Model Selection - death_2year

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Global parameters

```
k <- params$k # Number of folds for cross validation
grid_size <- params$grid_size # Number of parameter combination to tune on each model
repeats <- params$repeats
RUN_ALL_MODELS <- params$RUN_ALL_MODELS
Hmisc::list.tree(params)

## params = list 5 (952 bytes)
## . outcome_column = character 1= death_2year
## . k = double 1= 10
## . grid_size = double 1= 30
## . repeats = double 1= 2
## . RUN_ALL_MODELS = logical 1= TRUE</pre>
Minutes to run: 0
```

Imports

```
library(tidyverse)
library(yaml)
library(tidymodels)
library(usemodels)
library(vip)
library(bonsai)
library(lightgbm)
library(caret)
library(pROC)
source("aux_functions.R")
```

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

df <- mutate(df, across(where(is.character), as.factor))</pre>
```

Minutes to run: 0.007

Minutes to run: 0

Eligible features

```
cat_features_list = readRDS(sprintf(
  "./auxiliar/significant_columns/categorical_%s.rds",
  outcome_column
))
num_features_list = readRDS(sprintf(
  "./auxiliar/significant_columns/numerical_%s.rds",
  outcome_column
))
features_list = c(cat_features_list, num_features_list)
Minutes to run: 0
eligible_columns = df_names %>%
  filter(momento.aquisicao == 'Admissão t0') %>%
  .$variable.name
exception_columns = c('death_intraop', 'death_intraop_1', 'disch_outcomes_t0')
correlated_columns = c('year_procedure_1', # com year_adm_t0
                       'age_surgery_1', # com age
                       'admission_t0', # com admission_pre_t0_count
                       'atb', # com meds_antimicrobianos
                       'classe_meds_cardio_qtde', # com classe_meds_qtde
                       'suporte_hemod', # com proced_invasivos_qtde,
                       'radiografia', # com exames_imagem_qtde
                       'ecg' # com metodos_graficos_qtde
eligible_features = eligible_columns %>%
  base::intersect(c(columns_list$categorical_columns, columns_list$numerical_columns)) %>%
  setdiff(c(exception_columns, correlated_columns))
features = base::intersect(eligible_features, features_list)
gluedown::md_order(features, seq = TRUE, pad = TRUE)
## 01. sex
## 02. age
## 03. education_level
## 04. underlying_heart_disease
## 05. heart_disease
```

- ## 06. nyha_basal
- ## 07. hypertension
- ## 08. prior_mi
- ## 09. heart_failure
- ## 10. af
- ## 11. cardiac_arrest
- ## 12. valvopathy
- ## 13. diabetes
- ## 14. renal_failure
- ## 15. hemodialysis
- ## 16. stroke
- ## 17. copd
- ## 18. comorbidities_count
- ## 19. procedure_type_1
- ## 20. reop_type_1
- ## 21. procedure_type_new
- ## 22. cied_final_1
- ## 23. cied_final_group_1
- ## 24. admission_pre_t0_count
- ## 25. admission_pre_t0_180d
- ## 26. year_adm_t0
- ## 27. icu_t0
- ## 28. dialysis_t0
- ## 29. admission_t0_emergency
- ## 30. aco
- ## 31. antiarritmico
- ## 32. ieca_bra
- ## 33. dva
- ## 34. digoxina
- ## 35. estatina
- ## 36. diuretico
- ## 37. vasodilatador
- ## 38. insuf_cardiaca
- ## 39. espironolactona
- ## 40. antiplaquetario_ev
- ## 41. insulina
- ## 42. psicofarmacos
- ## 43. antifungico
- ## 44. antiviral
- ## 45. classe_meds_qtde
- ## 46. meds_cardiovasc_qtde
- ## 47. meds_antimicrobianos
- ## 48. vni
- ## 49. ventilacao_mecanica
- ## 50. transplante_cardiaco
- ## 51. outros_proced_cirurgicos
- ## 52. icp
- ## 53. angioplastia
- ## 54. cateterismo
- ## 55. cateter_venoso_central
- ## 56. proced_invasivos_qtde
- ## 57. transfusao
- ## 58. interconsulta
- ## 59. equipe_multiprof
- ## 60. holter
- ## 61. teste_esforco
- ## 62. tilt_teste
- ## 63. metodos_graficos_qtde
- ## 64. laboratorio
- ## 65. cultura
- ## 66. analises_clinicas_qtde

```
## 67. citologia
## 68. histopatologia_qtde
## 69. angio_tc
## 70. cintilografia
## 71. ecocardiograma
## 72. endoscopia
## 73. flebografia
## 74. pet_ct
## 75. ultrassom
## 76. tomografia
## 77. ressonancia
## 78. exames_imagem_qtde
## 79. bic
## 80. hospital_stay
```

Minutes to run: 0

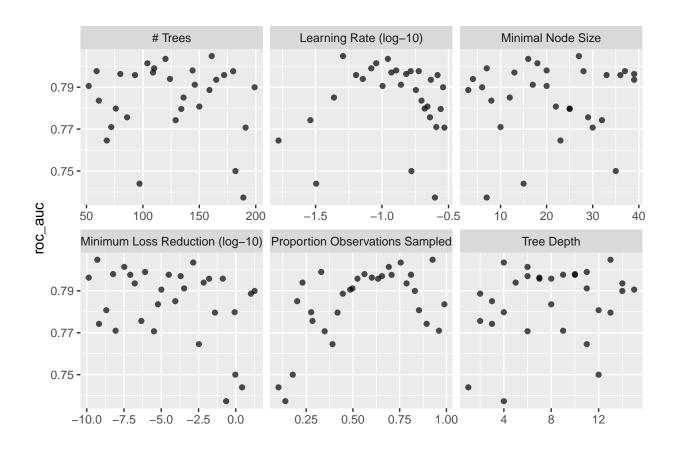
Train test split (70%/30%)

Minutes to run: 0.001

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())
xgboost_spec <- boost_tree(</pre>
 trees = tune(),
 \min_n = tune(),
 tree_depth = tune(),
 learn_rate = tune(),
 loss_reduction = tune(),
 sample_size = tune()
) %>%
  set_engine("xgboost",
             nthread = 8) %>%
  set_mode("classification")
```

```
xgboost_grid <- grid_latin_hypercube(</pre>
 trees(range = c(50L, 200L)),
 min n(),
 tree_depth(),
 learn_rate(range = c(0.01, 0.3), trans = NULL),
 loss_reduction(),
 sample_prop(range = c(1/10, 1), trans = NULL),
 size = grid_size
xgboost_workflow <-</pre>
 workflow() %>%
 add_recipe(xgboost_recipe) %>%
 add_model(xgboost_spec)
xgboost_tune <-</pre>
 xgboost_workflow %>%
 tune_grid(resamples = df_folds,
         grid = xgboost_grid)
xgboost_tune %>%
 show_best("roc_auc")
## # A tibble: 5 x 12
## trees min_n tree_depth learn_rate loss_reduction sample_size .metric .estimator mean n std_err .config
## <int> <int> <dbl> <dbl>
                                               <dbl> <chr> <dbl> <int> <dbl> <int> <dbl> <chr>
                                               161 27
                 13 0.0509
                                  5.16e-10
## 1
                  4 0.111
## 2 120 16
                                  1.40e- 3
                                             ## 3 104 18
                   6 0.0905
                                  3.29e- 8
                                               ## 4 110
          7
                  11
                        0.0829
                                  8.26e- 7
                                               0.331 roc_auc binary
                                                                   0.799
                                                                          10 0.00877 Preprod
                                               0.562 roc_auc binary
                                                                   0.798
## 5
     144
          20
                  10
                         0.128
                                   5.85e- 9
                                                                          10 0.0117 Preprod
best_xgboost <- xgboost_tune %>%
 select_best("roc_auc")
autoplot(xgboost_tune, metric = "roc_auc")
```

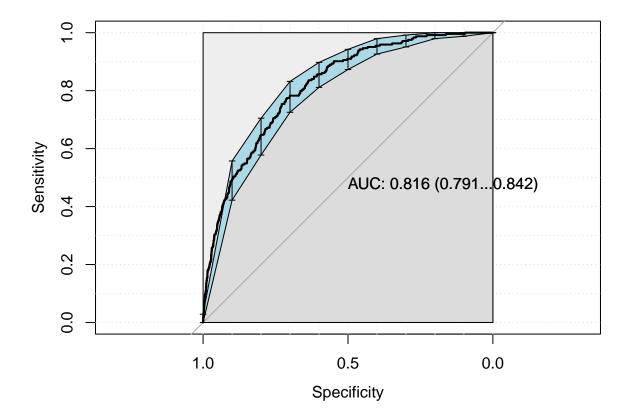


```
final_xgboost_workflow <-
    xgboost_workflow %>%
    finalize_workflow(best_xgboost)

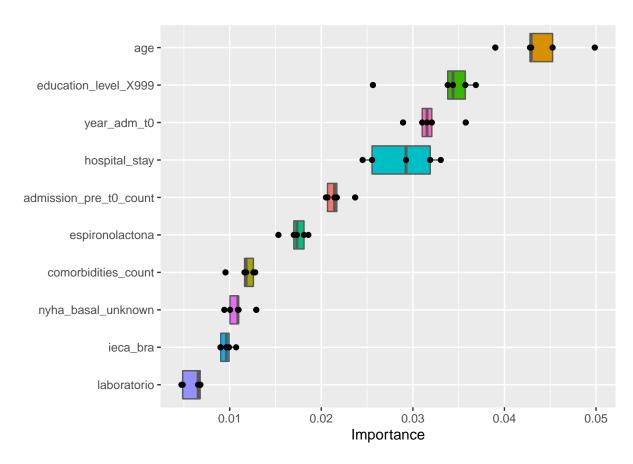
last_xgboost_fit <-
    final_xgboost_workflow %>%
    last_fit(df_split)

final_xgboost_fit <- extract_workflow(last_xgboost_fit)

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



##

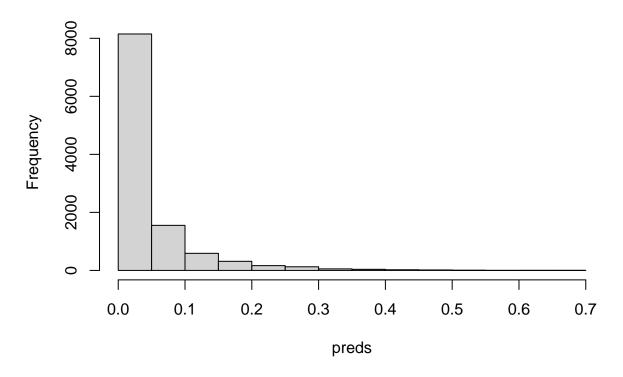


```
xgboost_parameters <- xgboost_tune %>%
    show_best("roc_auc", n = 1) %>%
    select(trees, min_n, tree_depth, learn_rate, loss_reduction) %>%
    as.list

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

preds <- predict(final_xgboost_fit, new_data = df_train, type = "prob") %>%
    rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
    .$`1`
hist(preds)
```

Histogram of preds



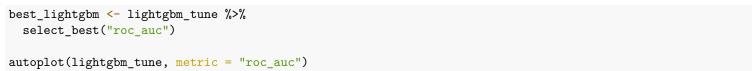
Minutes to run:

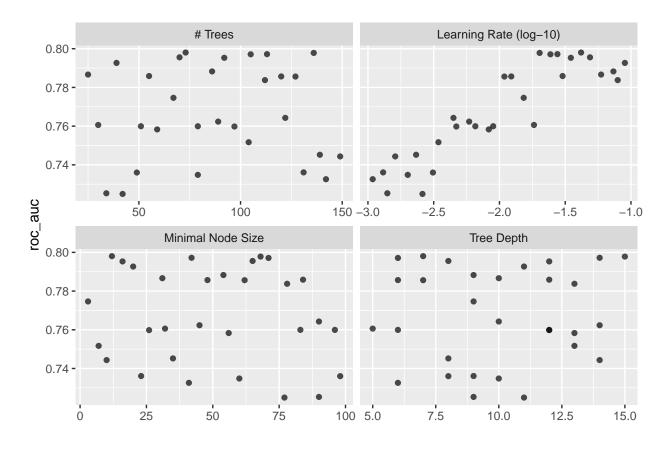
12.607

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_dummy(all_nominal_predictors())
lightgbm_spec <- boost_tree(</pre>
  trees = tune(),
 min_n = tune(),
  tree_depth = tune(),
  learn_rate = tune(),
  sample_size = 1
) %>%
  set_engine("lightgbm",
             nthread = 8) \%%
  set_mode("classification")
lightgbm_grid <- grid_latin_hypercube(</pre>
  trees(range = c(25L, 150L)),
 min_n(range = c(2L, 100L)),
  tree_depth(range = c(5L, 15L)),
  learn_rate(range = c(-3, -1), trans = log10_trans()),
  size = grid_size
)
lightgbm_workflow <-</pre>
```

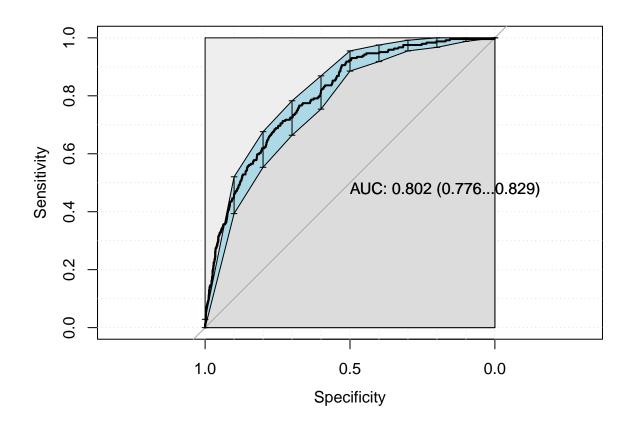
```
workflow() %>%
  add_recipe(lightgbm_recipe) %>%
  add_model(lightgbm_spec)
lightgbm_tune <-
  lightgbm_workflow %>%
  tune_grid(resamples = df_folds,
            grid = lightgbm_grid)
lightgbm_tune %>%
  show_best("roc_auc")
## # A tibble: 5 x 10
     trees min_n tree_depth learn_rate .metric .estimator
                                                            mean
                                                                      n std_err .config
##
     <int> <int>
                      <int>
                                  <dbl> <chr>
                                                <chr>
                                                            <dbl> <int>
                                                                           <dbl> <chr>
##
  1
        73
              12
                          7
                                 0.0417 roc_auc binary
                                                            0.798
                                                                     10 0.00793 Preprocessor1_Model04
  2
                                                            0.798
                                                                     10 0.00914 Preprocessor1_Model21
##
       136
              68
                          15
                                 0.0202 roc_auc binary
                                                                     10 0.00857 Preprocessor1_Model13
##
       113
              42
                          14
                                                            0.797
  3
                                 0.0276 roc_auc binary
       105
              71
                          6
                                 0.0244 roc_auc binary
                                                            0.797
                                                                     10 0.00757 Preprocessor1_Model22
##
  4
## 5
        70
              65
                          8
                                 0.0488 roc_auc binary
                                                            0.796
                                                                     10 0.00875 Preprocessor1_Model20
best_lightgbm <- lightgbm_tune %>%
  select_best("roc_auc")
```





```
final_lightgbm_workflow <-</pre>
  lightgbm_workflow %>%
  finalize_workflow(best_lightgbm)
last_lightgbm_fit <-</pre>
  final_lightgbm_workflow %>%
```

```
last_fit(df_split)
final_lightgbm_fit <- extract_workflow(last_lightgbm_fit)
lightgbm_auc <- validation(final_lightgbm_fit, df_test)</pre>
```

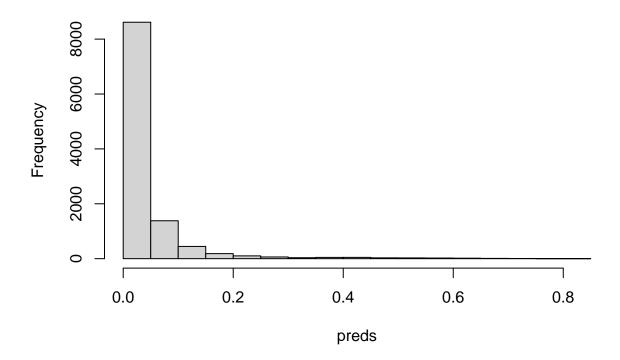


##

```
##
          'Positive' Class: 0
##
##
lightgbm_parameters <- lightgbm_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(-.metric, -.estimator, -.config, -mean, -n, -std_err) %>%
  as.list
Hmisc::list.tree(lightgbm_parameters)
   lightgbm_parameters = list 4 (736 bytes)
##
## . trees = integer 1= 73
## . min_n = integer 1= 12
## . tree_depth = integer 1= 7
## . learn_rate = double 1= 0.041746
saveRDS(
  lightgbm_parameters,
  file = sprintf(
    "./auxiliar/model_selection/hyperparameters/lightgbm_%s.rds",
    outcome_column
  )
)
```

Minutes to run: 3.638

Histogram of preds

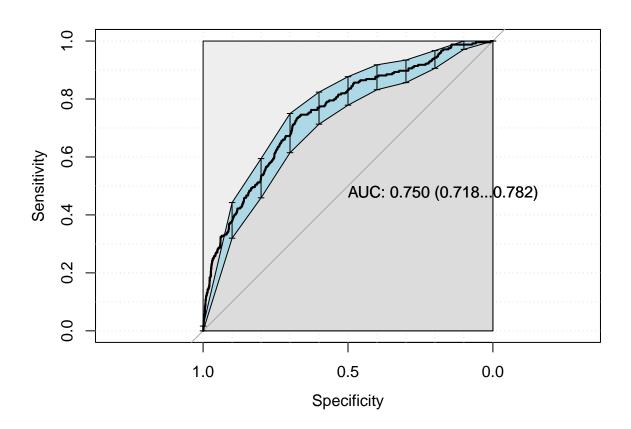


Minutes to run:

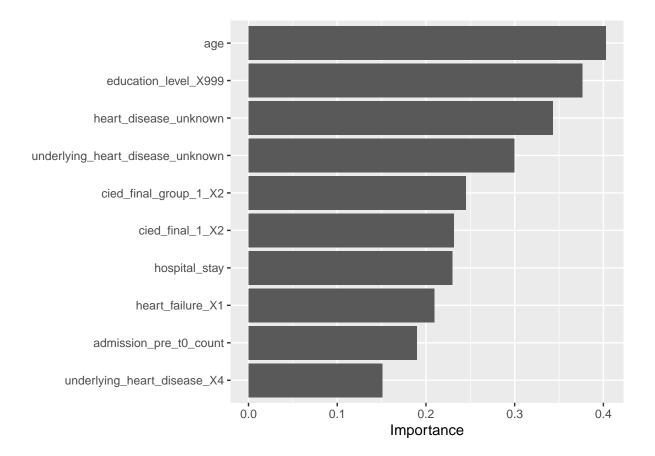
0.005

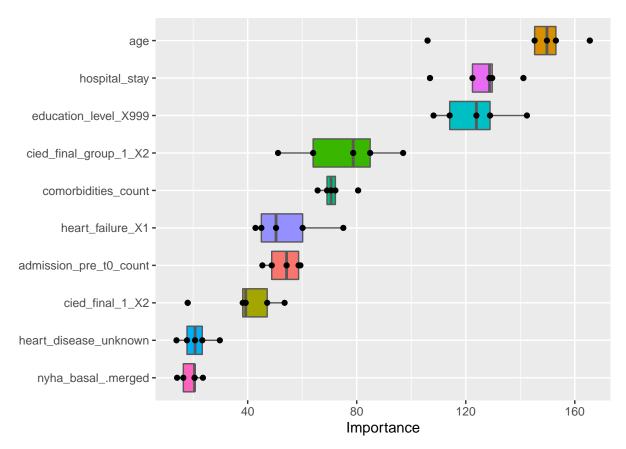
GLM

```
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()) %>%
  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)
glmnet_auc <- validation(glm_fit, df_test)</pre>
```



```
##
##
                  Accuracy : 0.6797
##
                    95% CI: (0.6662, 0.693)
##
      No Information Rate: 0.9484
      P-Value [Acc > NIR] : 1
##
##
##
                     Kappa : 0.1114
##
##
   Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.6768
               Specificity: 0.7336
##
##
            Pos Pred Value: 0.9790
##
            Neg Pred Value: 0.1099
##
                Prevalence: 0.9484
            Detection Rate: 0.6419
##
      Detection Prevalence: 0.6556
##
##
        Balanced Accuracy: 0.7052
##
##
          'Positive' Class : 0
##
```





Minutes to run:

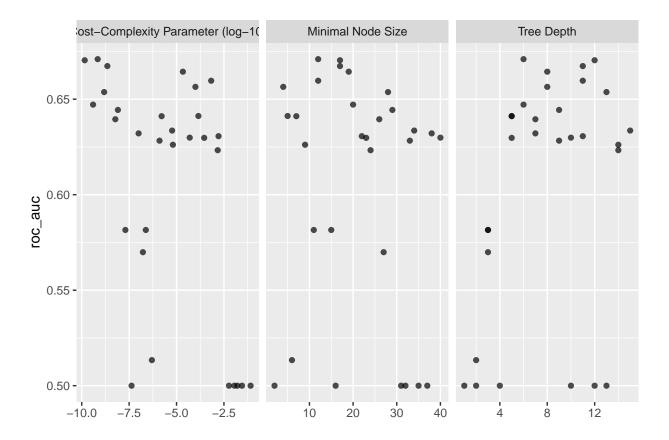
2.897

Decision Tree

```
tree_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()) %>%
  step_zv(all_predictors())
tree_spec <-
  decision_tree(cost_complexity = tune(),
                tree_depth = tune(),
                min_n = tune()) %>%
  set_mode("classification") %>%
  set_engine("rpart")
tree_grid <- grid_latin_hypercube(cost_complexity(),</pre>
                                   tree_depth(),
                                   min_n(),
                                   size = grid_size)
tree workflow <-
  workflow() %>%
  add_recipe(tree_recipe) %>%
  add_model(tree_spec)
tree_tune <-
 tree_workflow %>%
```

```
##
  # A tibble: 60 x 9
##
      cost_complexity tree_depth min_n .metric
                                                 .estimator mean
                                                                      n std_err .config
##
                <dbl>
                           <int> <int> <chr>
                                                            <dbl> <int>
                                                                          <dbl> <chr>
                                                 <chr>
##
             1.49e- 3
                            14
                                    24 accuracy binary
                                                            0.950
                                                                     10 0.00154 Preprocessor1 Model01
             1.49e- 3
                                                                     10 0.00941 Preprocessor1_Model01
##
   2
                              14
                                    24 roc_auc binary
                                                            0.623
##
   3
             6.73e-4
                              11
                                    12 accuracy binary
                                                            0.940
                                                                     10 0.00260 Preprocessor1_Model02
##
   4
             6.73e- 4
                              11
                                    12 roc_auc binary
                                                            0.660
                                                                     10 0.0142 Preprocessor1_Model02
             3.96e-10
                              6
                                                            0.950
                                                                     10 0.00142 Preprocessor1_Model03
   5
                                    20 accuracy binary
                               6
##
   6
             3.96e-10
                                    20 roc_auc binary
                                                            0.647
                                                                     10 0.0120 Preprocessor1_Model03
   7
             1.12e- 2
                              10
                                                            0.954
                                                                     10 0.00132 Preprocessor1_Model04
##
                                    37 accuracy binary
##
   8
             1.12e- 2
                              10
                                    37 roc_auc binary
                                                            0.5
                                                                     10 0
                                                                                Preprocessor1_Model04
             9.98e-8
                              7
                                                            0.952
                                                                     10 0.00147 Preprocessor1_Model05
##
   9
                                    38 accuracy binary
             9.98e- 8
                               7
                                    38 roc_auc binary
                                                            0.632
                                                                     10 0.00737 Preprocessor1_Model05
##
  10
  # ... with 50 more rows
```

autoplot(tree_tune, metric = "roc_auc")



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

```
##
  # A tibble: 5 x 9
##
     cost_complexity tree_depth min_n .metric .estimator mean
                                                                     n std_err .config
##
               <dbl>
                           <int> <int> <chr>
                                               <chr>>
                                                           <dbl> <int>
                                                                          <dbl> <chr>
##
  1
            6.95e-10
                               6
                                    12 roc_auc binary
                                                           0.671
                                                                    10 0.0116 Preprocessor1_Model20
## 2
            1.44e-10
                              12
                                    17 roc_auc binary
                                                           0.670
                                                                    10 0.0122 Preprocessor1_Model14
```

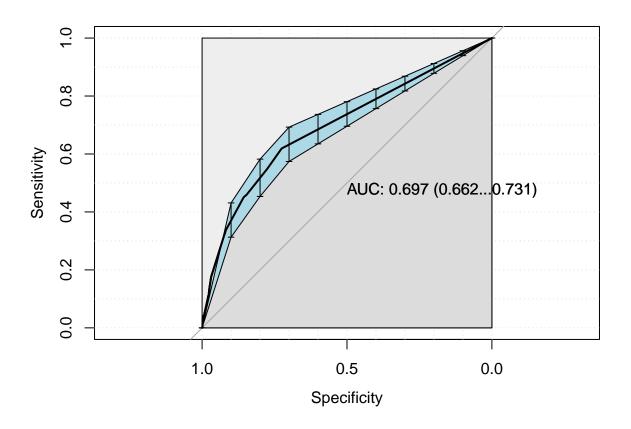
```
2.16e- 5
## 4
                                8
                                     19 roc_auc binary
                                                             0.664
                                                                       10 0.0147 Preprocessor1_Model06
             6.73e- 4
## 5
                               11
                                     12 roc_auc binary
                                                             0.660
                                                                       10 0.0142 Preprocessor1_Model02
best_tree <- tree_tune %>%
  select_best("roc_auc")
final_tree_workflow <-</pre>
  tree_workflow %>%
  finalize_workflow(best_tree)
last_tree_fit <-</pre>
  final_tree_workflow %>%
  last_fit(df_split)
final_tree_fit <- extract_workflow(last_tree_fit)</pre>
tree_auc <- validation(final_tree_fit, df_test)</pre>
```

0.667

10 0.0145 Preprocessor1_Model23

17 roc_auc binary

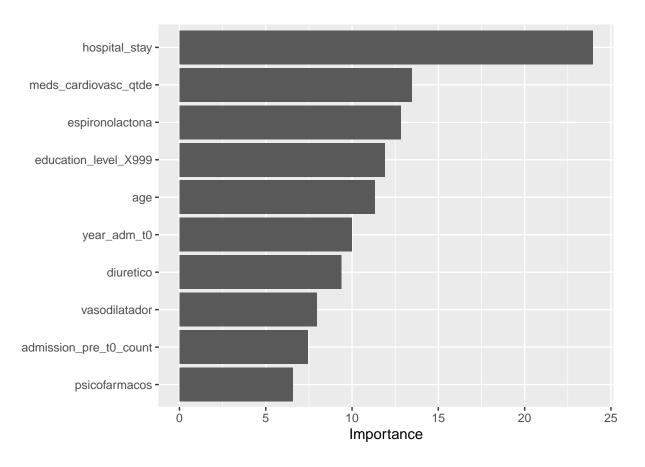
11



3

2.25e- 9

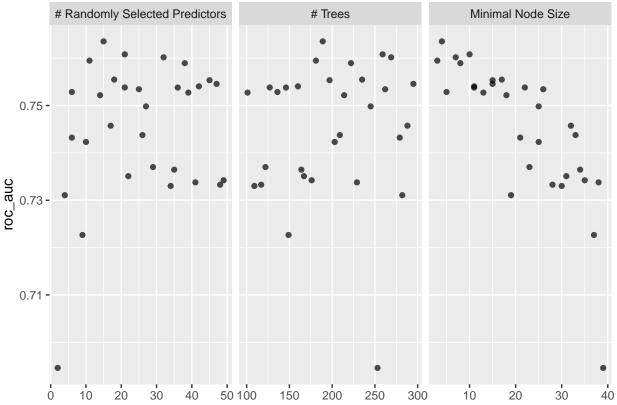
```
##
                     Kappa : 0.1075
##
##
   Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.7256
##
               Specificity: 0.6189
            Pos Pred Value : 0.9722
##
##
            Neg Pred Value: 0.1093
##
                Prevalence: 0.9484
##
            Detection Rate : 0.6882
      Detection Prevalence: 0.7078
##
##
         Balanced Accuracy: 0.6722
##
##
          'Positive' Class : 0
##
```



Minutes to run: 9.749

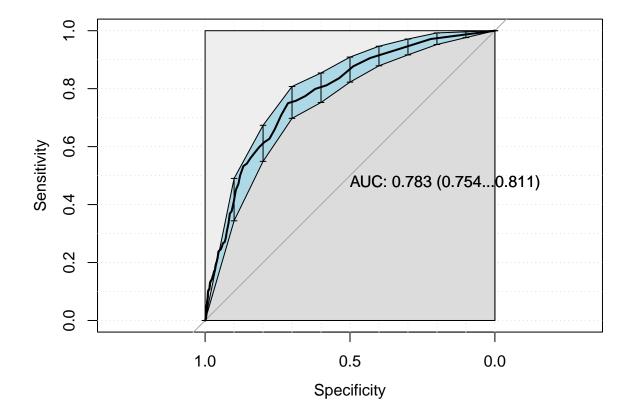
Random Forest

```
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()) %>%
 step_zv(all_predictors()) %>%
 step_impute_mean(all_numeric_predictors())
rf_spec <-
 rand_forest(mtry = tune(),
            trees = tune(),
            \min n = tune()) \%>\%
 set_mode("classification") %>%
 set_engine("randomForest",
            probability = TRUE,
            nthread = 8)
rf_grid <- grid_latin_hypercube(mtry(range = c(1L, 50L)),
                             trees(range = c(100L, 300L)),
                             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()
## # A tibble: 60 x 9
##
      mtry trees min_n .metric .estimator mean n std_err .config
##
     <int> <int> <int> <chr>
                              <chr> <dbl> <int>
                                                     <dbl> <chr>
      25 262 26 accuracy binary
## 1
                                        0.954 10 0.00134 Preprocessor1_Model01
                                        0.753 10 0.00754 Preprocessor1_Model01
        25
## 2
            262
                   26 roc_auc binary
## 3
      42 160 11 accuracy binary
                                        0.953 10 0.00111 Preprocessor1_Model02
## 4 42 160 11 roc_auc binary
                                        0.754 10 0.0103 Preprocessor1_Model02
## 5 15 189
                                        0.954 10 0.00133 Preprocessor1_Model03
                   4 accuracy binary
      15 189
                                        ## 6
                   4 roc_auc binary
## 7
       39 101 13 accuracy binary
                                        0.953 10 0.00131 Preprocessor1_Model04
## 8
       39 101
                   13 roc_auc binary
                                        0.753 10 0.00852 Preprocessor1_Model04
## 9
       11 181
                                        0.954 10 0.00135 Preprocessor1_Model05
                    3 accuracy binary
## 10
        11
            181
                    3 roc_auc binary
                                        0.759
                                                 10 0.0114 Preprocessor1_Model05
## # ... with 50 more rows
autoplot(rf_tune, metric = "roc_auc")
```



```
rf_tune %>%
  show_best("roc_auc")
## # A tibble: 5 x 9
                                                    n std_err .config
      mtry trees min_n .metric .estimator mean
##
     <int> <int> <chr> <chr>
                                          <dbl> <int>
                                                        <dbl> <chr>
                    4 roc_auc binary
                                                   10 0.0104 Preprocessor1_Model03
## 1
        15
            189
                                          0.764
                                                   10 0.00878 Preprocessor1_Model14
## 2
        21 259
                  10 roc_auc binary
                                         0.761
        32 269
                    7 roc_auc binary
                                                   10 0.00932 Preprocessor1_Model13
## 3
                                          0.760
## 4
        11 181
                    3 roc_auc binary
                                          0.759
                                                   10 0.0114 Preprocessor1_Model05
       38 222
                    8 roc_auc binary
                                          0.759
                                                   10 0.00982 Preprocessor1_Model10
## 5
best_rf <- rf_tune %>%
  select_best("roc_auc")
final_rf_workflow <-</pre>
  rf_workflow %>%
  finalize_workflow(best_rf)
last_rf_fit <-</pre>
  final_rf_workflow %>%
 last_fit(df_split)
final_rf_fit <- extract_workflow(last_rf_fit)</pre>
```

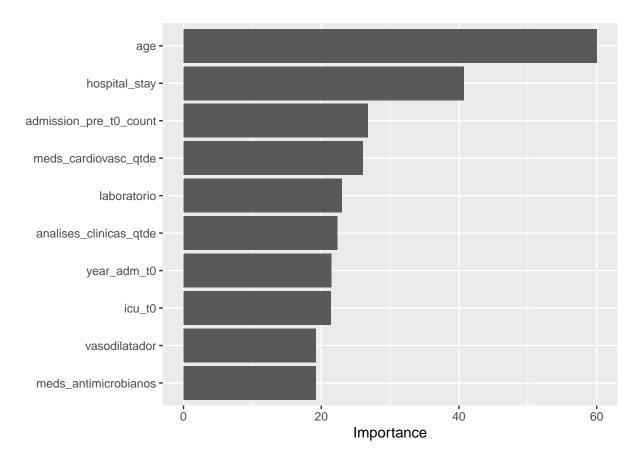
rf_auc <- validation(final_rf_fit, df_test)</pre>



##

pfun_rf <- function(object, newdata) predict(object, data = newdata)
extract_vip(final_rf_fit, pred_wrapper = predict,</pre>

```
reference_class = "1", use_matrix = FALSE,
method = 'model')
```

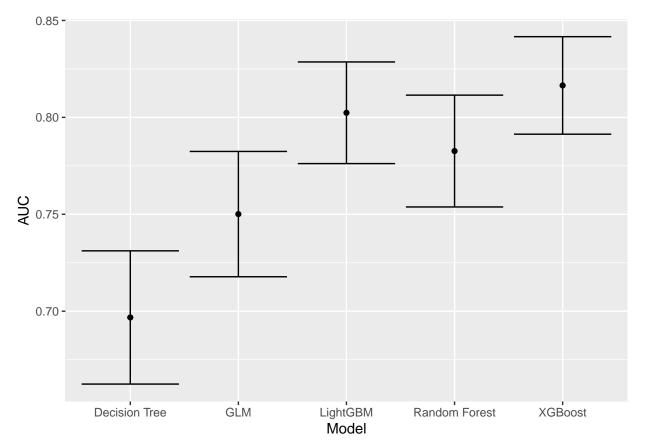


```
# extract_vip(final_rf_fit, pred_wrapper = predict,
# reference_class = "1", use_matrix = FALSE,
# method = 'permute')
```

Minutes to run: 129.867

Models Comparison

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



saveRDS(df_auc, sprintf("./auxiliar/model_selection/performance/%s.RData", outcome_column))

Minutes to run: 0.002