Bagging and Random Forests

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Math 243: Stat Learning

November 15th, 2021

Outline

In today's class, we will...

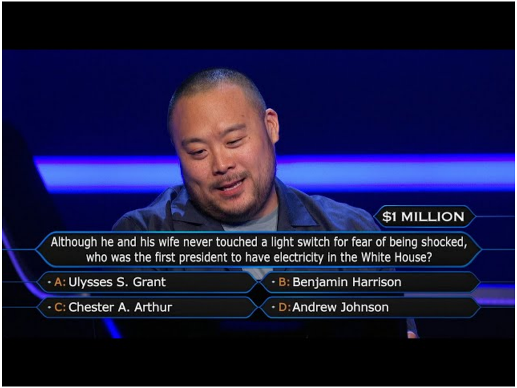
- Introduce ensemble modeling as means of improving low accuracy models
- Discuss bagging and random forests as methods for reducing variance in decision trees
- Implement random forests in R

Section 1

Ensemble Models

Who Wants to Be a Millionaire?

- *Who Wants to Be a Millionaire* is a television gameshow that debuted in the 1990s and in which contestants answer a series of increasingly difficult multiple choice questions in order to win the grand prize of $1,000,000.



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- The original show included 3 “lifeline” options contestants could use to answer questions:
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- Suppose we have m different models to predict Y based on $X_1, \ldots, X_n$. Suppose $\hat{Y}_i$ is the prediction made by the ith model.

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$$\hat{Y} = w_1 \hat{Y}_1 + \cdots + w_m \hat{Y}_m \qquad \text{where } w_1 + \ldots w_m = 1, \quad w_i \geq 0$$

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- Advantages of ensemble models?
  - Significantly more flexible than a single model
  - More efficient than single model
  - More resilient against model-building bias
- Disadvantages?
  - Making predictions is more computationally expensive
  - Favors models with low test time
  - Diminishing returns on the number models that can be incorporated in ensemble

Section 2

Bagging

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- Recall that decision trees tend to have high variance. But averaging the results of independent (or weakly dependent) variables decreases variance
  - Think about the Central Limit Theorem

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- Recall that decision trees tend to have high variance. But averaging the results of independent (or weakly dependent) variables decreases variance
  - Think about the Central Limit Theorem
- Unlike a single tree model, we do not prune (we instead control variance by averaging)

Test Error for Bagged Models

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- For each bootstrap, approximately $1/3$ of observations are not included (called *out-of-bag* observations)
- The out-of-bag observations can be used as a natural validation set for the bootstrap model.
- We get an overall estimate of test MSE for the bagged model by averaging the MSE of each bootstrap model on its out-of-bag observations

A Bag of Trees

We return to the pdxTrees data set, this time expanding both our data set size and number of predictors:

```
names(my_pdxTrees)
```

```
## [1] "DBH"                        "Condition"
## [3] "Tree_Height"                "Crown_Width_NS"
## [5] "Crown_Width_EW"             "Crown_Base_Height"
## [7] "Functional_Type"            "Mature_Size"
## [9] "Carbon_Sequestration_lb"
```

```
dim(my_pdxTrees)
```

```
## [1] 3015    9
```

```
set.seed(1)
library(rsample)
my_pdxTrees_split <- initial_split(my_pdxTrees )
my_pdxTrees_train <- training(my_pdxTrees_split)
my_pdxTrees_test <- testing(my_pdxTrees_split)
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- Can we improve on our previous model predicting `Carbon_Sequestration_lb`, now using more data and more predictors?

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library(rsample)
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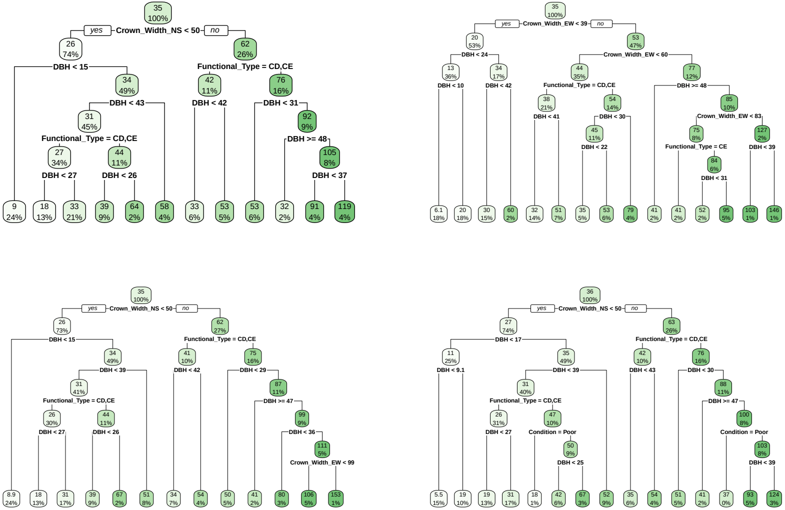
- And now build trees on each:

```
library(rpart)
get_tree <- function(split){
  bootstrap_sample <- analysis(split)
  model <- rpart(Carbon_Sequestration_lb ~., data = bootstrap_sample)
}
pdx_bootstrap$model <- map(pdx_bootstrap$splits, get_tree)
```

A few trees



Performance

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```
get_predictions <- function(model){
  predictions <- predict(model, my_pdxTrees_test)
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```

- And calculate rmse on each using yardstick

```
library(yardstick)
results <- map_dfr(pdx_bootstrap$predictions, rmse, obs, preds)
results
```

```
## # A tibble: 4 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        14.0
## 2 rmse    standard        13.2
## 3 rmse    standard        15.1
## 4 rmse    standard        12.8
```

```
mean(results$.estimate)
```

```
## [1] 13.75185
```

Variation in Model Predictions

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```
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## # Rowwise:
##   tree1 tree2 tree3 tree4 bagged
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## 1  91.3  79.9  95.5  93.4   90.0
## 2  39.5  39.2  19.6  42.5   35.2
## 3  91.3  79.9  95.5  93.4   90.0
## 4 119.  106.   78.8 124.   107.
## 5  53.1  50.2  52.3  50.9   51.6
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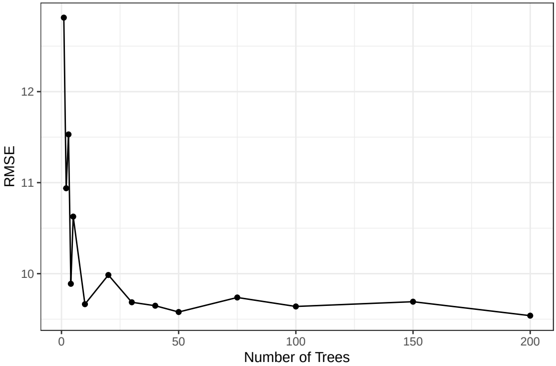
- Note that the RMSE for the bagged tree is **NOT** simply the average RMSE. It is significantly *lower*!

The more trees the merrier?

If 4 trees improved performance over 1, what if we bagged 10 trees? 100?



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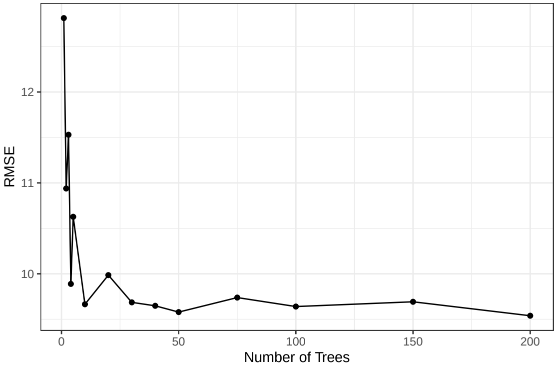

- Greatest gains by adding a small number of additional trees
- Moderately small gains thereafter

Section 3

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- When bagging trees, if one predictor accounts for large amount of deviation in the response, it will usually be selected as the first split (regardless of the bootstrap sample used)
- To artificially increase the variety among trees, we randomly restrict which predictors can be used at each split point.
- Although counterintuitive, this restriction tends to increase accuracy of the ensemble by breaking correlations among the participant trees

Random Forests

To create a random forest:

1. Select the number of models m to build and a number of predictors k to use at each step t
2. Generate a bootstrap sample for each model
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Disadvantages?

- Difficult to interpret
- Theoretically properties less well-studied (possible Senior Thesis project!)

Hand-drawn Example

Section 4

Bagging and Random Forests in R

Random Forest in R

- To create both bagged trees and random forests, we use the `randomForest` function in the `randomForest` package in R:

```
library(randomForest)
rfmodel <- randomForest(Carbon_Sequestration_lb ~ ., data = my_pdxTrees_train)
rfmodel
```

```
##
## Call:
##  randomForest(formula = Carbon_Sequestration_lb ~ ., data = my_pdxTrees_train)
##                Type of random forest: regression
##                      Number of trees: 500
## No. of variables tried at each split: 2
##
##           Mean of squared residuals: 123.172
##                     % Var explained: 84.48
```

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How can we create a bagged model using the `randomForest` function?

- Set `mtry= p`, where `p` is the total number predictors available