Decision Trees

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DATA 2010–Tools and Techniques in Data Science

Lecture Objectives

- Explain the decision tree algorithm.
- Fit decision trees in Python.
- Evaluate the model using different metrics.

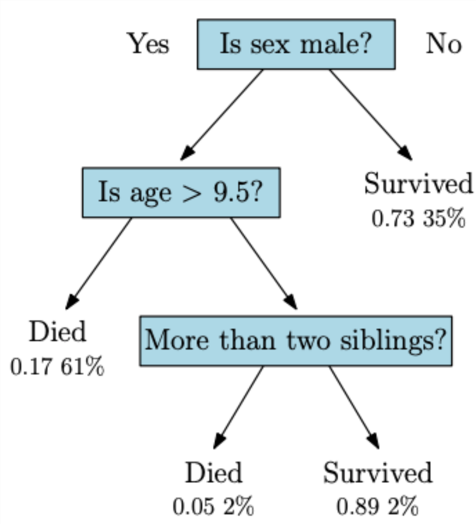
Motivation

- Last lecture, we discussed nearest neighbour classifiers.
    - Simple and sometimes powerful.
- To improve flexibility, we had to let go of interpretability.
    - We can't really tell which predictors are important.
- **Decision trees** are also very flexible, but they are more interpretable.

Decision Tree Classifiers i

- Let's consider the Titanic dataset, which contains several predictors:
    - Age and sex, how many siblings/parents a passenger had, which class they were in, whether they survived, etc.
- Given our knowledge of this tragedy, we can guess which variables are most important in predicting survival.
    - Women and children were more likely to survive.
    - First and second class were more likely to survive than third class and the crew.
    - Etc.
- These guesses could be encoded in a **decision tree**.

Decision Tree Classifiers ii



Decision Tree Classifiers iii

- Decision trees are binary trees (i.e. each node splits into two branches).
- Each node corresponds to a predicate (i.e. something that is either TRUE or FALSE) involving a *single* predictor.
- Each leaf corresponds to a single class.
- Starting from the root (i.e. the first node), we classify an observation by evaluating each predicate in succession until we reach a leaf. The class associated with this leaf is the prediction.

Properties

- Decision trees are really easy to interpret.
- They can model complex relationships between the target and the features.
- They easily account for categorical variables.
    - Ordinal (e.g. "Was the customer somewhat or extremely satisfied?")
    - Nominal (e.g. "Is the blood type A+ or A-?")

Non-Linear Relationships i

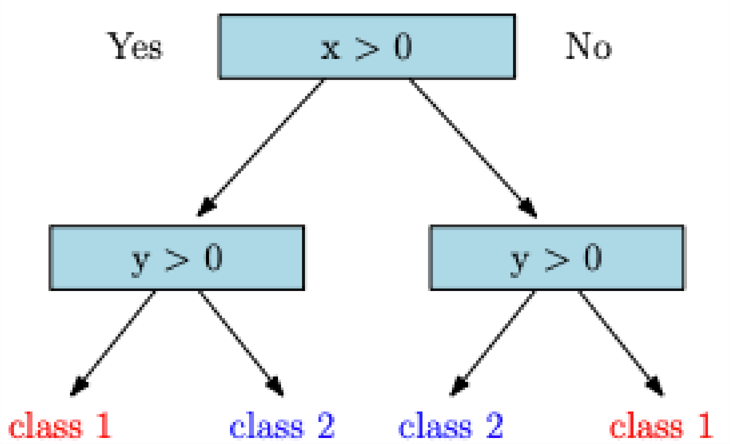
- Consider the following picture of a binary classification with two features.
- The data appears in four clusters, in each of the four quadrants of the plane, with opposite quadrants representing the same class.
    - This is also known as the *Exclusive OR* (XOR) classification problem.

Non-Linear Relationships ii

Non-Linear Relationships iii

- There is no way to draw a line that will perfectly classify this dataset.
- Similarly, logistic regression will also fail.
- On the other hand, it is very easy to construct a decision tree with perfect classification.

Non-Linear Relationships iv



- In fact, decision trees are known to be **universal approximators**, meaning they can approximate any smooth function to an arbitrary level of precision.
  - But keep in mind the bias-variance trade-off!

Fitting decision trees

- You can certainly build a decision tree from first principles.
    - Very common in medical sciences.
- But this is a data science course, so we will build them using training data.
- The general idea is to create a tree where each leaf is as pure as possible.
    - I.e. the only training data points reaching a given leaf have the same class.
- At the same time, we want to create balanced trees.
    - I.e. when we split a node, there should roughly be the same number of observations in each branch.
- We will quantify these two concepts using **entropy** and **information gain**.

Entropy i

- Let S be the subset of data at a particular node.
- Let f_k be the proportion of observations in S that are of class C_k, for $k = 1, \ldots, K$.
- The entropy is defined as

$$H(S) = -\sum_{k=1}^{K} f_k \log(f_k).$$

- **Note**: Different applications use different bases for the logarithm. We will use the natural logarithm, as is common in statistics.

Entropy ii

- A few observations:
  - Since $f_k \leq 1$, we have $\log(f_k) \leq 0$, which means $H(S) \geq 0$.
  - If $f_k = 0$ or $f_k = 1$, we have $f_k \log(f_k) = 0$. Therefore, if all observations are in a single class, we have $H(S) = 0$.
  - If all observations are equally distributed among the K classes, we have the following result:

Entropy iii

$$
\begin{aligned}
H(S) &= -\sum_{k=1}^{K} f_k \log(f_k) \\
&= -\sum_{k=1}^{K} \frac{1}{K} \log\left(\frac{1}{K}\right) \\
&= \log\left(K\right).
\end{aligned}
$$

- In decision trees, we want to minimize the entropy at each node.

Exercise

Assume we have 13 positive and 87 negative observations. Compute the entropy of this dataset, and compare it to the maximum entropy for two classes.

Solution

```
props <- c(13/100, 87/100)

-sum(props * log(props))
```

```
## [1] 0.3863867
```

```
# Compare to maximum
log(2)
```

```
## [1] 0.6931472
```

Information Gain

- The goal is therefore to find a predicate p that will maximize the drop in entropy.
- Suppose p separates the set S into two disjoint sets S_1, S_2.
- We define the **information gain** as follows:

$$IG_p(S) = H(S) - \sum_{j=1}^{2} \frac{|S_j|}{|S|} H(S_j).$$

- For each node, we look through **all** potential predicates to find the one that maximizes the information gain. That predicate is then used to split the node.

Exercise

Assume our 13 positive and 87 negative observations can be further broken down as follows:

	Positive	Negative
Male	8	22
Female	5	65

What is the information gain when splitting the dataset using the covariates "Sex"?

Solution i

```
props <- c(13/100, 87/100)
props_m <- c(8/30, 22/30)
props_f <- c(5/70, 65/70)

entropy_full <- -sum(props * log(props))
entropy_male <- -sum(props_m * log(props_m))
entropy_fem <- -sum(props_f * log(props_f))

c(entropy_full, entropy_male, entropy_fem)
```

```
## [1] 0.3863867 0.5799152 0.2573186
```

Solution ii

```
entropy_full - (29/100)*entropy_male -
    (71/100)*entropy_fem
```

```
## [1] 0.03551507
```

Stopping Rule

- We now have a way to grow a tree:
    - At each leaf, choose the predicate that maximizes the information gain.
- But we also need a **stopping rule**: when do we stop growing the tree?
- There are two main strategies:
    - Fix a tolerance level $\epsilon > 0$. If you can't find a predicate with information gain $IG_p(S) > \epsilon$, stop growing the tree.
    - Fix a positive integer D. Stop growing the tree once you've reached a depth D or if each leaf is pure (i.e. all observations from the same class).
- In practice, people usually use the second approach, and then prune the tree using another algorithm (details omitted).

Regression Trees

- Trees can also be used for regression.
- **Main idea**: Use the average outcome of all training observations at a leaf as the predicted value.
- Instead of maximizing the information gain, we look for a predicate that minimizes the Sum of Squares of Errors (SSE).

$$SSE = \sum_{y \in S_1} (y - \bar{y}_1)^2 + \sum_{y \in S_2} (y - \bar{y}_2)^2,$$

where $\bar{y}_j$ is the average outcome for the training observations in the subset S_j.

Final Comments

- Other splitting criterion can be used, and none are optimal.
    - Gini impurity, variance reduction, positive correctness, etc.
- Small trees may miss important aspects of the data, while large trees may overfit.
    - Bias-variance trade-off!
- When we have many covariates, finding the optimal predicate can be computationally expensive.
    - Same thing if a categorical variable has many levels.
- Two general strategies can be used to address these issues:
    - Bagging (next lecture)
    - Boosting