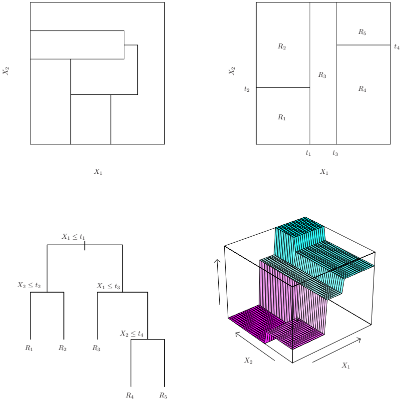
Lecture 8: Decision trees

Reading: Section 8.1

STATS 202: Data mining and analysis

Rajan Patel

Decision trees, 10,000 foot view



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2. Predict a constant in each set of the partition.

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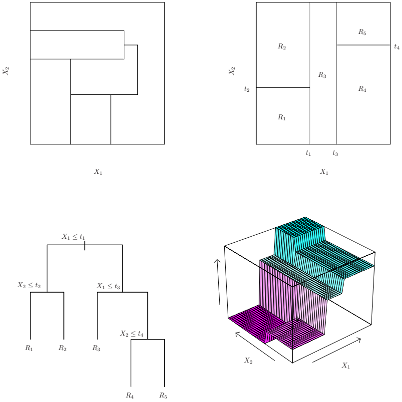

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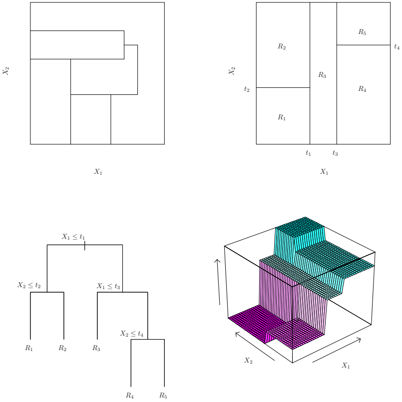

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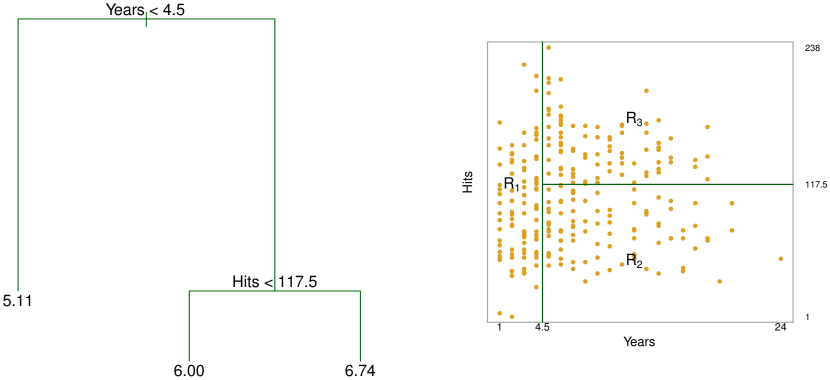
   $\rightarrow$ Not all partitions are possible.

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:

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

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

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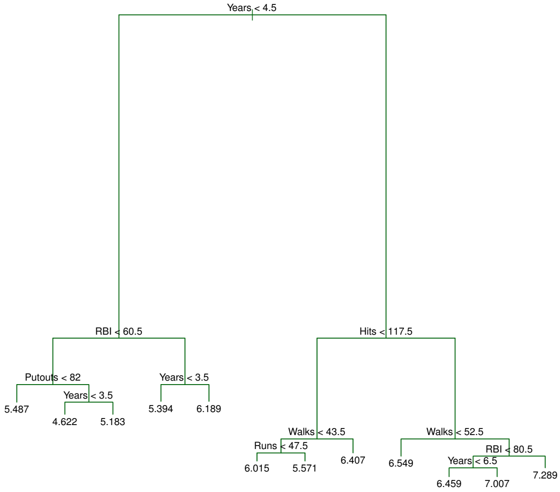

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  $\rightarrow$ In our greedy algorithm, it is possible to find good cuts after bad ones.

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  - Choose the optimal α (the optimal T_i) by cross validation.

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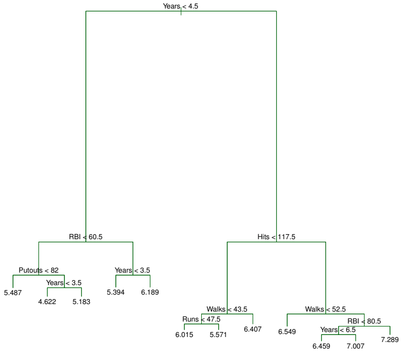
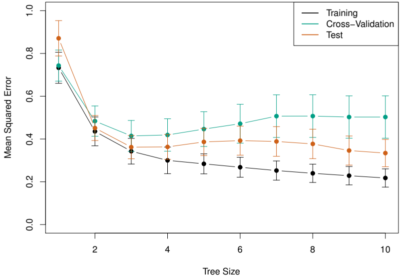
Note: We are doing all fitting, **including the construction of the trees**, using only the training data.

Example. Predicting baseball salaries





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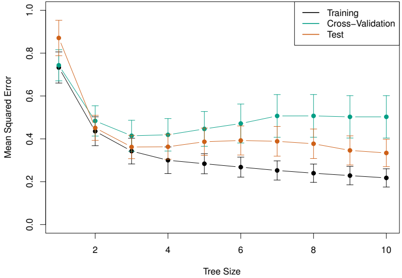

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- We predict the response by **majority vote**, i.e. pick the most common class in every region.
- Instead of trying to minimize the RSS:

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

we minimize a classification loss function.

Classification losses

- The 0-1 loss or misclassification rate:

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

- 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:

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

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- **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.

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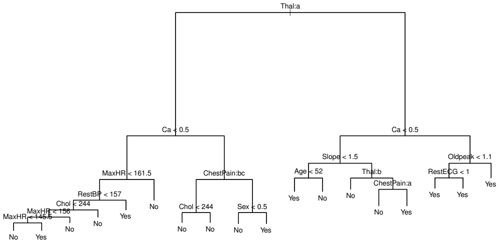
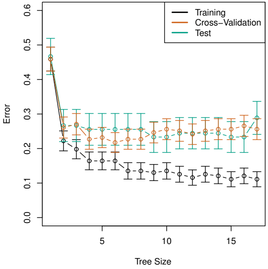
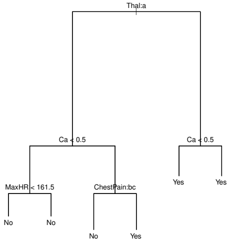
- It is typical to use the Gini index or cross-entropy for growing the tree, while using the misclassification rate when pruning the tree.

Example. Heart dataset.







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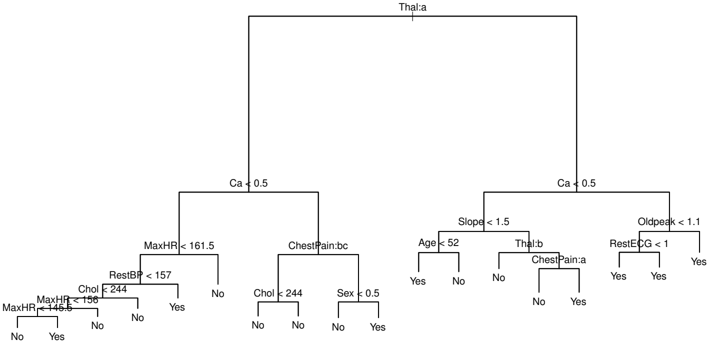
- Easy to visualize graphically.
- They easily handle qualitative predictors and missing data.

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.
- This is the optimal way of partitioning.

Missing data

Problem: If a sample is missing variable X_j, and a tree contains a split according to $X_j > s$, then we may not be able to assign the sample to a region.

Solution:

- 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, ...

Bagging

- Bagging = Bootstrap Aggregating
- In the Bootstrap, we replicate our dataset by sampling with replacement:
  - Original dataset: $\mathtt{x} = \mathtt{c}(\mathtt{x1}, \mathtt{x2}, \ldots, \mathtt{x100})$
  - Bootstrap samples:
    $\mathtt{boot1} = \mathtt{sample}(\mathtt{x}, 100, \mathtt{replace} = \mathtt{True})$, ...,
    $\mathtt{bootB} = \mathtt{sample}(\mathtt{x}, 100, \mathtt{replace} = \mathtt{True})$.
- We used these samples to approximate the Standard Error of a parameter estimate:

$$\mathsf{SE}(\hat{\beta}_1) \approx \mathsf{SD}(\hat{\beta}_1^{(1)}, \ldots, \hat{\beta}_1^{(B)})$$

Bagging

- In **Bagging** we average the predictions of a model fit to many Bootstrap samples.

  Example. Bagging the Lasso

  - Let $\hat{y}^{L,b}$ be the prediction of the Lasso applied to the bth bootstrap sample.
  - Bagging prediction:

$$\hat{y}^{\text{boot}} = \frac{1}{B} \sum_{b=1}^{B} \hat{y}^{L,b}.$$

When does Bagging make sense?

When a regression method or a classifier has a tendency to overfit, Bagging reduces the variance of the prediction.

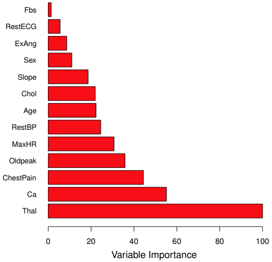
- When n is large, the empirical distribution is similar to the true distribution of the samples.
- Bootstrap samples are like independent realizations of the data.
- Bagging amounts to averaging the fits from many independent datasets, which would reduce the variance by a factor $1/B$.

Bagging decision trees

- **Disadvantage:** Every time we fit a decision tree to a Bootstrap sample, we get a different tree T^b.

  $\rightarrow$ Loss of interpretability

- For each predictor, add up the total amount by which the RSS (or Gini index) decreases every time we use the predictor in T^b.
- Average this total over each Boostrap estimate $T^1, \ldots, T^B$.



Out-of-bag (OOB) error

- To estimate the test error of a bagging estimate, we could use cross-validation.
- Each time we draw a Bootstrap sample, we only use 63% of the observations.
- **Idea:** use the rest of the observations as a test set.
- **OOB error:**
  - For each sample x_i, find the prediction $\hat{y}_i^b$ for all bootstrap samples b which do not contain x_i. There should be around $0.37B$ of them. Average these predictions to obtain $\hat{y}_i^{\text{oob}}$.
  - Compute the error $(y_i - \hat{y}_i^{\text{oob}})^2$.
  - Average the errors over all observations $i = 1, \ldots, n$.

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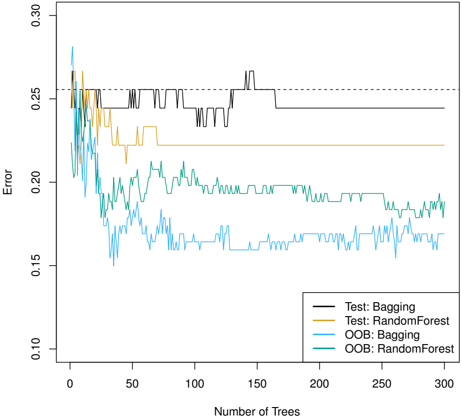


The test error decreases as we increase B
(dashed line is the error for a plain decision tree).

Random Forests

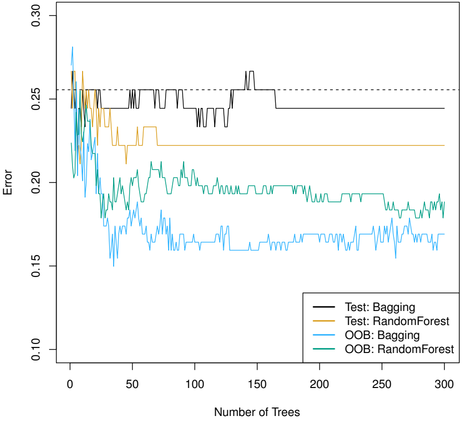
Bagging has a problem:

→ The trees produced by different Bootstrap samples can be very similar.

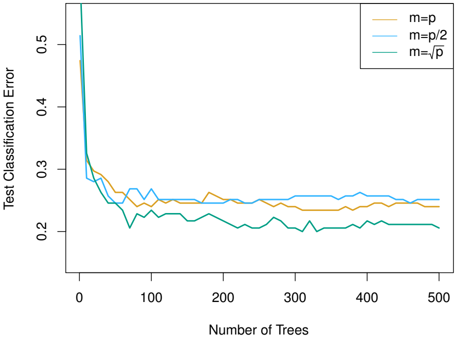
Random Forests:

- We fit a decision tree to different Bootstrap samples.
- When growing the tree, we select a random sample of $m < p$ predictors to consider in each step.
- This will lead to very different (or "uncorrelated") trees from each sample.
- Finally, average the prediction of each tree.

Random Forests vs. Bagging



Random Forests, choosing m



The optimal m is usually around $\sqrt{p}$,
but this can be used as a tuning parameter.