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: 0.007
```

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_t0
## 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: 0.005 Minutes to run: 0

Global parameters

Minutes to run: 0

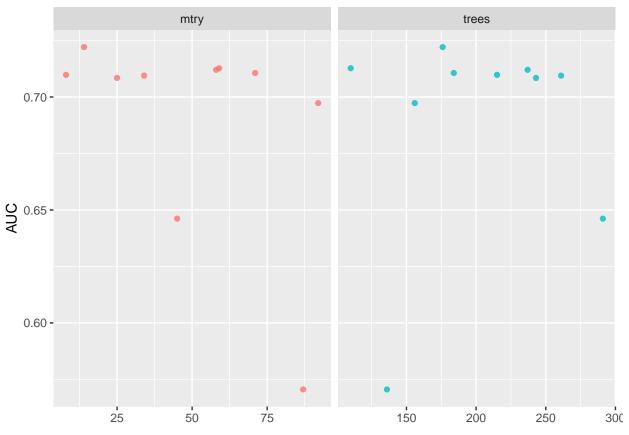
Functions

```
validation = function(model_fit, new_data, plot=TRUE) {
  library(pROC)
 library(caret)
 test_predictions_prob <-</pre>
    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)
}
```

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(</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 re~1 .metric .esti~2 mean
                                                                                   n std err .config
                            <int>
                                                                         <dbl> <int>
##
     <int> <int> <int>
                                        <dbl>
                                                  <dbl> <chr>
                                                                <chr>
                                                                                       <dbl> <chr>
## 1
        14
            176
                    27
                                9 0.0386
                                                2.01e-6 roc_auc binary 0.722
                                                                                   4 0.00270 Prepro~
## 2
        59
            110
                    12
                                6 0.000376
                                                3.01e-2 roc_auc binary 0.713
                                                                                   4 0.00656 Prepro~
## 3
        58 237
                    32
                               12 0.00000516
                                                6.37e-1 roc_auc binary 0.712
                                                                                   4 0.00689 Prepro~
## 4
        71
             184
                    18
                                5 0.00000269
                                                4.36e-3 roc_auc binary 0.711
                                                                                   4 0.00634 Prepro~
             215
                    22
                                                                                   4 0.00692 Prepro~
## 5
                               11 0.0000451
                                                1.00e-4 roc_auc binary 0.710
## # ... with abbreviated variable names 1: loss_reduction, 2: .estimator
```

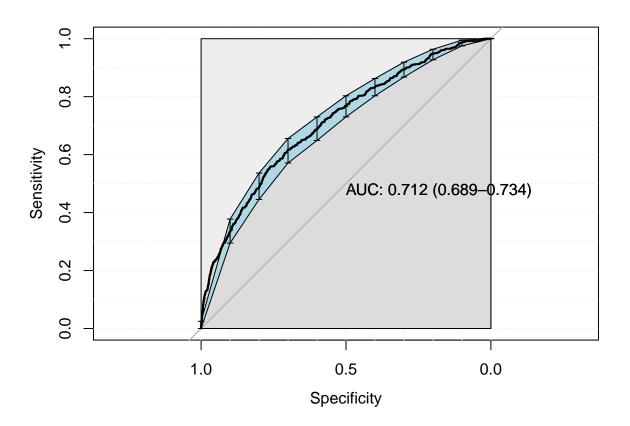


```
final_xgboost_workflow <-
    xgboost_workflow %>%
    finalize_workflow(best_xgboost)

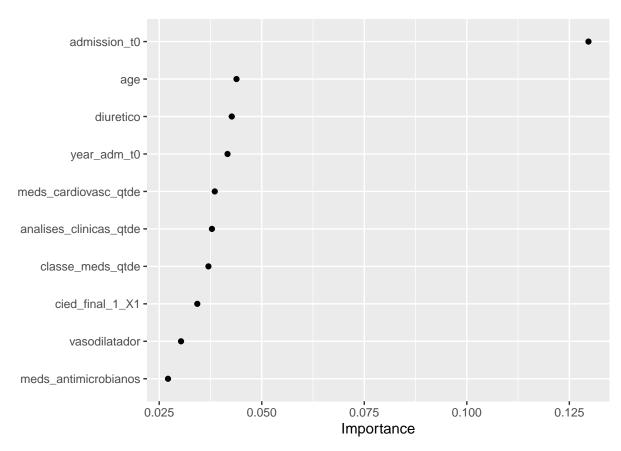
last_xgboost_fit <-
    final_xgboost_workflow %>%
    last_fit(df_split)

final_xgboost_fit <- extract_workflow(last_xgboost_fit)

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



```
Confusion Matrix and Statistics
##
##
##
   test_predictions_class
                                   1
##
                        0 4114
                                 580
##
                        1
                             13
                                  24
##
                  Accuracy : 0.8747
##
                    95% CI: (0.8649, 0.884)
##
       No Information Rate: 0.8723
##
       P-Value [Acc > NIR] : 0.3252
##
##
##
                     Kappa : 0.061
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.99685
##
               Specificity: 0.03974
##
            Pos Pred Value: 0.87644
##
            Neg Pred Value: 0.64865
                Prevalence: 0.87233
##
##
            Detection Rate: 0.86958
##
      Detection Prevalence: 0.99218
##
         Balanced Accuracy: 0.51829
##
##
          '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

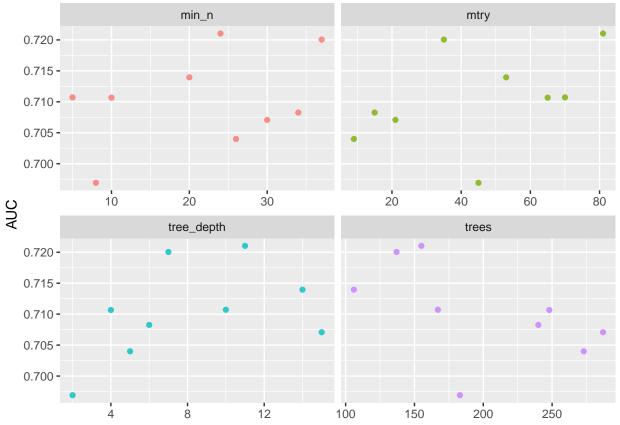
saveRDS(
    xgboost_parameters,
    file = sprintf(
        "../EDA/auxiliar/hyperparameters/model_selection/xgboost_parameters_%s.rds",
        outcome_column
    )
)
```

Boosted Tree (LightGBM)

```
lightgbm_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_impute_mean(all_numeric_predictors()) %>%
    step_zv(all_predictors())

lightgbm_spec <- boost_tree(
    mtry = tune(),
    trees = tune(),
    min_n = tune(),
    tree_depth = tune(),
    learn_rate = tune(),
    loss_reduction = tune(),
    sample_size = 1</pre>
```

```
) %>%
  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_re~1 .metric .esti~2 mean
                                                                                 n std_err .config
##
     <int> <int> <int>
                            <int>
                                       <dbl>
                                                 <dbl> <chr>
                                                               <chr>
                                                                       <dbl> <int>
                                                                                      <dbl> <chr>
## 1
                                    1.22e- 2
        81 155
                    24
                               11
                                               2.72e-9 roc_auc binary 0.721
                                                                                 4 0.00388 Prepro~
        35 137
                    37
                               7 1.97e- 2 1.77e-4 roc_auc binary 0.720
## 2
                                                                                 4 0.00287 Prepro~
## 3
        53 106
                    20
                               14
                                    1.01e- 6
                                               2.05e-1 roc_auc binary 0.714
                                                                                 4 0.00674 Prepro~
## 4
                                               2.36e-5 roc_auc binary 0.711
        70
             167
                     5
                               10
                                    3.98e- 9
                                                                                 4 0.00733 Prepro~
## 5
        65
             248
                    10
                                4
                                    5.73e-10
                                                                                 4 0.00650 Prepro~
                                               2.66e-7 roc_auc binary 0.711
## # ... with abbreviated variable names 1: loss_reduction, 2: .estimator
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")
```

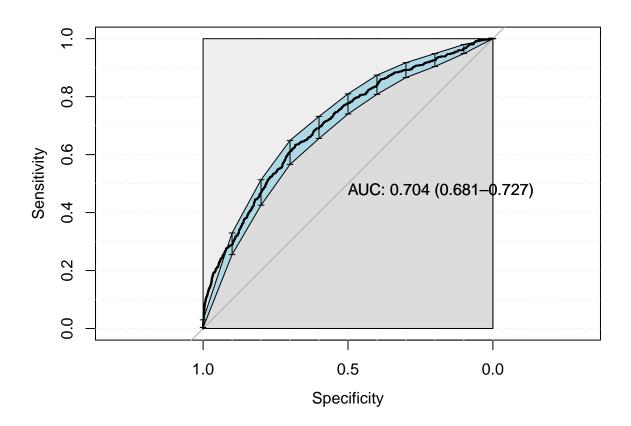


```
final_lightgbm_workflow <-
    lightgbm_workflow %>%
    finalize_workflow(best_lightgbm)

last_lightgbm_fit <-
    final_lightgbm_workflow %>%
    last_fit(df_split)

final_lightgbm_fit <- extract_workflow(last_lightgbm_fit)

lightgbm_auc <- validation(final_lightgbm_fit, df_test)</pre>
```



Confusion Matrix and Statistics

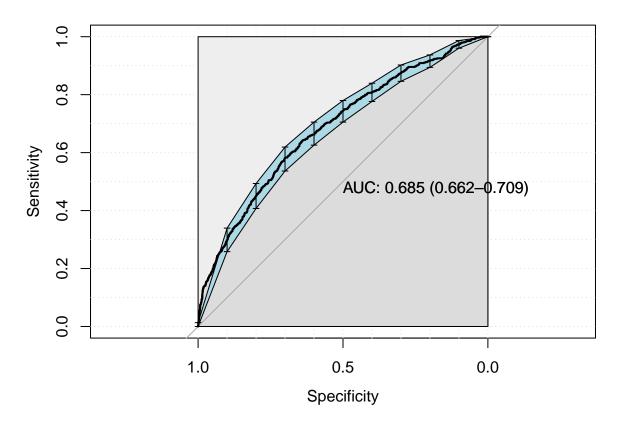
##

```
test_predictions_class
                                   1
                        0 4125
                                592
##
##
                        1
                                  12
##
                  Accuracy : 0.8744
##
                    95% CI: (0.8647, 0.8838)
##
       No Information Rate: 0.8723
##
       P-Value [Acc > NIR] : 0.3411
##
##
##
                     Kappa : 0.0332
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.99952
##
               Specificity: 0.01987
##
            Pos Pred Value: 0.87450
##
            Neg Pred Value: 0.85714
                Prevalence: 0.87233
##
##
            Detection Rate: 0.87191
##
      Detection Prevalence: 0.99704
##
         Balanced Accuracy: 0.50969
##
##
          '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
)
)
```

GLM

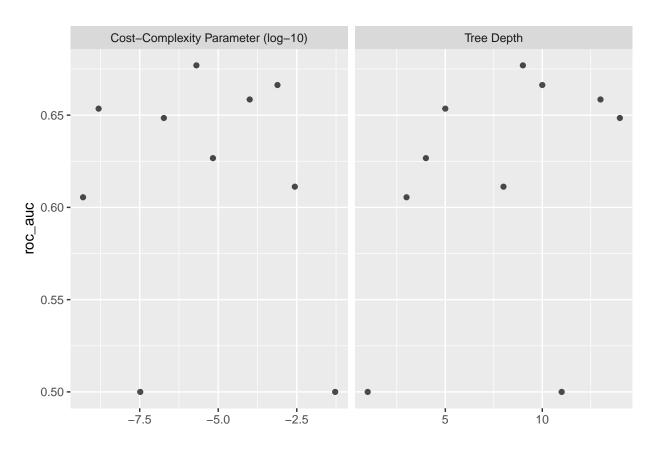
```
glmnet_recipe <-</pre>
  recipe(formula = sprintf("%s ~ .", outcome_column) %% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
  step_dummy(all_nominal_predictors(), 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
                                   1
##
                        0 4105
                                 571
                             22
##
                        1
                                  33
##
                  Accuracy : 0.8747
##
##
                    95% CI: (0.8649, 0.884)
       No Information Rate: 0.8723
##
       P-Value [Acc > NIR] : 0.3252
##
##
##
                     Kappa : 0.0806
##
    Mcnemar's Test P-Value : <2e-16
##
##
##
               Sensitivity: 0.99467
##
               Specificity: 0.05464
##
            Pos Pred Value: 0.87789
##
            Neg Pred Value : 0.60000
##
                Prevalence: 0.87233
##
            Detection Rate: 0.86768
##
      Detection Prevalence: 0.98837
##
         Balanced Accuracy : 0.52465
##
##
          '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(),</pre>
                                   tree_depth(),
                                   size = grid_size)
tree_workflow <-</pre>
 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")

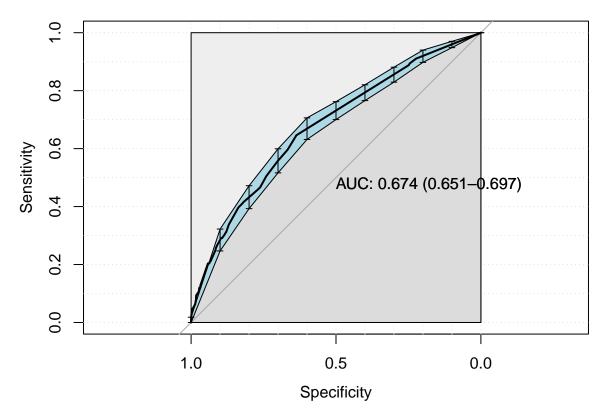
best_tree <- tree_tune %>%
    select_best("roc_auc")

final_tree_workflow <-
    tree_workflow %>%
    finalize_workflow(best_tree)

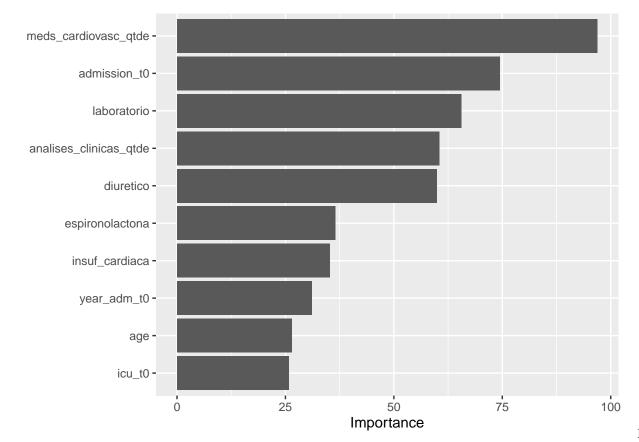
last_tree_fit <-
    final_tree_workflow %>%
    last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

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

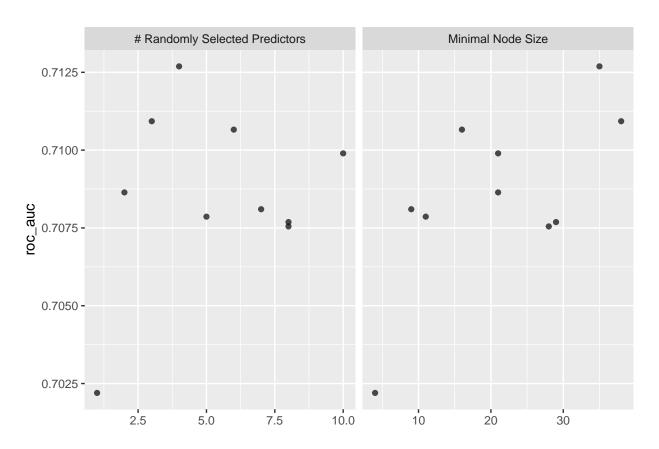


```
if (tree_auc$auc > 0.55){
  final_tree_fit %>%
    extract_fit_parsnip() %>%
    vip()
}
```



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)),</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")

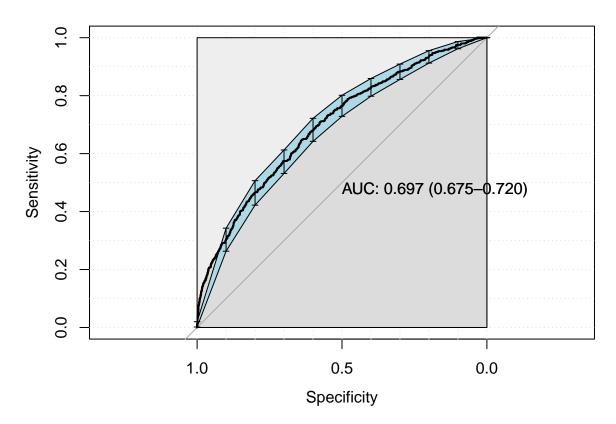
best_rf <- rf_tune %>%
    select_best("roc_auc")

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>
```



1.179

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 <-
   workflow() %>%
    add_recipe(knn_recipe) %>%
    add_model(knn_spec)
# knn_tune <-
   knn_workflow %>%
    tune\_grid(resamples = df\_folds,
```

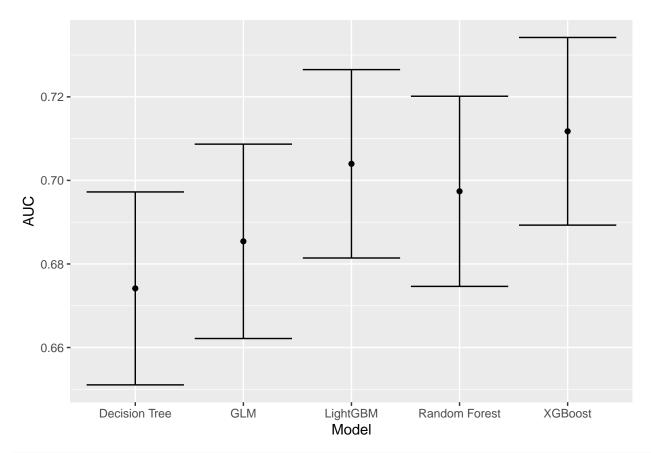
```
qrid = knn_qrid
#
# knn tune %>%
#
    collect_metrics()
# autoplot(knn_tune, metric = "roc_auc")
# knn_tune %>%
#
    show_best("roc_auc")
# best_knn <- knn_tune %>%
    select_best("roc_auc")
# final_knn_workflow <-</pre>
    knn_workflow %>%
    finalize_workflow(best_knn)
# last_knn_fit <-</pre>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

SVM

```
# svm_recipe <-
              recipe(formula = sprintf("%s ~ .", outcome\_column) \%>\% as.formula, data = df\_train) %>% as.formul
              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 <-</pre>
              workflow() %>%
              add_recipe(svm_recipe) %>%
              add_model(svm_spec)
# svm_tune <-
#
              sum_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_svm <- svm_tune %>%
# select_best("roc_auc")
#
# final_svm_workflow <-
# svm_workflow %>%
# finalize_workflow(best_svm)
#
# last_svm_fit <-
# final_svm_workflow %>%
# last_stm_fit <-
# final_svm_workflow %>%
# last_fit(af_split)
#
# final_svm_fit <- extract_workflow(last_svm_fit)
#
# svm_auc = validation(final_svm_fit, df_test)</pre>
```

Models Comparison



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