

# Lecture 9: Bagging, Random Forests, Boosting

Reading: Chapter 8

STATS 202: Data mining and analysis

Rajan Patel

Bagging = Bootstrap Aggregation

## Bagging = Bootstrap Aggregation

- ▶ Replicate the dataset by sampling with replacement.

## Bagging = Bootstrap Aggregation

- ▶ Replicate the dataset by sampling with replacement.
- ▶ We apply a learning method to each bootstrap replicate, to produce predictions  $\hat{f}^{(1)}, \dots, \hat{f}^{(B)}$ .

## Bagging = Bootstrap Aggregation

- ▶ Replicate the dataset by sampling with replacement.
- ▶ We apply a learning method to each bootstrap replicate, to produce predictions  $\hat{f}^{(1)}, \dots, \hat{f}^{(B)}$ .
- ▶ In Chapter 5, we were interested in the variability of these predictions:

$$\text{SE}(\hat{f}(x)) \approx \text{SD}(\hat{f}^{(1)}(x), \dots, \hat{f}^{(B)}(x)).$$

## Bagging = Bootstrap Aggregation

- ▶ Replicate the dataset by sampling with replacement.
- ▶ We apply a learning method to each bootstrap replicate, to produce predictions  $\hat{f}^{(1)}, \dots, \hat{f}^{(B)}$ .
- ▶ In Chapter 5, we were interested in the variability of these predictions:

$$\text{SE}(\hat{f}(x)) \approx \text{SD}(\hat{f}^{(1)}(x), \dots, \hat{f}^{(B)}(x)).$$

- ▶ Now, we will use the average of these predictions as an estimator with reduced variance:

$$\hat{f}^{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}^{(b)}(x)$$

## Bagging decision trees

- ▶ Replicate the dataset by sampling with replacement.

## Bagging decision trees

- ▶ Replicate the dataset by sampling with replacement.
- ▶ Fit a decision tree to each bootstrap replicate (growing the tree, and pruning).



## Bagging decision trees

- ▶ Replicate the dataset by sampling with replacement.
- ▶ Fit a decision tree to each bootstrap replicate (growing the tree, and pruning).
- ▶ **Regression:** To make a prediction for an input point  $x$ , average the predictions of all the trees:

$$\hat{f}^{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}^{(b)}(x)$$

## Bagging decision trees

- ▶ Replicate the dataset by sampling with replacement.
- ▶ Fit a decision tree to each bootstrap replicate (growing the tree, and pruning).
- ▶ **Regression:** To make a prediction for an input point  $x$ , average the predictions of all the trees:

$$\hat{f}^{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}^{(b)}(x)$$

- ▶ **Classification:** To make a prediction for an input point  $x_0$ , take the majority vote from the set of predictions:

$$\hat{y}_0^{(1)}, \dots, \hat{y}_0^{(B)}.$$

## Bagging decision trees

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

## Bagging decision trees

- ▶ **Disadvantage:** Every time we fit a decision tree to a Bootstrap sample, we get a different tree  $T^b$ .  
→ Loss of interpretability

## Bagging decision trees

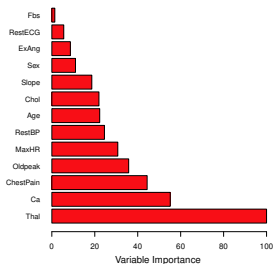
- ▶ **Disadvantage:** Every time we fit a decision tree to a Bootstrap sample, we get a different tree  $T^b$ .  
→ Loss of interpretability
- ▶ For each predictor, add up the total amount by which the RSS (or Gini index) decreases every time we use the predictor in  $T^b$ .

## Bagging decision trees

- ▶ **Disadvantage:** Every time we fit a decision tree to a Bootstrap sample, we get a different tree  $T^b$ .  
→ 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 Bootstrap estimate  $T^1, \dots, T^B$ .

## Bagging decision trees

- ▶ **Disadvantage:** Every time we fit a decision tree to a Bootstrap sample, we get a different tree  $T^b$ .  
→ 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 Bootstrap estimate  $T^1, \dots, T^B$ .



## Out-of-bag (OOB) error

- ▶ To estimate the test error of a bagging estimate, we could use cross-validation.



## 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.

## 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.

## 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  $\hat{y}_i^{\text{OOB}}$ .

## 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  $(y_i - \hat{y}_i^{\text{oob}})^2$ .

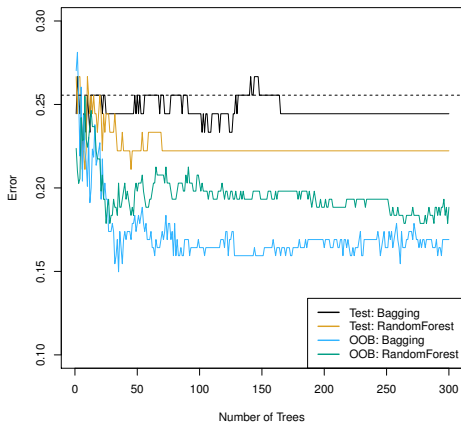
## Out-of-bag (OOB) error

- ▶ 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  $i = 1, \dots, n$ .

## 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  $i = 1, \dots, n$ .
- ▶ For  $B$  large, OOB error is virtually equivalent to LOOCV.

## 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:

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

**Random Forests:**



# 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.

# 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.

# 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.

# Random Forests

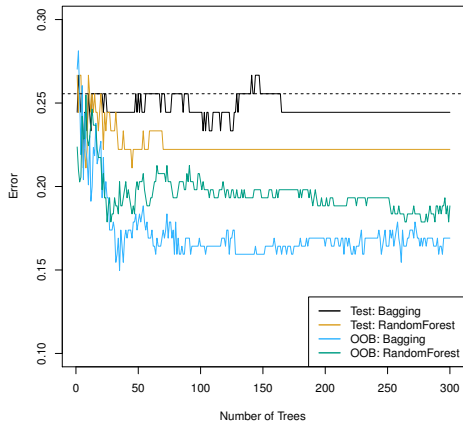
Bagging has a problem:

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

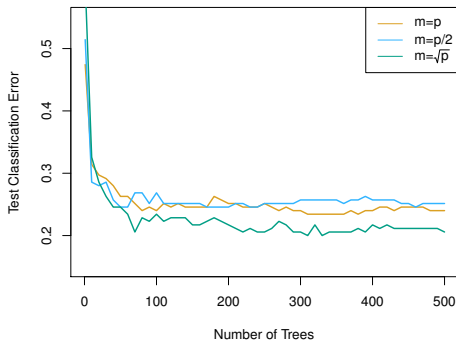
## Random Forests:

- ▶ 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.

# Boosting

# Boosting

1. Set  $\hat{f}(x) = 0$ , and  $r_i = y_i$  for  $i = 1, \dots, n$ .



# Boosting

1. Set  $\hat{f}(x) = 0$ , and  $r_i = y_i$  for  $i = 1, \dots, n$ .
2. For  $b = 1, \dots, B$ , iterate:

# Boosting

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

# Boosting

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

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

# Boosting

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

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

- 2.3 Update the residuals,

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

# Boosting

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

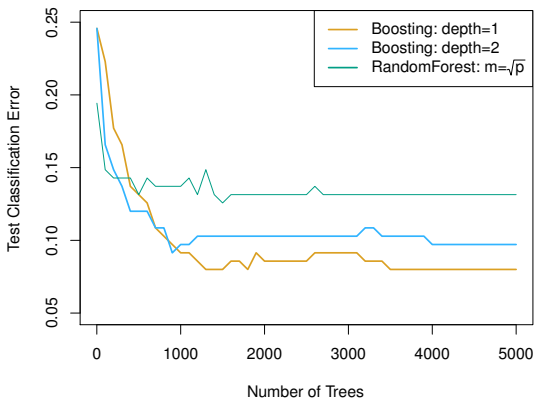
$$\hat{f}(x) = \sum_{b=1}^B \lambda \hat{f}^b(x).$$

## 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  $\lambda, d, B$ .