dm25s1

Topic 10 : Classification2

Part 01 : DecisionTree

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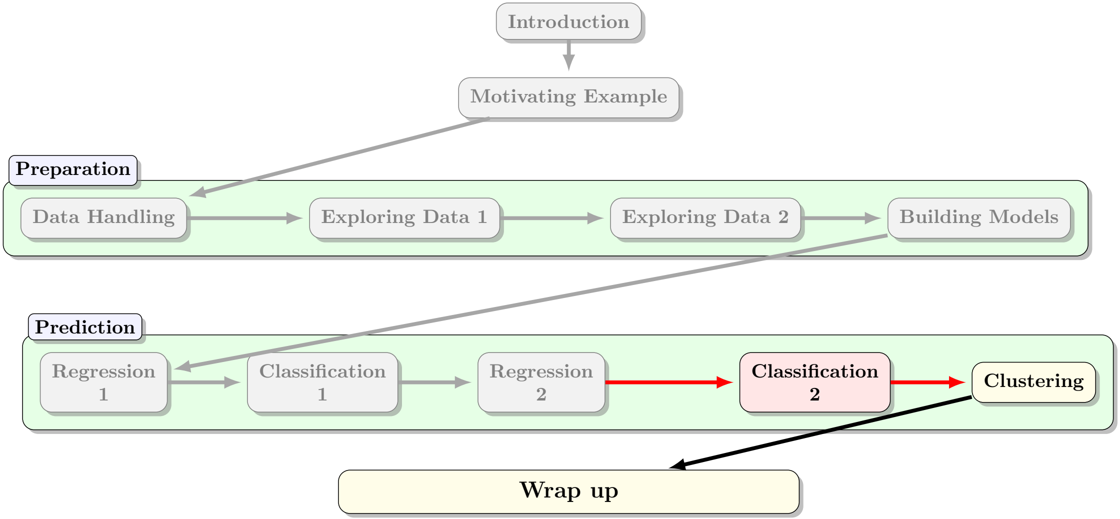
Autumn Semester, 2025

Outline

- How Decision Trees work
- How Decision Trees are used

Data Mining (Week 10)



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

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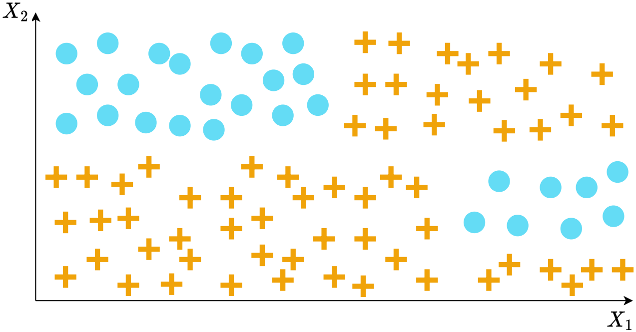
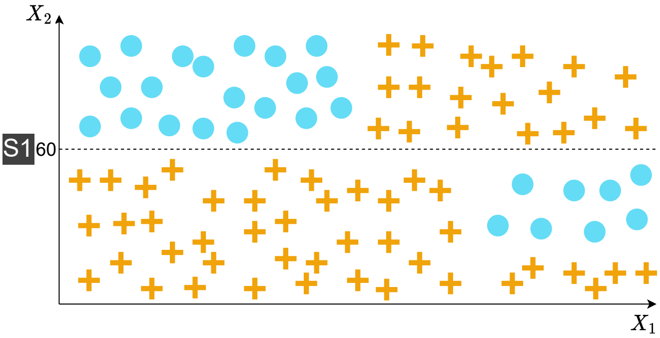
- the algorithm proceeds top-down from the root (all data), recursively generating rules as it goes
- Prediction is simple: the rules are applied along the path from root to leaf. The predicted class value is either the most frequent value at the leaf, or the leaf's probability vector.

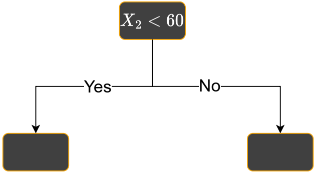
Classification tree: Example Data



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

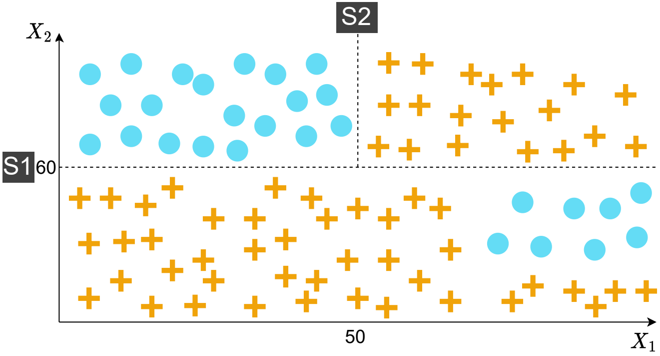
Classification tree: Example Data - First Split

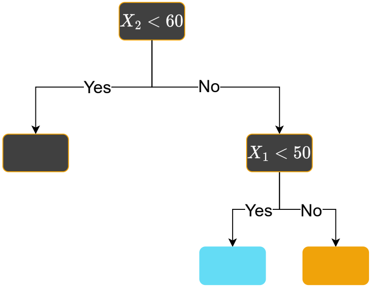




First split is on X_2; purity is improved (less mixing in each subset)

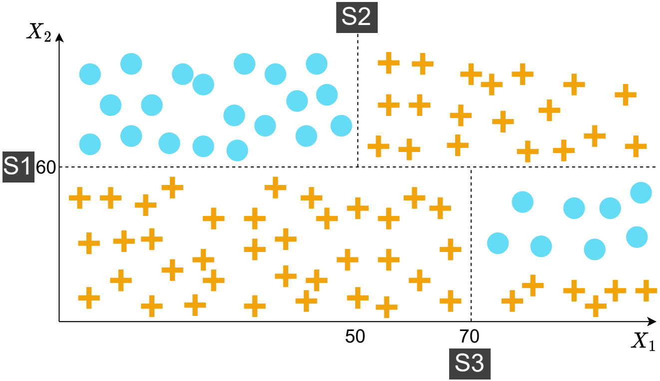
Classification tree: Example Data - Second Split

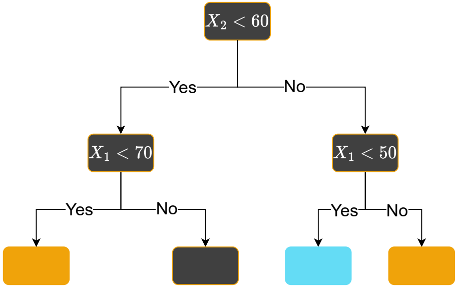




Second split is on X_1 so one region is pure (all blue disks) - can continue.

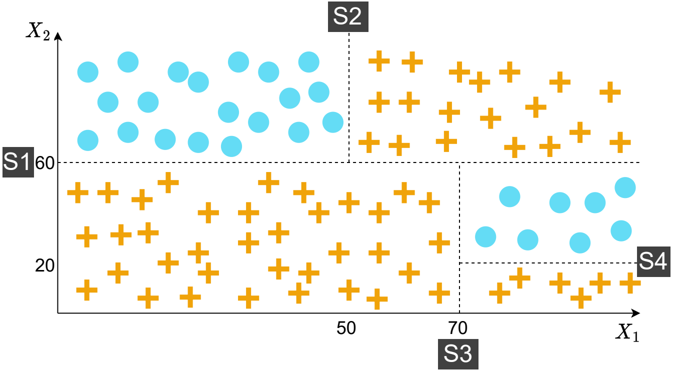
Classification tree: Example Data - Third Split

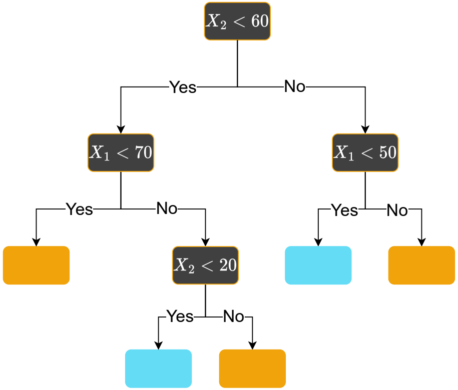




Third split on X_1 adds two extra pure regions.

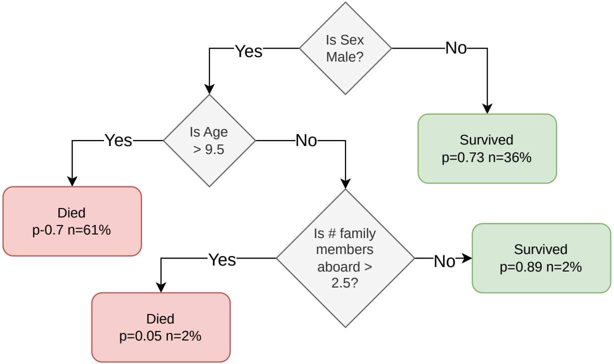
Classification tree: Example Data - Fourth Split





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.

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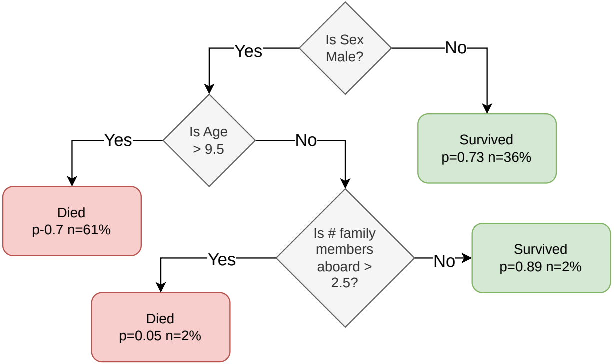

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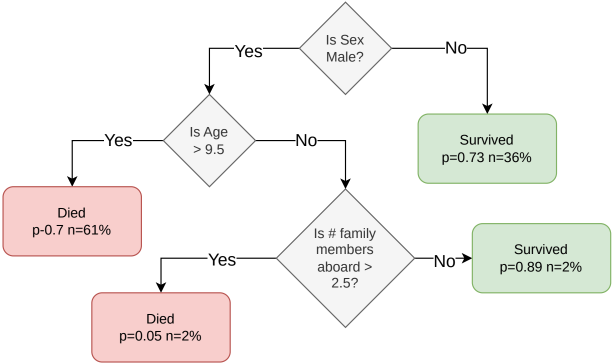

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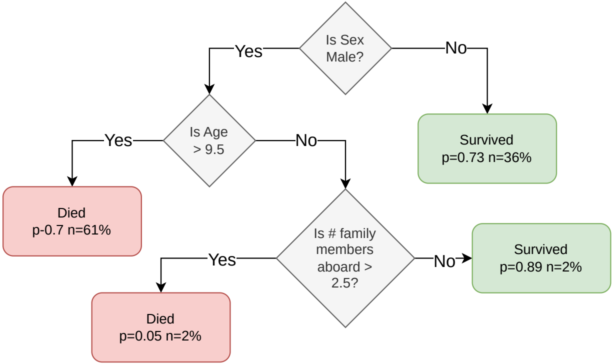

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- Leaf colour indicates p(survival) ≈ 1 (green) or p(survival) ≈ 0 (red)

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  - For each candidate split

Information Entropy: intuition

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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

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

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!

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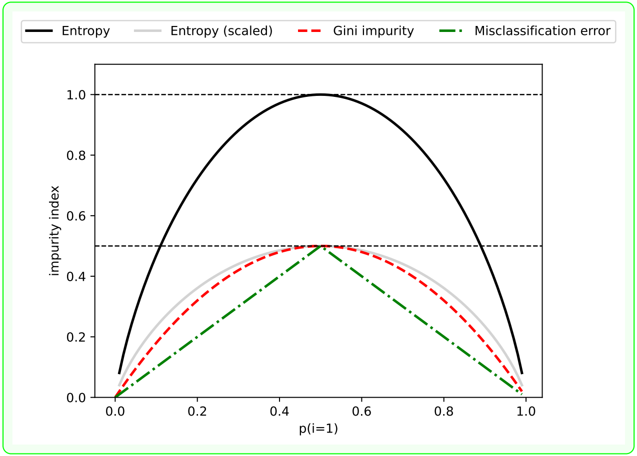
A decision tree recursively partitions a set so as to increase the purity (equivalently: reduce the mixing) of the set of observations X at each node as we move from the root to the leaves.

Classification tree metrics for rule building



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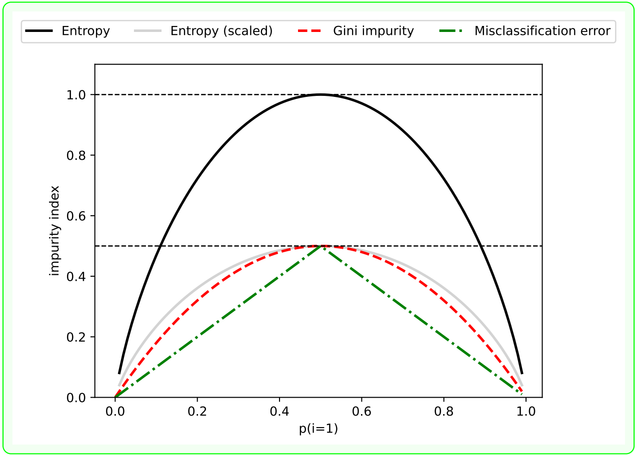

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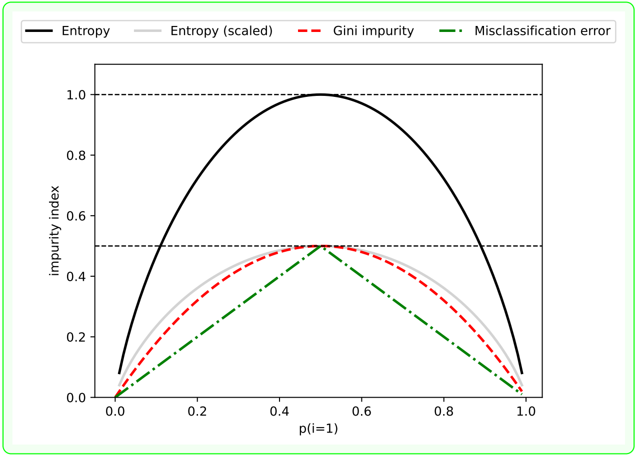

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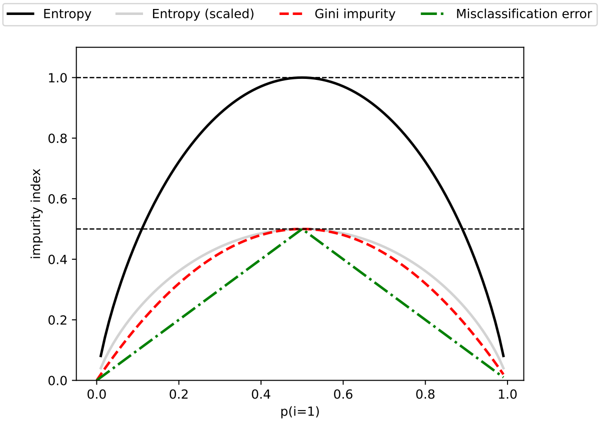

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- We wish to minimise this entropy.

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- 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.

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- 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.

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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
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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))

$$
\begin{aligned}
H(\text{play}) &= -\left(p(\text{play} = \text{yes}) \log_2 p(\text{play} = \text{yes}) + p(\text{play} = \text{no}) \log_2 p(\text{play} = \text{no})\right) \\
&= H_{9,5} \\
&= -\left(\frac{9}{14} \log_2\left(\frac{9}{14}\right) + \frac{5}{14} \log_2\left(\frac{5}{14}\right)\right) \approx 0.94
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$$\begin{aligned} H(\text{play},\text{outlook}) &= p(\text{outlook}=\text{sunny})H(\text{play}\&(\text{outlook}=\text{sunny})) + \dots \\ &= p(\text{outlook}=\text{sunny})H_{3,2} + p(\text{outlook}=\text{overcast})H_{4,0} + \dots \\ &\approx \frac{5}{14}0.97 + \frac{4}{14}0 + \frac{5}{14}0.97 \\ &\approx 0.69 \end{aligned}$$

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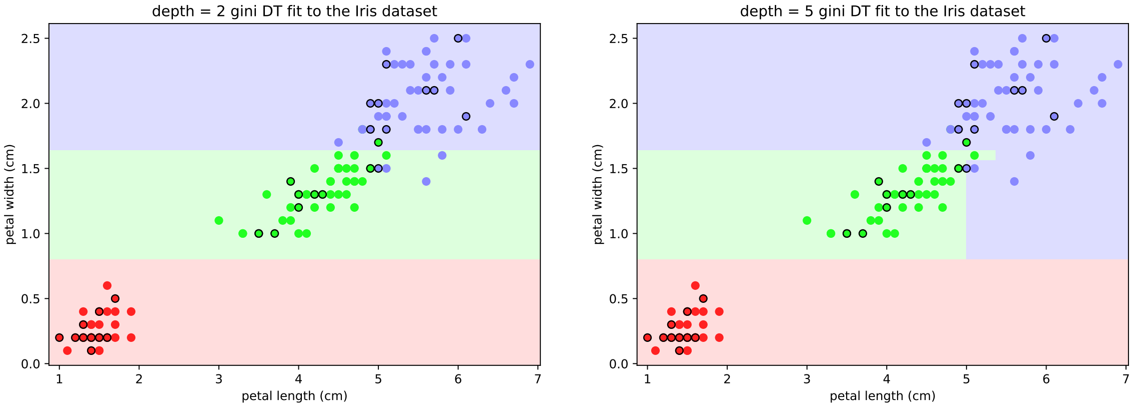
When growing decision trees, at a given node we search over the attributes for splitting, and choose the one that gives the maximum information gain, until we reach a leaf, which has an entropy of zero.

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.

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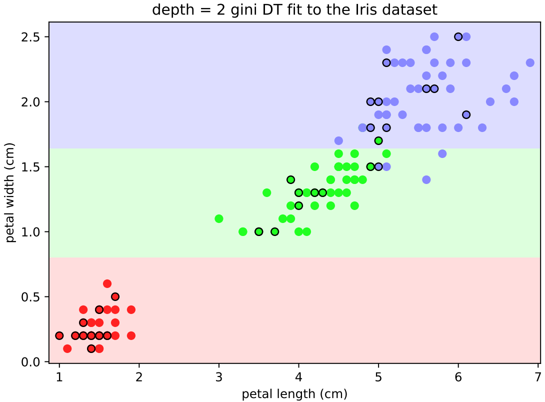

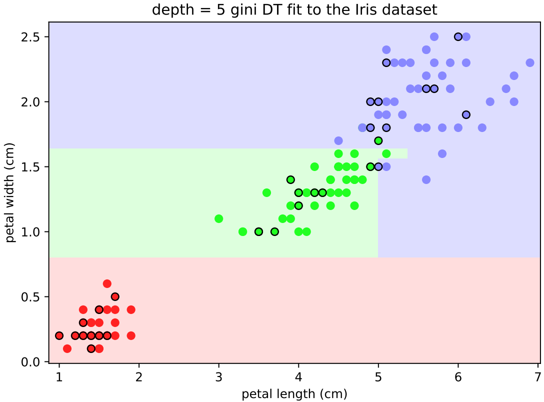

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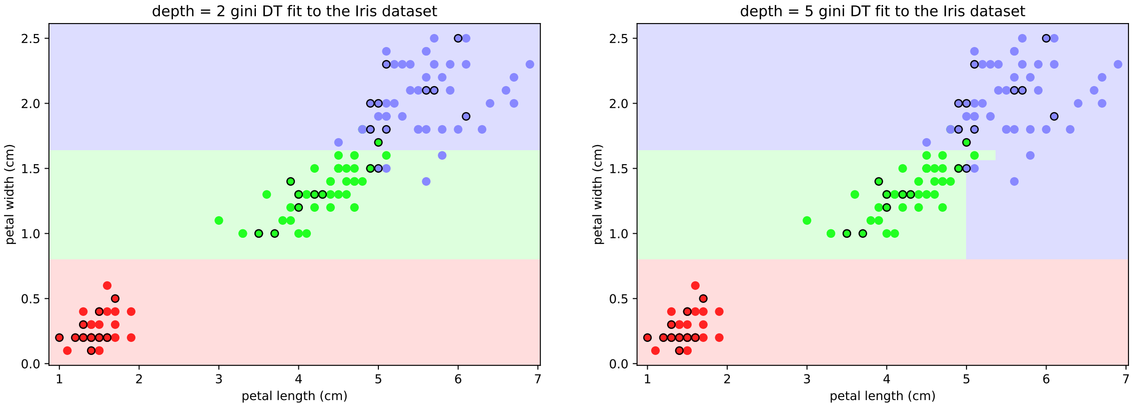

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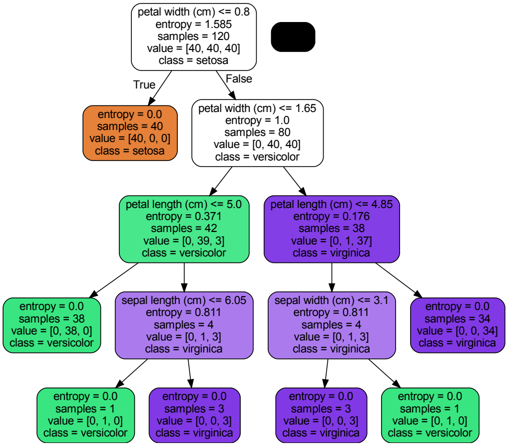
The choice of metric (Gini impurity or Information Gain) makes only slight changes to fit.

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*.
- Also, the maximum entropy occurs at the root, where there are 40 of each of the 3 species, resulting in entropy = $\log_2(3)$.



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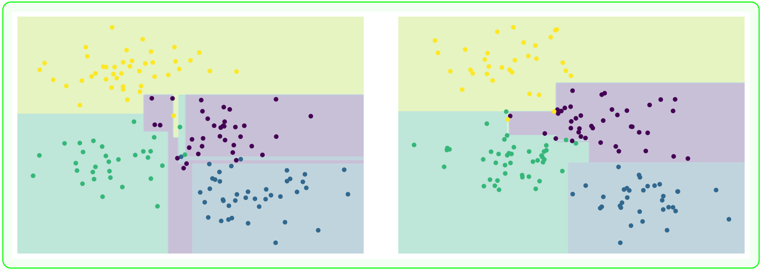
Python can extract paths from the root to each leaf as a set of if-then-else rules, to explain decisions.

Be careful of overfitting. . .



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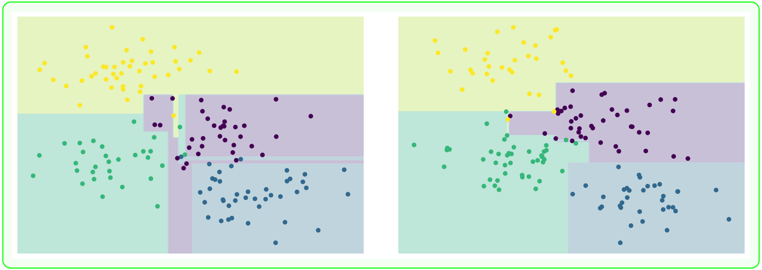

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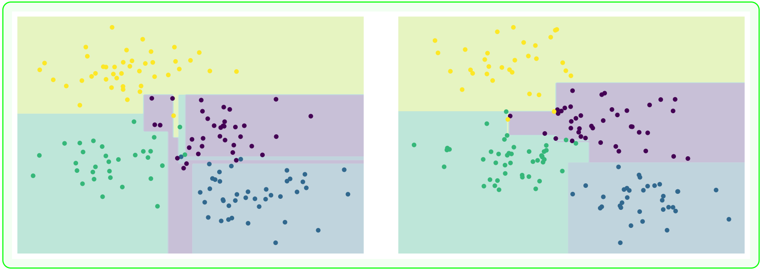

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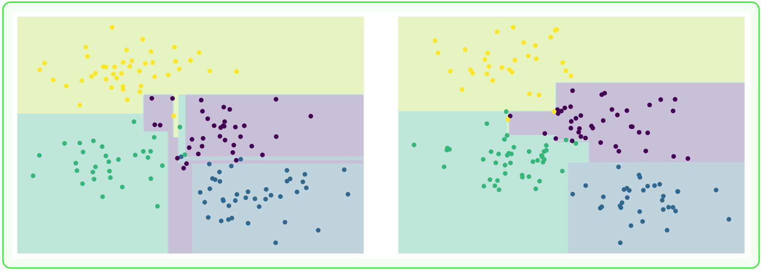

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- The resulting decision trees look very different, especially in the middle.
- This sensitivity to the noise in the data is characteristic of *overfitting* (high variance).
- Control by a) limiting depth or b) limiting number of leaves.

Classification trees in python

```python
criterion = "entropy"
treeDepth = 5
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.

Classification Trees - summary

- Classification trees learn recursive feature splits to predict categorical targets
- After training, they are relatively easy to use and to interpret (white-box, not black-box)
- Use stopping criteria (e.g., max depth of tree) to control bias and variance: e.g., early stopping results in shallower trees, resulting in higher bias and lower variance
- The goal is to maximise the purity in the leaves, as measured by the *entropy* of the distribution of the target class labels at each leaf.
- This *entropy at each leaf* is related, but different to, the *cross-entropy of the classifier model* (not just the leaves)
    - A parent node is split into children if the sum of their entropy scores is less than the entropy of the parent node. This occurs when the child nodes have less mixing of labels and so are more pure.
    - Each leaf node takes its predicted value (of the target) from the majority class label of the subset of training observations resulting in that node.
    - Cross-entropy loss measures the difference between the distributions of the true and predicted targets and can be calculated for any classifier.
- Classification tree "stumps" are commonly used as base models in ensemble techniques like bagging, boosting and stacking. For example, RandomForest models combine large numbers of classification trees using *bagging* and use random feature selection per base model.