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.

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
  - **Phone a Friend**: The contestant calls a friend and is given 30 seconds to discuss
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Why?

Ensemble Methods

- 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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- A simple ensemble model makes a prediction $\hat{Y}$ as the weighted average of the predictions from each model:

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

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  - More efficient than single model
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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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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

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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
- Unlike a single tree model, we do not prune (we instead control variance by averaging)

Test Error for Bagged Models

- Recall from a previous homework that an individual observation has probability $1 - e^{-1} \approx 0.632$ of appearing in a bootstrap sample.

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- The out-of-bag observations can be used as a natural validation set for the bootstrap model.

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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?

Bagged pdXTrees

- Let's get a few bootstrap samples using `rsample`:

Bagged pdXTrees

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library(rsample)
set.seed(1115)
pdx_bootstrap <- bootstraps(my_pdxTrees_train, times = 4)
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```
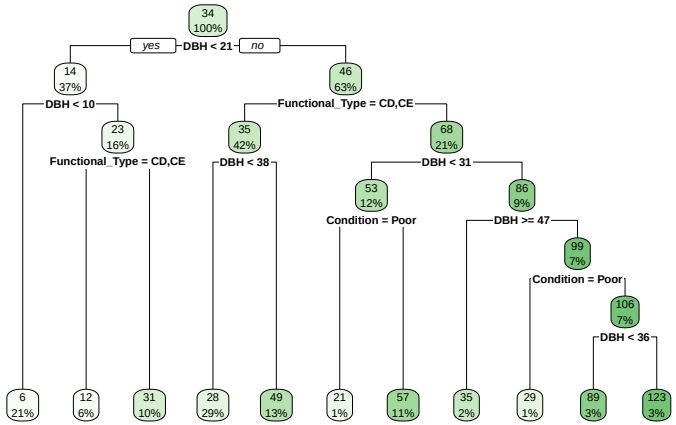
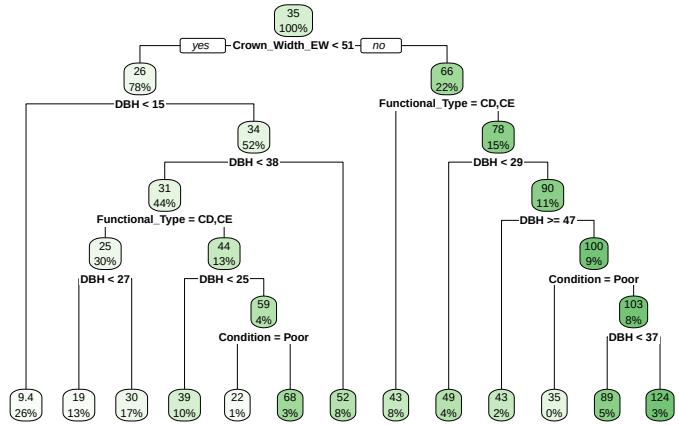
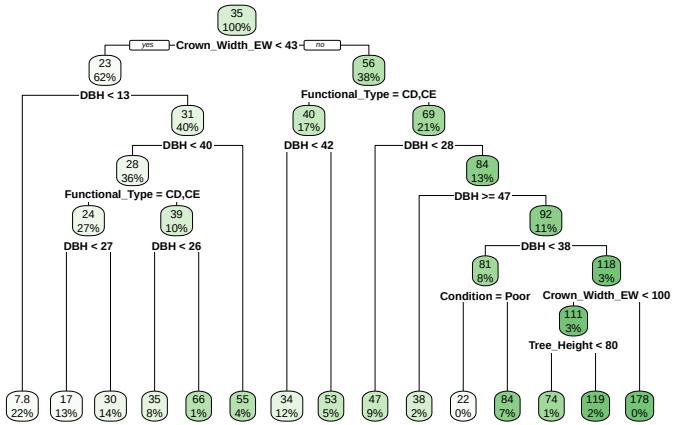

- And now build trees on each:

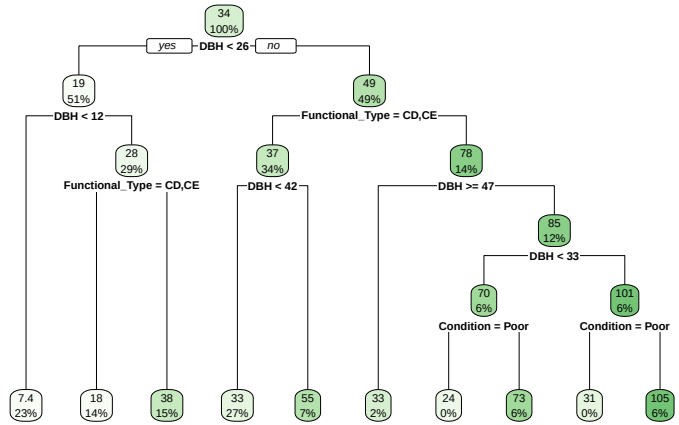
```
library(rpart)
get_tree <- function(split){
  bootstrap_sample <- analysis(split)
  model <- rpart(Carbon_Sequestration_lb ~., data = bootstrap_sample)
}
pdx_bootstrap$model <- map(pdx_bootstrap$splits, get_tree)
```

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%
Condition = Poor
DBH < 27
DBH < 25
59
4%
103
8%
Condition = Poor
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
Functional_Type = CD,CE
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%
119
2%
178
0%


34
100%
yes
DBH < 26
no
19
51%
49
49%
DBH < 12
Functional_Type = CD,CE
28
29%
37
34%
78
14%
Functional_Type = CD,CE
DBH < 42
DBH >= 47
85
12%
DBH < 33
70
6%
101
6%
Condition = Poor
Condition = Poor
7.4
23%
18
14%
38
15%
33
27%
55
7%
33
2%
24
0%
73
6%
31
0%
105
6%

Performance

- Let's get predictions for each bootstrap:

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```
get_predictions <- function(model){
  predictions <- predict(model, my_pdxTrees_test)
  tibble(obs = my_pdxTrees_test$Carbon_Sequestration_lb, preds = predictions)
}
pdx_bootstrap$predictions <- map(pdx_bootstrap$model, get_predictions)
```

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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        14.3
## 3 rmse    standard        14.3
## 4 rmse    standard        13.1
```

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

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

Variation in Model Predictions

- How do individual tree predictions compare?

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```
## # A tibble: 6 x 5
## # Rowwise:
##   tree1 tree2 tree3 tree4 bagged
##   <dbl> <dbl> <dbl> <dbl>  <dbl>
## 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
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```
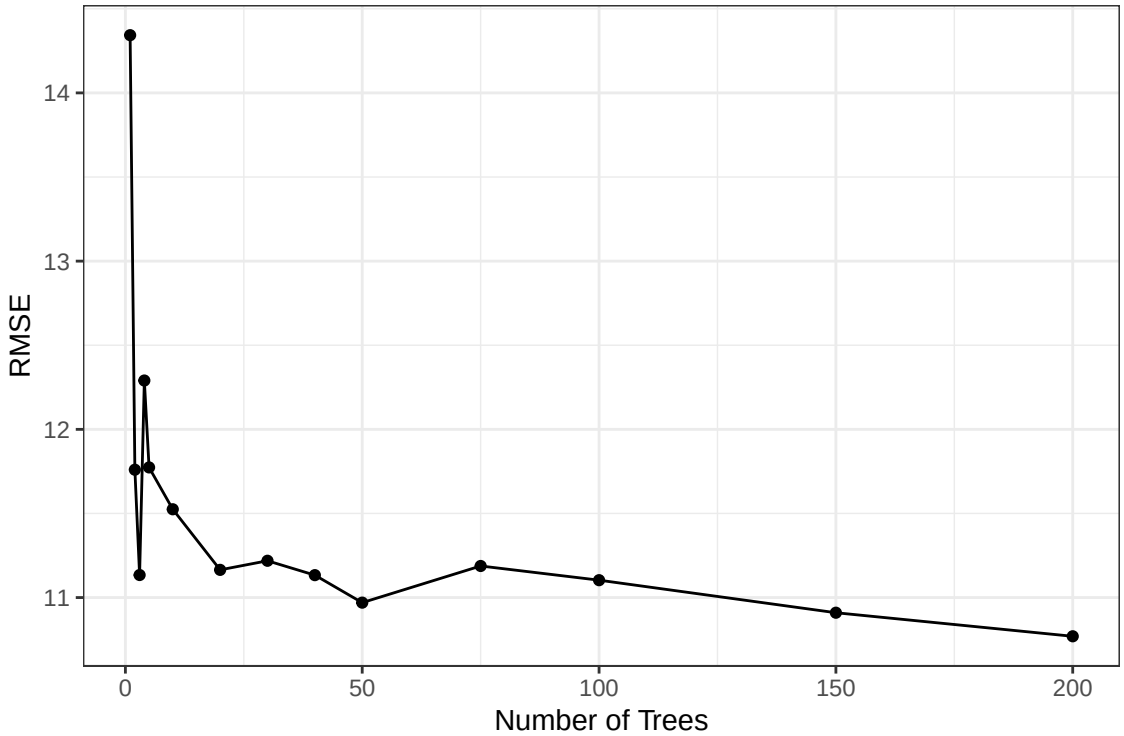

- Note that the RMSE for the bagged tree is **NOT** simply the average RMSE. It is significantly *lower*!

The more trees the merrier?

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



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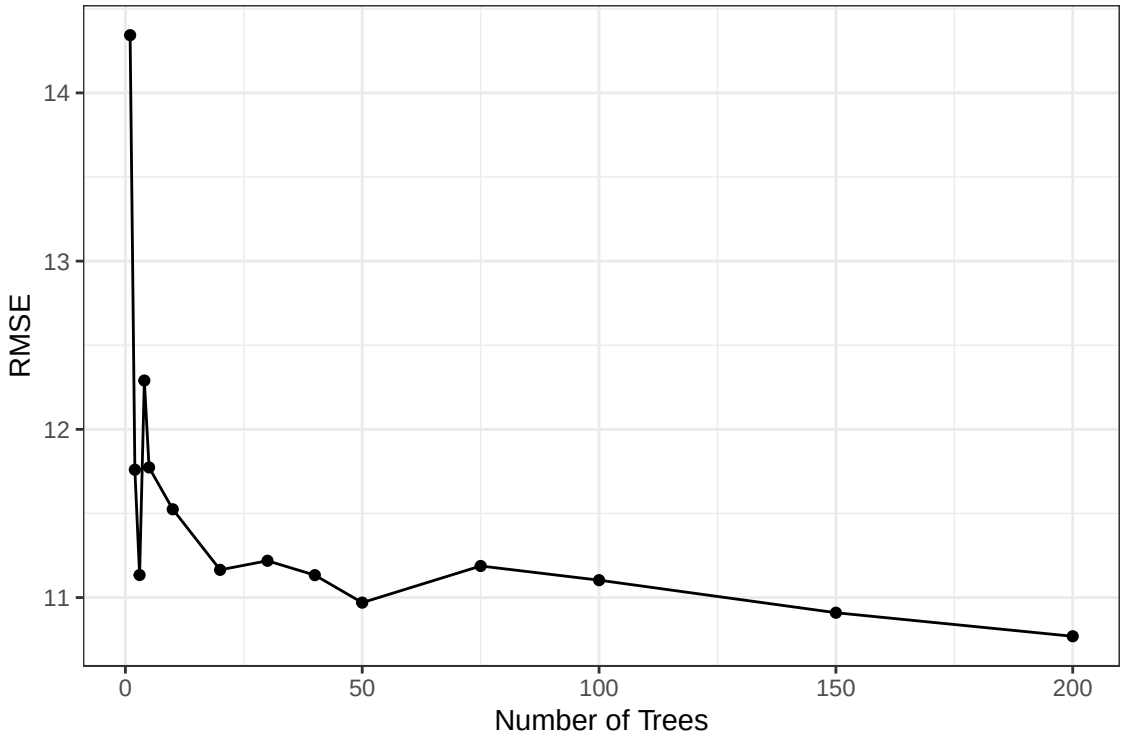

- Greatest gains by adding a small number of additional trees
- Moderately small gains thereafter

Section 3

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
3. Build a tree on the bootstrap sample where at each step, a random selection of k of the p predictors can be used (independent of prior predictors selected)
4. Aggregate the models to create an ensemble 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: 112.2864
##                     % Var explained: 85.74
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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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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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varImpPlot(rfmodel)
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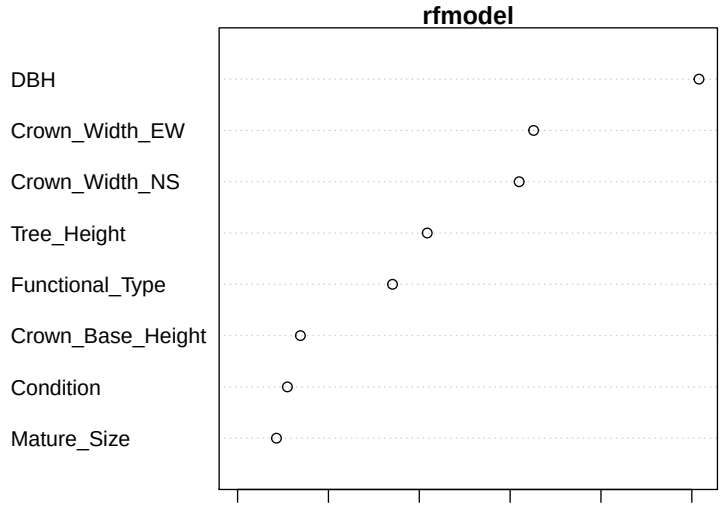

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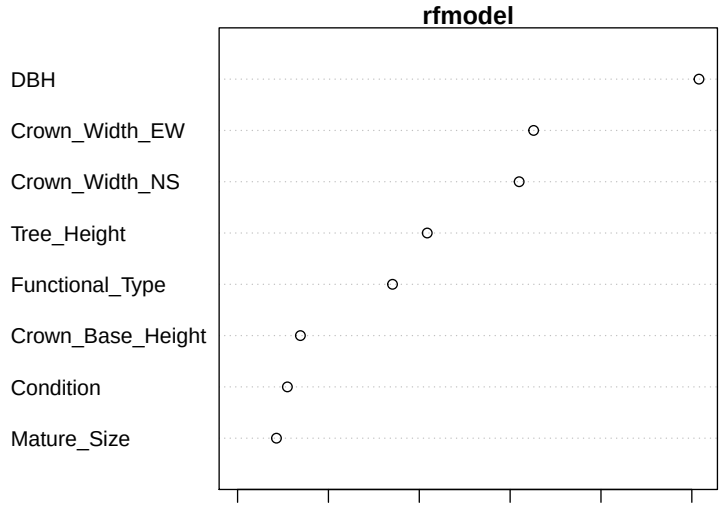

- For regression trees, node impurity is calculated using RSS.
- For classification trees, node impurity is calculated using Gini Index.

Comparison of Bagged Trees versus Random Forests