PSTAT 131 - Homework Assignment 6

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Tree Based Models

For this assignment, we will continue working with the file `"pokemon.csv"`, found in `/data`. The file is from Kaggle: https://www.kaggle.com/abcsds/pokemon.

The Pokémon franchise encompasses video games, TV shows, movies, books, and a card game. This data set was drawn from the video game series and contains statistics about 721 Pokémon, or "pocket monsters." In Pokémon games, the user plays as a trainer who collects, trades, and battles Pokémon to (a) collect all the Pokémon and (b) become the champion Pokémon trainer.

Each Pokémon has a primary type (some even have secondary types). Based on their type, a Pokémon is strong against some types, and vulnerable to others. (Think rock, paper, scissors.) A Fire-type Pokémon, for example, is vulnerable to Water-type Pokémon, but strong against Grass-type.

The goal of this assignment is to build a statistical learning model that can predict the **primary type** of a Pokémon based on its generation, legendary status, and six battle statistics.

Read in the file and familiarize yourself with the variables using pokemon_codebook.txt.

```
library(tidymodels)
library(tidyverse)
library(ggplot2)
library(corrr)
library(klaR)
library(glmnet)
library(MASS)
library(discrim)
library(poissonreg)
library(janitor)
library(corrplot)

library(rpart.plot)
library(vip)
library(randomForest)
library(xgboost)
tidymodels_prefer()
```

Exercise 1

Read in the data and set things up as in Homework 5:

```
data <- read_csv("data/pokemon.csv")
data %>% head(5)
```

```
## # A tibble: 5 x 13
##     `#` Name    `Type 1` `Type 2` Total    HP Attack Defense `Sp. Atk` `Sp. Def`
##   <dbl> <chr>   <chr>    <chr>    <dbl> <dbl>  <dbl>   <dbl>     <dbl>     <dbl>
## 1     1 Bulbas~ Grass    Poison     318    45     49      49        65        65
## 2     2 Ivysaur Grass    Poison     405    60     62      63        80        80
## 3     3 Venusa~ Grass    Poison     525    80     82      83       100       100
## 4     3 Venusa~ Grass    Poison     625    80    100     123       122       120
## 5     4 Charma~ Fire     <NA>       309    39     52      43        60        50
## # ... with 3 more variables: Speed <dbl>, Generation <dbl>, Legendary <lgl>
```

- Use `clean_names()`
- Filter out the rarer Pokémon types
- Convert `type_1` and `legendary` to factors

```
# Clean Names
data <- data %>% clean_names()

# Filter out rarer Pokemon types
data <- data %>% filter(type_1 == "Bug" | type_1 == "Fire" |
                          type_1 == "Grass" | type_1 == "Normal" |
                          type_1 == "Water" | type_1 == "Psychic")

# Convert type_1, legendary, generation to factors
data$type_1 <- as.factor(data$type_1)
data$generation <- as.factor(data$generation)
data$legendary <- as.factor(data$legendary)


data %>% head(5)
```

```
## # A tibble: 5 x 13
##   number name       type_1 type_2 total    hp attack defense sp_atk sp_def speed
##    <dbl> <chr>      <fct>  <chr>  <dbl> <dbl>  <dbl>   <dbl>  <dbl>  <dbl> <dbl>
## 1      1 Bulbasaur  Grass  Poison   318    45     49      49     65     65    45
## 2      2 Ivysaur    Grass  Poison   405    60     62      63     80     80    60
## 3      3 Venusaur   Grass  Poison   525    80     82      83    100    100    80
## 4      3 VenusaurM~ Grass  Poison   625    80    100     123    122    120    80
## 5      4 Charmander Fire   <NA>     309    39     52      43     60     50    65
## # ... with 2 more variables: generation <fct>, legendary <fct>
```

Do an initial split of the data; you can choose the percentage for splitting. Stratify on the outcome variable.

```
# Setting Seed
set.seed(3478)

# Stratified Initial Split
data_split <- initial_split(data = data,
                            prop = 0.8,
                            strata = type_1)
```

```
train <- training(data_split)
test <- testing(data_split)
```

Fold the training set using v-fold cross-validation, with `v = 5`. Stratify on the outcome variable.

```
folds <- vfold_cv(data = train,
                  v = 5,
                  strata = type_1)
```

Set up a recipe to predict `type_1` with `legendary`, `generation`, `sp_atk`, `attack`, `speed`, `defense`, `hp`, and `sp_def`:

- Dummy-code `legendary` and `generation`;
- Center and scale all predictors.

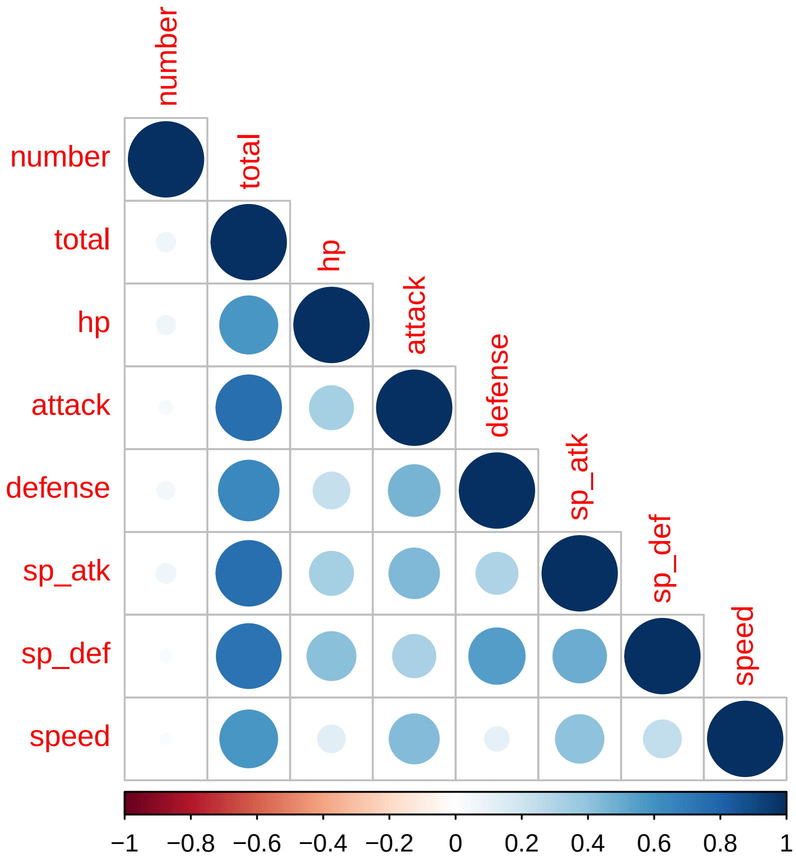
```
pokemon_recipe <- recipe(formula = type_1 ~ legendary + generation + sp_atk + attack + speed + defense +
                         data = train) %>%
  step_dummy(legendary) %>%
  step_dummy(generation) %>%
  step_normalize(all_predictors())
```

Exercise 2

Create a correlation matrix of the training set, using the `corrplot` package. *Note: You can choose how to handle the continuous variables for this plot; justify your decision(s).*

```
data %>%
  select(is.numeric) %>%
  cor() %>%
  corrplot(type = "lower")
```

```
## Warning: Predicate functions must be wrapped in `where()`.
##
##   # Bad
##   data %>% select(is.numeric)
##
##   # Good
##   data %>% select(where(is.numeric))
##
## i Please update your code.
## This message is displayed once per session.
```



What relationships, if any, do you notice? Do these relationships make sense to you?

The number of a Pokemon has no relation to any of the attributes of the Pokemon. Speed is slightly positively correlated with attack and special attack. Special defense is slightly correlated with defense and special attack. Special attack is slightly correlated with attack. Defense is slightly correlated with attack. When looking at the influence of individual attributes on the total score, it seems to be that attack, special attack, and special defense are the most important. There are no negatively correlated variables.

Exercise 3

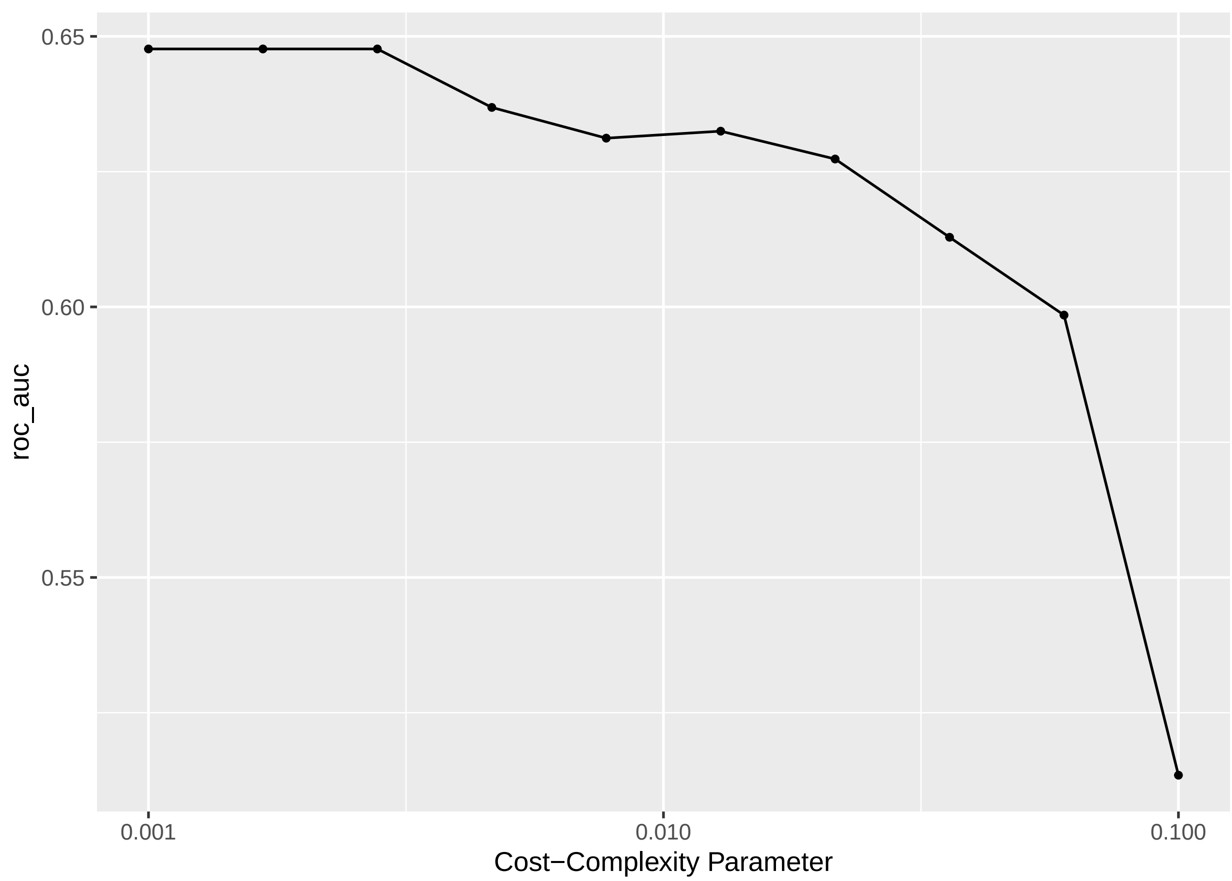
First, set up a decision tree model and workflow. Tune the `cost_complexity` hyperparameter. Use the same levels we used in Lab 7 – that is, `range = c(-3, -1)`. Specify that the metric we want to optimize is `roc_auc`.

```
pokemon_tree_spec <- decision_tree(cost_complexity = tune()) %>%
  set_mode("classification") %>%
  set_engine("rpart")

pokemon_tree_workflow <- workflow() %>%
  add_recipe(pokemon_recipe) %>%
  add_model(pokemon_tree_spec)

param_grid_tree <- grid_regular(cost_complexity(range = c(-3, -1)), levels = 10)

tune_res_tree <- tune_grid(
```

```
  pokemon_tree_workflow,
  resamples = folds,
  grid = param_grid_tree,
  metrics = metric_set(roc_auc))
```

Print an `autoplot()` of the results. What do you observe? Does a single decision tree perform better with a smaller or larger complexity penalty?

```
autoplot(tune_res_tree)
```



In general, as cost-complexity goes up the overall roc_auc of our model goes down. There seems to be no change in cost complexities of 0.001, 0.0016, 0.0027 (roc_auc of 0.6477), but after that the model starts preforming worse and worse until it eventually reaches an roc_auc of 0.5135 at the largest cost_complexity of 1.

Exercise 4

What is the `roc_auc` of your best-performing pruned decision tree on the folds? *Hint: Use `collect_metrics()` and `arrange()`.*

```
# the best cost_complexity in terms of roc_auc is the top result
collect_metrics(tune_res_tree) %>% arrange(desc(mean))
```

```
## # A tibble: 10 x 7
```

```
##    cost_complexity .metric .estimator  mean     n std_err .config
##              <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
##  1         0.001   roc_auc hand_till  0.648     5  0.0185 Preprocessor1_Model01
##  2         0.00167 roc_auc hand_till  0.648     5  0.0185 Preprocessor1_Model02
##  3         0.00278 roc_auc hand_till  0.648     5  0.0185 Preprocessor1_Model03
##  4         0.00464 roc_auc hand_till  0.637     5  0.0219 Preprocessor1_Model04
##  5         0.0129  roc_auc hand_till  0.632     5  0.0177 Preprocessor1_Model06
##  6         0.00774 roc_auc hand_till  0.631     5  0.0218 Preprocessor1_Model05
##  7         0.0215  roc_auc hand_till  0.627     5  0.0179 Preprocessor1_Model07
##  8         0.0359  roc_auc hand_till  0.613     5  0.0151 Preprocessor1_Model08
##  9         0.0599  roc_auc hand_till  0.598     5  0.0143 Preprocessor1_Model09
## 10         0.1     roc_auc hand_till  0.513     5  0.0135 Preprocessor1_Model10
```

The roc_auc of the best-performing pruned decision tree was 0.6477, which has a corresponding cost_complexity of 0.001, 0.001668, 0.002783 (all had the same performance).

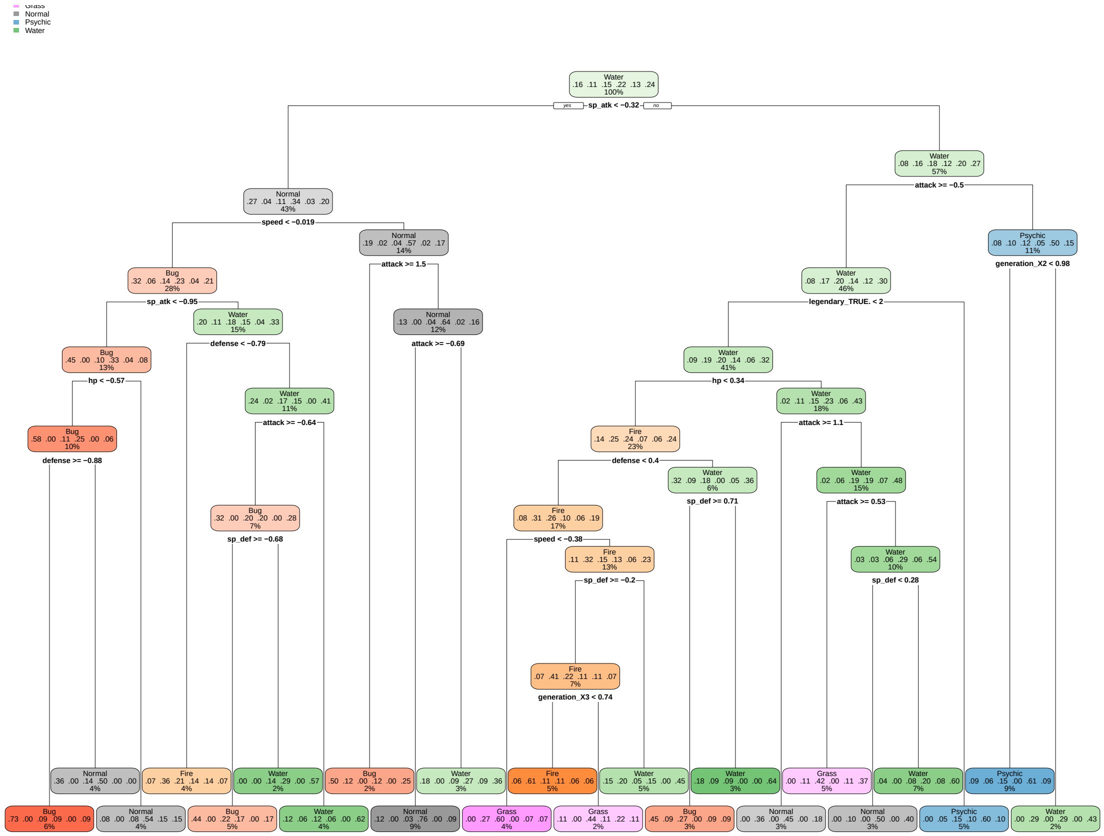
```
best_parameter_tree <- select_best(tune_res_tree, metric = "roc_auc")
best_parameter_tree
```

```
## # A tibble: 1 x 2
##   cost_complexity .config
##             <dbl> <chr>
## 1           0.001 Preprocessor1_Model01
```

Exercise 5

Using `rpart.plot`, fit and visualize your best-performing pruned decision tree with the *training* set.

```
#finalizing workflow and fitting that model to the training data
pokemon_tree_final <- finalize_workflow(pokemon_tree_workflow, best_parameter_tree)
pokemon_tree_final_fit <- fit(pokemon_tree_final, data = train)

# visualizing best performing pruned decision tree
pokemon_tree_final_fit %>% extract_fit_engine() %>% rpart.plot(roundint = FALSE)
```



Exercise 5

Now set up a random forest model and workflow. Use the `ranger` engine and set `importance = "impurity"`. Tune `mtry`, `trees`, and `min_n`. Using the documentation for `rand_forest()`, explain in your own words what each of these hyperparameters represent.

```
pokemon_rf_spec <- rand_forest(mtry=tune(), trees=tune(), min_n=tune()) %>%
  set_engine("randomForest", importance = TRUE) %>%
  set_mode("classification")

pokemon_rf_workflow <- workflow() %>%
  add_recipe(pokemon_recipe) %>%
  add_model(pokemon_rf_spec)
```

mtry represents the number of randomly selected variables we give each tree to make decisions with.

trees represents the number of trees we will create in our forest

min_n represents the minimum # data points in each node that are required for it to further split

Create a regular grid with 8 levels each. You can choose plausible ranges for each hyperparameter. Note that `mtry` should not be smaller than 1 or larger than 8. **Explain why not. What type of model would `mtry = 8` represent?**

```r
# create regular grid
param_grid_rf <- grid_regular(mtry(range = c(1, 8)),
                              trees(range = c(1, 10)),
                              min_n(range = c(1, 10)),
                              levels = 8)
param_grid_rf
```

```
## # A tibble: 512 x 3
##     mtry trees min_n
##    <int> <int> <int>
##  1     1     1     1
##  2     2     1     1
##  3     3     1     1
##  4     4     1     1
##  5     5     1     1
##  6     6     1     1
##  7     7     1     1
##  8     8     1     1
##  9     1     2     1
## 10     2     2     1
## # ... with 502 more rows
```

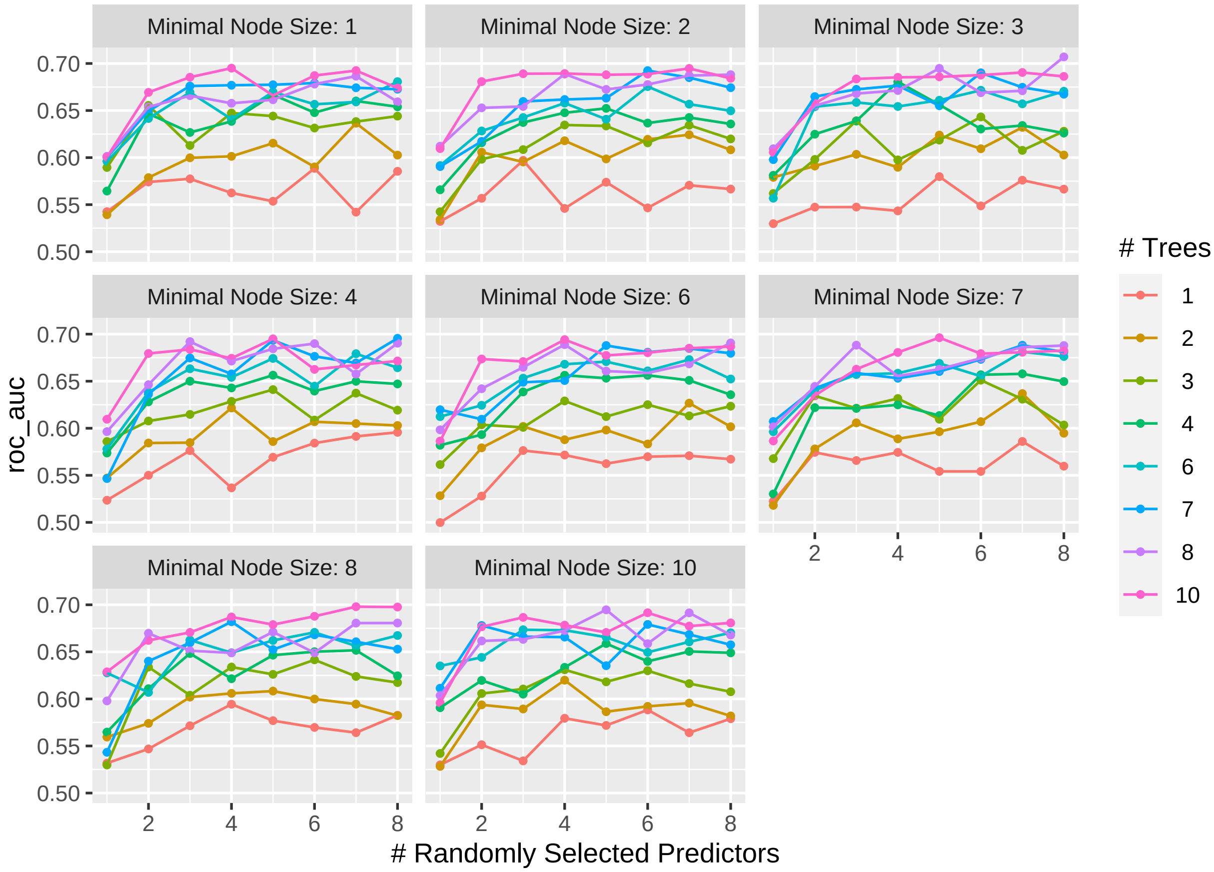
We have 9 predictors in our dataset, so if we set mtry = 9 we are no longer training a random forest model and instead are utilizing bagging, because there is no subset of the predictors that is randomly chosen (its using all available predictors).

Exercise 6

Specify `roc_auc` as a metric. Tune the model and print an `autoplot()` of the results. What do you observe? What values of the hyperparameters seem to yield the best performance?

```r
tune_res_rf <- tune_grid(
  pokemon_rf_workflow,
  resamples = folds,
  grid = param_grid_rf,
  metrics = metric_set(roc_auc))
```

```r
autoplot(tune_res_rf)
```



Across all values of of min_n, the best performing models had 7, 8, or 10 trees. Minimal node size of 3, 8, and 4 seemed to perform similarly well, with roc_auc very close to 0.7. For most models, increasing the # of randomly selected predictors to at least 3 seem to bring the greatest benefit in performance, after which some models flatten out and others go back and forth in terms of roc_auc.

Exercise 7

What is the `roc_auc` of your best-performing random forest model on the folds? *Hint: Use `collect_metrics()` and `arrange()`.*

```
# the best parameters are the top results
collect_metrics(tune_res_rf) %>% arrange(desc(mean))
```

```
## # A tibble: 512 x 9
##     mtry trees min_n .metric .estimator  mean     n std_err .config
##    <int> <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
##  1     8     8     3 roc_auc hand_till  0.707     5 0.0149  Preprocessor1_Model~
##  2     7    10     8 roc_auc hand_till  0.698     5 0.0198  Preprocessor1_Model~
##  3     8    10     8 roc_auc hand_till  0.698     5 0.00786 Preprocessor1_Model~
##  4     5    10     7 roc_auc hand_till  0.696     5 0.0141  Preprocessor1_Model~
##  5     8     7     4 roc_auc hand_till  0.696     5 0.0116  Preprocessor1_Model~
##  6     4    10     1 roc_auc hand_till  0.695     5 0.0185  Preprocessor1_Model~
##  7     5    10     4 roc_auc hand_till  0.695     5 0.0108  Preprocessor1_Model~
##  8     5     8     3 roc_auc hand_till  0.695     5 0.0117  Preprocessor1_Model~
##  9     7    10     2 roc_auc hand_till  0.695     5 0.0157  Preprocessor1_Model~
```

```
## 10     5     8    10 roc_auc hand_till  0.695     5 0.0181  Preprocessor1_Model~
## # ... with 502 more rows
```

The best performing random forest model (mtry = 8, trees = 8, min_n = 3) had an roc_auc of 0.7070.

```
best_parameter_rf <- select_best(tune_res_rf, metric = "roc_auc")
best_parameter_rf
```

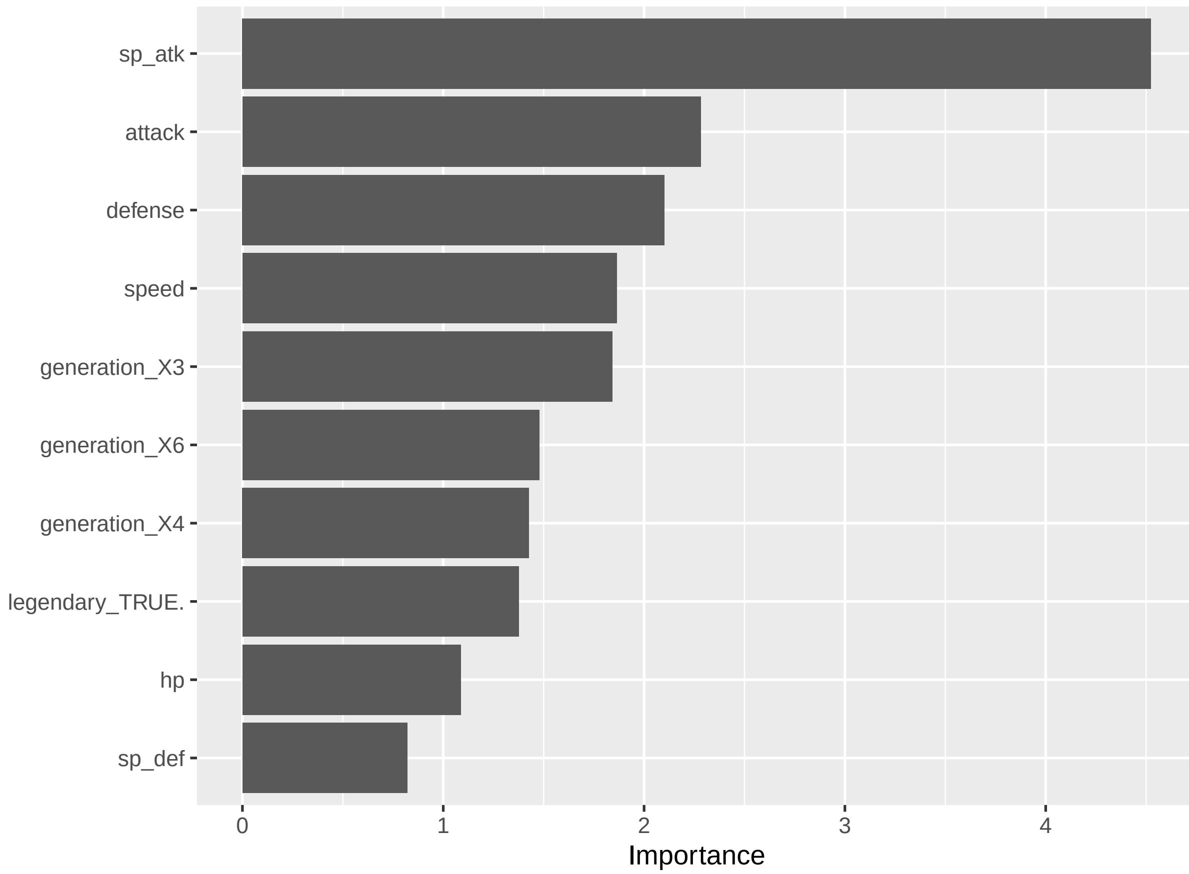
```
## # A tibble: 1 x 4
##    mtry trees min_n .config
##   <int> <int> <int> <chr>
## 1     8     8     3 Preprocessor1_Model184
```

Exercise 8

Create a variable importance plot, using `vip()`, with your best-performing random forest model fit on the *training* set.

Which variables were most useful? Which were least useful? Are these results what you expected, or not?

```
#finalizing workflow and fitting that model to the training data
pokemon_rf_final <- finalize_workflow(pokemon_rf_workflow, best_parameter_rf)
pokemon_rf_final_fit <- fit(pokemon_rf_final, data = train)

# visualizing decision tree
pokemon_rf_final_fit %>% extract_fit_engine() %>% vip()
```



The variables that is the most useful is by far special attack, which is almost 3x as important as the following variables of attack, special defense, and speed. The variables that are the least useful are generation_x2 and generation_x5. This is sort've what I expected because in the games certain pokemon are known for their special attack stats, so it would be a very useful predictor to be identifying the type of a pokemon based on that stat profile.

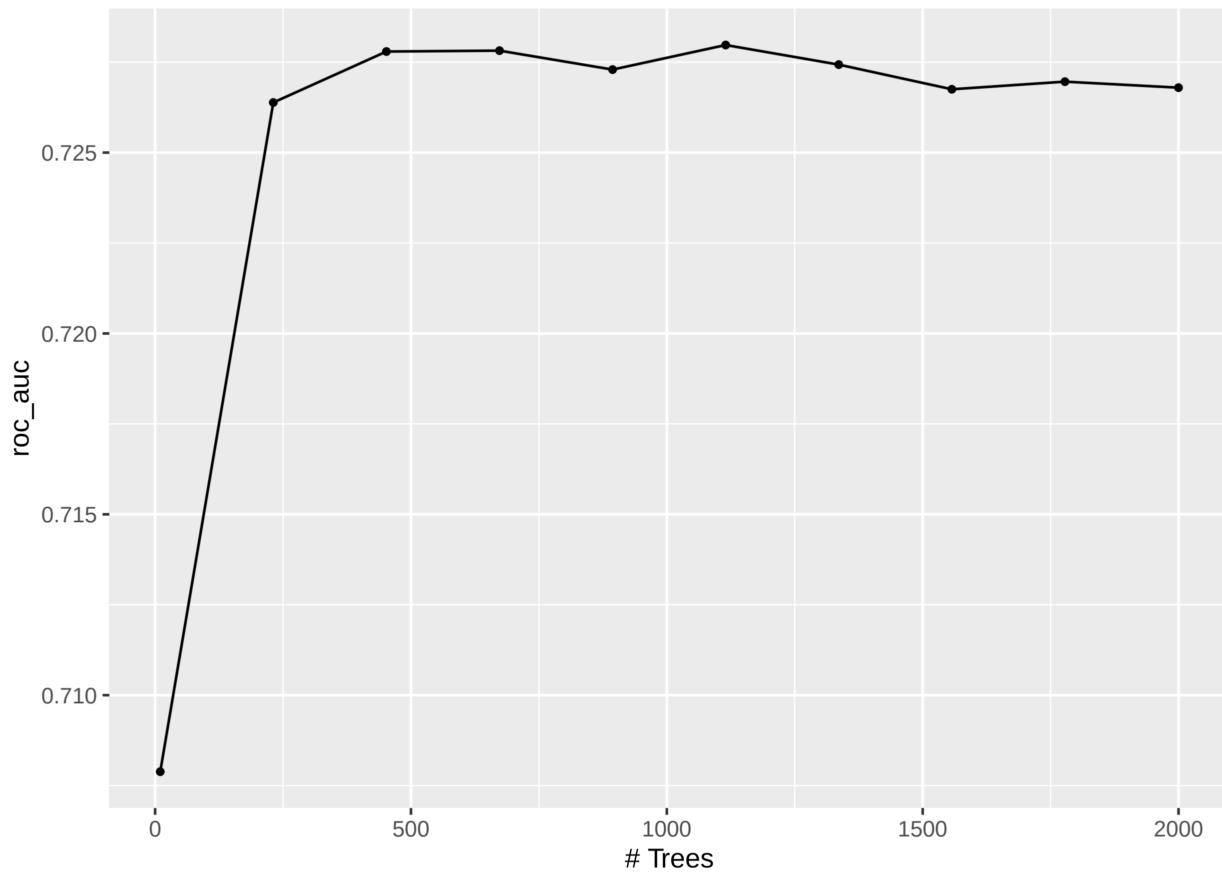
Exercise 9

Finally, set up a boosted tree model and workflow. Use the `xgboost` engine. Tune `trees`. Create a regular grid with 10 levels; let `trees` range from 10 to 2000. Specify `roc_auc` and again print an `autoplot()` of the results.

```
# Set up boosted tree specification
pokemon_boosted_spec <- boost_tree(trees=tune()) %>%
  set_engine("xgboost") %>%
  set_mode("classification")

#boosted tree workflow
pokemon_boosted_workflow <- workflow() %>%
  add_recipe(pokemon_recipe) %>%
  add_model(pokemon_boosted_spec)

#boosted tree tuning grid
param_grid_boosted <- grid_regular(trees(range = c(10, 2000)),
                                   levels = 10)
```

```
#resulting values with hyperparameter tuning across CV
tune_res_boosted <- tune_grid(
  pokemon_boosted_workflow,
  resamples = folds,
  grid = param_grid_boosted,
  metrics = metric_set(roc_auc))
```

```
autoplot(tune_res_boosted)
```



What do you observe?

We observe that there is an initial jump of roc_auc from the 0-300 tree range, after which we essentially get the same or even potentially worse roc_auc from 300-2000 trees.

What is the `roc_auc` of your best-performing boosted tree model on the folds? *Hint: Use `collect_metrics()` and `arrange()`.*

```
# the best parameters are the top results
collect_metrics(tune_res_boosted) %>% arrange(desc(mean))
```

```
## # A tibble: 10 x 7
##    trees .metric .estimator  mean     n std_err .config
##    <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
##  1  1115 roc_auc hand_till  0.728     5 0.00851 Preprocessor1_Model06
```

```
##  2   673 roc_auc hand_till  0.728     5 0.00865 Preprocessor1_Model04
##  3   452 roc_auc hand_till  0.728     5 0.00830 Preprocessor1_Model03
##  4  1336 roc_auc hand_till  0.727     5 0.00859 Preprocessor1_Model07
##  5   894 roc_auc hand_till  0.727     5 0.00821 Preprocessor1_Model05
##  6  1778 roc_auc hand_till  0.727     5 0.00838 Preprocessor1_Model09
##  7  2000 roc_auc hand_till  0.727     5 0.00833 Preprocessor1_Model10
##  8  1557 roc_auc hand_till  0.727     5 0.00860 Preprocessor1_Model08
##  9   231 roc_auc hand_till  0.726     5 0.00645 Preprocessor1_Model02
## 10    10 roc_auc hand_till  0.708     5 0.00965 Preprocessor1_Model01
```

```
best_paramater_boosted <- select_best(tune_res_boosted, metric = "roc_auc")
best_paramater_boosted
```

```
## # A tibble: 1 x 2
##   trees .config
##   <int> <chr>
## 1  1115 Preprocessor1_Model06
```

Exercise 10

Display a table of the three ROC AUC values for your best-performing pruned tree, random forest, and boosted tree models. Which performed best on the folds? Select the best of the three and use `select_best()`, `finalize_workflow()`, and `fit()` to fit it to the *testing* set.

```
roc_aucs <- bind_rows(best_parameter_tree, best_parameter_rf, best_paramater_boosted)
roc_aucs <- roc_aucs %>% add_column('model' = c("Pruned Decision Tree", "Random Forest", "Boosted Tree")
                        'roc_auc' = c(0.6477, 0.7070, 0.7280))
roc_aucs[, c("model", ".config", "cost_complexity", "mtry", "trees", "min_n", "roc_auc")]
```

```
## # A tibble: 3 x 7
##   model                .config         cost_complexity  mtry trees min_n roc_auc
##   <chr>                <chr>                     <dbl> <int> <int> <int>   <dbl>
## 1 Pruned Decision Tree Preprocessor1_~           0.001    NA    NA    NA   0.648
## 2 Random Forest        Preprocessor1_~          NA         8     8     3   0.707
## 3 Boosted Tree         Preprocessor1_~          NA        NA  1115    NA   0.728
```

```
pokemon_final <- finalize_workflow(pokemon_boosted_workflow, best_paramater_boosted)
pokemon_final_fit <- fit(pokemon_final, data = train)
```

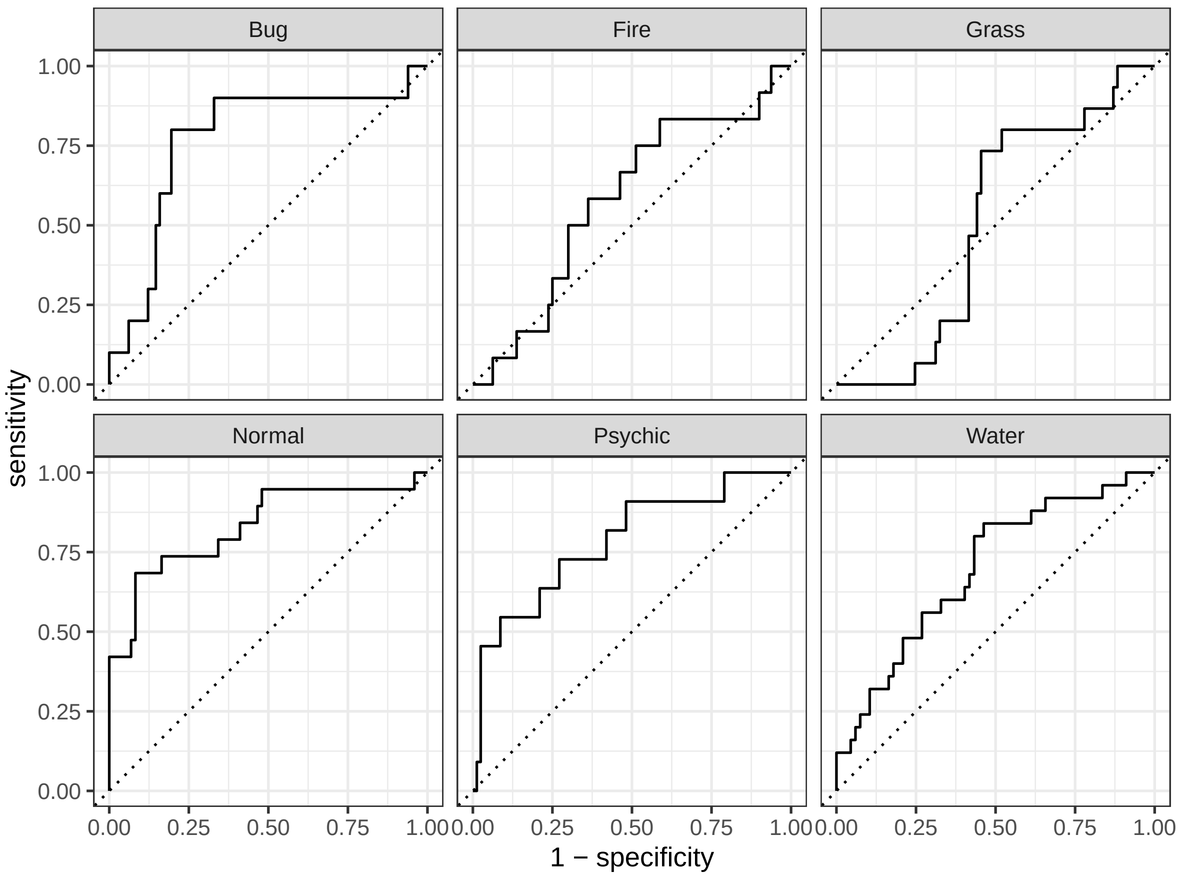
Of all the methods we trained, the Boosted Tree model with 1115 trees performed the best on the folds with an roc_auc of 0.7280.

Print the AUC value of your best-performing model on the testing set. Print the ROC curves. Finally, create and visualize a confusion matrix heat map.

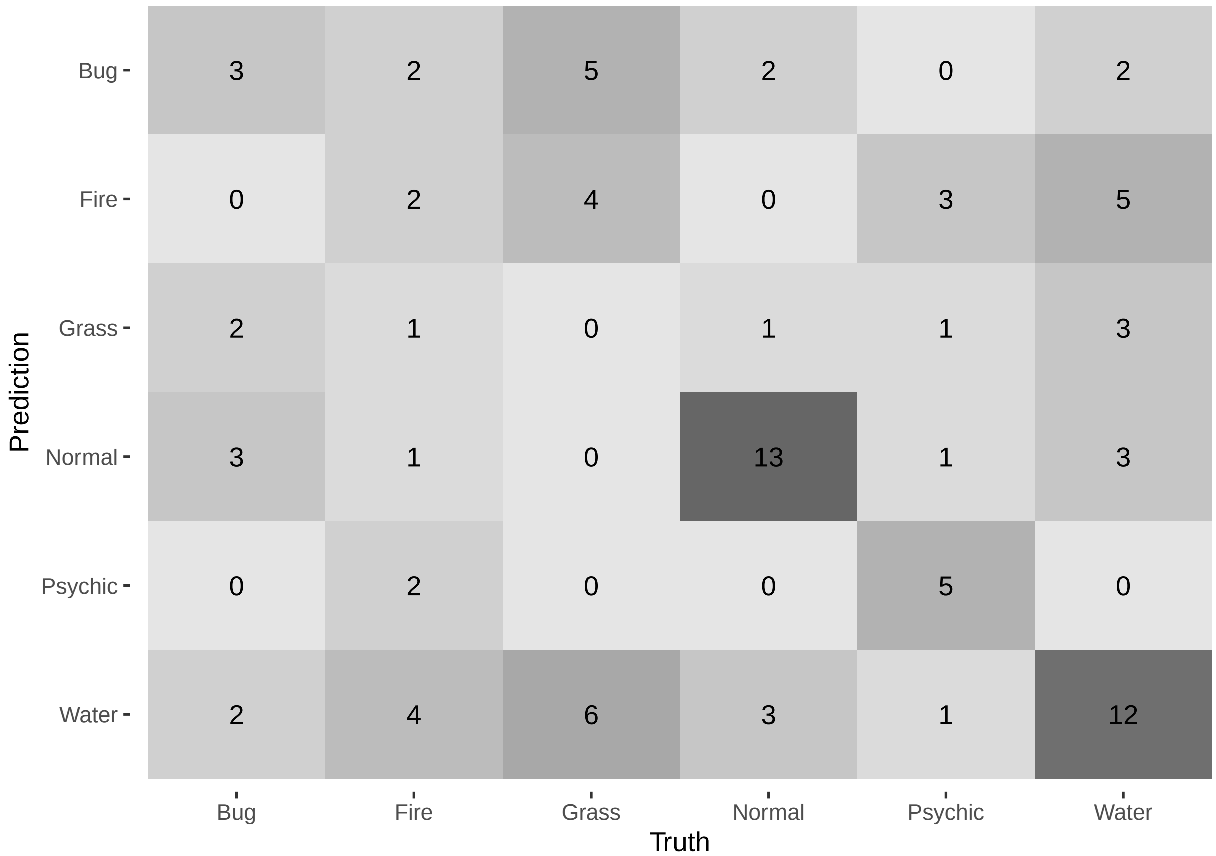
```
testing_roc_auc <- augment(pokemon_final_fit, new_data = test) %>%
  roc_auc(truth = type_1, estimate = c(.pred_Bug, .pred_Fire, .pred_Grass, .pred_Normal, .pred_Psychic,
testing_roc_auc
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 roc_auc hand_till      0.692
```

```
roc_curves <- augment(pokemon_final_fit, new_data = test) %>%
  roc_curve(truth = type_1, estimate = c(.pred_Bug, .pred_Fire, .pred_Grass, .pred_Normal, .pred_Psychic
  autoplot()
roc_curves
```




```
final_model_conf <- augment(pokemon_final_fit, new_data = test) %>%
  conf_mat(truth = type_1, estimate = .pred_class) %>%
  autoplot(type = "heatmap")
final_model_conf
```



Which classes was your model most accurate at predicting? Which was it worst at?

The model was extremely good at predicting Normal types with 6 misclassifications and 13 correct ones. This was followed by water with 13 misclassifications and 12 correct ones. Psychic was also very similar with 6 misclassifications and 5 correct ones. Bug types had 3 correct classifications with 7 misclassifications, and Fire had 2 correct classifications with 10 misclassifications. Grass was by far the worst class to predict because there were 0 correct classifications, and 15 misclassifications.