Model

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Imports

```
library(tidyverse)
library(yaml)
library(tidymodels)
library(usemodels)
library(vip)
```

Loading data

```
load('../dataset/processed_data.RData')
load('../dataset/processed_dictionary.RData')

columns_list <- yaml.load_file("./auxiliar/columns_list.yaml")

outcome_column <- params$outcome_column
```

Filtering eligible pacients

```
df = df %>%
  filter(disch_outcomes_t0 == 0)

df %>% dim
```

```
## [1] 15766   236
```

Eligible features

```
eligible_columns = df_names %>%
  filter(momento.aquisicao == 'Admissão t0') %>%
  .$variable.name

exception_columns = c('disch_outcomes_t0', 'icu_post_t0')

correlated_columns = c('year_procedure_1', # com year_adm_t0
                       'age_surgery_1', # com age
                       'admission_pre_t0_count', # com admission_t0
                       'atb', # com meds_antimicrobianos
                       'classe_meds_cardio_qtde', # com classe_meds_qtde
                       'suporte_hemod' # com proced_invasivos_qtde
                       )

features = eligible_columns %>%
  base::intersect(c(columns_list$categorical_columns, columns_list$numerical_columns)) %>%
  setdiff(c(exception_columns, correlated_columns))

length(features)
```

```
## [1] 119
```

Train test split (70%/30%)

```
set.seed(42)

df[columns_list$outcome_columns] <- lapply(df[columns_list$outcome_columns], factor)

df_split <- initial_split(df %>% dplyr::select(all_of(c(features, outcome_column))),
                          prop = .7, strata = all_of(outcome_column))
df_train <- training(df_split)
df_test <- testing(df_split)

dim(df_train)[1] / dim(df)[1]
```

```
## [1] 0.6999873
```

```
dim(df_test)[1] / dim(df)[1]
```

```
## [1] 0.3000127
```

Imputation

```
all_cores <- parallel::detectCores(logical = FALSE)

library(doParallel)
cl <- makePSOCKcluster(all_cores)
registerDoParallel(cl)

imputation_recipe <- recipe(sprintf("%s ~ .", outcome_column) %>% as.formula,
                            data = df_train) %>%
  step_zv(all_predictors()) %>%
  step_dummy(all_nominal_predictors()) %>%
  step_impute_mode(all_nominal_predictors()) %>%
  step_impute_mean(all_numeric_predictors())
  # step_impute_knn(all_predictors(), neighbors = 3)

trained_imputation_recipe <- prep(imputation_recipe,
                                  training = df_train)

df_train_imputed <- bake(trained_imputation_recipe, df_train)
df_test_imputed <- bake(trained_imputation_recipe, df_test)
```

Functions

```
validation = function(model_fit, new_data) {
  library(pROC)
  library(caret)

  test_predictions_prob <-
    predict(model_fit, new_data = new_data, type = "prob") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$`1`

  pROC_obj <- roc(
    new_data[[outcome_column]],
    test_predictions_prob,
    smoothed = TRUE,
    # arguments for ci
```

```
    ci = TRUE,
    ci.alpha = 0.9,
    stratified = FALSE,
    # arguments for plot
    plot = TRUE,
    auc.polygon = TRUE,
    max.auc.polygon = TRUE,
    grid = TRUE,
    print.auc = TRUE,
    show.thres = TRUE
  )

  sens.ci <- ci.se(pROC_obj)
  plot(sens.ci, type = "shape", col = "lightblue")
  plot(sens.ci, type = "bars")

  test_predictions_class <-
    predict(model_fit, new_data = new_data, type = "class") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$class

  conf_matrix = table(test_predictions_class, new_data[[outcome_column]])

  confusionMatrix(conf_matrix) %>% print

  return(pROC_obj)
}
```

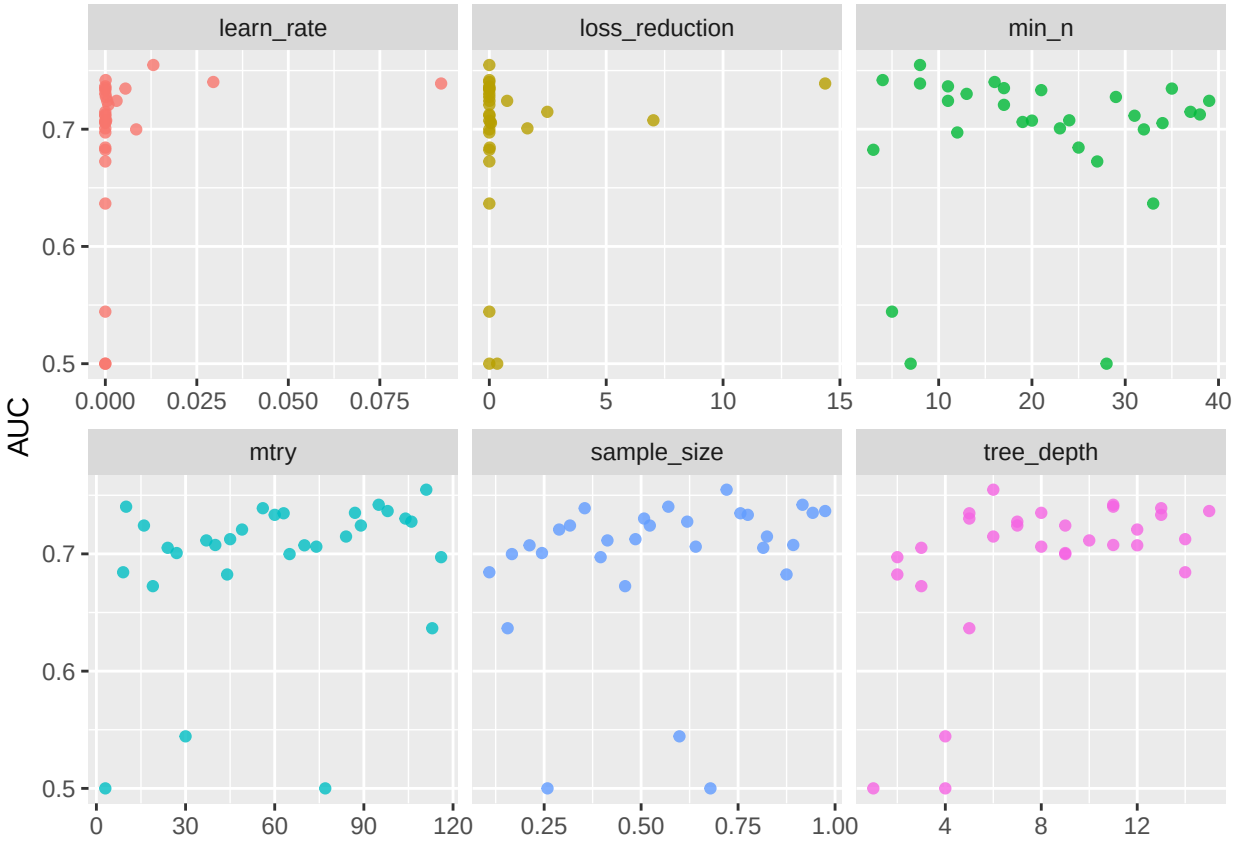
XGBoost

```
xgboost_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_string2factor(one_of("sex", "race", "education_level", "patient_state",
    "underlying_heart_disease", "heart_disease", "nyha_basal", "hypertension",
    "prior_mi", "heart_failure", "af", "cardiac_arrest", "transplant", "valvopathy",
    "endocardites", "diabetes", "renal_failure", "hemodialysis", "stroke",
    "copd", "cancer", "surgery_count", "procedure_type_1", "reop_type_1", "cied_final_1",
    "death_intraop_1", "dialysis_hosp", "icu_hosp", "admission_pre_t0_180d", "ventilacao_mecanica")) %>%
  step_novel(all_nominal_predictors()) %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors())

xgboost_spec <- boost_tree(
  trees = 500,
  tree_depth = tune(),
  min_n = tune(),
  loss_reduction = tune(),
  sample_size = tune(),
  mtry = tune(),
  learn_rate = tune()
) %>%
  set_engine("xgboost") %>%
  set_mode("classification")

xgboost_grid <- grid_latin_hypercube(
  tree_depth(),
  min_n(),
  loss_reduction(),
  sample_size = sample_prop(),
  finalize(mtry(), df_train),
```

```
  learn_rate(),
  size = 30
)

set.seed(234)
df_folds <- vfold_cv(df_train, v = 5, strata = all_of(outcome_column))

xgboost_workflow <-
  workflow() %>%
  add_recipe(xgboost_recipe) %>%
  add_model(xgboost_spec)

xgboost_tune <-
  xgboost_workflow %>%
  tune_grid(resamples = df_folds,
            grid = xgboost_grid)

xgboost_tune %>%
  show_best("roc_auc")
```

```
## # A tibble: 5 x 12
##    mtry min_n tree_depth learn_rate loss_reduction sample_size
##   <int> <int>      <int>      <dbl>          <dbl>       <dbl>
## 1   111     8          6 0.0131            1.25e-4       0.720
## 2    95     4         11 0.0000941         4.15e-9       0.916
## 3    10    16         11 0.0295            3.04e-9       0.570
## 4    56     8         13 0.0918            1.44e+1       0.355
## 5    98    11         15 0.00000457        3.15e-4       0.974
## # ... with 6 more variables: .metric <chr>, .estimator <chr>,
## #   mean <dbl>, n <int>, std_err <dbl>, .config <chr>
```

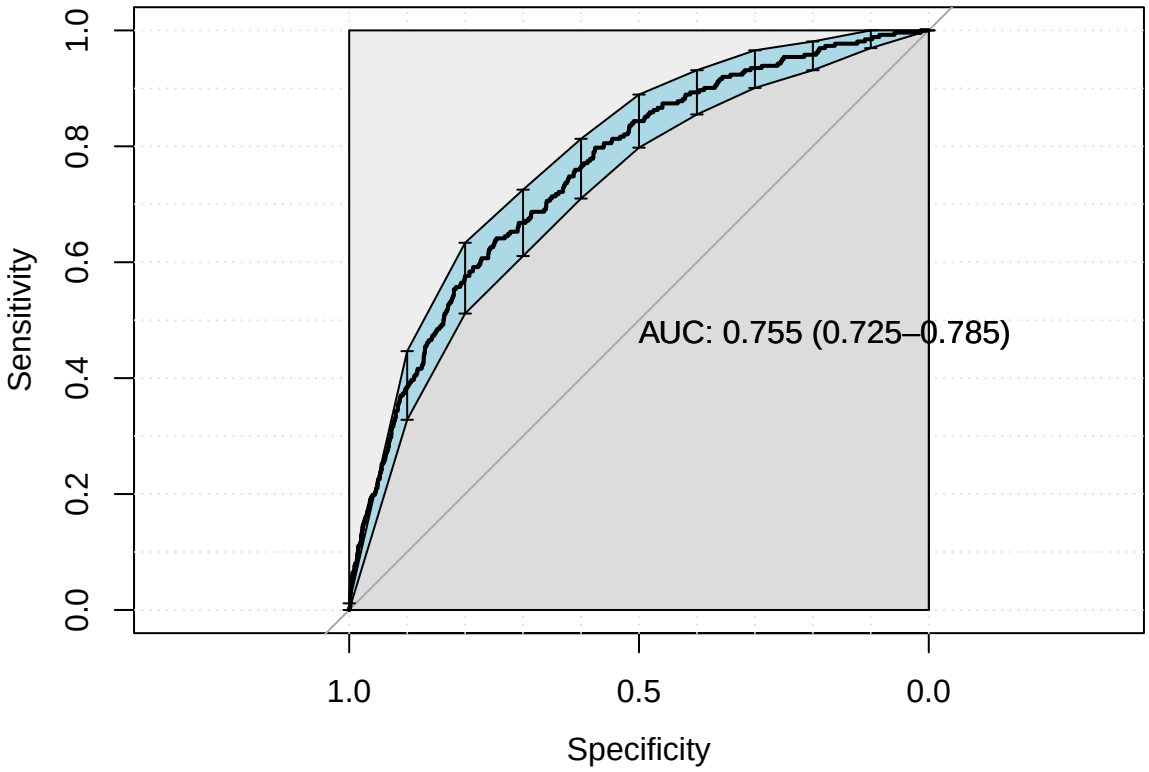
```
best_xgboost <- xgboost_tune %>%
  select_best("roc_auc")

xgboost_tune %>%
  collect_metrics() %>%
  filter(.metric == "roc_auc") %>%
  select(mean, mtry:sample_size) %>%
  pivot_longer(mtry:sample_size,
               values_to = "value",
               names_to = "parameter"
  ) %>%
  ggplot(aes(value, mean, color = parameter)) +
  geom_point(alpha = 0.8, show.legend = FALSE) +
  facet_wrap(~parameter, scales = "free_x") +
  labs(x = NULL, y = "AUC")
```




```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

last_xgboost_fit <-
  final_xgboost_workflow %>%
  last_fit(df_split)

final_xgboost_fit <- extract_workflow(last_xgboost_fit)

xgboost_auc = validation(final_xgboost_fit, df_test)
```

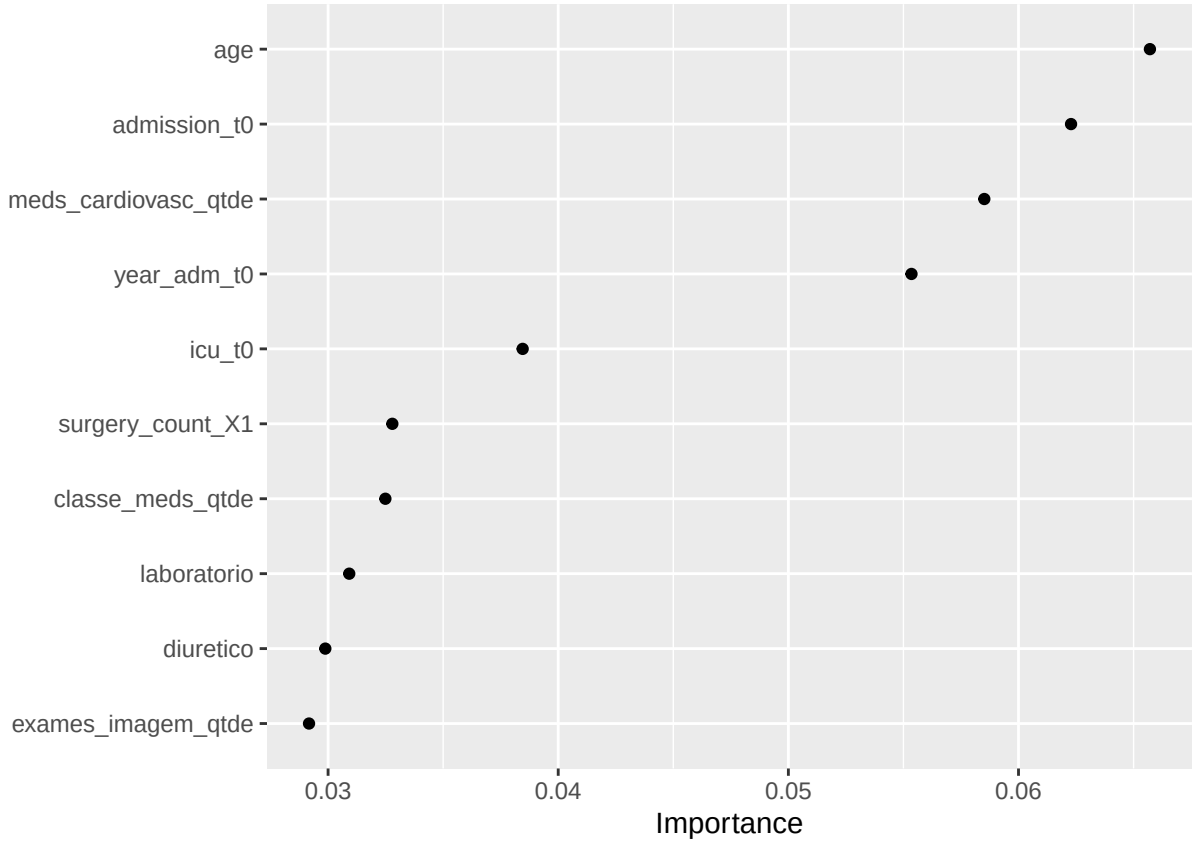
```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```




```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                       0 4461  261
##                       1    7    1
##
##                Accuracy : 0.9433
##                  95% CI : (0.9364, 0.9498)
##     No Information Rate : 0.9446
##     P-Value [Acc > NIR] : 0.6631
##
##                   Kappa : 0.0041
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.998433
##             Specificity : 0.003817
##          Pos Pred Value : 0.944727
##          Neg Pred Value : 0.125000
##              Prevalence : 0.944609
##          Detection Rate : 0.943129
##    Detection Prevalence : 0.998309
##       Balanced Accuracy : 0.501125
##
##        'Positive' Class : 0
##
```

```
final_xgboost_fit %>%
  fit(data = df_train) %>%
  extract_fit_parsnip() %>%
  vip(geom = "point")
```

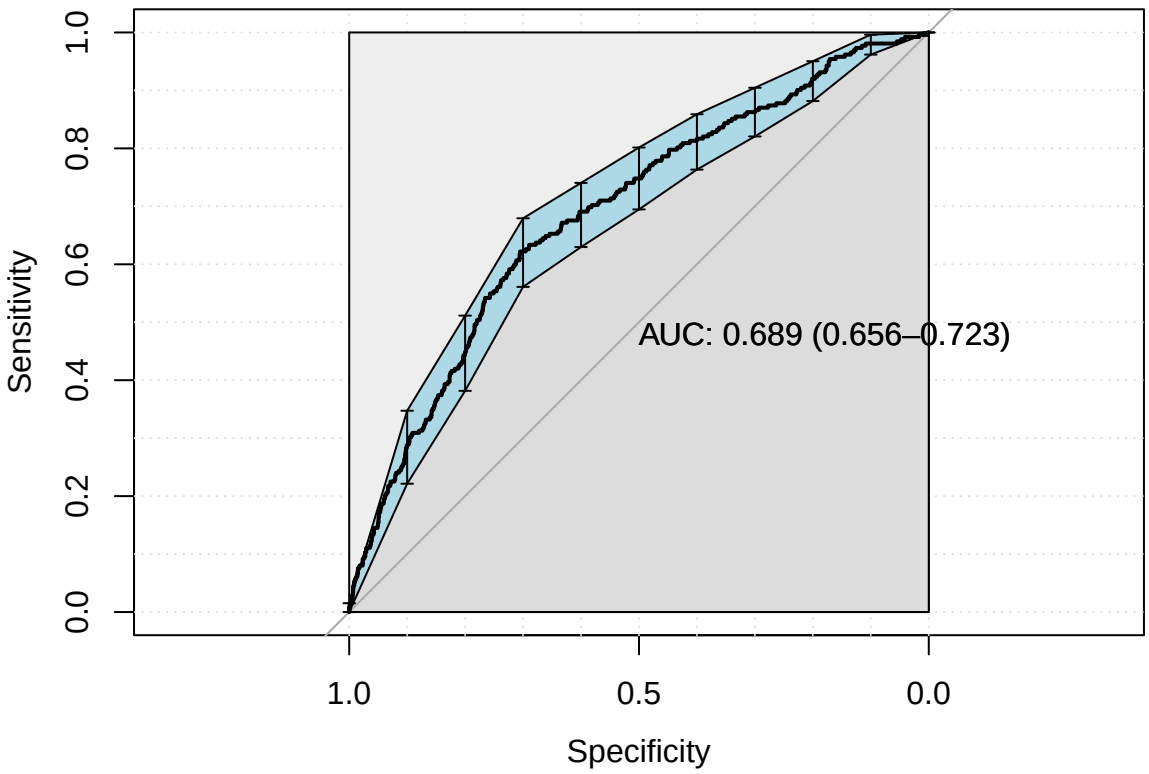


GLM

```
glmnet_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_string2factor(one_of("sex", "race", "education_level", "patient_state",
    "underlying_heart_disease", "heart_disease", "nyha_basal", "hypertension",
    "prior_mi", "heart_failure", "af", "cardiac_arrest", "transplant", "valvopathy",
    "endocardites", "diabetes", "renal_failure", "hemodialysis", "stroke",
    "copd", "cancer", "surgery_count", "procedure_type_1", "reop_type_1", "cied_final_1",
    "death_intraop_1", "dialysis_hosp", "icu_hosp", "admission_pre_t0_180d", "ventilacao_mecanica")) %>%
  step_novel(all_nominal_predictors()) %>%
  step_dummy(all_nominal_predictors()) %>%
  step_zv(all_predictors()) %>%
  step_normalize(all_numeric_predictors())

glmnet_spec <-
  logistic_reg(penalty = 0) %>%
  set_mode("classification") %>%
  set_engine("glmnet")

glmnet_workflow <-
  workflow() %>%
  add_recipe(glmnet_recipe) %>%
  add_model(glmnet_spec)

glm_fit <- glmnet_workflow %>%
  fit(df_train)

# glm_fit %>%
#   pull_workflow_fit() %>%
#   tidy()
```

```
glm_auc = validation(glm_fit, df_test)
```

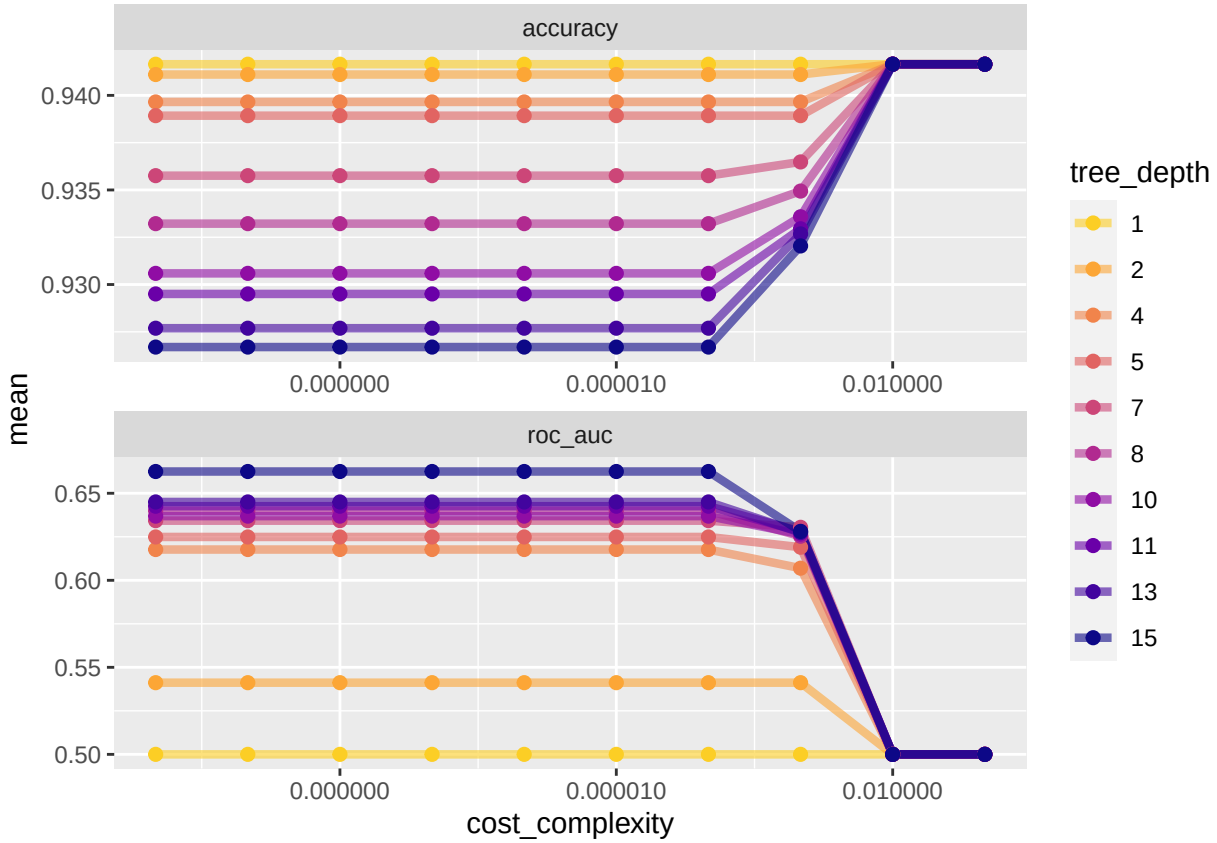
```
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
```



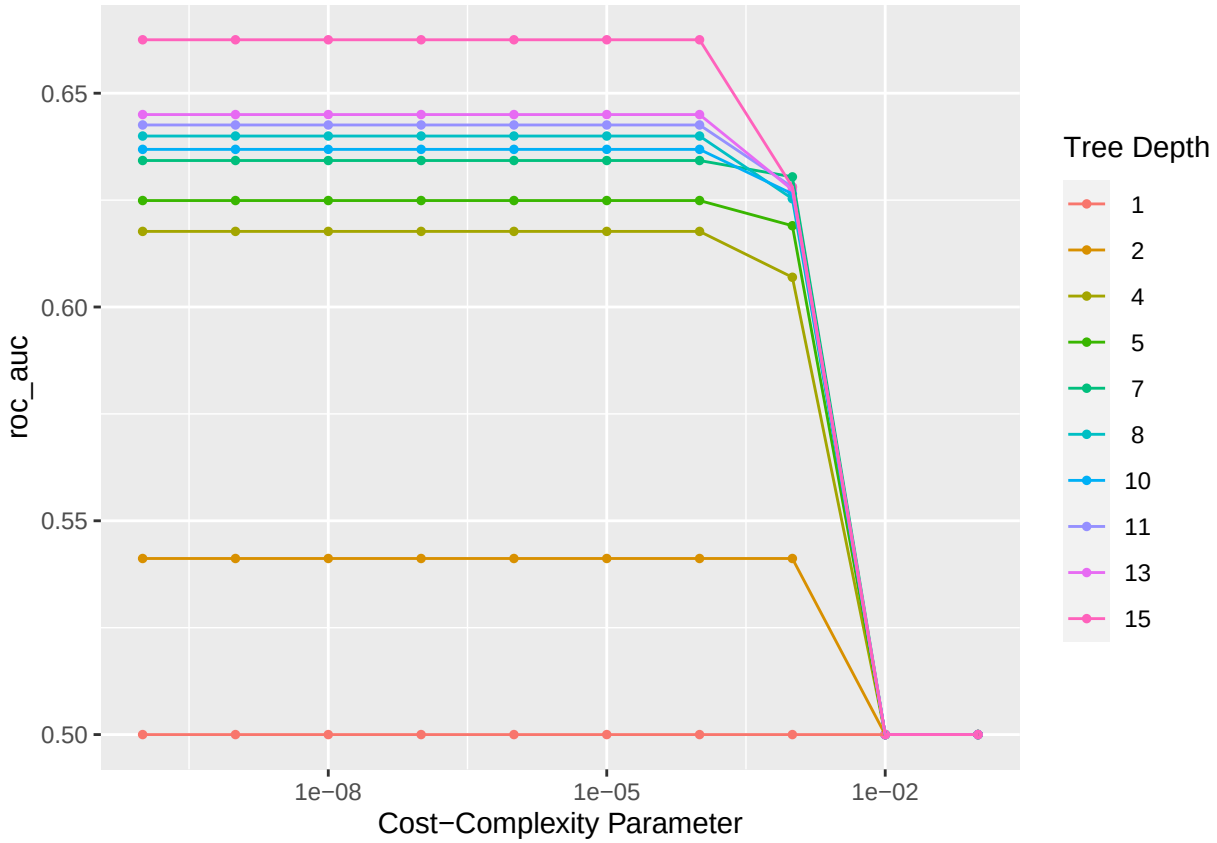

```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4466  260
##                      1    2    2
##
##                Accuracy : 0.9446
##                  95% CI : (0.9377, 0.951)
##     No Information Rate : 0.9446
##     P-Value [Acc > NIR] : 0.5164
##
##                   Kappa : 0.0134
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.999552
##             Specificity : 0.007634
##          Pos Pred Value : 0.944985
##          Neg Pred Value : 0.500000
##              Prevalence : 0.944609
##          Detection Rate : 0.944186
##    Detection Prevalence : 0.999154
##       Balanced Accuracy : 0.503593
##
##        'Positive' Class : 0
##
```

Decision Tree

```
tree_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_string2factor(one_of("sex", "race", "education_level", "patient_state",
    "underlying_heart_disease", "heart_disease", "nyha_basal", "hypertension",
    "prior_mi", "heart_failure", "af", "cardiac_arrest", "transplant", "valvopathy",
    "endocardites", "diabetes", "renal_failure", "hemodialysis", "stroke",
    "copd", "cancer", "surgery_count", "procedure_type_1", "reop_type_1", "cied_final_1",
    "death_intraop_1", "dialysis_hosp", "icu_hosp", "admission_pre_t0_180d", "ventilacao_mecanica")) %>%
  step_novel(all_nominal_predictors()) %>%
  step_zv(all_predictors())

tree_spec <-
  decision_tree(cost_complexity = tune(),
                tree_depth = tune()) %>%
  set_mode("classification") %>%
  set_engine("rpart")

tree_grid <- grid_regular(cost_complexity(),
                          tree_depth(),
                          levels = 10)

set.seed(234)
df_folds <- vfold_cv(df_train, v = 5, strata = all_of(outcome_column))

tree_workflow <-
  workflow() %>%
  add_recipe(tree_recipe) %>%
  add_model(tree_spec)

tree_tune <-
  tree_workflow %>%
  tune_grid(resamples = df_folds,
            grid = tree_grid)

tree_tune %>%
  collect_metrics()

tree_tune %>%
  collect_metrics() %>%
  mutate(tree_depth = factor(tree_depth)) %>%
  ggplot(aes(cost_complexity, mean, color = tree_depth)) +
  geom_line(size = 1.5, alpha = 0.6) +
  geom_point(size = 2) +
  facet_wrap(~ .metric, scales = "free", nrow = 2) +
  scale_x_log10(labels = scales::label_number()) +
  scale_color_viridis_d(option = "plasma", begin = .9, end = 0)
```




```
autoplot(tree_tune, metric = "roc_auc")
```

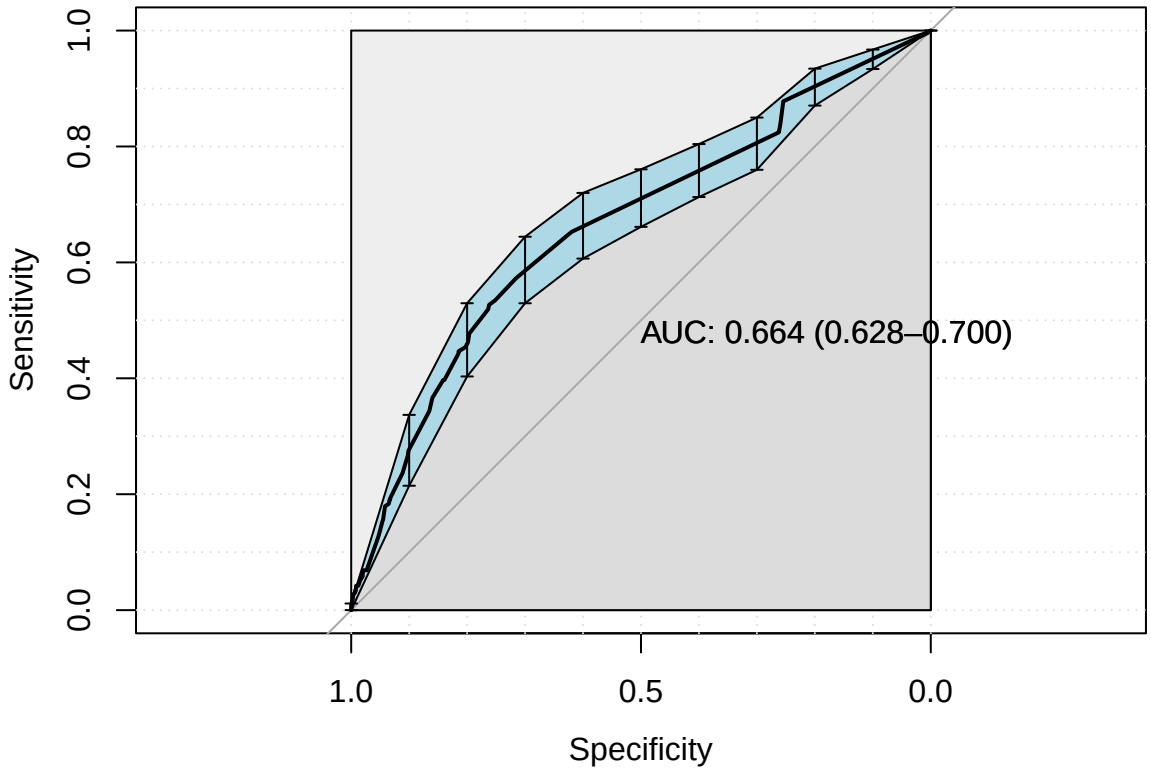



```
tree_tune %>%
  show_best("roc_auc")

best_tree <- tree_tune %>%
```

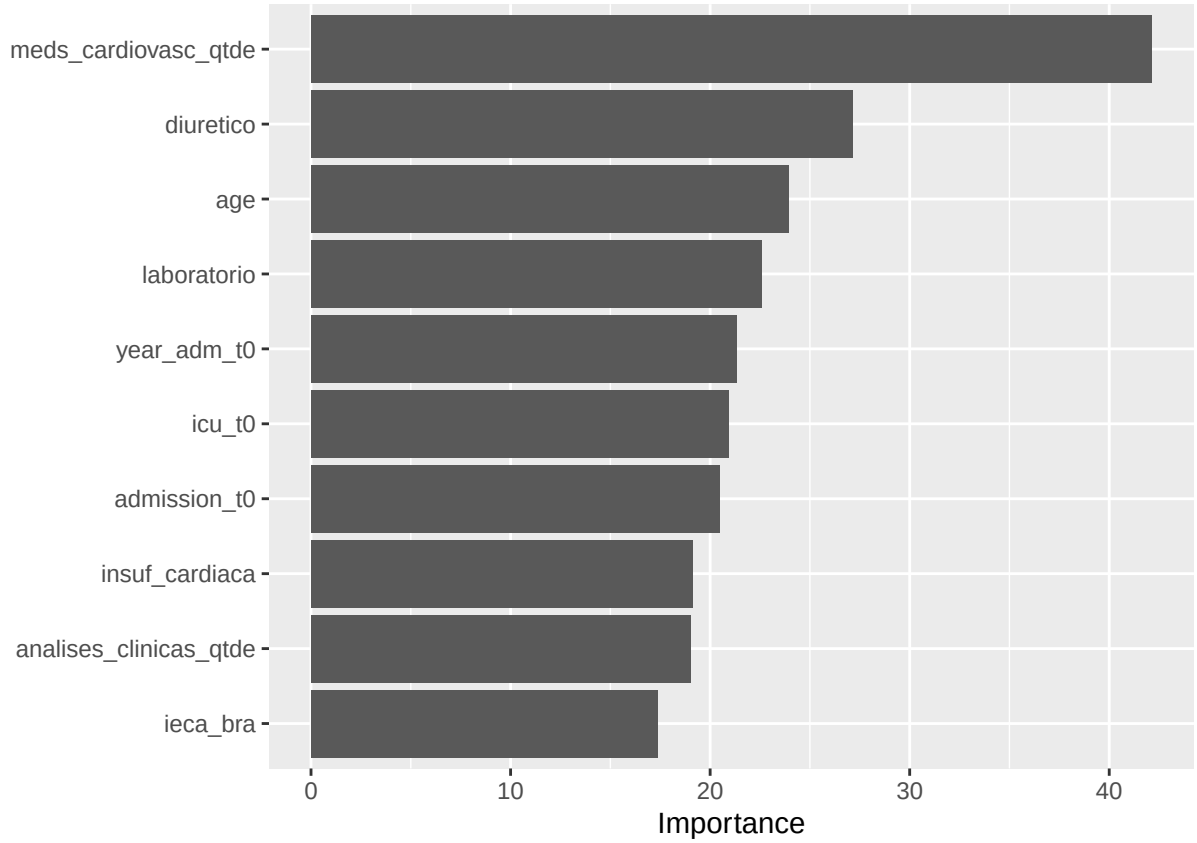
```
  select_best("roc_auc")

final_tree_workflow <-
  tree_workflow %>%
  finalize_workflow(best_tree)

last_tree_fit <-
  final_tree_workflow %>%
  last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

tree_auc = validation(final_tree_fit, df_test)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```



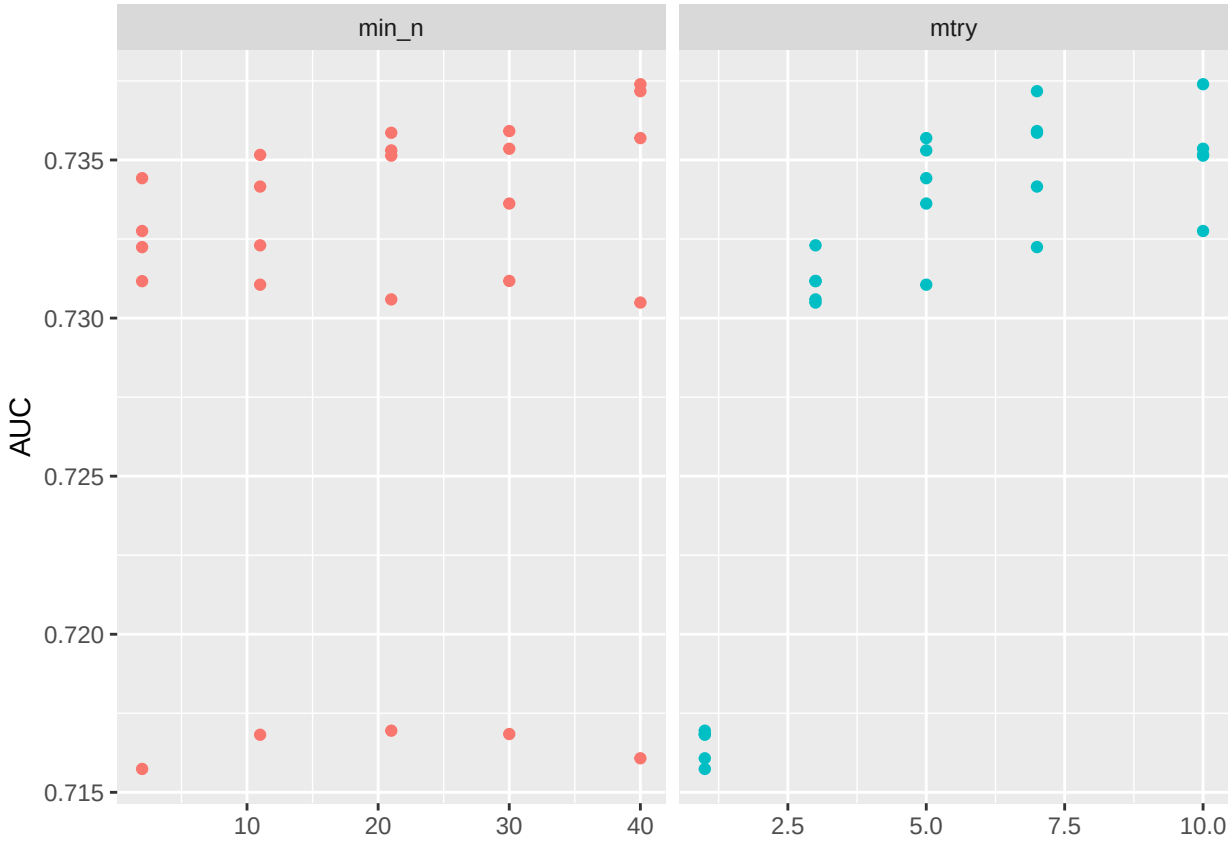

```
final_tree_fit %>%
  extract_fit_parsnip() %>%
  vip()
```



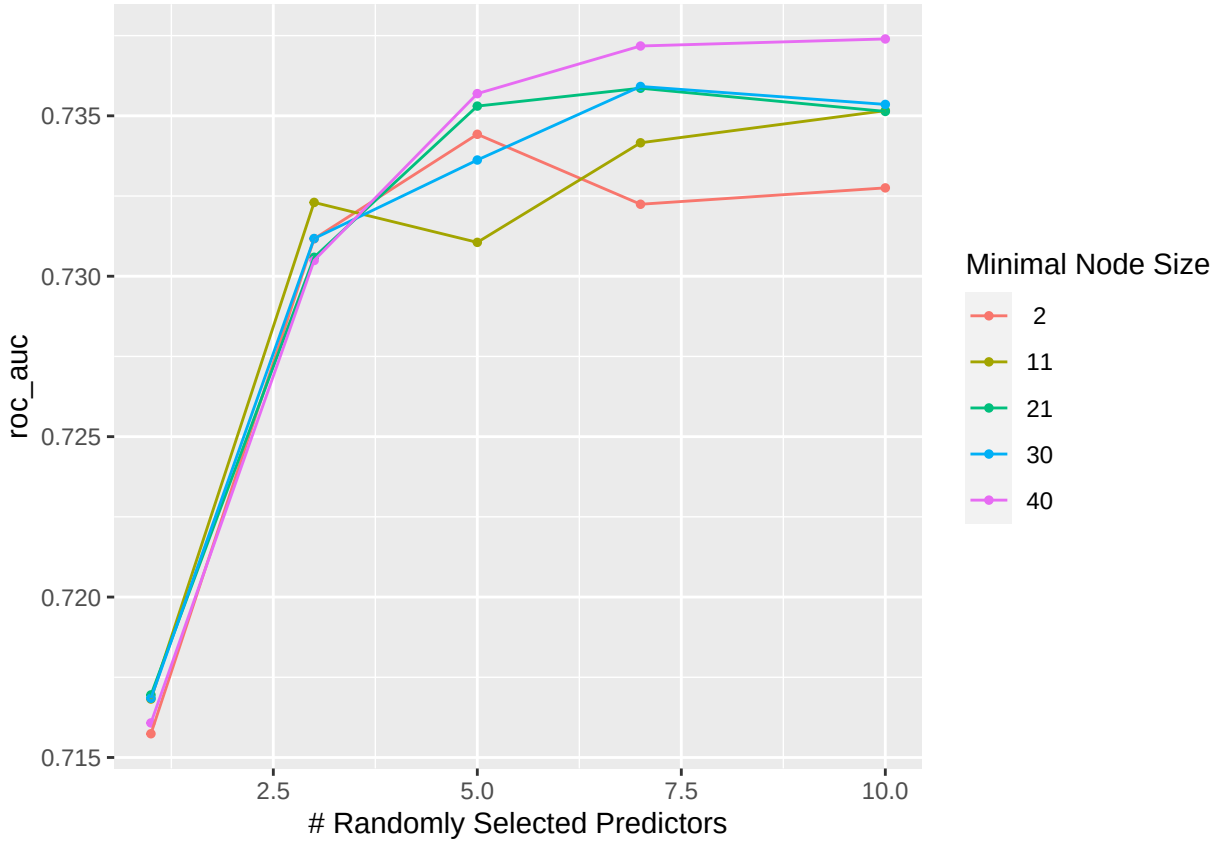
Random Forest

```
rf_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_string2factor(one_of("sex", "race", "education_level", "patient_state",
    "underlying_heart_disease", "heart_disease", "nyha_basal", "hypertension",
    "prior_mi", "heart_failure", "af", "cardiac_arrest", "transplant", "valvopathy",
    "endocardites", "diabetes", "renal_failure", "hemodialysis", "stroke",
    "copd", "cancer", "surgery_count", "procedure_type_1", "reop_type_1", "cied_final_1",
    "death_intraop_1", "dialysis_hosp", "icu_hosp", "admission_pre_t0_180d", "ventilacao_mecanica")) %>%
  step_novel(all_nominal_predictors()) %>%
  step_zv(all_predictors()) %>%
  step_dummy(all_nominal_predictors()) %>%
  step_impute_mode(all_nominal_predictors()) %>%
  step_impute_mean(all_numeric_predictors())

rf_spec <-
  rand_forest(mtry = tune(),
              trees = 1000,
              min_n = tune()) %>%
  set_mode("classification") %>%
  set_engine("ranger")

rf_grid <- grid_regular(mtry(range = c(1, 10)),
                        min_n(),
                        levels = 5)

set.seed(234)
df_folds <- vfold_cv(df_train, v = 5, strata = all_of(outcome_column))

rf_workflow <-
  workflow() %>%
```

```
  add_recipe(rf_recipe) %>%
  add_model(rf_spec)

rf_tune <-
  rf_workflow %>%
  tune_grid(resamples = df_folds,
            grid = rf_grid)

rf_tune %>%
  collect_metrics()

rf_tune %>%
  collect_metrics() %>%
  filter(.metric == "roc_auc") %>%
  select(mean, min_n, mtry) %>%
  pivot_longer(min_n:mtry,
    values_to = "value",
    names_to = "parameter"
  ) %>%
  ggplot(aes(value, mean, color = parameter)) +
  geom_point(show.legend = FALSE) +
  facet_wrap(~parameter, scales = "free_x") +
  labs(x = NULL, y = "AUC")
```



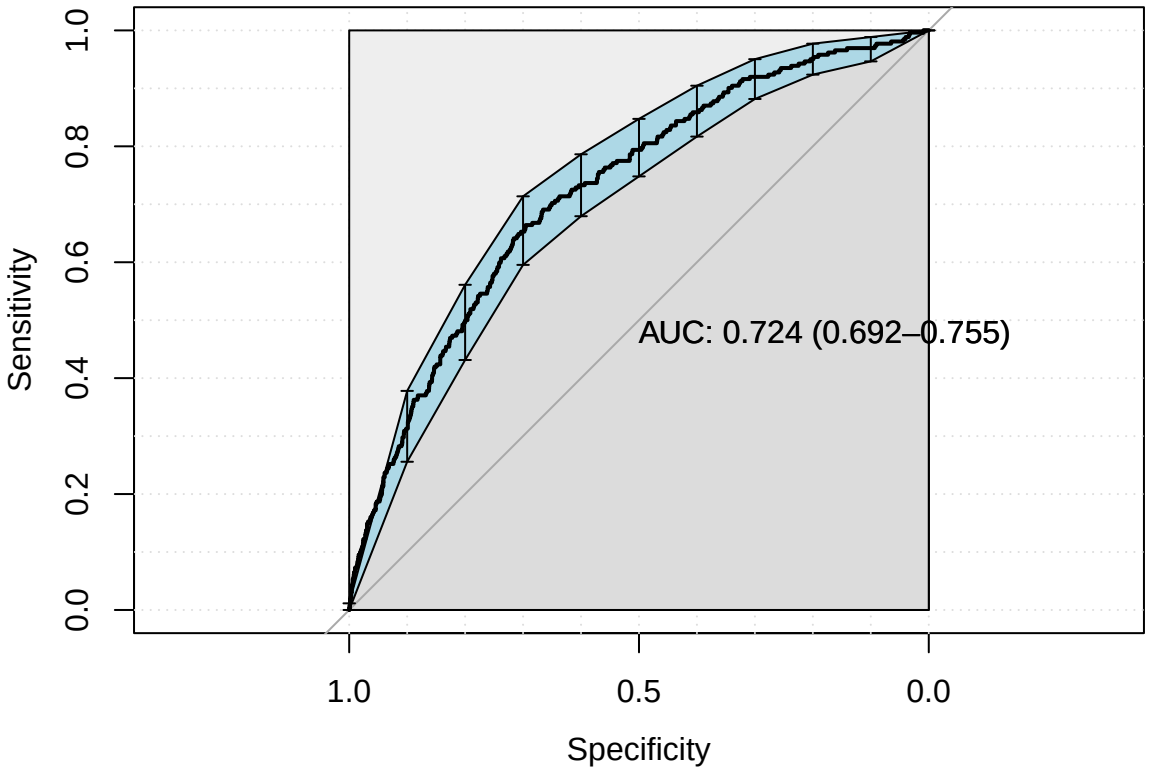

```
autoplot(rf_tune, metric = "roc_auc")
```




```
rf_tune %>%
  show_best("roc_auc")

best_rf <- rf_tune %>%
  select_best("roc_auc")

final_rf_workflow <-
  rf_workflow %>%
  finalize_workflow(best_rf)

last_rf_fit <-
  final_rf_workflow %>%
  last_fit(df_split)

final_rf_fit <- extract_workflow(last_rf_fit)

rf_auc = validation(final_rf_fit, df_test)
```

```
## Setting levels: control = 0, case = 1
```

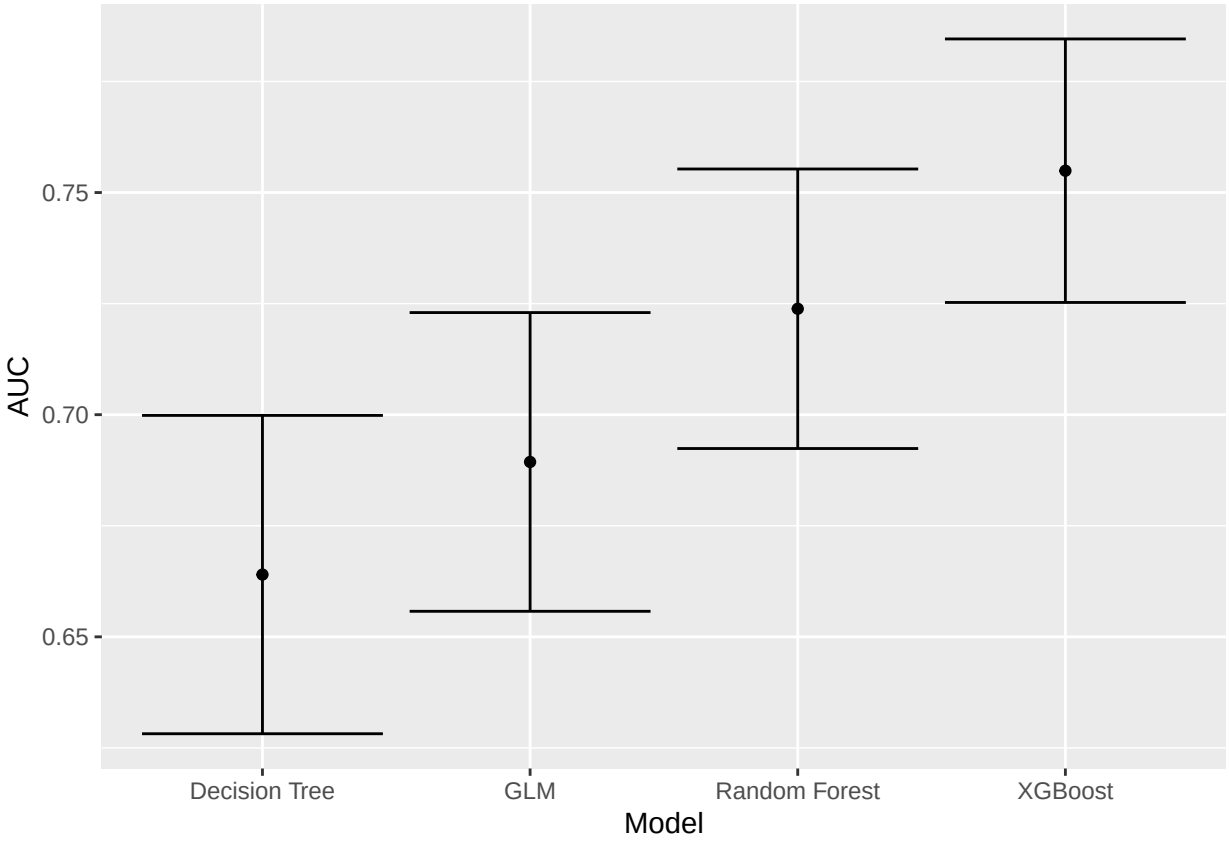
```
## Setting direction: controls < cases
```




```
# final_rf_fit %>%
#   extract_fit_parsnip() %>%
#   vip()
```

Models Comparison

```
df_auc <- tibble::tribble(
  ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
  'XGBoost', as.numeric(xgboost_auc$auc), xgboost_auc$ci[1], xgboost_auc$ci[3],
  'GLM', as.numeric(glm_auc$auc), glm_auc$ci[1], glm_auc$ci[3],
  'Decision Tree', as.numeric(tree_auc$auc), tree_auc$ci[1], tree_auc$ci[3],
  'Random Forest', as.numeric(rf_auc$auc), rf_auc$ci[1], rf_auc$ci[3]
) %>%
  mutate(Target = outcome_column)

df_auc %>%
  ggplot(aes(x = Model, y = AUC, ymin = `Lower Limit`, ymax = `Upper Limit`)) +
    geom_point() +
    geom_errorbar()
```




```
saveRDS(df_auc, sprintf("../EDA/auxiliar/performance/%s_auc_result.RData", outcome_column))
```