Model Selection

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Imports

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

Loading data

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

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

outcome_column <- params$outcome_column
features_list <- params$features_list
```

Filtering eligible pacients

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

df %>% dim
```

```
## [1] 15766   239
```

Eligible features

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

exception_columns = c('death_intraop', 'death_intraop_1')

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
                       )

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

```r
if (is.null(features_list)) {
  features = eligible_features
} else {
  features = base::intersect(eligible_features, features_list)
}

length(features)
```

```
## [1] 118
```

```r
print(features)
```

```
##   [1] "sex"                        "age"                        "race"
##   [4] "education_level"            "patient_state"              "underlying_heart_disease"
##   [7] "heart_disease"              "nyha_basal"                 "hypertension"
##  [10] "prior_mi"                   "heart_failure"              "af"
##  [13] "cardiac_arrest"             "transplant"                 "valvopathy"
##  [16] "endocardites"               "diabetes"                   "renal_failure"
##  [19] "hemodialysis"               "stroke"                     "copd"
##  [22] "cancer"                     "comorbidities_count"        "procedure_type_1"
##  [25] "reop_type_1"                "procedure_type_new"         "cied_final_1"
##  [28] "cied_final_group_1"         "admission_t0"               "admission_pre_t0_180d"
##  [31] "year_adm_t0"                "icu_t0"                     "dialysis_t0"
##  [34] "disch_outcomes_t0"          "n_procedure_t0"             "admission_t0_emergency"
##  [37] "aco"                        "antiarritmico"              "antihipertensivo"
##  [40] "betabloqueador"             "ieca_bra"                   "dva"
##  [43] "digoxina"                   "estatina"                   "diuretico"
##  [46] "vasodilatador"              "insuf_cardiaca"             "espironolactona"
##  [49] "bloq_calcio"                "trombolitico"               "antiplaquetario_vo"
##  [52] "antiplaquetario_ev"         "insulina"                   "hipoglicemiante"
##  [55] "hormonio_tireoidiano"       "broncodilatador"            "anticonvulsivante"
##  [58] "psicofarmacos"              "antifungico"                "antiviral"
##  [61] "antiretroviral"             "classe_meds_qtde"           "meds_cardiovasc_qtde"
##  [64] "meds_antimicrobianos"       "vni"                        "ventilacao_mecanica"
##  [67] "cec"                        "cir_cardiovascular"         "transplante_cardiaco"
##  [70] "cir_toracica"               "outros_proced_cirurgicos" "traqueostomia"
##  [73] "icp"                        "intervencao_cv"             "stent"
##  [76] "angioplastia"               "cateterismo"                "eletrofisiologia"
##  [79] "cateter_venoso_central"     "drenagem_torax"             "proced_invasivos_qtde"
##  [82] "cve_desf"                   "transfusao"                 "interconsulta"
##  [85] "equipe_multiprof"           "ecg"                        "holter"
##  [88] "teste_esforco"              "espiro_ergoespiro"          "tilt_teste"
##  [91] "polissonografia"            "metodos_graficos_qtde"      "laboratorio"
##  [94] "cultura"                    "analises_clinicas_qtde"     "citologia"
##  [97] "biopsia"                    "histopatologia_qtde"        "angio_rm"
## [100] "angio_tc"                   "angiografia"                "aortografia"
## [103] "arteriografia"              "cavografia"                 "cintilografia"
## [106] "ecocardiograma"             "endoscopia"                 "flebografia"
## [109] "pet_ct"                     "ultrassom"                  "tomografia"
## [112] "radiografia"                "ressonancia"                "exames_imagem_qtde"
## [115] "dieta_enteral"              "dieta_parenteral"           "bic"
## [118] "mpp"
```

Train test split (70%/30%)

```r
set.seed(42)

df[columns_list$outcome_columns] <- lapply(df[columns_list$outcome_columns], factor)
df <- mutate(df, across(where(is.character), as.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
```

Global parameters

```
k = 4 # Number of folds for cross validation
grid_size = 10 # Number of parameter combination to tune on each model

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

Functions

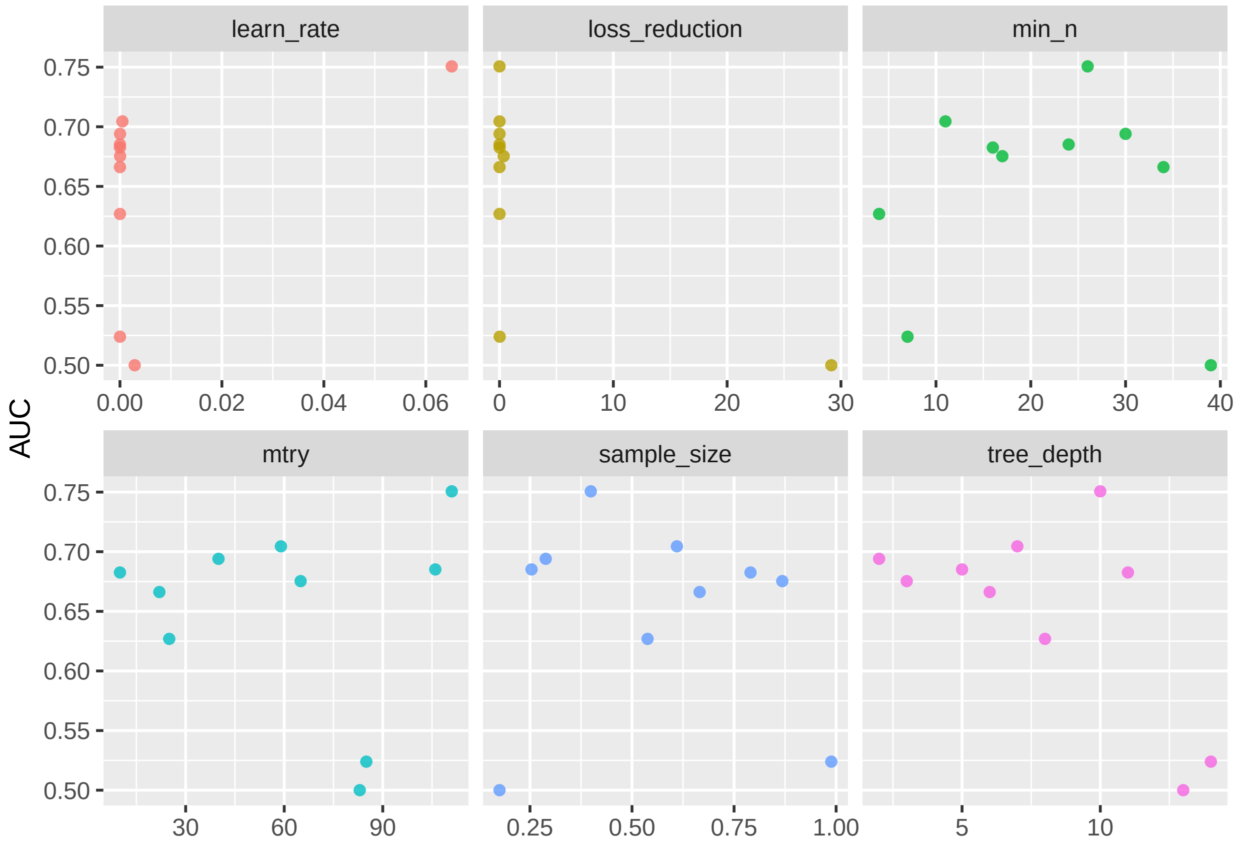
```
validation = function(model_fit, new_data) {
  library(pROC)
  library(caret)

  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)
}
```

Boosted Tree (XGBoost)

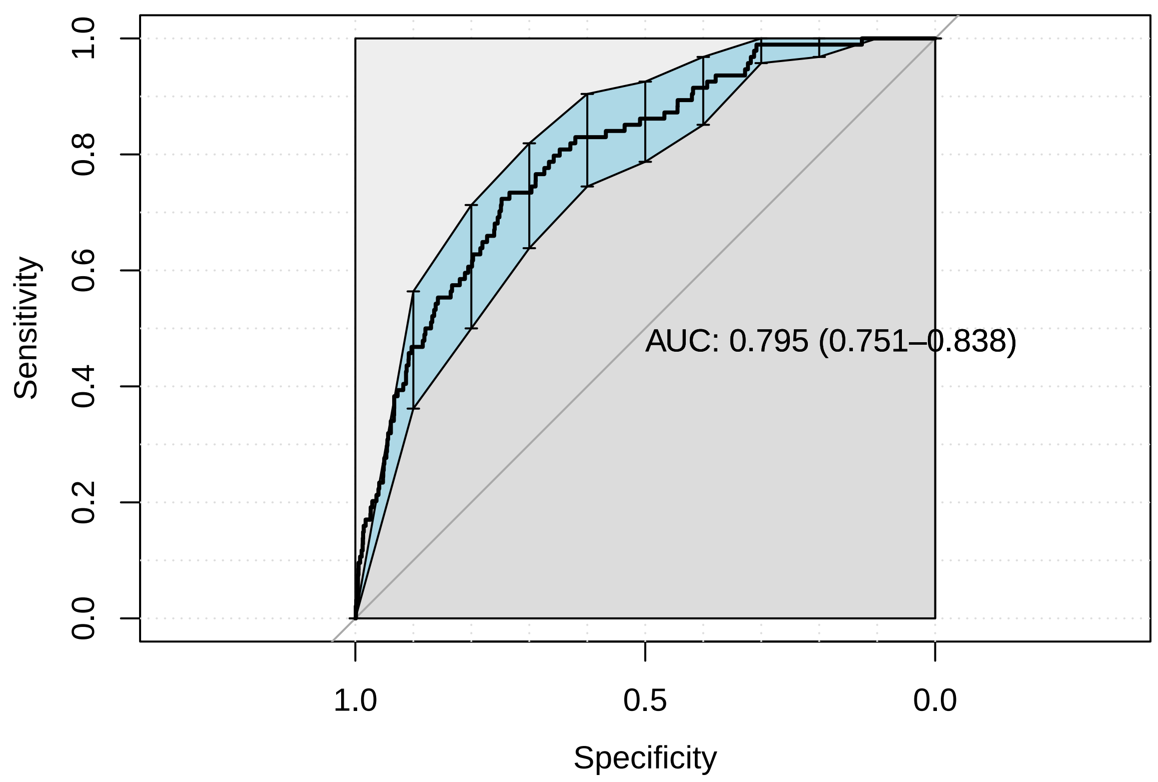
```
xgboost_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors())

xgboost_spec <- boost_tree(
  trees = 100,
  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 = grid_size
)

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_~1 sampl~2 .metric .esti~3  mean     n std_err .config
##   <int> <int>      <int>      <dbl>   <dbl>   <dbl> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1   111    26         10    6.51e-2 1.59e-4   0.399 roc_auc binary  0.751     4  0.0233 Prepro~
## 2    59    11          7    4.79e-4 4.05e-8   0.610 roc_auc binary  0.705     4  0.0166 Prepro~
## 3    40    30          2    1.40e-5 5.75e-7   0.289 roc_auc binary  0.694     4  0.0302 Prepro~
## 4   106    24          5    1.52e-6 2.40e-5   0.254 roc_auc binary  0.685     4  0.0208 Prepro~
## 5    10    16         11    1.57e-7 1.02e-2   0.790 roc_auc binary  0.683     4  0.0186 Prepro~
## # ... with abbreviated variable names 1: loss_reduction, 2: sample_size, 3: .estimator
```

```
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")
```

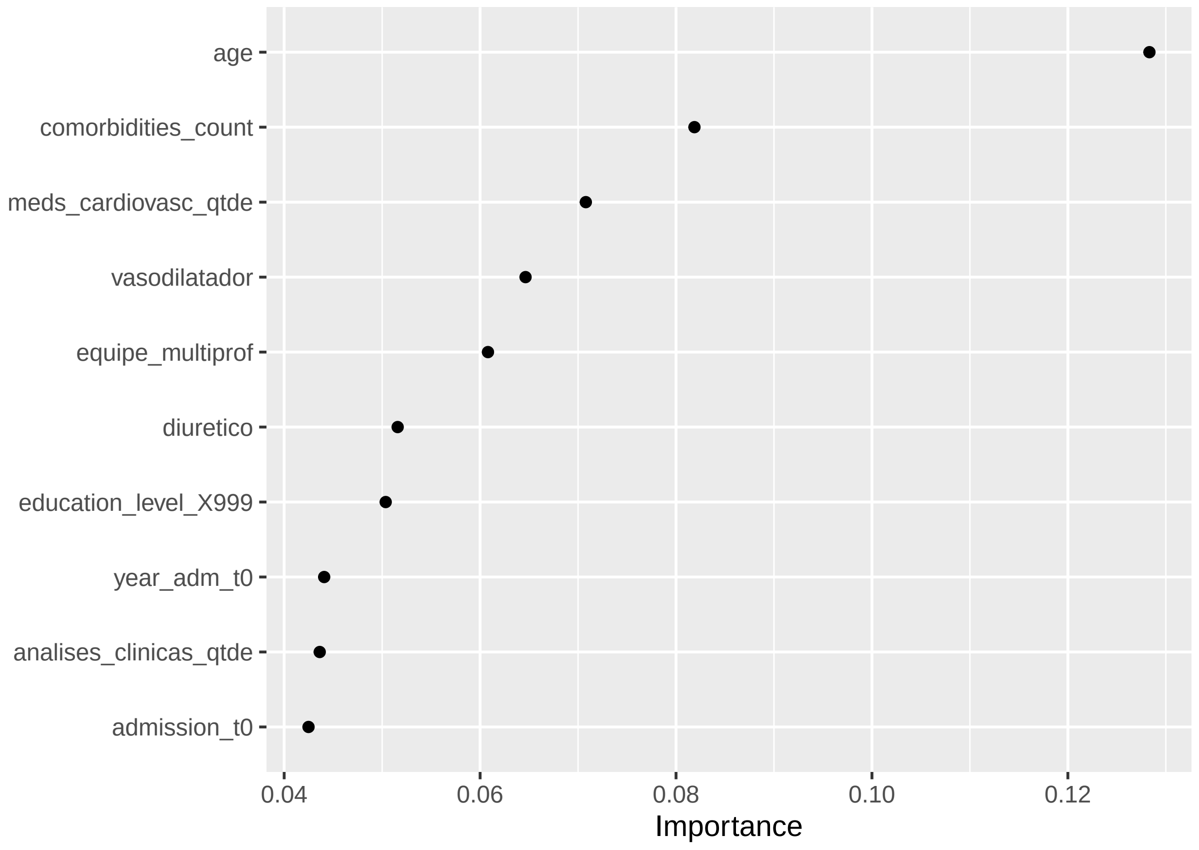


```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

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)
```



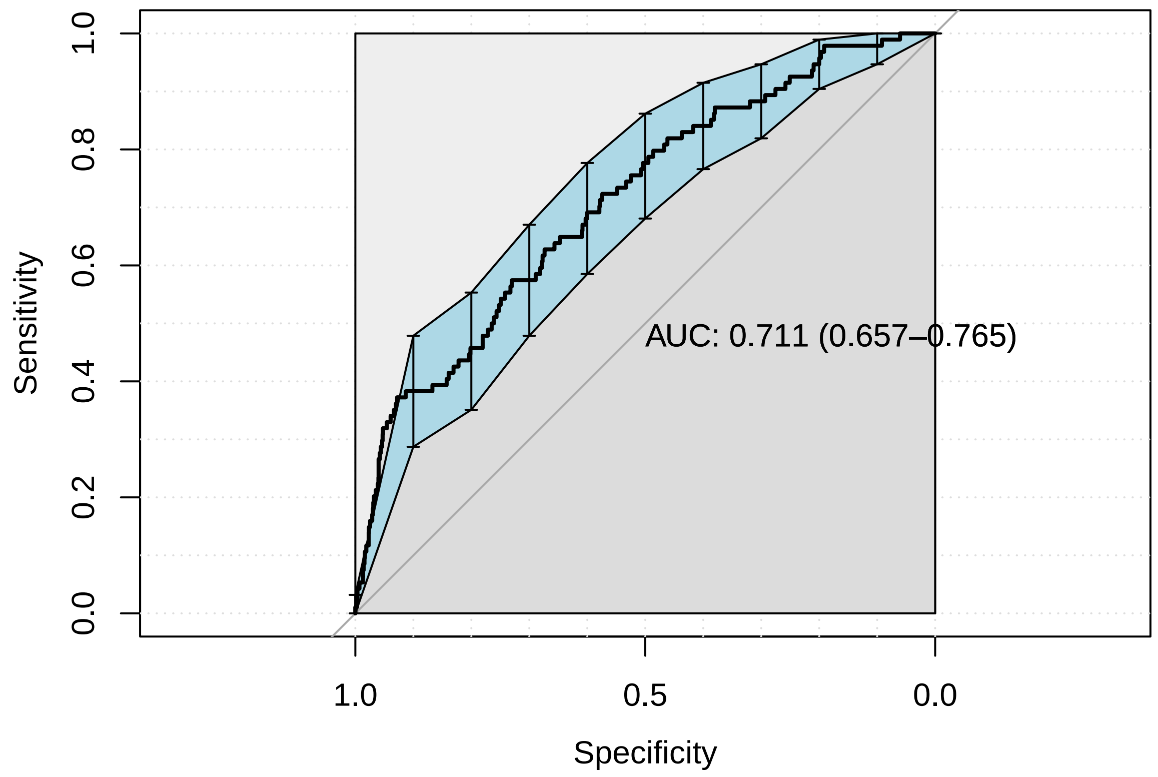
```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4636   94
##                      1    0    0
##
##                Accuracy : 0.9801
##                  95% CI : (0.9757, 0.9839)
##     No Information Rate : 0.9801
##     P-Value [Acc > NIR] : 0.5274
##
##                   Kappa : 0
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 1.0000
##             Specificity : 0.0000
##          Pos Pred Value : 0.9801
##          Neg Pred Value :    NaN
##              Prevalence : 0.9801
##          Detection Rate : 0.9801
##    Detection Prevalence : 1.0000
##       Balanced Accuracy : 0.5000
##
##        'Positive' Class : 0
##
```

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



GLM

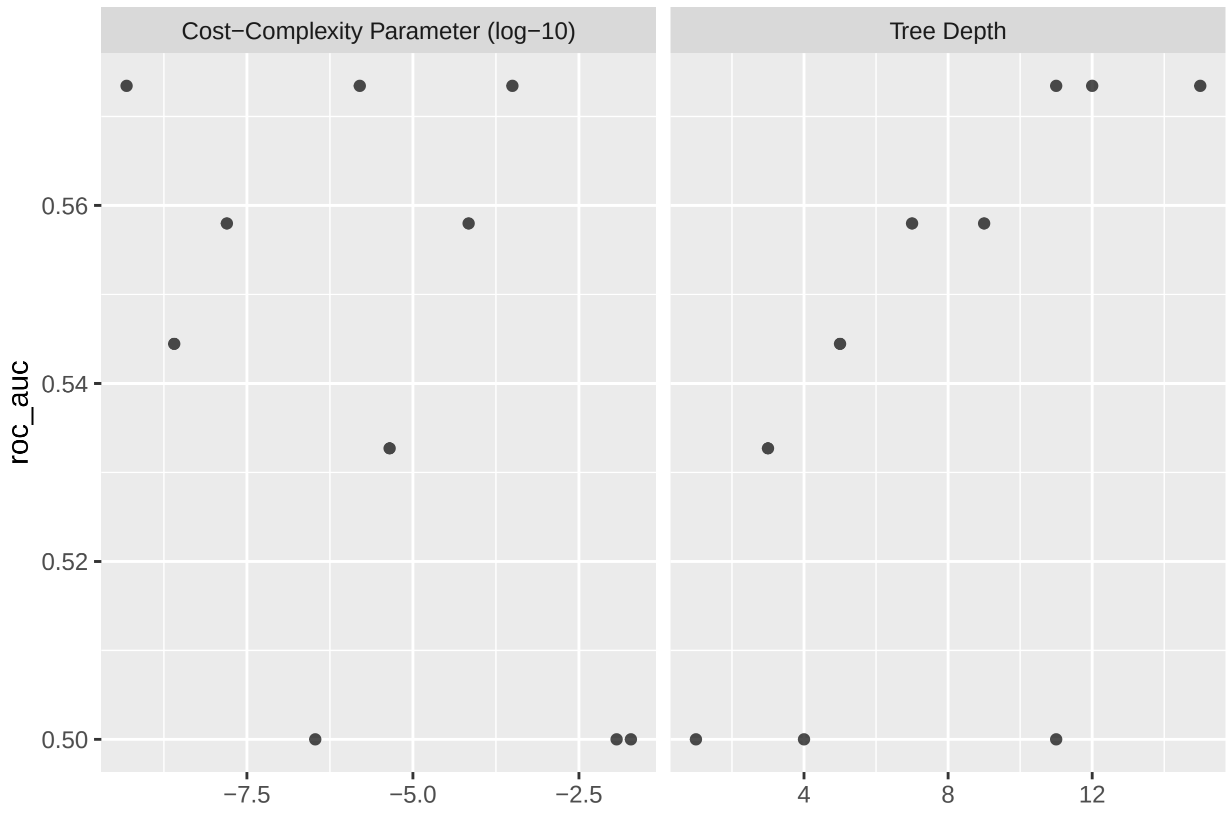
```
glmnet_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  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_auc = validation(glm_fit, df_test)
```



```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4636   93
##                      1    0    1
##
##                Accuracy : 0.9803
##                  95% CI : (0.976, 0.9841)
##     No Information Rate : 0.9801
##     P-Value [Acc > NIR] : 0.4859
##
##                   Kappa : 0.0206
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 1.00000
##             Specificity : 0.01064
##          Pos Pred Value : 0.98033
##          Neg Pred Value : 1.00000
##              Prevalence : 0.98013
##          Detection Rate : 0.98013
##    Detection Prevalence : 0.99979
##       Balanced Accuracy : 0.50532
##
##        'Positive' Class : 0
##
```

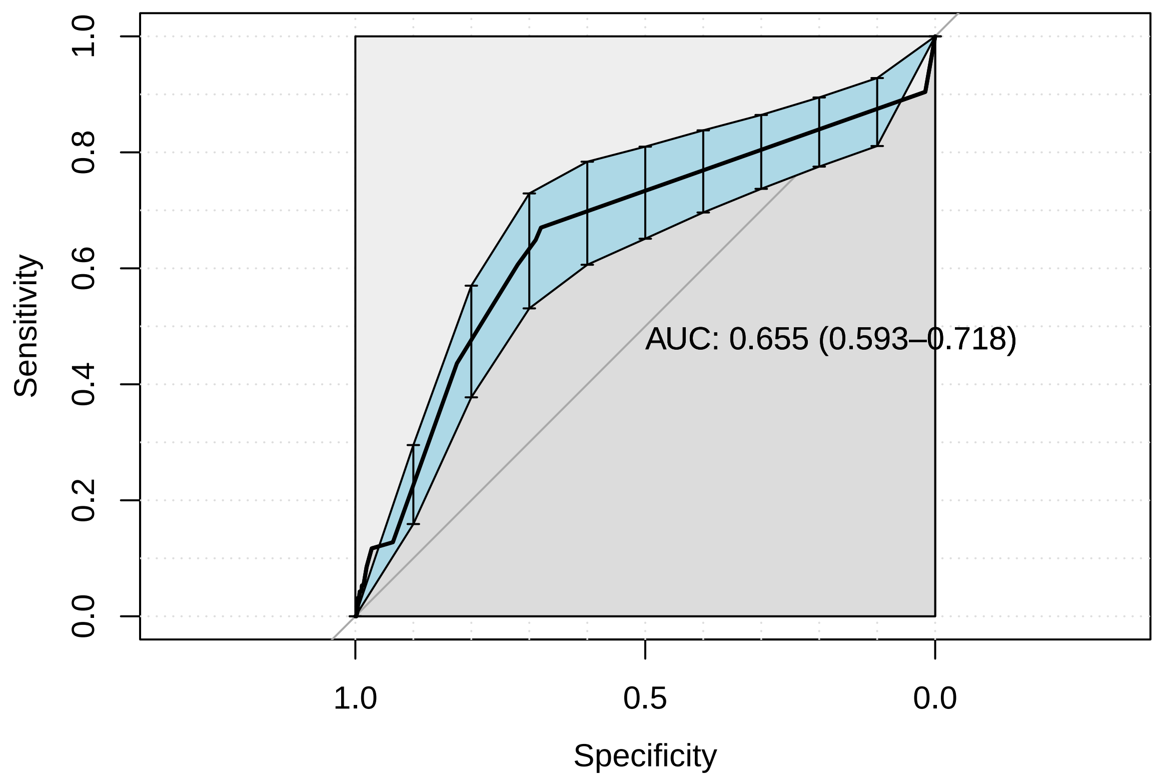
Decision Tree

```
tree_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors())

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

tree_grid <- grid_latin_hypercube(cost_complexity(),
                                  tree_depth(),
                                  size = grid_size)

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()

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

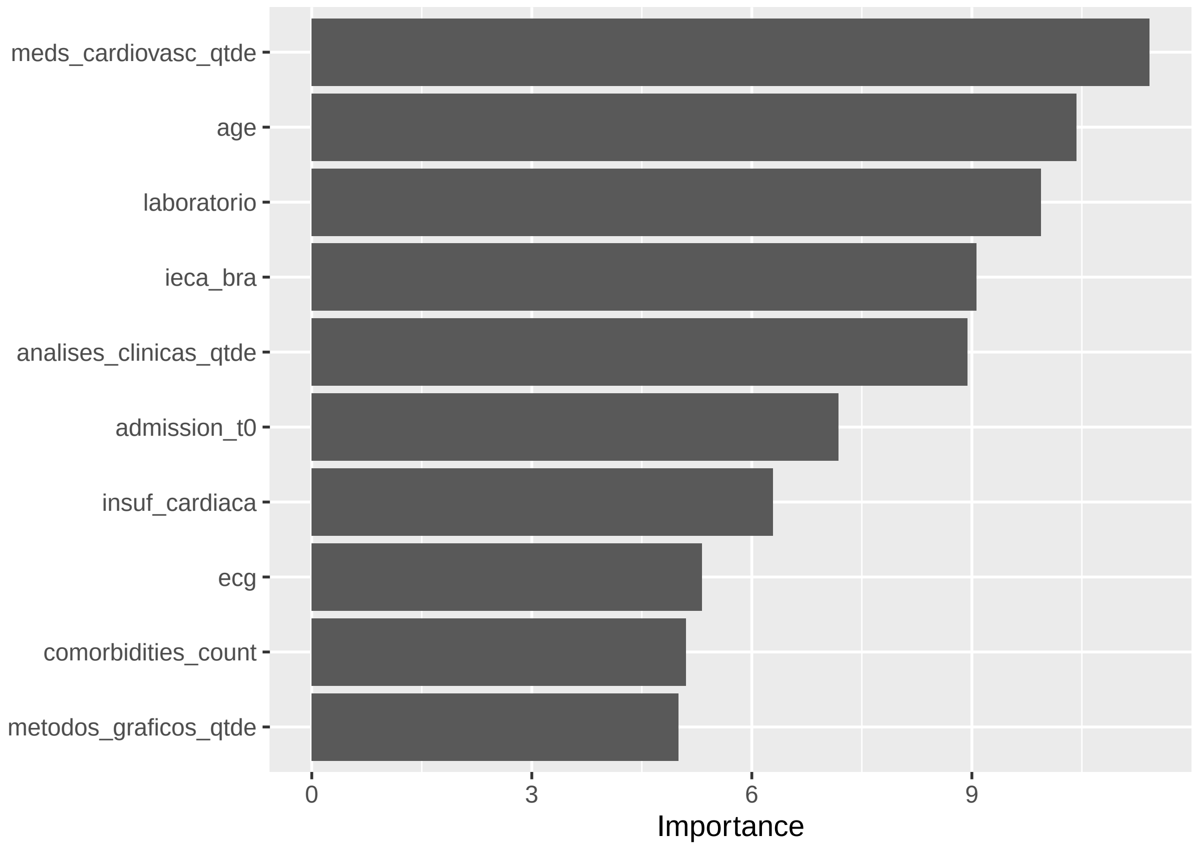


```
tree_tune %>%
  show_best("roc_auc")
```

```r
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)
```



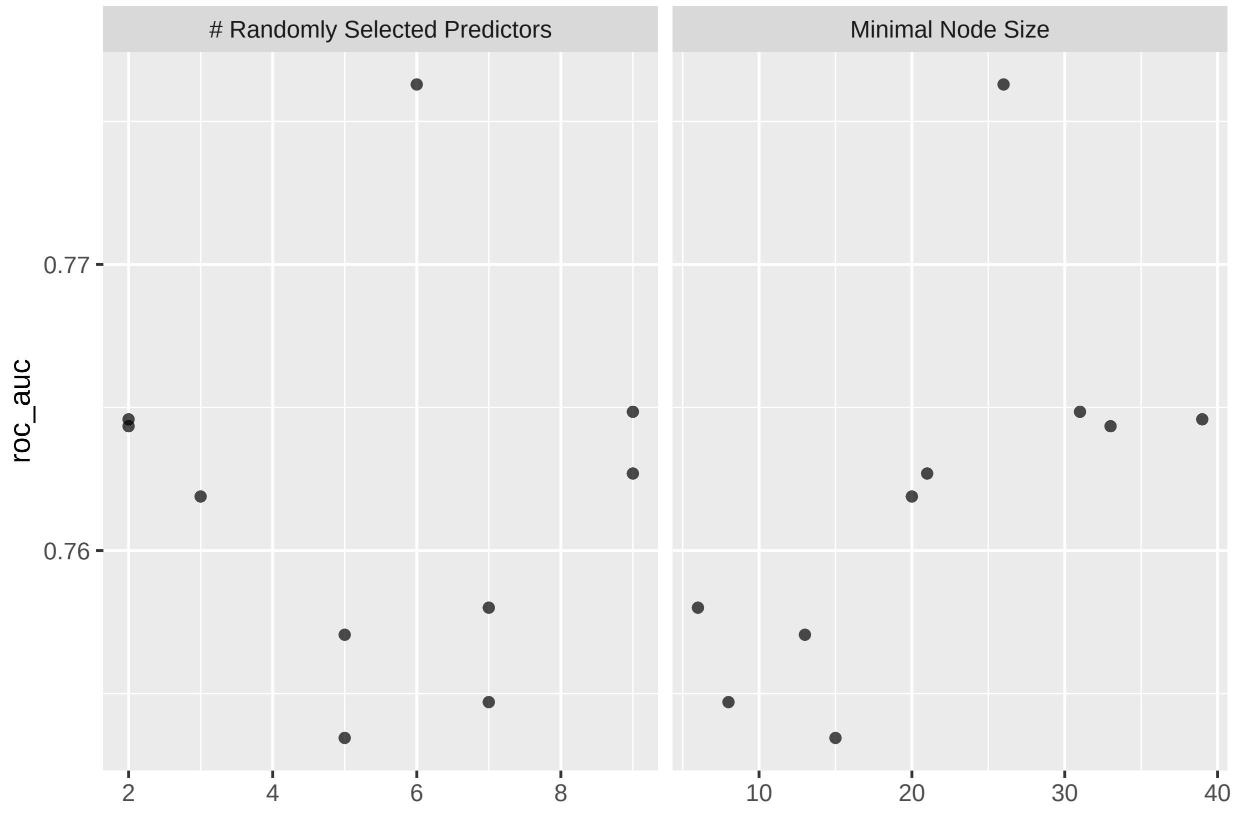
```r
if (tree_auc$auc > 0.55){
  final_tree_fit %>%
    extract_fit_parsnip() %>%
    vip()
}
```



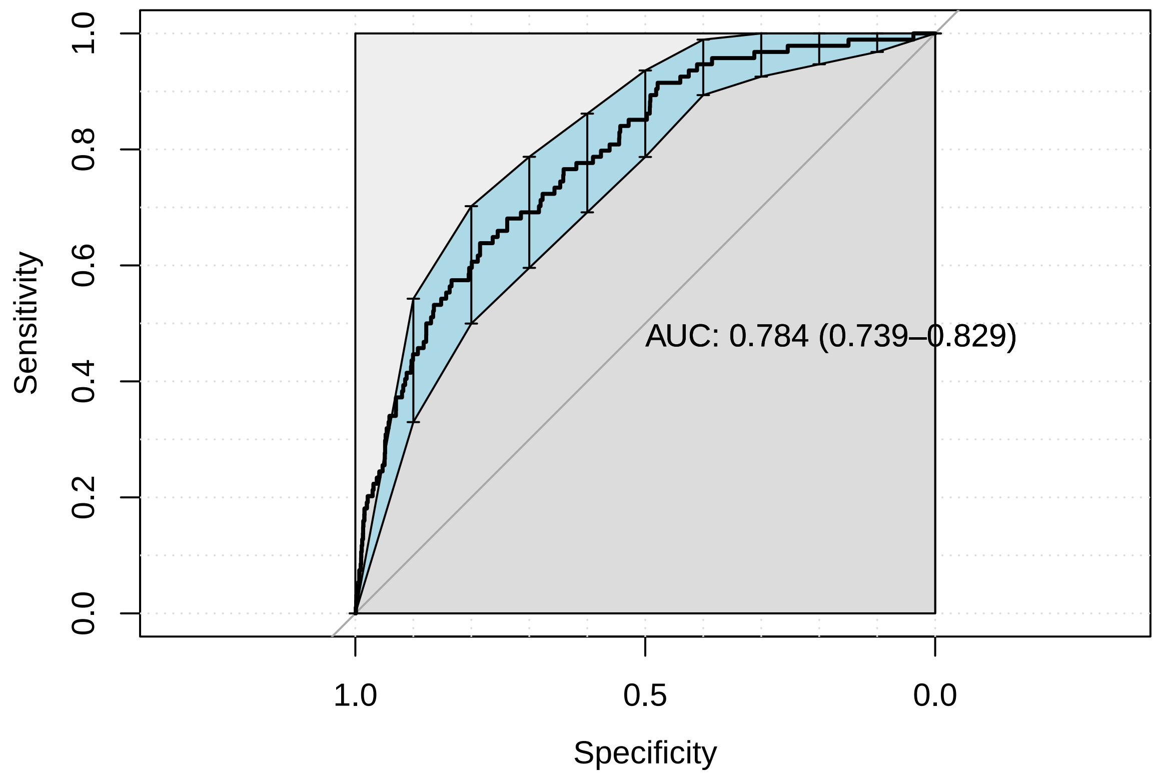
Random Forest

```
rf_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors()) %>%
  step_impute_mean(all_numeric_predictors())

rf_spec <-
  rand_forest(mtry = tune(),
              trees = 100,
              min_n = tune()) %>%
  set_mode("classification") %>%
  set_engine("ranger")

rf_grid <- grid_latin_hypercube(mtry(range = c(1, 10)),
                                min_n(),
                                size = grid_size)

rf_workflow <-
  workflow() %>%
  add_recipe(rf_recipe) %>%
  add_model(rf_spec)

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

```r
rf_tune %>%
  collect_metrics()

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



```r
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)
```



KNN

```
# knn_recipe <-
#   recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
#   step_novel(all_nominal_predictors()) %>%
#   step_unknown(all_nominal_predictors()) %>%
#   step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
#   step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
#   step_zv(all_predictors()) %>%
#   step_impute_mean(all_numeric_predictors())
#
# knn_spec <-
#   nearest_neighbor(neighbors = tune(),
#                    weight_func = tune(),
#                    dist_power = tune()) %>%
#   set_mode("classification") %>%
#   set_engine("kknn")
#
# knn_grid <- grid_latin_hypercube(neighbors(),
#                                  weight_func(),
#                                  dist_power(),
#                                  size = 5)
#
# knn_workflow <-
#   workflow() %>%
#   add_recipe(knn_recipe) %>%
#   add_model(knn_spec)
#
# knn_tune <-
#   knn_workflow %>%
#   tune_grid(resamples = df_folds,
#             grid = knn_grid)
```

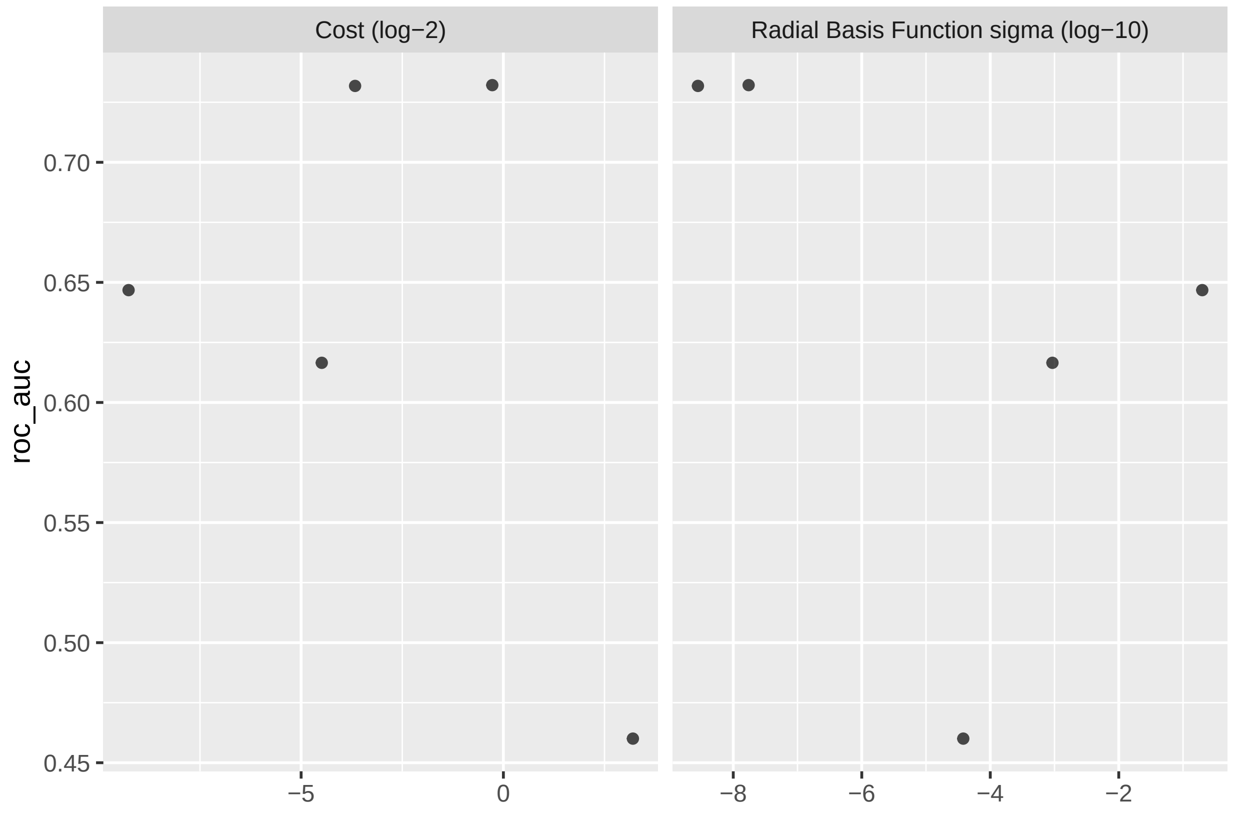
```r
#
# knn_tune %>%
#   collect_metrics()
#
# autoplot(knn_tune, metric = "roc_auc")
#
# knn_tune %>%
#   show_best("roc_auc")
#
# best_knn <- knn_tune %>%
#   select_best("roc_auc")
#
# final_knn_workflow <-
#   knn_workflow %>%
#   finalize_workflow(best_knn)
#
# last_knn_fit <-
#   final_knn_workflow %>%
#   last_fit(df_split)
#
# final_knn_fit <- extract_workflow(last_knn_fit)
#
# knn_auc = validation(final_knn_fit, df_test)
```

SVM

```r
svm_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors()) %>%
  step_impute_mean(all_numeric_predictors())

svm_spec <-
  svm_rbf(cost = tune(), rbf_sigma = tune()) %>%
  set_mode("classification") %>%
  set_engine("kernlab")

svm_grid <- grid_latin_hypercube(cost(),
                                 rbf_sigma(),
                                 size = grid_size)

svm_workflow <-
  workflow() %>%
  add_recipe(svm_recipe) %>%
  add_model(svm_spec)

svm_tune <-
  svm_workflow %>%
  tune_grid(resamples = df_folds,
            grid = 5)

svm_tune %>%
  collect_metrics()
```

```
## # A tibble: 10 x 8
##        cost     rbf_sigma .metric   .estimator  mean     n  std_err .config
##       <dbl>         <dbl> <chr>     <chr>      <dbl> <int>    <dbl> <chr>
##  1 0.0788  0.00000000282 accuracy binary     0.979     4 0.000993 Preprocessor1_Model1
##  2 0.0788  0.00000000282 roc_auc  binary     0.732     4 0.0154   Preprocessor1_Model1
##  3 0.0445  0.000929      accuracy binary     0.979     4 0.000993 Preprocessor1_Model2
##  4 0.0445  0.000929      roc_auc  binary     0.617     4 0.00683  Preprocessor1_Model2
##  5 0.827   0.0000000174  accuracy binary     0.979     4 0.000993 Preprocessor1_Model3
##  6 0.827   0.0000000174  roc_auc  binary     0.732     4 0.0166   Preprocessor1_Model3
##  7 9.20    0.0000380     accuracy binary     0.979     4 0.000993 Preprocessor1_Model4
##  8 9.20    0.0000380     roc_auc  binary     0.460     4 0.0173   Preprocessor1_Model4
##  9 0.00162 0.199         accuracy binary     0.979     4 0.000993 Preprocessor1_Model5
## 10 0.00162 0.199         roc_auc  binary     0.647     4 0.0194   Preprocessor1_Model5
```

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

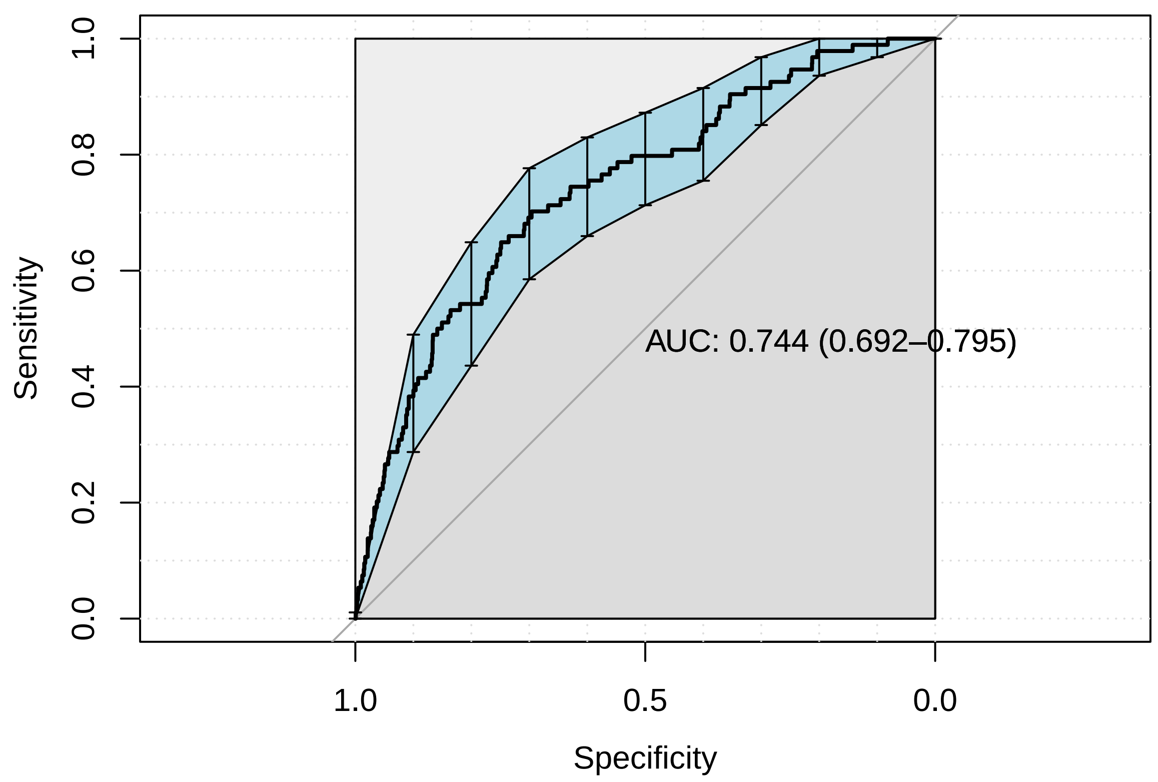


```
svm_tune %>%
  show_best("roc_auc")
```

```
## # A tibble: 5 x 8
##      cost     rbf_sigma .metric .estimator  mean     n std_err .config
##     <dbl>         <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1 0.827   0.0000000174  roc_auc binary     0.732     4 0.0166  Preprocessor1_Model3
## 2 0.0788  0.00000000282 roc_auc binary     0.732     4 0.0154  Preprocessor1_Model1
## 3 0.00162 0.199         roc_auc binary     0.647     4 0.0194  Preprocessor1_Model5
## 4 0.0445  0.000929      roc_auc binary     0.617     4 0.00683 Preprocessor1_Model2
## 5 9.20    0.0000380     roc_auc binary     0.460     4 0.0173  Preprocessor1_Model4
```

```
best_svm <- svm_tune %>%
  select_best("roc_auc")

final_svm_workflow <-
  svm_workflow %>%
  finalize_workflow(best_svm)

last_svm_fit <-
  final_svm_workflow %>%
  last_fit(df_split)
```

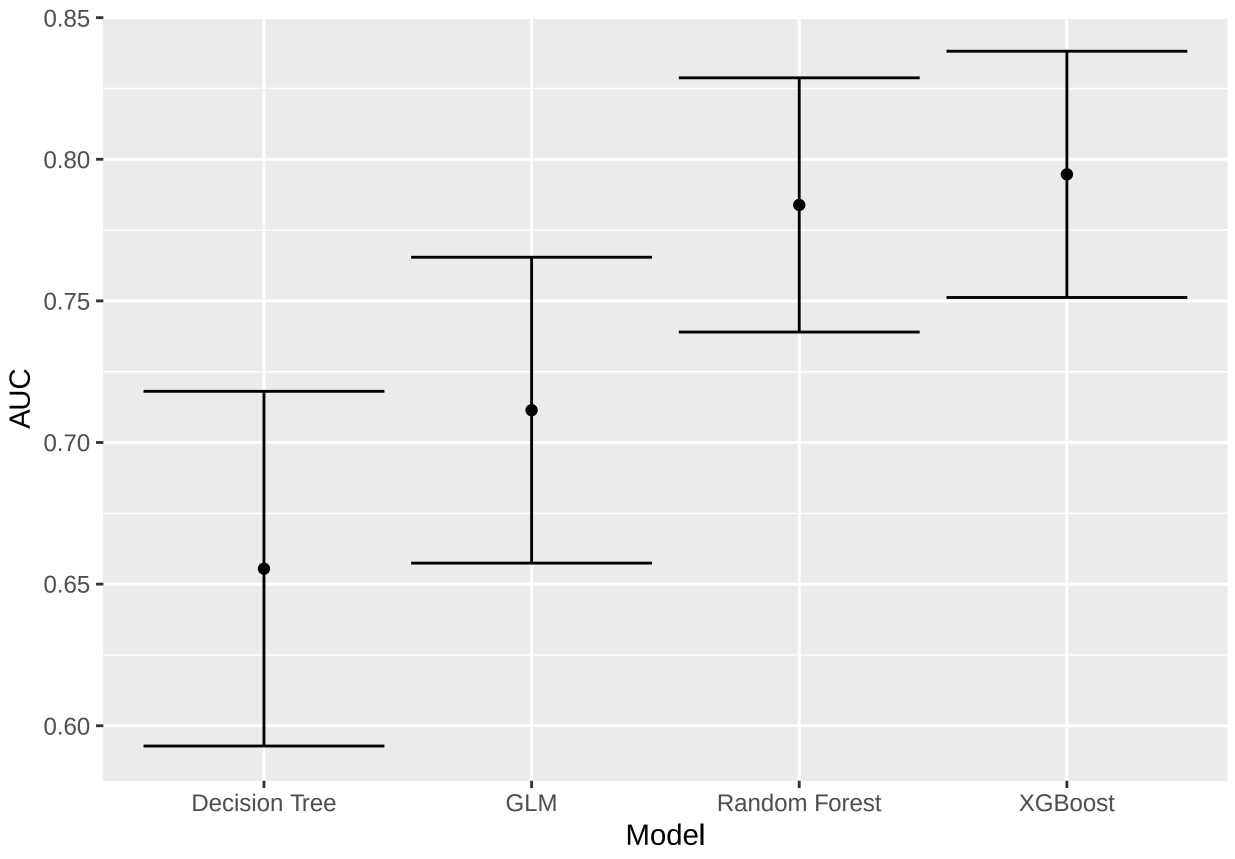
```
final_svm_fit <- extract_workflow(last_svm_fit)

svm_auc = validation(final_svm_fit, df_test)
```



```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4636   94
##                      1    0    0
##
##                Accuracy : 0.9801
##                  95% CI : (0.9757, 0.9839)
##     No Information Rate : 0.9801
##     P-Value [Acc > NIR] : 0.5274
##
##                   Kappa : 0
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 1.0000
##             Specificity : 0.0000
##          Pos Pred Value : 0.9801
##          Neg Pred Value :    NaN
##              Prevalence : 0.9801
##          Detection Rate : 0.9801
##    Detection Prevalence : 1.0000
##       Balanced Accuracy : 0.5000
##
##        'Positive' Class : 0
##
```

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))
```