Lecture 14: Decision trees

Reading: Section 9.2

GU4241/GR5241 Statistical Machine Learning

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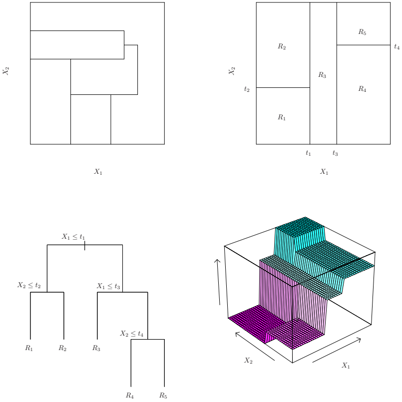
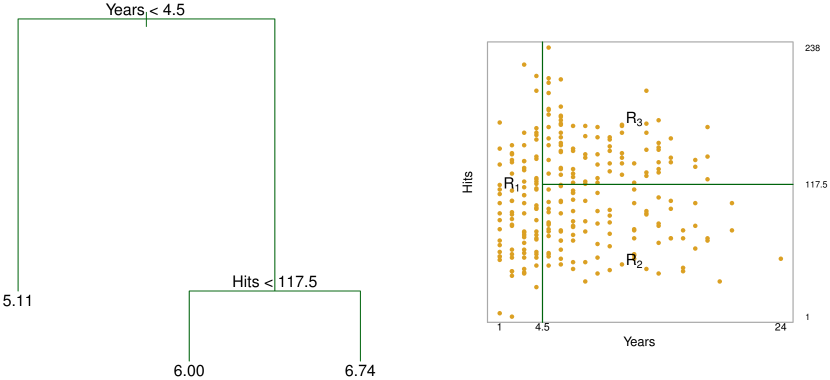
Decision trees, 10,000 foot view



1. Find a partition of the space of predictors.
2. Predict a constant in each set of the partition.
3. The partition is defined by splitting the range of one predictor at a time.

   $\rightarrow$ Not all partitions are possible.

Example: Predicting a baseball player's salary



The prediction for a point in R_i is the average of the training points in R_i.

How is a decision tree built?

- Start with a single region R_1, and iterate:

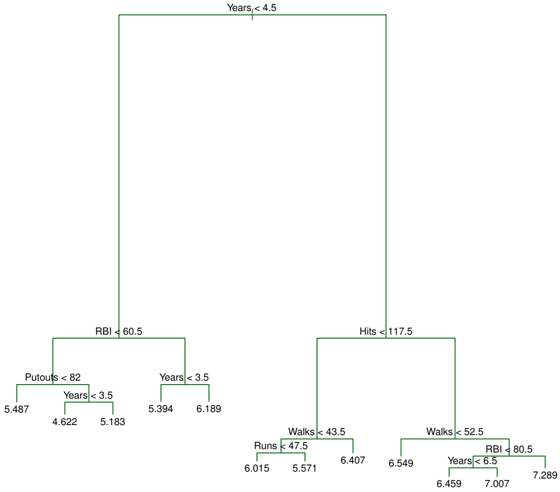
  1. Select a region R_k, a predictor X_j, and a splitting point s, such that splitting R_k with the criterion $X_j < s$ produces the largest decrease in RSS:

  $$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \bar{y}_{R_m})^2$$

  2. Redefine the regions with this additional split.

- Terminate when there are 5 observations or fewer in each region.
- This grows the tree from the root towards the leaves.

How is a decision tree built?



How do we control overfitting?

- **Idea 1:** Find the optimal subtree by cross validation.

  $\rightarrow$ There are too many possibilities, so we would still over fit.

- **Idea 2:** Stop growing the tree when the RSS doesn't drop by more than a threshold with any new cut.

  $\rightarrow$ In our greedy algorithm, it is possible to find good cuts after bad ones.

How do we control overfitting?

- **Cost complexity pruning:**
  - Solve the problem:

$$\text{minimize} \sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \bar{y}_{R_m})^2 + \alpha |T|.$$

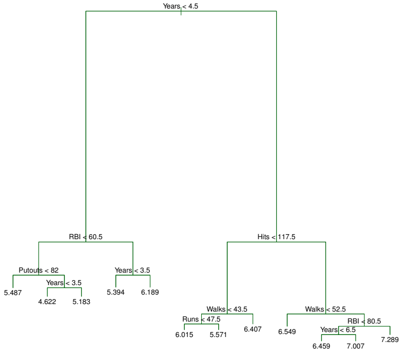
  - When $\alpha = \infty$, we select the null tree.
  - When $\alpha = 0$, we select the full tree.
  - The solution for each α is among $T_1, T_2, \ldots, T_m$ from weakest link pruning.
  - Choose the optimal α (the optimal T_i) by cross validation.

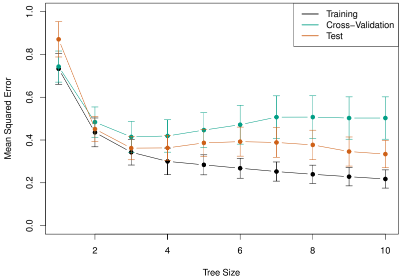
Cross validation

1. Split the training points into 10 folds.
2. For $k = 1, \ldots, 10$, using every fold except the kth:
   - Construct a sequence of trees $T_1, \ldots, T_m$ for a range of values of α, and find the prediction for each region in each one.
   - For each tree T_i, calculate the RSS on the test set.
3. Select the parameter α that minimizes the average test error.

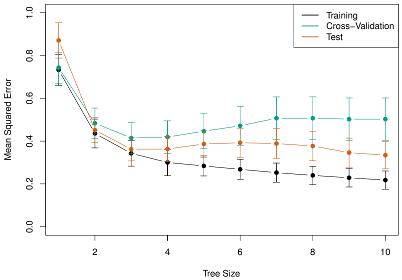
Note: We are doing all fitting, **including the construction of the trees**, using only the training data.

Example. Predicting baseball salaries





Example. Predicting baseball salaries



Classification trees

- They work much like regression trees.
- We predict the response by **majority vote**, i.e. pick the most common class in every region.
- Instead of trying to minimize the RSS:

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \bar{y}_{R_m})^2$$

we minimize a classification loss function.

Classification losses

- The 0-1 loss or misclassification rate:

$$\sum_{m=1}^{|T|} q_m \sum_{x_i \in R_m} \mathbf{1}(y_i \neq \hat{y}_{R_m})$$

- The Gini index:

$$\sum_{m=1}^{|T|} q_m \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}),$$

  where $\hat{p}_{m,k}$ is the proportion of class k within R_m, and q_m is the proportion of samples in R_m.

- The cross-entropy:

$$-\sum_{m=1}^{|T|} q_m \sum_{k=1}^{K} \hat{p}_{mk} \log(\hat{p}_{mk}).$$

Classification losses

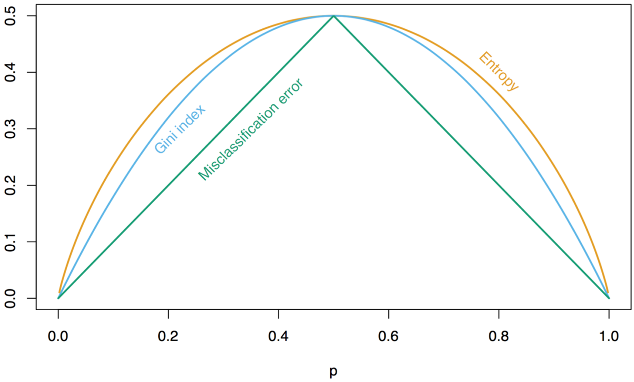


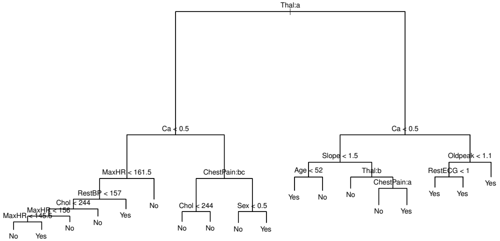
Figure: Node impurity measures for two-class classification

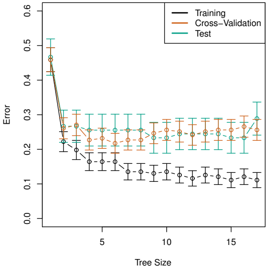
Classification losses

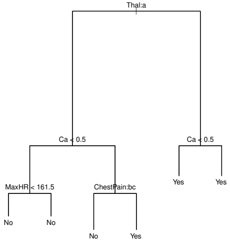
- The Gini index and cross-entropy are better measures of the purity of a region, i.e. they are low when the region is mostly one category.
- **Motivation for the Gini index:**

  If instead of predicting the most likely class, we predict a random sample from the distribution $(\hat{p}_{1,m}, \hat{p}_{2,m}, \ldots, \hat{p}_{K,m})$, the Gini index is the expected misclassification rate.
- It is typical to use the Gini index or cross-entropy for growing the tree, while using the misclassification rate when pruning the tree.

Example. Heart dataset.







Some advantages of decision trees

- Very easy to interpret!
- Closer to human decision-making.
- Easy to visualize graphically.
- They easily handle qualitative predictors and missing data.

Classification and Regression trees, in a nut shell

- Grow the tree by recursively splitting the samples in the leaf R_i according to $X_j > s$, such that (R_i, X_j, s) maximize the drop in RSS.

  $\rightarrow$ Greedy algorithm.

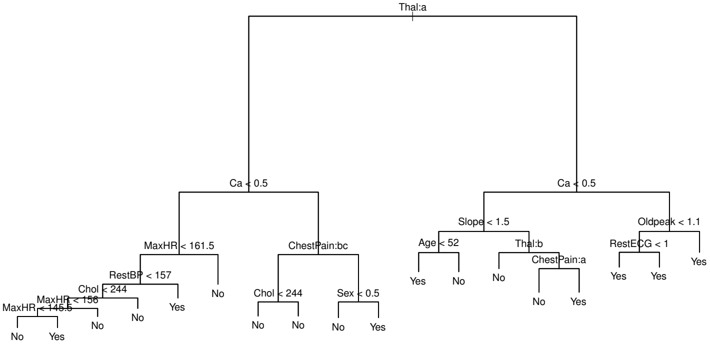
- Create a sequence of subtrees $T_0, T_1, \ldots, T_m$ using a **pruning** algorithm.

- Select the best tree T_i (or the best α) by cross validation.

  $\rightarrow$ Why might it be better to choose α instead of the tree T_i by cross-validation?

Example. Heart dataset.

How do we deal with categorical predictors?



Categorical predictors

- If there are only 2 categories, then the split is obvious. We don't have to choose the splitting point s, as for a numerical variable.
- If there are more than 2 categories:
  - Order the categories according to the average of the response:

    $$\texttt{ChestPain}:\texttt{a} > \texttt{ChestPain}:\texttt{c} > \texttt{ChestPain}:\texttt{b}$$

  - Treat as a numerical variable with this ordering, and choose a splitting point s.
- One can show that this is the optimal way of partitioning.

Missing data

- Suppose we can assign every sample to a leaf R_i despite the missing data.
- When choosing a new split with variable X_j (growing the tree):
  - Only consider the samples which have the variable X_j.
  - In addition to choosing the best split, choose a second best split using a different variable, and a third best, ...
- To propagate a sample down the tree, if it is missing a variable to make a decision, try the second best decision, or the third best, ...