# 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. sex
## 02. age
## 03. race
## 04. education_level
## 05. patient_state
## 06. underlying_heart_disease
## 07. heart_disease
## 08. nyha_basal
## 09. prior_mi
## 10. heart_failure
## 11. af
## 12. cardiac_arrest
## 13. transplant
## 14. valvopathy
## 15. endocardites
## 16. diabetes
## 17. renal_failure
## 18. hemodialysis
## 19. copd
## 20. comorbidities_count
## 21. procedure_type_1
## 22. reop_type_1
## 23. procedure_type_new
## 24. cied_final_1
## 25. cied_final_group_1
## 26. admission_pre_t0_count
## 27. admission_pre_t0_180d
## 28. year_adm_t0
## 29. icu_t0
## 30. dialysis_t0
## 31. disch_outcomes_t0
## 32. admission_t0_emergency
## 33. aco
## 34. antiarritmico
## 35. betabloqueador
## 36. ieca_bra
## 37. dva
## 38. digoxina
## 39. estatina
## 40. diuretico
## 41. vasodilatador
## 42. insuf cardiaca
## 43. espironolactona
## 44. bloq_calcio
## 45. antiplaquetario_ev
## 46. insulina
```

```
## 47. anticonvulsivante
## 48. psicofarmacos
## 49. antifungico
## 50. antiviral
## 51. antiretroviral
## 52. classe meds qtde
## 53. meds_cardiovasc_qtde
## 54. meds_antimicrobianos
## 55. vni
## 56. cec
## 57. transplante_cardiaco
## 58. outros_proced_cirurgicos
## 59. icp
## 60. intervencao_cv
## 61. angioplastia
## 62. cateterismo
## 63. eletrofisiologia
## 64. cateter_venoso_central
## 65. proced_invasivos_qtde
## 66. cve_desf
## 67. transfusao
## 68. interconsulta
## 69. equipe_multiprof
## 70. ecg
## 71. holter
## 72. teste_esforco
## 73. espiro_ergoespiro
## 74. tilt_teste
## 75. metodos_graficos_qtde
## 76. laboratorio
## 77. cultura
## 78. analises_clinicas_qtde
## 79. citologia
## 80. biopsia
## 81. histopatologia_qtde
## 82. angio_rm
## 83. angio_tc
## 84. arteriografia
## 85. cintilografia
## 86. ecocardiograma
## 87. endoscopia
## 88. flebografia
## 89. pet_ct
## 90. ultrassom
## 91. tomografia
## 92. radiografia
## 93. ressonancia
## 94. exames_imagem_qtde
## 95. bic
## 96. mpp
Minutes to run: 0
```

# Train test split (70%/30%)

```
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)</pre>
```

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_")) %>%
    .$`1`
 pROC_obj <- roc(</pre>
    new_data[[outcome_column]],
    test_predictions_prob,
    direction = "<",
    levels = c(0, 1),
    smoothed = TRUE,
    ci = TRUE,
    ci.alpha = 0.9,
   stratified = FALSE,
    plot = plot,
    auc.polygon = TRUE,
   max.auc.polygon = TRUE,
    grid = TRUE,
   print.auc = TRUE,
    show.thres = TRUE
  test_predictions_class <-</pre>
    predict(model_fit, new_data = new_data, type = "class") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$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
```

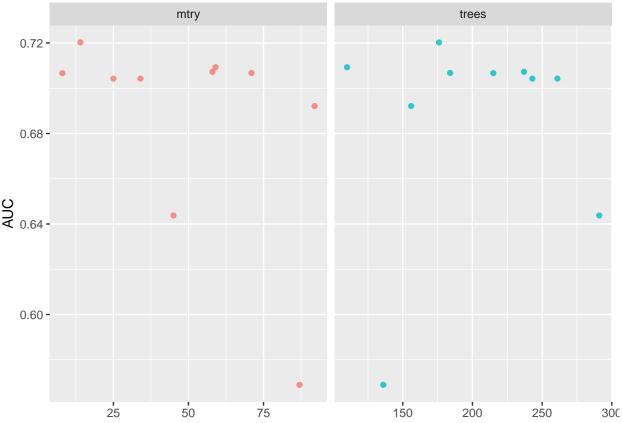
```
}
return(pROC_obj)
}
```

Minutes to run: 0

xgboost\_recipe <-

## Boosted Tree (XGBoost)

```
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
                                                                                           n std_err .config
     mtry trees min n tree depth learn rate loss reduction .metric .estimator mean
                             <int>
##
     <int> <int> <int>
                                        <dbl>
                                                       <dbl> <chr>
                                                                      <chr>
                                                                                 <dbl> <int>
                                                                                                <dbl> <chr>
## 1
        14
             176
                    27
                                9 0.0386
                                                  0.00000201 roc_auc binary
                                                                                 0.720
                                                                                           4 0.00199 Preprocessor
## 2
        59
            110
                    12
                                6 0.000376
                                                  0.0301
                                                             roc_auc binary
                                                                                 0.709
                                                                                           4 0.00690 Preprocessor
## 3
        58 237
                    32
                               12 0.00000516
                                                  0.637
                                                             roc_auc binary
                                                                                 0.707
                                                                                           4 0.00722 Preprocessor
        71
             184
                    18
                                                                                 0.707
## 4
                                5 0.00000269
                                                  0.00436
                                                                                           4 0.00647 Preprocessor
                                                             roc_auc binary
## 5
             215
                    22
                               11 0.0000451
                                                  0.000100
                                                             roc_auc binary
                                                                                 0.707
                                                                                           4 0.00631 Preprocessor
```

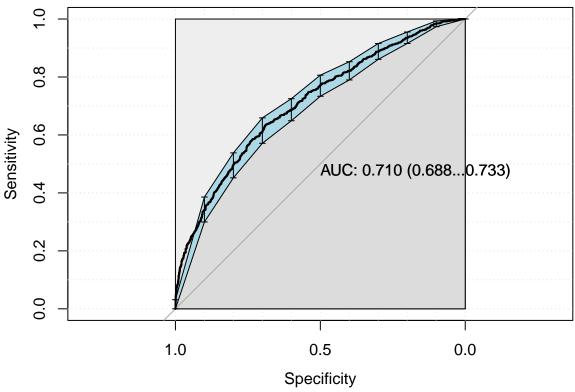


```
final_xgboost_workflow <-
    xgboost_workflow %>%
    finalize_workflow(best_xgboost)

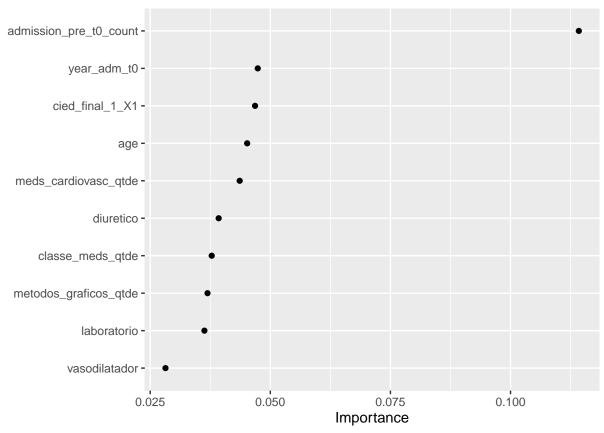
last_xgboost_fit <-
    final_xgboost_workflow %>%
    last_fit(df_split)

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 4118
                                573
                        1
                             9
                                  31
##
##
##
                  Accuracy: 0.877
##
                    95% CI: (0.8673, 0.8862)
##
       No Information Rate : 0.8723
       P-Value [Acc > NIR] : 0.1746
##
##
##
                     Kappa: 0.0817
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.99782
##
               Specificity: 0.05132
##
            Pos Pred Value : 0.87785
##
            Neg Pred Value: 0.77500
##
                Prevalence: 0.87233
##
            Detection Rate: 0.87043
##
      Detection Prevalence : 0.99155
##
         Balanced Accuracy: 0.52457
##
##
          '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

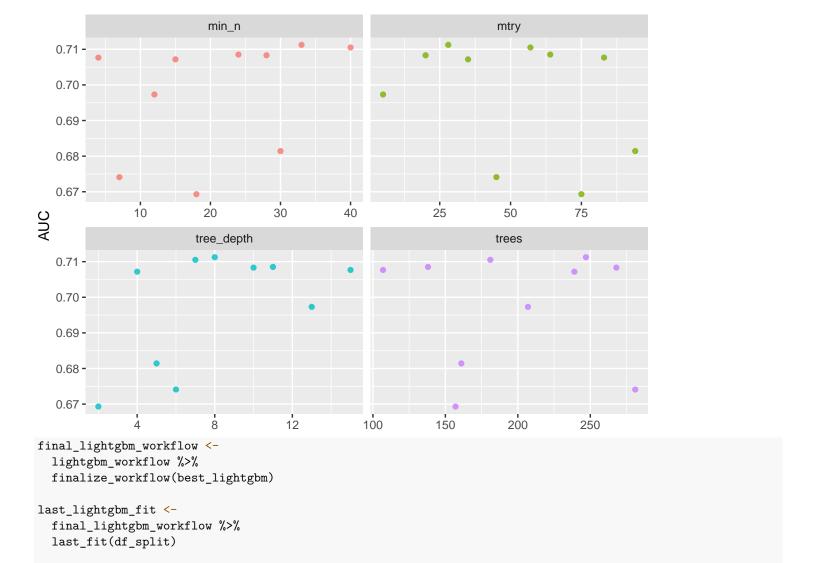
saveRDS(
    xgboost_parameters,
    file = sprintf(
        "../EDA/auxiliar/hyperparameters/model_selection/xgboost_parameters_%s.rds",
        outcome_column
    )
)
```

Minutes to run: 4.169

# 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>
                            8 8.71e- 7
       28 247
                                                  1.22e-10 roc_auc binary
## 1
                 33
                                                                             0.711 4 0.00583 Preprocessor
                              7 3.26e-10
## 2
       57 181
                   40
                                                  1.38e- 3 roc_auc binary
                                                                             0.711
                                                                                       4 0.00727 Preprocessor
       64 138
                   24
                             11 1.88e- 4
## 3
                                                  6.16e- 8 roc_auc binary
                                                                             0.709
                                                                                       4 0.00624 Preprocessor
## 4
       20
            268
                   28
                              10
                                  1.80e- 8
                                                  1.29e- 4 roc_auc binary
                                                                             0.708
                                                                                       4 0.00637 Preprocessor
                                   2.89e- 3
                                                                                       4 0.00674 Preprocessori
## 5
       83
           107
                    4
                              15
                                                  2.66e+ 0 roc_auc binary
                                                                             0.708
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")
```



final\_lightgbm\_fit <- extract\_workflow(last\_lightgbm\_fit)</pre>

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

```
Sensitivity

AUC: 0.703 (0.681...0.726)

1.0 0.5 0.0

Specificity
```

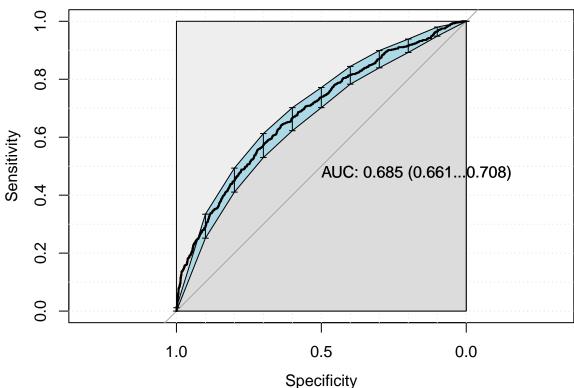
```
##
   Confusion Matrix and Statistics
##
##
##
   test_predictions_class
##
                        0 4127
                                 604
##
                        1
##
##
                  Accuracy : 0.8723
                    95% CI : (0.8625, 0.8817)
##
##
       No Information Rate: 0.8723
##
       P-Value [Acc > NIR] : 0.5108
##
##
                     Kappa: 0
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 1.0000
##
               Specificity: 0.0000
##
            Pos Pred Value : 0.8723
##
            Neg Pred Value :
##
                Prevalence: 0.8723
##
            Detection Rate: 0.8723
##
      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: 0.602

### 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)
```



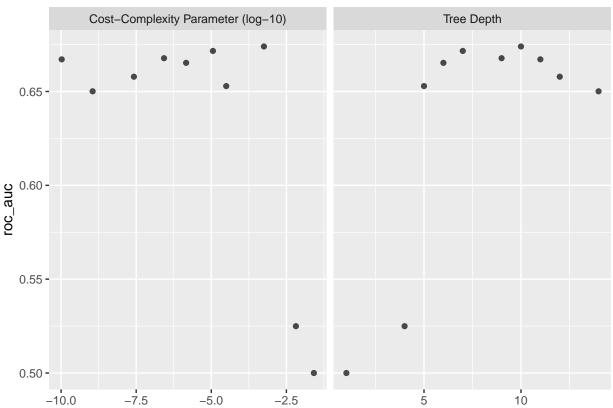
```
## |
## Confusion Matrix and Statistics
##
```

```
##
## test_predictions_class
##
                        0 4106 574
##
                            21
                                 30
##
##
                  Accuracy : 0.8742
##
                    95% CI: (0.8644, 0.8836)
##
       No Information Rate: 0.8723
##
      P-Value [Acc > NIR] : 0.3573
##
##
                     Kappa: 0.0732
##
##
   Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.99491
##
               Specificity: 0.04967
            Pos Pred Value: 0.87735
##
##
            Neg Pred Value: 0.58824
##
                Prevalence: 0.87233
##
            Detection Rate: 0.86789
##
      Detection Prevalence: 0.98922
##
        Balanced Accuracy: 0.52229
##
          'Positive' Class : 0
##
##
```

Minutes to run: 0.087

### **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")

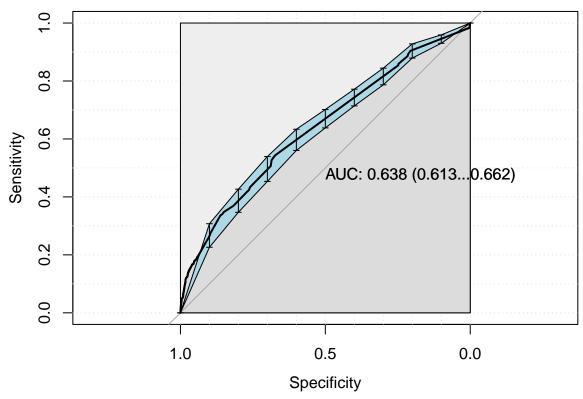
best_tree <- tree_tune %>%
    select_best("roc_auc")

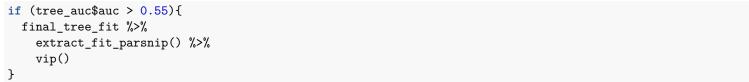
final_tree_workflow <-
    tree_workflow %>%
    finalize_workflow(best_tree)

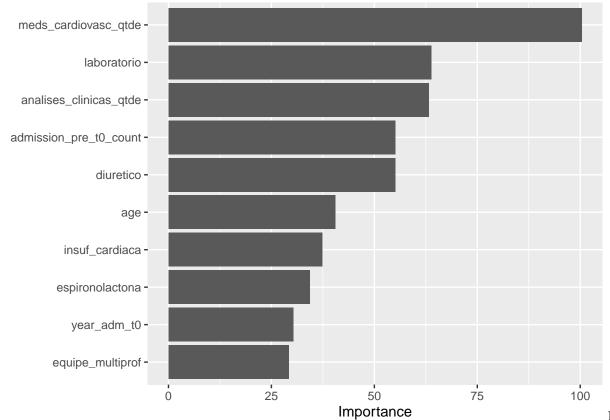
last_tree_fit <-
    final_tree_workflow %>%
    last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

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

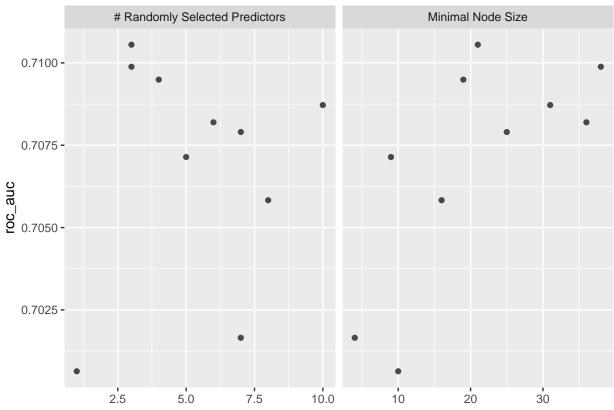






### **Random Forest**

```
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")

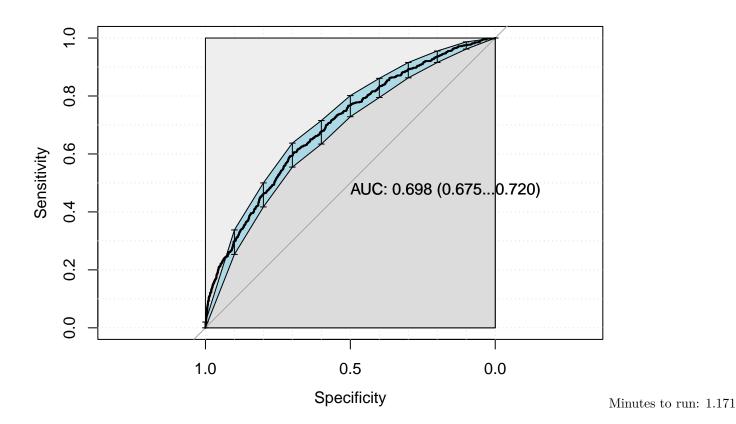
best_rf <- rf_tune %>%
    select_best("roc_auc")

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

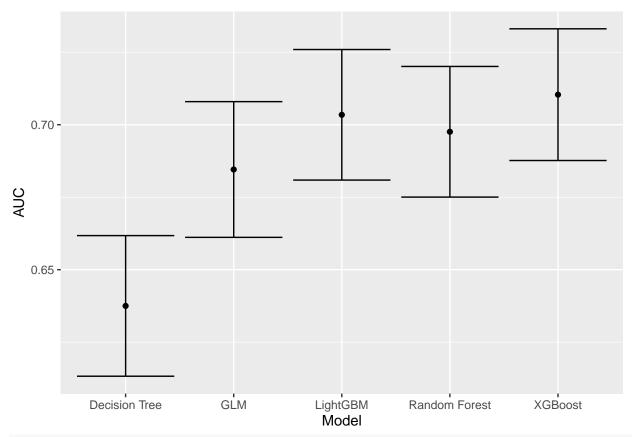
### SVM

```
# 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