 - \left(\frac{8}{20} \right)^2 \right] + \frac{80}{100} \left[1 - \left(\frac{18}{80} \right)^2 - \left(\frac{62}{80} \right)^2 \right] \\ &= 0.2 \times 0.48 + 0.8 \times 0.34875 = 0.375\end{aligned}$$

$$\begin{aligned}\text{Gini}(\text{Split 2}) &= \frac{10}{100} \left[1 - \left(\frac{8}{10} \right)^2 - \left(\frac{2}{10} \right)^2 \right] + \frac{90}{100} \left[1 - \left(\frac{22}{90} \right)^2 - \left(\frac{68}{90} \right)^2 \right] \\ &= 0.1 \times 0.32 + 0.9 \times 0.3693827 = 0.3644\end{aligned}$$

⇒ **Lower Gini impurity** is better. ∴ Split 2 is preferred. I is wrong.

$$\begin{aligned}\text{H}(\text{Split 1}) &= -\frac{20}{100} \left[\frac{12}{20} \log_2 \frac{12}{20} + \frac{8}{20} \log_2 \frac{8}{20} \right] - \frac{80}{100} \left[\frac{18}{80} \log_2 \frac{18}{80} + \frac{62}{80} \log_2 \frac{62}{80} \right] \\ &= -0.2 \times (-0.9710) - 0.8 \times (-0.7692) = 0.8096\end{aligned}$$

$$\begin{aligned}\text{H}(\text{Split 2}) &= -\frac{10}{100} \left[\frac{8}{10} \log_2 \frac{8}{10} + \frac{2}{10} \log_2 \frac{2}{10} \right] - \frac{90}{100} \left[\frac{22}{90} \log_2 \frac{22}{90} + \frac{68}{90} \log_2 \frac{68}{90} \right] \\ &= -0.1 \times (-0.7219) - 0.9 \times (-0.8024) = 0.7944\end{aligned}$$

⇒ **Smaller entropy** (vs larger information gain) is better. ∴ Split 2 is preferred. II is wrong.

Remark: SRM Answer is different because they use natural log.

For Split 1, there are 8+18=26 errors while for Split 2 there are 2+22 = 24 errors. With fewer errors, Split 2 is preferred.

Answer: (E)

Gain Ratio (cont)

Example 9: (Final Exam Jan 2019, Q2(d))

A classification tree is being constructed to predict if an insurance policy will lapse. A random sample of 1000 policies contains 320 that lapsed. You are considering two splits:

Split 1: One node has 260 observations with 140 lapses and one node has 740 observations with 180 lapses.

Split 2: One node has 120 observations with 70 lapses and one node has 880 observations with 250 lapses.

Gain Ratio (cont)

Example 9: (cont)

Determine which split is preferred based on

- (i) Gini impurity (4 marks)
- (ii) Information gain (4 marks)
- (iii) Gain ratio (3 marks)
- (iv) Classification errors (3 marks)

Gain Ratio (cont)

Example 9: (cont)

Can you get the results?

- (i) $G(S_1) = 0.4017$; $G(S_2) = 0.4163$ ($S_1 \checkmark$)
- (ii) $IG(S_1) = 0.0532$; $IG(S_2) = 0.0291$ ($S_1 \checkmark$)
- (iii) $R(S_1) = 0.0644$; $R(S_2) = 0.0550$ ($S_1 \checkmark$)
- (iv) Classification error (also known as Misclassification error, ME), i.e. $1 - \max_j \{p_j\}$ (vs Gini $1 - \sum_j p_j^2$ and IG $-\sum_j p_j \log_2 p_j$).

$$\text{ME before split} = 1 - \max\left\{\frac{320}{1000}, \frac{680}{1000}\right\} = 0.68$$

$$\text{ME for Split 1} = \frac{260}{1000} \left(1 - \max\left\{\frac{140}{260}, \frac{120}{260}\right\}\right) + \frac{740}{1000} \left(1 - \max\left\{\frac{180}{740}, \frac{560}{740}\right\}\right) = 0.3$$

$$\text{ME for Split 2} = \frac{120}{1000} \left(1 - \max\left\{\frac{70}{120}, \frac{50}{120}\right\}\right) + \frac{880}{1000} \left(1 - \max\left\{\frac{250}{880}, \frac{630}{880}\right\}\right) = 0.3$$

Gain Ratio (cont)

From this example, we can see that misclassification error (smaller is better) is not able to distinguish between the two splits. In general, it is not able to generate a good decision tree compare to the Information Gain, the Gini impurity index and the Gain Ratio. Therefore it is ignored in this course except being mentioned in the past year final exam.

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Decision Tree Implementations

The evolution of various classification (and regression*) tree algorithms is shown below:

1st generation: node splitting

- THAID [MM72]
- CHAID [Kas80]

2nd generation: tree-pruning, CV, gain ratio.

- CART (Breiman et al., 1984)
- ID3 (Quinlan, 1986)
- M5 (Quinlan, 1992)*
- C4.5 (Quinlan, 1993)
- FACT (Loh and Vanichsetakul, 1988)

Decision Tree Implementations (cont)

3rd generation: more enhanced split rules.

- QUEST (Loh and Shih, 1997)
- CRUISE (Kim and Loh, 2001, 2003)
- Bayesian CART (Chipman et al., 1998; Denison et al., 1998)*

4th generation: ensemble methods

- GUIDE (Loh, 2002, 2009; Loh and Zheng, 2013; Loh et al., 2015)
- CTREE (Hothorn et al., 2006)
- MOB (Zeileis et al., 2008)*
- Random forest [Bre01]
- TARGET (Fan and Gray, 2005)
- BART (Chipman et al., 2010)

Decision Tree Implementations (cont)

Aspect	Original ID3	C4.5	CART
Features	Discrete features only; cannot handle numeric features	continuous and discrete features	continuous and discrete features
missing values	Not supported	Handles missing attributes by ignoring them in Gain Ratio (or IG)	Surrogate variables are used (see rpart documentation)
splitting criteria	Multi-category split which max. IG / min. entropy	Multi-category split which maximises gain ratio	uses Gini impurity to perform binary split
shape	short and wide tree	short and wide tree	taller tree
pruning	no pruning, prone to overfitting	performs post-pruning (bottom-up pruning)	prunes the tree to a size with the lowest cross-validation estimate of error

ID3 Algorithm

ID3 (Iterative Dichotomiser 3) was developed in 1986 by Ross Quinlan. The training observations are sorted to the corresponding internal nodes. If the nodes only contain observations from a single class, then the node will become a leaf node. Otherwise, it will be further expanded, by selecting the predictor with highest information gain relative to the new subsets of observations.

ID3 Algorithm (cont)

Example 10: (Final Exam May 2019, Q5(b))

A decision tree model is built to detect whether an online transaction is a fraud transaction (Yes/No), based on three variables – credit card association, transaction amount and country. Table Q5(b) – i to Q5(b) – iii shows the number of observations for different variables with different levels, for fraud and not fraud cases respectively.

Credit Card Associations	Fraud = Yes	Fraud = No
Amex	11	20
Master	34	47
Visa	25	33

Table Q5(b) – i

ID3 Algorithm (cont)

Example 10: (cont)

Transaction Amount	Fraud = Yes	Fraud = No
<1000	52	21
≥ 1000	18	79

Table Q5(b) – ii

Country	Fraud = Yes	Fraud = No
A	25	32
B	17	46
C	28	22

Table Q5(b) – iii

ID3 Algorithm (cont)

Example 10: (cont)

Construct a decision tree with leaves purity of at least 70% by using gain ratio. State the prediction and respective purity for each terminal node. (15 marks)

Solution: Let S be the whole table of Fraud, Fraud=Yes be positive (+) class and Fraud=No be negative (-) class.

To answer this question, we need to recall the Gain ratio, Equation (7) on Page 34:

$$R(S^A) = IG(S^A)/H(A).$$

ID3 Algorithm (cont)

Example 10: (cont)

Total, $S = [70+, 100-] \Rightarrow H(S) = - \left[\frac{70}{170} \log_2 \frac{70}{170} + \frac{100}{170} \log_2 \frac{100}{170} \right] = 0.9774$

For $X_1 =$ Credit card association [Amex= A ; Master= M ; Visa= V]:

$$\begin{aligned} A = [11+, 20-] &\Rightarrow H(\text{Fraud} | X_1 = A) \\ &= - \left[\frac{11}{31} \log_2 \frac{11}{31} + \frac{20}{31} \log_2 \frac{20}{31} \right] = 0.9383 \end{aligned}$$

$$M = [34+, 47-] \Rightarrow H(S_M) = 0.9813$$

$$V = [25+, 33-] \Rightarrow H(S_V) = 0.9862$$

$$IG(S^{X_1}) = 0.9774 - \left[\frac{31}{170} \times 0.9383 + \frac{81}{170} \times 0.9813 + \frac{58}{170} \times 0.9862 \right] = 0.0023$$

$$H(X_1) = - \left[\frac{31}{170} \log_2 \frac{31}{170} + \frac{81}{170} \log_2 \frac{81}{170} + \frac{58}{170} \log_2 \frac{58}{170} \right] = 1.4866$$

$$R(S^{X_1}) = \frac{0.0023}{1.4866} = 0.0015$$

ID3 Algorithm (cont)

Example 10: (cont)

For $X_2 = \text{Transaction amount}$ [$< 1000 = L$; $\geq 1000 = H$]:

$$L = [52+, 21-] \Rightarrow H(S_L) = 0.8657$$

$$H = [18+, 79-] \Rightarrow H(S_H) = 0.6921$$

$$IG(S^{X_2}) = 0.9774 - \left[\frac{73}{170} \times 0.8657 + \frac{97}{170} \times 0.6921 \right] = 0.2108$$

$$H(X_2) = - \left[\frac{73}{170} \log_2 \frac{73}{170} + \frac{97}{170} \log_2 \frac{97}{170} \right] = 0.9856$$

$$R(S^{X_2}) = 0.2139$$

For $X_3 = \text{Country}$ [A ; B ; C]:

$$A = [25+, 32-] \Rightarrow H(S_A) = 0.9891$$

$$B = [17+, 46-] \Rightarrow H(S_B) = 0.8412$$

$$C = [28+, 22-] \Rightarrow H(S_C) = 0.9896$$

$$IG(S^{X_3}) = 0.0430$$

$$H(X_3) = - \left[\frac{57}{170} \log_2 \frac{57}{170} + \frac{63}{170} \log_2 \frac{63}{170} + \frac{50}{170} \log_2 \frac{50}{170} \right] = 1.5786$$

$$R(S^{X_3}) = 0.0272$$

ID3 Algorithm (cont)

Example 10: (cont)

The transaction amount, X_2 , has the highest gain ratio, hence it should be chosen as the root node.

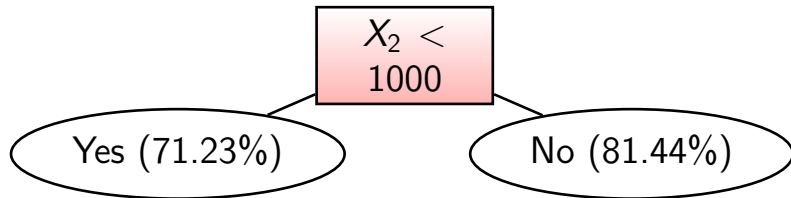
For $X_2 = L(< 1000)$: prediction=Yes; purity = $\frac{52}{52+21} = 0.7123$ (the “purity” is more than 70%)

For $X_2 = H(\geq 1000)$: prediction=No; purity = $\frac{79}{18+79} = 0.8144$ (the “purity” is more than 70%)

ID3 Algorithm (cont)

Example 10: (cont)

Therefore, we have the classification tree below.



ID3 Algorithm (cont)

The ID3 algorithm is restricted in dealing with categorical data only. However, [Mit97, §3.7.2] mentioned it is possible to introduce a threshold to turn the numeric feature to a binary categorical data. [Mit97, §3.7.3] also pointed out that ID3 can be extended to use gain ratio. Note that decision trees are myopic in general and ID3-trees are prone to overfitting as the tree depth increases. Therefore, we need more sophisticated tree algorithms.

ID3 Algorithm (cont)

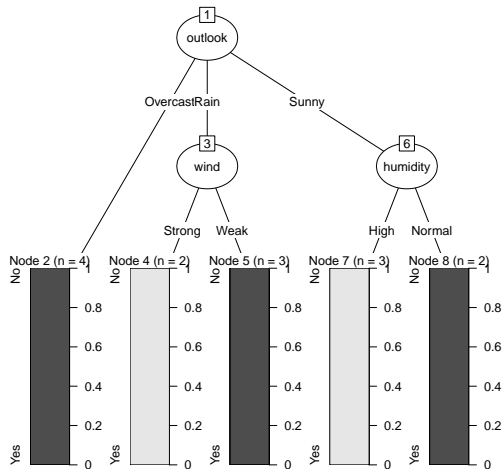
Since ID3 cannot handle numeric data, C4.5 is a successor to ID3 which removed the restriction that features must be categorical by dynamically defining a discrete attribute (based on numerical variables) that partitions the continuous attribute value into a discrete set of intervals. The C4.5 algorithm (https://en.wikipedia.org/wiki/C4.5_algorithm) constructs a decision tree based on the gain ratio. C4.5 is superseded in 1997 by a commercial system See5/C5.0 according to <https://rulequest.com/see5-comparison.html> and CART.

ID3 Algorithm (cont)

C5.0 is Quinlan's latest version release under a proprietary license. It uses less memory and builds smaller rulesets than C4.5 while being more accurate. The C50 library implements C5.0 decision trees and rule-based models for pattern recognition extend the work of [Qui86]. The company <https://www.rulequest.com> has the pattern of C5.0 and provides Cubist (Rule- And Instance-Based Regression Modelling) and outlier tree (Explainable outlier detection through decision tree conditioning based on GritBot) for statistical inference with tree models.

ID3 Algorithm (cont)

Example 11: Use C5.0 to construct the ID3 tree for the tennis data in **Example 3**.



C4.5 Algorithm

Example 12: Construct the C4.5 tree for the 'Numeric' Tennis / Golf Data below:

Day	Outlook	Temperature	Humidity	Wind	Play
D1	Sunny	85	85	Weak	No
D2	Sunny	80	90	Strong	No
D3	Overcast	83	78	Weak	Yes
D4	Rain	70	96	Weak	Yes
D5	Rain	68	80	Weak	Yes
D6	Rain	65	70	Strong	No
D7	Overcast	64	65	Strong	Yes
D8	Sunny	72	95	Weak	No
D9	Sunny	69	70	Weak	Yes
D10	Rain	75	80	Weak	Yes
D11	Sunny	75	70	Strong	Yes
D12	Overcast	72	90	Strong	Yes
D13	Overcast	81	75	Weak	Yes
D14	Rain	71	80	Strong	No

C4.5 Algorithm (cont)

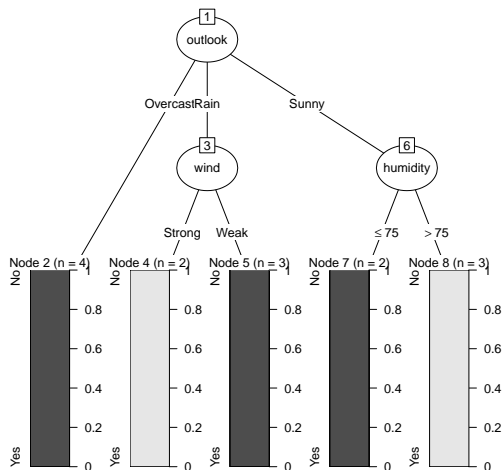
Example 12: (cont)

Solution:

```
library(C50)
tennis.data = read.csv("playtennis2.csv", skip=1,
  stringsAsFactors=TRUE)
names(tennis.data) = c("day","outlook","temperature","humidity",
  "wind","playtennis")
#tennis.data = read.csv("playtennis.csv", stringsAsFactors=TRUE)
tennis.data$day = NULL
model = C5.0(playtennis ~., data=tennis.data)
plot(model)
#model2 = C5.0(playtennis ~., data=tennis.data,
#  control=C5.0Control(subset=FALSE,noGlobalPruning=TRUE,
#  earlyStopping=FALSE,minCases=1,CF=1))
#plot(model2)
```

C4.5 Algorithm (cont)

Example 12: (cont)



C4.5 Algorithm (cont)

The handling of numeric feature humidity (for outlook=Sunny) in **Example 12** is roughly shown below (the C5.0 is a complex):

Day	Outlook	Temperature	Humidity	Wind	Play
D1	Sunny	85	85	Weak	No
D2	Sunny	80	90	Strong	No
D8	Sunny	72	95	Weak	No
D9	Sunny	69	70	Weak	Yes
D11	Sunny	75	70	Strong	Yes

Humidity	≤ 70	> 70	≤ 85	> 85	≤ 90	> 90	≤ 95	> 95
No	3	0	2	1	1	2	0	3
Yes	0	2	0	2	0	2	0	2
Entropy	0		0.5510		0.8		0.9710	

Minimum entropy is the same as maximum information gain. So we should pick 70 (we are close but not sure how C5.0 get 75).

CART

Classification And Regression Tree (CART) is a binary tree generation algorithm using Gini index as its splitting criteria which can handle both categorical and numeric predictors. CART handles missing values by surrogating tests to approximate outcomes.

A detail account of the algorithm is given in [BFSO84].

CART (cont)

CART is very similar to C4.5, but it differs in that it supports numerical target variables, i.e. it supports regression. CART constructs **binary trees** using the feature and threshold that yield the largest information gain at each node.

CART (in `rpart`) and CTree (conditionally inference tree, in the `party` and the `partykit`) are two available regression trees in R.

The scikit-learn uses an optimised version of the CART algorithm (`sklearn.tree.DecisionTreeRegressor`); however, the implementation does not support categorical variables for now (if the input is categorical, it will convert to number?).

CART (cont)

In R, CART is supported by `tree`, `rpart` and `party`. The `tree` library provides a limited functions of constructing, plotting and pruning trees. The `rpart`, which stands for “recursive partitioning” for classification (`method="class"`), regression (`method="anova"`) and survival (`method="exp"`) trees, implements most of the functionality of [BFSO84]. The `rpart.plot` or `partykit::plot.party` can be used to draw nice diagrams for `rpart`.

```
rpart(formula, data, weights, subset,
      na.action=na.rpart,
      method, model = FALSE, x = FALSE, y = TRUE,
      parms, control, cost, ...)
```

CART (cont)

The `ctree()` from `party` library is designed based on continuous input(s) X_i , however, it supports nominal, ordinal, numeric, censored as well as multivariate response variables Y . It implements the conditional inference trees which embed tree-structured regression models:

- 1 Test the global null hypothesis of independence between X_i and Y ;
- 2 Perform binary split in the selected X_i ;
- 3 Recursively repeat steps 1. & 2.

```
ctree(formula, data, subset=NULL, weights=NULL,  
      controls = ctree_control(), xtrafo = ptrao,  
      ytrafo = ptrao, scores = NULL)
```

CART (cont)

The `ctree()` from `partykit` library is a reimplementation of (most of) `'party::ctree'`. It treats nominal variables as ordered variables.

```
ctree(formula, data, subset, weights,
      na.action=na.pass, offset, cluster,
      control = ctree_control(...), ytrafo = NULL,
      converged = NULL, scores = NULL, doFit = TRUE, ...)
```

Benefits: `ctree` avoids certain variable selection bias of `rpart` (which tends to select variables that have many possible splits or many missing values) and uses a (permutation-based) significance test procedure in order to select variables instead of selecting the variable that maximises the impurity (e.g. Gini coefficient).

CART (cont)

The decision trees C5.0, CART/rpart, ctree are based on impurity measures or statistics on the individual input against the output.

The **model-based recursive partitioning** yields a decision tree with fitted parametric models (such as GLM) associated with each terminal node.

It is available in R with the syntax:

```
party::mob(formula, weights, data = list(),
  na.action=na.omit, model=glinearModel,
  control=mob_control(), ...)
partykit::mob(formula, data, subset, na.action,
  weights, offset, cluster, fit,
  control=mob_control(), ...)
```

CART (cont)

In Python, CART for classification is implemented as `sklearn.tree.DecisionTreeClassifier`, which is capable of both binary classification with labels $\{-1, 1\}$ and multiclass classification with labels $\{0, \dots, K - 1\}$.

```
DecisionTreeClassifier(*, criterion='gini', splitter='best',  
    max_depth=None, min_samples_split=2, min_samples_leaf=1,  
    min_weight_fraction_leaf=0.0, max_features=None,  
    random_state=None, max_leaf_nodes=None,  
    min_impurity_decrease=0.0, class_weight=None, ccp_alpha=0.0)
```

CART (cont)

Example 13: Use CART to construct a decision tree for the tennis data in **Example 3**.

Solution: We can either use tree library:

```
1 library(tree)
2 tennis.data = read.csv("playtennis.csv")
3 tennis.data = tennis.data[,2:ncol(tennis.data)] # Remove 'day'
4 t.m = tree(playtennis~., data=tennis.data, control=tree.control(
5     nobs=nrow(tennis.data),minsize=1))
6 print(t.m); plot(t.m); text(t.m, cex=0.8)
```

or the rpart library:

```
1 library(rpart)
2 tennis.data = read.csv("playtennis.csv")
3 tennis.data$day = NULL
4 dt = rpart(playtennis ~ ., data=tennis.data,
5     control=rpart.control(minsplit=2, minbucket=1, cp=0.001))
6 print(dt); plot(dt, margin=0.05); text(dt, use.n=TRUE, cex=0.8)
```

CART (cont)

Example 13: (cont)

Text/Logic representation of tree::tree:

```
node), split, n, deviance, yval, (yprob)
```

```
* denotes terminal node
```

```
1) root 14 18.250 Yes ( 0.3571 0.6429 )
  2) outlook: Rain,Sunny 10 13.860 No ( 0.5000 0.5000 )
    4) humidity: High 5 5.004 No ( 0.8000 0.2000 )
      8) outlook: Rain 2 2.773 Yes ( 0.5000 0.5000 )
        16) wind: Strong 1 0.000 No ( 1.0000 0.0000 ) *
        17) wind: Weak 1 0.000 Yes ( 0.0000 1.0000 ) *
      9) outlook: Sunny 3 0.000 No ( 1.0000 0.0000 ) *
    5) humidity: Normal 5 5.004 Yes ( 0.2000 0.8000 )
      10) wind: Strong 2 2.773 No ( 0.5000 0.5000 )
        20) outlook: Rain 1 0.000 No ( 1.0000 0.0000 ) *
        21) outlook: Sunny 1 0.000 Yes ( 0.0000 1.0000 ) *
      11) wind: Weak 3 0.000 Yes ( 0.0000 1.0000 ) *
    3) outlook: Overcast 4 0.000 Yes ( 0.0000 1.0000 ) *
```

CART (cont)

Example 13: (cont)

Text/Logic representation of `rpart::rpart`:

```
node), split, n, loss, yval, (yprob)
```

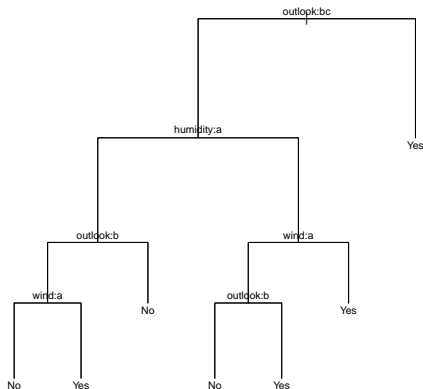
```
* denotes terminal node
```

```
1) root 14 5 Yes (0.3571429 0.6428571)
  2) outlook=Rain,Sunny 10 5 No (0.5000000 0.5000000)
    4) humidity=High 5 1 No (0.8000000 0.2000000)
      8) outlook=Sunny 3 0 No (1.0000000 0.0000000) *
      9) outlook=Rain 2 1 No (0.5000000 0.5000000)
        18) wind=Strong 1 0 No (1.0000000 0.0000000) *
        19) wind=Weak 1 0 Yes (0.0000000 1.0000000) *
    5) humidity=Normal 5 1 Yes (0.2000000 0.8000000)
      10) wind=Strong 2 1 No (0.5000000 0.5000000)
        20) outlook=Rain 1 0 No (1.0000000 0.0000000) *
        21) outlook=Sunny 1 0 Yes (0.0000000 1.0000000) *
      11) wind=Weak 3 0 Yes (0.0000000 1.0000000) *
  3) outlook=Overcast 4 0 Yes (0.0000000 1.0000000) *
```

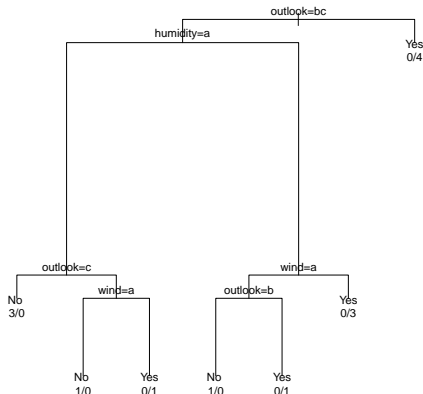
CART (cont)

Example 13: (cont)

Graphical representation of CART trees:



(a) tree



(b) rpart

CART (cont)

Example 14: (2D numeric inputs with R's tree library)
Training the tree's decision tree on the "flame" data produces the CART tree:

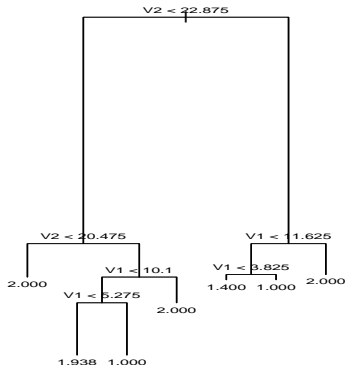
```
node), split, n, deviance, yval
  * denotes terminal node

1) root 240 55.4600 1.638
  2) V2 < 22.875 165 16.8100 1.885
    4) V2 < 20.475 113 0.0000 2.000 *
    5) V2 > 20.475 52 12.0600 1.635
      10) V1 < 10.1 34 8.3820 1.441
        20) V1 < 5.275 16 0.9375 1.938 *
        21) V1 > 5.275 18 0.0000 1.000 *
      11) V1 > 10.1 18 0.0000 2.000 *
  3) V2 > 22.875 75 6.3470 1.093
    6) V1 < 11.625 70 1.9430 1.029
      12) V1 < 3.825 5 1.2000 1.400 *
      13) V1 > 3.825 65 0.0000 1.000 *
    7) V1 > 11.625 5 0.0000 2.000 *
```

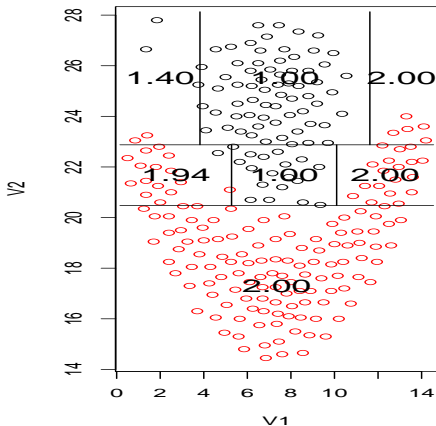
CART (cont)

Example 14: (cont)

plot.tree



partition.tree



For numeric inputs, the feature space can be regarded as being 'recursively' partitioned, therefore the name 'rpart'.

CART (cont)

Example 15: (2D numeric inputs with R's rpart library)
Training the rpart's decision tree on the “flame” data produces the CART tree:

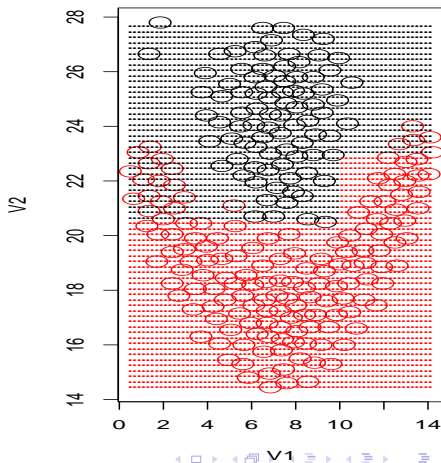
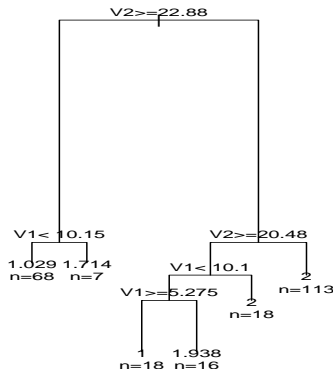
```
node), split, n, deviance, yval
  * denotes terminal node
```

```
1) root 240 55.462500 1.637500
  2) V2>=22.875 75 6.346667 1.093333
    4) V1< 10.15 68 1.941176 1.029412 *
    5) V1>=10.15 7 1.428571 1.714286 *
  3) V2< 22.875 165 16.812120 1.884848
    6) V2>=20.475 52 12.057690 1.634615
      12) V1< 10.1 34 8.382353 1.441176
        24) V1>=5.275 18 0.000000 1.000000 *
        25) V1< 5.275 16 0.937500 1.937500 *
      13) V1>=10.1 18 0.000000 2.000000 *
    7) V2< 20.475 113 0.000000 2.000000 *
```

CART (cont)

Example 15: (cont)

The decision tree of the “flame” data can be analysed using rpart’s CART tree and produces:



CART (cont)

Example 16: (SRM-02-18, Q33)

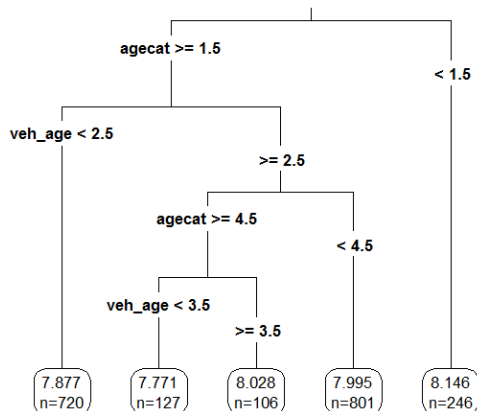
The regression tree shown below was produced from a dataset of auto claim payments. Age Category (agecat: 1, 2, 3, 4, 5, 6) and Vehicle Age (veh_age: 1, 2, 3, 4) are both predictor variables, and log of claim amount (LCA) is the dependent variable.

Consider three autos I, II, III:

- i. An Auto in Age Category 1 and Vehicle Age 4
- ii. An Auto in Age Category 5 and Vehicle Age 5
- iii. An Auto in Age Category 5 and Vehicle Age 3

CART (cont)

Example 16: (cont)



CART (cont)

Example 16: (cont)

Rank the estimated LCA of Autos I, II, and III.

- (A) $LCA(I) < LCA(II) < LCA(III)$
- (B) $LCA(I) < LCA(III) < LCA(II)$
- (C) $LCA(II) < LCA(I) < LCA(III)$
- (D) $LCA(II) < LCA(III) < LCA(I)$
- (E) $LCA(III) < LCA(II) < LCA(I)$

Answer: (E) Do you know why?

Outline

1 Theory and Terminologies

2 Impurity Measures

3 Implementations

4 Practical Considerations

Practical Considerations

- overfitting
- tree pruning
- complexity

Example 17: (SRM-02-18, Q29) Determine which of the following considerations may make decision trees preferable to other statistical learning methods.

- i. Decision trees are easily interpretable.
- ii. Decision trees can be displayed graphically.
- iii. Decision trees are easier to explain than linear regression methods.

Practical Considerations (cont)

Example 17: (cont)

- (A) None
- (B) I and II only
- (C) I and III only
- (D) II and III only
- (E) The correct answer is not given by (A), (B), (C), or (D).

Solution: All three statements are true. See [JWHT13, Section 8.1]. The statement that trees are easier to explain than linear regression methods may not be obvious. For those familiar with regression but just learning about trees, the reverse may be the case. However, for those not familiar with regression, relating the dependent variable to the independent variables, especially if the dependent variable has been transformed, can be difficult to explain.

Answer: (E)

Practical Considerations (cont)

Tree Pruning:

A smaller tree with fewer splits may lead to a lower variance, better interpretation and slightly more “generalisation”. There are two approaches in “pruning” a complex decision tree:

- **Pre-pruning:** This type of algorithms will stop growing the tree earlier, before it perfectly classifies the training set.
- **Post-pruning:** This type of algorithms will allow the tree to perfectly classify training set, and post prune the tree.

Practical Considerations (cont)




Complexity:

Let n be the number of samples and p be the number of features (which are used throughout the lecture).




According to [https:](https://scikit-learn.org/stable/modules/tree.html)

[//scikit-learn.org/stable/modules/tree.html](https://scikit-learn.org/stable/modules/tree.html), the run time cost to construct a balanced binary tree is $O(p \times n \log(n))$ and query time $O(\log(n))$. Although the tree construction algorithm attempts to generate balanced trees, they will not always be balanced.



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