## Model Selection

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### **Imports**

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

Minutes to run: 0

## Loading data

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

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

outcome_column <- params$outcome_column
features_list <- params$features_list</pre>
```

Minutes to run: 0.001

## Filtering eligible pacients

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

df %>% dim

## [1] 15766 239

Minutes to run: 0.005
```

# Eligible features

```
'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))
if (is.null(features_list)) {
  features = eligible_features
} else {
  features = base::intersect(eligible_features, features_list)
}
gluedown::md_order(features, seq = TRUE, pad = TRUE)
## 01. age
## 02. education_level
## 03. underlying_heart_disease
## 04. heart_disease
## 05. nyha_basal
## 06. prior_mi
## 07. heart_failure
## 08. af
## 09. cardiac_arrest
## 10. transplant
## 11. valvopathy
## 12. diabetes
## 13. hemodialysis
## 14. comorbidities_count
## 15. procedure_type_1
## 16. reop_type_1
## 17. procedure_type_new
## 18. cied_final_1
## 19. cied_final_group_1
## 20. admission_pre_t0_count
## 21. admission_pre_t0_180d
## 22. icu_t0
## 23. dialysis t0
## 24. disch_outcomes_t0
## 25. admission_t0_emergency
## 26. aco
## 27. antiarritmico
## 28. betabloqueador
## 29. ieca_bra
## 30. dva
## 31. digoxina
## 32. estatina
## 33. diuretico
## 34. vasodilatador
## 35. insuf_cardiaca
## 36. espironolactona
## 37. bloq_calcio
## 38. antiplaquetario_ev
## 39. insulina
## 40. anticonvulsivante
## 41. psicofarmacos
## 42. antifungico
## 43. antiviral
## 44. classe_meds_qtde
## 45. meds_cardiovasc_qtde
## 46. meds_antimicrobianos
```

```
## 47. cec
## 48. transplante_cardiaco
## 49. cir_toracica
## 50. outros_proced_cirurgicos
## 51. icp
## 52. angioplastia
## 53. cateterismo
## 54. eletrofisiologia
## 55. cateter_venoso_central
## 56. proced_invasivos_qtde
## 57. cve_desf
## 58. transfusao
## 59. equipe_multiprof
## 60. ecg
## 61. holter
## 62. teste_esforco
## 63. espiro_ergoespiro
## 64. tilt_teste
## 65. metodos_graficos_qtde
## 66. laboratorio
## 67. cultura
## 68. analises_clinicas_qtde
## 69. citologia
## 70. biopsia
## 71. histopatologia_qtde
## 72. angio_rm
## 73. angio_tc
## 74. arteriografia
## 75. cintilografia
## 76. ecocardiograma
## 77. endoscopia
## 78. pet_ct
## 79. ultrassom
## 80. tomografia
## 81. radiografia
## 82. ressonancia
## 83. exames_imagem_qtde
## 84. bic
Minutes to run: 0
```

# Train test split (70%/30%)

Minutes to run: 0.003 Minutes to run: 0

## Global parameters

Minutes to run: 0

### **Functions**

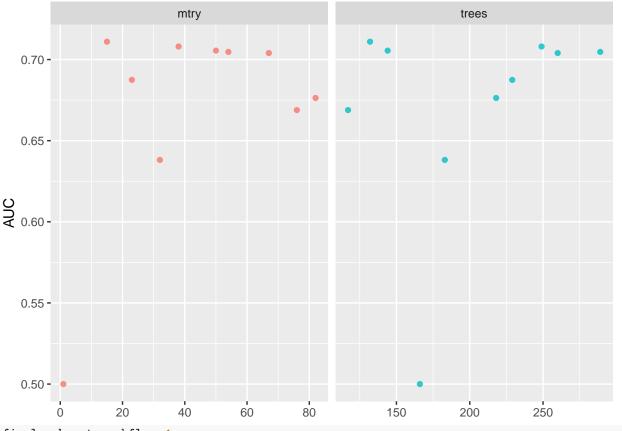
```
validation = function(model_fit, new_data, plot=TRUE) {
  library(pROC)
  library(caret)
  test_predictions_prob <-
    predict(model_fit, new_data = new_data, type = "prob") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$`1`
  pROC_obj <- roc(
    new_data[[outcome_column]],
    test_predictions_prob,
    direction = "<",
    levels = c(0, 1),
    smoothed = TRUE,
    ci = TRUE,
    ci.alpha = 0.9,
    stratified = FALSE,
    plot = plot,
    auc.polygon = TRUE,
    max.auc.polygon = TRUE,
    grid = TRUE,
    print.auc = TRUE,
    show.thres = TRUE
  )
  test_predictions_class <-</pre>
    predict(model_fit, new_data = new_data, type = "class") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$class
  conf_matrix <- table(test_predictions_class, new_data[[outcome_column]])</pre>
  if (plot) {
    sens.ci <- ci.se(pROC_obj)</pre>
    plot(sens.ci, type = "shape", col = "lightblue")
    plot(sens.ci, type = "bars")
    confusionMatrix(conf_matrix) %>% print
  }
  return(pROC_obj)
```

Minutes to run: 0

### Boosted Tree (XGBoost)

```
xgboost_recipe <-</pre>
  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(</pre>
  mtry = tune(),
  trees = tune(),
 min_n = tune(),
 tree_depth = tune(),
  learn_rate = tune(),
  loss_reduction = tune()
) %>%
  set_engine("xgboost") %>%
  set_mode("classification")
xgboost_grid <- grid_latin_hypercube(</pre>
  finalize(mtry(), df_train),
  dials::trees(range = c(100L, 300L)),
  min_n(),
  tree_depth(),
  learn rate(),
 loss_reduction(),
  size = grid_size
)
xgboost_workflow <-</pre>
  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 trees min_n tree_depth learn_rate loss_reduction .metric .estimator mean
##
                                                                                           n std_err .config
##
     <int> <int> <int>
                            <int>
                                       <dbl>
                                                       <dbl> <chr>
                                                                      <chr>
                                                                                 <dbl> <int> <dbl> <chr>
## 1
             132
        15
                    6
                                7 0.0208
                                                    5.12e- 8 roc_auc binary
                                                                                 0.711
                                                                                          4 0.0195 Preprocessor
## 2
        38
             249
                    30
                                5 0.00269
                                                    1.41e+ 0 roc_auc binary
                                                                                 0.708
                                                                                           4 0.0172 Preprocessor
                    26
## 3
        50 144
                               15 0.00000173
                                                    5.15e-10 roc_auc binary
                                                                                 0.705
                                                                                           4 0.0167 Preprocessor
## 4
        54
             289
                     6
                               13 0.0000222
                                                    2.81e- 4 roc_auc binary
                                                                                 0.705
                                                                                           4 0.0156 Preprocessor
## 5
        67
             260
                    40
                                                                                 0.704
                               11 0.0000974
                                                    3.79e- 7 roc_auc binary
                                                                                           4 0.0173 Preprocessor
best_xgboost <- xgboost_tune %>%
  select_best("roc_auc")
xgboost_tune %>%
  collect_metrics() %>%
  filter(.metric == "roc_auc") %>%
  select(mean, mtry:trees) %>%
  pivot_longer(mtry:trees,
               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")
```

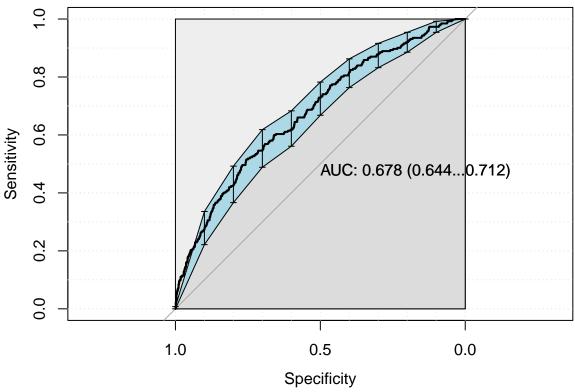


```
final_xgboost_workflow <-
    xgboost_workflow %>%
    finalize_workflow(best_xgboost)

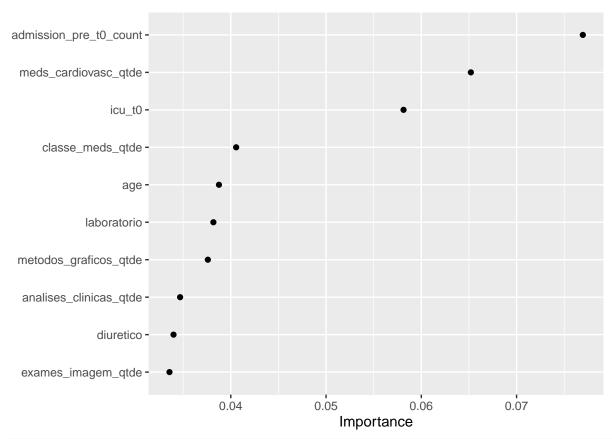
last_xgboost_fit <-
    final_xgboost_workflow %>%
    last_fit(df_split)

final_xgboost_fit <- extract_workflow(last_xgboost_fit)

xgboost_auc <- validation(final_xgboost_fit, df_test)</pre>
```



```
##
   Confusion Matrix and Statistics
##
##
##
   test_predictions_class
##
                        0 4466
                                 262
##
                        1
                             2
##
##
                  Accuracy : 0.9442
##
                    95% CI: (0.9373, 0.9506)
##
       No Information Rate : 0.9446
       P-Value [Acc > NIR] : 0.5667
##
##
##
                     Kappa : -8e-04
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.9996
               Specificity: 0.0000
##
##
            Pos Pred Value : 0.9446
##
            Neg Pred Value: 0.0000
##
                Prevalence: 0.9446
##
            Detection Rate: 0.9442
##
      Detection Prevalence : 0.9996
##
         Balanced Accuracy: 0.4998
##
##
          'Positive' Class : 0
##
final_xgboost_fit %>%
  fit(data = df_train) %>%
  extract_fit_parsnip() %>%
  vip(geom = "point")
```



```
xgboost_parameters <- xgboost_tune %>%
    show_best("roc_auc", n=1) %>%
    select(trees, mtry, min_n, tree_depth, learn_rate, loss_reduction) %>%
    as.list

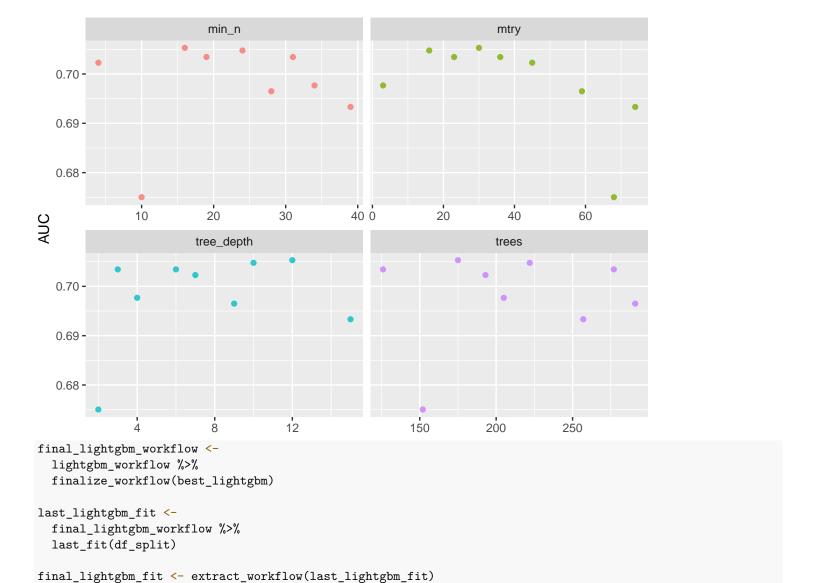
saveRDS(
    xgboost_parameters,
    file = sprintf(
        "../EDA/auxiliar/hyperparameters/model_selection/xgboost_parameters_%s.rds",
        outcome_column
    )
)
```

Minutes to run: 3.728

# Boosted Tree (LightGBM)

```
lightgbm_recipe <-</pre>
  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_impute_mean(all_numeric_predictors()) %>%
  step_zv(all_predictors())
lightgbm_spec <- boost_tree(</pre>
 mtry = tune(),
  trees = tune(),
 min_n = tune(),
  tree_depth = tune(),
  learn_rate = tune(),
  loss_reduction = tune(),
  sample size = 1
) %>%
```

```
set_engine("lightgbm") %>%
  set_mode("classification")
lightgbm_grid <- grid_latin_hypercube(</pre>
  finalize(mtry(), df_train),
  dials::trees(range = c(100L, 300L)),
 min_n(),
 tree_depth(),
 learn_rate(),
 loss_reduction(),
 size = grid_size
)
lightgbm_workflow <-</pre>
  workflow() %>%
  add_recipe(lightgbm_recipe) %>%
  add_model(lightgbm_spec)
lightgbm_tune <-
  lightgbm_workflow %>%
  tune_grid(resamples = df_folds,
           grid = lightgbm_grid)
lightgbm_tune %>%
  show_best("roc_auc")
## # A tibble: 5 x 12
##
     mtry trees min_n tree_depth
                                    learn_rate loss_reduction .metric .estimator mean
                                                                                         n std_err .config
##
    <int> <int> <int> <int>
                                         <dbl>
                                                       <dbl> <chr>
                                                                    <chr>
                                                                                <dbl> <int> <dbl> <chr>
                                                                                0.705 4 0.0189 Preprocess
       30 175 16
                            12 0.00000000638
                                                     2.70e+ 0 roc_auc binary
## 1
                             10 0.000121
## 2
       16 222
                   24
                                                     4.07e- 8 roc_auc binary
                                                                                0.705
                                                                                         4 0.0189 Preprocess
       23 277
                  19
## 3
                              3 0.0000000649
                                                     8.90e- 7 roc_auc binary
                                                                                0.703
                                                                                          4 0.0170 Preprocess
## 4
       36 126
                   31
                              6 0.00000269
                                                     8.31e-10 roc_auc binary
                                                                                0.703
                                                                                          4 0.0183 Preprocess
## 5
       45 193
                    4
                               7 0.00535
                                                     1.01e- 3 roc_auc binary
                                                                                0.702
                                                                                          4 0.0164 Preprocess
best_lightgbm <- lightgbm_tune %>%
  select_best("roc_auc")
lightgbm_tune %>%
  collect_metrics() %>%
 filter(.metric == "roc_auc") %>%
  select(mean, mtry:tree_depth) %>%
 pivot_longer(mtry:tree_depth,
              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")
```



lightgbm\_auc <- validation(final\_lightgbm\_fit, df\_test)</pre>

```
Sensitivity

AUC: 0.665 (0.630...0.699)

1.0 0.5 0.0

Specificity
```

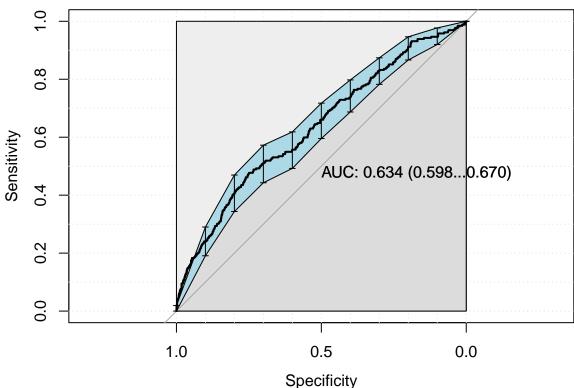
```
##
   Confusion Matrix and Statistics
##
##
##
   test_predictions_class
##
                        0 4468
                                 262
##
                        1
                             0
##
##
                  Accuracy: 0.9446
                    95% CI : (0.9377, 0.951)
##
##
       No Information Rate: 0.9446
##
       P-Value [Acc > NIR] : 0.5164
##
##
                     Kappa: 0
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 1.0000
##
               Specificity: 0.0000
##
            Pos Pred Value : 0.9446
##
            Neg Pred Value :
##
                Prevalence: 0.9446
##
            Detection Rate: 0.9446
##
      Detection Prevalence : 1.0000
##
         Balanced Accuracy: 0.5000
##
##
          'Positive' Class : 0
##
lightgbm_parameters <- lightgbm_tune %>%
  show_best("roc_auc", n=1) %>%
  select(trees, mtry, min_n, tree_depth, learn_rate, loss_reduction) %>%
  as.list
saveRDS(
  lightgbm_parameters,
  file = sprintf(
```

```
"../EDA/auxiliar/hyperparameters/model_selection/lightgbm_parameters_%s.rds",
   outcome_column
)
```

Minutes to run: 0.525

#### GLM

```
glmnet_recipe <-</pre>
  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 <-</pre>
  logistic_reg(penalty = 0) %>%
  set_mode("classification") %>%
  set_engine("glmnet")
glmnet_workflow <-</pre>
  workflow() %>%
  add_recipe(glmnet_recipe) %>%
  add_model(glmnet_spec)
glm_fit <- glmnet_workflow %>%
  fit(df_train)
glm_auc = validation(glm_fit, df_test)
```



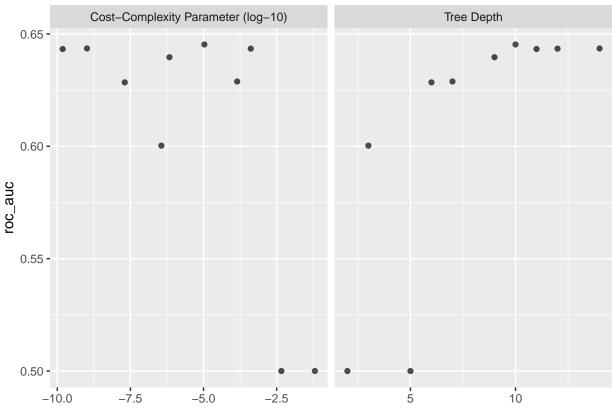
```
## |
## Confusion Matrix and Statistics
##
```

```
##
## test_predictions_class
##
                        0 4467
                                260
##
##
##
                  Accuracy: 0.9448
##
                    95% CI: (0.9379, 0.9512)
##
       No Information Rate: 0.9446
##
      P-Value [Acc > NIR] : 0.4911
##
##
                     Kappa: 0.0139
##
##
   Mcnemar's Test P-Value : <2e-16
##
               Sensitivity: 0.999776
##
##
               Specificity: 0.007634
##
            Pos Pred Value : 0.944997
##
            Neg Pred Value: 0.666667
##
                Prevalence: 0.944609
##
            Detection Rate: 0.944397
##
      Detection Prevalence: 0.999366
##
        Balanced Accuracy: 0.503705
##
          'Positive' Class : 0
##
##
```

Minutes to run: 0.086

### **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(),</pre>
                                  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()
```



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

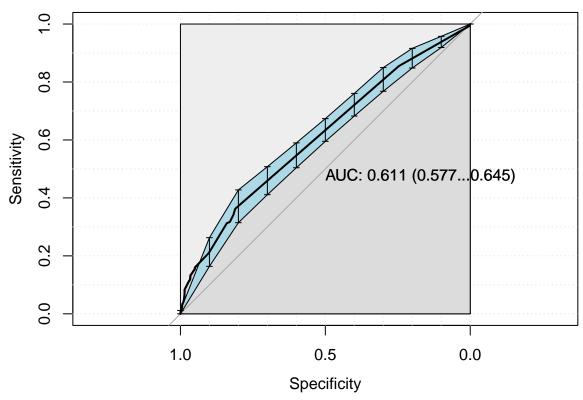
best_tree <- tree_tune %>%
    select_best("roc_auc")

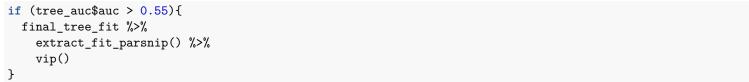
final_tree_workflow <-
    tree_workflow %>%
    finalize_workflow(best_tree)

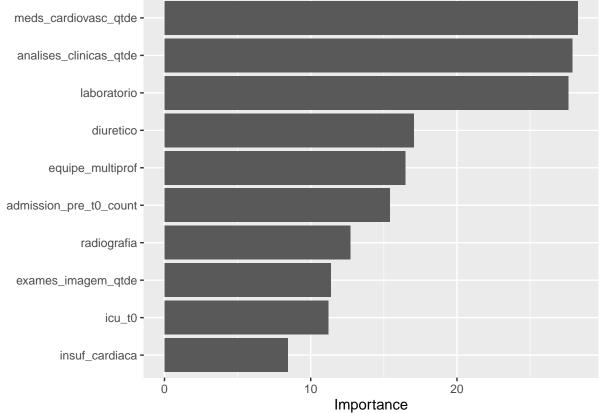
last_tree_fit <-
    final_tree_workflow %>%
    last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

tree_auc = validation(final_tree_fit, df_test)</pre>
```

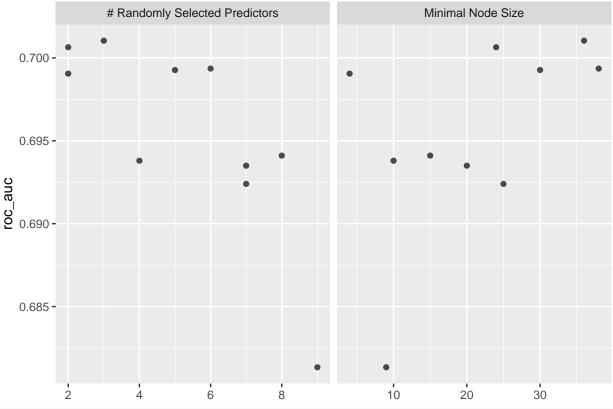






### **Random Forest**

```
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)),</pre>
                                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)
rf_tune %>%
  collect_metrics()
autoplot(rf_tune, metric = "roc_auc")
```



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

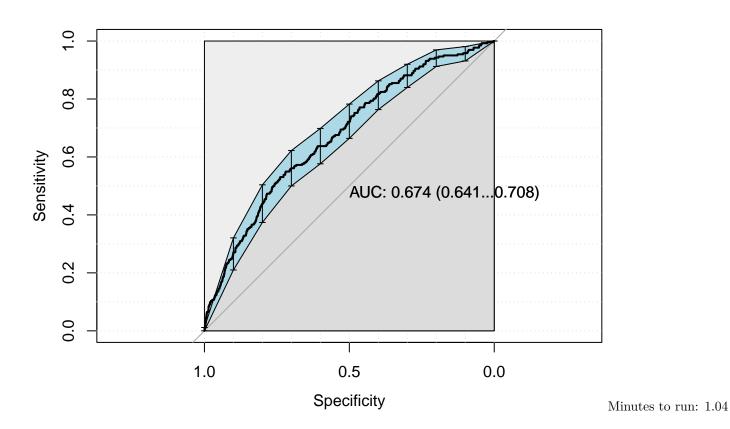
best_rf <- rf_tune %>%
    select_best("roc_auc")

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)</pre>
```



## **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(),</pre>
                                    weight_func(),
#
                                    dist_power(),
#
                                    size = 5)
#
# knn_workflow <-</pre>
    workflow() %>%
#
    add_recipe(knn_recipe) %>%
    add_model(knn_spec)
# knn_tune <-
#
    knn_workflow %>%
#
    tune_grid(resamples = df_folds,
#
              grid = knn_grid
# 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)</pre>
```

Minutes to run: 0

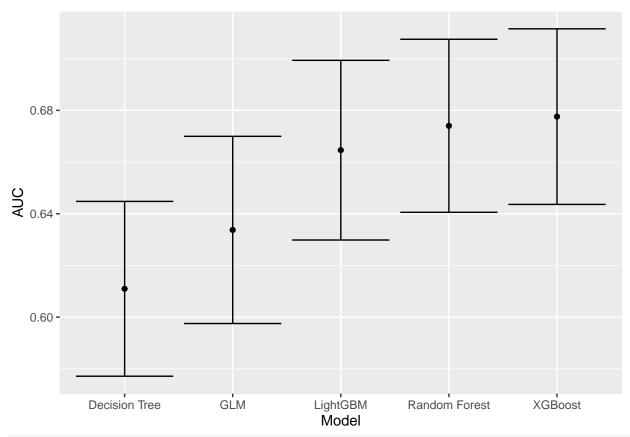
#### SVM

```
# 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(),</pre>
#
                                    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()
# autoplot(svm_tune, metric = "roc_auc")
# svm_tune %>%
   show_best("roc_auc")
```

```
# best_sum <- sum_tune %>%
# select_best("roc_auc")
#
# final_sum_workflow <-
# sum_workflow %>%
# finalize_workflow(best_sum)
#
# last_sum_fit <-
# final_sum_workflow %>%
# last_fit(df_split)
#
# final_sum_fit <- extract_workflow(last_sum_fit)
#
# sum_auc = validation(final_sum_fit, df_test)</pre>
```

Minutes to run: 0

# **Models Comparison**



saveRDS(df\_auc, sprintf("../EDA/auxiliar/performance/%s\_auc\_result.RData", outcome\_column))

Minutes to run: 0.002