Random Forests and Boosted Trees

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STA 295: Stat Learning

April 23rd, 2024

Outline

- Discuss random forests and boosted trees as methods for reducing variance in decision trees
- Implement random forests and boosted trees in R

Section 1

Random Forests

Review: Bagging

- To create a bagged model, first create many bootstrap samples from the original training set (i.e. sample with replacement to create a sample of same size as original)
    - Then fit a decision tree to each bootstrap sample. Average the resulting predictions to get the bagged prediction.
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- However, in bagged trees, since we average large number of (full) decision trees, we reduce variance
  - Additionally, averaging models with low bias will produce a model with low bias
- This a a rare case in stat learning in which there is no bias-variance trade-off. Bagged trees allow us to reduce variance with no increase in bias!

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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

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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
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Disadvantages?

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

Hand-made Random Forests

I have a data set of 50 observations on a binary response Y and 3 quantitative predictors.

- 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 2

Bagging and Random Forests in R

A Forest of Trees

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

```r
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"
```

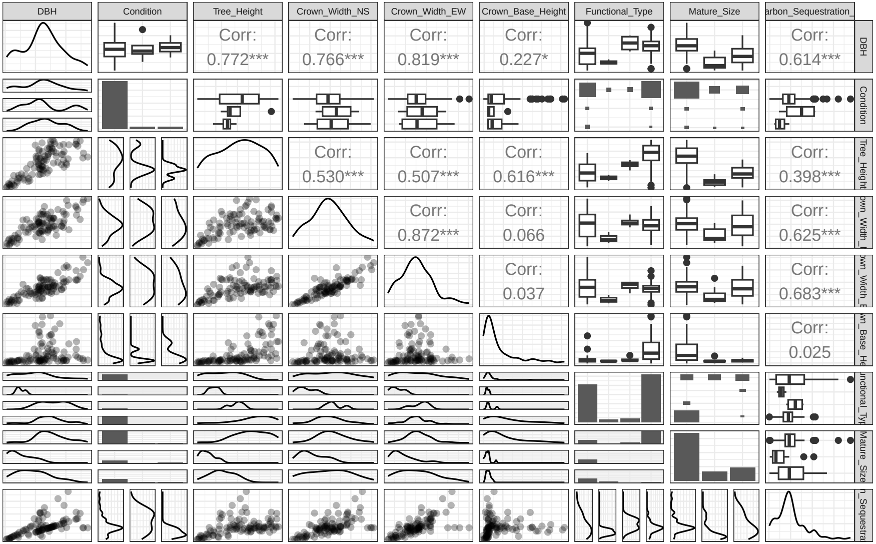
```r
dim(my_pdxTrees)
```

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

```r
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)
```

```r
library(GGally)
ggpairs(my_pdxTrees_train)
```

Exploratory Analysis



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: 111.5371
##                     % Var explained: 85.84
```

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?

```r
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 38.26301
## 2 110.2 66.90372
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Let's compute test rMSE

```
library(yardstick)
results %>% rmse(truth = obs, estimate = preds)
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        11.3
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- For reference, the bagged model had rMSE of 12.3, while the average rMSE for single trees was 13.9

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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                    506807.58
## Condition               54752.15
## Tree_Height            204541.39
## Crown_Width_NS         311571.85
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varImpPlot(rfmodel)
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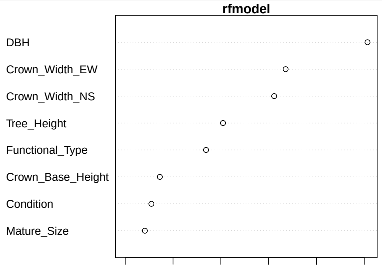

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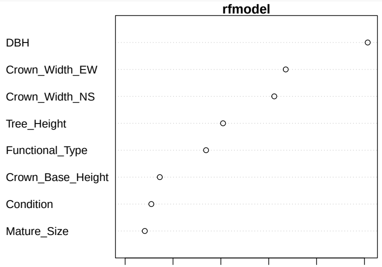
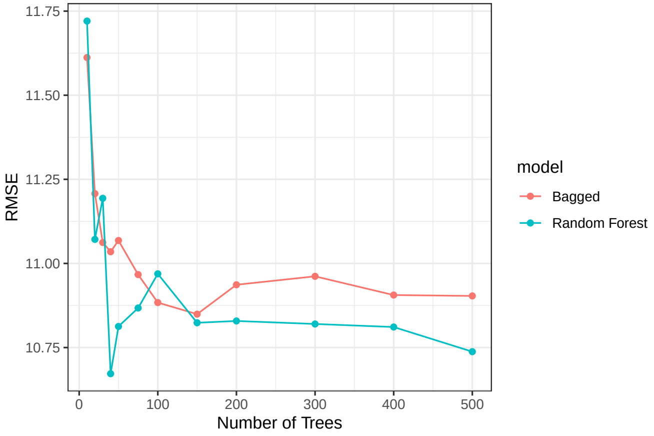


- For regression trees, node impurity is calculated using RSS.
- For classification trees, node impurity is calculated using Gini Index.

Comparison of Bagged Trees versus Random Forests



Section 3

Boosting

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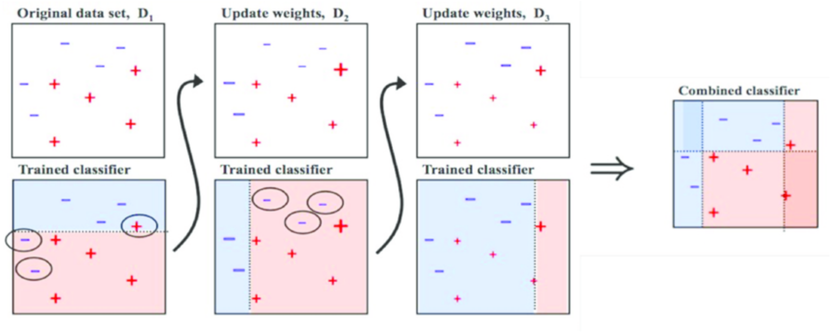
- The overall sequence of classifiers are combined into an ensemble which as high chance of classifying more accurately than any individaul model in the list.
- The algorithm relies on using a sequence of **weak** learners (low variance, high bias)
  - In the tree setting, we can create weak learners by restricting the depth of the tree.

AdaBoost Graphic



Boosting for regression

Boosting also works in the regression setting. The **gradient boosting machine** is a boosting algorithm that works as follows:

1. Select tree depth D and number of iterations K.
2. Compute the average response $\hat{y}$ and use this as the initial predicted value for each observation
3. Compute the residual for each observation.
4. Fit a regression tree of depth D, using the **residuals** as the response.
5. Predict each observation using the regression tree from the previous step.
6. Update the predicted value of each observation by adding the previous iteration's predicted value to the predicted value generated in the previous step.
7. Repeat at total of K times.

Brief Example

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## [1] 34.49668
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Fit a new tree

```
boost_tree_model<- rpart(residuals1 ~ Crown_Base_Height,
                        data = my_pdxTrees_train_boost,
                        control = rpart.control(maxdepth = 2))
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  - Instead of adding the full value for a sample to the previous iteration's predicted value, only a fraction of the current predicted value is added.
  - This fraction is called the *learning rate* λ, with $0 < \lambda < 1$. (Typical values range from 0.001 to 0.01)

Boosting in R

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- For regression problems, we use the argument `distribution = "gaussian"` and for classification problems, we use `distribution = "bernoulli"`

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- For regression problems, we use the argument `distribution = "gaussian"` and for classification problems, we use `distribution = "bernoulli"`
- The argument `n.trees` controls the number of iterations
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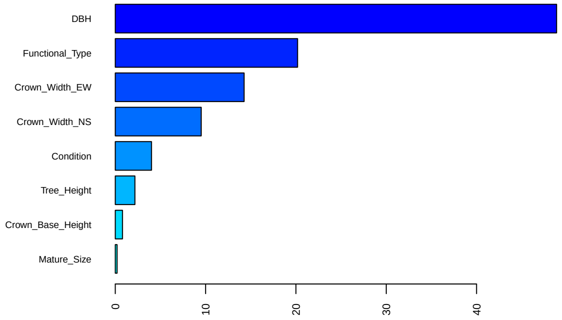
- The argument shrinkage controlls the learning rate λ

```r
library(gbm)
set.seed(10101)
boosted_tree<-gbm(Carbon_Sequestration_lb ~., my_pdxTrees_train,
                  distribution = "gaussian",
                  n.trees=5000,
                  interaction.depth = 3,
                  shrinkage = .0025)
```

Summary Information

```
summary(boosted_tree )
```

```
##                               var    rel.inf
## DBH                           DBH 48.8607778
## Functional_Type     Functional_Type 20.1833428
## Crown_Width_EW       Crown_Width_EW 14.2618538
## Crown_Width_NS       Crown_Width_NS  9.5128157
## Condition                 Condition  4.0105335
## Tree_Height             Tree_Height  2.1739086
## Crown_Base_Height Crown_Base_Height  0.7980455
## Mature_Size             Mature_Size  0.1987224
```



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results %>% group_by(model) %>% rmse(truth = obs, estimate = preds) %>% arrange(.estimate)
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## # A tibble: 4 x 4
##   model         .metric .estimator .estimate
##   <chr>         <chr>   <chr>          <dbl>
## 1 random_forest rmse    standard        10.8
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- Note that boosted trees have a number of important parameters: `n.trees`, `interaction.depth`, `shrinkage`.
  - How do we find the best values of these hyperparameters?
  - Cross-validation!

Cross-Validating gbm

Warning! fitting a single `gbm` models can be time and computing intensive.

- Using cross-validation to compare multiple models can be VERY time and computing intensive
- Cross-validation for `gbm` models is NOT RECOMMENDED if using the RStudio Server

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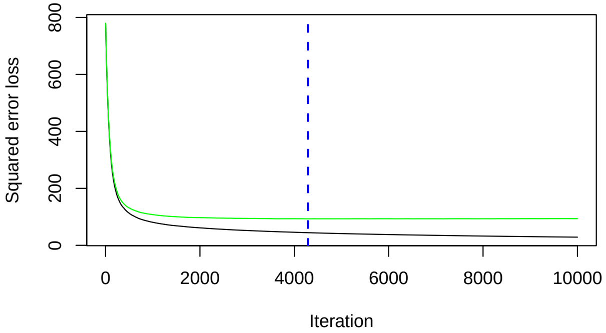
- Using cross-validation to compare multiple models can be VERY time and computing intensive
- Cross-validation for gbm models is NOT RECOMMENDED if using the RStudio Server
- We can include an additional cross-validation term in our boosted tree model.
    - It may be helpful to include a number of CPU cores as well. First verify your number of available cores using `parallel::decectCores()`

```
library(gbm)
set.seed(10101)
cv_boosted_tree<-gbm(Carbon_Sequestration_lb ~., my_pdxTrees_train,
                  distribution = "gaussian",
                  n.trees=10000,
                  interaction.depth = 3,
                  shrinkage = .01,
                  cv.folds = 10,
                  n.cores = 8)
```

CV Results

- We can plot cross-validated performance using `gbm.perf()`

```
gbm.perf(cv_boosted_tree, method = "cv")
```



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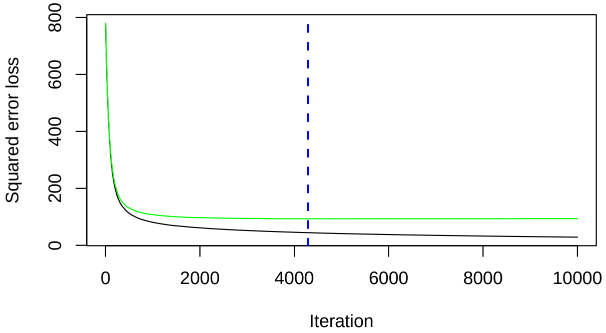

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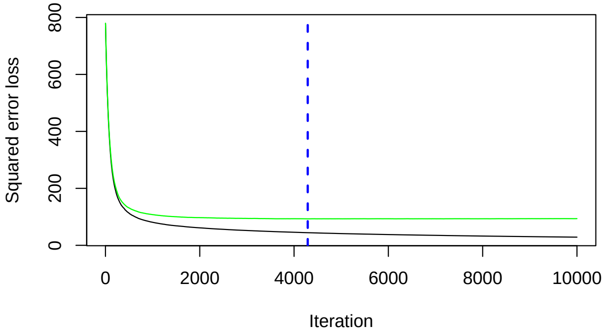

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- The green curve is the cross-validated error, while the black curve is the training error.
- The blue vertical line is the optimal value of the cross-validated error

Recording CV Error

- The `gbm` object also stores the values of the cross-validated errors for each number of trees used, accessible via `$cv.errors`

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```
my_errors <- cv_boosted_tree$cv.error
best_n <- which.min(cv_boosted_tree$cv.error)
data.frame(best_n, cv_error = my_errors[best_n])
```

```
##   best_n cv_error
## 1   4290 93.01164
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- This is particularly useful if we want to record the error for a model with certain parameters

General Strategy for finding best Parameters

1. Choose a relatively high initial learning rate. A rate of 0.1 is a reasonable starting point.
2. Determine the optimal number of trees for this learning rate using cross-validation.
3. Fix other tree-specific parameters and tune the learning rate, assessed by computation speed and model accuracy.
4. Tune tree-specific parameters for fixed learning rate.
5. Once tree-specific parameters have been found, lower learning rate and increase number of trees to assess improvements in accuracy.

Warning! This search can take considerable time (minutes to hours), depending on computing power, number of variables in model, and number of observations. DO NOT ATTEMPT ON RSTUDIO SERVER!!

Cross-Validation along a Grid

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```
my_grid <- expand.grid(
  n.trees = 5000,
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- Then we create a model fitting function:

```
model_fit <- function(n.trees, shrinkage, interaction.depth, n.minobsinnode){
  set.seed(40)
  library(gbm)
  gbm_mod <- bm(Carbon_Sequestration_lb ~., my_pdxTrees_train,
                distribution = "gaussian",
                n.trees=n.trees,
                interaction.depth = interaction.depth,
                shrinkage = shrinkage,
                cv.folds = 10,
                n.cores = 8,
              n.minobsinnode = n.minobsinnode)
  rMSE <- sqrt(min(gbm_mod$cv.error))
  rMSE
}
```

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Implementing the Grid Search

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library(purrr)
my_grid$rmse <- pmap_dbl(
  my_grid,
  ~ model_fit(
    n.trees = ..1,
    shrinkage = ..2,
    interaction =..3,
    n.minobsinnode = ..4
  )
)
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  )
)
```

We can then view results of the exhuastive search:

```
head(arrange(my_grid, rmse))
```

```
##   n.trees shrinkage interaction.depth n.minobsinnode     rmse
## 1    5000      0.01                 7              5 9.389038
## 2    5000      0.01                 7             10 9.486088
## 3    5000      0.01                 5              5 9.557491
## 4    5000      0.01                 7             15 9.610702
## 5    5000      0.01                 5             10 9.708710
## 6    5000      0.01                 5             15 9.708723
```