Decision Trees for Classification

Overview

- Classification is widely used for prediction purposes.
- For example, by building a classifier on the transcripts of United States Congressional floor debates, it can be determined whether the speeches represent support or opposition to proposed legislation.
- Classification can help health care professionals diagnose heart disease patients.
- Based on an email's content, email providers also use classification to decide whether the incoming email messages are spam.
- Decision tree is a classification method with two varieties: **classification tree** and **regression tree**. We focus more on the first one.

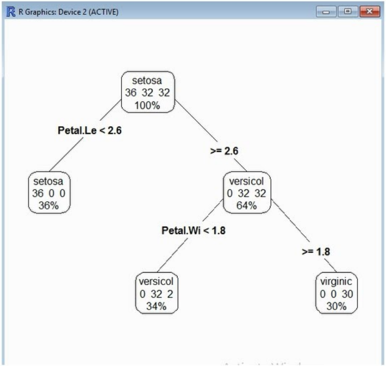
Decision Trees (DT)

- A decision tree (also called prediction tree) uses a tree structure to specify sequences of decisions and consequences.

- Given a set of features $X = (x_1, x_2, ..., x_n)$, here, each x_i is denoted for a feature, the goal is to predict a response or output variable Y.

- Each member of the set $(x_1, x_2, ..., x_n)$ is called an input variable or feature.

Decision Tree Classification in R



Example of a decision tree

General idea of a DT

- Prediction can be achieved by constructing a decision tree with test points and branches.
- At each test point, a decision is made to pick a specific branch and traverse down the tree.
- Eventually, a final point is reached, and a prediction can be made.
- Each test point in a decision tree involves testing a particular input variable (or attribute), and each branch represents the decision being made.
- Due to its flexibility and easy visualization, decision trees are commonly deployed in data mining applications for classification purposes.

General idea of a DT

- The input values of a decision tree can be categorical or continuous.
- A decision tree employs a structure of test points, called **nodes**, and **branches**—which represent the decision being made.
- A node without further branches is called a **leaf node**.
- The leaf nodes return class labels and, in some implementations, they return the probability scores.

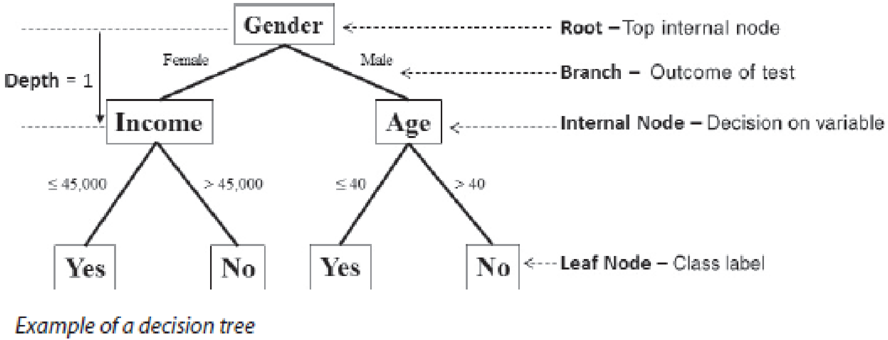
General idea of a DT

- Classification trees usually apply to output variables that are categorical (often binary) in nature, such as yes or no, purchase or not purchase, and so on.

- They can be easily represented in a visual way, and the corresponding decision rules are quite straightforward.

- We will start with an example with predicting whether customers will buy a product.

An Example



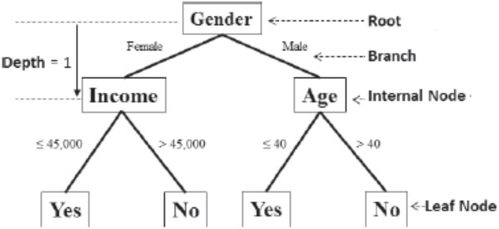
Example of a decision tree. Source: *Data Science & Big Data Analytics*

Decision Trees

- 'Branch' refers to the outcome of a decision and is visualized as a line connecting two nodes.
- If a decision is numerical, the "greater than" branch is usually placed on the right, and the "less than" branch is placed on the left.
- Depending on the nature of the variable, one of the branches may need to include an "equal to" component.

Example of a Decision Tree

- Internal nodes are the decision or test points.
- Each internal node refers to an input variable or an attribute.
- The top internal node is called the root.
- The decision tree on the right is a binary tree in that each internal node has no more than two branches.
- The branching of a node is referred to as a split.



General idea of a DT

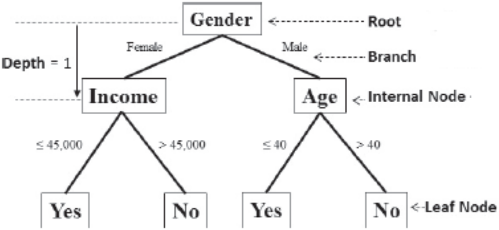
- Sometimes decision trees may have more than two branches stemming from a node.

- For example, suppose an input variable `Weather` is categorical and has three choices: Sunny, Rainy, and Snowy.

- Then the corresponding node `Weather` in the decision tree may have three branches labelled as Sunny, Rainy, and Snowy, respectively.

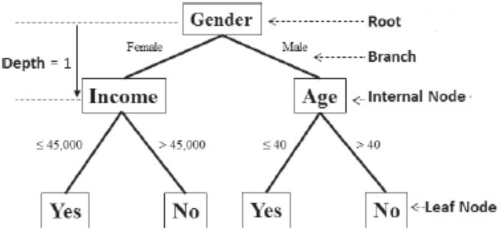
Example of a Decision Tree

- The depth of a node is the minimum number of steps required to reach the node from the root.
- In the decision tree on the left, nodes `Income` and `Age` have a depth of one, and the four nodes on the bottom of the tree have a depth of two.



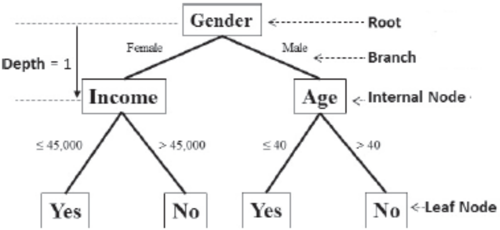
Example of a Decision Tree

- Leaf nodes are at the end of the last branches on the tree.
- They represent class labels: the outcome of all the prior decisions.
- The path from the root to a leaf node contains a series of decisions made at various internal nodes.



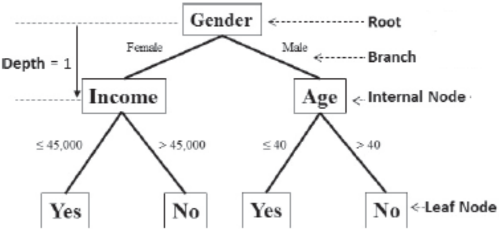
Example of a Decision Tree

- In this figure, the root node splits into two branches with a `Gender` test. The right branch contains all those records with the variable `Gender` equal to `Male`, and the left branch contains all those records with the variable `Gender` equal to `Female` to create the depth 1 internal nodes.
- Each internal node effectively acts as the root of a sub-tree, and a best test for each node is determined independently of the other internal nodes.



Example of a Decision Tree

- The left-hand side (LHS) internal node splits on a question based on the `Income` to create leaf nodes at depth 2, whereas the right-hand side (RHS) splits on a question on the `Age` variable.
- This decision tree shows that **females with income less than or equal to $45,000 and males 40 years old or younger are classified as people who would purchase the product**.
- In traversing this tree, age does not matter for females, and income does not matter for males.



Examples of DT

- Decision trees are widely used in practice.

- For example, to classify animals, questions like cold-blooded or warm-blooded, mammal or not mammal, etc. are answered to arrive at a certain classification.

- Another example is a checklist of symptoms during medical evaluation of a patient.

- The artificial intelligence (AI) engine of a video game commonly uses decision trees to control the autonomous actions of a character in response to various scenarios.

Examples of DT

- Retailers can use decision trees to segment customers or predict response rates to marketing and promotions.

- Financial institutions can use decision trees to help decide if a loan application should be approved or denied. In the case of loan approval, computers can use the logical if-then statements to predict whether the customer will default on the loan.

- For customers with a clear (strong) outcome, no human interaction is required; for observations that may not generate a clear response, a human is needed for the decision.

Some Questions

- Question 1: Why `Gender` was selected as the root? Why not `Age` or `Income` be selected?

- Question 2: How do we implement/run DT in R when a data set is given?

Who would subscribe to a term deposit?

- Our first example of decision trees in in R concerns a bank that wants to market its term deposit products (such as Certificates of Deposit) to the appropriate customers.
- Given the demographics of clients and their reactions to previous campaign phone calls, the bank's goal is to predict which clients would subscribe to a term deposit.
- The data set `bank-sample.csv` contains records of 2000 customers.

'bank-sample.csv' Data Set

- The variables include (1) job, (2) marital status, (3) education level, (4) if the credit is in default, (5) if there is a housing loan, (6) if the customer currently has a personal loan, (7) contact type, (8) result of the previous marketing campaign contact (poutcome), and finally (9) if the client actually subscribed to the term deposit.
- Attributes (1) through (8) are the input variables or features.
- (9) is considered the (binary) outcome: The outcome subscribed is either yes (meaning the customer will subscribe to the term deposit) or no (meaning the customer won't subscribe).
- All the variables listed earlier are categorical.

'bank-sample.csv' Data Set

```
> bankdata = read.csv("C:/Data/bank-sample.csv", header = TRUE)
> head(bankdata[,2:8])
          job  marital education default balance housing loan
1  management   single  tertiary      no       0     yes   no
2 entrepreneur  married  tertiary      no    1752     yes  yes
3     services divorced secondary      no    4329      no   no
4  management  married  tertiary      no    1108     yes   no
5  management  married secondary      no    1410     yes   no
6  management   single  tertiary      no     499     yes   no
> head(bankdata[,c(9,16,17)])
   contact poutcome subscribed
1 cellular  unknown         no
2 cellular  unknown         no
3 cellular  unknown        yes
4 cellular  unknown         no
5  unknown  unknown         no
6  unknown  unknown         no
```

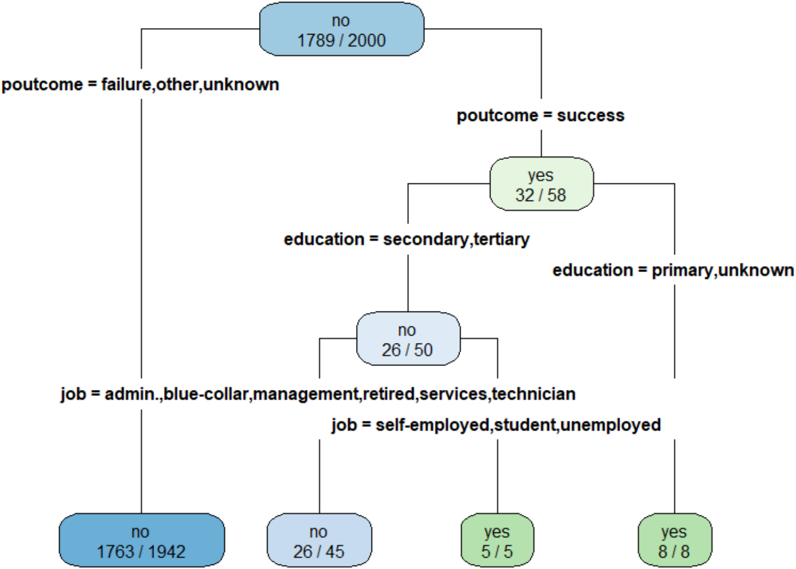
```
> table(bankdata$job)

       admin.   blue-collar  entrepreneur     housemaid    managemen
          235           435            70            63           42
      retired self-employed      services       student    technicia
           92            69           168            36           33
   unemployed       unknown
           60            10
> table(bankdata$marital)

divorced  married   single
     228     1201      571
> table(bankdata$education)

  primary secondary  tertiary   unknown
      335      1010       564        91
> table(bankdata$default)

  no  yes
1961   39
```

```
> table(bankdata$housing)

  no  yes
 916 1084

> table(bankdata$loan)

  no  yes
1717  283

> table(bankdata$contact)

 cellular telephone   unknown
     1287       136       577

> table(bankdata$poutcome)

failure   other success unknown
    210      79      58    1653
```

- We will build a decision tree to predict the response subscribed based on the features: `job`, `marital`, `education`, `default`, `housing`, `loan`, `contact` and `poutcome`.

```
> #install.packages("rpart")
> #install.packages("rpart.plot")
> library("rpart")
> library("rpart.plot")
> fit <- rpart(subscribed ~job + marital + education+default +
+ housing + loan + contact+poutcome,
+ method="class",
+ data=bankdata,
+ control=rpart.control(minsplit=1),
+ parms=list(split='information'))
> # To plot the fitted tree:
> rpart.plot(fit, type=4, extra=2, clip.right.labs=FALSE)#, faclen=(
```

Plot of a fitted tree



Decision Tree Algorithm

- *Question*: Why is the variable `poutcome` selected as the decision variable at the root node?

- *Question*: Traversing down the tree, how are the subsequent decision variables at each node selected?

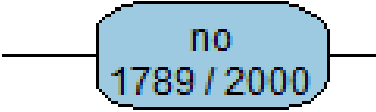
Questions

- *Question*: Why is the variable `poutcome` selected as the decision variable at the root node?

- *Question*: Traversing down the tree, how are the subsequent decision variables at each node selected?

The Root Node

- The *purity* of a node is defined as its probability of the corresponding class
- For example, in the root node of the decision tree built earlier,
  $P(\text{subscribed} = 0) = \frac{1789}{2000} \approx 89.45\%$
- Therefore, the root is 89.45% pure on the subscribed $= 0$ class and 10.55% pure on the subscribed $= 1$ class



Choosing Internal Node

- The first step after the Root Node is to choose the **most informative attribute**.

- A common way to identify the most informative attribute is to use entropy-based methods, which are used by decision tree learning algorithms such as ID3 (or Iterative Dichotomiser 3) and C4.5.

- The entropy methods select the most informative attribute based on two basic measures:

(i) *Entropy*, which measures the impurity of an attribute

(ii) *Information gain*, which measures the purity of an attribute

Entropy

- Given variable Y and and the set of possible categorical values it can take, $(y_1, y_2, ..., y_K)$, the entropy of Y is defined as

$$D_Y = -\sum_{j=1}^{K} P(Y = y_j) \log_2 P(Y = y_j),$$

where $P(Y = y_j)$ denotes the purity or the probability of the class $Y = y_j$, and $\sum_{j=1}^{K} P(Y = y_j) = 1$.

Entropy

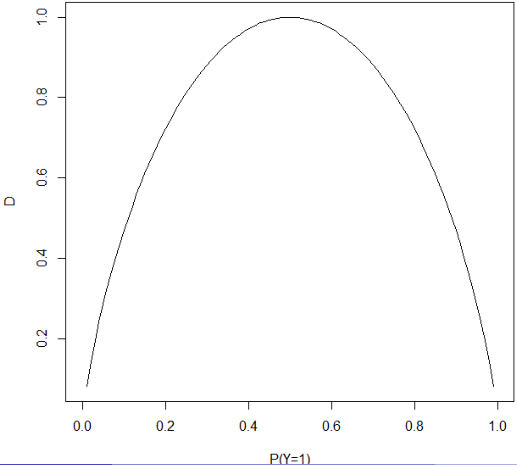
- If the variable Y is binary and only take on two values 0 or 1, the entropy of Y is
$$-\left\{P(Y=1)\log_2 P(Y=1) + P(Y=0)\log_2 P(Y=0)\right\}.$$
- For example, let Y denote the outcome of a coin toss, where $Y = 1$ for head and $Y = 0$ for tail.
- If the coin if a fair one, then $P(Y=0) = P(Y=1) = \frac{1}{2}$, so that the entropy is calculated as
$$-\left\{0.5\log_2 0.5 + 0.5\log_2 0.5\right\} = 1$$
- On the other hand, if the coin is biased, then suppose $P(Y=0) = \frac{3}{4}$, $P(Y=1) = \frac{1}{4}$, so that the entropy is now
$$-\left\{0.25\log_2 0.25 + 0.75\log_2 0.75\right\} \approx 0.81$$

Entropy

- Heuristically, entropy is a measure of unpredictability.
- When the coin is biased, we have less "uncertainty" in predicting the outcome of its next toss, so that the entropy is lower.
- When the coin is fair, we are much more less able to predict the next toss, and so the entropy is at its highest value.
- For a binary variable Y, we can plot in R its entropy.

Entropy Plot

```
> p=seq(0,1,0.01)
> D=-(p*log2(p)+(1-p)*log2(1-p))
> plot(p,D,ylab="D", xlab="P(Y=1)", type="l")
```



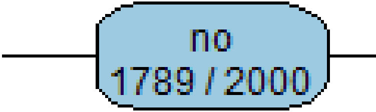
A good supplement before continuing

- A very simple example yet the general idea of Entropy is well explained.

`https://www.youtube.com/watch?v=ZVR2Way4nwQ&t=11s`

Bank Sample: Base Entropy

- The base entropy is defined as the entropy of the output variable at the root node.
- Recall: $P(\text{subscribed} = 0) = \frac{1789}{2000} \approx 89.45\%$ and $P(\text{subscribed} = 1) = 1 - \frac{1789}{2000} \approx 10.55\%$
- Therefore, the base entropy is $D_{\text{subscribed}} = -\{0.1055 log_2(0.1055) + 0.8945 log_2(0.8945)\} \approx$ $\color{red}{0.4862}$.



- Ideally, we would like to reduce this base entropy by leveraging on feature variables X for prediction.

- Recall that lower entropy is associated with less "uncertainty" in predicting the outcome, which is something that we want.

- So we select the feature that reduces entropy the most.

- We consider binary tree algorithm. Suppose feature X has split values (x_1, x_2). The conditional entropy given feature X and the split points (x_1, x_2) is defined as

$$
\begin{aligned}
D_{Y|X} &= \sum_{i=1}^{2} P(X = x_i) D(Y|X = x_i) \\
&= -\sum_{i=1}^{2} \left\{ P(X = x_i) \sum_{j=1}^{K} P(Y = y_j|X = x_i) log_2[P(Y = y_j|X = x_i)] \right\}
\end{aligned}
$$

Conditional Entropy

- We will illustrate the calculation of conditional entropy for the decision variable in the root node, `poutcome`.

- Recall that the split categories are x_1 : `failure,other,unknown` and x_2: `success`.

```
> length(bankdata$poutcome)
[1] 2000
> table(bankdata$poutcome)
failure   other success unknown
    210      79      58    1653
```

- Probabilities of two categories of `poutcome`:

	poutcome (X)	
	x_1 : `failure,other,unknown`	x_2: `success`
$P(X = x_i)$	$\frac{210+79+1653}{2000} = 0.971$	$\frac{58}{2000} = 0.029$

Conditional Entropy

```
> x1=which(bankdata$poutcome!="success")
> x2=which(bankdata$poutcome=="success")
> table(bankdata$subscribed[x1])

  no   yes
1763   179

> table(bankdata$subscribed[x2])

 no yes
 26  32
```

- Conditional probabilities:

	poutcome (X)	
	x_1 : failure,other,unknown	x_2: success
$P(X = x_i)$	$\frac{210+79+1653}{2000} = \frac{1942}{2000} = 0.971$	$\frac{58}{2000} = 0.029$
$P(Y = 1 \mid X = x_i)$	$\frac{179}{1942} \approx 0.092$	$\frac{32}{58} \approx 0.552$
$P(Y = 0 \mid X = x_i)$	$\frac{1763}{1942} \approx 0.908$	$\frac{26}{58} \approx 0.448$

Conditional Entropy

- Therefore the conditional entropy for selecting `poutcome` as decision variable with the split at x_1 and x_2 is

$$
\begin{aligned}
&D_{subscribed|poutcome}\\
&= -\sum_{i=1}^{2}\left\{P(X=x_i)\sum_{j=1}^{2}P(Y=y_j|X=x_i)log_2[P(Y=y_j|X=x_i)]\right\}\\
&= -\{0.971\times[0.092log_2(0.092)+0.908log_2(0.908)]\\
&+0.029\times[0.552log_2(0.552)+0.448log_2(0.448)]\}\\
&\approx 0.459
\end{aligned}
$$

- Hence, there is a reduction of about $0.4862-0.459\approx 0.027$ from the base entropy.

- This reduction in entropy is also known as **information gain**.

Entropy Reduction

- Hence, there is a reduction of about $0.4862 - 0.459 \approx 0.027$ from the base entropy.
- This reduction in entropy is also known as **information gain**.
- We can calculate the reduction for other feature variables and /or split points and show that they are all less than the entropy reduction of approximately 0.027.
- For example, using the same feature variable `poutcome`, let us instead calculate the conditional entropy for splitting at the values x_1 : `other,success,unknown` and x_2: **failure**.
- We shall show why this split is not the one in the decision tree built earlier, in terms of entropy reduction.

Different split for poutcome

```
> length(bankdata$poutcome)
[1] 2000
> table(bankdata$poutcome)
failure   other success unknown
    210      79      58    1653
```

- Split poutcome at x_1 : other, success, unknown and x_2: **failure**. Probabilities of two categories:

	poutcome (X)	
	x_1 : success, other, unknown	x_2: failure
$P(X = x_i)$	$\frac{58+79+1653}{2000} = 0.895$	$\frac{210}{2000} = 0.105$

Conditional Probabilities

```
> x1=which(bankdata$poutcome!="failure")
> x2=which(bankdata$poutcome=="failure")
> table(bankdata$subscribed[x1])

  no  yes
1600  190

> table(bankdata$subscribed[x2])

 no yes
189  21
```

- Conditional probabilities:

	poutcome (X)	
	x_1 : success, other, unknown	x_2: failure
$P(X = x_i)$	$\frac{58+79+1653}{2000} = \frac{1790}{2000} = 0.895$	$\frac{210}{2000} = 0.105$
$P(Y = 1 \mid X = x_i)$	$\frac{190}{1790} \approx 0.106$	$\frac{21}{210} = 0.10$
$P(Y = 0 \mid X = x_i)$	$\frac{1600}{1790} \approx 0.894$	$\frac{189}{210} = 0.90$

Entropy

- The conditional entropy for selecting `poutcome` as decision variable with the split at $x_1 =$ **success, other, unknown** and $x_2 =$ **failure** is

$$
\begin{aligned}
& D_{subscribed|poutcome} \\
&= -\sum_{i=1}^{2}\left\{P(X=x_i)\sum_{j=1}^{2}P(Y=y_j|X=x_i)log_2[P(Y=y_j|X=x_i)]\right\} \\
&= -\{0.895 \times [0.106log_2(0.106)+0.894log_2(0.894)] \\
&+0.105 \times [0.10log_2(0.10)+0.90log_2(0.90)]\} \\
&\approx 0.486
\end{aligned}
$$

- Hence, there is a reduction of about $0.4862 - 0.486 \approx 0.0002$ from the base entropy.
- This information gain is far less than splitting at x_1 : `failure,other,unknown` and x_2: `success`.

Entropy

- We can calculate the reduction for other feature variables and /or split points and show that they are all less than the entropy reduction of approximately 0.027.

- For example, instead of the feature variable `poutcome`, let us calculate the conditional entropy for choosing feature variable `education` at the split points x_1 : `tertiary` and x_2 : `secondary,primary,unknown`.

- We shall show why `education` is not the decision variable for the root node by calculating the reduction from the base entropy for `education`.

If Education...

```
> length(bankdata$education)
[1] 2000
> table(bankdata$education)
  primary secondary  tertiary   unknown
      335      1010       564        91
```

-

	education (X)	
	x_1 : tertiary	x_2: secondary,primary,unknown
$P(X = x_i)$	$\frac{564}{2000} = 0.282$	$\frac{335 + 1010 + 91}{2000} = 0.718$

If Education...

```
> x1=which(bankdata$education=="tertiary")
> x2=which(bankdata$education!="tertiary")
> table(bankdata$subscribed[x1])
```

```
 no yes
494  70
```

```
> table(bankdata$subscribed[x2])
```

```
  no  yes
1295  141
```

	education (X)	
	x_1 : tertiary	x_2: secondary,primary,unknown
$P(X = x_i)$	$\frac{564}{2000} = 0.282$	$\frac{335 + 1010 + 91}{2000} = \frac{1436}{2000} = 0.718$
$P(Y = 1 \mid X = x_i)$	$\frac{70}{564} \approx 0.124$	$\frac{141}{1436} = 0.098$
$P(Y = 0 \mid X = x_i)$	$\frac{494}{564} \approx 0.876$	$\frac{1295}{1436} = 0.902$

If Education, then Information Gain is

- Therefore the conditional entropy for selecting `education` as decision variable with the split at x_1 : `tertiary` and x_2: `secondary,primary,unknown` is

$$
\begin{aligned}
& D_{subscribed|poutcome} \\
& = -\sum_{i=1}^{2}\left\{P(X=x_i)\sum_{j=1}^{2}P(Y=y_j|X=x_i)log_2[P(Y=y_j|X=x_i)]\right\} \\
& = -\{0.282\times[0.124log_2(0.124)+0.876log_2(0.876)] \\
& +0.718\times[0.098log_2(0.098)+0.902log_2(0.902)]\} \\
& \approx 0.485
\end{aligned}
$$

- Therefore, there is a reduction of about $0.4862 - 0.485 \approx 0.0012$ from the base entropy.
- This information gain is far less than selecting `poutcome` as decision variable splitting at x_1 : `failure,other,unknown` and x_2: `success`

Conclusion

- Therefore, the decision tree algorithm proceeds at the root node by calculating the conditional entropy for (i) each feature variable X and (ii) its different split points.
- Then, the decision variable and its split points are selected based on the largest information gain (or decrease from base entropy).
- At internal nodes, the decision tree algorithm proceeds similarly by calculating the conditional entropy for (i) each feature variable X and (ii) its different split points.
- However, the sample for calculating the base and conditional entropies is restricted to the one at the node.

Conclusion

- The tree is built recursively until a criteria is met, for example

(i) All the leaf nodes in the tree satisfy the minimum purity threshold.

(ii) The tree cannot be further split with the preset minimum purity threshold.

(iii) Any other stopping criterion is satisfied (such as the maximum depth of the tree).

Gini Index

- Another commonly used criteria for selecting decision variable and split points is the Gini index.

- Given variable Y and and the set of possible categorical values it can take, $(y_1, y_2, ..., y_K)$, the Gini index of Y is defined as

$$G_Y = \sum_{j=1}^{K} P(Y = y_j)[1 - P(Y = y_j)],$$

  where $P(Y = y_j)$ denotes the purity or the probability of the class $Y = y_j$, and $\sum_{j=1}^{K} P(Y = y_j) = 1$.

- We will look at a few more examples of *decision trees* in R and also take a look at the decision or prediction surface that arise from fitting *decision trees*.

Example: Playing Golf?

- The goal of this illustrative example is to predict whether to play golf given factors such as weather outlook, temperature, humidity, and wind.
- Data set is `DTdata.csv` which contains five attributes: Play, Outlook, Temperature, Humidity, and Wind.
- Play would be the output variable (or the predicted class), and Outlook, Temperature, Humidity, and Wind would be the input variables.

Source: *The Straits Times*

Data Set

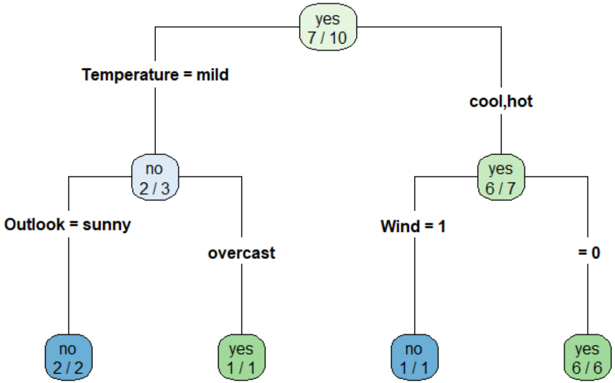
```
> library("rpart") # load libraries
> library("rpart.plot")
> play_decision <- read.table("C:/Data/DTdata.csv",header=TRUE,sep='
> head(play_decision)
  Play  Outlook Temperature Humidity  Wind
1  yes    rainy        cool   normal FALSE
2   no    rainy        cool   normal  TRUE
3  yes overcast         hot     high FALSE
4   no    sunny        mild     high FALSE
5  yes    rainy        cool   normal FALSE
6  yes    sunny        cool   normal FALSE
```

Aim

- We will build a *decision tree* to predict golf play based on feature variables such as weather outlook, temperature, humidity, and wind, using entropy reduction (or information gain) to determine the split variables.

```
> fit <- rpart(Play ~ Outlook + Temperature + Humidity + Wind,
+ method="class",
+ data=play_decision,
+ control=rpart.control(minsplit=1),
+ parms=list(split='information'))
> rpart.plot(fit, type=4, extra=2)
```

Output: The fitted decision tree



Prediction

- The decision tree can be used to predict outcomes for new data sets.
- Consider a testing set that contains the following record: Outlook='rainy', Temperature='mild', Humidity='high', Wind=FALSE.
- The goal is to predict the play decision of this record. The following code loads the data into R as a data frame `newdata`.

```
> newdata <- data.frame(Outlook="rainy", Temperature="mild",
+ Humidity="high", Wind=FALSE)
> newdata
  Outlook Temperature Humidity  Wind
1   rainy        mild     high FALSE
```

Prediction

```
> predict(fit,newdata=newdata,type="prob")
  no yes
1  1   0
> predict(fit,newdata=newdata,type="class")
 1
no
Levels: no yes
```

- High probability for `Play` to fall into category 'no' given the condition as in `newdata`.
- If to classify the decision, then the prediction should be in category 'no'.