

Model Selection - death_180days

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Imports

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

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))
```

Minutes to run: 0.006

Eligible features

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

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

correlated_columns = c('year_procedure_1', # com year_adm_t0
  'age_surgery_1', # com age
  'admission_t0', # com admission_pre_t0_count
  'atb', # com meds_antimicrobianos
  'classe_meds_cardio_qtde', # com classe_meds_qtde
  'suporte_hemod' # com proced_invasivos_qtde
)

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

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. 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. cancer
## 19. comorbidities_count
## 20. procedure_type_1
## 21. reop_type_1
## 22. procedure_type_new
## 23. cied_final_1
## 24. cied_final_group_1
## 25. admission_pre_t0_count
## 26. admission_pre_t0_180d
## 27. year_adm_t0
## 28. icu_t0
## 29. dialysis_t0
## 30. admission_t0_emergency
## 31. aco
## 32. antiarritmico
## 33. ieca_bra
## 34. dva
## 35. digoxina
## 36. estatina
## 37. diuretico
## 38. vasodilatador
## 39. insuf_cardiaca
## 40. espironolactona
## 41. antiplaquetario_ev
## 42. insulina
## 43. psicofarmacos
## 44. antifungico
## 45. classe_meds_qtde
## 46. meds_cardiovasc_qtde
## 47. meds_antimicrobianos
## 48. vni
## 49. outros_proced_cirurgicos
## 50. icp
## 51. cateterismo
## 52. cateter_venoso_central
## 53. proced_invasivos_qtde
## 54. transfusao
## 55. interconsulta

```

```
## 56. equipe_multiprof
## 57. ecg
## 58. holter
## 59. teste_esforco
## 60. metodos_graficos_qtde
## 61. laboratorio
## 62. cultura
## 63. analises_clinicas_qtde
## 64. citologia
## 65. histopatologia_qtde
## 66. angiografia
## 67. aortografia
## 68. arteriografia
## 69. cintilografia
## 70. ecocardiograma
## 71. endoscopia
## 72. ultrassom
## 73. tomografia
## 74. radiografia
## 75. ressonancia
## 76. exames_imagem_qtde
## 77. bic
```

Minutes to run: 0

Train test split (70%/30%)

```
set.seed(42)

if (outcome_column == 'readmission_30d') {
  df_split <- readRDS("../dataset/split_object.rds")
} else {
  df_split <- initial_split(df, prop = .7, strata = all_of(outcome_column))
}

df_train <- training(df_split) %>% dplyr::select(all_of(c(features, outcome_column)))
df_test <- testing(df_split) %>% dplyr::select(all_of(c(features, outcome_column)))
```

Minutes to run: 0.001

Global parameters

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

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

Minutes to run: 0.001

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 <-
  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]])

if (plot) {
  sens.ci <- ci.se(pROC_obj)
  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 <-
  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(
  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(
  finalize(mtry(), df_train),
  dials::trees(range = c(100L, 300L)),
  min_n(),
  tree_depth(),
  learn_rate(),
  loss_reduction(),
  size = grid_size
)

xgboost_workflow <-
  workflow() %>%
  add_recipe(xgboost_recipe) %>%
  add_model(xgboost_spec)

xgboost_tune <-
  xgboost_workflow %>%
  tune_grid(resamples = df_folds,
            grid = xgboost_grid)

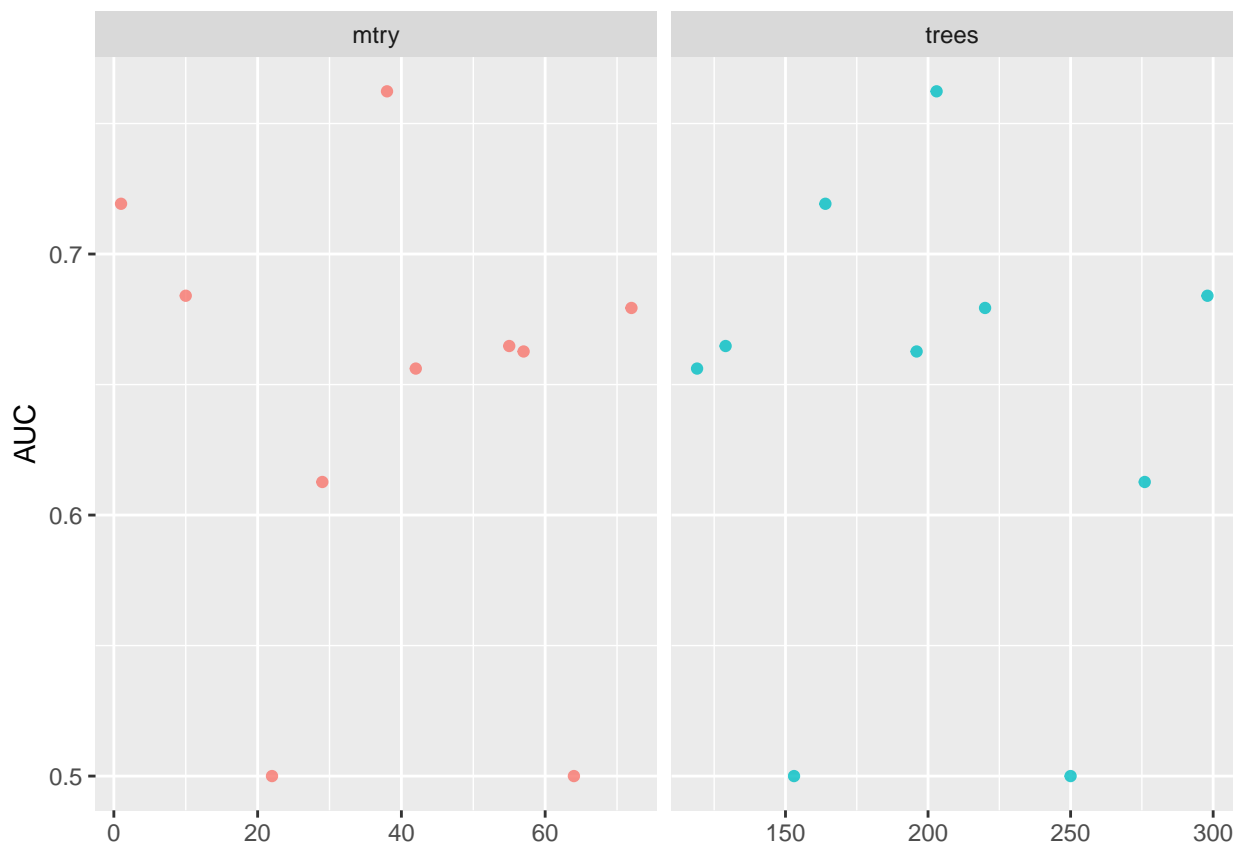
xgboost_tune %>%
  show_best("roc_auc")

## # A tibble: 5 x 12
##   mtry 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     38   203    13         5  0.0141    5.19e- 9 roc_auc binary  0.762     4  0.0230 Prepro~
## 2      1   164    34        15  0.00935    3.66e- 2 roc_auc binary  0.719     4  0.0160 Prepro~
## 3     10   298     8        11  0.0000235  8.98e- 7 roc_auc binary  0.684     4  0.0198 Prepro~
## 4     72   220    38         8  0.000222    6.10e-10 roc_auc binary  0.679     4  0.0227 Prepro~
## 5     55   129    16         4  0.0000622  5.53e- 3 roc_auc binary  0.665     4  0.0168 Prepro~
## # ... with abbreviated variable names 1: loss_reduction, 2: .estimator

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")

```

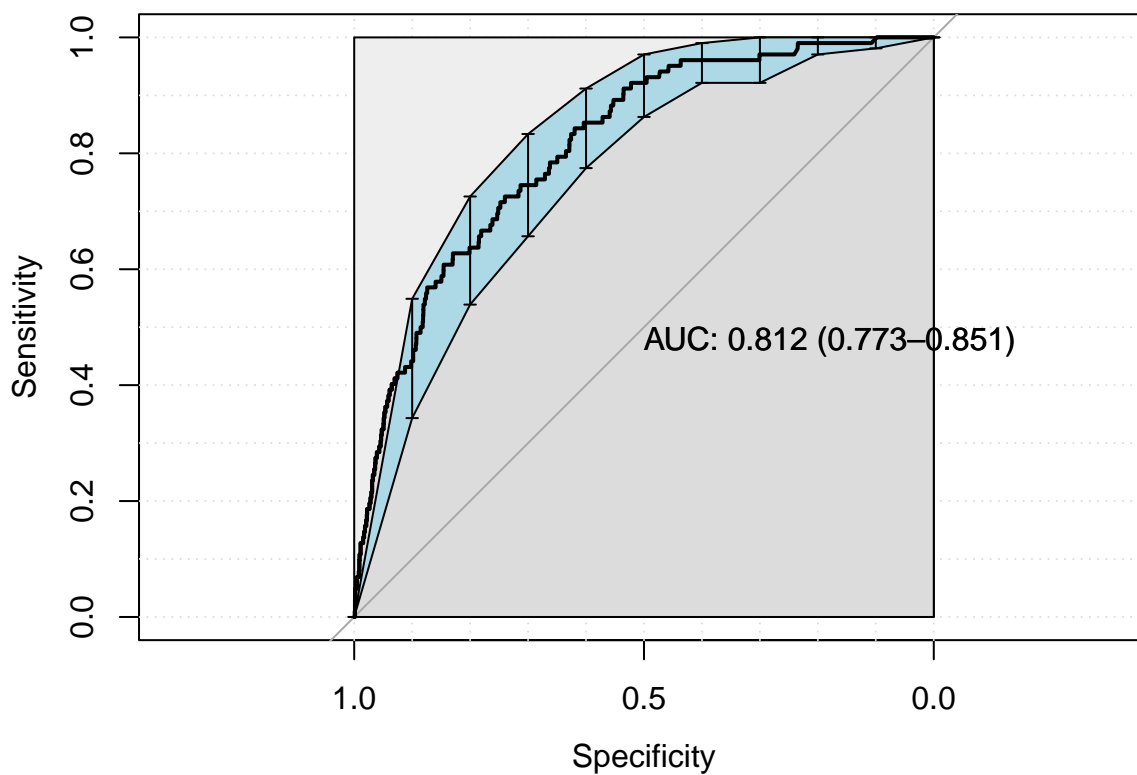


```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

last_xgboost_fit <-
  final_xgboost_workflow %>%
  last_fit(df_split)

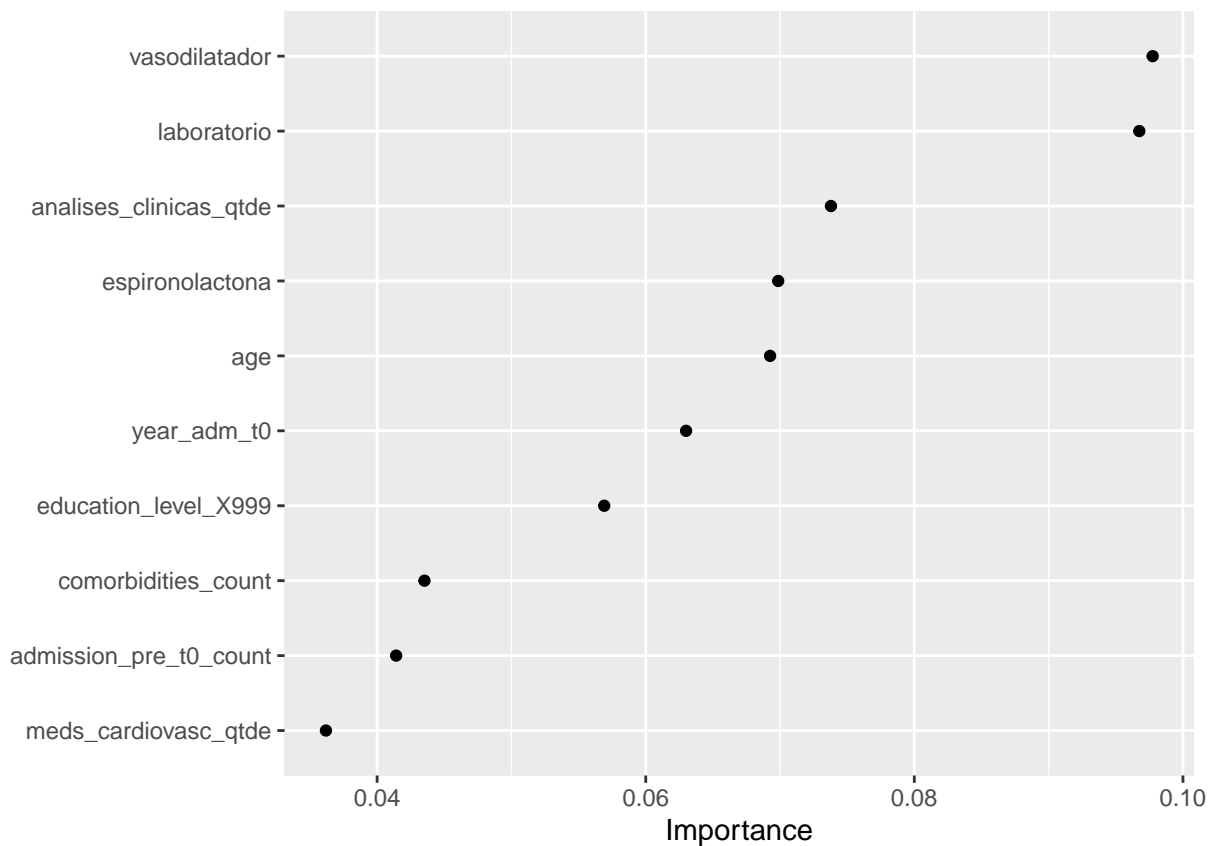
final_xgboost_fit <- extract_workflow(last_xgboost_fit)

xgboost_auc <- validation(final_xgboost_fit, df_test)
```



```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                0 4628  102
##                1    0    0
##
##          Accuracy : 0.9784
##          95% CI   : (0.9739, 0.9824)
##    No Information Rate : 0.9784
##    P-Value [Acc > NIR] : 0.5263
##
##          Kappa : 0
##
##  McNemar's Test P-Value : <2e-16
##
##          Sensitivity : 1.0000
##          Specificity : 0.0000
##    Pos Pred Value : 0.9784
##    Neg Pred Value :    NaN
##    Prevalence : 0.9784
##    Detection Rate : 0.9784
##    Detection Prevalence : 1.0000
##    Balanced Accuracy : 0.5000
##
##    '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/model_selection/hyperparameters/xgboost_%s.rds",
    outcome_column
  )
)
```

Minutes to run: 1.986

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
)
```



```

) %>%
  set_engine("lightgbm") %>%
  set_mode("classification")

lightgbm_grid <- grid_latin_hypercube(
  finalize(mtry(), df_train),
  dials::trees(range = c(100L, 300L)),
  min_n(),
  tree_depth(),
  learn_rate(),
  loss_reduction(),
  size = grid_size
)

lightgbm_workflow <-
  workflow() %>%
  add_recipe(lightgbm_recipe) %>%
  add_model(lightgbm_spec)

lightgbm_tune <-
  lightgbm_workflow %>%
  tune_grid(resamples = df_folds,
            grid = lightgbm_grid)

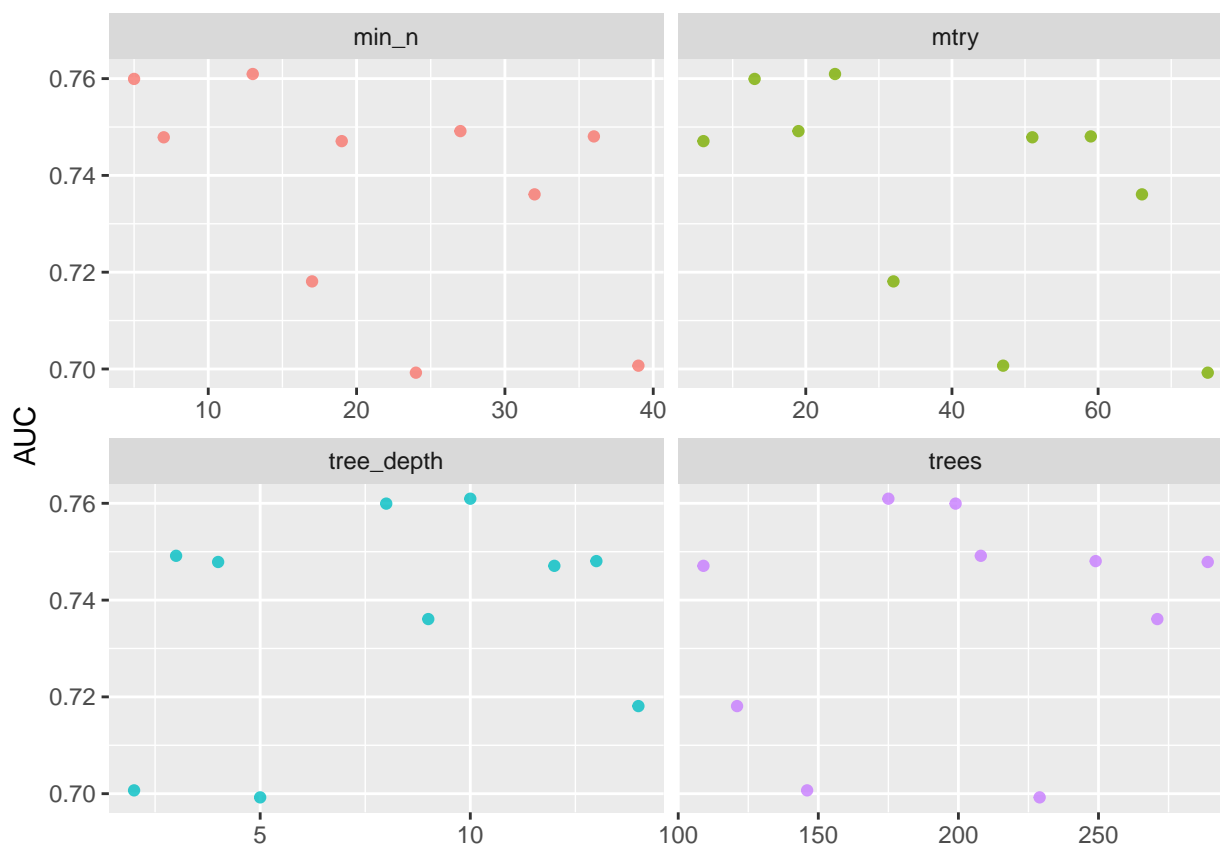
lightgbm_tune %>%
  show_best("roc_auc")

## # A tibble: 5 x 12
##   mtry trees min_n tree_depth   learn_rate loss_~1 .metric .esti~2   mean     n std_err .config
##   <int> <int> <int>     <int>       <dbl>   <dbl> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1     24   175    13         10    4.68e-8  3.97e-2 roc_auc binary  0.761     4  0.0217 Prepro~
## 2     13   199     5          8    2.62e-6  2.43e-5 roc_auc binary  0.760     4  0.0185 Prepro~
## 3     19   208    27          3    8.31e-4  3.15e-6 roc_auc binary  0.749     4  0.0197 Prepro~
## 4     59   249    36         13    1.44e-9  1.20e-8 roc_auc binary  0.748     4  0.0240 Prepro~
## 5     51   289     7          4    4.34e-2  1.91e-4 roc_auc binary  0.748     4  0.0173 Prepro~
## # ... 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")

```

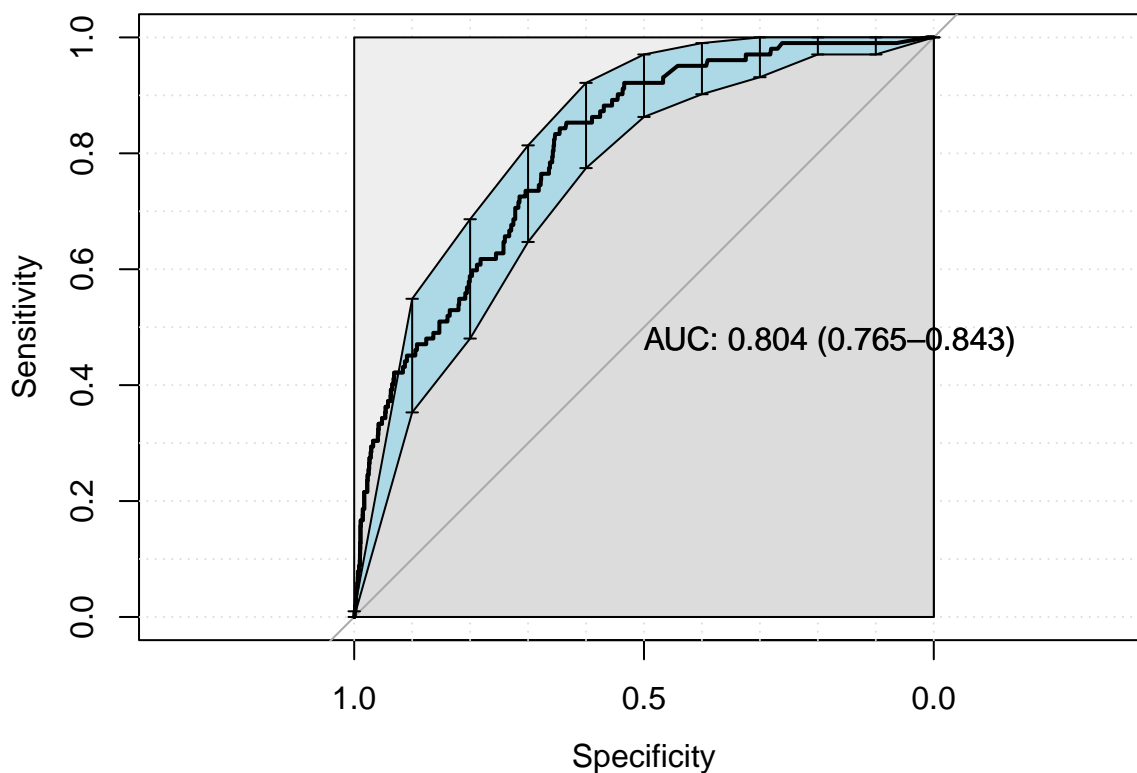


```
final_lightgbm_workflow <-
  lightgbm_workflow %>%
  finalize_workflow(best_lightgbm)

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)
```



Confusion Matrix and Statistics

```
##
##
## test_predictions_class    0    1
##                0 4628  102
##                1    0    0
##
##          Accuracy : 0.9784
##          95% CI   : (0.9739, 0.9824)
##    No Information Rate : 0.9784
##    P-Value [Acc > NIR] : 0.5263
##
##          Kappa : 0
##
##  McNemar's Test P-Value : <2e-16
##
##          Sensitivity : 1.0000
##          Specificity : 0.0000
##    Pos Pred Value : 0.9784
##    Neg Pred Value :      NaN
##    Prevalence : 0.9784
##    Detection Rate : 0.9784
##    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/model_selection/hyperparameters/lightgbm_%s.rds",
  outcome_column
)
)

```

Minutes to run: 1.193

GLM

```

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

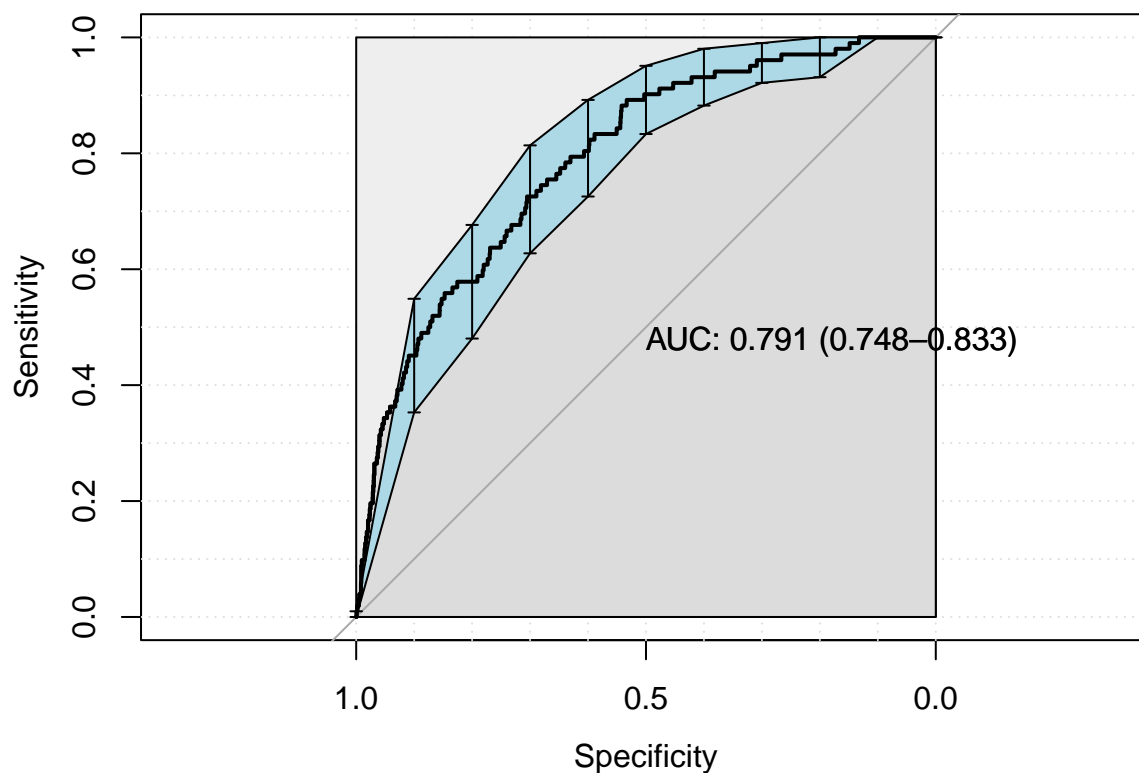
glmnet_spec <-
  logistic_reg(penalty = 0) %>%
  set_mode("classification") %>%
  set_engine("glmnet")

glmnet_workflow <-
  workflow() %>%
  add_recipe(glmnet_recipe) %>%
  add_model(glmnet_spec)

glm_fit <- glmnet_workflow %>%
  fit(df_train)

glm_auc = validation(glm_fit, df_test)

```

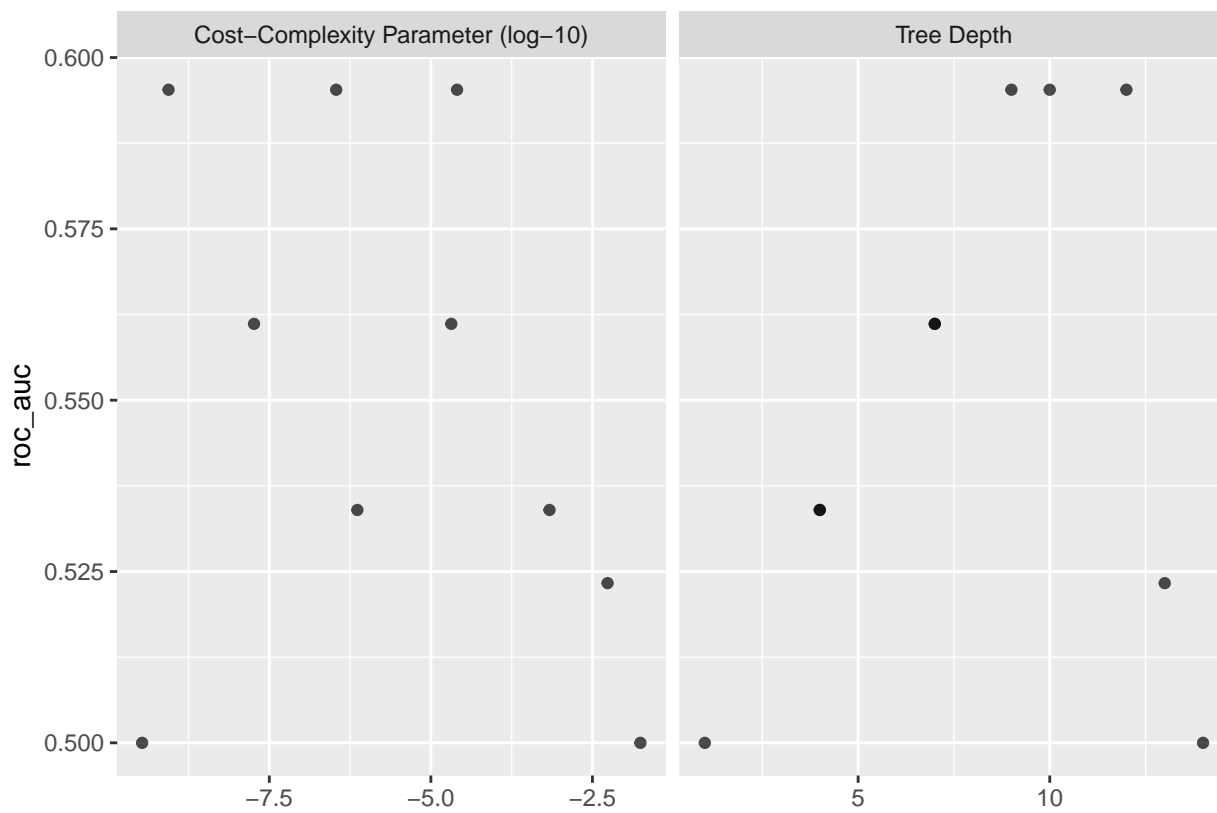


```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                0 4625  102
##                1    3    0
##
##                Accuracy : 0.9778
##                95% CI : (0.9732, 0.9818)
##      No Information Rate : 0.9784
##      P-Value [Acc > NIR] : 0.6422
##
##                Kappa : -0.0012
##
## McNemar's Test P-Value : <2e-16
##
##                Sensitivity : 0.9994
##                Specificity : 0.0000
##      Pos Pred Value : 0.9784
##      Neg Pred Value : 0.0000
##      Prevalence : 0.9784
##      Detection Rate : 0.9778
##      Detection Prevalence : 0.9994
##      Balanced Accuracy : 0.4997
##
##      'Positive' Class : 0
##
```

Minutes to run: 0.152

Decision Tree

```
tree_recipe <-  
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%  
  step_nominal(all_nominal_predictors()) %>%  
  step_unknown(all_nominal_predictors()) %>%  
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%  
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%  
  step_zv(all_predictors())  
  
tree_spec <-  
  decision_tree(cost_complexity = tune(),  
                tree_depth = tune()) %>%  
  set_mode("classification") %>%  
  set_engine("rpart")  
  
tree_grid <- grid_latin_hypercube(cost_complexity(),  
                                   tree_depth(),  
                                   size = grid_size)  
  
tree_workflow <-  
  workflow() %>%  
  add_recipe(tree_recipe) %>%  
  add_model(tree_spec)  
  
tree_tune <-  
  tree_workflow %>%  
  tune_grid(resamples = df_folds,  
            grid = tree_grid)  
  
tree_tune %>%  
  collect_metrics()  
  
autoplot(tree_tune, metric = "roc_auc")
```



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

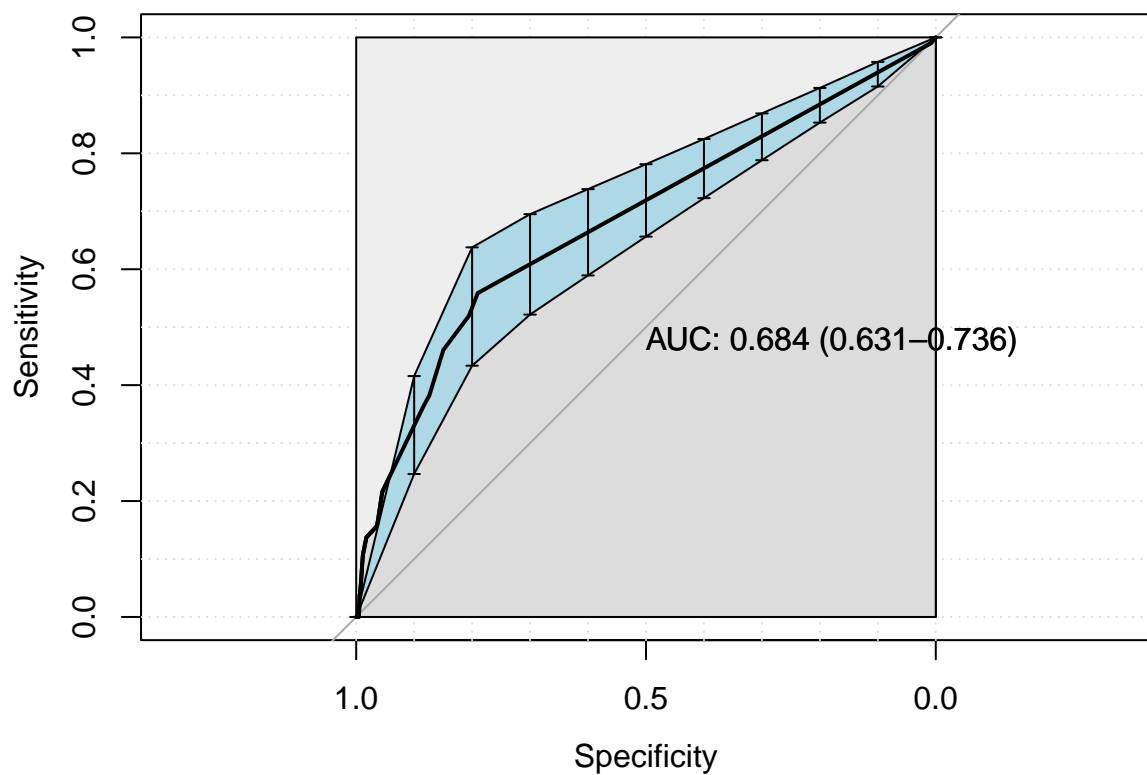
best_tree <- tree_tune %>%
  select_best("roc_auc")

final_tree_workflow <-
  tree_workflow %>%
  finalize_workflow(best_tree)

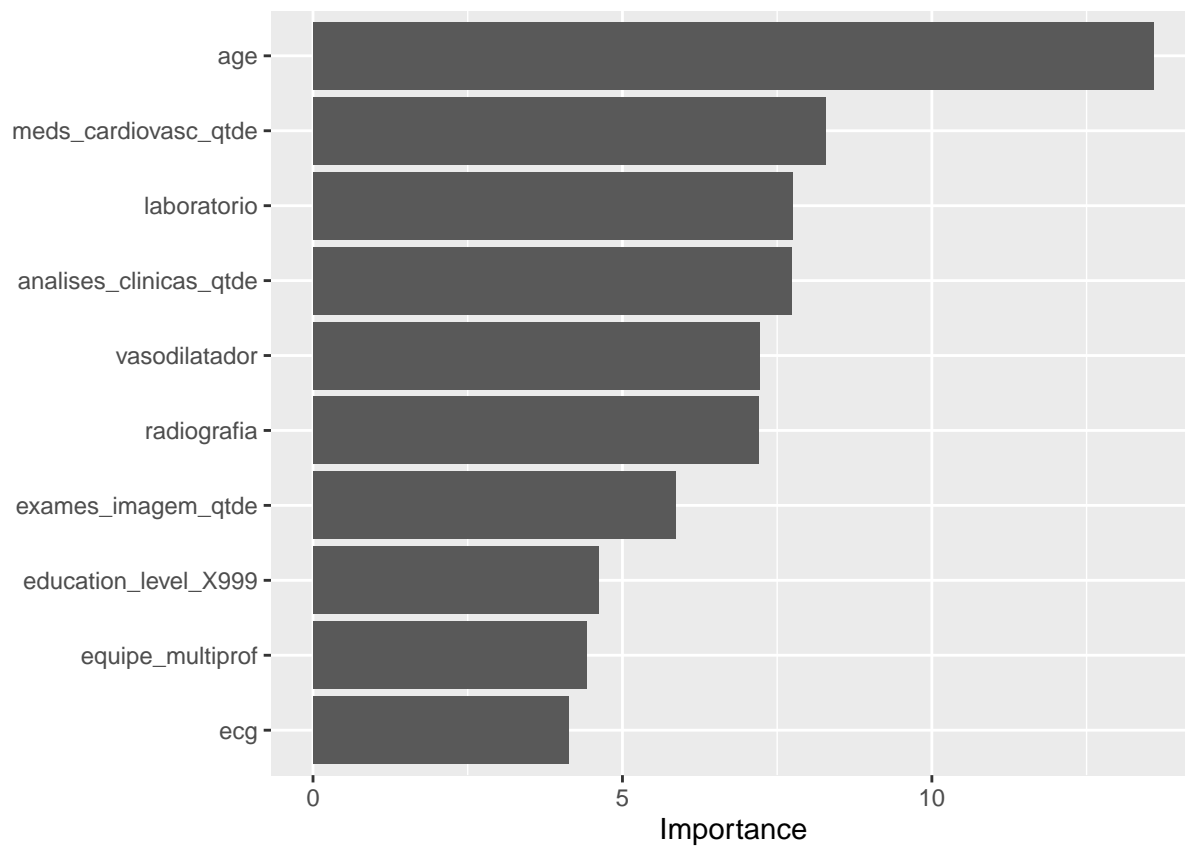
last_tree_fit <-
  final_tree_workflow %>%
  last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

tree_auc = validation(final_tree_fit, df_test)
```



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

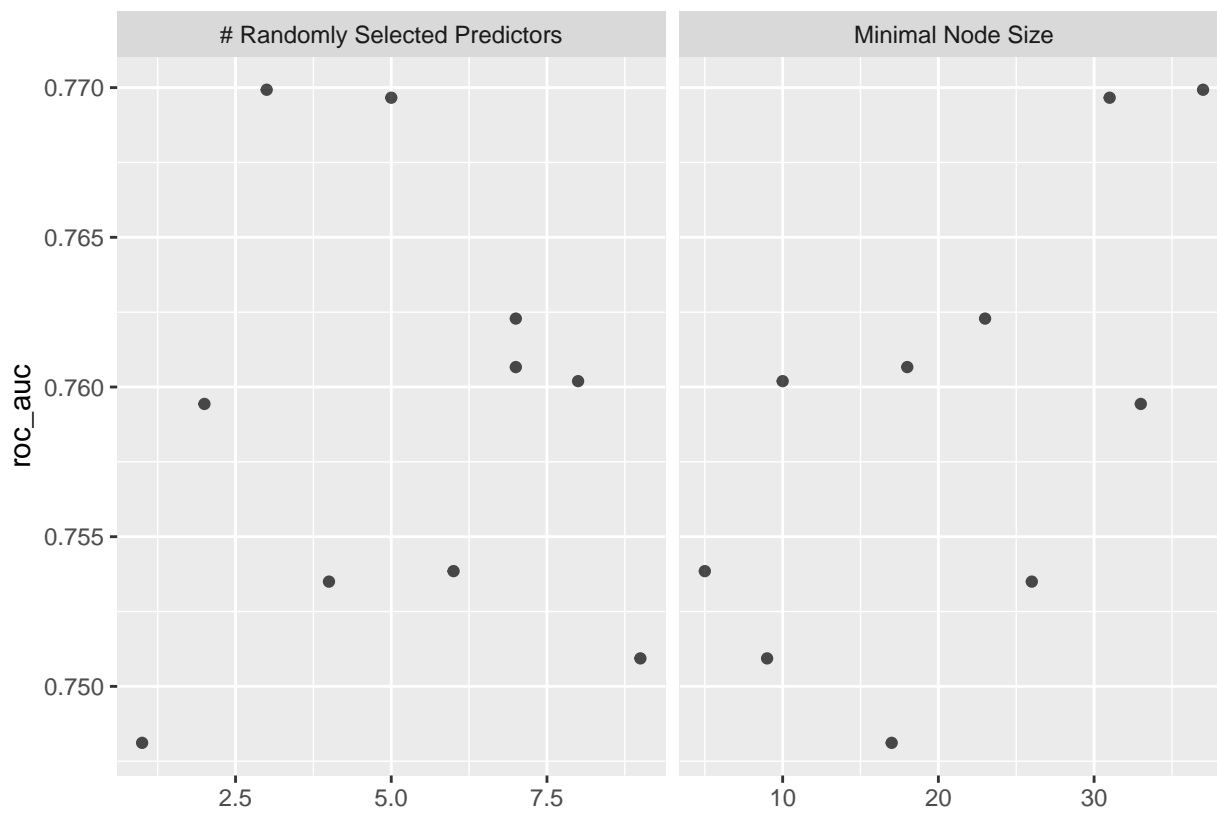


0.949

Minutes to run:

Random Forest

```
rf_recipe <-  
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%  
  step_nominal(all_nominal_predictors()) %>%  
  step_unknown(all_nominal_predictors()) %>%  
  step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%  
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%  
  step_zv(all_predictors()) %>%  
  step_impute_mean(all_numeric_predictors())  
  
rf_spec <-  
  rand_forest(mtry = tune(),  
              trees = 100,  
              min_n = tune()) %>%  
  set_mode("classification") %>%  
  set_engine("ranger")  
  
rf_grid <- grid_latin_hypercube(mtry(range = c(1, 10)),  
                                min_n(),  
                                size = grid_size)  
  
rf_workflow <-  
  workflow() %>%  
  add_recipe(rf_recipe) %>%  
  add_model(rf_spec)  
  
rf_tune <-  
  rf_workflow %>%  
  tune_grid(resamples = df_folds,  
            grid = rf_grid)  
  
rf_tune %>%  
  collect_metrics()  
  
autoplot(rf_tune, metric = "roc_auc")
```



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

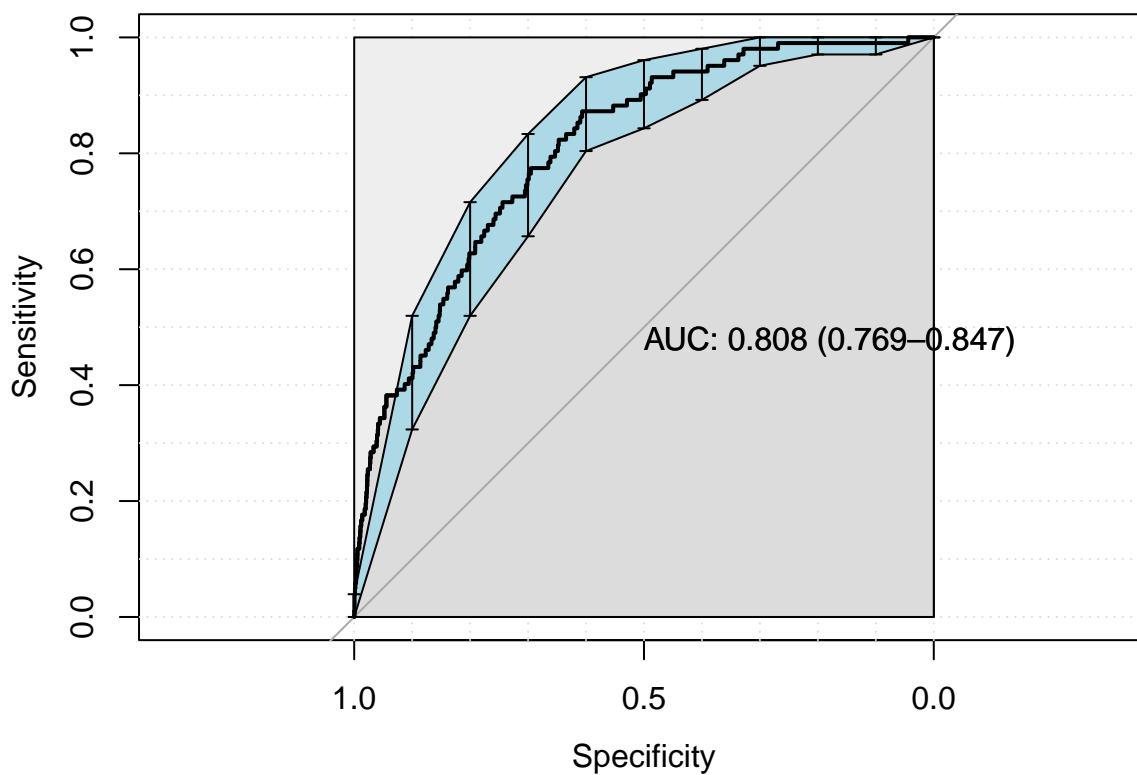
best_rf <- rf_tune %>%
  select_best("roc_auc")

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)
```



0.807

Minutes to run:

KNN

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

```

#           grid = knn_grid)
#
# 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)

```

Minutes to run: 0

SVM

```

# svm_recipe <-
#   recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
#   step_nominal(all_nominal_predictors()) %>%
#   step_unknown(all_nominal_predictors()) %>%
#   step_other(all_nominal_predictors(), threshold = 0.05, other=".merged") %>%
#   step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
#   step_zv(all_predictors()) %>%
#   step_impute_mean(all_numeric_predictors())
#
# svm_spec <-
#   svm_rbf(cost = tune(), rbf_sigma = tune()) %>%
#   set_mode("classification") %>%
#   set_engine("kernlab")
#
# svm_grid <- grid_latin_hypercube(cost(),
#                                   rbf_sigma(),
#                                   size = grid_size)
#
# svm_workflow <-
#   workflow() %>%
#   add_recipe(svm_recipe) %>%
#   add_model(svm_spec)
#
# svm_tune <-
#   svm_workflow %>%
#   tune_grid(resamples = df_folds,
#             grid = 5)
#
# svm_tune %>%
#   collect_metrics()
#

```

```

# autoplot(sum_tune, metric = "roc_auc")
#
# sum_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)

```

Minutes to run: 0

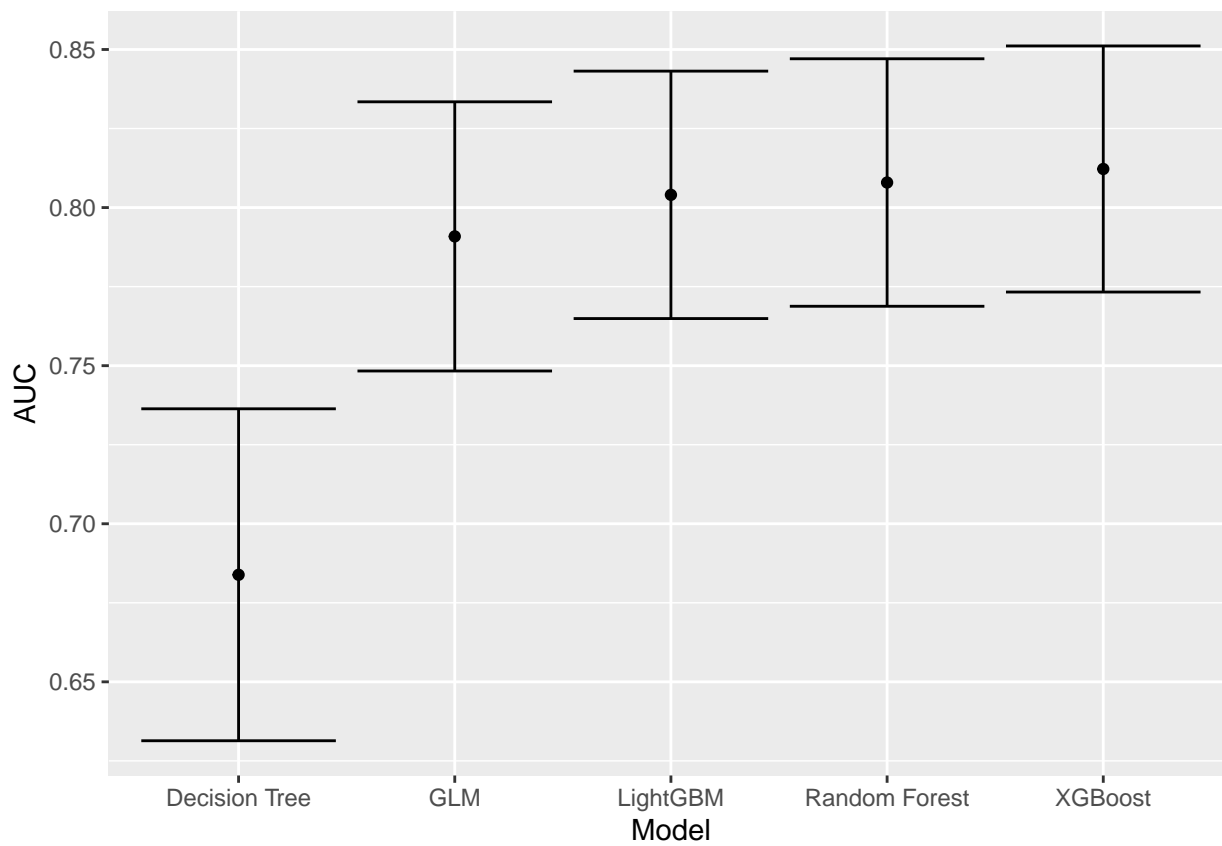
Models Comparison

```

df_auc <- tibble::tribble(
  ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
  'XGBoost', as.numeric(xgboost_auc$auc), xgboost_auc$ci[1], xgboost_auc$ci[3],
  'LightGBM', as.numeric(lightgbm_auc$auc), lightgbm_auc$ci[1], lightgbm_auc$ci[3],
  'GLM', as.numeric(glm_auc$auc), glm_auc$ci[1], glm_auc$ci[3],
  'Decision Tree', as.numeric(tree_auc$auc), tree_auc$ci[1], tree_auc$ci[3],
  'Random Forest', as.numeric(rf_auc$auc), rf_auc$ci[1], rf_auc$ci[3]
) %>%
  mutate(Target = outcome_column)

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

```



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

Minutes to run: 0.009