Bagging and Random Forests

Prof Wells

STA 295: Stat Learning

April 23rd, 2024

Outline

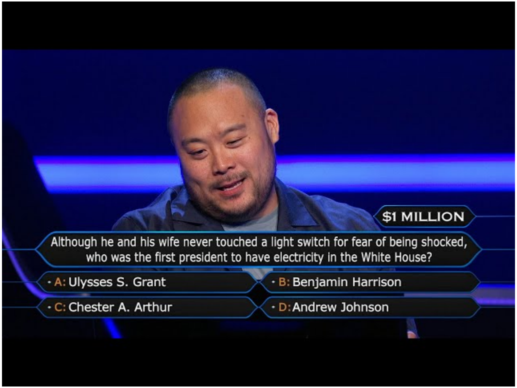
- Introduce ensemble modeling as means of improving low accuracy models
- Discuss bagging and random forests as methods for reducing variance in decision trees
- Implement random forests in R

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.



$1 MILLION

Although he and his wife never touched a light switch for fear of being shocked, who was the first president to have electricity in the White House?

A: Ulysses S. Grant
B: Benjamin Harrison
C: Chester A. Arthur
D: Andrew Johnson

Who Wants to Be a Millionaire?

- The original show included 3 “lifeline” options contestants could use to answer questions:
  - **50:50**: Two randomly selected incorrect answers are eliminated
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- How many grocery aisles are there?
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- A survey of 30 current STEM students in STA 209 were asked the same question.
    - The average value of their guess was 28.4, with standard deviation of 16.2

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  - The average value of their guess was 28.4, with standard deviation of 16.2
- The rMSE for individual students was 15.9.
- However, the rMSE for the class was only 0.4.
- What factors about the class would cause such a drastic reduction in rMSE?

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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

Bootstrapping

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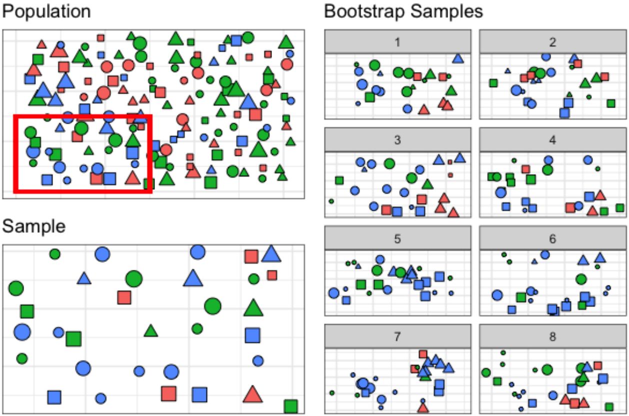
  - Variability in statistics depends on sample size
- Instead, we create **bootstrap** samples by sampling *with replacement* from the original sample a number of times equal to the original sample size
  - Since we sample with replacement, some observations from original sample are included more than once while others are omitted, which introduces a source of variability
  - Bootstrap sample is same size as original, and so can be used to estimate variability in statistic

Bootstrap Visualization



Bootstrap Sample Computations

Suppose we have a sample with 4 unique observations $\{x_1, x_2, x_3, x_4\}$ and create a bootstrap sample.

- What is the probability that x_1 is not the 1st element in the bootstrap sample? What is the probability that it is not the 2nd?
- What is the probability that x_1 is not in the bootstrap sample at all?
- What is the probability that x_2 is not in the bootstrap sample?

Now suppose we have n unique observations $\{x_1, \ldots, x_n\}$ and we create a bootstrap sample.

- What is the probability that x_1 is not in the bootstrap sample?
- What is the probability that an arbitrary observation x_i is not in the bootstrap sample?

What happens to the probability that an arbitrary observation is not in the sample, as n goes to infinity?

Bootstrap Sample Computations Solutions

Suppose we have a sample with 4 unique observations $\{x_1, x_2, x_3, x_4\}$ and create a bootstrap sample.

- What is the probability that x_1 is not the 1st element in the bootstrap sample? What is the probability that it is not the 2nd? $1 - \frac{1}{4}$
- What is the probability that x_1 is not in the bootstrap sample at all? $(1 - \frac{1}{4})^4$
- What is the probability that x_2 is not in the bootstrap sample? $(1 - \frac{1}{4})^4$

Now suppose we have n unique observations $\{x_1, \ldots, x_n\}$ and we create a bootstrap sample.

- What is the probability that x_1 is not in the bootstrap sample? $(1 - \frac{1}{n})^n$
- What is the probability that an arbitrary observation x_i is not in the bootstrap sample? $(1 - \frac{1}{n})^n$

What happens to the probability that an arbitrary observation is not in the sample, as n goes to infinity? $\lim_{n\to\infty} \left(1 - \frac{1}{n}\right)^n = e^{-1}$

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Why?

- 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:
    - For large n, $\bar{X}$ is approximately Normal, with mean μ and standard deviation $\frac{\sigma}{\sqrt{n}}$

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    - Think about the Central Limit Theorem:
    - For large n, $\bar{X}$ is approximately Normal, with mean μ and standard deviation $\frac{\sigma}{\sqrt{n}}$
- 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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- Let’s get a few bootstrap samples using `rsample`:

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set.seed(1115)
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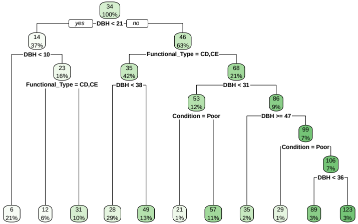
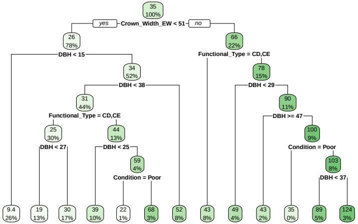
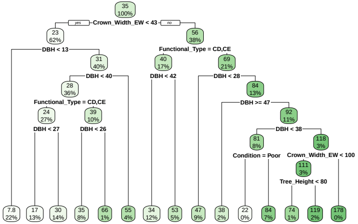
- And now build trees on each:

```
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


34 100%
yes DBH < 21 no
14 37%
46 63%
DBH < 10
Functional_Type = CD,CE
23 16%
35 42%
68 21%
Functional_Type = CD,CE
DBH < 38
DBH < 31
53 12%
86 9%
Condition = Poor
DBH >= 47
99 7%
Condition = Poor
106 7%
DBH < 36
6 21%
12 6%
31 10%
28 29%
49 13%
21 1%
57 11%
35 2%
29 1%
89 3%
123 3%


35 100%
yes Crown_Width_EW < 51 no
26 78%
66 22%
DBH < 15
Functional_Type = CD,CE
34 52%
78 15%
DBH < 38
DBH < 29
31 44%
90 11%
Functional_Type = CD,CE
DBH >= 47
25 30%
44 13%
100 9%
DBH < 27
DBH < 25
59 4%
Condition = Poor
Condition = Poor
103 8%
DBH < 37
9.4 26%
19 13%
30 17%
39 10%
22 1%
68 3%
52 8%
43 8%
49 4%
43 2%
35 0%
89 5%
124 3%


35 100%
yes Crown_Width_EW < 43 no
23 62%
56 38%
DBH < 13
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31 40%
40 17%
69 21%
DBH < 40
DBH < 42
DBH < 28
28 36%
84 13%
Functional_Type = CD,CE
DBH >= 47
24 27%
39 10%
92 11%
DBH < 27
DBH < 26
DBH < 38
81 8%
118 3%
Condition = Poor
Crown_Width_EW < 100
111 3%
Tree_Height < 80
7.8 22%
17 13%
30 14%
35 8%
66 1%
55 4%
34 12%
53 5%
47 9%
38 2%
22 0%
84 7%
74 1%
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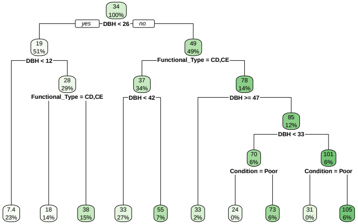
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19 51%
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DBH < 12
Functional_Type = CD,CE
28 29%
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78 14%
DBH < 42
DBH >= 47
85 12%
DBH < 33
70 6%
101 6%
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55 7%
33 2%
24 0%
73 6%
31 0%
105 6%

Performance

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```
get_predictions <- function(model){
  predictions <- predict(model, my_pdxTrees_test)
  data.frame(obs = my_pdxTrees_test$Carbon_Sequestration_lb, preds = predictions)
}
pdx_bootstrap$predictions <- map(pdx_bootstrap$model, get_predictions)
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```
library(yardstick)
results <- map_dfr(pdx_bootstrap$predictions, rmse, obs, preds)
results
```

```
## # A tibble: 4 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        14.0
## 2 rmse    standard        14.3
## 3 rmse    standard        14.3
## 4 rmse    standard        13.1
```

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

```
## [1] 13.89024
```

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## # Rowwise:
##   tree1 tree2 tree3 tree4 bagged
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## 1  49.0  30.4  52.2  32.5   41.0
## 2  34.7  38.0  43.3  32.8   37.2
## 3  56.8  84.0  67.6  72.9   70.3
## 4  30.6  46.6  38.8  37.8   38.4
## 5  56.8  65.7  67.6  72.9   65.7
## 6  56.8  84.0  89.1  72.9   75.7
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##   <chr>  <chr>   <chr>          <dbl>
## 1 tree 1 rmse    standard        14.0
## 2 tree 2 rmse    standard        14.3
## 3 tree 3 rmse    standard        14.3
## 4 tree 4 rmse    standard        13.1
## 5 bagged rmse    standard        12.3
```

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## # A tibble: 5 x 4
##   model  .metric .estimator .estimate
##   <chr>  <chr>   <chr>          <dbl>
## 1 tree 1 rmse    standard        14.0
## 2 tree 2 rmse    standard        14.3
## 3 tree 3 rmse    standard        14.3
## 4 tree 4 rmse    standard        13.1
## 5 bagged rmse    standard        12.3
```
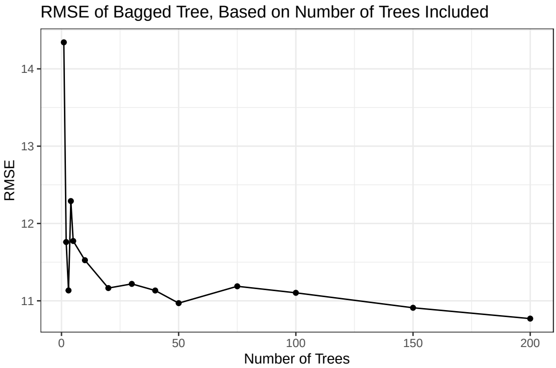

- Note that the RMSE for the bagged tree is **NOT** simply the average RMSE. It is significantly *lower*!

The more trees the merrier?

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



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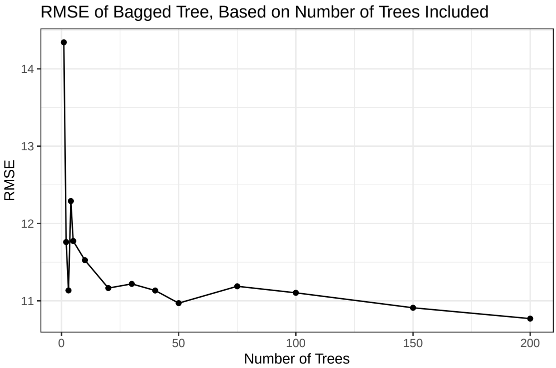

- Greatest gains by adding a small number of additional trees
- Moderately small gains thereafter

Section 3

Random Forests

Further Performance Improvements

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- 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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- Each tree is quicker to build (why?)

Disadvantages?

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

Hand-made Random Forests

I have a data set with categorical response Y with two, with 3 quantitative predictors and with 50 observations.

- Our goal is to build, as a class, a random forest for predicting Y.
- Each table will be tasked with building (by hand) a single decision tree for predicting Y.
- Each table will be randomly assigned 2 of the 3 predictors, and will have a bootstrap sample of the 50 observations.
- Each table will be given a scatterplot showing the relationship between their 2 predictors and the response, on their bootstrap sample.
- Each table should work together to decide where to make cuts in the scatterplot to create a decision tree with between 3 and 6 leaves (group's choice)
- I will give each group the same 10 test points to classify. And as a class, we will average the predictions to create a random forest prediction.

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: 112.2864
##                     % Var explained: 85.74
```

Modifications

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```
set.seed(1)
rfmodel2 <- randomForest(Carbon_Sequestration_lb ~ ., data = my_pdxTrees_train,
                         ntree = 10, mtry = 5)
rfmodel2
```

```
##
## Call:
##  randomForest(formula = Carbon_Sequestration_lb ~ ., data = my_pdxTrees_train,      ntree = 1
##                Type of random forest: regression
##                      Number of trees: 10
## No. of variables tried at each split: 5
##
##           Mean of squared residuals: 106.4475
##                     % Var explained: 86.48
```

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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

Making predictions

- So you have your `randomForest` model. How do you make predictions?

```
my_preds<- predict(rfmodel, my_pdxTrees_test)
results <- data.frame(obs =  my_pdxTrees_test$Carbon_Sequestration_lb, preds = my_preds)

results %>% head()
```

```
##     obs    preds
## 1  39.0 38.85781
## 2 110.2 66.09302
## 3  61.2 75.53011
## 4  34.0 33.41863
## 5  75.4 51.02538
## 6  96.1 82.35864
```

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- How can we determine which predictors are most influential?

One possibility is to record the total amount of RSS/Purity that is decreased due to splits of the given predictor, averaged across all trees in the random forest.

Importance in R

```
importance(rfmodel)
```

```
##                   IncNodePurity
## DBH                   507862.05
## Condition              54821.17
## Tree_Height           208750.74
## Crown_Width_NS        309930.48
## Crown_Width_EW        325846.81
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## Functional_Type       170538.17
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```r
varImpPlot(rfmodel)
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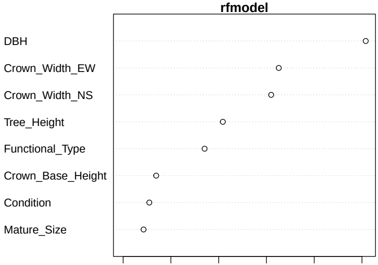

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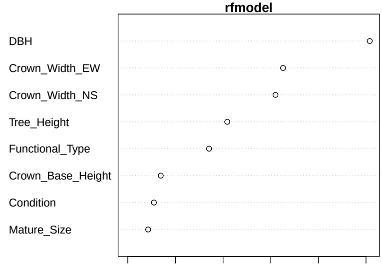

- For regression trees, node impurity is calculated using RSS.
- For classification trees, node impurity is calculated using Gini Index.

Comparison of Bagged Trees versus Random Forests