# dm24s1

## Topic 10 : Classification2

## Part 01 : Classification2-Overview

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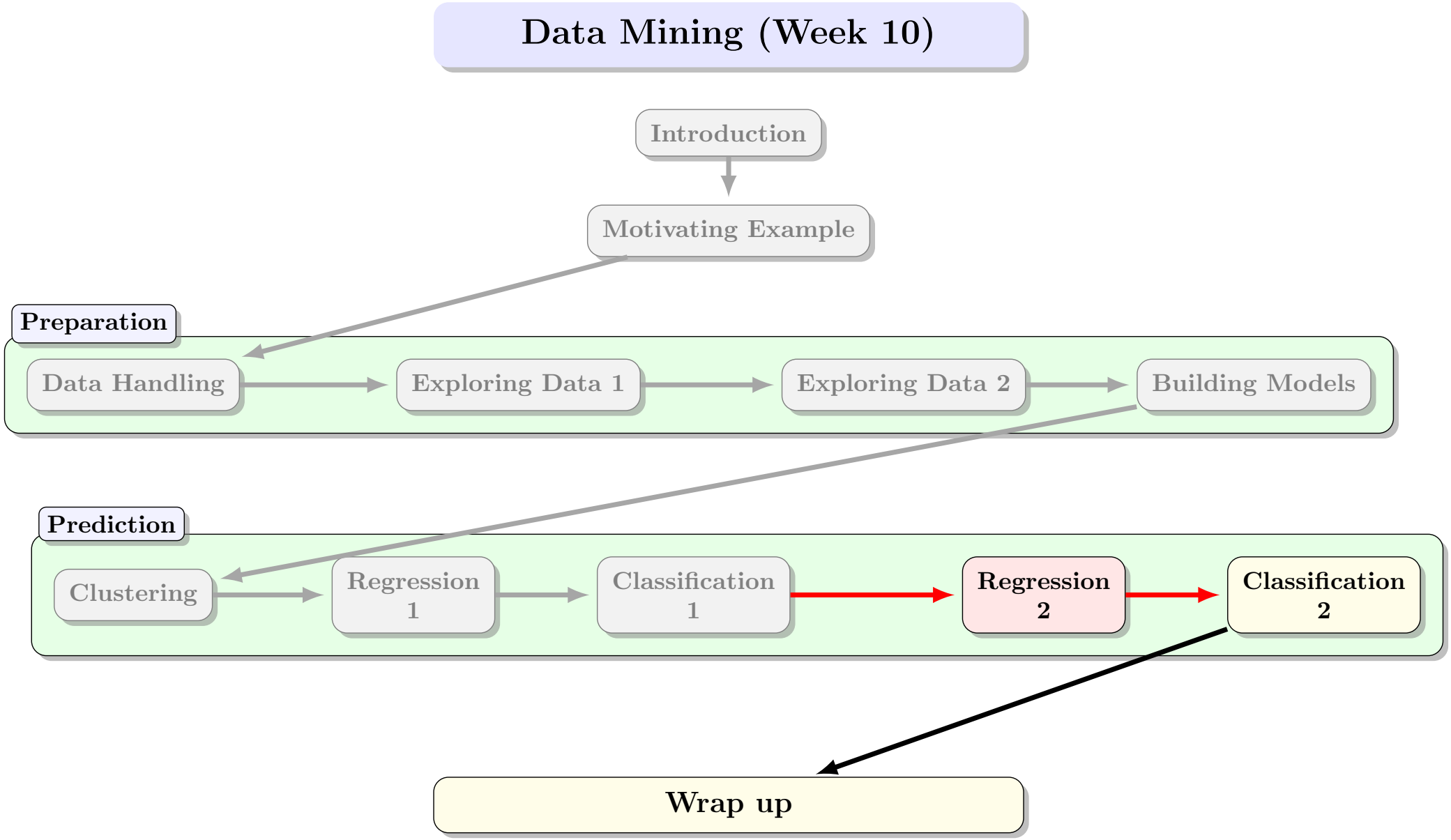
### Outline

- Decision Trees
- Naive Bayes


Data Mining (Week 10)
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Motivating Example
Preparation
Data Handling
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Exploring Data 2
Building Models
Prediction
Clustering
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Classification 1
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# Classification2-Overview — Summary

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# Objectives

In this topic, you are introduced to some more advanced techniques used for classification. Remember: you have already met *logistic regression* and *k nearest neighbours* in Topics 8 and 2, respectively.
The new approaches are:

- A technique that uses a series of questions to classify a data set (Decision Trees)
- A technique that uses probability directly to classify a data set (Naive Bayes)

These are two of the Top 10 algorithms in data mining (**WuKumarRossQuinlanEtAl2008**), each with its own strengths and weaknesses.

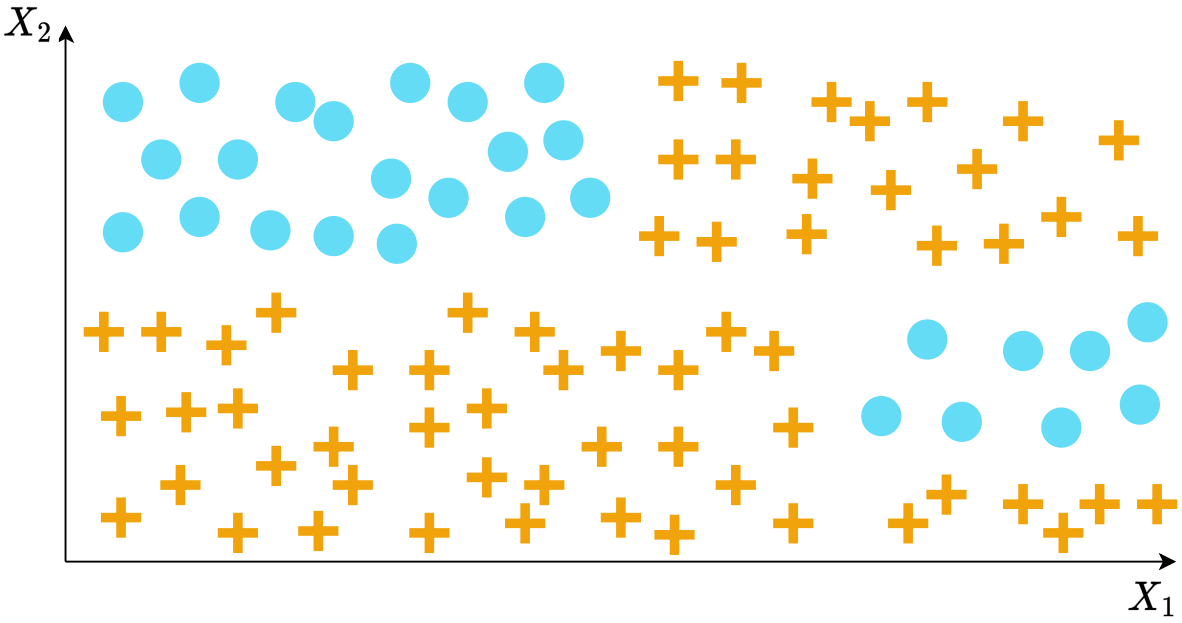
# Motivation

Twenty Questions is a powerful way of learning (identifying something)

**Can it be used to predict categorical variables?**

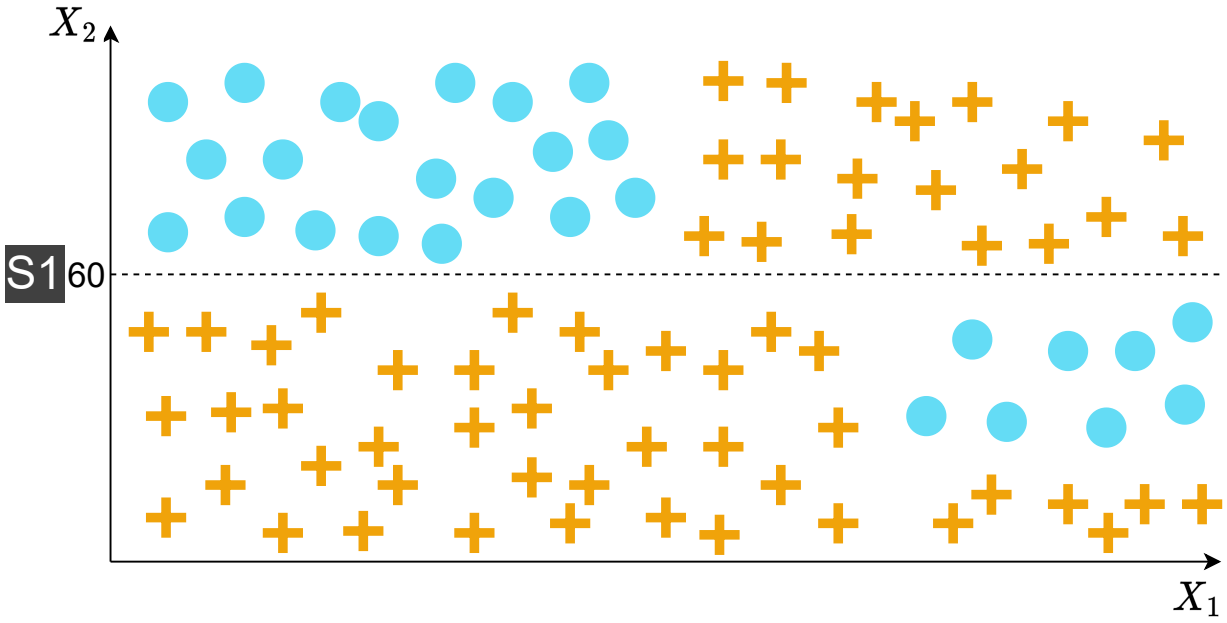
- Assume we have a set of $l$ labels to assign to $n_{\text{test}}$ data observations
- During training we repeatedly partition the training set using a sequence of ever finer rules
- The resulting decision tree generates a mapping from *attributes* of an item (the mapping is defined by a path from root to leaf) to conclusions about the item's target value (represented in the leaves).
- The rules which generate the binary splits are applied in a greedy fashion and are intended to reduce the *impurity* in each nodes' children as quickly as possible
- the algorithm proceeds top-down from the root (all data), recursively generating rules as it goes
- Prediction is simple: the rules are applied along the path from root to leaf. The predicted class value is either the most frequent value at the leaf, or the leaf's probability vector.

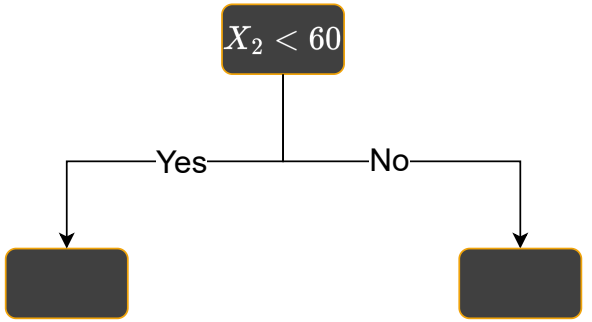
# Classification tree: Example Data




Task: learn from this training data, to classify new data as either orange cross or blue disk

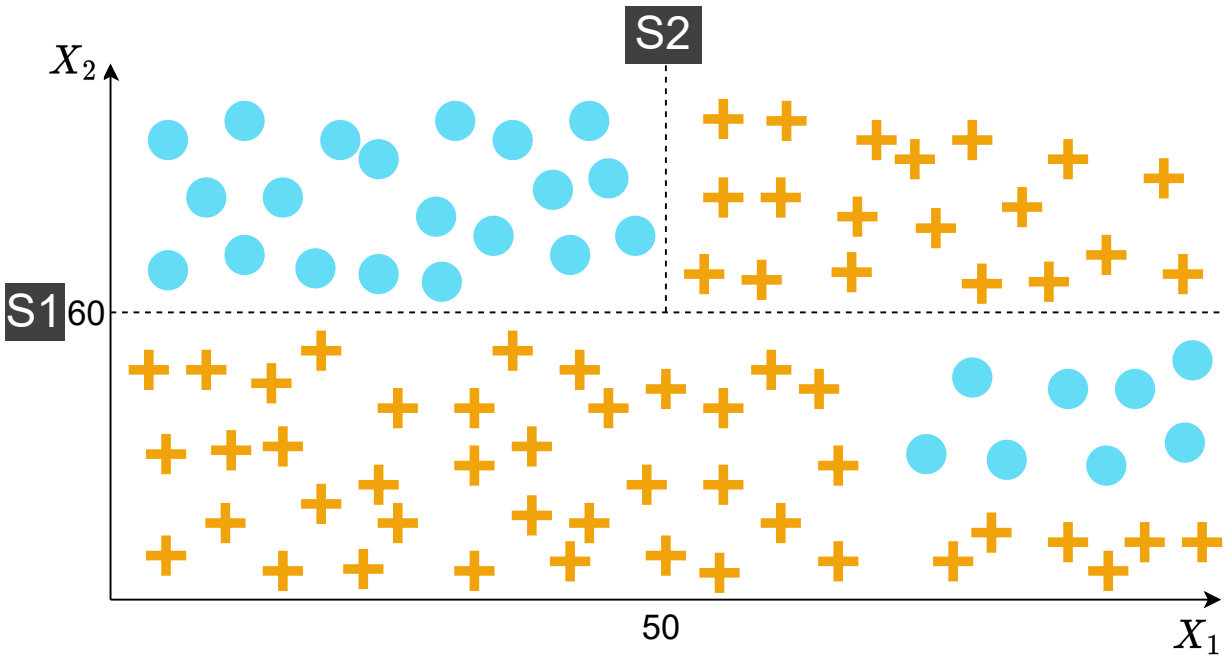
# Classification tree: Example Data - First Split

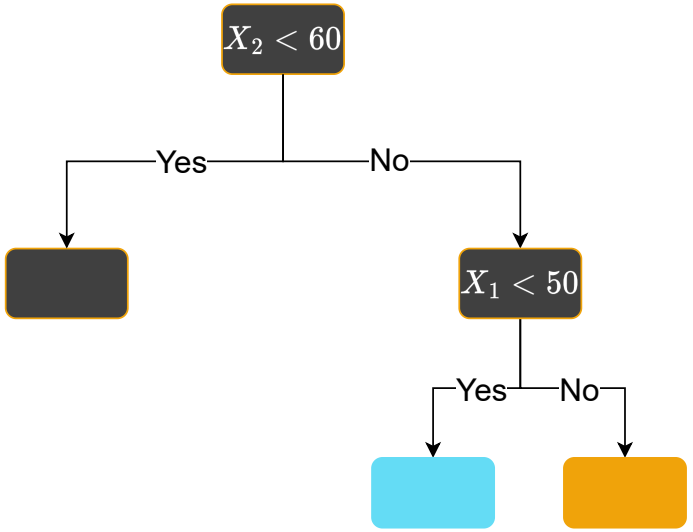



First split is on $X_2$; purity is improved (less mixing in each subset)

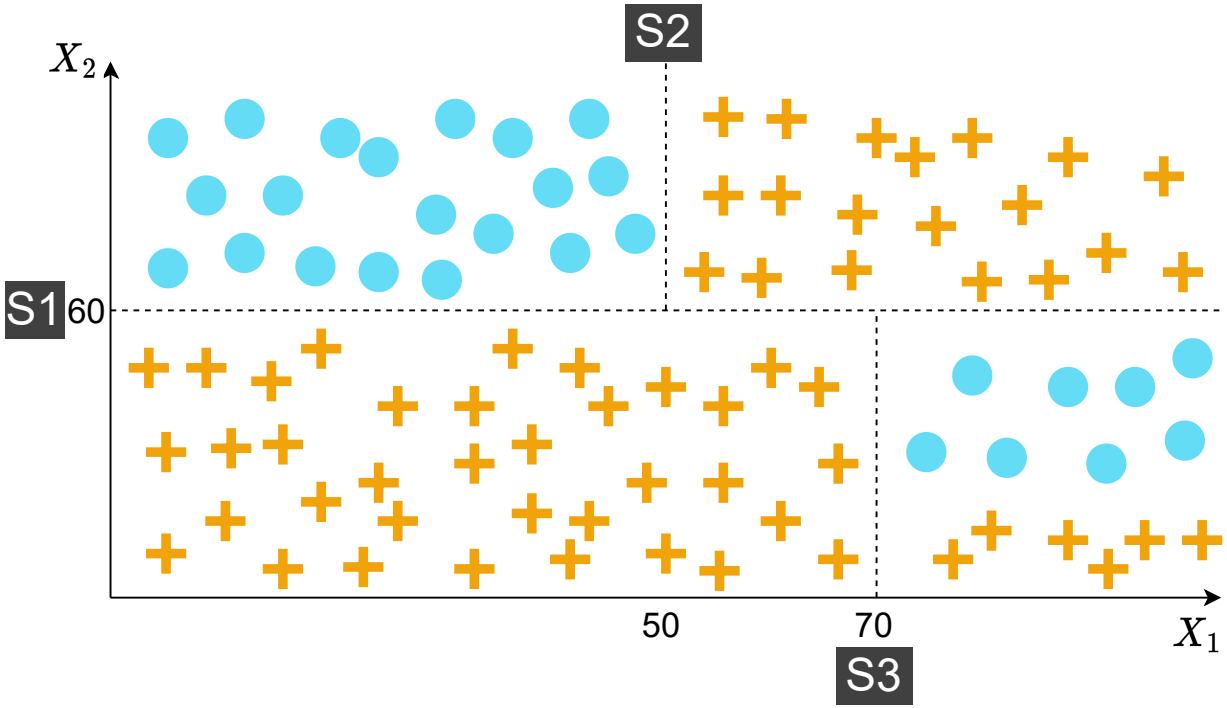
# Classification tree: Example Data - Second Split

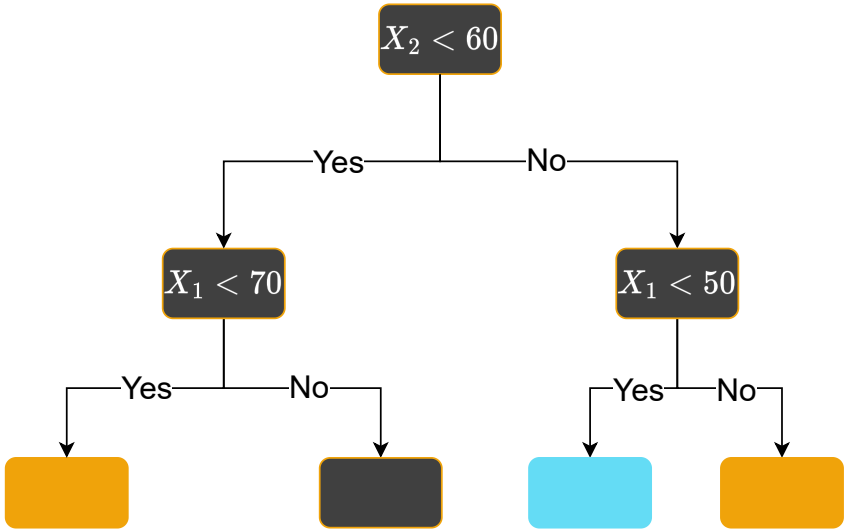



Second split is on $X_1$ so one region is pure (all blue disks) - can continue.

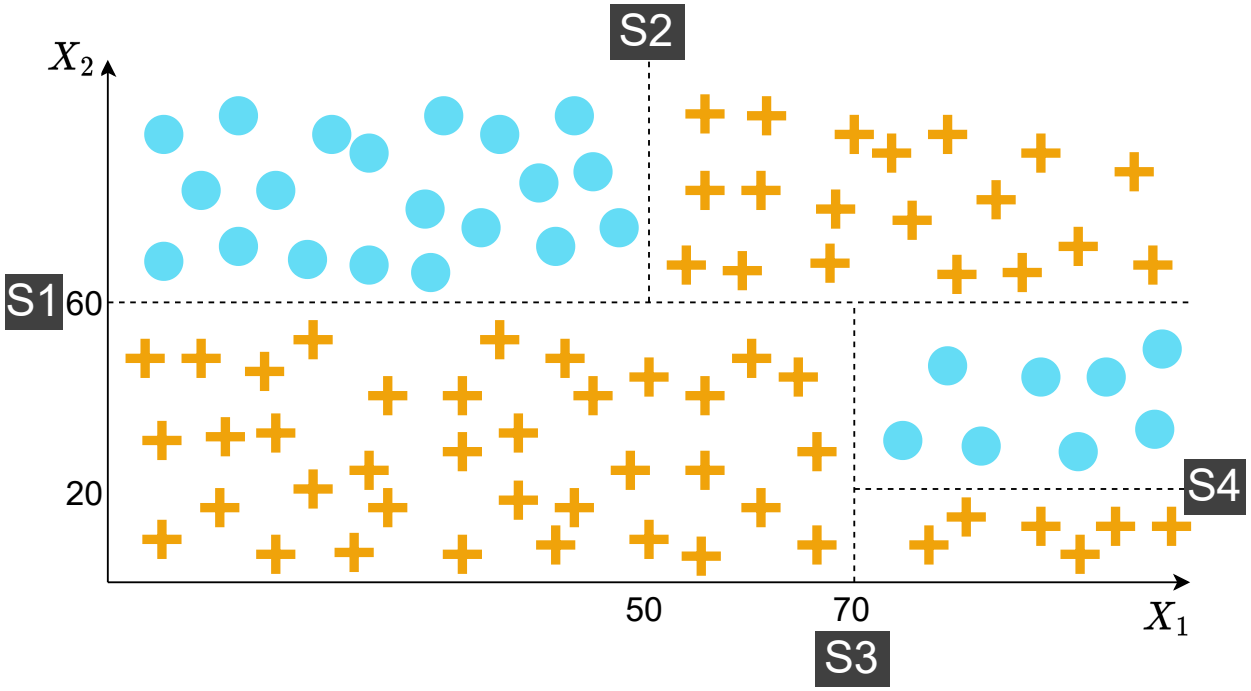
# Classification tree: Example Data - Third Split

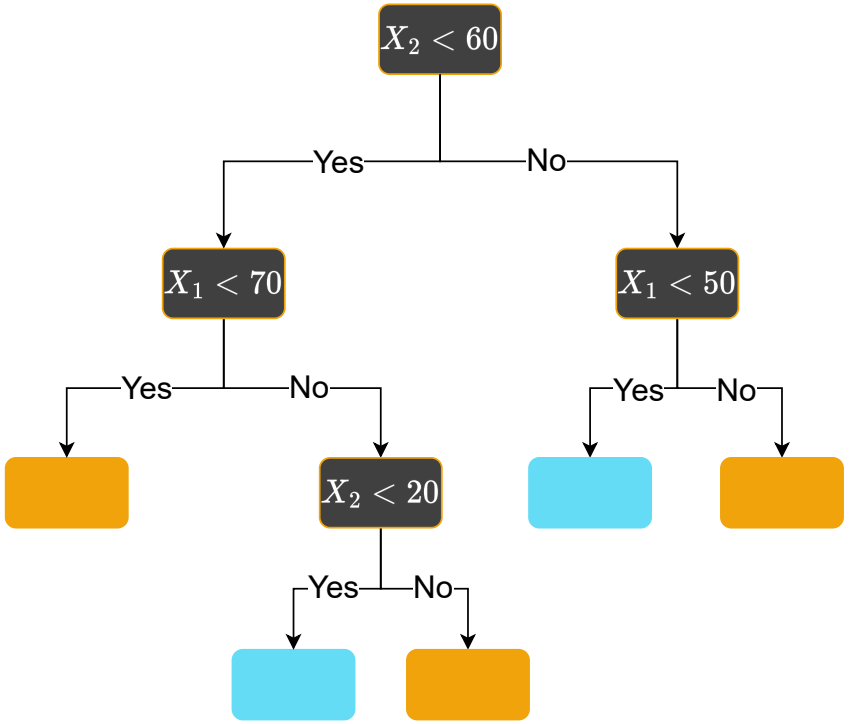



Third split on $X_1$ adds two extra pure regions.

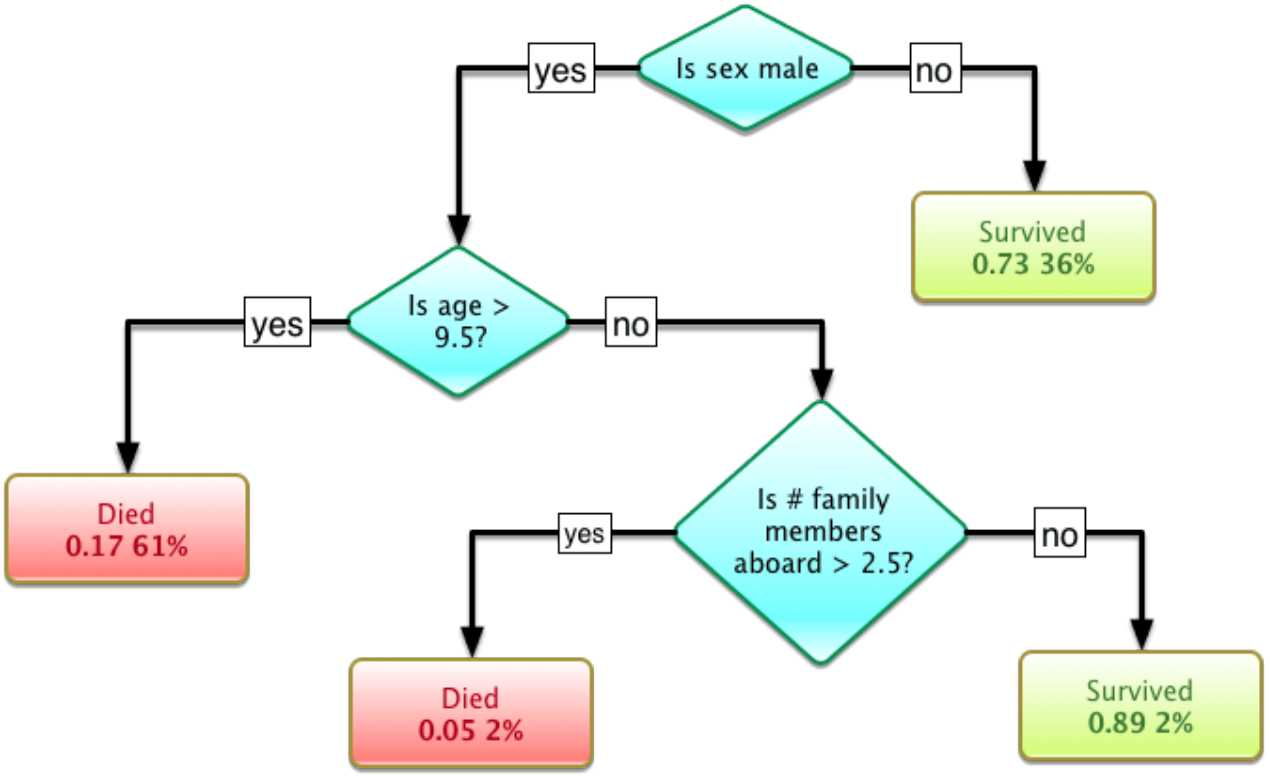
# Classification tree: Example Data - Fourth Split




After fourth split on $X_2$, all regions are pure, so we stop.

# Classification tree example: Titanic survival




- First split is on Sex, as that attribute was the most important predictor of survival.
- Leaves show the probability of survival and the percentage of training observations in the leaf.
- Percentages sum to 100% (approximately), as the leaves partition the training data.
- Leaf colour indicates p(survival) $\approx$ 1 (green) or p(survival) $\approx$ 0 (red)

# Classification tree notes

- At each step, we choose a feature and split a data subset using that feature
- Each split is parallel to one of the feature axes
- Aim of splitting is to maximise progress to purity at each step
- But how do we choose the feature to split? Or the value of that featurei for splitting?
- The algorithm needs a suitable metric and criterion that can be calculated
  - For each impure set
  - For each candidate split

# Information Entropy: intuition

| Probability | Information | Perceived as |
|---|---|---|
| Low | High | Surprising |
| High | Low | Unsurprising |

## Example

If it is winter in Ireland, and Met Eireann forecast that tomorrow will have a temperature of 10 degrees C, nobody would pay much attention. If, on the other hand, they said it would be 40 degrees C, everyone would notice!

Entropy is average amount of information conveyed by an event, considering all possible outcomes.

## How information is measured

Information is measured in bits, and is computed from the probability $P(x)$ using $h(x) = -\log_2(P(x))$.

# Information Entropy: Applied to classification

## Classification and entropy

- Given a set of observations with the same label, we wish to make membership of that set as unsurprising as possible as possible, given the training set.
- Can we partition a set of observations to achieve this, so that it is "obvious" that the label assignments are correct? In other words, we want as many elements as possible to have a label that matches the label given to the set partition to which they belong. This increases the *purity* of that partition.

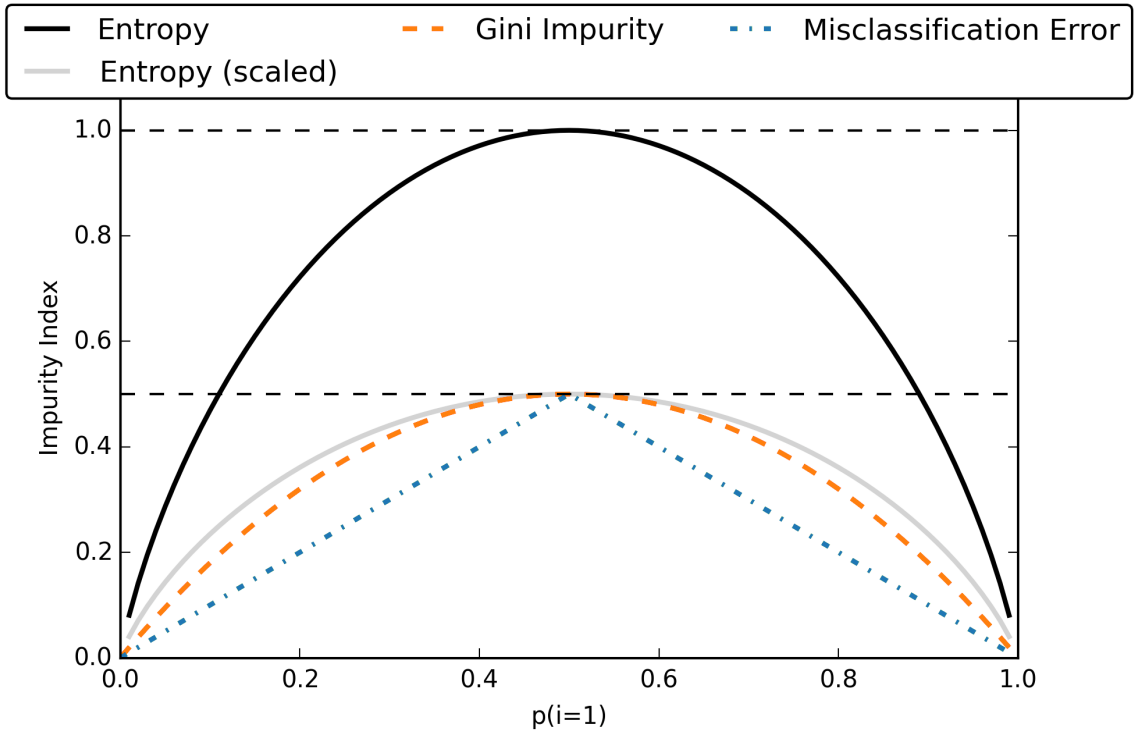
## Definition 1 ((Information) Entropy)

$$H(X) = -\sum_{i=1}^{n} P(x_i)\log_2(P(x_i))$$

where $X = \{x_i\}$. If all probabilities are equal (X is uniformly distributed), $H(X) = 1$. If they differ, $H(X) < 1$. Remember the weather forecasting example!

A decision tree recursively partitions a set so as to increase the purity (equivalently: reduce the mixing) of the set of observations $X$ at each node as we move from the root to the leaves.

# Classification tree metrics for rule building




Let $p_i$ be the probability of an item with label $1 < i < J$ being chosen. Then the *GINI* impurity is $1 - \sum_{i=1}^{J} p_i^2$. Worst case (maximum impurity): labels are uniformly distributed (entropy of the set is maximum: each value of the label appears the same number of times in the set of observations at that node). We wish to minimise this entropy.

# Sidebar: Entropy

## Definition 2 (Entropy)

- Entropy is a concept from *thermodynamics* and *information theory*.
- Here it measures the *impurity* of a collection of items.
- It ranges from 0 (only 1 item, possibly repeated) to 1 (equal numbers of each item type).
- Mathematically, it is defined for *one attribute* $T$ as $H(T) = -\sum_{j=1}^{J} p_j \log_2 p_j$, in a collection of size $N$ where there are $J$ unique elements of $T$, hence $p_j = \frac{n_j}{N}$ where there are $n_j$ elements of type $j$.
- For *two attributes* $T$ and $X$, $H(T,X) = \sum_{c \in X} P(c)E(c)$ where each $c$ represents a level of the $X$ attribute.

# Sidebar: Information Gain

## Definition 3 (Information Gain)

- Information Gain measures the decrease in entropy (equivalently: increase in purity) after a dataset is split on an attribute.
- It is defined as $G(T, X) = H(T) - H(T, X)$, where
  - $H(T)$ is the entropy at the parent node, and
  - $H(T, X)$ is the entropy after the split by candidate attribute $X$.

# Example: PlayTennis example data

| outlook | temp | humidity | windy | play |
|---|---|---|---|---|
| sunny | hot | high | false | no |
| sunny | hot | high | true | no |
| overcast | hot | high | false | yes |
| rainy | mild | high | false | yes |
| rainy | cool | normal | false | yes |
| rainy | cool | normal | true | no |
| overcast | cool | normal | true | yes |
| sunny | mild | high | false | no |
| sunny | cool | normal | false | yes |
| rainy | mild | normal | false | yes |
| sunny | mild | normal | true | yes |
| overcast | mild | high | true | yes |
| overcast | hot | normal | false | yes |
| rainy | mild | high | true | no |

*Source:* Mitchell, *Machine Learning*, 1997.

# PlayTennis example calculations

## Example 4 (H(play))

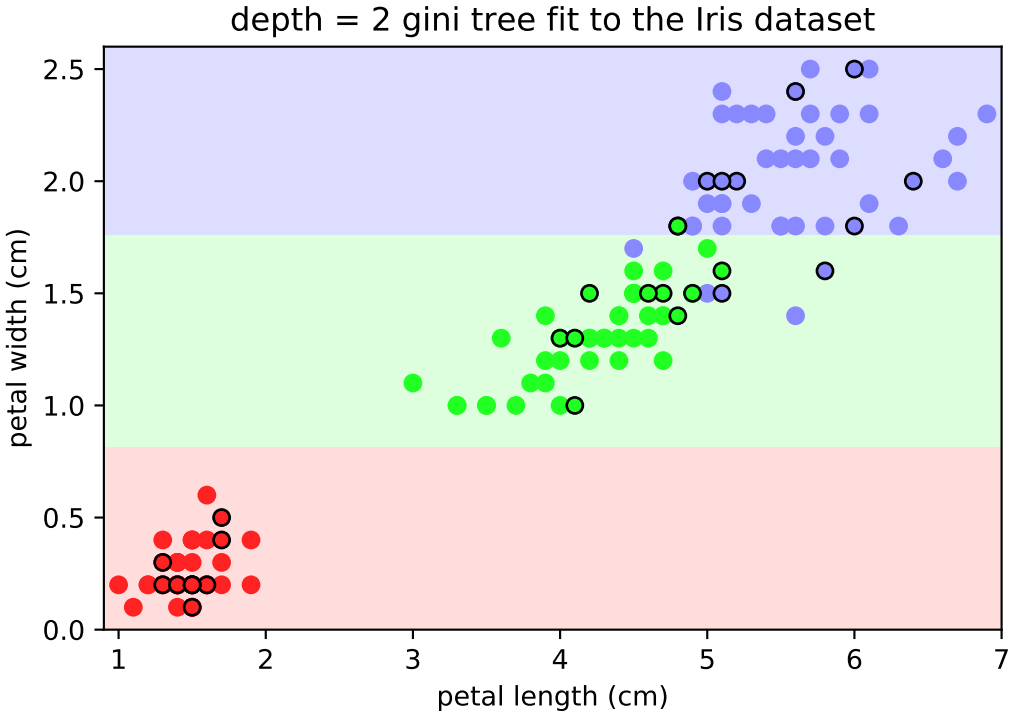
$$\begin{aligned} H(\text{play}) &= -\left(p(\text{play}=\text{yes})\log_2 p(\text{play}=\text{yes}) + p(\text{play}=\text{no})\log_2 p(\text{play}=\text{no})\right) \\ &= H_{9,5} \\ &= -\left(\frac{9}{14}\log_2\left(\frac{9}{14}\right) + \frac{5}{14}\log_2\left(\frac{5}{14}\right)\right) \approx 0.94 \end{aligned}$$

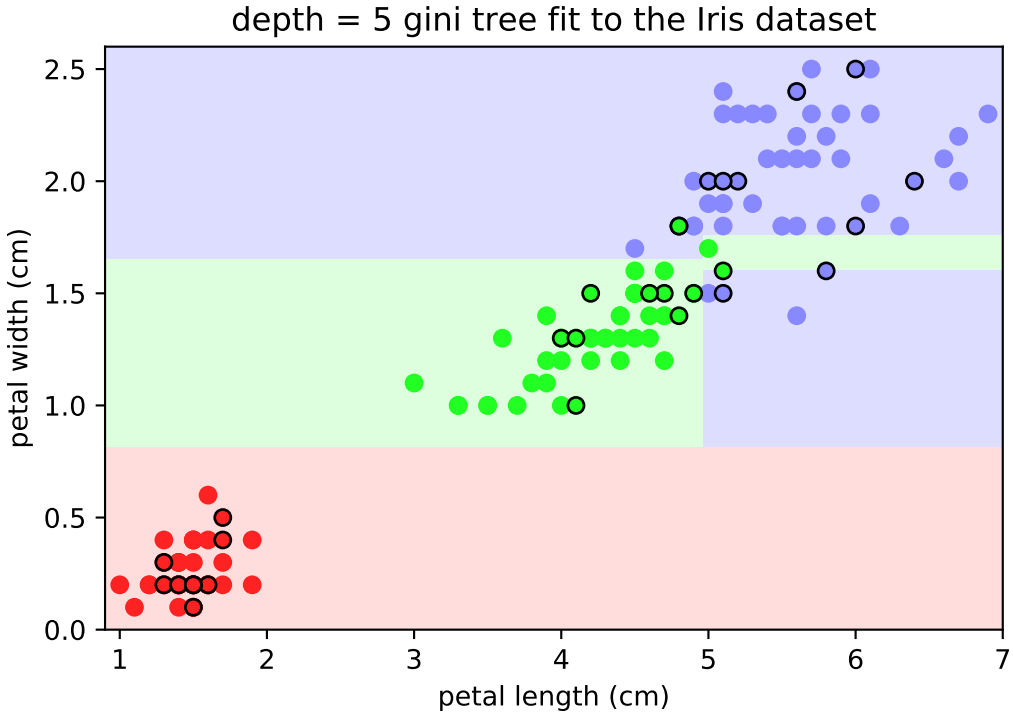
## Example 5 (H(play,outlook))

$$\begin{aligned} H(\text{play},\text{outlook}) &= p(\text{outlook}=\text{sunny})H(\text{play}\&(\text{outlook}=\text{sunny})) + \ldots \\ &= p(\text{outlook}=\text{sunny})H_{3,2} + p(\text{outlook}=\text{overcast})H_{4,0} + \ldots \\ &\approx \frac{5}{14}0.97 + \frac{4}{14}0 + \frac{5}{14}0.97 \\ &\approx 0.69 \end{aligned}$$

When growing decision trees, at a given node we search over the attributes for splitting, and choose the one that gives the maximum information gain, until we reach a leaf, which has an entropy of zero.

# Classification tree examples: Iris Data



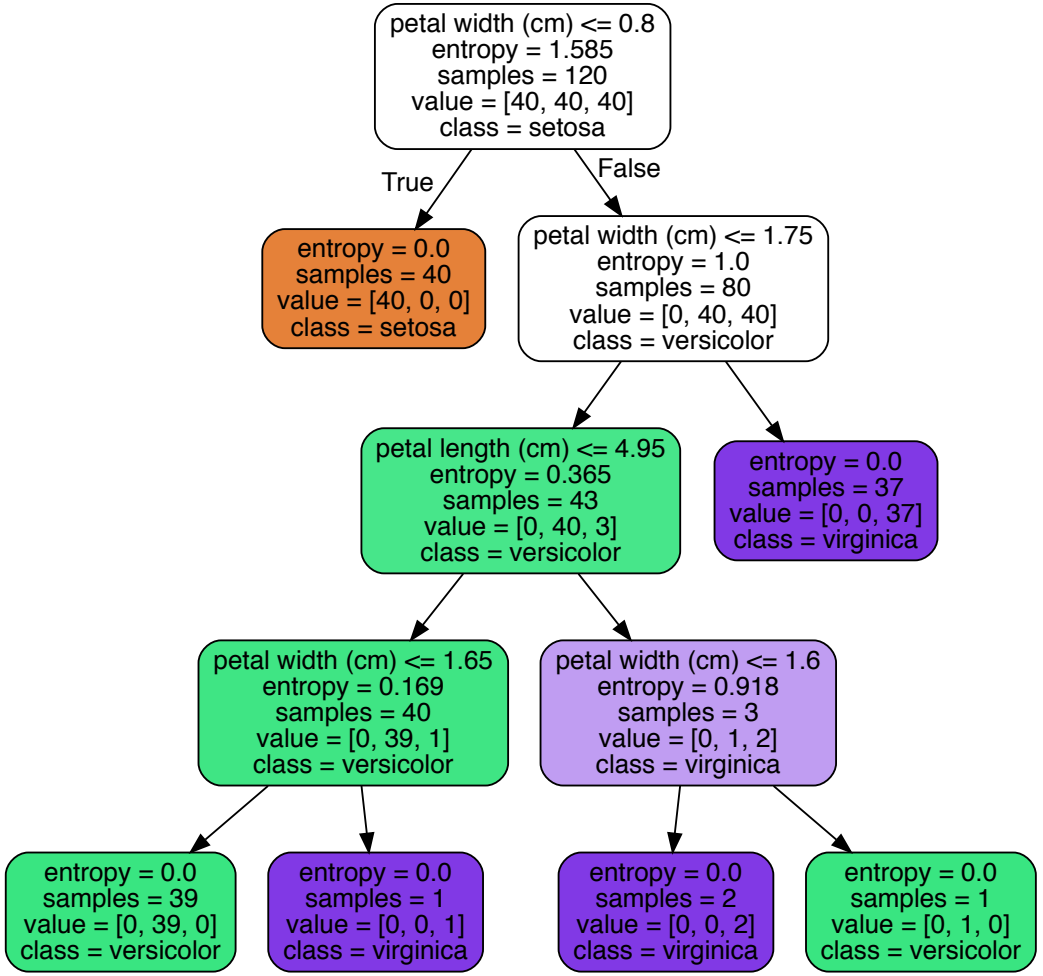

Note the rectangular regions (because each split is over one variable) and the greater complexity when the maximum depth of the tree increases.

Points within a dark circle represent test data, with the main colour of the point indicating its species label.

The choice of metric (Gini impurity or Information Gain) makes only slight changes to fit.

# Classification tree view: Iris Data

Note that the leaf nodes are pure (entropy=0) and are coloured according to predicted value (species label): brown for *I. setosa*, green for *I. versicolor* and purple for *I. virginica*.



# Classification tree: Use for Prediction

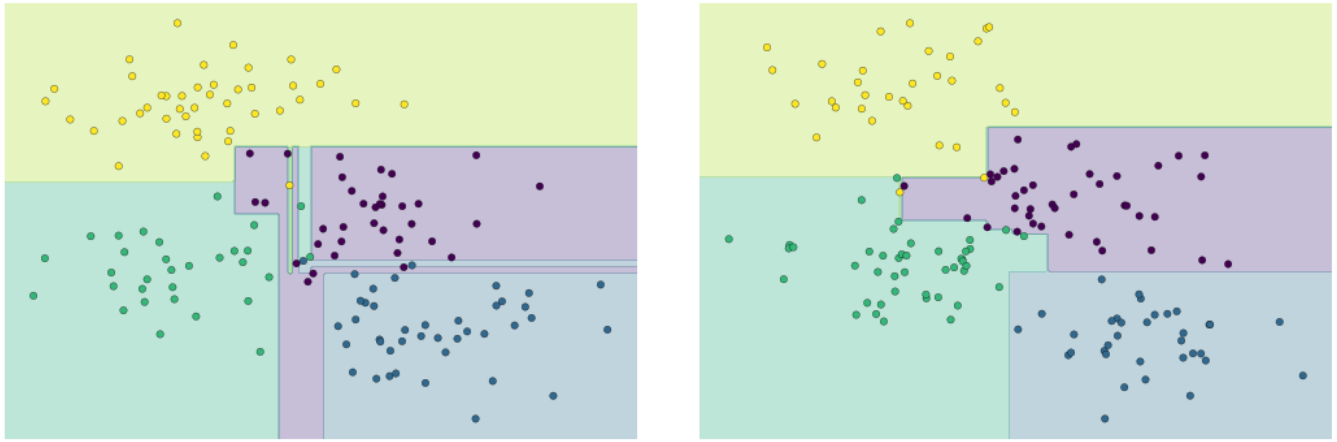
Now that we have a decision tree, how do we use it to predict the label?

## Example: estimating the species of an iris plant

- Let Petal_Width = 1.5cm and Petal_Length = 5cm. The other (sepal) dimensions are ignored by the decision tree because they were not as useful for classification.
- The first split (Petal_Width $\leq 0.8$) is `False` so we take the *right* branch.
- The second split (Petal_Width $\leq 1.75$ is `True` so we take the *left* branch.
- The third split (Petal_Length $\leq 4.95$ is `False` so we take the *right* branch.
- The fourth split (Petal_Width $\leq 1.6$ is `True` so we take the *left* branch.
- We have reached a leaf (entropy = 0) and connot split any further.
- Depending on where we stop, we would assign the prevalent label for that node (`versicolor`, `versicolor`, `virginica` or `virginica` if the `max_depth` was 2, 3, 4 or 5, respectively).

Python can extract paths from the root to each leaf as a set of if-then-else rules, to explain decisions.

# Be careful of overfitting. . .



- Given two very similar (generated) data sets, all leaves in each fitted decision tree are *pure*.
- The resulting trees look very different.
- This sensitivity to the noise in the data is characteristic of *overfitting* (high variance).
- Control by a) limiting depth or b) limiting number of leaves.

# Classification trees in python

```
tree = DecisionTreeClassifier(criterion=criterion, max_depth=treeDepth, random_state=0)
tree.fit(Xtrain, ytrain)
y_treeTest = tree.predict(Xtest)
print(accuracy_score(ytest, y_treeTest))
print(confusion_matrix(ytest, y_treeTest))
print(classification_report(ytest, y_treeTest, digits=3))
```

After creating the classifier object, fit the training data and then use the fit to predict yTest from xTest. I have also shown how to get some diagnostic output. Similar diagnostics can be obtained for other classifiers.

# Rev. Bayes and his theorem

*Rev. Thomas Bayes, 1702–1761*

## Usage

Given $P(E|H)$ (Probability of Evidence (attributes) given the Hypothesis (the known classes) in the *training* set), Bayes theorem shows how to invert this relationship to get $P(H|E)$ (Probability of the Hypothesis (class) given the evidence (attributes) with an (unseen) *test case*).

## Bayes' Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \tag{1}$$

where $P(X|Y)$ is the conditional probability of $X$ given that we know $Y$ is true.

## Application to classification

By convention, $A = H$ and $B = E$, where $H$ is the hypothesis and $E$ is the evidence in support of that hypothesis.
With this interpretation, the Bayes identity can be used to predict class probabilities (hypothesis) from features (evidence).

# Conditional probabilities and Bayes terminology

## Definition 6 (Conditional Probability)

If $A$ and $B$ are events, the Probability of $A$, given that $B$ is true (has happened), written $P(A|B)$ is defined as follows:

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \tag{2}$$

where $P(A \cap B)$ is the probability that both $A$ and $B$ are true.

Given Bayes Theorem 1, we have

| Term | Description |
|---|---|
| $P(A)$ | Class prior; Prior probability |
| $P(B)$ | Predictor prior; evidence |
| $P(A\|B)$ | Posterior probability; Updated Class Prior |
| $P(B\|A)$ | Likelihood |

- In courtrooms, $B$ might represent the available evidence in favour of guilt, and $A$ might represent the verdict "is guilty".
- In data mining, $B$ might represent the features (derived from the Data) for a given instance and $A$ might represent the *predicted label* for these features.
- If $A$ and $B$ are independent events, $P(A \cap B) \equiv P(A)P(B)$, so $P(A|B) = P(A)$ and $P(B|A) = P(B)$.

# Extended and Bayes

In practice, there would be multiple features/evidence so $B = \{B_1, B_2, \ldots, B_n\}$

.

## Definition 7 (Extended Bayes Theorem)

The extended form, when $\{B_j\}$ partition $B$, so $B = \cup_j B_j$ and $B_p \cap B_q \equiv \emptyset$ unless $p = q$, is

$$P(A|\{B_i\}) = \frac{P(\{B_i\}|A)P(A)}{P(\{B_i\})} \tag{3}$$

which is the component-wise version of the standard Bayes Theorem.

## Side note: Prosecutor's Fallacy

Note that $P(A|B) \neq P(B|A)$ in general. If the ratio $\frac{P(A)}{P(B)}$ is not close to 1, lawyers can mislead jurors regarding guilt or innocence. *Probability of Guilt given the evidence is not the same as the probability of the evidence assuming the defendant is guilty.*

# Naive Extended Bayes

## Definition 8 (Naive Bayes)

If the features $B$ are assumed to be independent of each other, it can be shown that

$$P(B) = P(B_1 \cap B_2 \cap \ldots B_n) = \prod_i P(B_i) \tag{4}$$

$$P(B|A_j) = \prod_k P(B_i|A_j) \tag{5}$$

The naïve form of Bayes theorem becomes

$$P(A_j|B) = \frac{\prod_i P(B_i|A_j)P(A_j)}{\prod_i P(B_i)} \tag{6}$$

# Naive Bayes classifier

## Definition 9 (Naive Bayes classifier)

- The Naive Bayes algorithm predicts a class, given a set of set of features, using probability principles.
- It is naive because it assumes the features are statistically independent (rarely true in practice).
- The training data is used to estimate the probabilities and likelihood.
- Bayes theorem is used to predict the observation's membership of each class (associated with a label).
- It is then assigned to the class for which its conditional probability is greatest.

# Naive Bayes Interpretation

- Both the simple and extended Bayes Theorem provide a formula to flip between "B given A" (data given labels) to "A given B" (labels given data).
- From the Training set, we can calculate
  - $P(A_j)$ (prior probability of each class label),
  - $P(B_i)$ (the predictor prior) and
  - $P(B_i|A_j)$ (the evidence that the feature valued $B_i$ predicts the class label $A_j$).
- From this, we can use the naive version of the extended Bayes Theorem 6 to predict $P(A_j|B)$, the posterior probability of class label $A_j$ given all the evidence from the features $B$.

# Overview of Naïve Bayes algorithm

- In the *Training Phase*, the method precomputes various probabilities $P(A_j)$ and conditional probabilities $P(B_k|A_j)$.
- In the *Prediction Phase*
  - the extended form of Bayes' Theorem 6 is used to compute the posterior class probabilities $P(A_j|B)$ for the given observation.
  - according to the *Maximum A Posteriori* (MAP) criterion, the observation is assigned to the class with the highest probability from $P(A_j|B)$.
- One of the features of Naïve Bayes (with $P(A|B)$), like decision trees (with $P(A \cap B)$), is the direct role played by probability
- When training Naïve Bayes, it is convenient to compute a table of *marginal counts*, as seen in the next slide, and to use these for prediction.

# Fruit classification example

## Example: Fruit classification

| Type | Long | ¬Long | Sweet | ¬Sweet | Yellow | ¬Yellow | *Total* |
|---|---|---|---|---|---|---|---|
| Banana | 400 | 100 | 350 | 150 | 450 | 50 | *500* |
| Orange | 0 | 300 | 150 | 150 | 300 | 0 | *300* |
| Other | 100 | 100 | 150 | 50 | 50 | 150 | *200* |
| *Total* | *500* | *500* | *650* | *350* | *800* | *200* | *1000* |

*Source:* stackoverflow

## Fruit classification : Precalculations

P(<Fruit>) = Total_<Fruit> / Total_*
P(<Feature>) = Total_<Feature> / Total_*
P(<Feature> | <Fruit>) = <Fruit,Feature> / Total_<Fruit>

→ P(Other) = 200/1000 = 0.2
→ P(Sweet) = 650/1000 = 0.65
→ P(Sweet | Other) = 150/200 = 0.75

# Fruit classification example: prediction

Given observation: Long=L, Sweet=S, Yellow=Y fruit, which is it?

## Banana - B

$$P(\mathrm{B}|L,S,Y) = \frac{P(\mathrm{L}|\mathrm{B})P(\mathrm{S}|\mathrm{B})P(\mathrm{Y}|\mathrm{B})P(\mathrm{B})}{P(\mathrm{L})P(\mathrm{S})P(\mathrm{Y})}$$

$$= \frac{0.8 \times 0.7 \times 0.9 \times 0.5}{0.5 \times 0.65 \times 0.8}$$

$$= 0.97$$

## Orange - O

$$P(\mathrm{O}|L,S,Y) = \frac{P(\mathrm{L}|\mathrm{O})P(\mathrm{S}|\mathrm{O})P(\mathrm{Y}|\mathrm{O})P(\mathrm{O})}{P(\mathrm{L})P(\mathrm{S})P(\mathrm{Y})}$$

$$= \frac{0.0 \times 0.5 \times 1.0 \times 0.3}{0.5 \times 0.65 \times 0.8}$$

$$= 0$$

## Other = R

$$P(\mathrm{R}|L,S,Y) = \frac{P(\mathrm{L}|\mathrm{R})P(\mathrm{S}|\mathrm{R})P(\mathrm{Y}|\mathrm{R})P(\mathrm{R})}{P(\mathrm{L})P(\mathrm{S})P(\mathrm{Y})}$$

$$= \frac{0.5 \times 0.75 \times 0.25 \times 0.2}{0.5 \times 0.65 \times 0.8}$$

$$= 0.07$$

According to the MAP criterion, the observation (mystery fruit) is a banana!

Given the 3 binary-valued attributes, there are $2^3 = 8$ possible combinations - Naïve Bayes will classify each of these 8 combinations as one of the 3 fruit classes.

# Naïve Bayes Classifier summary

- Advantages
  - Conceptually simple and easy to implement
  - Fast and scalable
  - Variants exist for numeric (Gaussian-), binary (Bernoulli-) and multi-class (mulinomial-) featured Naïve Bayes
  - Particularly good for text classification and email spam detection
- Disadvantages
  - Ignores feature relationships, so #(feature) + #(¬feature) is the same for all features
  - Be careful of zero-valued conditional probabilities and numerical underflow
  - Prone to underfitting (high bias)
- For prediction $F(X) \rightarrow Y$
  - Most classifiers are discriminative—they learn $P(Y|X)$: "Given data $X$, what class $Y$ is it?"
  - Naïve Bayes is generative—it learns $P(X|Y)$ and $P(Y)$: "Given classes $Y$, what data $X$ fits each class, and how often do those classes occur?"
- Implementations exist in `sklearn`: `from sklearn.naive_bayes import GaussianNB`, etc.

# Ordinal regression vs Ordinal Classification

- Should ordinal targets be predicted using regression?
  - Yes, because like numbers, they have a natural order...
  - No, because differences don't work the same way...
- Should ordinal targets be predicted using classification?
  - Yes, because the targets are categories, not numbers...
  - No, because the difference between two categories depends on their order, and classificatuion ignores this
- scikit-learn does not offer Ordinal Regression/Ordinal Classification directly
- But there are proposals to wrap existing classifiers and to solve an extended problem that predicts the target while considering ordinal target values.

In the meantime, either Regression or Classification is used, with caveats...

# Summary

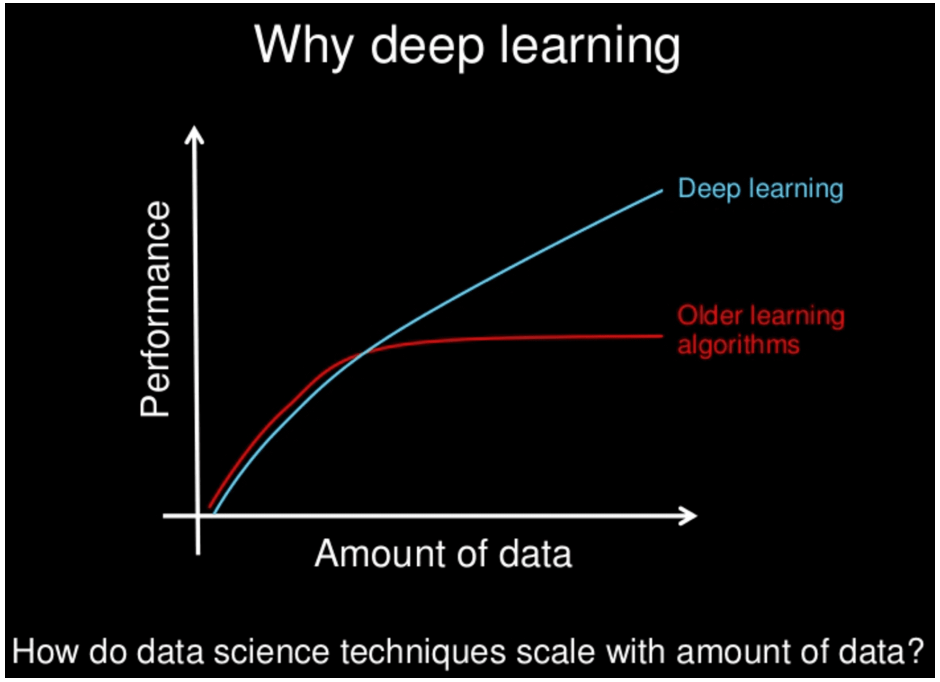
- Classification is one of the main tasks in data mining, and is a mature and well-studied field
  - k-nearest-neighbours is conceptually simple (based on voting) and the lack of a model (lazy learning) means it responds better to data drift
  - Logistic regression is an extension of linear regression and benefits from its strengths
  - Decision trees learn a representation that is often easily interpretable, but works better with linear boundaries
  - Naïve Bayes offers a probability-based generative model, able to work from data summaries, ideal for text and email classification
- More advanced classifiers have their own advantages, especially in relation to high dimensional data:
  - Ensemble methods (such as RandomForest and AdaBoost) were state of the art (2000-2012, say) and sacrifice interpretability for good performance with high dimensional data
  - SVM was state of the art (1985-2000, say) and is still extremely effective for very high dimensional problems like document classification

# Other considerations

- KNN uses *lazy* learning, all other techniques above use *eager* learning (derive model from training data)
- Naive Bayes uses *generative* learning to learn how the data was generated, all other techniques above use *discriminative* learning to derive the function that assigns class labels
- For KNN and Decision Trees, the representation grows with the size of the data - that is not generally true in all other techniques above

Classification is sometimes confused with clustering - will cover this clustering next lecture.

# But is that the last word on Classification?




*Source*: Andrew Ng, *Why Deep Learning*

## Learning from big data

- Traditional classification algorithms eventually run out of steam as data size increases
- Shallow neural networks had been discounted in the 1980s and 1990s when trained with small data
- Deep learning to the rescue!
- Kernel SVM and logistic regression lead nicely to perceptron models, hence ANNs, hence deep learning
- Deep learning requires lots of data but the models can scale better to take account of extra data

Deep Learning will probably be covered in semester 2...

# General References