Tree-Based Methods

Last modified on February 20, 2025 10:23:55 Eastern Standard Time

> Crediting the materials
>
> The descriptions of tree-based methods in this document are taken primarily from *An Introduction to Statistical Learning with Applications in R* while most of the coding ideas for `tidymodels` are gleaned from *Tidy Modeling with R: A framework for Modeling in the Tidyverse*.

Advantages and Disadvantages of Trees

Pros

- Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- Some people believe that decision trees more closely mirror human decision-making than do regression and classification approaches.
- Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small).
- Trees can easily handle qualitative predictors without the need to create dummy variables (`model.matrix()`).

Cons

- Trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches.

- Trees suffer from *high variance*. This means if we split the training data into two parts at random, and fit a decision tree to both halves, the results that we get could be quite different. In contrast, a procedure with *low variance* will yield similar results if applied repeatedly to distinct data sets.

> How do we improve on a single tree?
>
> By aggregating many decision trees, using methods like *bagging*, *random forests*, and *boosting*, the predictive performance of trees can be substantially improved!

The Basics of Decision Trees

Decision trees can be applied to both **regression** and **classifcation** problems. We first consider regression problems, and then move on to classification problems.

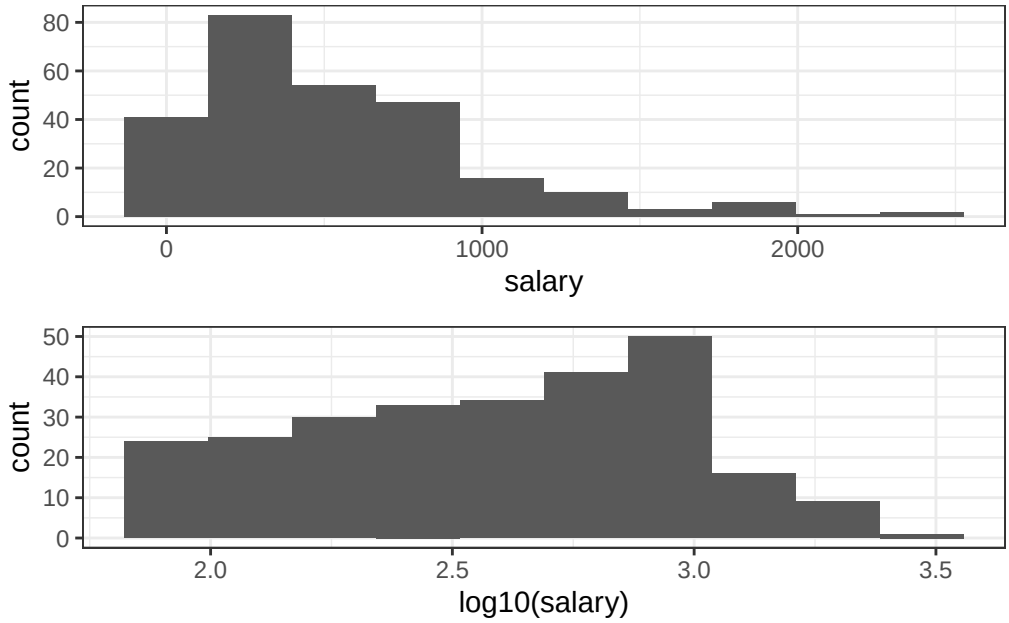
Predicting Baseball Players' Salaries Using Regression Trees

We use the `Hitters` data set to predict a baseball player's `Salary` based on `Years` (the number of years that he has played in the major leagues) and `Hits` (the number of hits that he made in the previous year). We first remove observations that are missing `Salary` values, and log-transform `Salary` so that its distribution has more of a typical bell-shape. (Recall that Salary is measured in thousands of dollars.)

```
library(tidymodels)
library(tidyverse)
library(ISLR2)
library(janitor) # standardize variable names
tidymodels_prefer()
Hitters <- na.omit(Hitters) |>
  clean_names() |>
  as_tibble()
names(Hitters)
```

```
 [1] "at_bat"     "hits"       "hm_run"     "runs"       "rbi"
 [6] "walks"      "years"      "c_at_bat"   "c_hits"     "c_hm_run"
[11] "c_runs"     "crbi"       "c_walks"    "league"     "division"
[16] "put_outs"   "assists"    "errors"     "salary"     "new_league"
```

```
ggplot(data = Hitters, aes(x = salary)) +
  geom_histogram(bins = 10) +
  theme_bw() -> p1
ggplot(data = Hitters, aes(x = log10(salary))) +
  geom_histogram(bins = 10) +
  theme_bw() -> p2
library(patchwork)
p1/p2
```




```
# Put salary on log10 scale
Hitters <- Hitters |>
  mutate(salary = log10(salary))
```

We start by creating a tree "specification" using the `parsnip` package which was loaded with the `tidymodels` bundle.

```
tree_spec <- decision_tree() |>
  set_engine("rpart") |>
  set_mode("regression")
tree_spec
```

```
Decision Tree Model Specification (regression)
```

```
Computational engine: rpart
```

With a model specification and data we are ready to fit a model. The first model we will consider uses both `year` and `hits` as predictors.

```
tree_fit <- tree_spec |>
  fit(salary ~ years + hits, data = Hitters)
```

When we look at the model output, we see an informative summary of the model.

```
tree_fit
```

```
parsnip model object

n= 263

node), split, n, deviance, yval
      * denotes terminal node

 1) root 263 39.0716200 2.574160
   2) years< 4.5 90  7.9883020 2.217851
     4) years< 3.5 62  4.3397050 2.124487
       8) hits< 114 43  3.2338760 2.053078 *
       9) hits>=114 19  0.3903227 2.286097 *
     5) years>=3.5 28  1.9114650 2.424585 *
   3) years>=4.5 173 13.7130700 2.759523
     6) hits< 117.5 90  5.2988020 2.605063
      12) years< 6.5 26  1.3651130 2.470669 *
      13) years>=6.5 64  3.2733010 2.659661
        26) hits< 50.5 12  0.5072597 2.488515 *
        27) hits>=50.5 52  2.3334350 2.699156 *
     7) hits>=117.5 83  3.9387920 2.927009 *
```

Once the tree gets more than a couple of nodes, it can become hard to read the printed diagram. The `rpart.plot` package provides functions to let us easily visualize the decision tree. The function `rpart.plot` only works with `rpart` trees so we will use the `extract_fit_engine()` from the `parsnip` package.

```
tree_fit |>
  extract_fit_engine() |>
```

```
rpart.plot::rpart.plot()
```

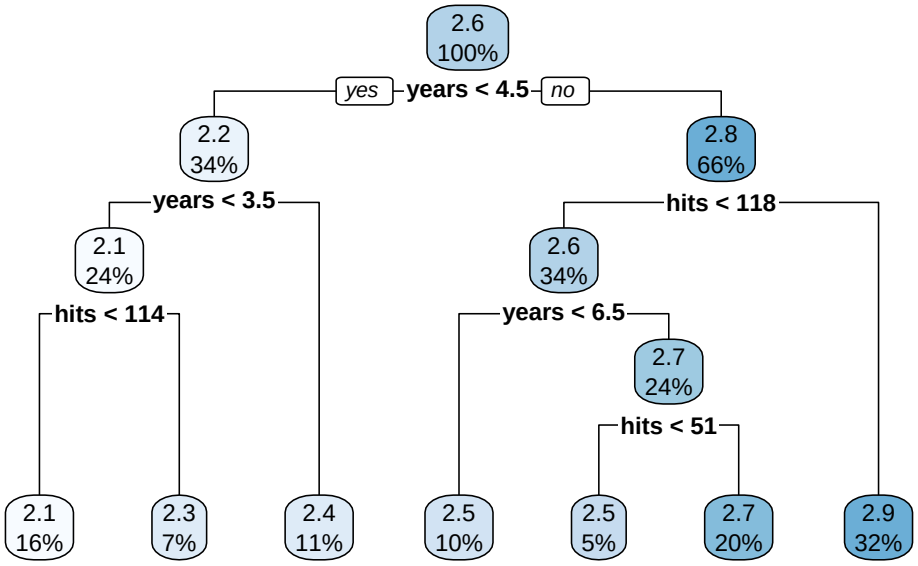


Figure 1: Tree Model for predicting `salary` based on `years` and `hits`

```
# Print Rules
tree_fit |>
  extract_fit_engine() |>
  rpart.plot::rpart.rules()
```

```
salary
   2.1 when years <  3.5        & hits <  114
   2.3 when years <  3.5        & hits >=        114
   2.4 when years is 3.5 to 4.5
   2.5 when years is 4.5 to 6.5 & hits <  118
   2.5 when years >=        6.5 & hits <   51
   2.7 when years >=        6.5 & hits is  51 to 118
   2.9 when years >=        4.5 & hits >=        118
```

Tip

Each node in Figure 1 shows:

- the predicted value,
- the percentage of observations in the node.

For example, all observations (100%) are in the first node and the top number (2.6) is the average salary (in log10) of all players in `Hitters`. That is $10^{2.574160} = 375.1112$ and remembering that `salary` is in thousands of dollars, the average `salary` for all 263 players is \$375,111. Moving to the left for players with fewer than 4.5 years in the league we see that note contains 34% of the players and their predicted salary is $10^{2.217851} \times 1000 = \$165{,}140$.

Next we consider a model that uses all of the variables in `Hitters`.

```
tree_fit2 <- tree_spec |>
  fit(salary ~ ., data = Hitters)
```

```
tree_fit2 |>
  extract_fit_engine() |>
  rpart.plot::rpart.plot()
```

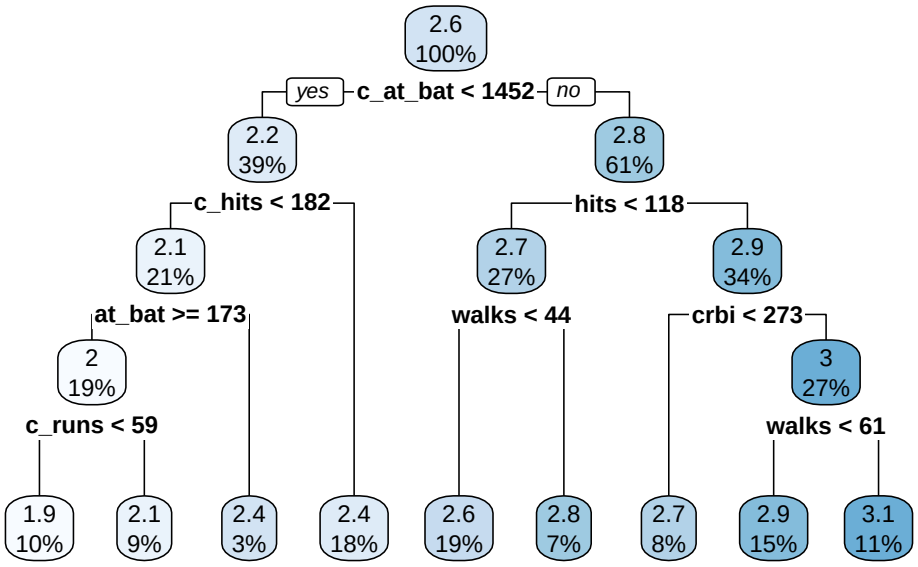


Figure 2: Tree Model for predicting `salary` based on all predictors in `Hitters`

Evaluating the Performance of your Model

To evaluate model performance, we will use the `metrics()` function from the `yardstick` package which was loaded with the `tidyverse` bundle.

```
augment(tree_fit2, new_data = Hitters) |>
  metrics(truth = salary, estimate = .pred) -> R1
```

```
R1 |>
  knitr::kable()
```

.metric	.estimator	.estimate
rmse	standard	0.1823249
rsq	standard	0.7762381
mae	standard	0.1339507

The mean absolute error (`mae`) is $10^{0.1339507} \cdot 1000 = \$1{,}361.29$ and the model's R^2 value is 77.62% which is not bad. However, this model was fit on the entire data set and the model is likely **overfitting** the data. Next we refit the model using a **training** set and **tune** the model's complexity parameter (`cost_complexity`). After tuning the `cost_complexity`, we evaluate the model's performance on the **test** set to get an idea of how the model will perform on data it has not seen.

Splitting the Data

```
set.seed(314)
hitters_split <- initial_split(Hitters)
hitters_train <- training(hitters_split)
hitters_test <- testing(hitters_split)
dim(hitters_train)
```

```
[1] 197  20
```

```
dim(hitters_test)
```

```
[1] 66 20
```

```
hitters_folds <- vfold_cv(hitters_train, v = 10, repeats = 5)
```

```
tree_spec <- decision_tree(cost_complexity = tune()) |>
  set_engine("rpart") |>
  set_mode("regression")
tree_spec
```

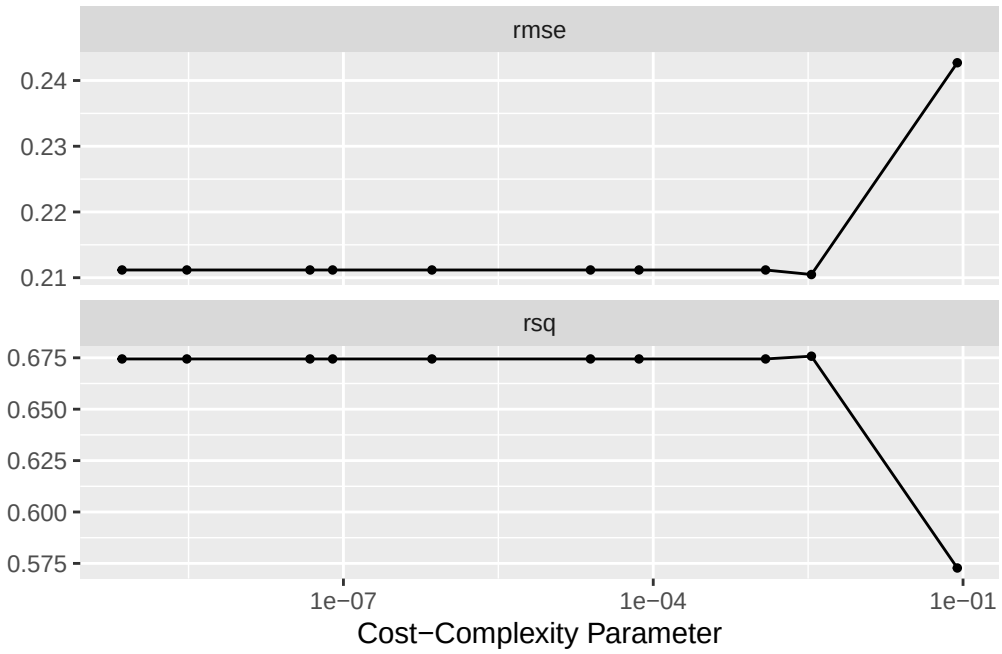
```
Decision Tree Model Specification (regression)

Main Arguments:
  cost_complexity = tune()

Computational engine: rpart
```

```
tree_recipe <- recipe(formula = salary ~ ., data = hitters_train)
tree_wkfl <- workflow() |>
  add_recipe(tree_recipe) |>
  add_model(tree_spec)
```

```
set.seed(8675)
tree_tune <-
  tune_grid(tree_wkfl, resamples = hitters_folds, grid = 10)
tree_tune
```

```
# Tuning results
# 10-fold cross-validation repeated 5 times
# A tibble: 50 x 5
   splits           id      id2    .metrics          .notes
   <list>           <chr>   <chr>  <list>            <list>
 1 <split [177/20]> Repeat1 Fold01 <tibble [20 x 5]> <tibble [0 x 3]>
 2 <split [177/20]> Repeat1 Fold02 <tibble [20 x 5]> <tibble [0 x 3]>
 3 <split [177/20]> Repeat1 Fold03 <tibble [20 x 5]> <tibble [0 x 3]>
 4 <split [177/20]> Repeat1 Fold04 <tibble [20 x 5]> <tibble [0 x 3]>
 5 <split [177/20]> Repeat1 Fold05 <tibble [20 x 5]> <tibble [0 x 3]>
 6 <split [177/20]> Repeat1 Fold06 <tibble [20 x 5]> <tibble [0 x 3]>
 7 <split [177/20]> Repeat1 Fold07 <tibble [20 x 5]> <tibble [0 x 3]>
 8 <split [178/19]> Repeat1 Fold08 <tibble [20 x 5]> <tibble [0 x 3]>
 9 <split [178/19]> Repeat1 Fold09 <tibble [20 x 5]> <tibble [0 x 3]>
10 <split [178/19]> Repeat1 Fold10 <tibble [20 x 5]> <tibble [0 x 3]>
# i 40 more rows
```

```
autoplot(tree_tune)
```




```
show_best(tree_tune, metric = "rmse")
```

```
# A tibble: 5 x 7
  cost_complexity .metric .estimator  mean     n std_err .config
            <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1   0.00340       rmse    standard   0.210    50 0.00774 Preprocessor1_Model10
2   0.0000247     rmse    standard   0.211    50 0.00760 Preprocessor1_Model01
3   0.0000728     rmse    standard   0.211    50 0.00760 Preprocessor1_Model02
4   0.00000000305 rmse    standard   0.211    50 0.00760 Preprocessor1_Model04
5   0.000000719   rmse    standard   0.211    50 0.00760 Preprocessor1_Model05
```

```
tree_param <- tibble(cost_complexity = 0.00340)
final_tree_wkfl <- tree_wkfl |>
  finalize_workflow(tree_param)
final_tree_wkfl
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: decision_tree()

-- Preprocessor ----------------------------------------------------------------
```

```
0 Recipe Steps

-- Model ---------------------------------------------------------------------
Decision Tree Model Specification (regression)

Main Arguments:
  cost_complexity = 0.0034

Computational engine: rpart
```

```
final_tree_fit <- final_tree_wkfl |>
  fit(hitters_train)
```

We used 10 fold cross validation repeated 5 times to determine the best value of $\alpha = 0.0034$ (`cost_complexity`) based on the model with the smallest RMSE (0.210). Then we created the final model (`final_tree_fit`) using cost complexity pruning and show the model in Figure 3.

```
final_tree_fit |>
  extract_fit_engine() |>
  rpart.plot::rpart.plot()
```

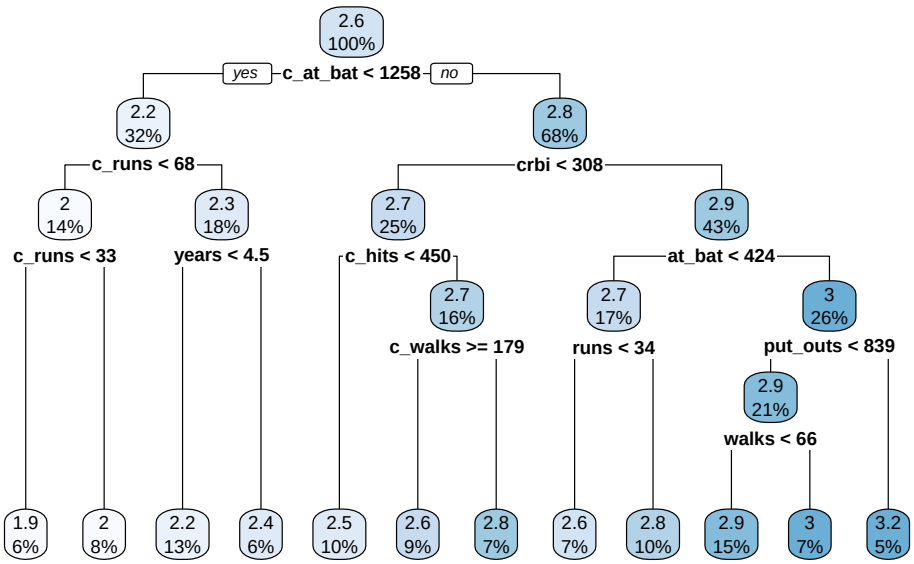


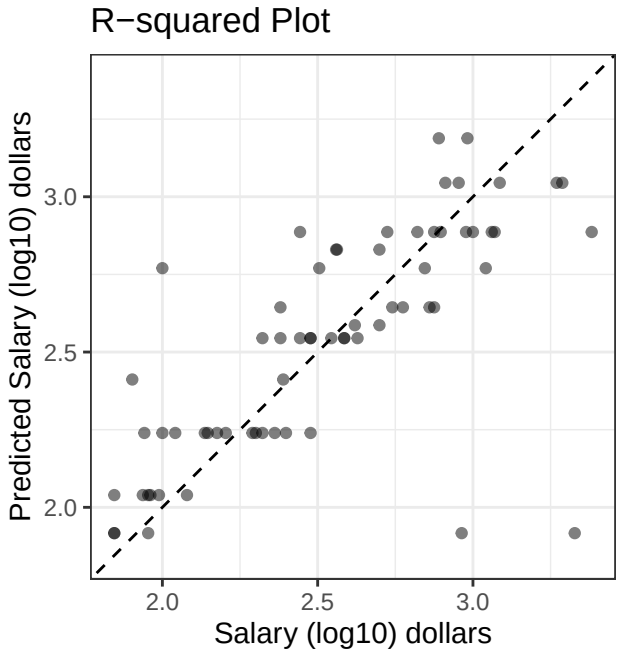
Figure 3: Final tree model after tuning the cost complexity parameter

Evaluating the Perfomance of your Final Tuned Model on the Test set

```
augment(final_tree_fit, new_data = hitters_test) |>
  metrics(truth = salary, estimate = .pred) -> R2
R2 |>
  knitr::kable()
```

.metric	.estimator	.estimate
rmse	standard	0.2962029
rsq	standard	0.5143753
mae	standard	0.1874979

```
augment(final_tree_fit, new_data = hitters_test) |>
  ggplot(aes(x = salary, y = .pred)) +
  geom_abline(lty = "dashed") +
  coord_obs_pred() +
  geom_point(alpha = 0.5) +
  theme_bw() +
  labs(x = "Salary (log10) dollars",
       y = "Predicted Salary (log10) dollars",
       title = "R-squared Plot")
```



Unfortunately, the model does not perform that well on the test set. The final tuned model has an R^2 value of 51.44% and a mean absolute error of $1,539.92.

Bagging

Decision trees suffer from high variance. This means that if we split the training data into two parts at random, and fit a decision tree to both halves, the results that we get could be quite different. In contrast, a procedure with low variance will yield similar results if applied repeatedly to distinct data sets; linear regression tends to have low variance, if the ratio of n to p is moderately large. Bootstrap aggregation, or **bagging**, is a general-purpose procedure for reducing the variance of a statistical learning method; we introduce it here because it is particularly useful and frequently used in the context of decision trees.

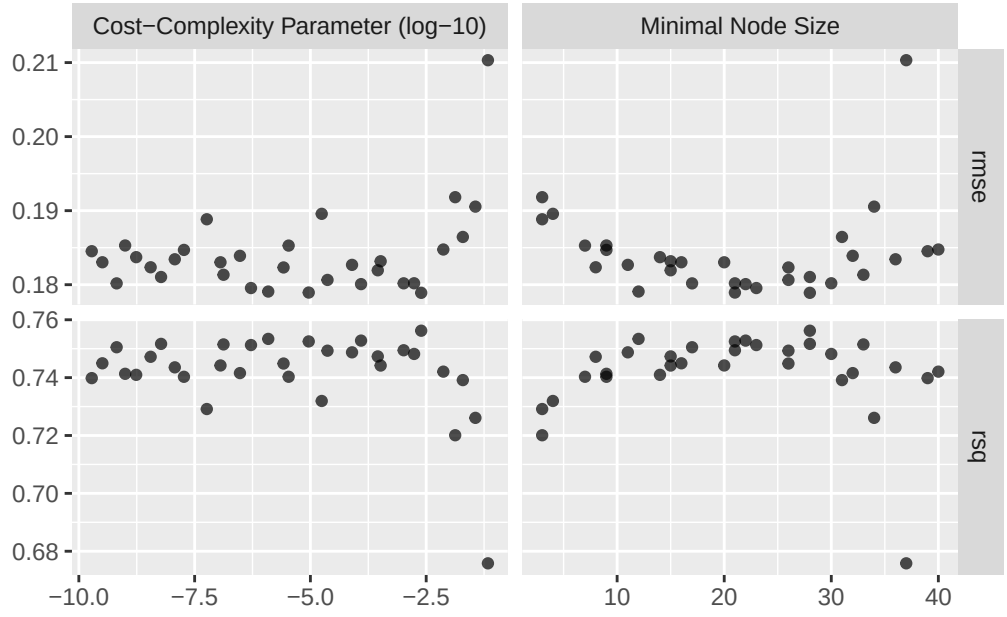
```
library(baguette)
bag_spec <-
  bag_tree(cost_complexity = tune(), min_n = tune())  |>
  set_engine('rpart')  |>
  set_mode('regression')
bag_recipe <- recipe(formula = salary ~ ., data = hitters_train)
bag_wkfl <- workflow() |>
  add_recipe(bag_recipe) |>
  add_model(bag_spec)
bag_wkfl
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: bag_tree()

-- Preprocessor ----------------------------------------------------------------
0 Recipe Steps

-- Model -----------------------------------------------------------------------
Bagged Decision Tree Model Specification (regression)

Main Arguments:
  cost_complexity = tune()
  min_n = tune()

Computational engine: rpart
```

```r
set.seed(8675)
bag_tune <-
  tune_grid(bag_wkfl, resamples = hitters_folds, grid = 32)
bag_tune
```

```
# Tuning results
# 10-fold cross-validation repeated 5 times
# A tibble: 50 x 5
   splits           id      id2    .metrics          .notes
   <list>           <chr>   <chr>  <list>            <list>
 1 <split [177/20]> Repeat1 Fold01 <tibble [64 x 6]> <tibble [0 x 3]>
 2 <split [177/20]> Repeat1 Fold02 <tibble [64 x 6]> <tibble [0 x 3]>
 3 <split [177/20]> Repeat1 Fold03 <tibble [64 x 6]> <tibble [0 x 3]>
 4 <split [177/20]> Repeat1 Fold04 <tibble [64 x 6]> <tibble [0 x 3]>
 5 <split [177/20]> Repeat1 Fold05 <tibble [64 x 6]> <tibble [0 x 3]>
 6 <split [177/20]> Repeat1 Fold06 <tibble [64 x 6]> <tibble [0 x 3]>
 7 <split [177/20]> Repeat1 Fold07 <tibble [64 x 6]> <tibble [0 x 3]>
 8 <split [178/19]> Repeat1 Fold08 <tibble [64 x 6]> <tibble [0 x 3]>
 9 <split [178/19]> Repeat1 Fold09 <tibble [64 x 6]> <tibble [0 x 3]>
10 <split [178/19]> Repeat1 Fold10 <tibble [64 x 6]> <tibble [0 x 3]>
# i 40 more rows
```

```r
autoplot(bag_tune)
```



```
show_best(bag_tune, metric = "rmse")
```

```
# A tibble: 5 x 8
  cost_complexity min_n .metric .estimator  mean     n std_err .config
            <dbl> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1     0.00247        28 rmse    standard   0.179    50 0.00739 Preprocessor1_Mo~
2     0.00000920     21 rmse    standard   0.179    50 0.00781 Preprocessor1_Mo~
3     0.00000123     12 rmse    standard   0.179    50 0.00772 Preprocessor1_Mo~
4     0.000000522    23 rmse    standard   0.180    50 0.00793 Preprocessor1_Mo~
5     0.000124       22 rmse    standard   0.180    50 0.00764 Preprocessor1_Mo~
```

```
bag_param <- tibble(cost_complexity = 0.002470553, min_n = 28)
final_bag_wkfl <- bag_wkfl |>
  finalize_workflow(bag_param)
final_bag_wkfl
```

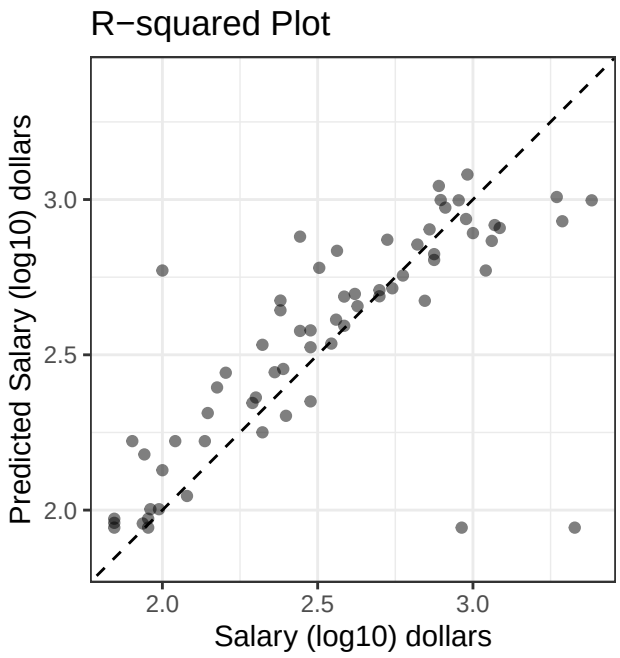
```
== Workflow ====================================================================
Preprocessor: Recipe
Model: bag_tree()

-- Preprocessor ----------------------------------------------------------------
0 Recipe Steps

-- Model -----------------------------------------------------------------------
Bagged Decision Tree Model Specification (regression)

Main Arguments:
  cost_complexity = 0.002470553
  min_n = 28

Computational engine: rpart
```

```
final_bag_fit <- final_bag_wkfl |>
  fit(hitters_train)
```

```
augment(final_bag_fit, new_data = hitters_test) |>
  metrics(truth = salary, estimate = .pred) -> R3
R3 |>
  knitr::kable()
```

.metric	.estimator	.estimate
rmse	standard	0.2811434
rsq	standard	0.5537454
mae	standard	0.1679286

```
augment(final_bag_fit, new_data = hitters_test) |>
  ggplot(aes(x = salary, y = .pred)) +
  geom_abline(lty = "dashed") +
  coord_obs_pred() +
  geom_point(alpha = 0.5) +
  theme_bw() +
  labs(x = "Salary (log10) dollars",
       y = "Predicted Salary (log10) dollars",
       title = "R-squared Plot")
```



The bagged model is an improvement over the decision tree model since the R^2 value increased to 55.37% and the mean absolute error decreased to \$1,472.07. While bagging can improve predictions for many regression methods, it is particularly useful for decision trees. To apply bagging to regression trees, we simply construct B regression trees using B bootstrapped training sets, and average the resulting predictions. Each individual tree has high variance, but low bias. Averaging these B trees reduces the variance. Bagging has been demonstrated to

give impressive improvements in accuracy by combining together hundreds or even thousands of trees into a single procedure.

Random Forests

Random forests provide an improvement over bagged trees by way of a small tweak that decorrelates the trees. As in bagging, we build a number of decision trees on bootstrapped training samples. But when building these decision trees, each time a split in a tree is considered, a random sample of m predictors is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors. A fresh sample of m predictors is taken at each split, and typically we choose $m = \sqrt{p}$ for classification problems and $p/3$ for regression problems—that is, the number of predictors considered at each split is approximately equal to the square root of the total number of predictors for classification problems or the number of predictors is roughly $p/3$ at each split for regression problems.

In other words, in building a. random forest, at each split in the tree, the algorithm is not even allowed to consider a majority of the available predictors. This may sound crazy, but it has a clever rationale. Suppose that there is one very strong predictor in the data set, along with a number of other moderately stromg predictors. Then in the collection of bagged trees, most or all of the trees will use this strong predictor in the top split. Consequently, all of the bagged trees will look quite similar to each other. Hence the predictions from the bagged trees will be highly correlated. Unfortunately, averaging many highly correlated trees does not lead to as large of a reduction in variance as averaging many uncorrelated quantities. In particular, this means that bagging will not lead to a substantial reduction in variance over a single tree in this setting.

Random forest overcome this problem by forcing each split to consider only a subset of the rpedictors. There fore, on average $(p - m)/p$ of the splits will not even consider the strong predictor, and so other predictors will have more of a chance. We can think of this process as **decorrelating** the trees, thereby making the average of the resulting trees less variable and hence more reliable.

```
ranger_spec <- rand_forest(mtry = tune(),
                           min_n = tune(),
                           trees = 500) |>
  set_mode("regression")  |>
  set_engine("ranger",
             importance = "impurity")
ranger_spec
```

```
Random Forest Model Specification (regression)
```

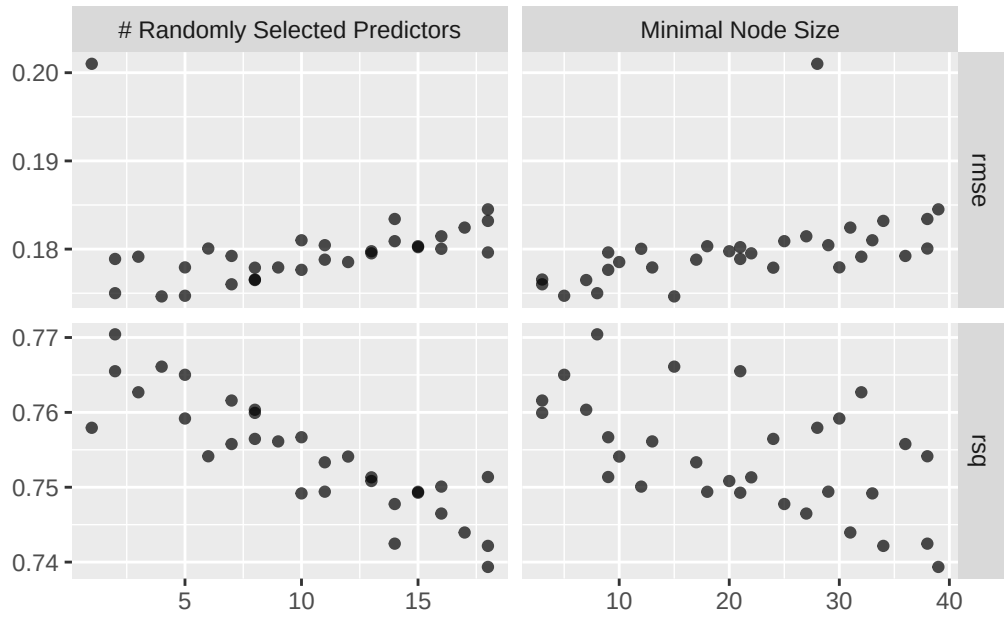
```
Main Arguments:
  mtry = tune()
  trees = 500
  min_n = tune()

Engine-Specific Arguments:
  importance = impurity

Computational engine: ranger
```

```
ranger_recipe <- recipe(formula = salary ~ ., data = hitters_train)

ranger_workflow <-
  workflow()  |>
  add_recipe(ranger_recipe)  |>
  add_model(ranger_spec)
```

```
set.seed(8675309)
ranger_tune <-
  tune_grid(ranger_workflow, resamples = hitters_folds, grid = 32)
ranger_tune
```

```
# Tuning results
# 10-fold cross-validation repeated 5 times
# A tibble: 50 x 5
   splits           id      id2    .metrics          .notes
   <list>           <chr>   <chr>  <list>            <list>
 1 <split [177/20]> Repeat1 Fold01 <tibble [62 x 6]> <tibble [0 x 3]>
 2 <split [177/20]> Repeat1 Fold02 <tibble [62 x 6]> <tibble [0 x 3]>
 3 <split [177/20]> Repeat1 Fold03 <tibble [62 x 6]> <tibble [0 x 3]>
 4 <split [177/20]> Repeat1 Fold04 <tibble [62 x 6]> <tibble [0 x 3]>
 5 <split [177/20]> Repeat1 Fold05 <tibble [62 x 6]> <tibble [0 x 3]>
 6 <split [177/20]> Repeat1 Fold06 <tibble [62 x 6]> <tibble [0 x 3]>
 7 <split [177/20]> Repeat1 Fold07 <tibble [62 x 6]> <tibble [0 x 3]>
 8 <split [178/19]> Repeat1 Fold08 <tibble [62 x 6]> <tibble [0 x 3]>
 9 <split [178/19]> Repeat1 Fold09 <tibble [62 x 6]> <tibble [0 x 3]>
10 <split [178/19]> Repeat1 Fold10 <tibble [62 x 6]> <tibble [0 x 3]>
# i 40 more rows
```

```
autoplot(ranger_tune)
```




```
show_best(ranger_tune, metric = "rmse")
```

```
# A tibble: 5 x 8
   mtry min_n .metric .estimator  mean     n std_err .config
  <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1     4    15 rmse    standard   0.175    50 0.00729 Preprocessor1_Model21
2     5     5 rmse    standard   0.175    50 0.00742 Preprocessor1_Model25
3     2     8 rmse    standard   0.175    50 0.00676 Preprocessor1_Model04
4     7     3 rmse    standard   0.176    50 0.00754 Preprocessor1_Model16
5     8     7 rmse    standard   0.176    50 0.00760 Preprocessor1_Model20
```

```
ranger_param <- tibble(mtry = 4, min_n = 15)
final_ranger_wkfl <- ranger_workflow |>
  finalize_workflow(ranger_param)
final_ranger_wkfl
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: rand_forest()

-- Preprocessor ----------------------------------------------------------------
0 Recipe Steps
```

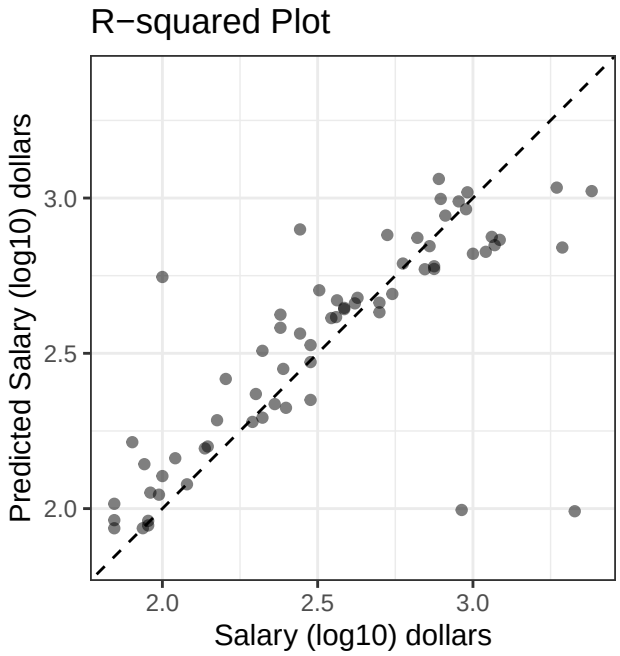
```
-- Model -----------------------------------------------------------------------
Random Forest Model Specification (regression)

Main Arguments:
  mtry = 4
  trees = 500
  min_n = 15

Engine-Specific Arguments:
  importance = impurity

Computational engine: ranger
```

```
final_ranger_fit <- final_ranger_wkfl |>
  fit(hitters_train)
```

```
augment(final_ranger_fit, new_data = hitters_test) |>
  metrics(truth = salary, estimate = .pred) -> R4
R4 |>
  knitr::kable()
```

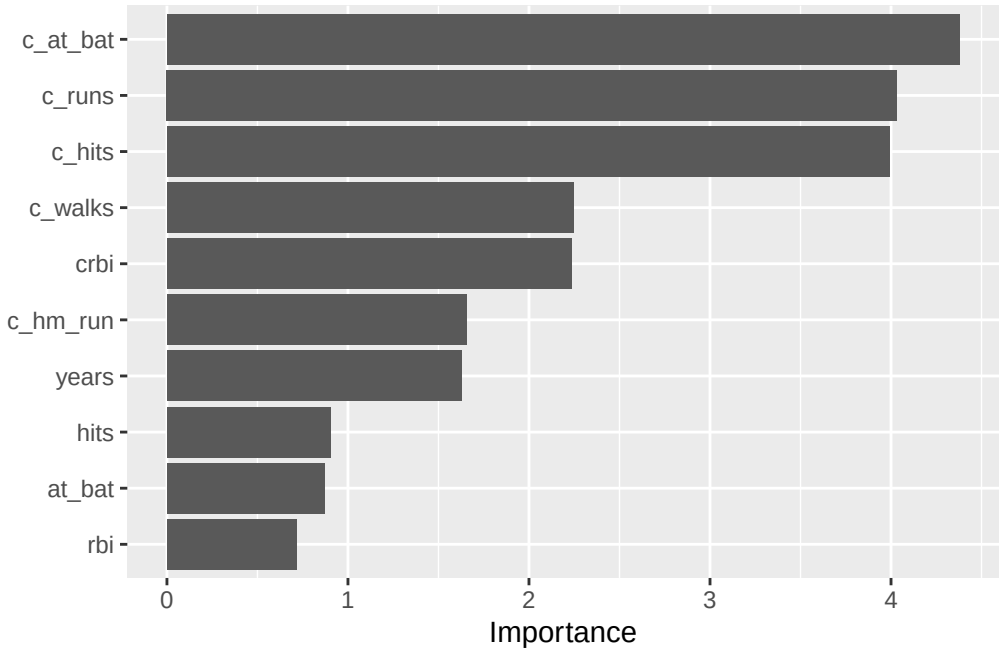
.metric	.estimator	.estimate
rmse	standard	0.2676943
rsq	standard	0.5891579
mae	standard	0.1542156

```
augment(final_ranger_fit, new_data = hitters_test) |>
  ggplot(aes(x = salary, y = .pred)) +
  geom_abline(lty = "dashed") +
  coord_obs_pred() +
  geom_point(alpha = 0.5) +
  theme_bw() +
  labs(x = "Salary (log10) dollars",
       y = "Predicted Salary (log10) dollars",
       title = "R-squared Plot")
```



The random forest model is an improvement over the bagged tree model since the R^2 value increased to 58.92% and the mean absolute error decreased to \$1,426.32.

```
vip::vip(final_ranger_fit)
```



Boosting

Recall that baggin involves creating multiple copies of the original training data set using the bootstrap, fittin a separate decision tree to each copy, and then combining all of the trees in order to create a single predictive model.. Notably, each tree is built on a bootstrap data set, independent of the other trees. Boosting works in a similar way, except that the trees are grown **sequentially**: each tree is grown using information from previously grown trees. Boosting does not involve bootstrap sampling; instead each tree is fit on a modified version of the original data set.

Like bagging, boosting involves combining a large number of decision trees $\hat{f}^1, \ldots, \hat{f}^B$.

Boosting for Regression Trees Algorithm

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   (a) Fit a tree $\hat{f}^b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   (b) Update $\hat{f}$ by adding a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$$
   (c) Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x).$$
3. Output the boosted model,
   $$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$$

What is the idea behind this procedure? Unlike fitting a single large decision tree to the data, which amounts to **fitting the data hard** and potentially overfitting, the boosting approach instead **learns slowly**. Given the current model, we fit a decision tree to the residuals from the model. That is, we fir a tree using the current residuals, rather than the outcome Y, as the response. We then add this new decision tree into the fitted function in order to update the residuals. Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm. By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals. In general, statistical learning approaches the **learn slowly** tend to perform well. Note that in boosting, unlike in bagging, the construction of each tree depends strongly on the trees that have already been grown.

Boosting Tuning Parameters

1. The number of trees B. Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select B.

2. The shrinkage parameter λ, a small positive number. This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.

3. The number d of splits in each tree, which controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree is a stump, consisting of a single split. In this case, the boosted ensembel is fitting and additive model, since each term involves only a single variable. More generally d is the **interaction depth**, and controls the interaction order of the boosted model, since d splits can involve at most d variables.

```
xgboost_spec <-
  boost_tree(trees = tune(), min_n = tune(), tree_depth = tune(),
             learn_rate = tune(), loss_reduction = tune(),
             sample_size = tune()) |>
  set_mode("regression") |>
  set_engine("xgboost")
xgboost_spec
```

```
Boosted Tree Model Specification (regression)

Main Arguments:
  trees = tune()
  min_n = tune()
  tree_depth = tune()
  learn_rate = tune()
  loss_reduction = tune()
  sample_size = tune()

Computational engine: xgboost
```

```
xgboost_recipe <-
  recipe(formula = salary ~  . , data = hitters_train) |>
  step_normalize(all_numeric_predictors()) |>
```

```
  step_dummy(all_nominal_predictors(), one_hot = TRUE) |>
  step_zv(all_predictors())
xgboost_recipe
```

```
xgboost_workflow <-
  workflow() |>
  add_recipe(xgboost_recipe) |>
  add_model(xgboost_spec)
xgboost_workflow
```

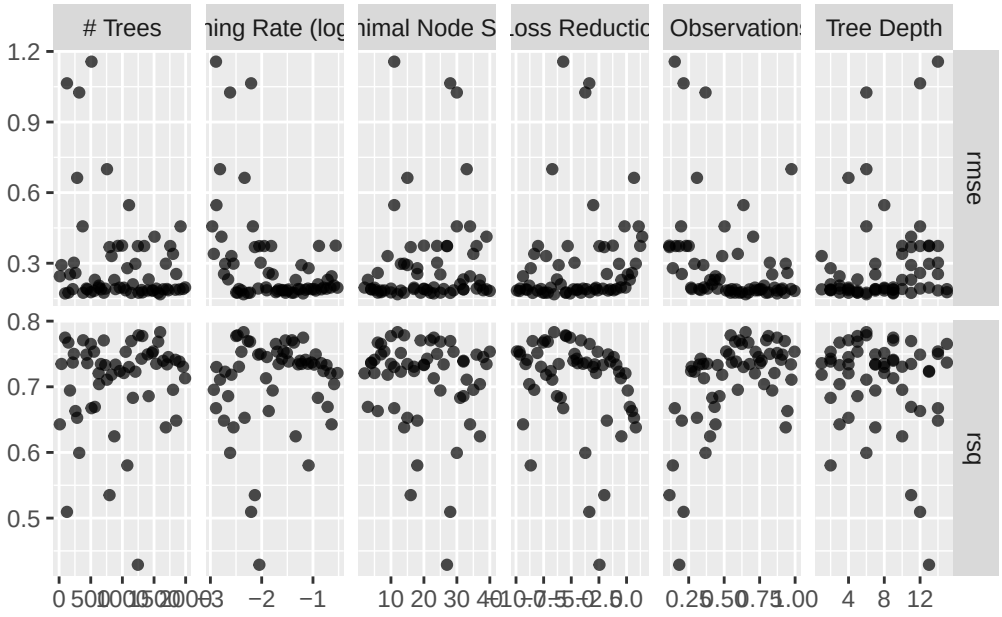
```
== Workflow ====================================================================
Preprocessor: Recipe
Model: boost_tree()

-- Preprocessor ----------------------------------------------------------------
3 Recipe Steps

* step_normalize()
* step_dummy()
* step_zv()

-- Model -----------------------------------------------------------------------
Boosted Tree Model Specification (regression)

Main Arguments:
  trees = tune()
  min_n = tune()
  tree_depth = tune()
  learn_rate = tune()
  loss_reduction = tune()
  sample_size = tune()

Computational engine: xgboost
```

```
set.seed(8675309)
xgboost_tune <-
  tune_grid(xgboost_workflow, resamples = hitters_folds, grid = 64)
xgboost_tune
```

```
# Tuning results
```

```
# 10-fold cross-validation repeated 5 times
# A tibble: 50 x 5
   splits           id      id2    .metrics            .notes
   <list>           <chr>   <chr>  <list>              <list>
 1 <split [177/20]> Repeat1 Fold01 <tibble [128 x 10]> <tibble [1 x 3]>
 2 <split [177/20]> Repeat1 Fold02 <tibble [128 x 10]> <tibble [1 x 3]>
 3 <split [177/20]> Repeat1 Fold03 <tibble [128 x 10]> <tibble [1 x 3]>
 4 <split [177/20]> Repeat1 Fold04 <tibble [128 x 10]> <tibble [1 x 3]>
 5 <split [177/20]> Repeat1 Fold05 <tibble [128 x 10]> <tibble [1 x 3]>
 6 <split [177/20]> Repeat1 Fold06 <tibble [128 x 10]> <tibble [1 x 3]>
 7 <split [177/20]> Repeat1 Fold07 <tibble [128 x 10]> <tibble [1 x 3]>
 8 <split [178/19]> Repeat1 Fold08 <tibble [128 x 10]> <tibble [1 x 3]>
 9 <split [178/19]> Repeat1 Fold09 <tibble [128 x 10]> <tibble [1 x 3]>
10 <split [178/19]> Repeat1 Fold10 <tibble [128 x 10]> <tibble [1 x 3]>
# i 40 more rows

There were issues with some computations:

  - Warning(s) x50: A correlation computation is required, but `estimate` is constant...

Run `show_notes(.Last.tune.result)` for more information.
```

```
autoplot(xgboost_tune)
```



```
show_best(xgboost_tune, metric = "rmse")
```

```
# A tibble: 5 x 12
  trees min_n tree_depth learn_rate loss_reduction sample_size .metric
  <int> <int>      <int>      <dbl>          <dbl>       <dbl> <chr>
1  1597    12          6    0.00444  0.000000282         0.651 rmse
2    94    23          9    0.0642   0.00000786          0.873 rmse
3  1141    28         11    0.00539  0.00000000320       0.927 rmse
4   380    22          4    0.0389   0.0000000404        0.796 rmse
5   706    19          9    0.0291   0.0000752           0.609 rmse
# i 5 more variables: .estimator <chr>, mean <dbl>, n <int>, std_err <dbl>,
#   .config <chr>
```

```
xgboost_param <- tibble(trees = 1597, min_n = 12, tree_depth = 6,
                        learn_rate = 0.00444 ,loss_reduction = 0.000000282,
                        sample_size = 0.651)
final_xgboost_wkfl <- xgboost_workflow |>
  finalize_workflow(xgboost_param)
final_xgboost_wkfl
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: boost_tree()

-- Preprocessor ----------------------------------------------------------------
3 Recipe Steps

* step_normalize()
* step_dummy()
* step_zv()

-- Model -----------------------------------------------------------------------
Boosted Tree Model Specification (regression)

Main Arguments:
  trees = 1597
  min_n = 12
  tree_depth = 6
  learn_rate = 0.00444
  loss_reduction = 2.82e-07
```

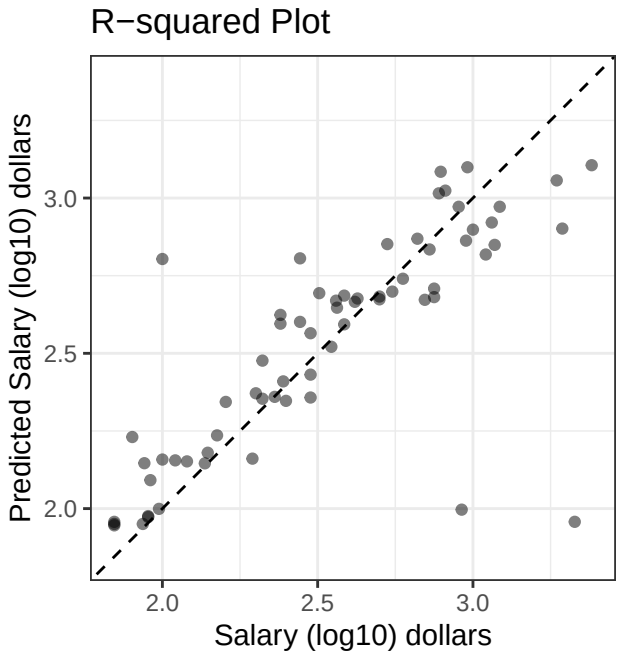
```
  sample_size = 0.651

Computational engine: xgboost
```

```
final_xgboost_fit <- final_xgboost_wkfl |>
  fit(hitters_train)
```

```
augment(final_xgboost_fit, new_data = hitters_test) |>
  metrics(truth = salary, estimate = .pred) -> R5
R5 |>
  knitr::kable()
```

.metric	.estimator	.estimate
rmse	standard	0.2684125
rsq	standard	0.5891675
mae	standard	0.1556772

```
augment(final_xgboost_fit, new_data = hitters_test) |>
  ggplot(aes(x = salary, y = .pred)) +
  geom_abline(lty = "dashed") +
  coord_obs_pred() +
  geom_point(alpha = 0.5) +
  theme_bw() +
  labs(x = "Salary (log10) dollars",
       y = "Predicted Salary (log10) dollars",
       title = "R-squared Plot")
```



The boosted model is very similar to the random forest model with an R^2 value of 58.92% and a mean absolute error of \$1,431.12.