

## Tree-Based Models

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# Homework 6

PSTAT 131/231

Code ▼

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```
library(tidymodels)
library(tidyverse)
library(ISLR) # For the Smarket data set
library(ISLR2) # For the Bikeshare data set
library(discrim)
library(poissonreg)
library(corr)
library(klaR) # for naive bayes
library(forcats)
library(corrplot)
library(pROC)
library(recipes)
library(rsample)
library(parsnip)
library(workflows)
library(janitor)
library(glmnet)
library(rpart.plot)
library(vip)
library(janitor)
library(randomForest)
library(xgboost)
tidymodels_prefer()
```

## 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> (<https://www.kaggle.com/abcsds/pokemon>).

The Pokémon (<https://www.pokemon.com/us/>) 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 (<https://bulbapedia.bulbagarden.net/wiki/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.



Fig 1. Houndoom, a Dark/Fire-type canine Pokémon from Generation II.

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.

**Note: Fitting ensemble tree-based models can take a little while to run. Consider running your models outside of the .Rmd, storing the results, and loading them in your .Rmd to minimize time to knit.**

## Exercise 1

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

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

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

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

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.

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```

# read dataset
pokemon_raw <- read.csv("Pokemon.csv")

# clean_name()
pokemon1 <- clean_names(pokemon_raw)

# filter out rarer
pokemon <- pokemon1[which(pokemon1$type_1 == "Bug" | pokemon1$type_1 == "Fire" |
                          pokemon1$type_1 == "Grass" | pokemon1$type_1 == "Normal" |
                          pokemon1$type_1 == "Water" | pokemon1$type_1 == "Psychic"), ]

# convert factors
pokemon <- pokemon %>%
  mutate(type_1 = factor(type_1),
         legendary = factor(legendary))

# initial split
set.seed(2022)
pokemon_split <- pokemon %>%
  initial_split(strata = type_1, prop = 0.7)
pokemon_train <- training(pokemon_split)
pokemon_test <- testing(pokemon_split)

# set up cross-validation
pokemon_fold <- vfold_cv(pokemon_train, v = 5, strata = type_1)

# set up recipe
pokemon_recipe <- recipe(type_1 ~ legendary + generation + sp_atk +
                          attack + speed + defense + hp + sp_def, pokemon_train) %>%
  step_dummy(legendary, generation) %>%
  step_center(all_predictors()) %>%
  step_scale(all_predictors())

```

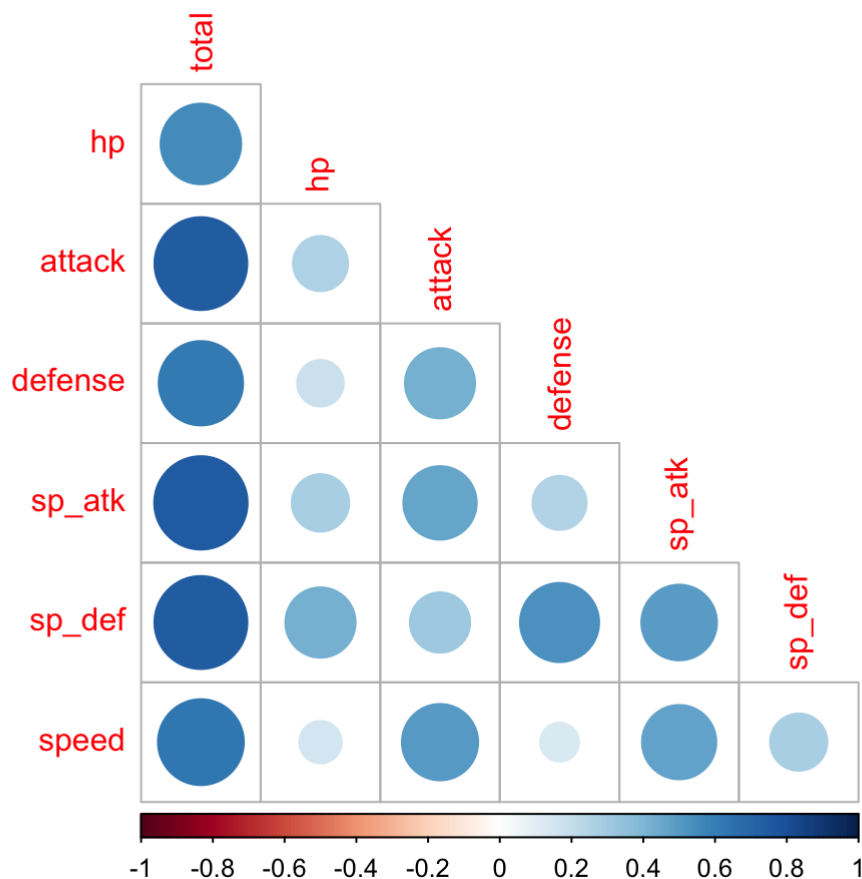
## Exercise 2

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).*

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

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```
pokemon_train %>%  
  select(where(is.numeric), -x,-generation) %>%  
  cor(use = "complete.obs") %>%  
  corrplot(type = "lower", diag = FALSE)
```



*I remove variable x and generation since x is index and generation is not continuous.*

*Almost all the variables have positive relationship to other, especially, all variables are high positive relate to total which make sense to me that the higher variable a pokemon has the more stronger pokemon is.*

## 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`.

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

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```
# set up model and workflow
tree_spec <- decision_tree() %>%
  set_engine("rpart")

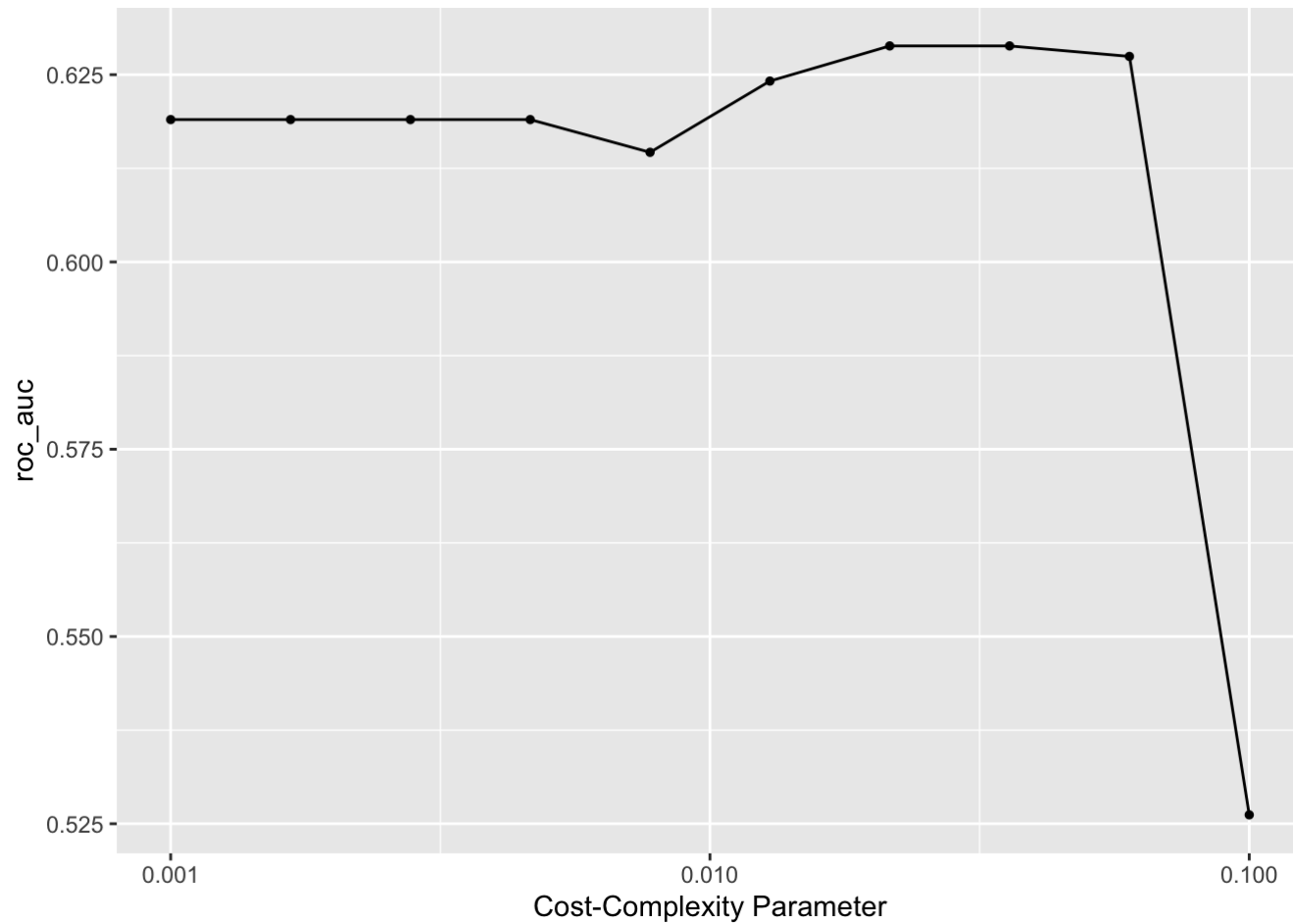
class_tree_spec <- tree_spec %>%
  set_mode("classification")

class_tree_wf <- workflow() %>%
  add_recipe(pokemon_recipe) %>%
  add_model(class_tree_spec %>%
    set_args(cost_complexity = tune()))

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

tune_res <- tune_grid(
  class_tree_wf,
  resamples = pokemon_fold,
  grid = param_grid,
  metrics = metric_set(roc_auc)
)

# print results
autoplot(tune_res)
```



The `roc_auc` stay 0.615 and doesn't change a lot with the parameter increasing, and reach the peak when parameter around 0.02. The `roc_auc` start dropping after parameter around 0.075.

We can see a single decision tree perform better with a larger complexity penalty.

## Exercise 4

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

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```
arrange(collect_metrics(tune_res), desc(mean))
```

```
## # A tibble: 10 × 7
##   cost_complexity .metric .estimator mean      n std_err .config
##   <dbl> <chr>    <chr>    <dbl> <int>   <dbl> <chr>
## 1      0.0215 roc_auc hand_till 0.629     5 0.0110 Preprocessor1_Model07
## 2      0.0359 roc_auc hand_till 0.629     5 0.0110 Preprocessor1_Model08
## 3      0.0599 roc_auc hand_till 0.627     5 0.0131 Preprocessor1_Model09
## 4      0.0129 roc_auc hand_till 0.624     5 0.0153 Preprocessor1_Model06
## 5      0.001  roc_auc hand_till 0.619     5 0.00885 Preprocessor1_Model01
## 6      0.00167 roc_auc hand_till 0.619     5 0.00885 Preprocessor1_Model02
## 7      0.00278 roc_auc hand_till 0.619     5 0.00885 Preprocessor1_Model03
## 8      0.00464 roc_auc hand_till 0.619     5 0.00885 Preprocessor1_Model04
## 9      0.00774 roc_auc hand_till 0.615     5 0.0141 Preprocessor1_Model05
## 10     0.1      roc_auc hand_till 0.526     5 0.0262 Preprocessor1_Model10
```

The best model is 0.6288 roc\_auc along with 0.0215 parameter.

## Exercise 5

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

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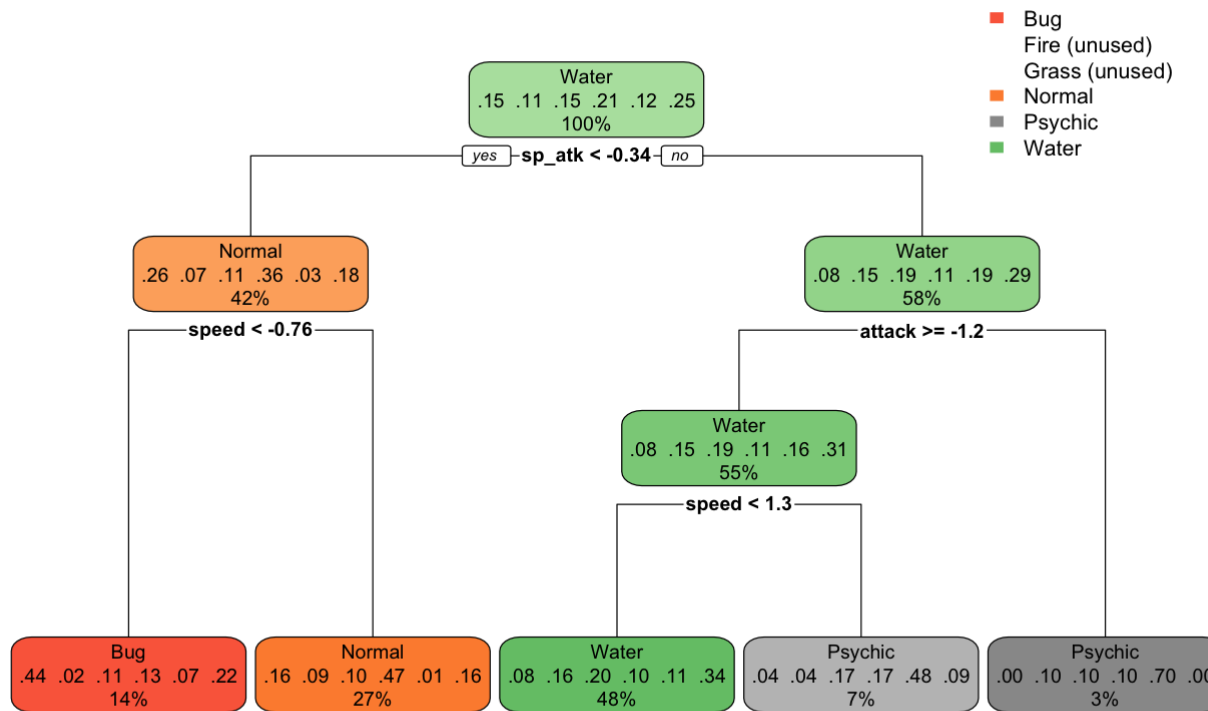
```
best_complexity <- select_best(tune_res)

class_tree_final <- finalize_workflow(class_tree_wf, best_complexity)

class_tree_final_fit <- fit(class_tree_final, data = pokemon_train)

class_tree_final_fit %>%
  extract_fit_engine() %>%
  rpart.plot()
```





## 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.

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?**

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```
rf_spec <- rand_forest(mtry = tune(), trees = tune(), min_n = tune()) %>%
  set_engine("ranger", importance = "impurity") %>%
  set_mode("classification")

rf_wf <- workflow() %>%
  add_model(rf_spec) %>%
  add_recipe(pokemon_recipe)

param_grid2 <- grid_regular(mtry(range = c(1, 8)),
                           trees(range = c(10, 1000)),
                           min_n(range = c(1, 8)),
                           levels = 8)
```

- `mtry`: The number of predictors that will be randomly sampled with each split of the tree models.
- `trees`: The number of trees in the ensemble tree models.
- `min_n`: minimum number of data points in a node required to make a split. *mtry should not be smaller than 1 or larger than 8, since we only have 8 predictors. If we set it to 8, it will represent the bagging model.*

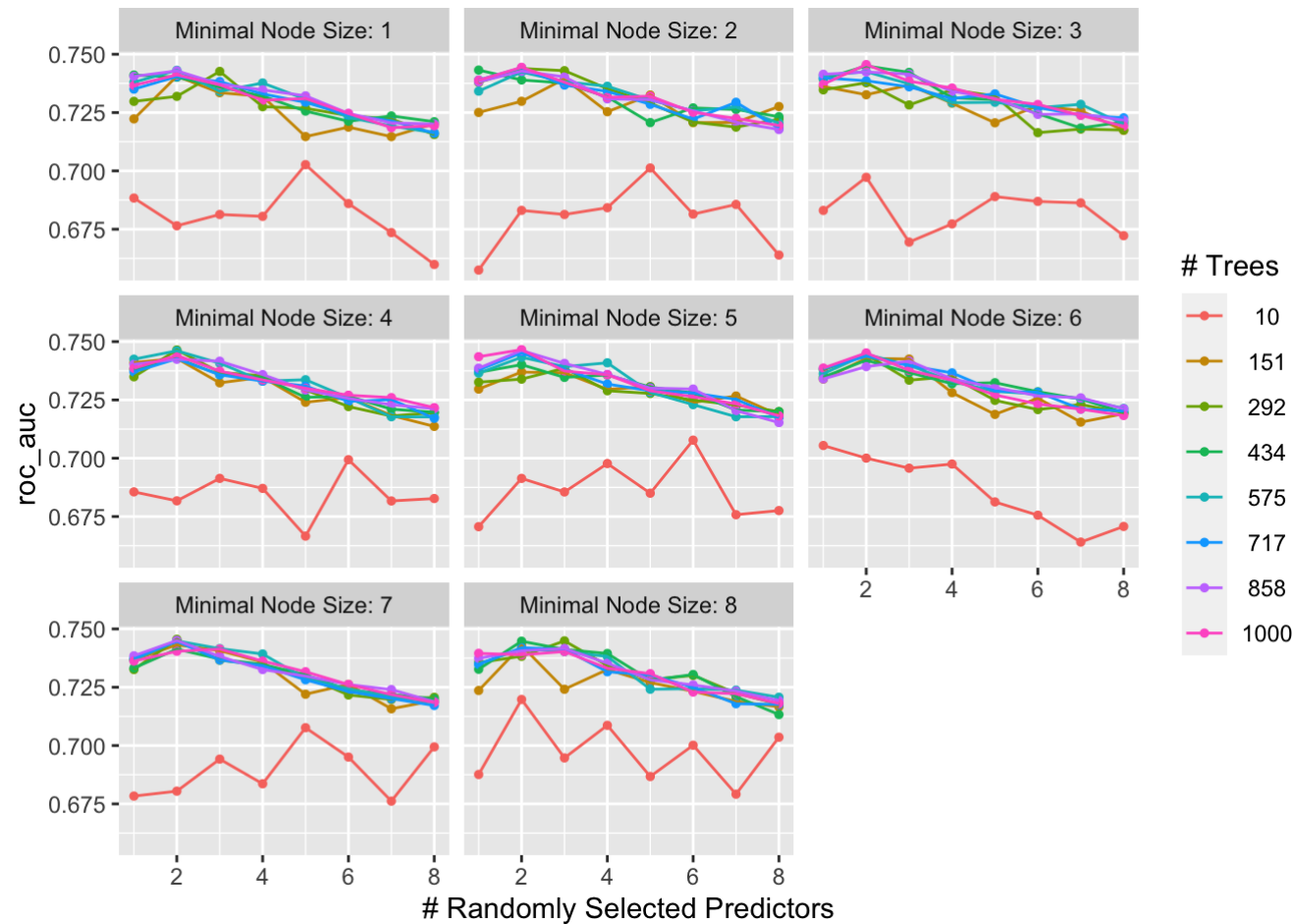
## Exercise 6

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?

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```
tune_res <- tune_grid(
  rf_wf,
  resamples = pokemon_fold,
  grid = param_grid2,
  metrics = metric_set(roc_auc)
)

# print results
autoplot(tune_res)
```



The best model's roc\_auc is 0.7489 which contains 2 mtry, 574 trees, and 4 min\_n.

In general, The more trees we add the better performance we have, and the roc\_auc and the number of predictors are negative relative.

## Exercise 7

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

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```
arrange(collect_metrics(tune_res), desc(mean))
```

```
## # A tibble: 512 × 9
##   mtry trees min_n .metric .estimator mean      n std_err .config
##   <int> <int> <int> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1     2  1000     5 roc_auc hand_till 0.747     5  0.0128 Preprocessor1_Model...
## 2     2   292     4 roc_auc hand_till 0.746     5  0.0138 Preprocessor1_Model...
## 3     2   858     5 roc_auc hand_till 0.746     5  0.0125 Preprocessor1_Model...
## 4     2   575     4 roc_auc hand_till 0.746     5  0.0134 Preprocessor1_Model...
## 5     2  1000     3 roc_auc hand_till 0.746     5  0.0111 Preprocessor1_Model...
## 6     2   292     7 roc_auc hand_till 0.746     5  0.0131 Preprocessor1_Model...
## 7     2   717     5 roc_auc hand_till 0.745     5  0.0123 Preprocessor1_Model...
## 8     2  1000     6 roc_auc hand_till 0.745     5  0.0110 Preprocessor1_Model...
## 9     2   858     7 roc_auc hand_till 0.745     5  0.0125 Preprocessor1_Model...
## 10    2   434     3 roc_auc hand_till 0.745     5  0.0130 Preprocessor1_Model...
## # ... with 502 more rows
```

The best model's `roc_auc` is 0.7489 which contains 2 `mtry`, 575 `trees`, and 4 `min_n`.

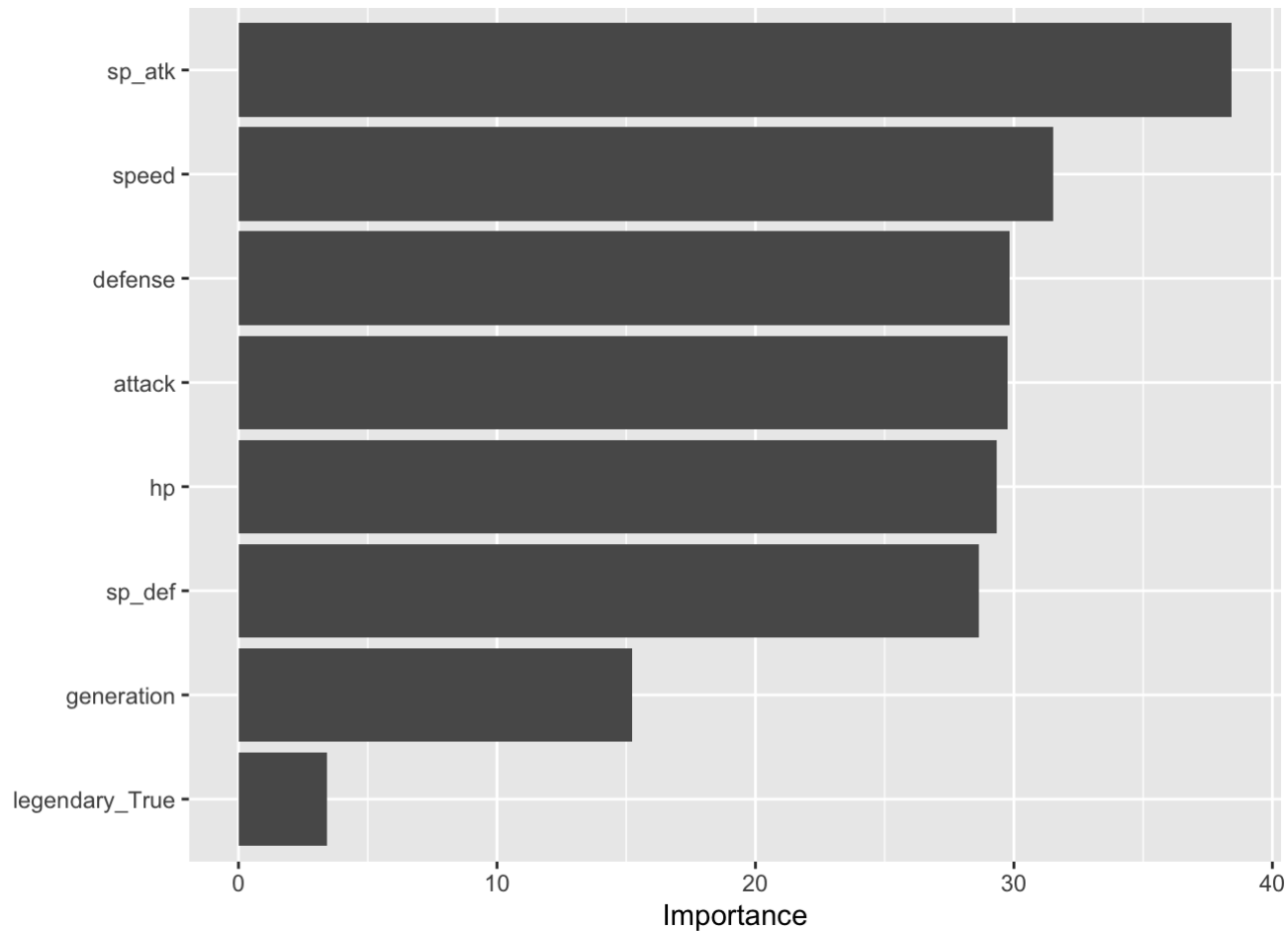
## Exercise 8

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?

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```
best_complexity <- select_best(tune_res, metric = "roc_auc")
pokemon_final <- finalize_workflow(rf_wf, best_complexity)
rf_fit <- fit(pokemon_final, data = pokemon_train)
rf_fit %>%
  extract_fit_engine() %>%
  vip()
```



*The most useful variable is `sp_atk` and the least useful variable is `legendary_True`, I'm so surprise that the `sp_atk` is the most useful variable, and the other variables are under my consideration.*

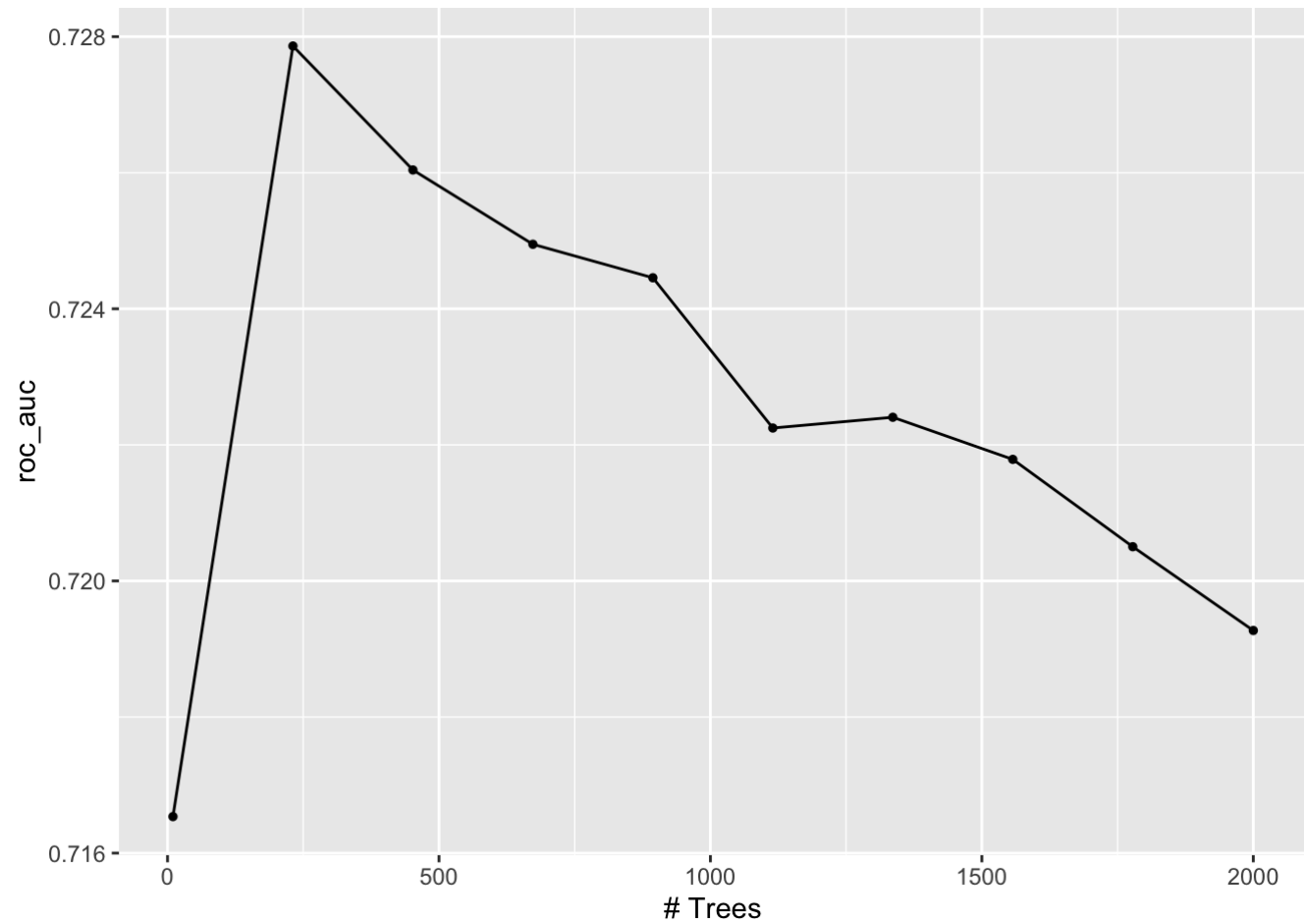
## Exercise 9

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.

What do you observe?

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

```
boost_tree_spec <- boost_tree(trees = tune()) %>%  
  set_engine("xgboost") %>%  
  set_mode("classification")  
  
boost_tree_grid <- grid_regular(trees(c(10,2000)),levels = 10)  
  
boost_tree_wf <- workflow() %>%  
  add_model(boost_tree_spec) %>%  
  add_formula(type_1 ~ sp_atk + attack + speed +  
    defense + hp + sp_def + legendary + generation)  
  
boost_tune_res <- tune_grid(  
  boost_tree_wf,  
  resamples = pokemon_fold,  
  grid = boost_tree_grid,  
  metrics = metric_set(roc_auc),  
)  
  
autoplot(boost_tune_res)
```



*The roc\_auc keep increasing until around 250 reach the peak and decrease with the tree number increasing.*

Hide

```
arrange(collect_metrics(boost_tune_res), desc(mean))
```

```
## # A tibble: 10 × 7
##   trees .metric .estimator mean      n std_err .config
##   <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1    231 roc_auc hand_till  0.728     5  0.0179 Preprocessor1_Model02
## 2    452 roc_auc hand_till  0.726     5  0.0178 Preprocessor1_Model03
## 3    673 roc_auc hand_till  0.725     5  0.0171 Preprocessor1_Model04
## 4    894 roc_auc hand_till  0.724     5  0.0174 Preprocessor1_Model05
## 5   1336 roc_auc hand_till  0.722     5  0.0187 Preprocessor1_Model07
## 6   1115 roc_auc hand_till  0.722     5  0.0181 Preprocessor1_Model06
## 7   1557 roc_auc hand_till  0.722     5  0.0190 Preprocessor1_Model08
## 8   1778 roc_auc hand_till  0.721     5  0.0199 Preprocessor1_Model09
## 9   2000 roc_auc hand_till  0.719     5  0.0201 Preprocessor1_Model10
## 10     10 roc_auc hand_till  0.717     5  0.0167 Preprocessor1_Model01
```

The best model has 0.727 roc\_auc and 231 trees.

## 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.

Hide

```
best_boost_tree <- select_best(boost_tune_res)
boost_tree_final <- finalize_workflow(boost_tree_wf, best_boost_tree)
boost_tree_final_fit <- fit(boost_tree_final, data = pokemon_train)
```

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```

final_class_model = augment(class_tree_final_fit, new_data = pokemon_train)
final_rand_model = augment(rf_fit, new_data = pokemon_train)
final_boost_model = augment(boost_tree_final_fit, new_data = pokemon_train)
results<- bind_rows(
  roc_auc(final_class_model, truth = type_1, .pred_Bug, .pred_Fire, .pred_Grass,
    .pred_Normal, .pred_Water, .pred_Psychic),
  roc_auc(final_rand_model, truth = type_1, .pred_Bug, .pred_Fire, .pred_Grass,
    .pred_Normal, .pred_Water, .pred_Psychic),
  roc_auc(final_boost_model, truth = type_1, .pred_Bug, .pred_Fire, .pred_Grass,
    .pred_Normal, .pred_Water, .pred_Psychic)
)
results

```

```

## # A tibble: 3 × 3
##   .metric .estimator .estimate
##   <chr>   <chr>       <dbl>
## 1 roc_auc hand_till     0.598
## 2 roc_auc hand_till     0.797
## 3 roc_auc hand_till     0.795

```

So we see that the best model is random forest which has roc\_auc is 0.79566.

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```

final_rand_model_test = augment(rf_fit, new_data = pokemon_test)
roc_auc(final_rand_model_test, truth = type_1, .pred_Bug, .pred_Fire, .pred_Grass, .pred_Normal, .pred_Water, .pred_Psychic)

```

```

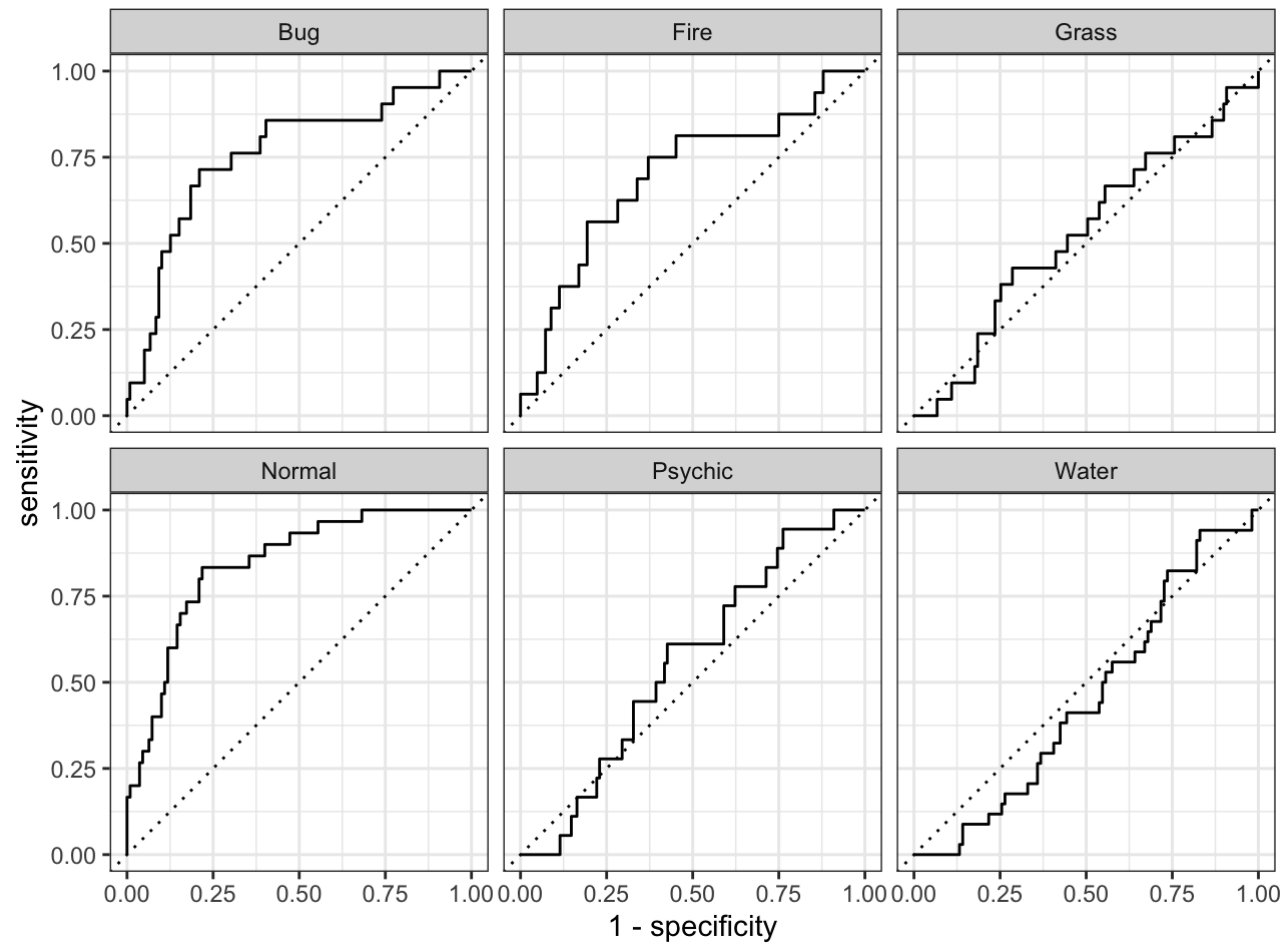
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>   <chr>       <dbl>
## 1 roc_auc hand_till     0.635

```

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.

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```
autoplot(roc_curve(final_rand_model_test, truth = type_1, .pred_Bug, .pred_Fire, .pred_Grass, .pred_Normal, .pred_Water, .pred_Psychic))
```



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```
conf_mat(final_rand_model_test, truth = type_1, estimate = .pred_class) %>% #calclate confusion matri
  autoplot(type = "heatmap")
```

Prediction	Bug -	6	0	4	2	1	2
	Fire -	0	1	1	0	0	2
	Grass -	2	3	1	0	3	3
	Normal -	8	1	3	20	0	10
	Psychic -	1	0	3	1	7	1
	Water -	4	11	9	7	7	16
		Bug	Fire	Grass	Normal	Psychic	Water
		Truth					

Which classes was your model most accurate at predicting? Which was it worst at?  
*The model is most accurate at Bug and Normal, and worst at Grass, Psychic, Water.*