Decision Trees and Random Forest

Stat 220

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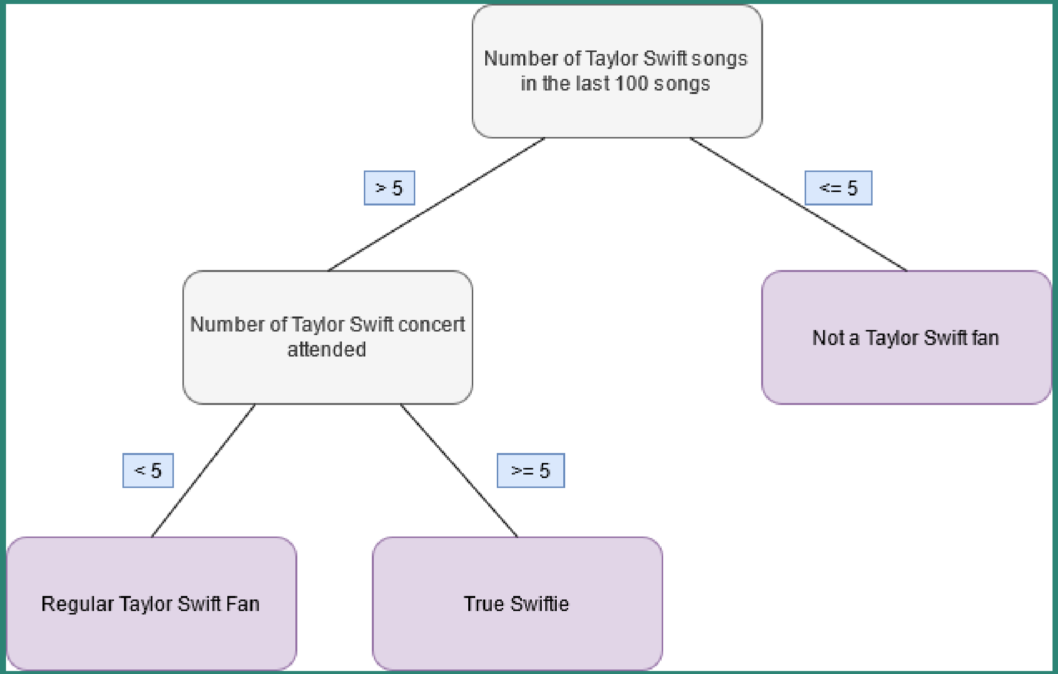
Decision Tree

- trains a model based on known values and uses the model to predict unknown values that have the same associated explanatory variables

- Data is continuously split according to a certain parameter
- Two main entities:
  - nodes: where the data is split
  - leaves: decisions or final outcomes



Decision Tree

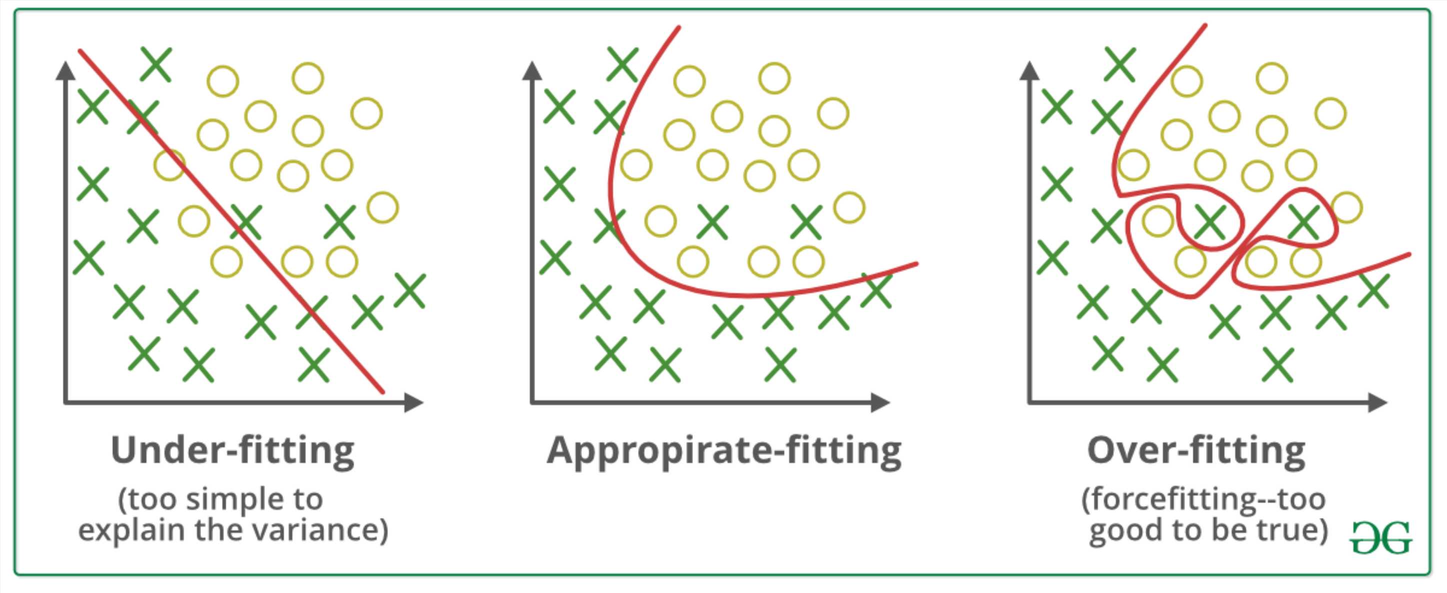
Use explanatory variables to make subsets of cases that are as similar (“pure”) as possible with respect to the response

- Start with all observations in one group
- Find the variable/split that best separates the outcome
- Divide the data into two groups (leaves) on the split (node)
- Within each split, find the best variable/split that separates the outcomes
- Continue until the groups are too small or sufficiently “pure”

```r
data(PimaIndiansDiabetes2)
db <- PimaIndiansDiabetes2 %>% na.omit() %>%
  mutate(diabetes = fct_relevel(diabetes, "pos"))
```

```
glimpse(db)
Rows: 392
Columns: 9
$ pregnant <dbl> 1, 0, 3, 2, 1, 5, 0, 1, 1, 3, 11, 10, 1, 13, 3, 3, 4, 4, 3
$ glucose  <dbl> 89, 137, 78, 197, 189, 166, 118, 103, 115, 126, 143, 125,
$ pressure <dbl> 66, 40, 50, 70, 60, 72, 84, 30, 70, 88, 94, 70, 66, 82, 76
$ triceps  <dbl> 23, 35, 32, 45, 23, 19, 47, 38, 30, 41, 33, 26, 15, 19, 36
$ insulin  <dbl> 94, 168, 88, 543, 846, 175, 230, 83, 96, 235, 146, 115, 14
$ mass     <dbl> 28.1, 43.1, 31.0, 30.5, 30.1, 25.8, 45.8, 43.3, 34.6, 39.3
$ pedigree <dbl> 0.167, 2.288, 0.248, 0.158, 0.398, 0.587, 0.551, 0.183, 0.
$ age      <dbl> 21, 33, 26, 53, 59, 51, 31, 33, 32, 27, 51, 41, 22, 57, 28
$ diabetes <fct> neg, pos, pos, pos, pos, pos, pos, neg, pos, neg, pos, pos
```

Overfitting and underfitting



- **Overfitting:** Good performance on the training data, poor generliazation to other data.
- **Underfitting:** Poor performance on the training data and poor generalization to other data

```r
set.seed(314)
db_split <- initial_split(db, prop = 0.80,
                             strata = diabetes)
db_train <- db_split %>% training()
db_test <- db_split %>% testing()
```

```r
# Scaling not needed
db_recipe <- recipe(diabetes ~ ., data = db_train) %>%
 step_dummy(all_nominal(), -all_outcomes()) %>%
 prep()
```

Model Specification

- **cost_complexity:** The cost complexity parameter
- **tree_depth:** The maximum depth of a tree
- **min_n:** The minimum number of data points in a node that are required for the node to be split further.

```
tree_model <- decision_tree(cost_complexity = tune(),
                            tree_depth = tune(),
                            min_n = tune()) %>%
              set_engine('rpart') %>%
              set_mode('classification')
```

Workflow

```
# Combine the model and recipe into a workflow
tree_workflow <- workflow() %>%
                 add_model(tree_model) %>%
                 add_recipe(db_recipe)
```

Hyperparameter tuning

```r
# Create folds for cross validation on the training data set
db_folds <- vfold_cv(db_train, v = 5, strata = diabetes)
```

```r
## Create a grid of hyperparameter values to test
tree_grid <- grid_regular(cost_complexity(),
                          tree_depth(),
                          min_n(),
                          levels = 2)
```

View grid

```
tree_grid
# A tibble: 8 × 3
  cost_complexity tree_depth min_n
            <dbl>      <int> <int>
1    0.0000000001          1     2
2    0.1                   1     2
3    0.0000000001         15     2
4    0.1                  15     2
5    0.0000000001          1    40
6    0.1                   1    40
7    0.0000000001         15    40
8    0.1                  15    40
```

Tuning Hyperparameters with `tune_grid()`

```
# Tune decision tree workflow
set.seed(314)
tree_tuning <- tree_workflow %>%
               tune_grid(resamples = db_folds,
                         grid = tree_grid)
```

Best model

```
# Select best model based on roc_auc
best_tree <- tree_tuning %>%
             select_best(metric = 'roc_auc')
```

```
# View the best tree parameters
best_tree
# A tibble: 1 × 4
  cost_complexity tree_depth min_n .config
            <dbl>      <int> <int> <chr>
1    0.0000000001         15    40 Preprocessor1_Model7
```

Finalize workflow

```
final_tree_workflow <- tree_workflow %>%
                       finalize_workflow(best_tree)
```

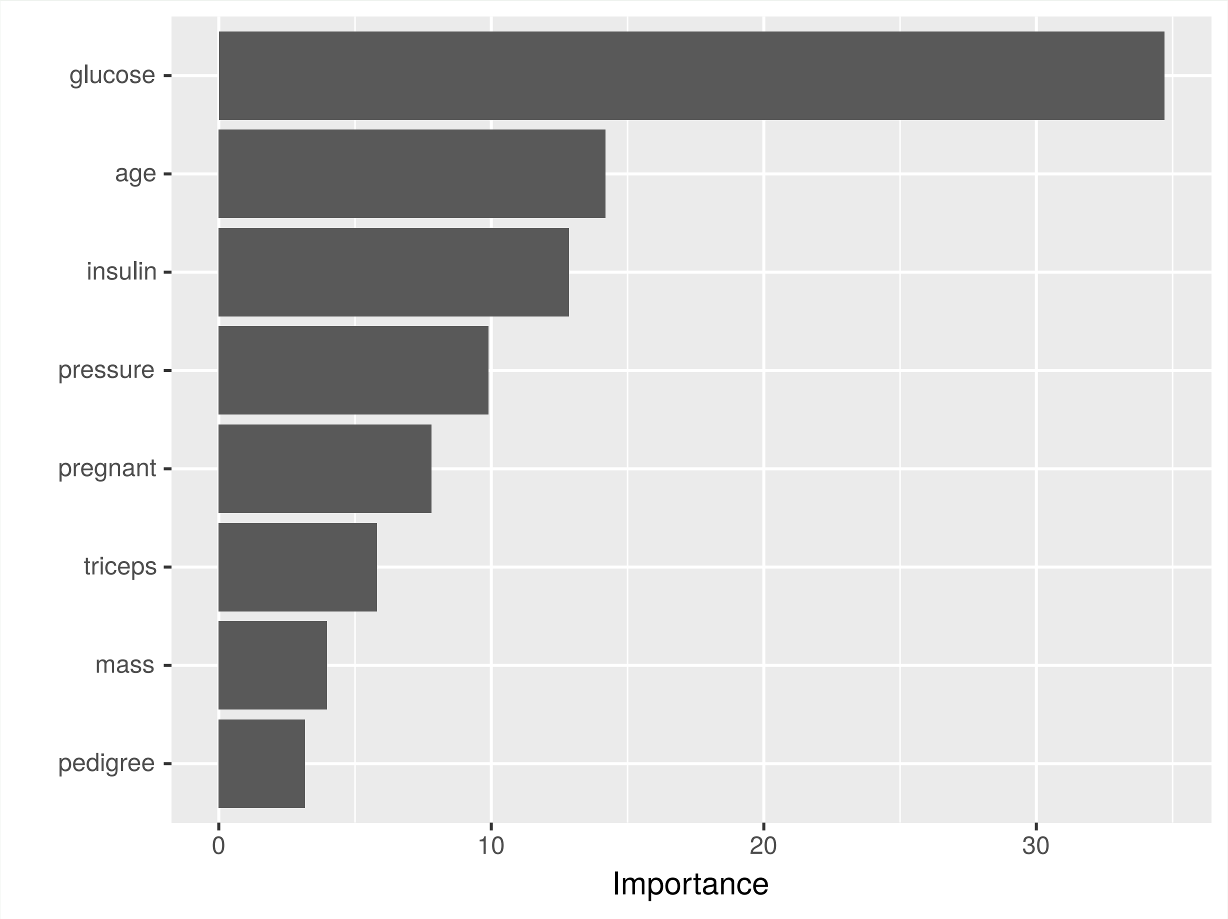
Fit the model

```
tree_wf_fit <- final_tree_workflow %>%
               fit(data = db_train)
```

Extract fit

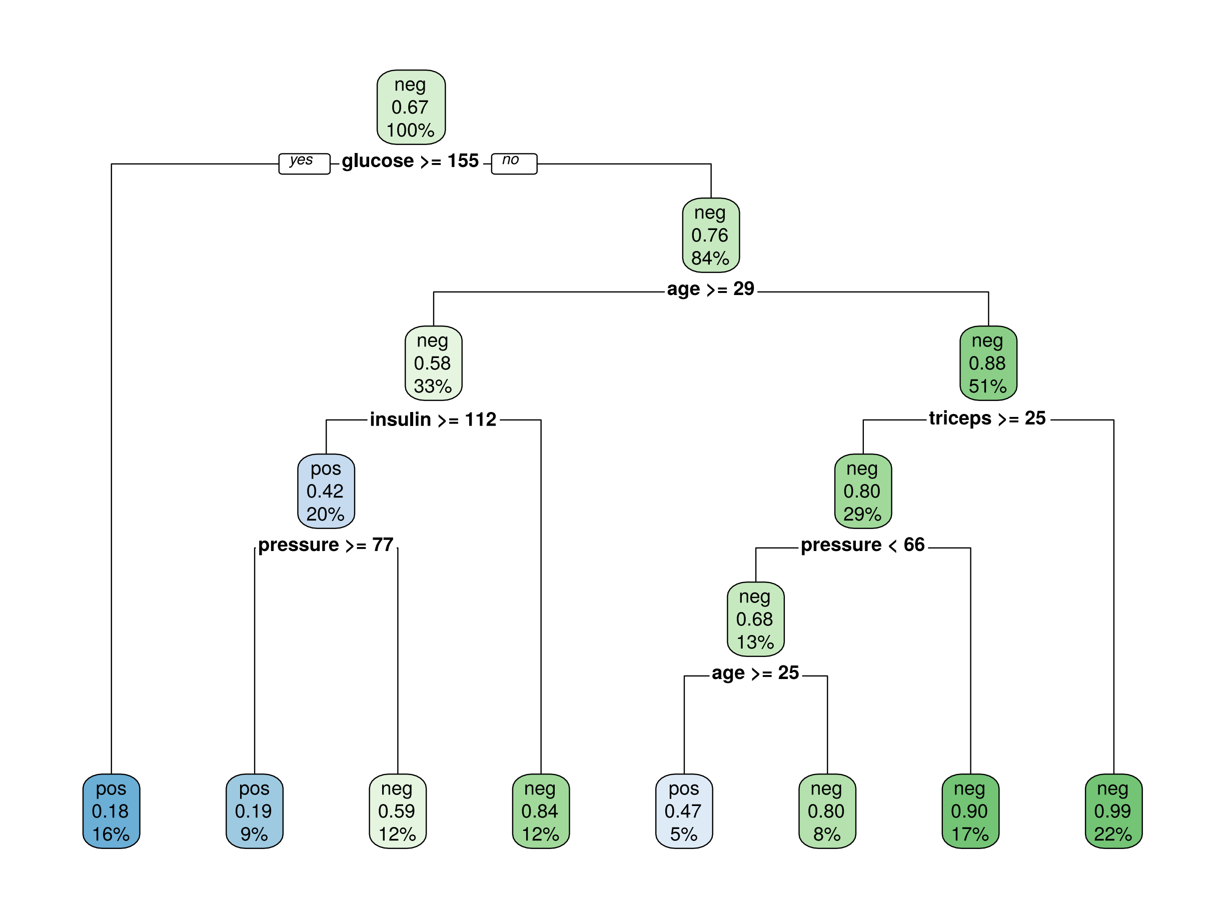
```
tree_fit <- tree_wf_fit %>%
            extract_fit_parsnip()
```

```r
vip(tree_fit)
```



Variable Importance

```r
rpart.plot(tree_fit$fit, roundint = FALSE)
```



Decision Tree

Train and Evaluate With `last_fit()`

```
tree_last_fit <- final_tree_workflow %>%
                 last_fit(db_split)
```

```
tree_last_fit %>% collect_metrics()
# A tibble: 2 × 4
  .metric  .estimator .estimate .config
  <chr>    <chr>          <dbl> <chr>
1 accuracy binary         0.785 Preprocessor1_Model1
2 roc_auc  binary         0.808 Preprocessor1_Model1
```

Confusion matrix

```
tree_predictions <- tree_last_fit %>% collect_predictions()
conf_mat(tree_predictions, truth = diabetes, estimate = .pred_class)
          Truth
Prediction pos neg
       pos  15   6
       neg  11  47
```

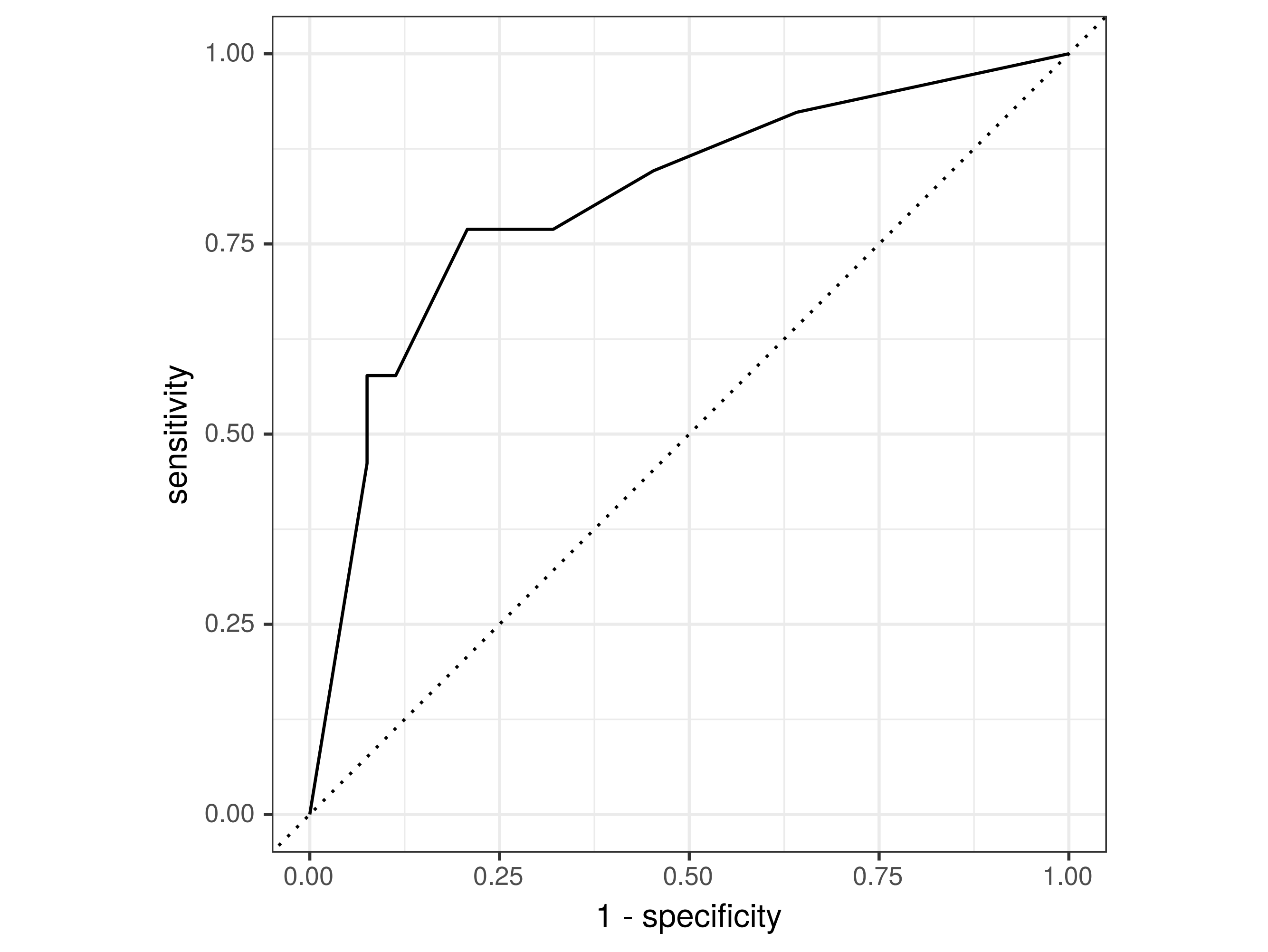
Assessing Accuracy

Accuracy = How often the classifier is correct out of the total possible predictions?

Accuracy = True Positives + True Negatives / (True Positives + True Negatives + False Positives + False Negatives)

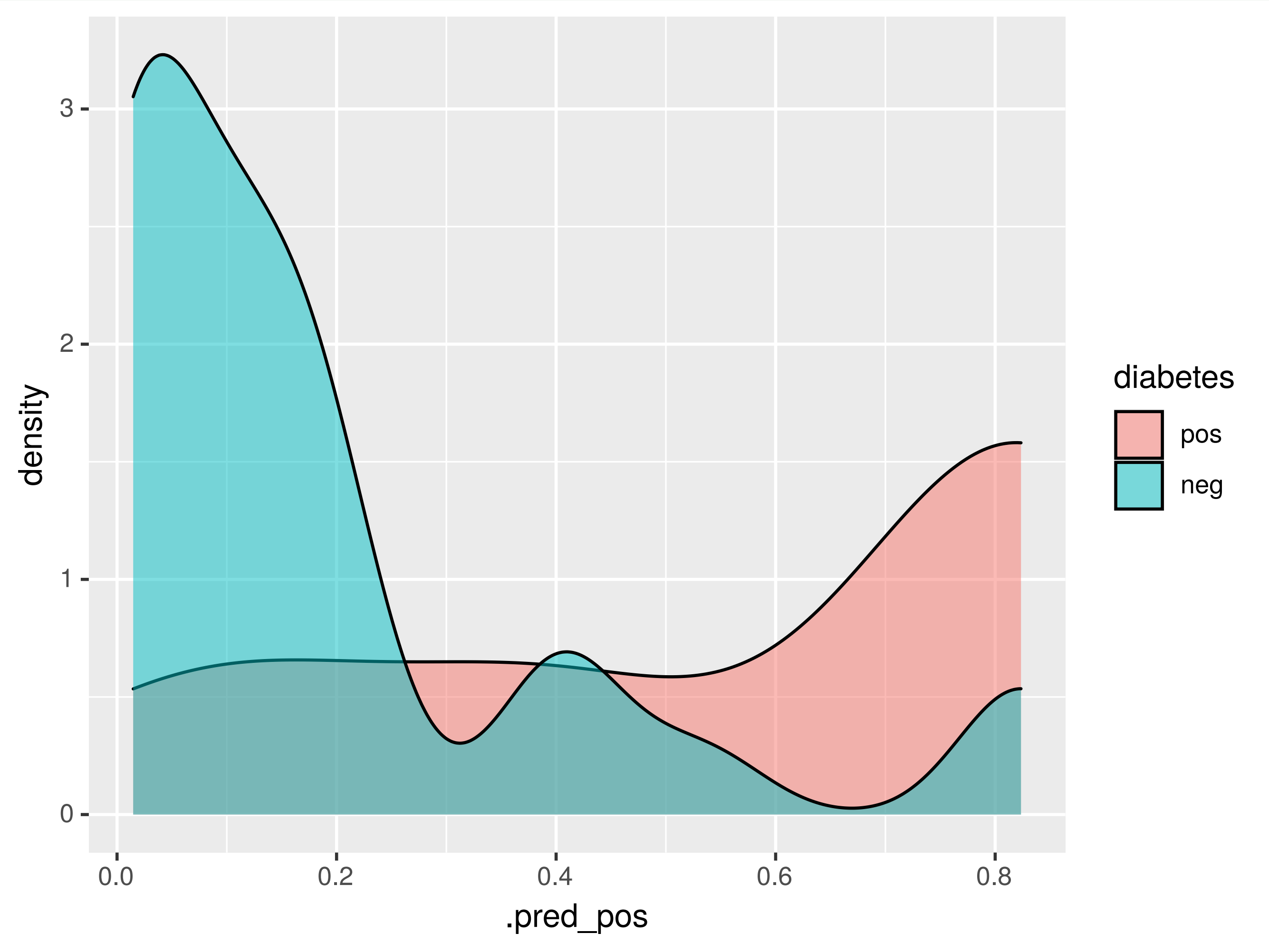
- True Positive Rate (Sensitivity/Recall):
  - Out of all true positives, how many did you predict right?
  - True Positives / (True Positives + False Negatives)
- True Negative Rate (Specificity):
  - Out of all true negatives, how many did you predict right?
  - True Negatives / (True Negatives + False Positives)

ROC-AUC



1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 - specificity

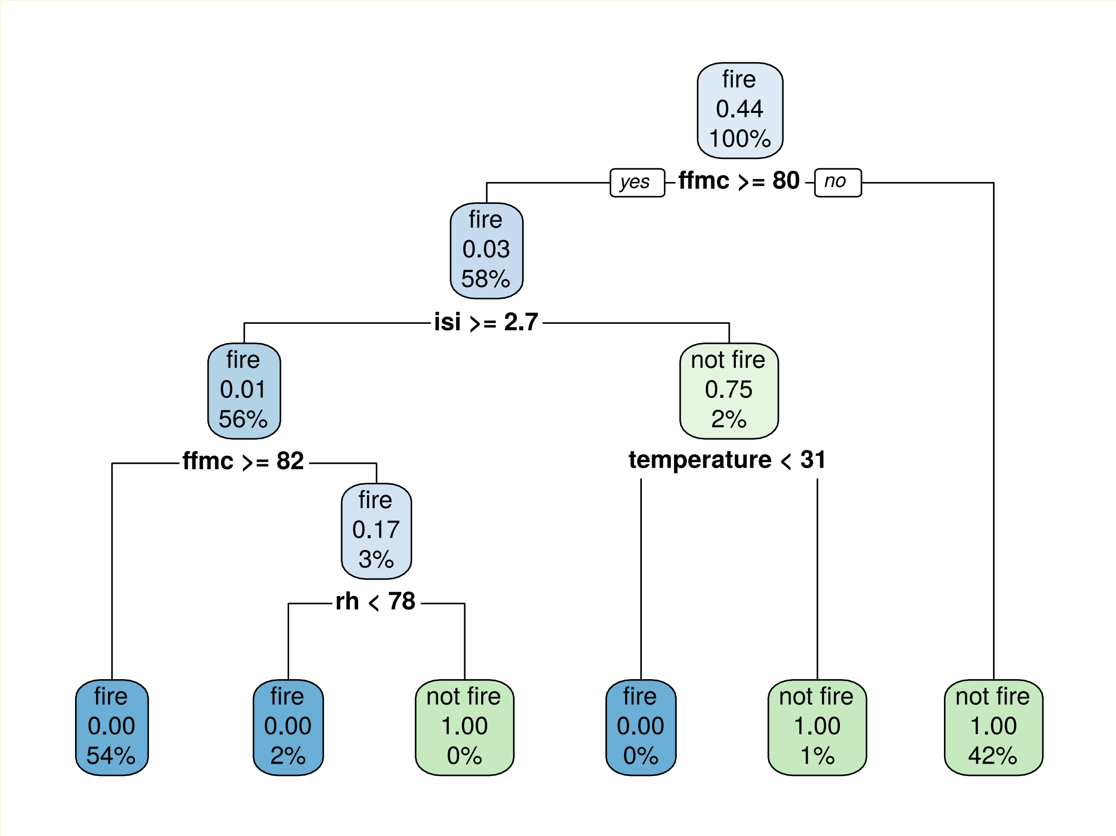
Predicted probability distributions for each class



Your Turn 1

10:00

Please clone the repository on decision tree and random forest to your local folder.



Follow the questionnaires to make a decision tree for the `fire` dataset.

Random Forest

Random forests take decision trees and construct more powerful models in terms of prediction accuracy.

- Repeated sampling (with replacement) of the training data to produce a sequence of decision tree models.
- These models are then averaged to obtain a single prediction for a given value in the predictor space.
- The random forest model selects a random subset of predictor variables for splitting the predictor space in the tree building process.

Model Specification

- **mtry:** The number of predictors that will be randomly sampled at each split when creating the tree models
- **trees:** The number of decision trees to fit and ultimately average
- **min_n:** The minimum number of data points in a node that are required for the node to be split further

Model Specification

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

Workflow

```
rf_workflow <- workflow() %>%
               add_model(rf_model) %>%
               add_recipe(db_recipe)
```

Hyperparameter Tuning

```
## Create a grid of hyperparameter values to test
set.seed(314)
rf_grid <- grid_random(mtry() %>% range_set(c(2, 7)),
                       trees(),
                       min_n(),
                       size = 15)
```

View Grid

```
rf_grid
# A tibble: 15 × 3
    mtry trees min_n
   <int> <int> <int>
 1     7   609    32
 2     5  1235     6
 3     4  1822    29
 4     5   678    16
 5     4   138    14
 6     3  1218    19
 7     7   228    14
 8     5   873     4
 9     6  1387    10
10     7  1717     5
11     5   436     4
12     3  1175    16
13     6  1909    33
14     6   118     4
15     2  1003    24
```

Tuning Hyperparameters with `tune_grid()`

```r
## Tune random forest workflow
set.seed(314)

rf_tuning <- rf_workflow %>%
             tune_grid(resamples = db_folds,
                       grid = rf_grid)
```

Select best

```
## Select best model based on roc_auc
best_rf <- rf_tuning %>%
           select_best(metric = 'roc_auc')
```

```
# View the best parameters
best_rf
# A tibble: 1 × 4
   mtry trees min_n .config
  <int> <int> <int> <chr>
1     2  1003    24 Preprocessor1_Model15
```

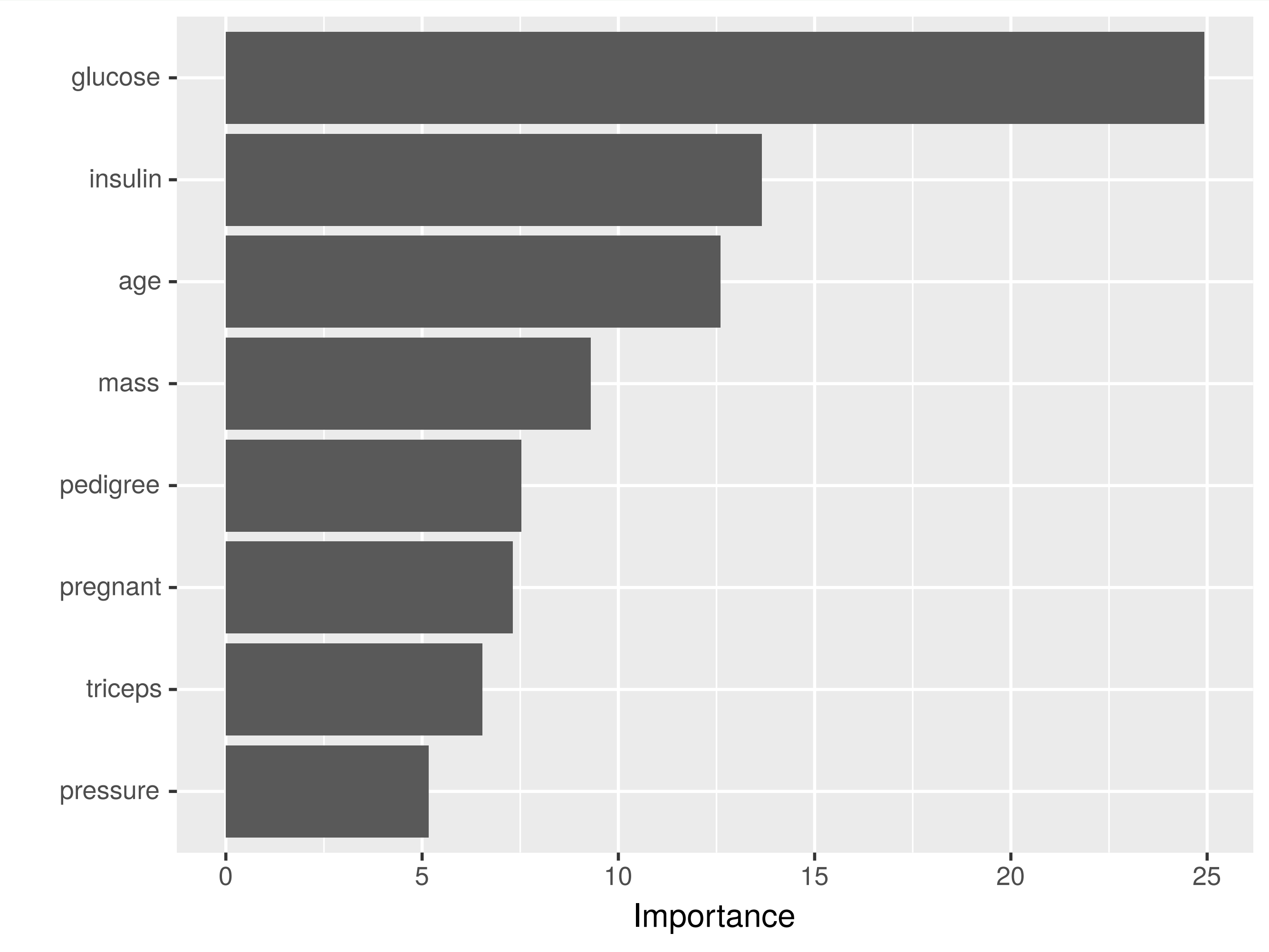
Finalize workflow

```
final_rf_workflow <- rf_workflow %>%
                     finalize_workflow(best_rf)
```

Variable Importance

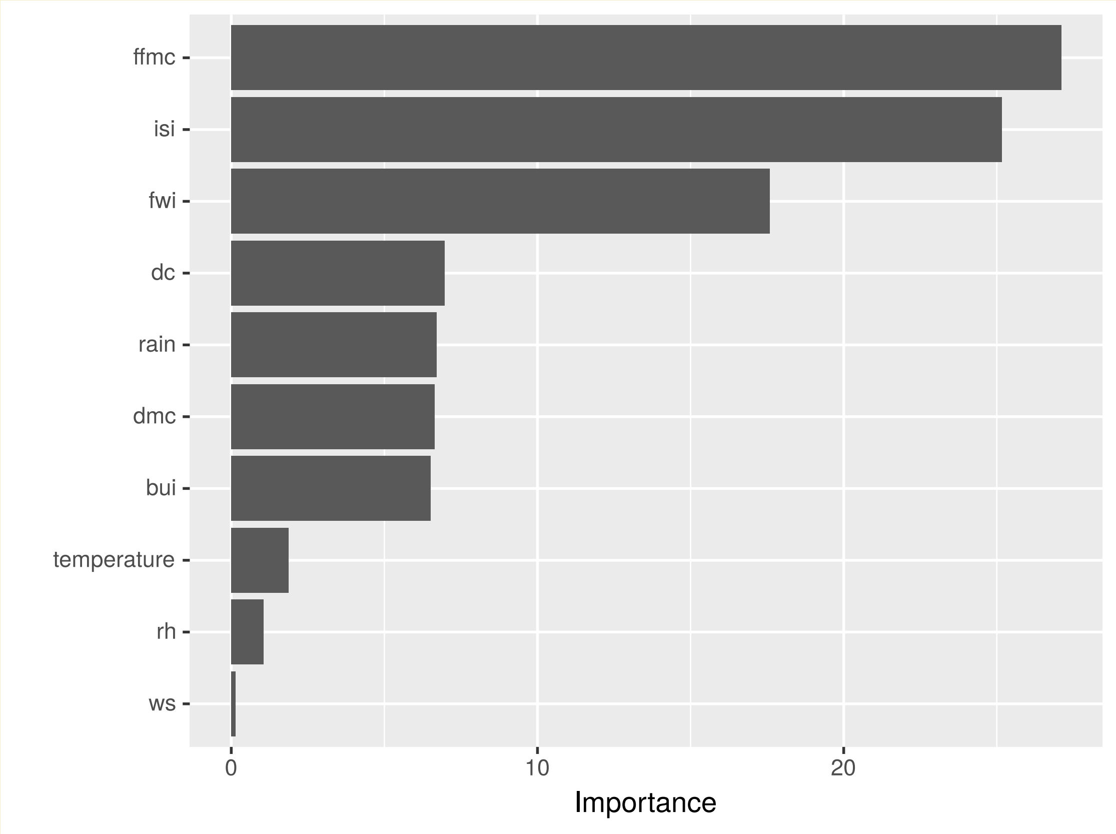
```
rf_wf_fit <- final_rf_workflow %>%
             fit(data = db_train)

rf_fit <- rf_wf_fit %>%
          extract_fit_parsnip()
```

Variable Importance



Your Turn 2

05:00



Use random forest model to find out the most important variables in predicting fire.