Lecture 20: Bagging, Random Forests, Boosting

Reading: Chapter 8

STATS 202: Data mining and analysis

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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.

  $\longrightarrow$ Greedy algorithm.

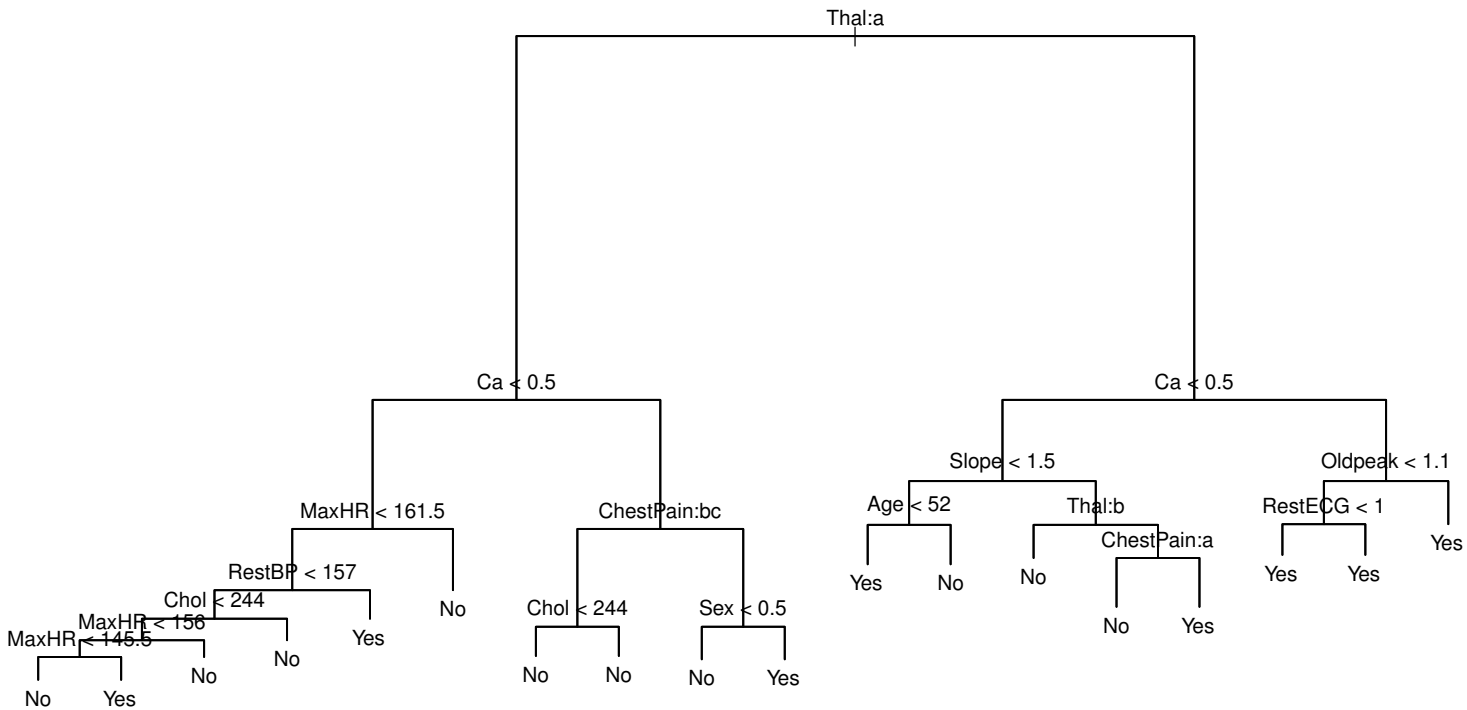
- Create a sequence of subtrees $T_0, T_1, \ldots, T_m$ using a **pruning** algorithm.

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

  $\longrightarrow$ 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, ...

Bagging

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

$$\mathsf{SE}(\hat{\beta}_1) \approx \frac{1}{B} \sum_{b=1}^{B} \hat{\beta}_1^{(b)}$$

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.

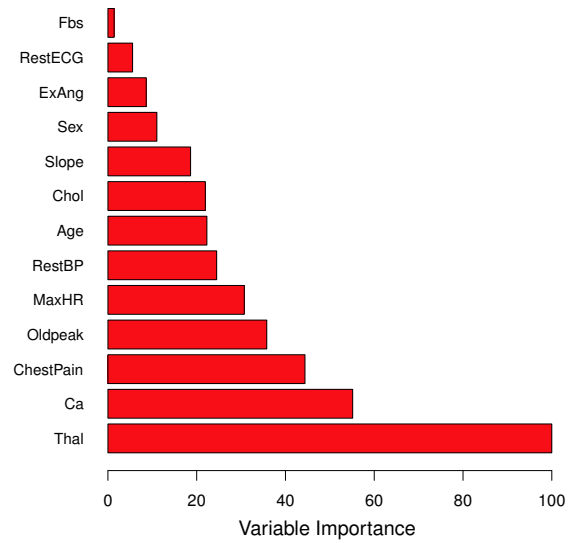
- When n is large, the empirical distribution is similar to the true distribution of the samples.
- Bootstrap samples are like independent realizations of the data.
- Bagging amounts to averaging the fits from many independent datasets, which would reduce the variance by a factor $1/B$.

Bagging decision trees

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

  $\longrightarrow$ Loss of interpretability

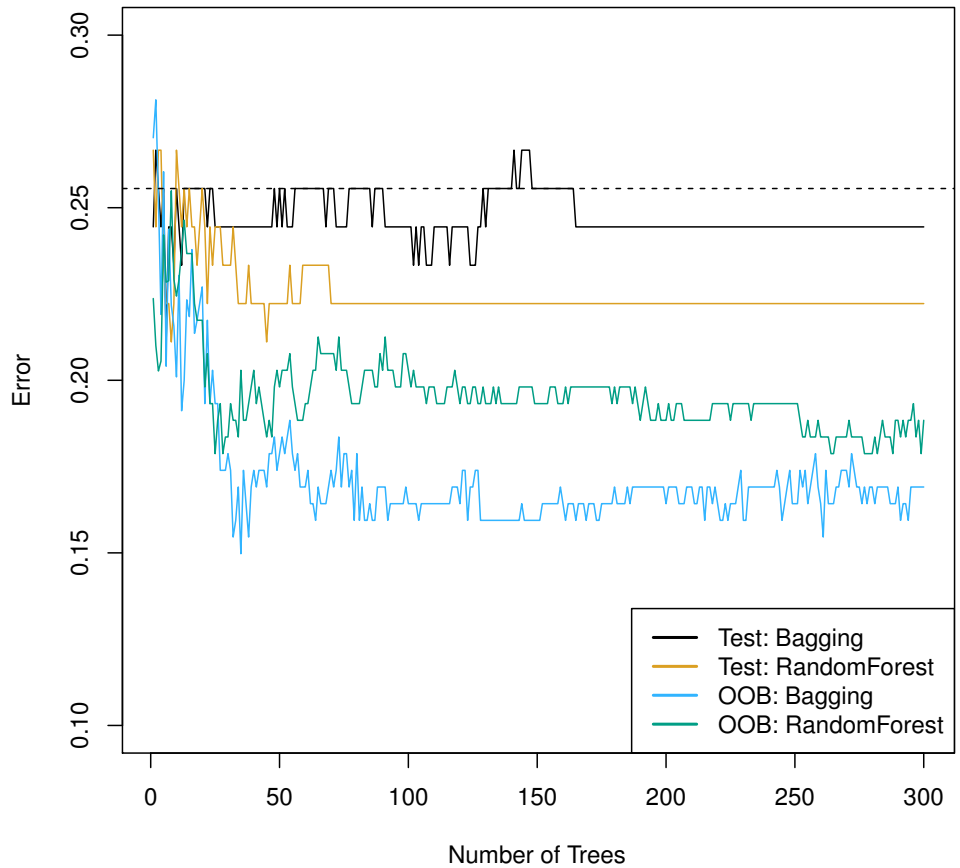
- For each predictor, add up the total amount by which the RSS (or Gini index) decreases every time we use the predictor in T^b.
- Average this total over each Boostrap estimate $T^1, \ldots, T^B$.



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 $i = 1, \ldots, n$.

Out-of-bag (OOB) error



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

Random Forests

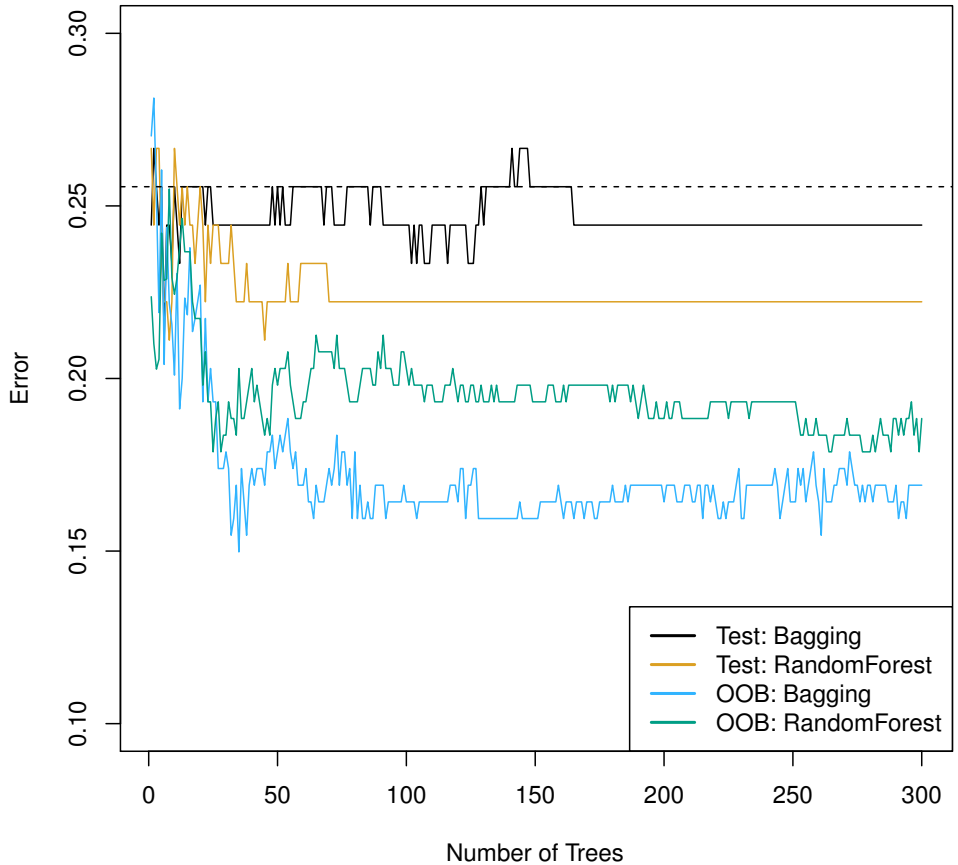
Bagging has a problem:

$\longrightarrow$ The trees produced by different Bootstrap samples can be very similar.

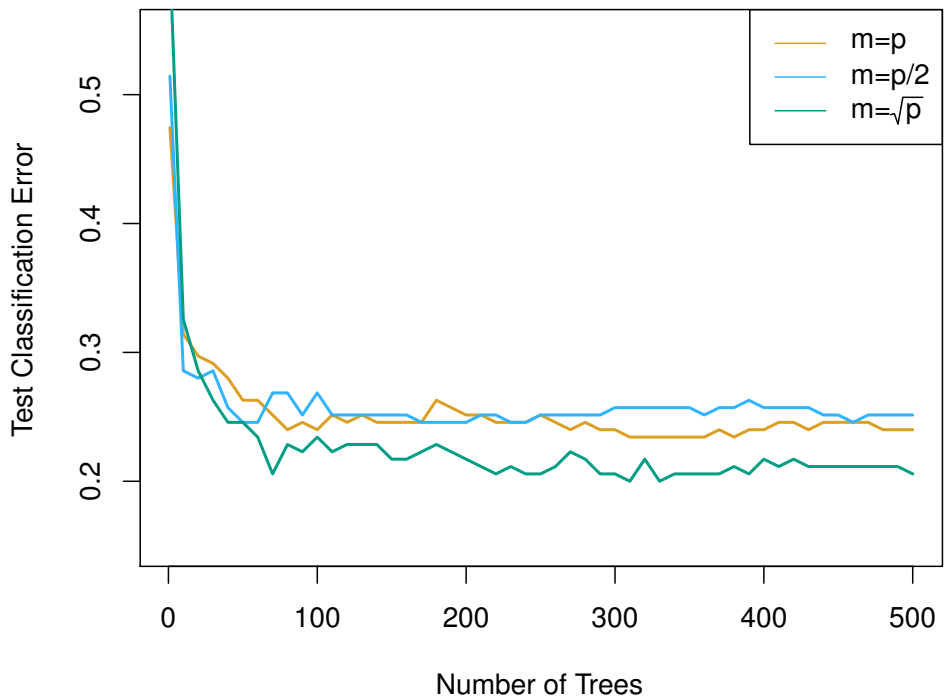
Random Forests:

- 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.

Boosting

1. Set $\hat{f}(x) = 0$, and $r_i = y_i$ for $i = 1, \ldots, n$.
2. For $b = 1, \ldots, B$, iterate:
   - 2.1 Fit a decision tree $\hat{f}^b$ with d splits to the response $r_1, \ldots, r_n$.
   - 2.2 Update the prediction to:

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$$

   - 2.3 Update the residuals,

$$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$$

3. Output the final model:

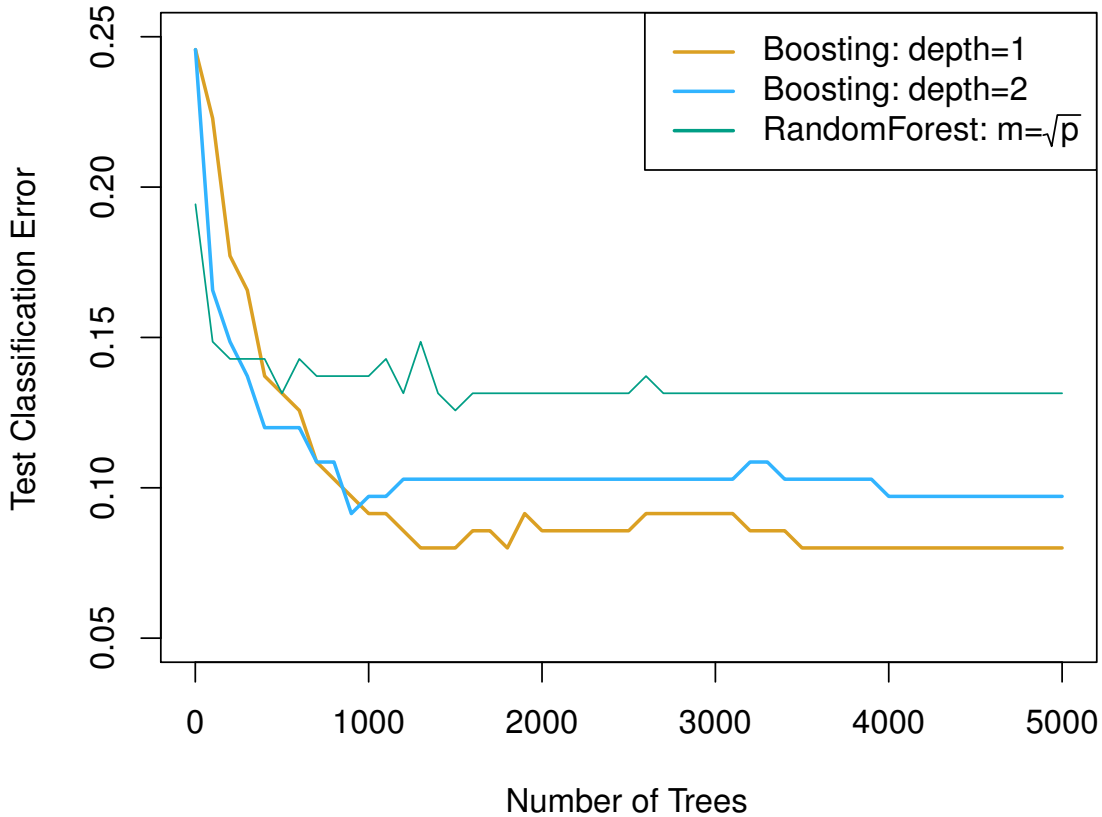
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$$

Boosting, intuitively

Boosting learns *slowly*:

We first use the samples that are easiest to predict, then slowly down weigh these cases, moving on to harder samples.

Boosting vs. random forests



The parameter $\lambda = 0.01$ in each case.
We can tune the model by CV using λ, d, B.