FIT3152 Data analytics – Lecture 7

Introduction to decision trees

- Overview: machine learning
- Introduction to classification and decision trees
- A specific decision tree algorithm: ID3
- Entropy and information gain
- Model accuracy; training and testing
- Decision trees in R

Consultations

Consultations have commenced.

Most are on Zoom.

Check Moodle for days/times:

https://lms.monash.edu/course/view.php?id=153815&section=2

Note: no consultation Tuesday 25th April (ANZAC Day).

Unit outline (week-by-week)

Clayton lecture is Wednesday 11:00am – 1:00pm (AEDT).

Updates for Weeks 11 and 12 highlighted.

Week Starting	Lecture	Topic	Tutorial	A1 25	A2 30	Q/P 25	A3 20	Due	
27/2/2023	1	Intro to Data Science, review of basic statistics using R	...						
6/3/2023	2	Exploring data using graphics in R	T1						
13/3/2023	3	Data manipulation in R	T2						
20/3/2023	4	Regression modelling	T3						
27/3/2023	5	Clustering	T4						
3/4/2023	6	Data Science methodologies, dirty/clean/tidy data	T5						
10/4/2023	-	Mid-semester Break	-	-	-	-	-	-	
17/4/2023	7	Classification using decision trees	T6					17/4/2023	Mo
24/4/2023	8	Naïve Bayes, evaluating classifiers	T7						
1/5/2023	9	Ensemble methods, artificial neural networks	T8						
8/5/2023	10	Text analysis	T9					12/5/2023	Fr
15/5/2023	11	Network analysis	Quiz/Prac					19/5/2023	Fr
22/5/2023	12	Text and Network Activities. Brief review of course	T10 & T11						
29/5/2023		SWOT VAC							
5/6/2023		EXAM PERIOD						9/6/2023	Fr

Assignment 2

Assignment 2 will be released during this week and discussed at next week's lecture.

Review questions from last lecture

Print

> niris = iris; niris *# = print(niris)*

```
    Sepal.Length Sepal.Width Petal.Length Petal.Width    Species
1            5.1         3.5          1.4         0.2     setosa
2            4.9         3.0          1.4         0.2     setosa
3            4.7         3.2          1.3         0.2     setosa
4            4.6         3.1          1.5         0.2     setosa
5            5.0         3.6          1.4         0.2     setosa
6            5.4         3.9          1.7         0.4     setosa
7            4.6         3.4          1.4         0.3     setosa
8            5.0         3.4          1.5         0.2     setosa
9            4.4         2.9          1.4         0.2     setosa
10           4.9         3.1          1.5         0.1     setosa
11           5.4         3.7          1.5         0.2     setosa
12           4.8         3.4          1.6         0.2     setosa
13           4.8         3.0          1.4         0.1     setosa
14           4.3         3.0          1.1         0.1     setosa
15           5.8         4.0          1.2         0.2     setosa
...
```

Question 1

Predict the output from the following command:

```
> niris$Species = recode(niris$Species," 'versicolor' = '0';'virginica' = '0';'setosa' = '1' ")
```

(a) **Replace data in species column with 0 for I.versicolor and virginica, 1 for I.setosa.**

(b) **Add a new column of 0 and 1s**

(c) **Add a 0 or 1 to each species name**

(d) **Recode “setosa” = 1, leave others unchanged**

Question 2

Which of the following is not a data science workflow methodology?

(a) CRISP-DM
(b) EDA
(c) KDD
(d) SEMMA

Question 3

Which of the following data types is not dirty data – in its strictest sense?

(a) `Duplicate data`
(b) `Business rule violation`
(c) `Inconsistent data`
(d) `Inexact data`

Question 4

Which of the following is not true: Tidy data has:

(a) Each value in its own cell
(b) Each observation in its own row
(c) Each factor level in its own column
(d) Each variable in its own column

Machine learning

Machine Learning

We can think of Machine Learning (ML) as the automated (statistical) learning of a concept from labelled sample data.

- For example: Spam filtering with an algorithm that takes some examples of spam and makes a rule to predict whether an email should go to the spam folder.

How can a model "learn" a concept?

- Descriptive: captures the "behaviour" of the training data;
- Predictive: generalizes to unseen data;
- Explanatory: describes the concept to be learned.

A common application of ML is classification.

ML classification example – tax return

- Given the following data about people who submitted a tax return, we want to automatically create a model that will classify people into cheats or non-cheats.
- We then want to be able to Use the model to classify 'new' people into cheats or non-cheats.

Tid	Refund (categorical)	Marital Status (categorical)	Taxable Income (continuous)	Cheat (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
10	No	Single	90K	Yes

Classification

Using a collection of records containing a set of *attributes* where one of the attributes is the *class*, find a model to predict class as a function of the other attributes.

- Goal: previously unseen records should be assigned a class as accurately as possible.
- Data is usually divided into a *training set* to build the model, and a *test set* used to validate (test the accuracy) of the model.

ML classification example – tax return

categorical categorical continuous class

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

Refund	Marital Status	Taxable Income	Cheat
No	Single	75K	?
Yes	Married	50K	?
No	Married	150K	?
Yes	Divorced	90K	?
No	Single	40K	?
No	Married	80K	?

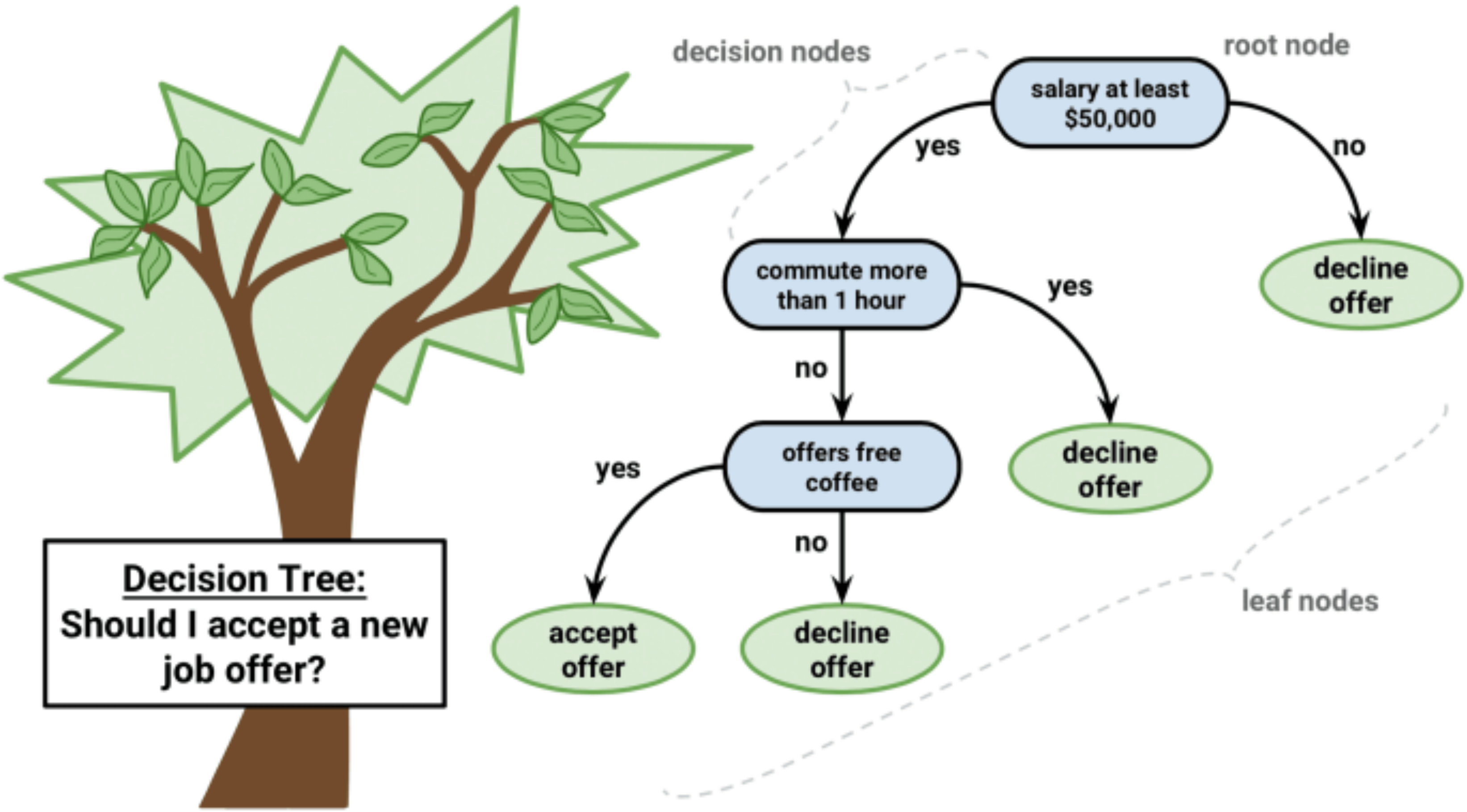
Classification

Machine Learning classification techniques include:

- Decision Tree based methods
- Naïve Bayes and Bayesian Belief Networks
- Ensemble methods
- Artificial Neural Networks
- Rule-based methods
- Memory based reasoning
- Support Vector Machines

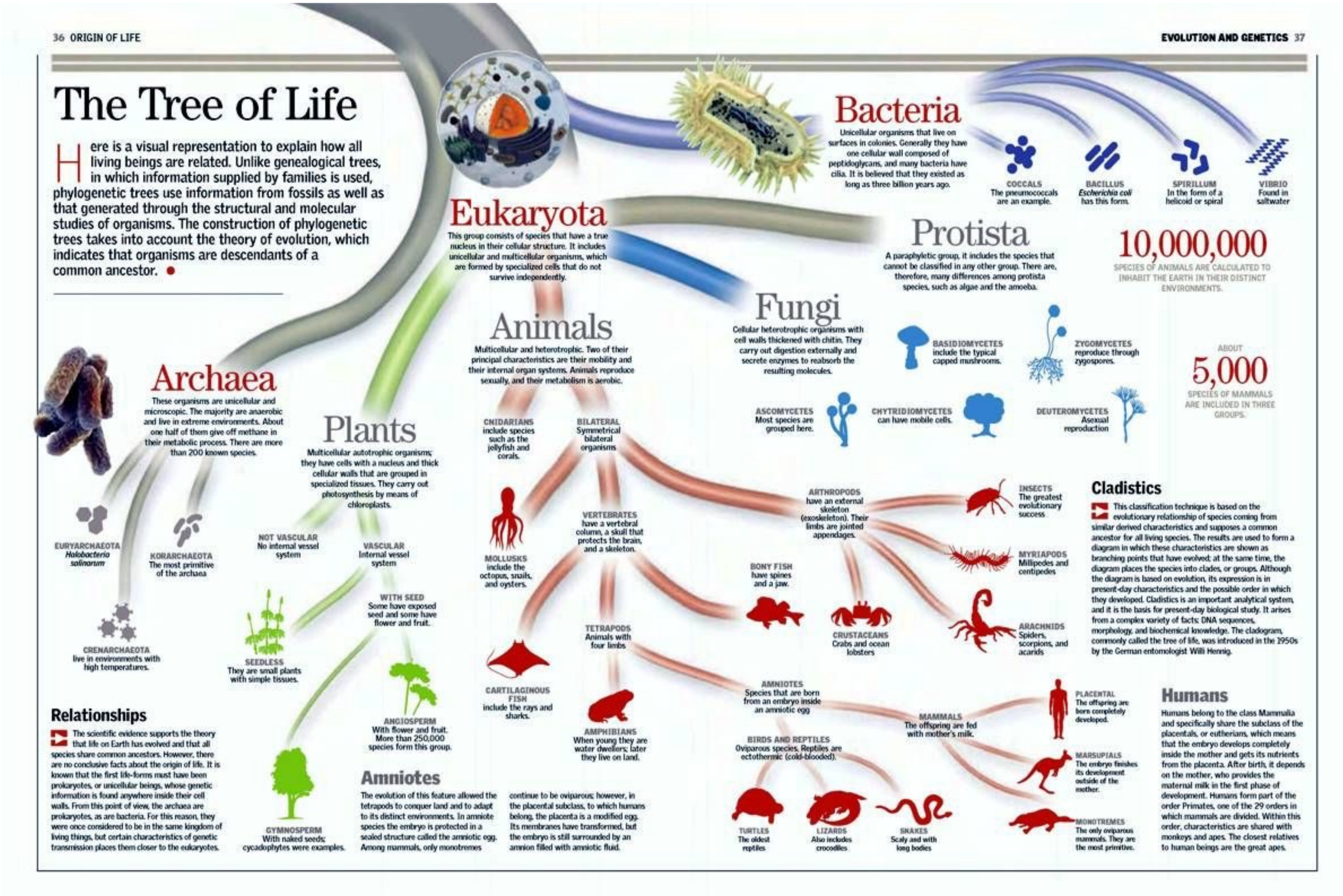
In each of these cases the model “learns” the classification rules from the data.

Decision tree: should I accept job?



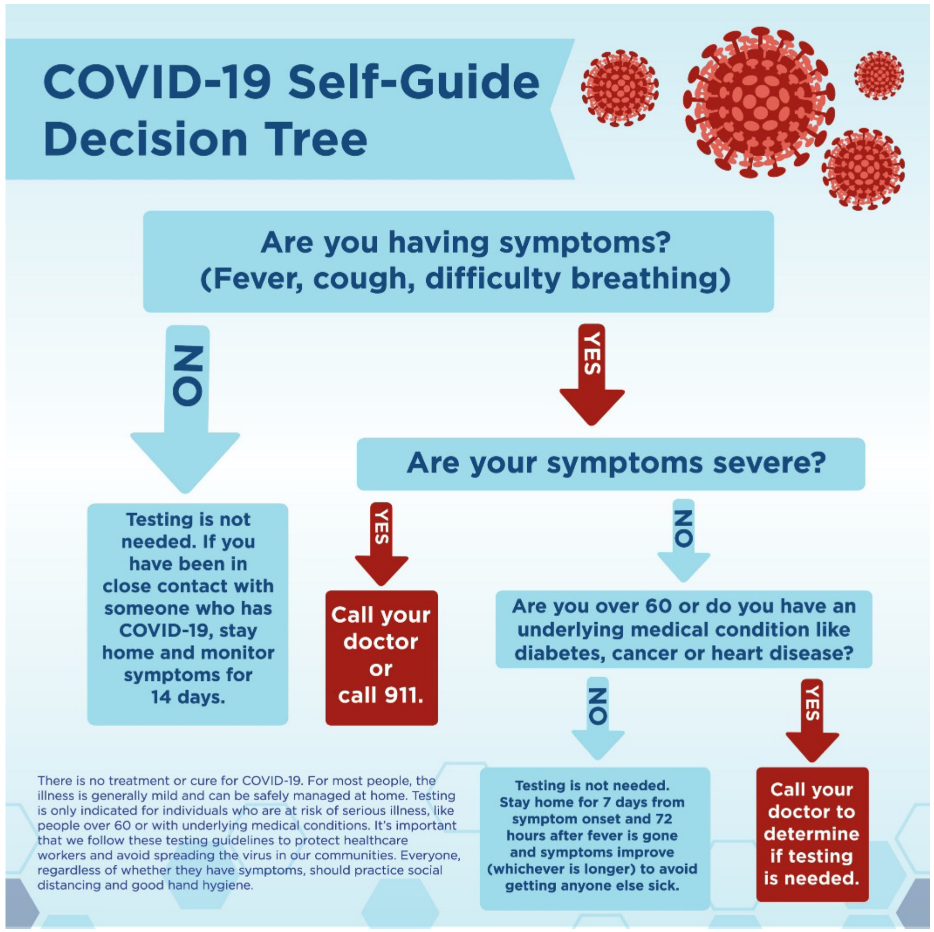
towardsdatascience.com/

Classification tree: life forms



medium.com/

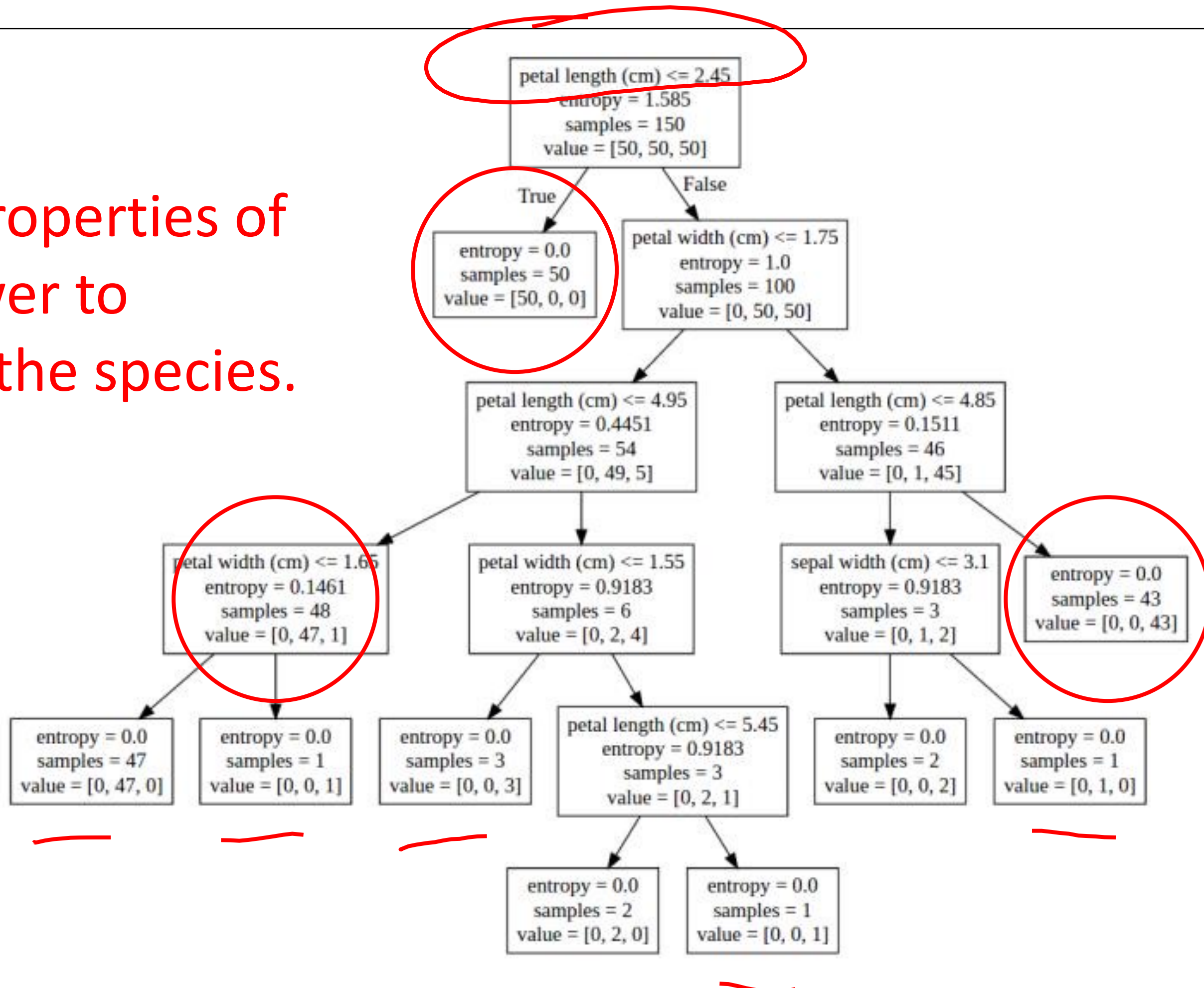
COVID-19 Self-diagnosis



holzer.org/

Iris species classification

Using properties of the flower to classify the species.



kdnuggets.com/

Decision Trees

Decision trees are one of the most widely used and practical methods in machine learning:

- Model uses existing data attributes and values
- Can be used to classify new instances
- Can be used to profile existing data
- Robust to noise and missing values
- Each tree can be viewed as a sequence of "if – then – else" statements, this readability is highly desirable.
- *We can construct simple decision trees by hand!*

Decision Trees

Tree constitutes:

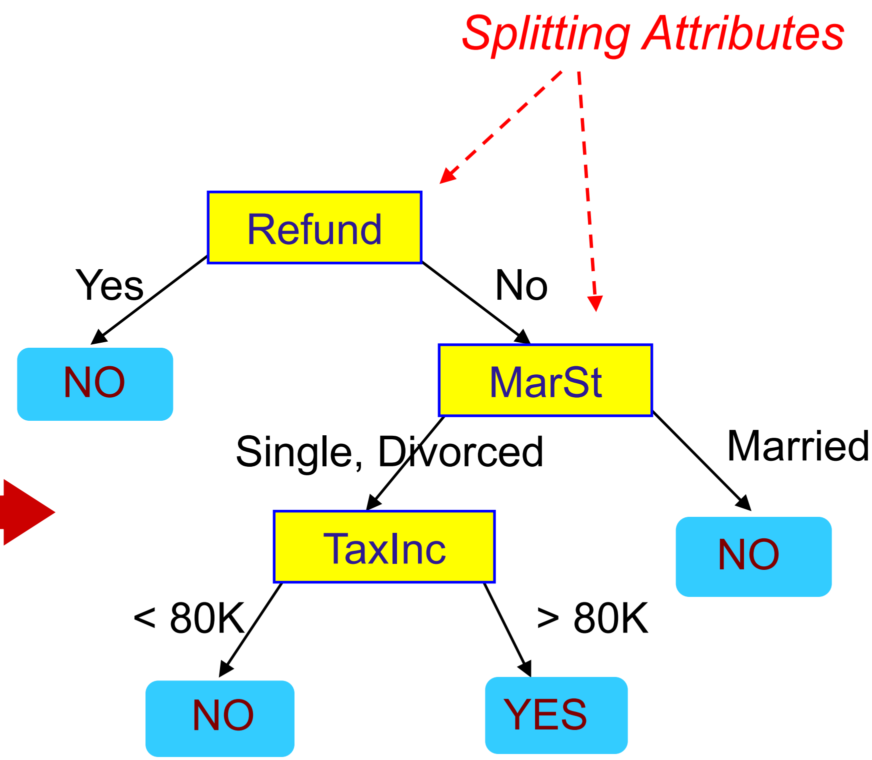
- Leaf nodes (of each class) and non-leaf nodes, corresponding to the decision attributes,
- Branches – corresponding to the values of the decision attributes having either binary or multi-way splits.
- To classify an object, each decision node (starting from the root) compares an attribute of the object with a specific attribute value (or range) and takes the corresponding branch.
- A path from the root to a leaf node gives the class of the object.

Classification example – tax return

categorical categorical continuous class

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**

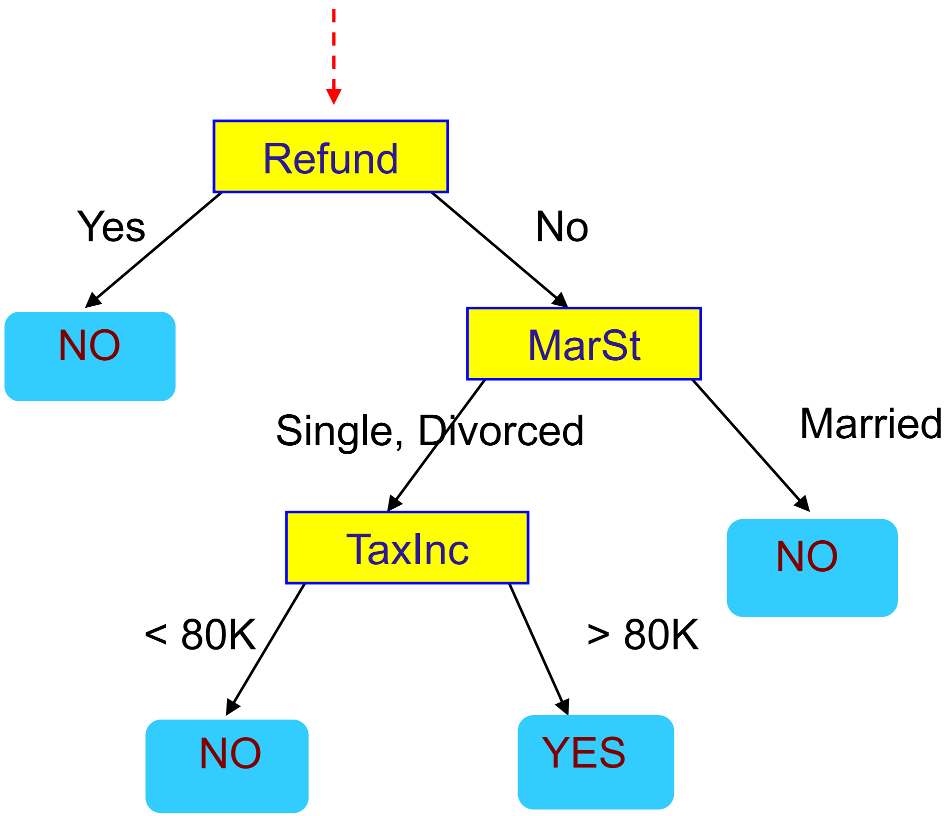
Training Data



Model: Decision Tree
(One of many possible trees)

Apply Model to Test Data

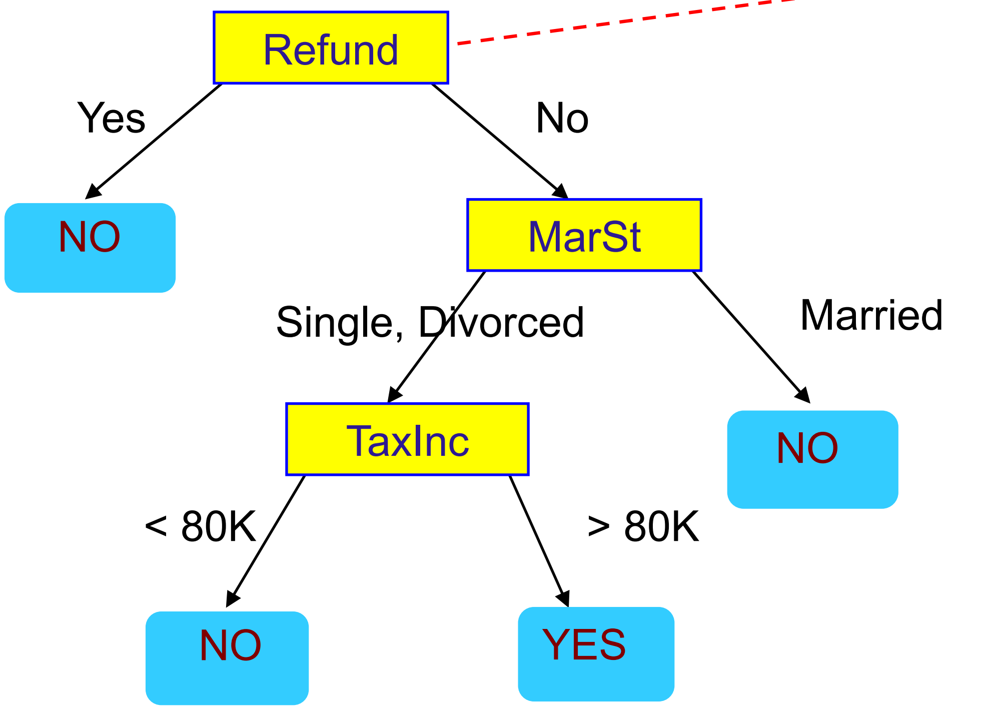
Start from the root of tree.



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



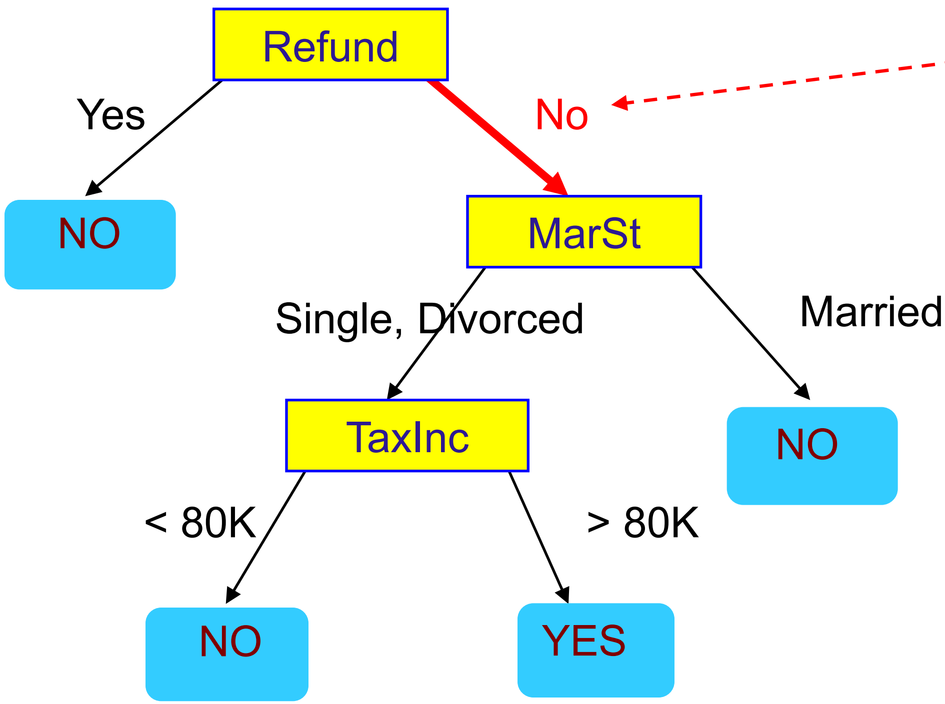
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

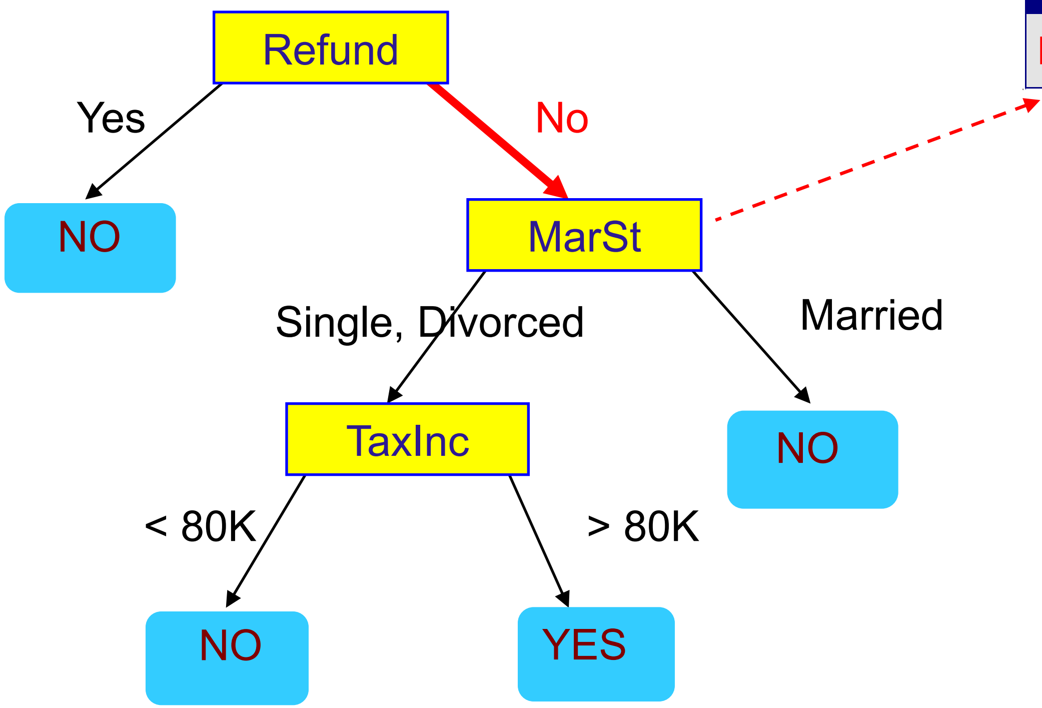
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



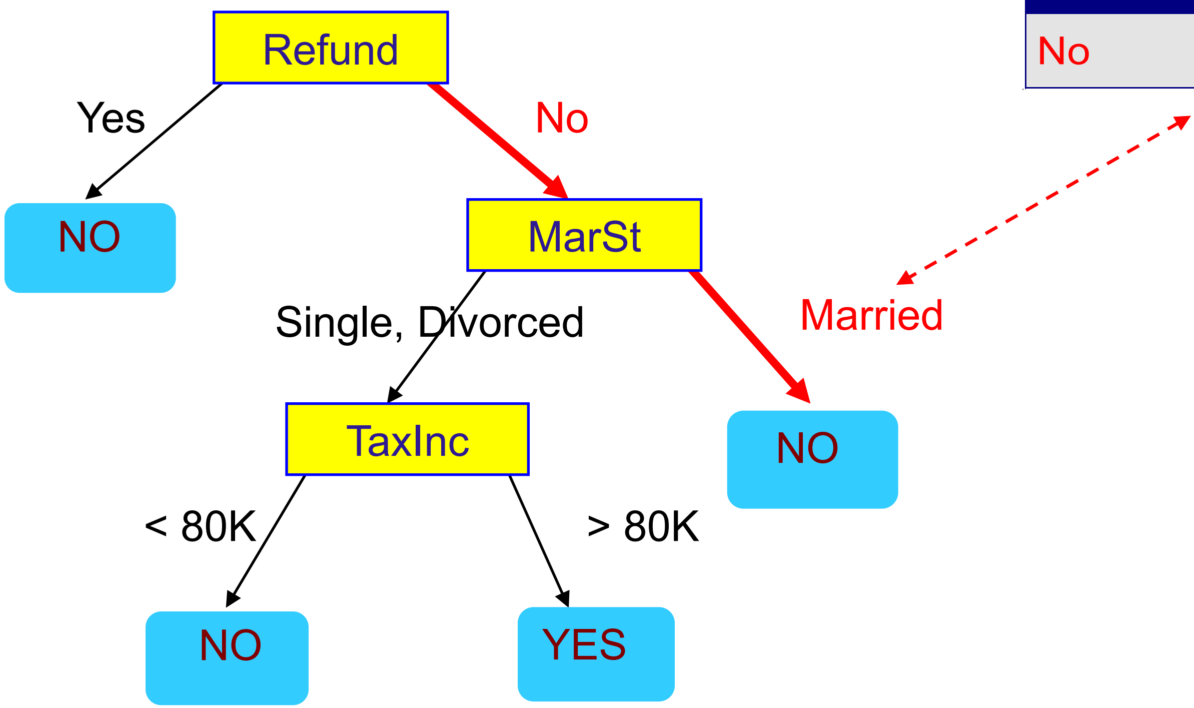
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



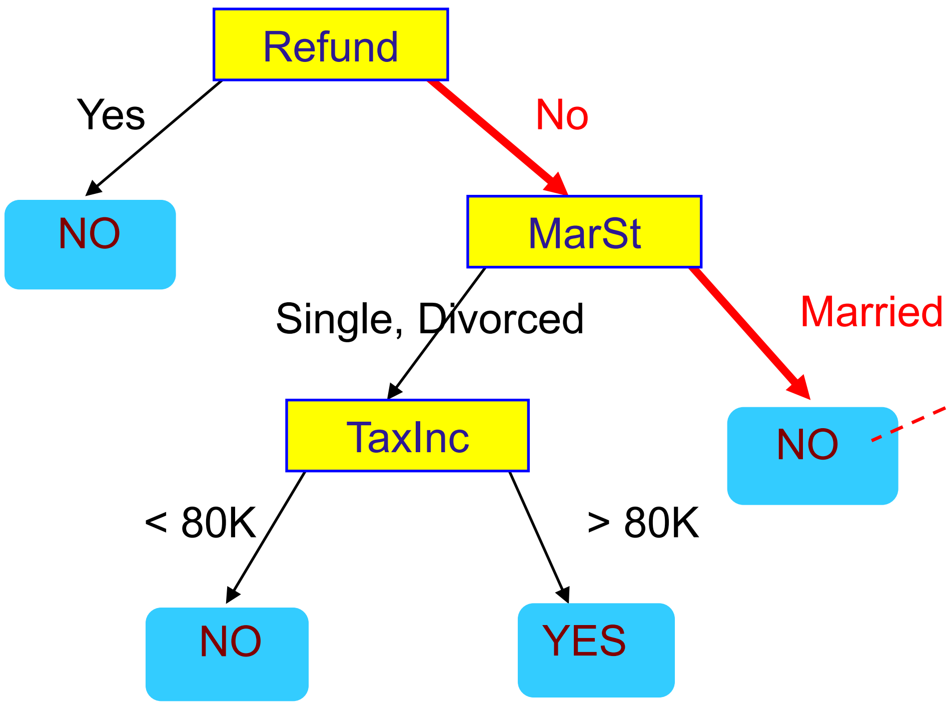
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to "No"

Building a decision tree

Building a decision tree requires answering:

- Which attribute should be tested at a node?
- When should a node be declared a leaf?
- What if tree becomes too large?
- How to handle missing values?
- Should the properties be restricted to binary-valued or allowed to be multi-valued?
- Answering these questions leads to different variants of decision trees: ID3, C4.5, C5, CART, etc.

Top-down induction: ID3

The algorithm (*Iterative Dichotomiser 3*):

- At each step, determine the "best" decision attribute, *A*.
- Assign *A* as decision attribute for node.
- For each value of *A* create new descendant.
- Sort training examples according to the attribute value.
- If all training examples are homogenous (i.e., perfectly classified), stop, else iterate over new leaf nodes.

For this algorithm assume class attribute is categorical.

en.wikipedia.org/

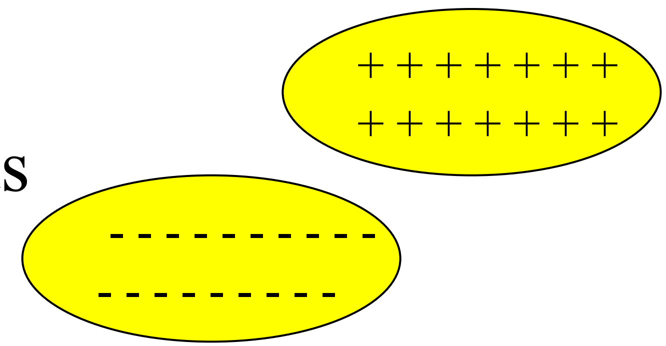
Which attribute to split on?

- At each stage of the process, we try to find the 'best' attribute and split to partition the data.
- That decision may not be the best overall – but once it is made, we stay with it for the rest of the tree.
- This is generally called a *greedy* approach and may not result in the best overall decision tree.
- At each split the goal is to increase the *homogeneity* of the resulting datasets with respect to the *class* or *target* variable (which we are trying to classify).

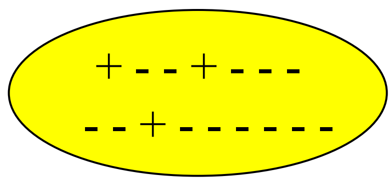
Homogeneity

Suppose we have a binary target attribute with values ‘+’ and ‘–’.

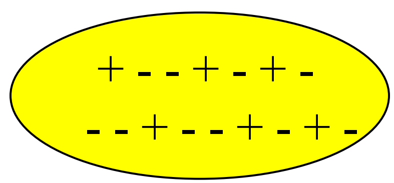
- These two sets are homogeneous



- This one is not



- This one even less so



Information gain

Which attribute to choose for splitting?

- A statistical property called *information gain* measures how well a given attribute separates the training examples into homogeneous groups according to target classification.
- ID3 uses information gain as the splitting criteria for building a tree and chooses the attribute which provides the greatest information gain.
- Information gain is determined using a measure from Information Theory called *Entropy*.

Entropy

In Thermodynamics:

- It gives a measure of the amount of chaos present in a system (or a measure of the disorder in a system).

In Information Theory:

- Entropy measures the uncertainty in a random variable or message or indicates how much information (or impurity) there is in an event.
- In general, the more uncertain or random the event is, the more information it will contain.

Entropy cont… *

See Wikipedia:

https://en.wikipedia.org/wiki/Entropy_(information_theory))

- In information theory, systems are modeled by a transmitter, channel, and receiver… The receiver attempts to infer which message was sent. In this context, entropy (more specifically, Shannon entropy) is the expected value (average) of the information contained in each message. 'Messages' can be modeled by any flow of information…

Calculating entropy

For a two-class problem: c_1 and c_2:

- P indicates the probability of belonging to each class, the number in each class is $N_{c1} + N_{c2} = N$.

$$
\begin{aligned}
\mathrm{Entropy(S)} &= -\mathrm{P}_{c1}\log_2(\mathrm{P}_{c1}) - \mathrm{P}_{c2}\log_2(\mathrm{P}_{c2}) \\
&= -\frac{\mathrm{N}_{c1}}{\mathrm{N}}\log_2(\frac{\mathrm{N}_{c1}}{\mathrm{N}}) - \frac{\mathrm{N}_{c2}}{\mathrm{N}}\log_2(\frac{\mathrm{N}_{c2}}{\mathrm{N}})
\end{aligned}
$$

For a multi-class problem

$$
\begin{aligned}
\mathrm{Entropy(S)} &= -\sum_{i=1}^{C}\mathrm{P}_i\log_2(\mathrm{P}_i) \\
&= -\sum_{i=1}^{C}\frac{\mathrm{N}_i}{\mathrm{N}}\log_2(\frac{\mathrm{N}_i}{\mathrm{N}})
\end{aligned}
$$

Calculating entropy

Suppose S is a collection of 14 examples, 9 positive and 5 negative → [9+ ,5-]

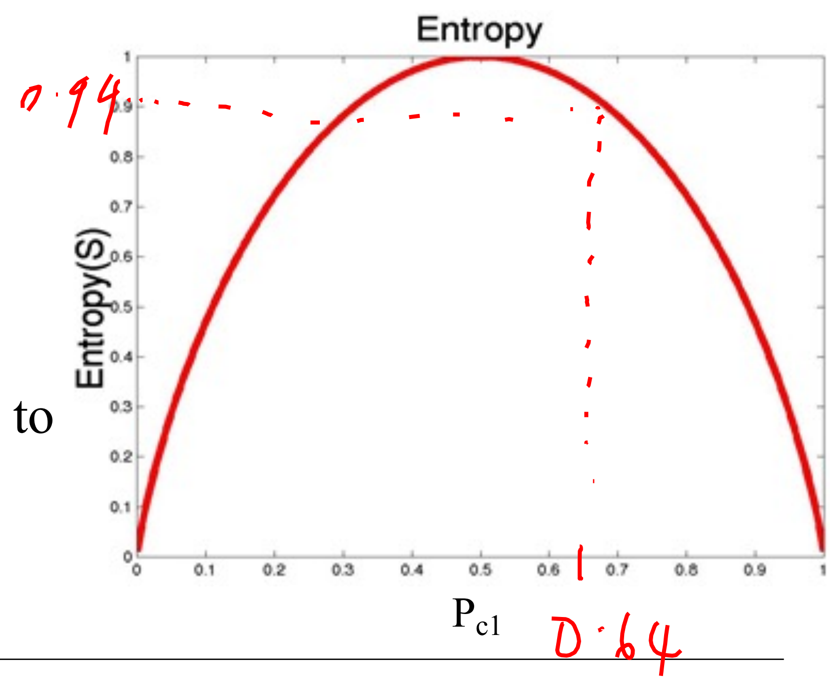
(+, -, +, -, +, -, +, +, +, -, -, +, +, +)

$$\begin{aligned}
\text{Entropy}(S) &= -P_{c1}\log_2(P_{c1}) - P_{c2}\log_2(P_{c2}) \\
&= -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) \\
&= 0.940
\end{aligned}$$

Suppose S has all positive or all negative Examples, then Entropy(S) = 0

(+, +, +, +, +, +, +, +, +), or

(-, -, -, -, -, -, -, -, -, -, -, -, -, -, -, -)



Entropy is 0 (minimum) if all members belong to the same class. Entropy is 1 (maximum) if the collection consists of equal number of positive and negative examples. Assume: $0\text{Log}_2 0 = 0$.

Calculating entropy

The previous example as a spreadsheet:

- If your calculator can't work out logs to base 2 then use the following:

$$\log_2(x) = \frac{\log_{10}(x)}{\log_{10}(2)} \approx \frac{\log_{10}(x)}{0.3010}$$

Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
9	5	0.6429	-0.6374	0.3571	-1.4854	0.9403

- Note: $\log_2$ yields entropy in units called "shannons".

Information gain

Information gain is the expected reduction in entropy caused by partitioning the examples according to an attribute A.

- Gain(S,A) of an attribute A, relative to a collection of examples S (with v groups having $|S_v|$ elements) is:

$$\mathrm{Gain}(S,A) = \mathrm{Entropy}(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} \times \mathrm{Entropy}(S_v)$$

Entropy before split

Expected entropy after split

How ID3 uses information gain

The algorithm ‘splits’ on the attribute that provides the most information gain – that is, gives the purest class breakdown at each step in the decision tree.

Recall: purer class = entropy reduction!

How ID3 uses information gain

The algorithm:

- At each step, determine the “best” decision attribute, A, for next node.
- Assign A as decision attribute for node.
- For each value of A create a new descendant.
- Sort training examples to that node according to the attribute value of the branch.
- If all training examples are perfectly classified (same value of target attribute) stop, else iterate over new leaf nodes.

Example: playing tennis

Build a decision tree for playing tennis based on weather conditions.

Training set (S):

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

First split on: Outlook, Temperature, Humidity or Wind?

Terminology

- *Instance*: single row in a data set. (each observation).
- *Attribute*: an aspect of an instance. Also called feature, variable. (usually each column variable).
- *Value*: category that an attribute can take.
- *Class*: the thing to be learned. (This is what we are trying to classify from the attributes).
- It is usual to have several decision attributes and one target attribute.

Playing tennis: initial entropy

Training set (S): Initial entropy before splitting based on 9 Yes/5 No:

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

Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
9	5	0.6429	-0.6374	0.3571	-1.4854	0.9403

Initial entropy

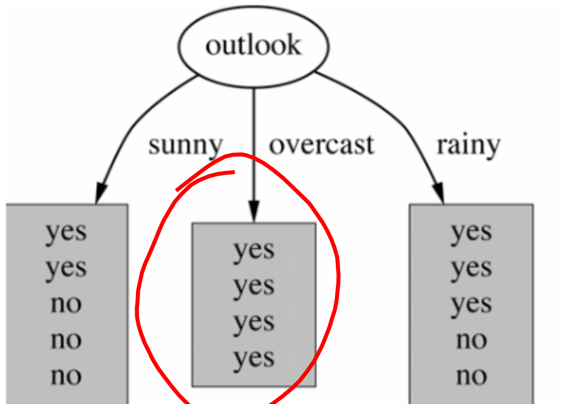
- Without any knowledge of the weather there are 9 Yes and 5 No cases. Initial entropy is:
- $E(S) = -\frac{9}{14} \cdot log_2\left(\frac{9}{14}\right) - \frac{5}{14} \cdot log_2\left(\frac{5}{14}\right)$
- $E(S) = 0.9403$

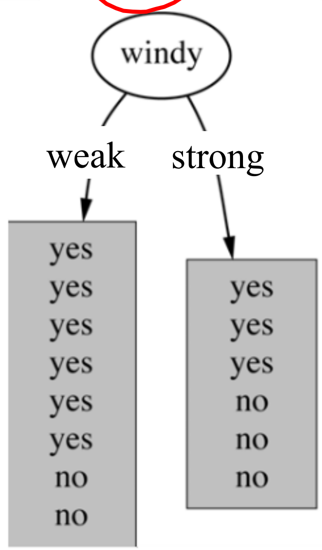
Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
9	5	0.6429	-0.6374	0.3571	-1.4854	0.9403

Which attribute to select?

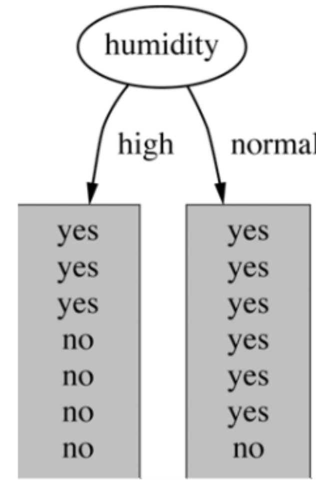
Remember - ID3 chooses the attribute which gives the greatest information gain (reduction in Entropy), or the 'purest' result.

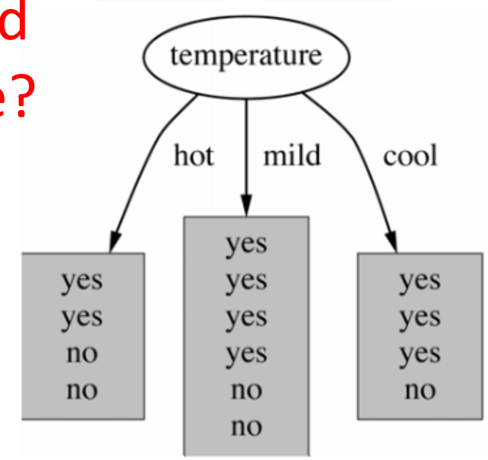
We next calculate the information gain for each attribute in turn.





What would you choose?

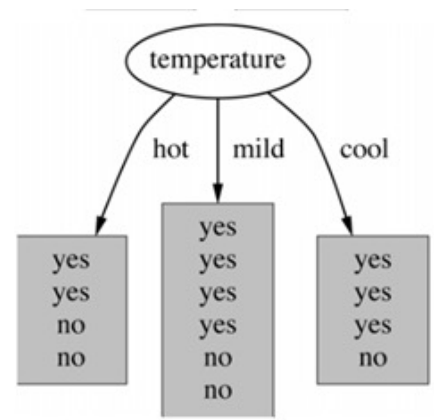




Information gain: Temperature

Calculate entropy for each branch first:

- $E(S_{hot}) = -\frac{2}{4} \cdot log_2\left(\frac{2}{4}\right) - \frac{2}{4} \cdot log_2\left(\frac{2}{4}\right) = 1$
- $E(S_{mild}) = -\frac{4}{6} \cdot log_2\left(\frac{4}{6}\right) - \frac{2}{6} \cdot log_2\left(\frac{2}{6}\right) = 0.918$
- $E(S_{cool}) = -\frac{3}{4} \cdot log_2\left(\frac{3}{4}\right) - \frac{1}{4} \cdot log_2\left(\frac{1}{4}\right) = 0.811$



Now calculate expected entropy and information gain

- $Gain(S, Temp) = E(S) - E(S, Temp)$
- $Gain(S, Temp) = E(S) - \left(\frac{4}{14}1 + \frac{6}{14}0.918 + \frac{4}{14}0.811\right)$
- $= 0.9403 - 0.910$
- $= 0.0292$

Expected entropy is the sum of entropy * probability for each branch.

Information gain: Temperature

As a spreadsheet showing initial entropy and subsequent information gain:

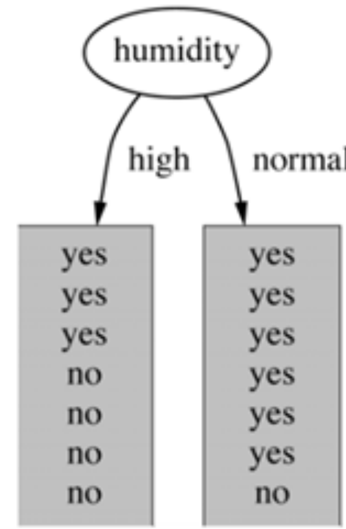
Initial State	**Yes**	**No**	**P(Yes)**	**Log2(Yes)**	**P(No)**	**Log2(No)**	**Entropy**
Entropy(S)	9	5	0.6429	-0.6374	0.3571	-1.4854	0.9403

Temperature	**Yes**	**No**	**P(Yes)**	**Log2(Yes)**	**P(No)**	**Log2(No)**	**Entropy**
Hot	2	2	0.5000	-1.0000	0.5000	-1.0000	1.0000
Mild	4	2	0.6667	-0.5850	0.3333	-1.5850	0.9183
Cool	3	1	0.7500	-0.4150	0.2500	-2.0000	0.8113
EEntropy(Temp)							0.9111
Gain(S, Temp)							**0.0292**

Information gain: Humidity

Calculate entropy for each branch first:

- $E(S_{high}) = -\frac{3}{7} \cdot log_2\left(\frac{3}{7}\right) - \frac{4}{7} \cdot log_2\left(\frac{4}{7}\right) = 0.9852$
- $E(S_{normal}) = -\frac{6}{7} \cdot log_2\left(\frac{6}{7}\right) - \frac{1}{7} \cdot log_2\left(\frac{1}{7}\right) = 0.5917$

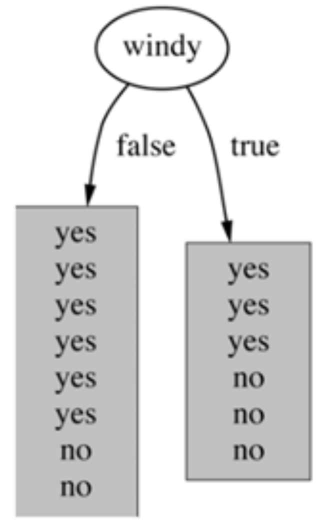


Now calculate expected entropy and information gain

- $Gain(S, Humidity) = E(S) - E(S, Humidity)$
- $Gain(S, Humidity) = E(S) - \left(\frac{7}{14}0.9852 + \frac{7}{14}0.5917\right)$
- $= 0.9403 - 0.7885$
- $= 0.1518$

Information gain: Windy (for you to do)

Calculate entropy for each branch first:



- $E(S_{false}) = -\frac{6}{8} \cdot log_2\left(\frac{6}{8}\right) - \frac{2}{8} \cdot log_2\left(\frac{2}{8}\right) = \boxed{\quad\quad}$
- $E(S_{true}) = -\frac{3}{6} \cdot log_2\left(\frac{3}{6}\right) - \frac{3}{6} \cdot log_2\left(\frac{3}{6}\right) = \boxed{\quad\quad}$

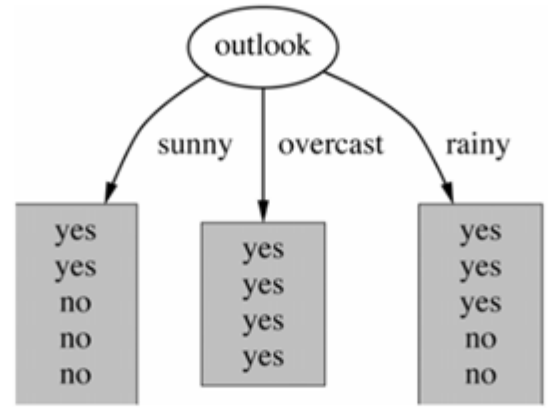
Now calculate expected entropy and information gain

- $Gain(S, Windy) = E(S) - E(S, Windy)$
- $Gain(S, Windy) = E(S) - \left(\frac{8}{14}\boxed{\quad\quad} + \frac{6}{14}\boxed{\quad\quad}\right) = \boxed{\quad\quad}$
- $= 0.9403 - \boxed{\quad\quad} = \boxed{\quad\quad}$

Information gain: Outlook (for you to do)

Calculate entropy for each branch first:

- $E(S_{sunny}) = -\frac{2}{5} \cdot log_2\left(\frac{2}{5}\right) - \frac{3}{5} \cdot log_2\left(\frac{3}{5}\right) = \boxed{}$
- $E(S_{overcast}) = 0$
- $E(S_{rainy}) = -\frac{3}{5} \cdot log_2\left(\frac{3}{5}\right) - \frac{2}{5} \cdot log_2\left(\frac{2}{5}\right) = \boxed{}$



Now calculate expected entropy and information gain

- $Gain(S, Outlook) = E(S) - E(S, Outlook)$
- $Gain(S, Outlook) = E(S) - \left(\frac{5}{14}\boxed{} + \frac{4}{14}\boxed{0} + \frac{5}{14}\boxed{}\right)$
- $= 0.9403 - \boxed{} = \boxed{}$

Calcs: Humidity, Windy, Outlook

Humidity	**Yes**	**No**	**P(Yes)**	**Log2(Yes)**	**P(No)**	**Log2(No)**	**Entropy**
High	3	4	0.4286	-1.2224	0.5714	-0.8074	0.9852
Normal	6	1	0.8571	-0.2224	0.1429	-2.8074	0.5917
EEntropy(Humidity)							0.7885
Gain(S, Humidity)							**0.1518**

Wind	**Yes**	**No**	**P(Yes)**	**Log2(Yes)**	**P(No)**	**Log2(No)**	**Entropy**
Weak	6	2	0.7500	-0.4150	0.2500	-2.0000	0.8113
Strong	3	3	0.5000	-1.0000	0.5000	-1.0000	1.0000
EEntropyWind)							0.8922
Gain(S, Wind)							**0.0481**

Outlook	**Yes**	**No**	**P(Yes)**	**Log2(Yes)**	**P(No)**	**Log2(No)**	**Entropy**
Sunny	2	3	0.4000	-1.3219	0.6000	-0.7370	0.9710
Overcast	4	0	1.0000	0.0000	0.0000	0.0000	0.0000
Rain	3	2	0.6000	-0.7370	0.4000	-1.3219	0.9710
EEntropy(Outlook)							0.6935
Gain(S, Outlook)							**0.2467**

Attribute giving greatest information gain

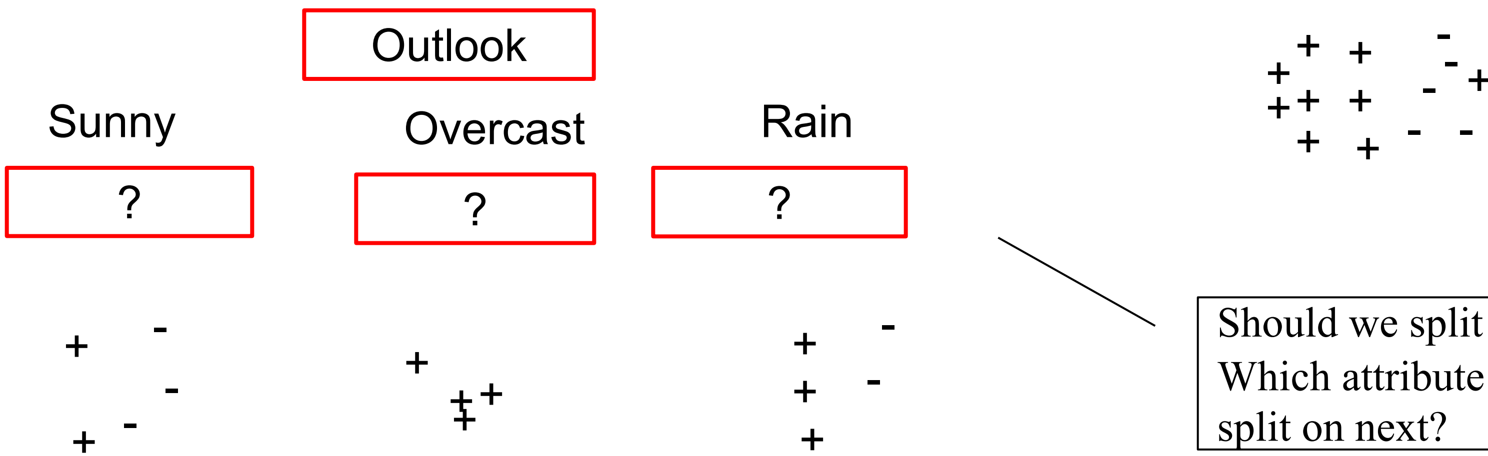
Which attribute to choose? Outlook, Temperature, Humidity or Wind?

Gain(S, Temperature) = 0.029

Gain(S, Humidity) = 0.151

Gain(S, Wind) = 0.048

Gain(S, Outlook) = 0.247 ← Choose this one!



Should we split again? If so Which attribute should we split on next?

Impure, non-leaf node. Apply splitting procedure again.

Pure, make it a leaf node.

Impure, non-leaf node. Apply splitting procedure again.

Entropy after "Outlook"

The entropy of each branch of the decision tree after split on Outlook is shown below.

- Information gain in descendent trees is now measured as change in the entropy of each branch.
- For example, Entropy(Sunny) = 0.971

Outlook	Yes	No	P(Yes)	og2(Yes)	P(No)	og2(No)	Entropy
Sunny	2	3	0.400	-1.322	0.600	-0.737	0.971
Overcast	4	0	1.000	0.000	0.000	0.000	0.000
Rain	3	2	0.600	-0.737	0.400	-1.322	0.971
EEntropy(Outlook)							0.694

Which attribute to split on next?

Now, starting with Sunny, which attribute should be split on next? Temperature, Humidity or Wind?

Outlook

Sunny

Overcast

Rain

?

?

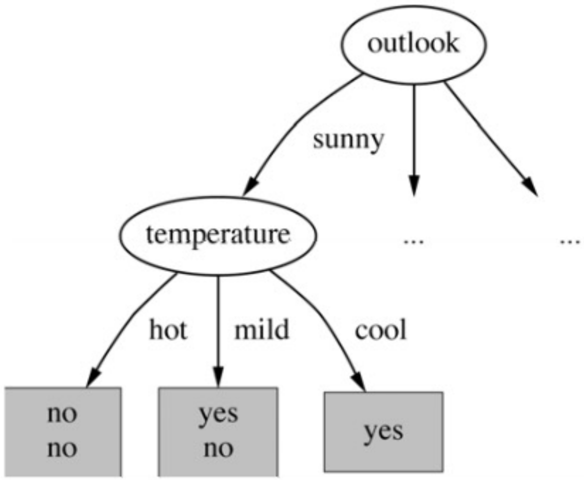
Yes

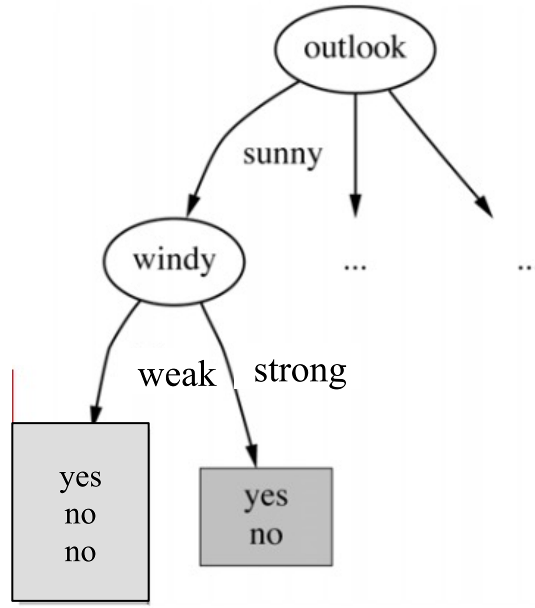
ID3 Step 2: gain(S_sunny, ???)

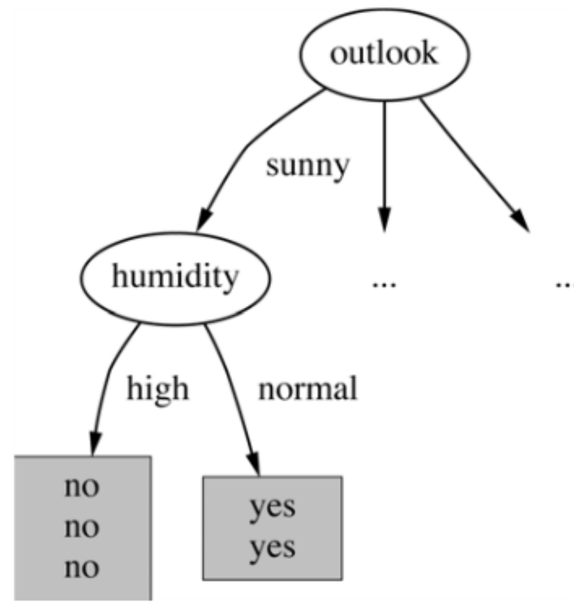
Now consider subset corresponding to “Sunny”:

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~~

Which attribute to split on next?







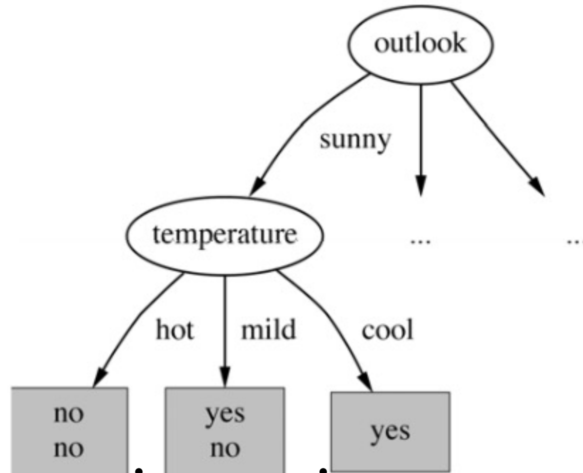
What attribute would you choose?

Do you need to do any calculations?

ID3 Step 2: Gain Sunny, Temperature

Calculate entropy for each branch first:

- $E\left(S_{sunny,\,hot}\right) = -\frac{0}{2} \cdot log_2\left(\frac{0}{2}\right) - \frac{2}{2} \cdot log_2\left(\frac{2}{2}\right) = 0$
- $E\left(S_{sunny,mild}\right) = -\frac{1}{2} \cdot log_2\left(\frac{1}{2}\right) - \frac{1}{2} \cdot log_2\left(\frac{1}{2}\right) = 1$
- $E\left(S_{sunny,cool}\right) = -\frac{1}{1} \cdot log_2\left(\frac{1}{1}\right) - \frac{0}{1} \cdot log_2\left(\frac{0}{1}\right) = 0$



Now calculate expected entropy and information gain

- $Gain(S, Sunny, Temp) = E(S, Sunny) - E(S, Sunny, Temp)$
- $Gain(S, Sunny, Temp) = E(S, Sunny) - \left(\frac{2}{5}0 + \frac{2}{5}1 + \frac{1}{5}0\right)$
- $= 0.971 - 0.4 = 0.571$

Calculations for all attributes shown on the next slide…

ID3 Step 2: Gain for Sunny Outlook

Sunny, Temp	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Hot	0	2	0.0000	0.0000	1.0000	0.0000	0.0000
Mild	1	1	0.5000	-1.0000	0.5000	-1.0000	1.0000
Cool	1	0	1.0000	0.0000	0.0000	0.0000	0.0000
EEntropy(Temp)							0.4000
Gain(Sunny, Temp)							**0.5710**

Sunny, Humid	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
High	0	3	0.0000	0.0000	1.0000	0.0000	0.0000
Normal	2	0	1.0000	0.0000	0.0000	0.0000	0.0000
EEntropy(Temp)							0.0000
Gain(Sunny, Humid)							**0.9710**

Sunny, Wind	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Weak	1	2	0.3333	-1.5850	0.6667	-0.5850	0.9183
Strong	1	1	0.5000	-1.0000	0.5000	-1.0000	1.0000
EEntropyWind)							0.9510
Gain(Sunny, Wind)							**0.0200**

ID3 Step 2: Gain for Sunny Outlook

Which attribute to choose? Temperature, Humidity or Wind?

- Gain(S_{sunny},Wind) = 0.020
- Gain(S_{sunny},Humidity) = 0.971
- Gain(S_{sunny},Temperature) = 0.570

Choose this one!

Repeat the process to find which attribute is the best to split on at this step

Outlook

Sunny

Overcast

Rain

Humidity

?

High

Normal

Yes

No

Yes

Not all leaves need to be 'pure'.
Splitting stops when the data can't be split any further.

Class activity

Now consider subset after "Rain Outlook":

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

Class activity

Class counts and expected entropy after rain outlook.

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

Rain, Temp	Yes	No
Hot		
Mild		
Cool		

Rain, Humid	Yes	No
High		
Normal		

Rain, Wind	Yes	No
Weak	3	0
Strong	0	2

What would you choose?

ID3 Step 3: Gain for Rain Outlook

Rain, Temp	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Hot							
Mild							
Cool							
EEntropy(Temp)							
Gain(Rain, Temp)							

$$\text{Entropy}(S) = -P_{C_1}\log_2\left(P_{C_1}\right) - P_{C_2}\log_2\left(P_{C_2}\right) = -\frac{N_{C_1}}{N}\log_2\left(\frac{N_{C_1}}{N}\right) - \frac{N_{C_2}}{N}\log_2\left(\frac{N_{C_2}}{N}\right)$$

Rain, Humid	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
High							
Normal							
EEntropy(Temp)							
Gain(Rain, Humid)							

$$\log_2(x) = \frac{\log_{10}(x)}{\log_{10}(2)} \approx \frac{\log_{10}(x)}{0.3010}$$

Rain, Wind	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Weak							
Strong							
EEntropyWind)							
Gain(Rain, Wind)							

ID3 Step 3: Gain for Rain Outlook

Rain, Temp	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Hot	0	0	0.0000	0.0000	0.0000	0.0000	0.0000
Mild	2	1	0.6667	-0.5850	0.3333	-1.5850	0.9183
Cool	1	1	0.5000	-1.0000	0.5000	-1.0000	1.0000
EEntropy(Temp)							0.9510
Gain(Rain, Temp)							**0.0200**

Rain, Humid	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
High	1	1	0.5000	-1.0000	0.5000	-1.0000	1.0000
Normal	2	1	0.6667	-0.5850	0.3333	-1.5850	0.9183
EEntropy(Temp)							0.9510
Gain(Rain, Humid)							**0.0200**

Rain, Wind	Yes	No	P(Yes)	Log2(Yes)	P(No)	Log2(No)	Entropy
Weak	3	0	1.0000	0.0000	0.0000	0.0000	0.0000
Strong	0	2	0.0000	0.0000	1.0000	0.0000	0.0000
EEntropyWind)							0.0000
Gain(Rain, Wind)							**0.9710**

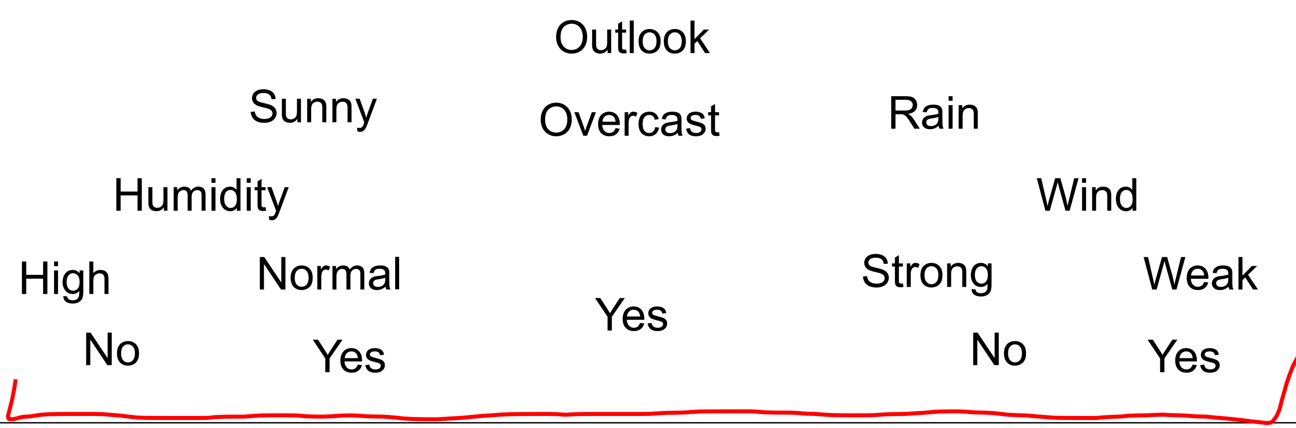
The Final tree

The process of selecting a new attribute and partitioning the training examples is repeated for each non-leaf node, this time only using the examples associated with that node.

Attributes that have been incorporated higher in the tree are excluded, so that any given attribute can appear at most once along any path through the tree.

The process continues for each leaf node until:

- every attribute has been included along that path through the tree or
- the training examples associated with this leaf node all have the same class.



5 Leaves

The Decision Tree Rules

In addition to generating a tree structure, explicit rules for classifying ‘play/don’t play’ are also generated:

If outlook = Overcast Then Play= Yes {No=0, Yes=4}

If outlook = Rain And wind = Strong Then Play= No {No=2, Yes=0}

If outlook = Rain And wind = Weak Then Play = Yes {No=0, Yes=3}

If outlook = Sunny And humidity = High Then Play = No {No=3, Yes=0}

If outlook = Sunny And humidity = Normal Then Play = Yes {No=0, Yes=2}

Further considerations *

Types of decision trees?

- Classification Trees (categorical – nominal attributes)
- Regression Trees (numerical – continuous attributes)

How do we specify the splitting conditions?

How do we evaluate the decision tree model?

Further considerations *

Classification Trees *vs* Regression Trees

- Target variable types

Splitting criteria:

- Information gain
- Gain ratio (reduces bias for highly branched attributes)
- Gini index

Decision tree algorithms

- ID3 (discrete), C4.5, C5 (continuous) target attributes
- CART, Chaid etc.
- See: https://en.wikipedia.org/wiki/Decision_tree_learning

Metrics for Performance Evaluation

How to evaluate the performance of a model?

- Training and testing
- Confusion matrix
- Cross validation

Training and testing

- You can measure a classifier's performance in terms of the error rate (proportion of errors made over a whole set of instances).
- Due to desirability of generalization, low error on the training data is not a good measure.
- To predict the performance of a classifier on a new data, we need to assess its error on data that was not used to build the model.
- In general, the data set is divided into two subsets: training and testing. Training for learning the model and testing for determining how well it will do on unseen data.

Training Data Testing Data

Performance evaluation of the Model

Focus on the predictive capability of a model

- Rather than how fast it takes to classify or build models, scalability, etc.

How to determine accuracy of decision tree in classifying/predicting?

- Usual to have two data sets:
    - A *Training Set* and a *Test Set*
    - This can be created by dividing the data set into two sets – e.g. 70%/30%
- We create the decision tree model using the training set.
- Then run the test set through the model to find out what the predicted class is.
- Then compare the predicted class with the actual class to see how accurate the model is.

Metrics for Performance Evaluation

One way of assessing performance is to calculate accuracy based on a *confusion matrix* (for the test data classification).

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Also:

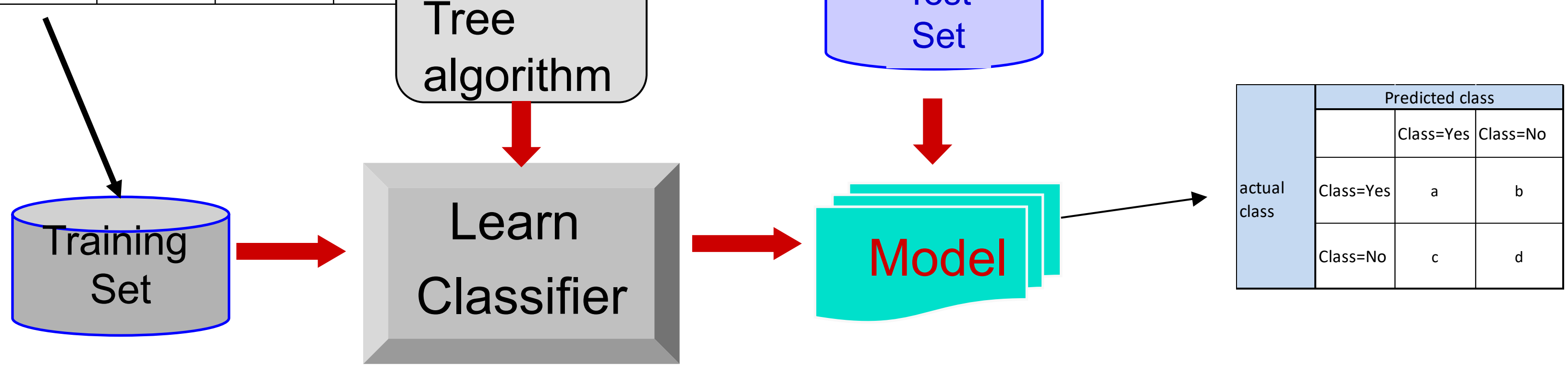
Precision = TP/(TP + FP)

Sensitivity = TP /(TP + FN)

The Play Tennis example

ID	outlook	temp	humidity	wind	play
D1	Sunny	Hot	High	Weak	No
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
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	Cold	Normal	Weak	Yes

ID	outlook	temp	humidity	wind	play
D15	Sunny	Mild	Normal	Strong	No
D16	Sunny	Hot	High	Weak	Yes
D17	Rain	Hot	High	Weak	No
D18	Overcast	Cool	High	Strong	No
D19	Overcast	Mild	Normal	Weak	Yes
D20	Rain	Mild	Normal	Weak	Yes



The play tennis example

Let's see what our model would predict using the test data:

Outlook

Sunny Overcast Rain

Humidity Wind

High Normal Yes Strong Weak

No Yes No Yes

Day	Outlook	Temperature	Humidity	Wind	Play	Predict
D15	Sunny	Mild	Normal	Strong	No	yes
D16	Sunny	Hot	High	Weak	Yes	no
D17	Rain	Hot	High	Weak	No	yes
D18	Overcast	Cool	High	Strong	No	yes
D19	Overcast	Mild	Normal	Weak	Yes	yes
D20	Rain	Mild	Normal	Weak	Yes	yes

Metrics for Performance Evaluation…

	PREDICTED CLASS	
	Class=Yes	Class=No
ACTUAL CLASS: Class=Yes	2 (TP)	1 (FN)
ACTUAL CLASS: Class=No	3 (FP)	0 (TN)

The most widely-used metric:

$$Accuracy = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN} = \frac{2+0}{6} = 33.3\%$$

More ways to measure classification performance next lecture...

Decision trees in R

Decision trees in R

There are a number of packages to create decision trees in R. We will start with the "tree" package.

```
>   install.packages("tree")
>   library(tree)
```

Note: "tree" aims to minimise 'impurity' by binary splitting. Similar, but not identical, to ID3 in effect.

https://cran.r-project.org/web/packages/tree/index.html

tree: details

- A tree is grown by binary recursive partitioning using the response in the specified formula and choosing splits from the terms of the right-hand-side. Numeric variables are divided into $X < a$ and $X > a$;
- The levels of an unordered factor are divided into two non-empty groups.
- The split which maximizes the reduction in impurity is chosen, the data set split, and the process repeated.
- Splitting continues until the terminal nodes are too small or too few to be split.

https://cran.r-project.org/web/packages/tree/index.html

Classification tree: data

Build and test a model using the playtennis data.

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

Classification tree: data

Build and test a model using the playtennis data.

- Ensure inputs are factors – not character vars.

  > ptt <- read.csv(“playtennistrain.csv”, stringsAsFactors = T)

- As the training set has too few instances for tree package to fit a model, a larger synthetic data set is created by resampling with replacement.

  > set.seed(9999) #make random selection repeatable

  > # resampling with replacement

  > pttrain = ptt[sample(nrow(ptt), 100, replace = TRUE),]

  Training data has been resampled to make 100 rows.

Classification tree: building the tree

Build the tree using “Play” as the response and all input variables except “Day” as predictors.

Syntax is very similar to linear model function.

Output is a list.

```
>   ptfit = tree(Play ~. -Day, data = pttrain)
```

Fit model to all attributes except “Day”.

? tree *

- Description

  A tree is grown by binary recursive partitioning using the response in the specified formula and choosing splits from the terms of the right-hand-side.

- Usage

```
tree(formula, data, weights, subset,
na.action = na.pass, control =
tree.control(nobs, ...),
method = "recursive.partition",
split = c("deviance", "gini"),
model = FALSE, x = FALSE, y = TRUE, wts = TRUE,
...)
```

Classification tree: summary

Use "summary" to get a basic idea of model performance: terminal nodes, error measures.

```
> summary(ptfit)
Classification tree:
tree(formula = Play ~ . - Day, data = pttrain)
Number of terminal nodes:  7
Residual mean deviance:  0 = 0 / 93
Misclassification error rate: 0 = 0 / 100
```

Classification tree: details

Details of each split, root to leaf, left to right.

- ptfit

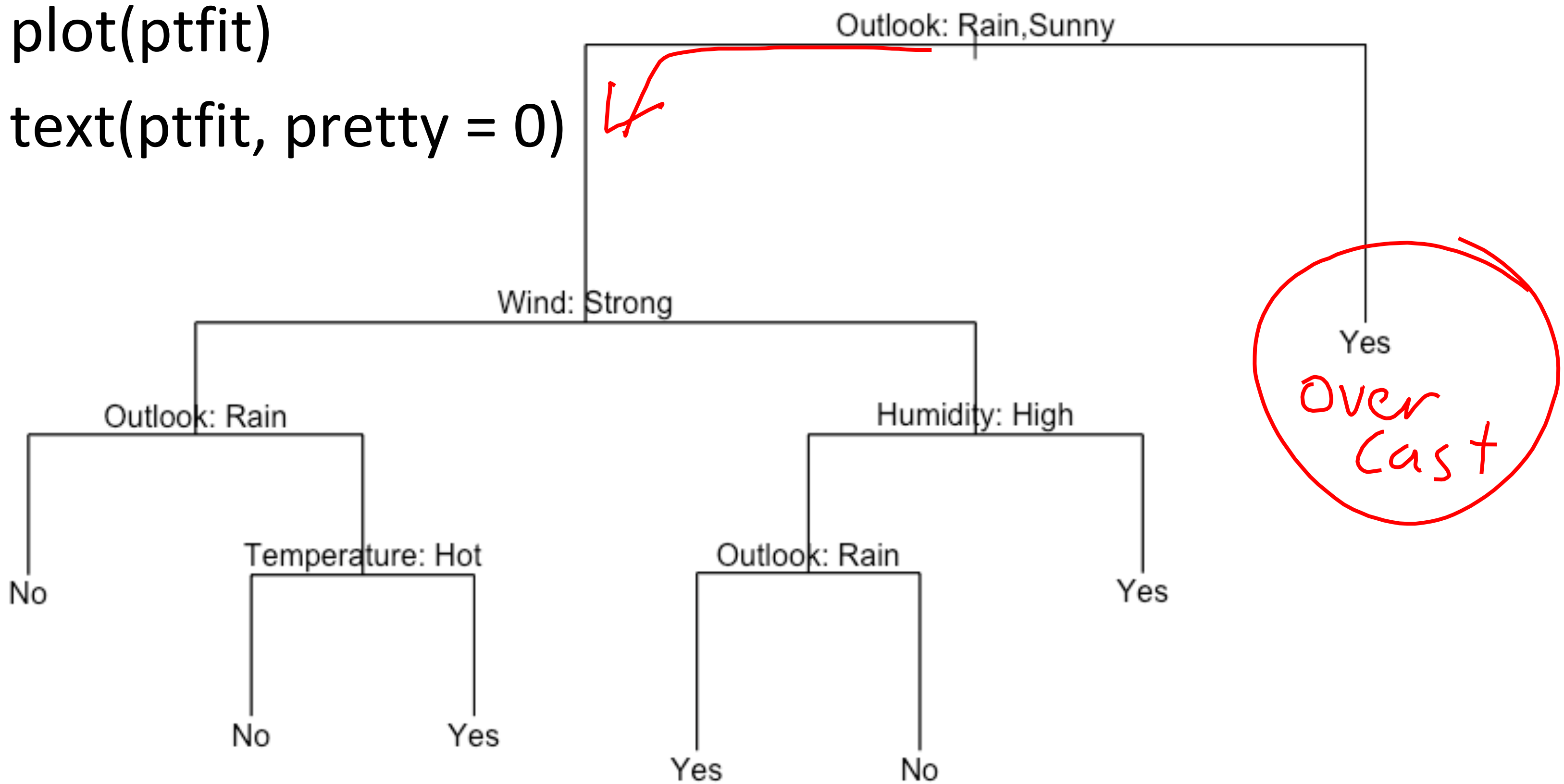
```
> ptfit
node), split, n, deviance, yval, (yprob)
      * denotes terminal node

 1) root 100 100 Yes ( 0.4 0.6 )
   2) Outlook: Rain,Sunny 70 100 No ( 0.6 0.4 )
     4) Wind: Strong 36  40 No ( 0.8 0.2 )
       8) Outlook: Rain 22   0 No ( 1.0 0.0 ) *
       9) Outlook: Sunny 14  20 Yes ( 0.4 0.6 )
        18) Temperature: Hot 6   0 No ( 1.0 0.0 ) *
        19) Temperature: Mild 8   0 Yes ( 0.0 1.0 ) *
     5) Wind: Weak 34  40 Yes ( 0.3 0.7 )
      10) Humidity: High 18  20 No ( 0.6 0.4 )
        20) Outlook: Rain 7   0 Yes ( 0.0 1.0 ) *
        21) Outlook: Sunny 11   0 No ( 1.0 0.0 ) *
      11) Humidity: Normal 16   0 Yes ( 0.0 1.0 ) *
   3) Outlook: Overcast 30   0 Yes ( 0.0 1.0 ) *
```

Classification tree: plot

Headers give rule for left branching.

> plot(ptfit)

> text(ptfit, pretty = 0)



Classification tree: testing the model

To test the model, make a prediction for each input from the test data set and cross tabulate with the actual classification in the test data:

```
> pttest <- read.csv("playtennistest.csv", stringsAsFactors = T)
> tpredict = predict(ptfit, pttest, type = "class")
> Tpredict
[1] Yes No  Yes Yes Yes Yes
Levels: No Yes
```

Tree

Data

classify

Classification tree: testing the model

Comparing predicted with actual values as a Confusion Matrix:

```
> tpredict
[1] Yes No  Yes Yes Yes Yes
> pttest$Play
[1] No  Yes No  No  Yes Yes
> table(observed = pttest$Play, predicted = tpredict)
         predicted
observed No Yes
     No   0   3
     Yes  1   2
```

Edgar Anderson's Iris data

50 samples from 3 species:

- Iris setosa, – virginica, – versicolor

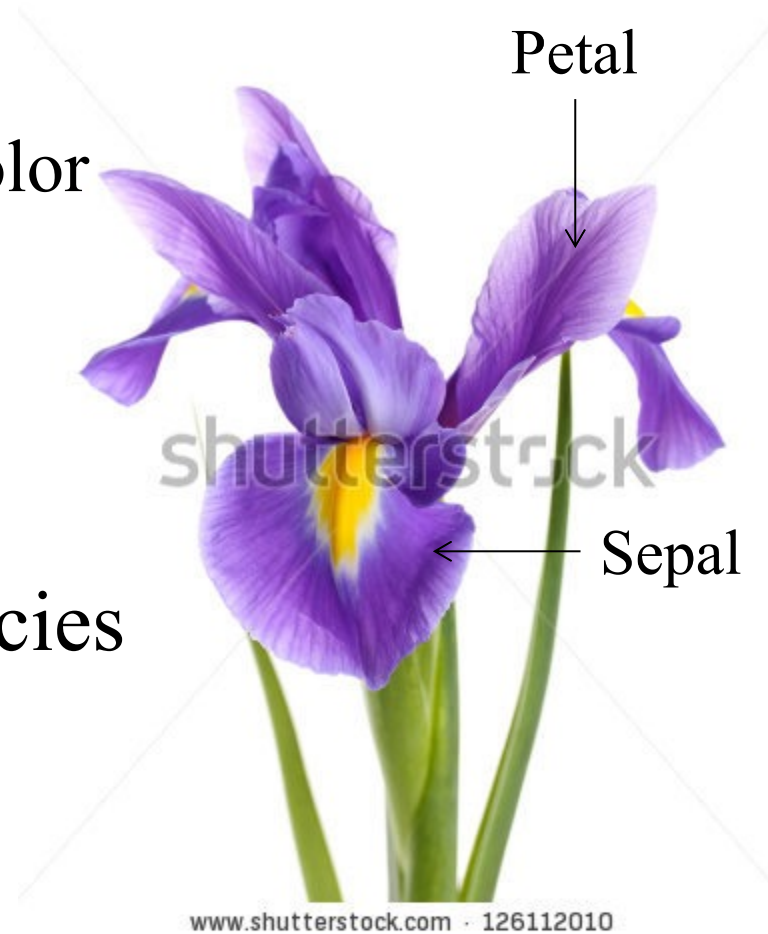
Four features measured:

- Sepal width and length
- Petal width and length

Is it possible to distinguish species using physical measurements?

- Data is packaged with R: "iris"

http://en.wikipedia.org/wiki/Iris_flower_data_set



Regression tree: data

Build and test a model using the iris data.

Subset the data into training and test data sets.

```
>   # to select 70% of rows
>   set.seed(9999) # make random selection repeatable
>   # create vector of row indices for train/test
>   train.row = sample(1:nrow(iris), 0.7*nrow(iris))
>   # assign train/test using row index
>   iris.train = iris[train.row,]  Row indices for training
>   iris.test = iris[-train.row,]  Row indices for testing
```

Regression tree: building and testing

Adapting the same commands used for the tennis example:

```
> itree = tree(Species ~., data = iris.train)
> itree
> summary(itree)
> plot(itree)
> text(itree, pretty = 0)
> ipredict = predict(itree, iris.test, type = "class")
> table(observed = iris.test$Species, predicted = ipredict)
```

Regression tree: summary

Summary of terminal nodes, variables actually used, error measures.

> summary(itree)

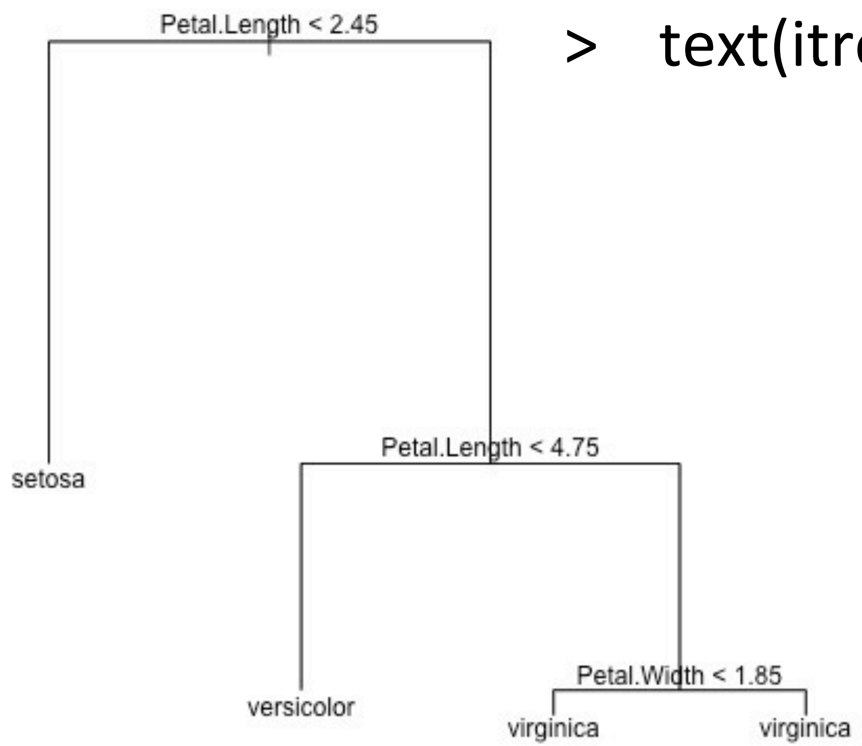
```
Classification tree:
tree(formula = Species ~ ., data = iris.train)
Variables actually used in tree construction:
[1] "Petal.Length" "Petal.Width"
Number of terminal nodes:  5
Residual mean deviance:  0.1332 = 13.32 / 100
Misclassification error rate: 0.0381 = 4 / 105
```

Regression tree: details

> itree

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

 1) root 105 200 setosa ( 0.36 0.30 0.34 )
   2) Petal.Length < 2.45 38   0 setosa ( 1.00 0.00 0.00 ) *
   3) Petal.Length > 2.45 67  90 virginica ( 0.00 0.46 0.54 )
     6) Petal.Length < 4.75 27   0 versicolor ( 0.00 1.00 0.00 ) *
     7) Petal.Length > 4.75 40  30 virginica ( 0.00 0.10 0.90 )
      14) Petal.Width < 1.7 6   8 virginica ( 0.00 0.50 0.50 ) *
      15) Petal.Width > 1.7 34   9 virginica ( 0.00 0.03 0.97 )
        30) Petal.Length < 4.95 5   5 virginica ( 0.00 0.20 0.80 ) *
        31) Petal.Length > 4.95 29   0 virginica ( 0.00 0.00 1.00 ) *
```

Regression tree: plot




```
> plot(itree)
> text(itree, pretty = 0)
```

Classification tree: testing the model

To test the model, make a prediction for each and draw the confusion matrix.

```
>   table(observed = iris.test$Species, predicted = ipredict)
                 predicted
observed         setosa versicolor virginica
  setosa             13          0         0
  versicolor          0         14         3
  virginica           0          1        14
```

Discussion

How good is each model?

Could the models be improved?

Are they too specific, based on the training set?

Note that previous examples are sensitive to the value of the random seed. If this changed the decision tree model and/or accuracy may change.

More on decision devlopment and testing as well as other classifcation methods next lecture.

Answers to the quiz questions

1. A
2. B
3. D
4. C

Reading/Notes on the presentation

Further Reading: FREE BOOK!!

- An Introduction to Statistical Learning with applications in R, 2nd Ed, 2021. (Springer Texts in Statistics), James, Witten, Hastie and Tibshirani, Chapter 8 (available on-line from Monash Library)

Notes:

- This presentation contains some slides created to accompany: *Introduction to Data Mining*, Tan, Steinbach, Kumar. Pearson Education Inc., 2006.
- Presentation originally created by Dr. Sue Bedingfield.