# Decision Trees and Random Forest

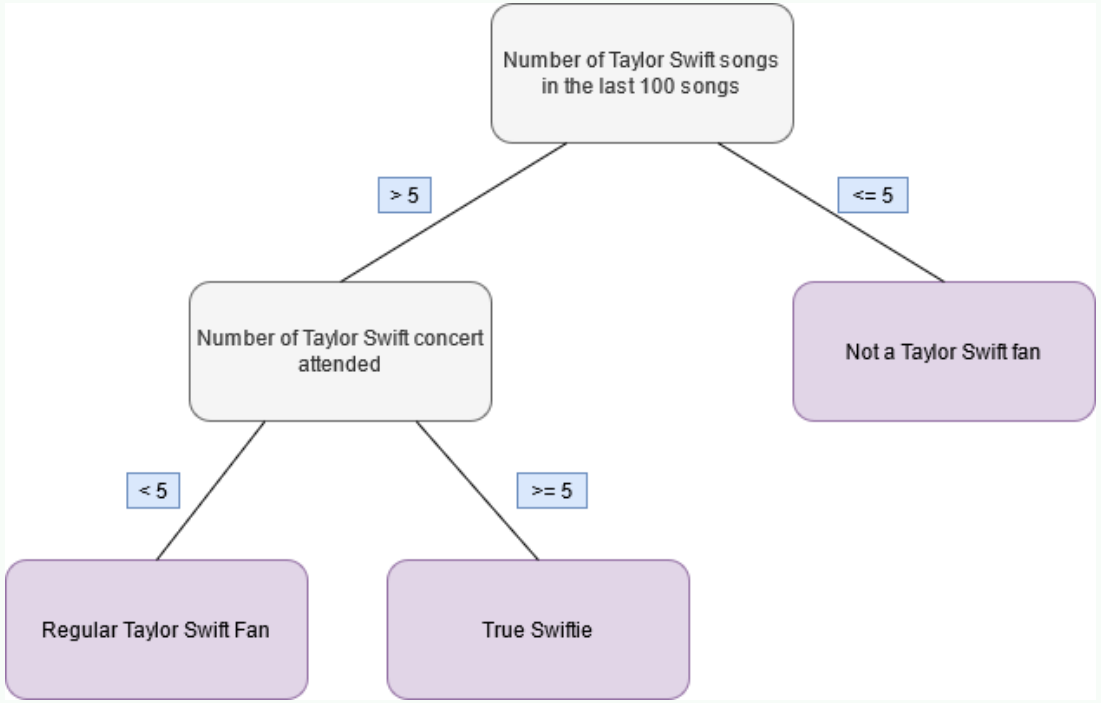
**Spring 2023**

May 24 2023

## Decision Tree

- ***learns how to best split the dataset into smaller and smaller subsets to predict the target value***

- 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 features to make subsets of cases that are as similar (“pure”) as possible with respect to the outcome

- **Start with all observations in one group**
- **Find the variable/feature/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”**

# Dataset

```
data(PimaIndiansDiabetes2)
db <- PimaIndiansDiabetes2 %>% drop_na() %>%
  mutate(diabetes = fct_relevel(diabetes, ref = "neg"))
```

```
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, 9…
$ glucose  <dbl> 89, 137, 78, 197, 189, 166, 118, 103, 115, 126, 143, 125, 97,…
$ pressure <dbl> 66, 40, 50, 70, 60, 72, 84, 30, 70, 88, 94, 70, 66, 82, 76, 5…
$ triceps  <dbl> 23, 35, 32, 45, 23, 19, 47, 38, 30, 41, 33, 26, 15, 19, 36, 1…
$ insulin  <dbl> 94, 168, 88, 543, 846, 175, 230, 83, 96, 235, 146, 115, 140, …
$ mass     <dbl> 28.1, 43.1, 31.0, 30.5, 30.1, 25.8, 45.8, 43.3, 34.6, 39.3, 3…
$ pedigree <dbl> 0.167, 2.288, 0.248, 0.158, 0.398, 0.587, 0.551, 0.183, 0.529…
$ age      <dbl> 21, 33, 26, 53, 59, 51, 31, 33, 32, 27, 51, 41, 22, 57, 28, 2…
$ diabetes <fct> neg, pos, pos, pos, pos, pos, pos, neg, pos, neg, pos, pos, n…
```

## Data preparation and pre-processing

```
set.seed(314)
db_split <- initial_split(db, prop = 0.75)
db_train <- db_split %>% training()
db_test <- db_split %>% testing()
```

```
# 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, the minimum improvement in the model needed at each node
- `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

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

```
## Create a grid of hyperparameter values to test
tree_grid <- grid_random(cost_complexity(),
                         tree_depth(),
                         min_n(),
                         size = 10)
```

# View grid

```
tree_grid
# A tibble: 10 × 3
   cost_complexity tree_depth min_n
             <dbl>      <int> <int>
 1        5.28e-10          7    40
 2        2.99e- 6          3     7
 3        1.30e- 8          1    17
 4        1.94e- 2         13    19
 5        1.74e- 7         11    22
 6        8.11e- 7          6     3
 7        2.41e- 6          4    10
 8        1.01e- 5         14    40
 9        2.38e- 2          4    18
10        2.68e- 6         15    39
```

## 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 accuracy
best_tree <- tree_tuning %>%
             select_best(metric = 'accuracy')
```

```
# View the best tree parameters
best_tree
# A tibble: 1 × 4
  cost_complexity tree_depth min_n .config
            <dbl>      <int> <int> <chr>
1        5.28e-10          7    40 Preprocessor1_Model01
```

## Finalize workflow

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

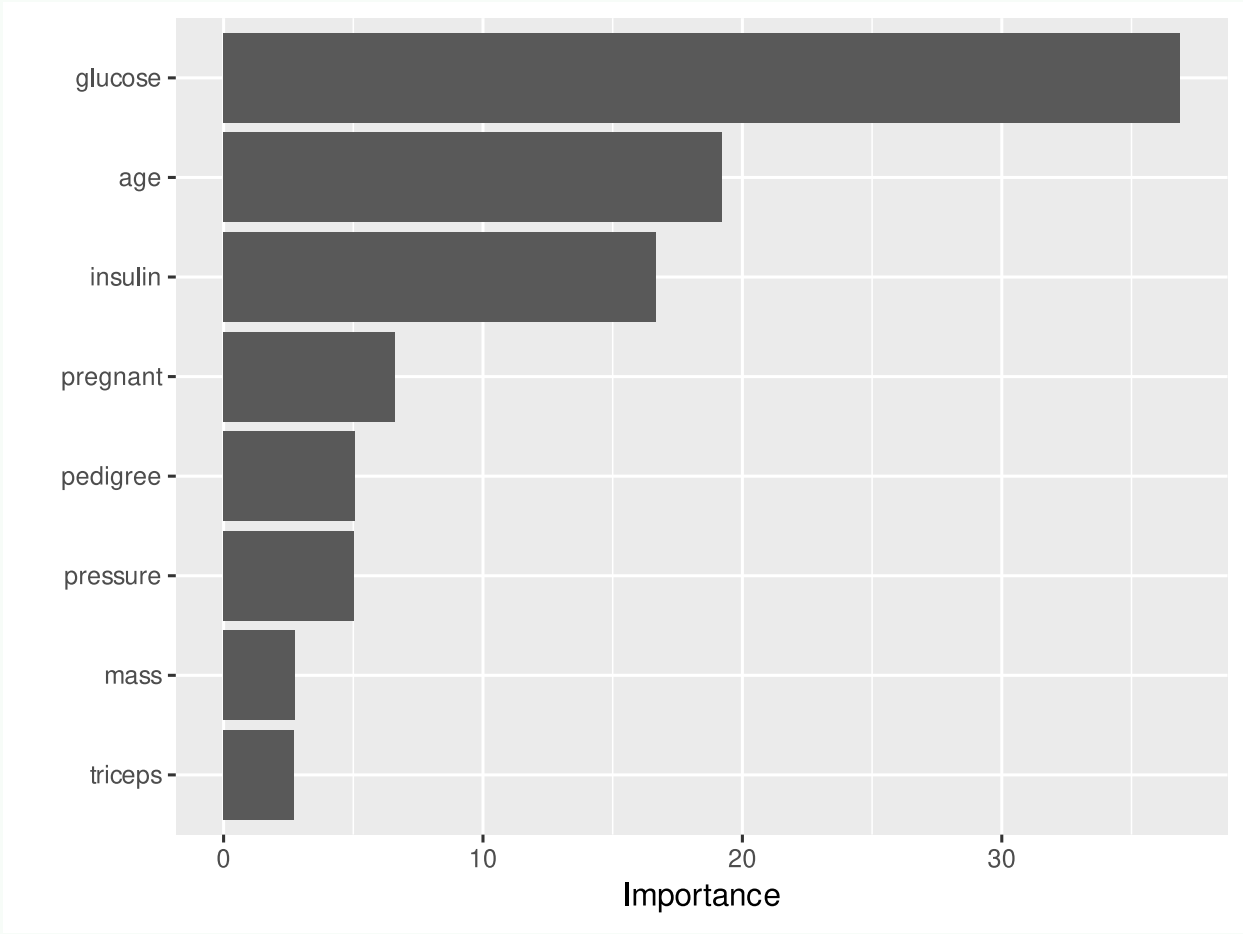
## Fit the model

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

## Extract fit

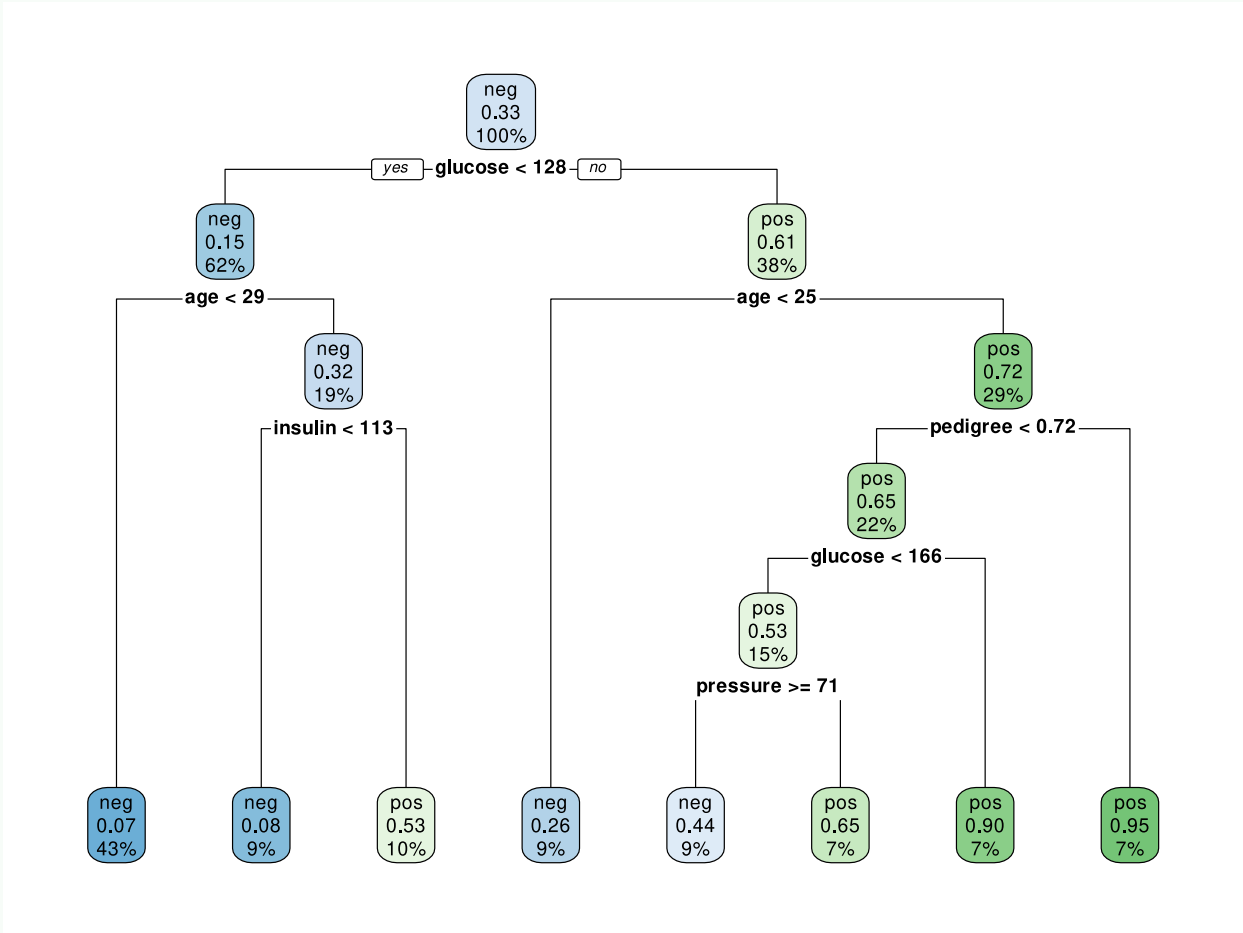
```
tree_fit <- tree_wf_fit %>%
            extract_fit_parsnip()
```

```
vip(tree_fit)
```




## Variable Importance

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



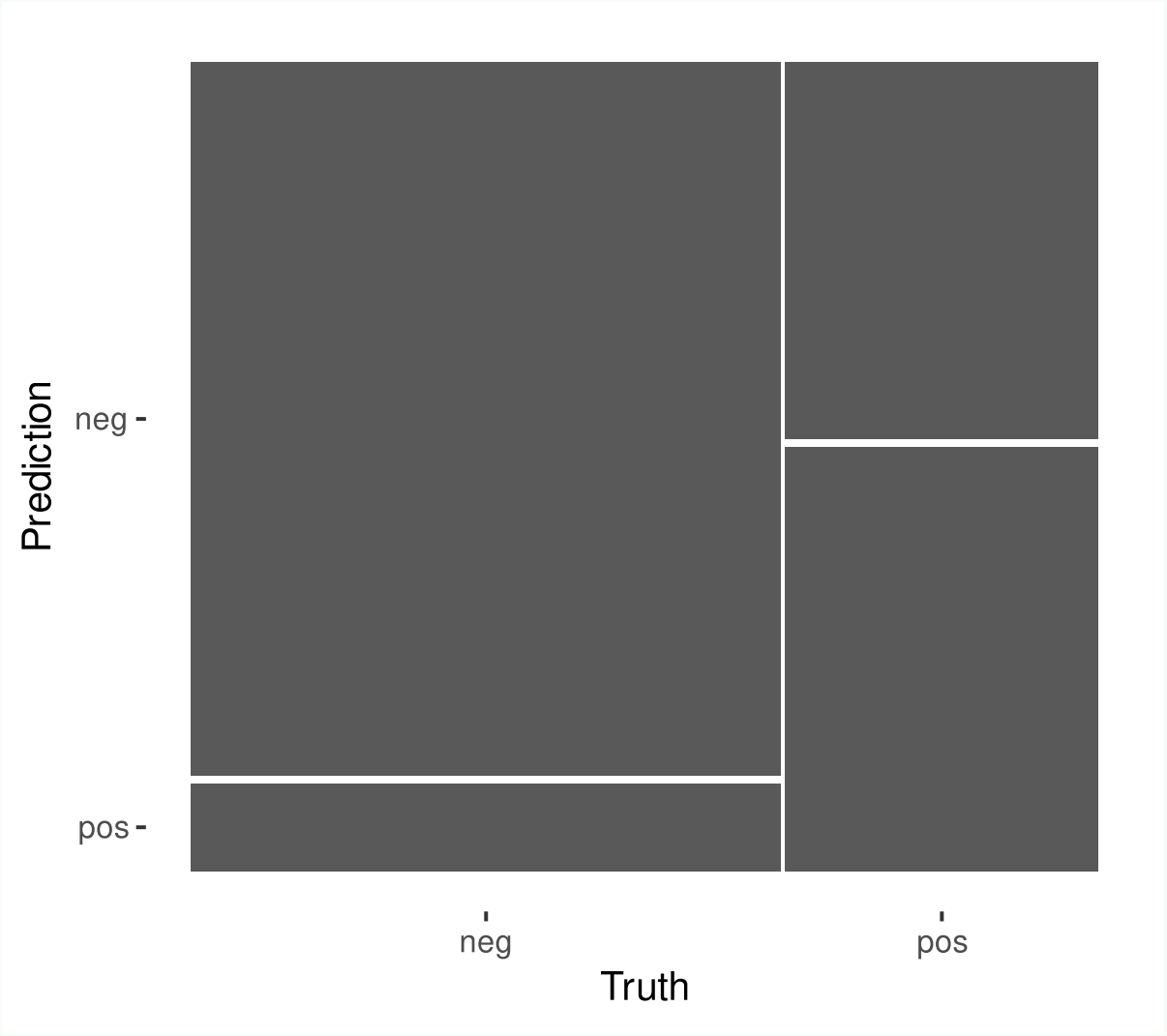

Decision Tree

# Train and Evaluate With `last_fit()`

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

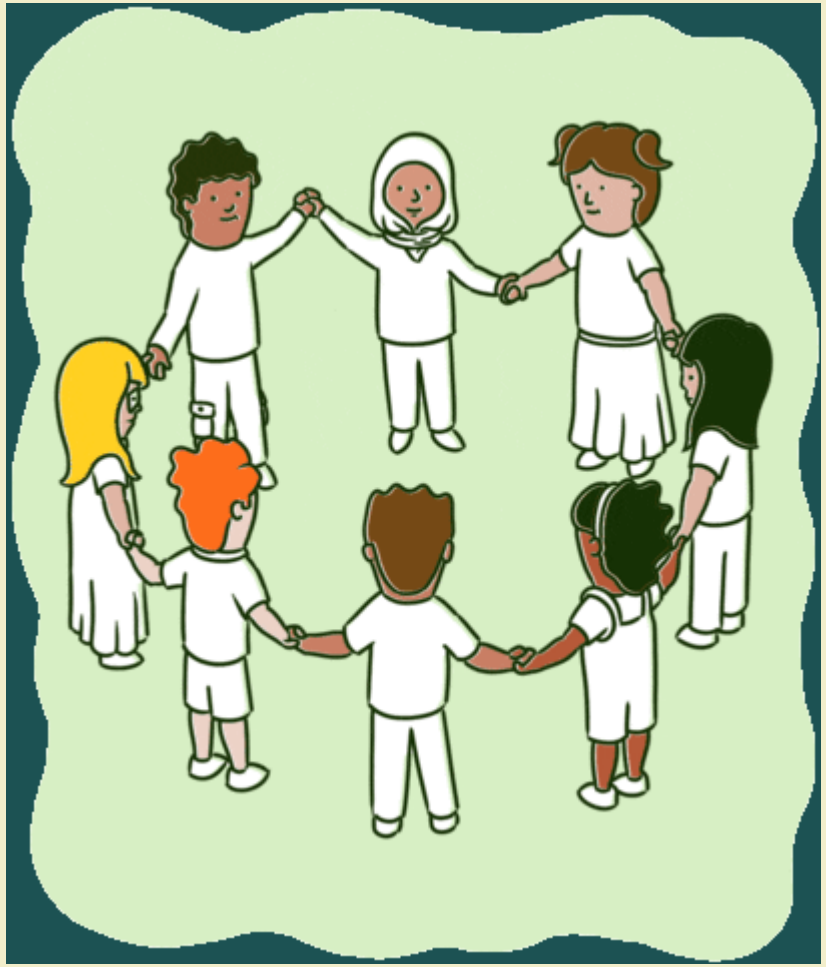
```
tree_last_fit %>% collect_metrics()
# A tibble: 2 × 4
  .metric  .estimator .estimate .config
  <chr>    <chr>          <dbl> <chr>
1 accuracy binary         0.765 Preprocessor1_Model1
2 roc_auc  binary         0.824 Preprocessor1_Model1
```

# Confusion matrix



# GROUP ACTIVITY 1

05:00



- Get the class activity 26.Rmd file from moodle
- Let's work on group activity 1 together

*Now, let's talk about random forest*

## 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()`

```
## 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 = 'accuracy')
```

```
# 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
```

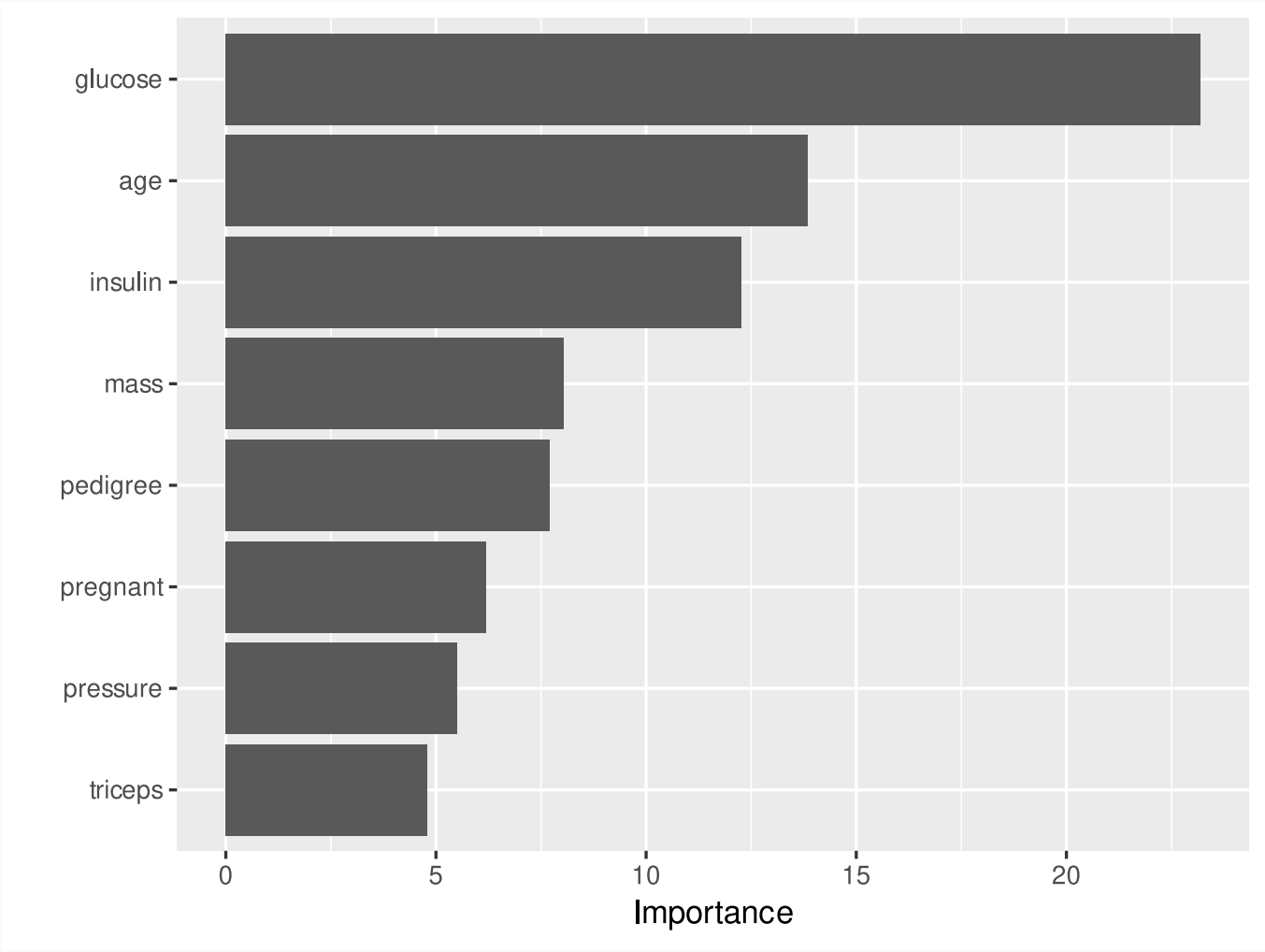
## Finalize workflow

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

## Variable Importance

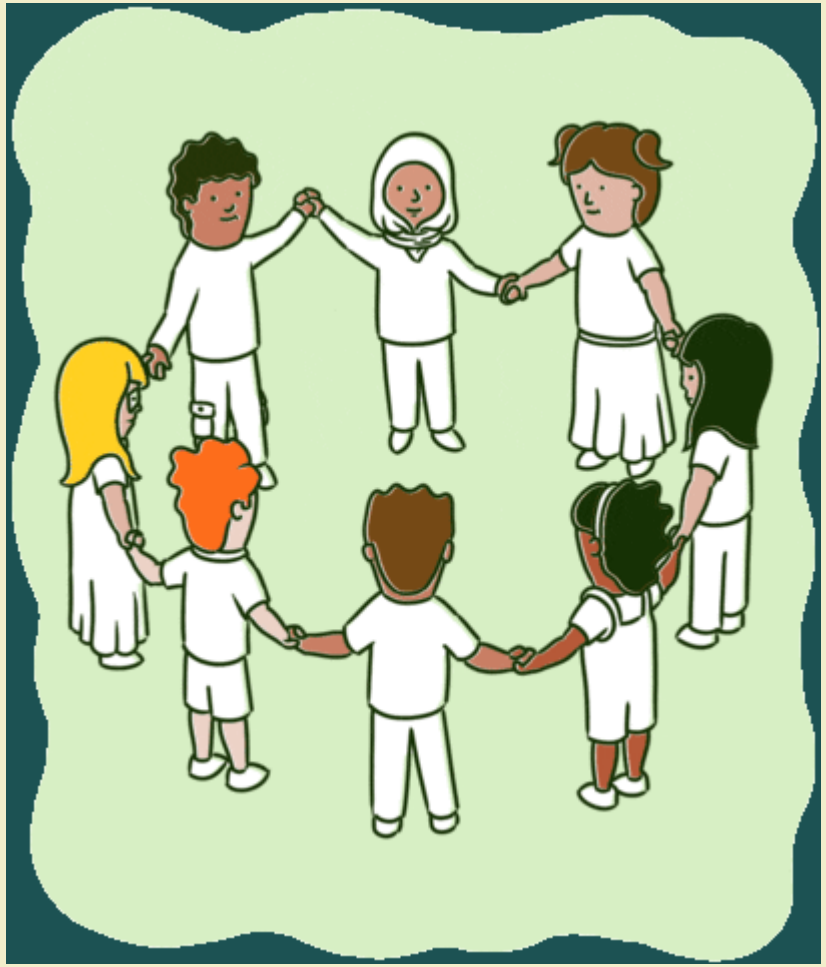
```
rf_wf_fit <- final_rf_workflow %>%
             fit(data = db_train)

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

# Variable Importance



# GROUP ACTIVITY 2

10:00



- Please continue working on group activity 2