Model Selection - death_30days

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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
```

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))
```

Minutes to run: 0.005

```
dir.create(file.path("./auxiliar/model_selection/hyperparameters/"),
           showWarnings = FALSE,
           recursive = TRUE)

dir.create(file.path("./auxiliar/model_selection/performance/"),
           showWarnings = FALSE,
           recursive = TRUE)
```

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))

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. valvopathy
## 12. diabetes
## 13. renal_failure
## 14. hemodialysis
## 15. cancer
## 16. comorbidities_count
## 17. procedure_type_1
## 18. reop_type_1
```

```
## 19. procedure_type_new
## 20. cied_final_1
## 21. cied_final_group_1
## 22. admission_pre_t0_count
## 23. admission_pre_t0_180d
## 24. year_adm_t0
## 25. icu_t0
## 26. antiarritmico
## 27. antihipertensivo
## 28. betabloqueador
## 29. dva
## 30. diuretico
## 31. vasodilatador
## 32. espironolactona
## 33. antiplaquetario_ev
## 34. insulina
## 35. psicofarmacos
## 36. antifungico
## 37. classe_meds_qtde
## 38. meds_cardiovasc_qtde
## 39. meds_antimicrobianos
## 40. vni
## 41. ventilacao_mecanica
## 42. intervencao_cv
## 43. cateter_venoso_central
## 44. proced_invasivos_qtde
## 45. transfusao
## 46. interconsulta
## 47. equipe_multiprof
## 48. holter
## 49. metodos_graficos_qtde
## 50. laboratorio
## 51. cultura
## 52. analises_clinicas_qtde
## 53. citologia
## 54. histopatologia_qtde
## 55. angio_tc
## 56. angiografia
## 57. cintilografia
## 58. ecocardiograma
## 59. flebografia
## 60. ultrassom
## 61. tomografia
## 62. ressonancia
## 63. exames_imagem_qtde
## 64. bic
## 65. hospital_stay
```

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)))

df_folds <- vfold_cv(df_train, v = k,
                     strata = all_of(outcome_column))
```

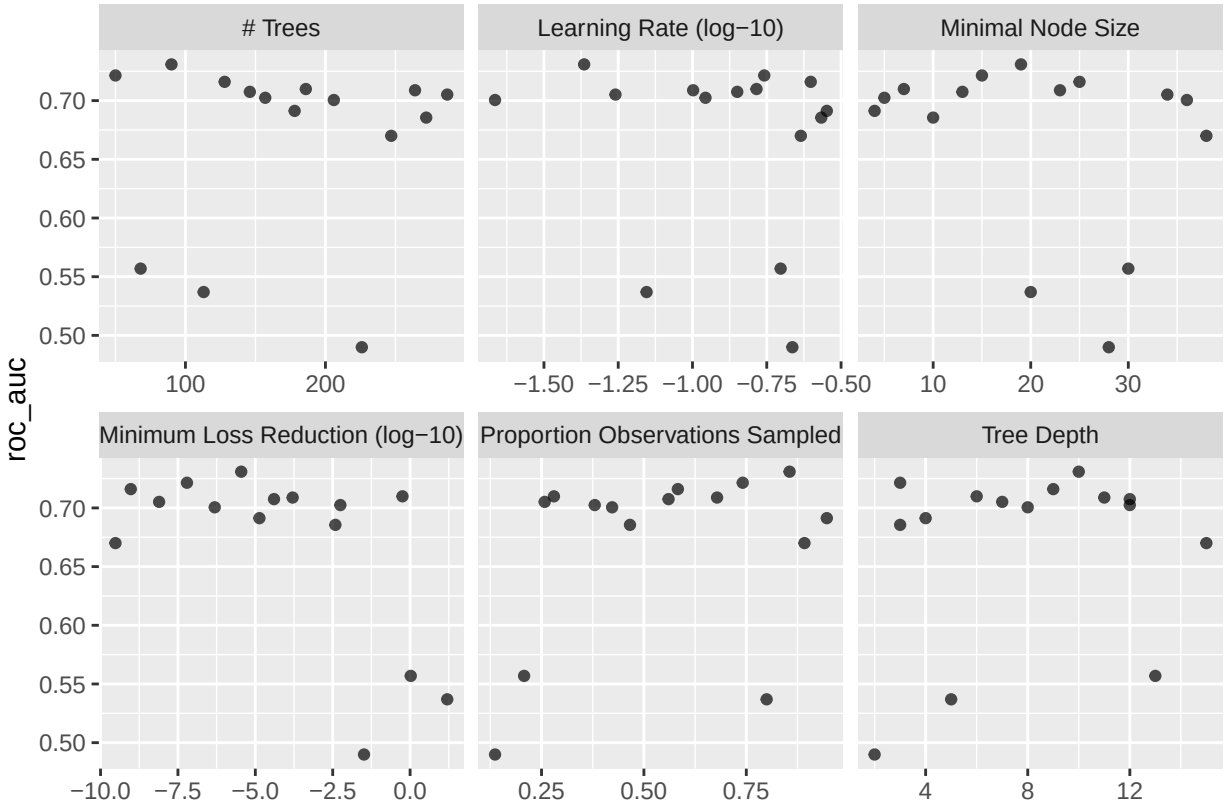
Minutes to run: 0.001

Boosted Tree (XGBoost)

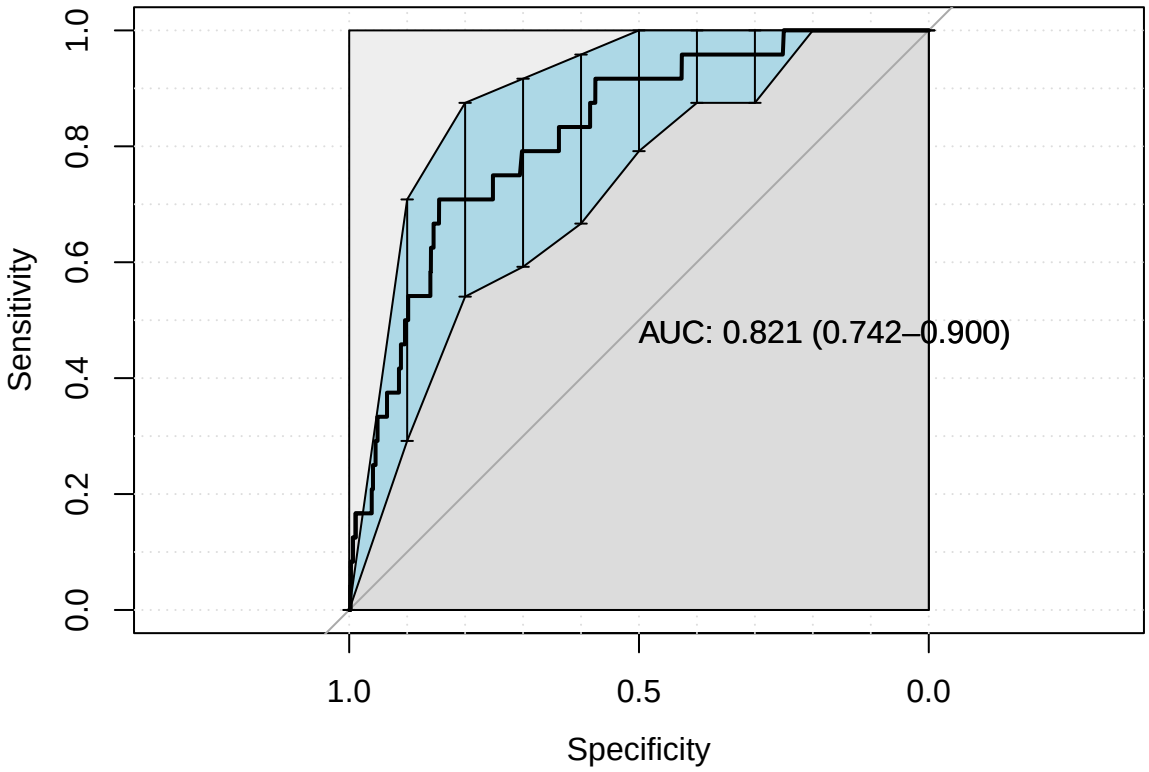
```
xgboost_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other = ".merged") %>%
  step_dummy(all_nominal_predictors())

xgboost_spec <- boost_tree(
  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(
  trees(range = c(50L, 300L)),
  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 <-
  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
##   trees min_n tree_depth learn_rate loss_reduction sample~1 .metric .esti~2  mean     n std_err .config
##   <int> <int>      <int>      <dbl>          <dbl>    <dbl> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1    90    19         10     0.0432       3.50e- 6    0.856 roc_auc binary  0.731     5  0.0272 Prepro~
## 2    50    15          3     0.174        6.19e- 8    0.741 roc_auc binary  0.721     5  0.0500 Prepro~
## 3   128    25          9     0.250        9.47e-10    0.583 roc_auc binary  0.716     5  0.0395 Prepro~
## 4   186     7          6     0.164        5.68e- 1    0.280 roc_auc binary  0.710     5  0.0483 Prepro~
## 5   264    23         11     0.100        1.61e- 4    0.679 roc_auc binary  0.709     5  0.0473 Prepro~
## # ... with abbreviated variable names 1: sample_size, 2: .estimator
```

```
best_xgboost <- xgboost_tune %>%
  select_best("roc_auc")

autoplot(xgboost_tune, metric = "roc_auc")
```

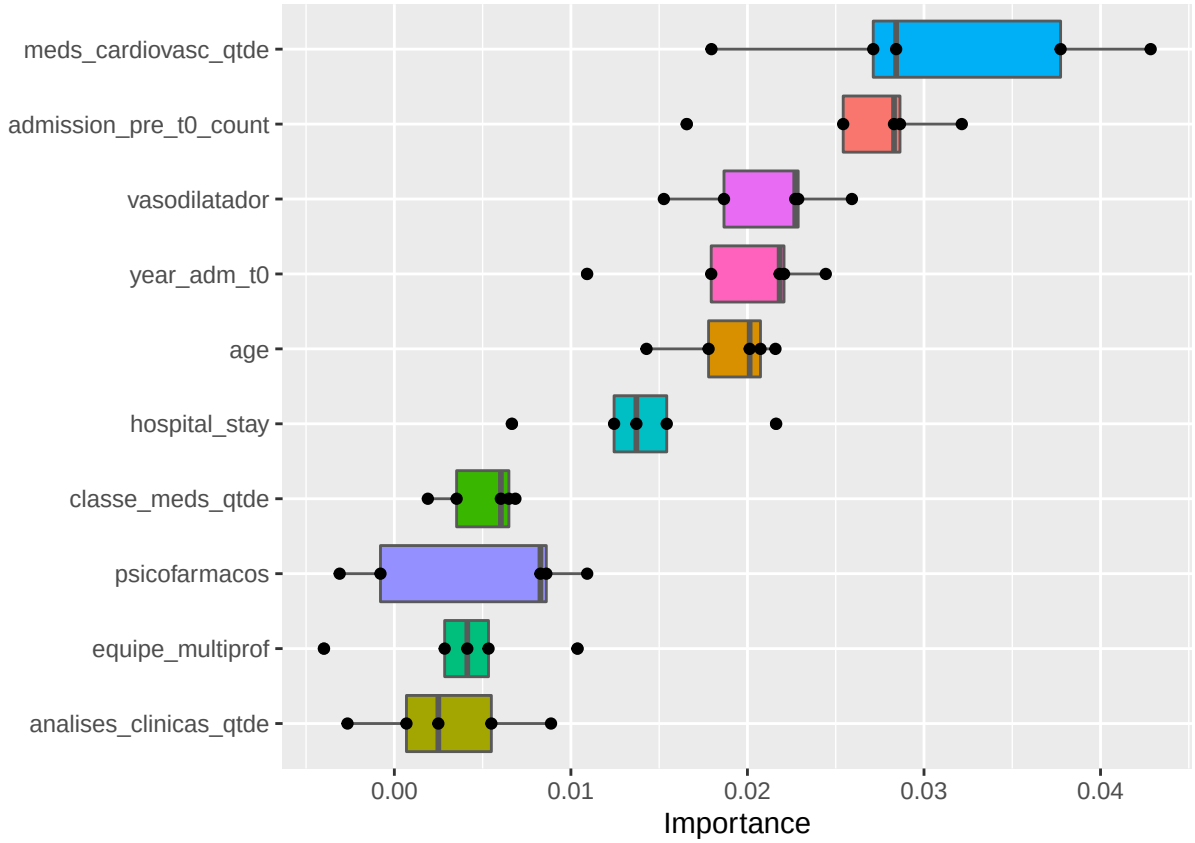



```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

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)
```



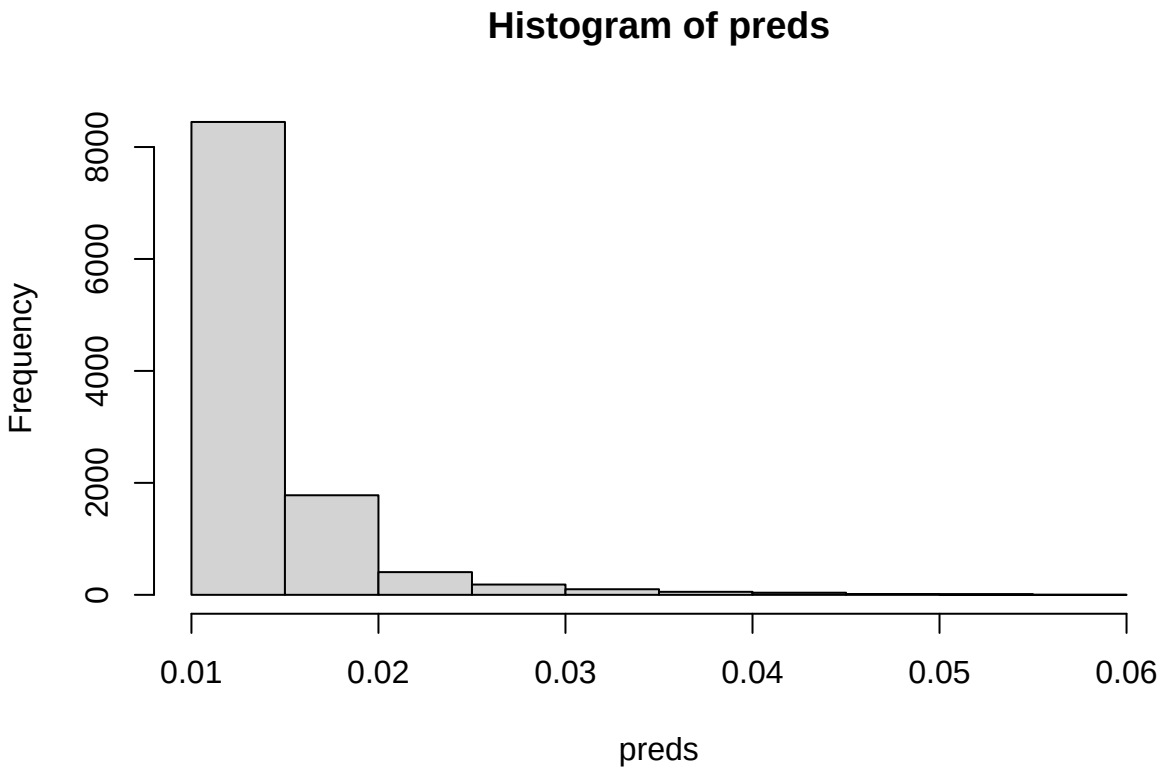

```
## [1] "Optimal Threshold: 0.02"
## Confusion Matrix and Statistics
##
##     reference
## data    0    1
##    0 3976    7
##    1  730   17
##
##                Accuracy : 0.8442
##                  95% CI : (0.8335, 0.8544)
##     No Information Rate : 0.9949
##     P-Value [Acc > NIR] : 1
##
##                   Kappa : 0.0346
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.84488
##             Specificity : 0.70833
##          Pos Pred Value : 0.99824
##          Neg Pred Value : 0.02276
##              Prevalence : 0.99493
##          Detection Rate : 0.84059
##    Detection Prevalence : 0.84207
##       Balanced Accuracy : 0.77661
##
##        'Positive' Class : 0
##
```

```
extract_vip(final_xgboost_fit, pred_wrapper = predict,
            reference_class = "0")
```




```
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
  )
)
```

Minutes to run: 1.469



Minutes to run: 0.005

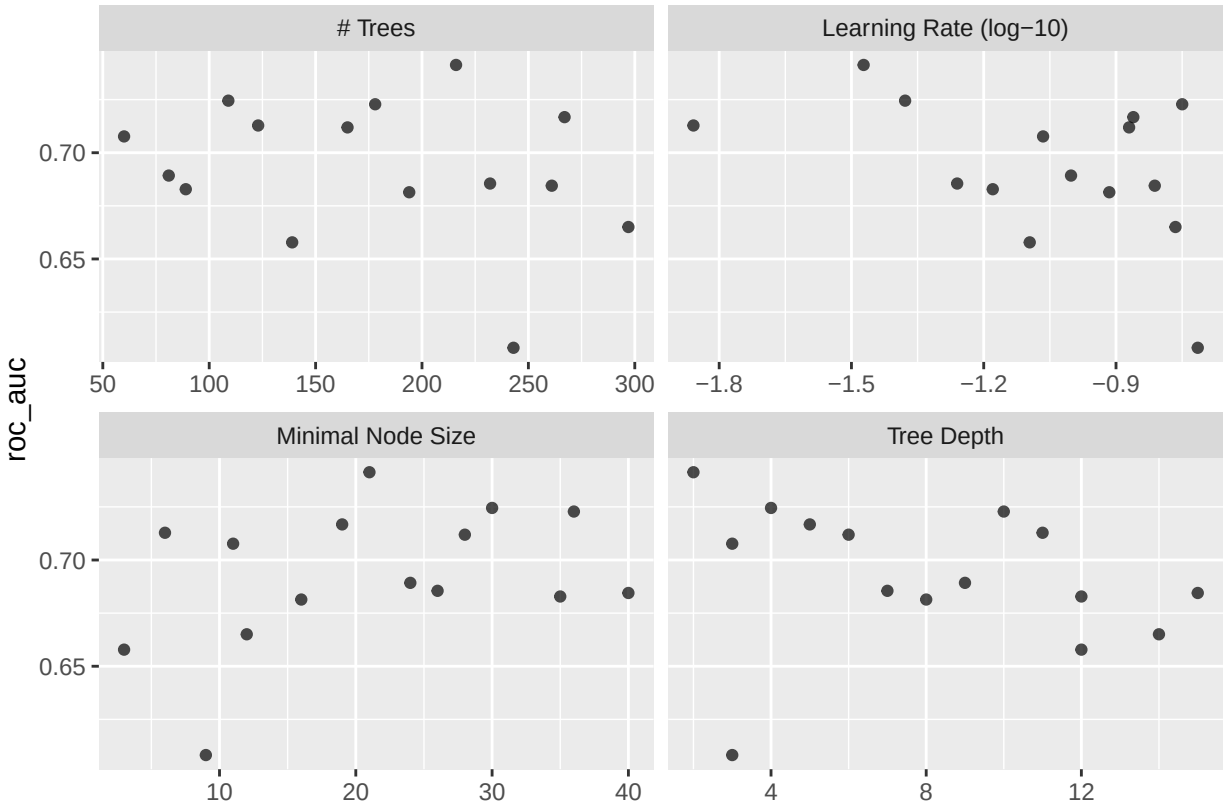
Boosted Tree (LightGBM)

```
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_dummy(all_nominal_predictors())

lightgbm_spec <- boost_tree(
  trees = tune(),
  min_n = tune(),
  tree_depth = tune(),
  learn_rate = tune(),
  # loss_reduction = tune(),
  sample_size = 1
) %>%
  set_engine("lightgbm",
             nthread = 8) %>%
  set_mode("classification")

lightgbm_grid <- grid_latin_hypercube(
  trees(range = c(50L, 300L)),
  min_n(),
  tree_depth(),
  learn_rate(range = c(0.01, 0.2), trans = NULL),
  # 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")
```

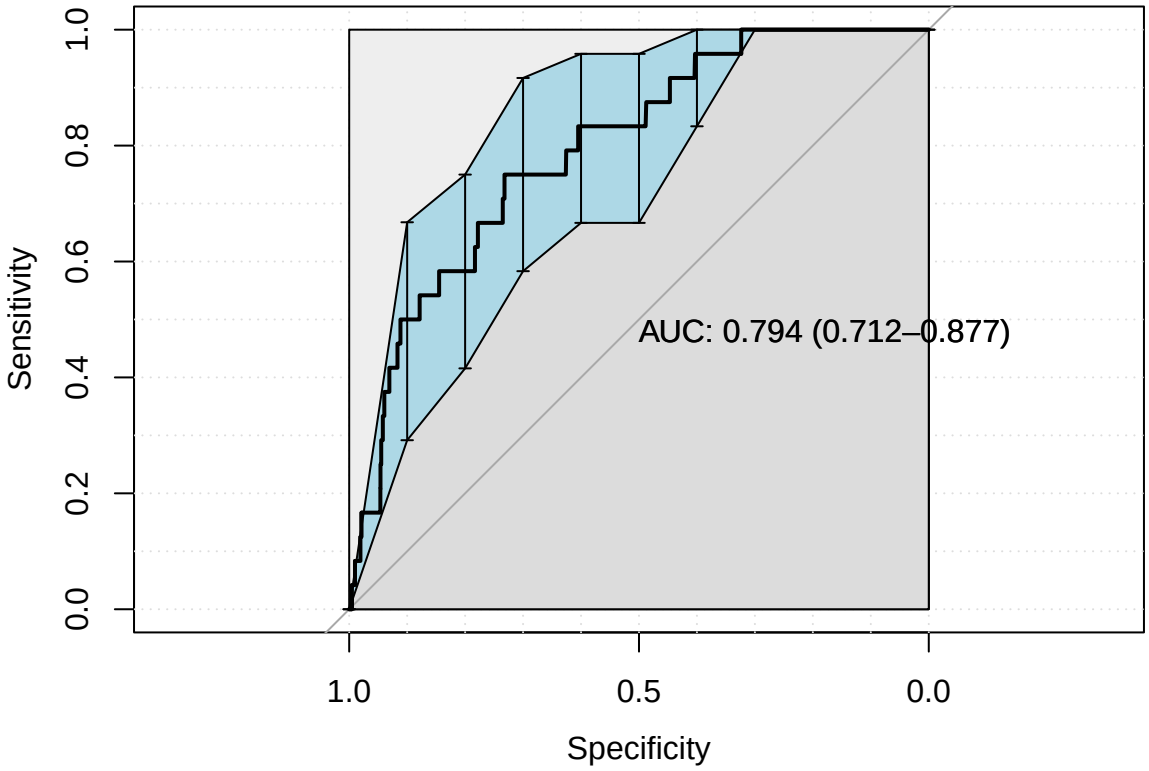
```
## # A tibble: 5 x 10
##   trees min_n tree_depth learn_rate .metric .estimator  mean     n std_err .config
##   <int> <int>      <int>      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1   216    21          2     0.0337 roc_auc binary     0.741     5  0.0503 Preprocessor1_Model08
## 2   109    30          4     0.0419 roc_auc binary     0.725     5  0.0514 Preprocessor1_Model12
## 3   178    36         10     0.178  roc_auc binary     0.723     5  0.0376 Preprocessor1_Model14
## 4   267    19          5     0.138  roc_auc binary     0.717     5  0.0346 Preprocessor1_Model07
## 5   123     6         11     0.0139 roc_auc binary     0.713     5  0.0508 Preprocessor1_Model02
```

```
best_lightgbm <- lightgbm_tune %>%
  select_best("roc_auc")

autoplot(lightgbm_tune, metric = "roc_auc")
```




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

last_lightgbm_fit <-
  final_lightgbm_workflow %>%
  last_fit(df_split)
```

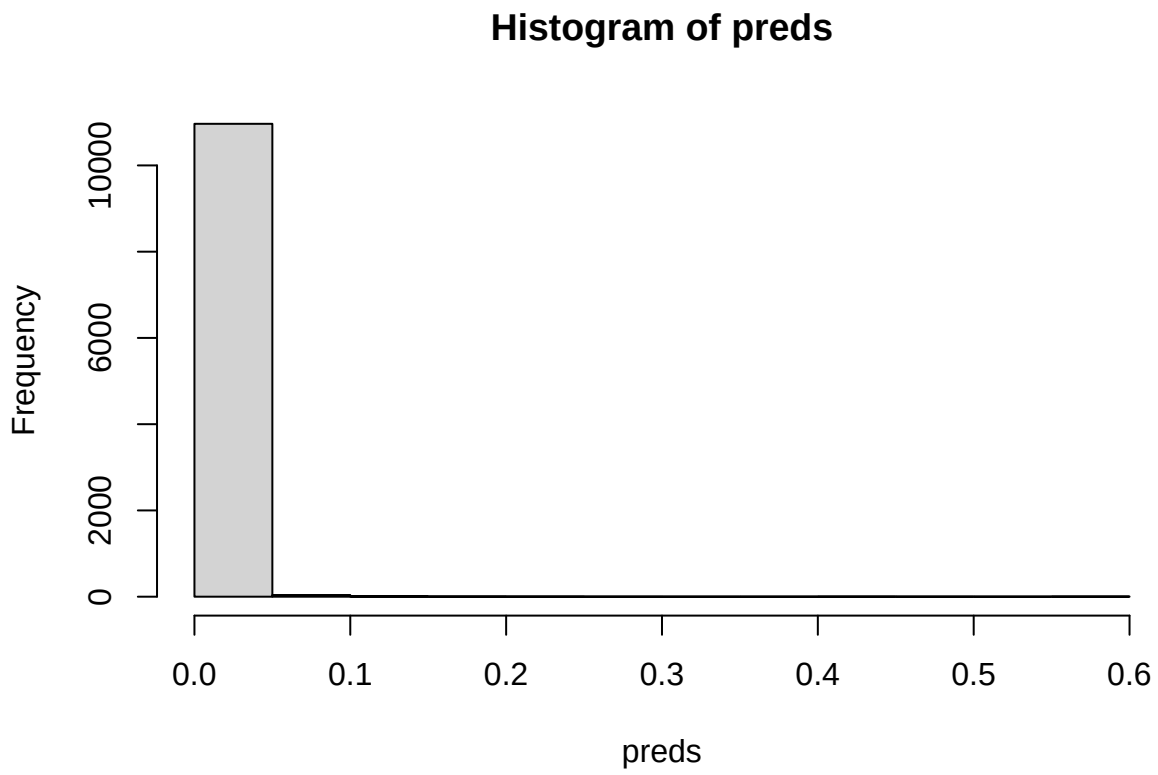
```
final_lightgbm_fit <- extract_workflow(last_lightgbm_fit)

lightgbm_auc <- validation(final_lightgbm_fit, df_test)
```




```
## [1] "Optimal Threshold: 0.00"
## Confusion Matrix and Statistics
##
##     reference
## data    0    1
##    0 3445    6
##    1 1261   18
##
##                Accuracy : 0.7321
##                  95% CI : (0.7193, 0.7447)
##     No Information Rate : 0.9949
##     P-Value [Acc > NIR] : 1
##
##                   Kappa : 0.0178
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.73204
##             Specificity : 0.75000
##          Pos Pred Value : 0.99826
##          Neg Pred Value : 0.01407
##              Prevalence : 0.99493
##          Detection Rate : 0.72833
##    Detection Prevalence : 0.72960
##       Balanced Accuracy : 0.74102
##
##        'Positive' Class : 0
##
```

```r
# pfun_lightgbm <- function(object, newdata) predict(object, data = newdata)
# extract_vip(final_lightgbm_fit, pred_wrapper = pfun_lightgbm,
#             reference_class = "1")

lightgbm_parameters <- lightgbm_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(trees, min_n, tree_depth, learn_rate) %>%
  as.list

saveRDS(
  lightgbm_parameters,
  file = sprintf(
    "./auxiliar/model_selection/hyperparameters/lightgbm_%s.rds",
    outcome_column
  )
)
```

Minutes to run: 2.057

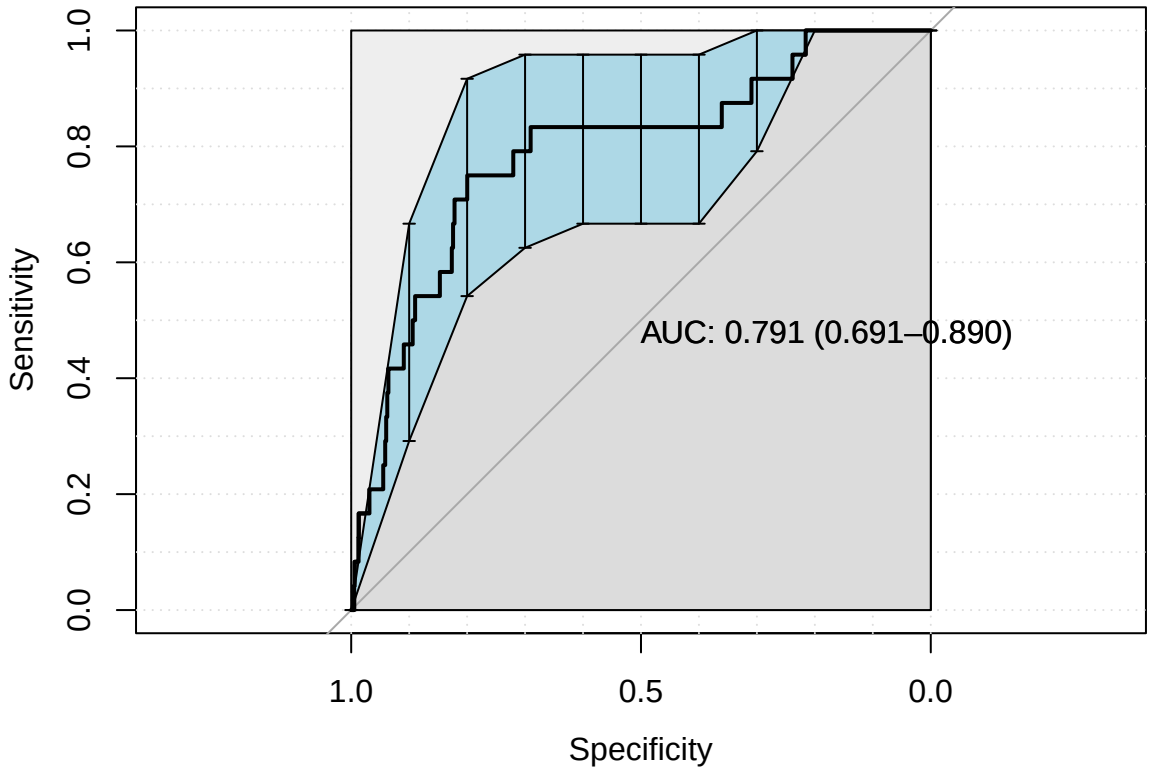


Minutes to run: 0.007

GLM

```r
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()) %>%
  step_zv(all_predictors()) %>%
  step_normalize(all_numeric_predictors())

glmnet_spec <-
```

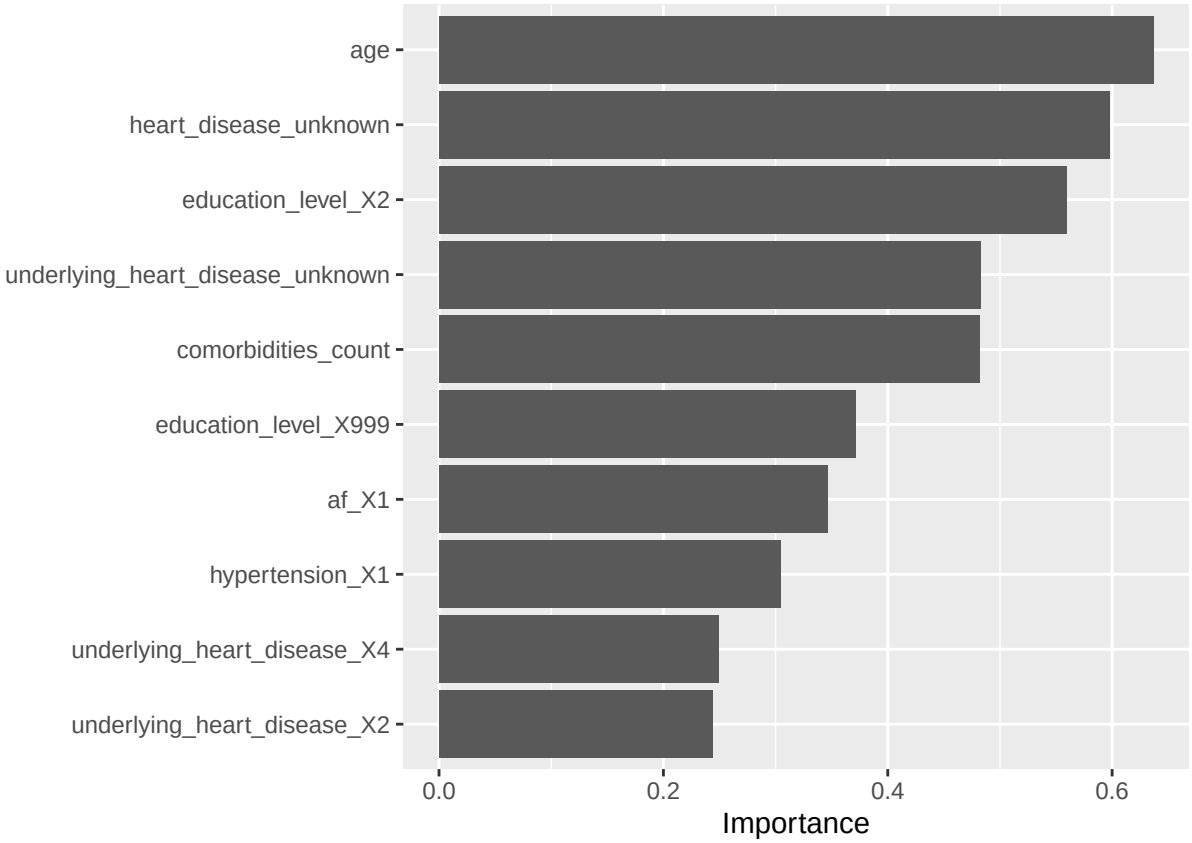
```
  logistic_reg(penalty = 0) %>%
  set_mode("classification") %>%
  set_engine("glmnet")

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

glm_fit <- glmnet_workflow %>%
  fit(df_train)

glmnet_auc <- validation(glm_fit, df_test)
```



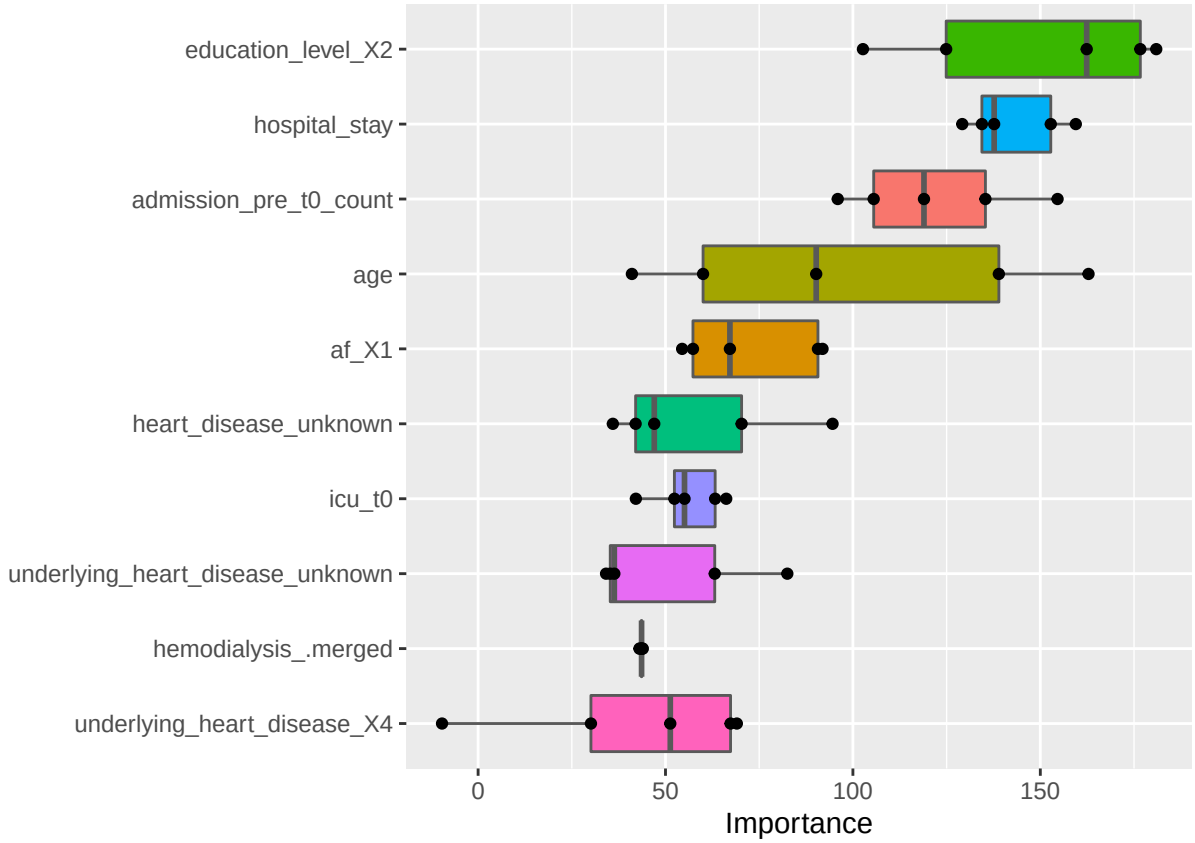

```
## [1] "Optimal Threshold: 0.01"
## Confusion Matrix and Statistics
##
##     reference
## data    0    1
##    0 3764    6
##    1  942   18
##
##                Accuracy : 0.7996
##                  95% CI : (0.7879, 0.8109)
##     No Information Rate : 0.9949
##     P-Value [Acc > NIR] : 1
##
##                   Kappa : 0.027
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.79983
##             Specificity : 0.75000
```

```
##          Pos Pred Value : 0.99841
##          Neg Pred Value : 0.01875
##              Prevalence : 0.99493
##          Detection Rate : 0.79577
##    Detection Prevalence : 0.79704
##       Balanced Accuracy : 0.77492
##
##        'Positive' Class : 0
##
```

```
pfun_glmnet <- function(object, newdata) predict(object, newx = newdata)

extract_vip(glm_fit, pred_wrapper = pfun_glmnet,
            reference_class = "1", method = 'model')
```




```
extract_vip(glm_fit, pred_wrapper = pfun_glmnet,
            reference_class = "1", method = 'permute')
```

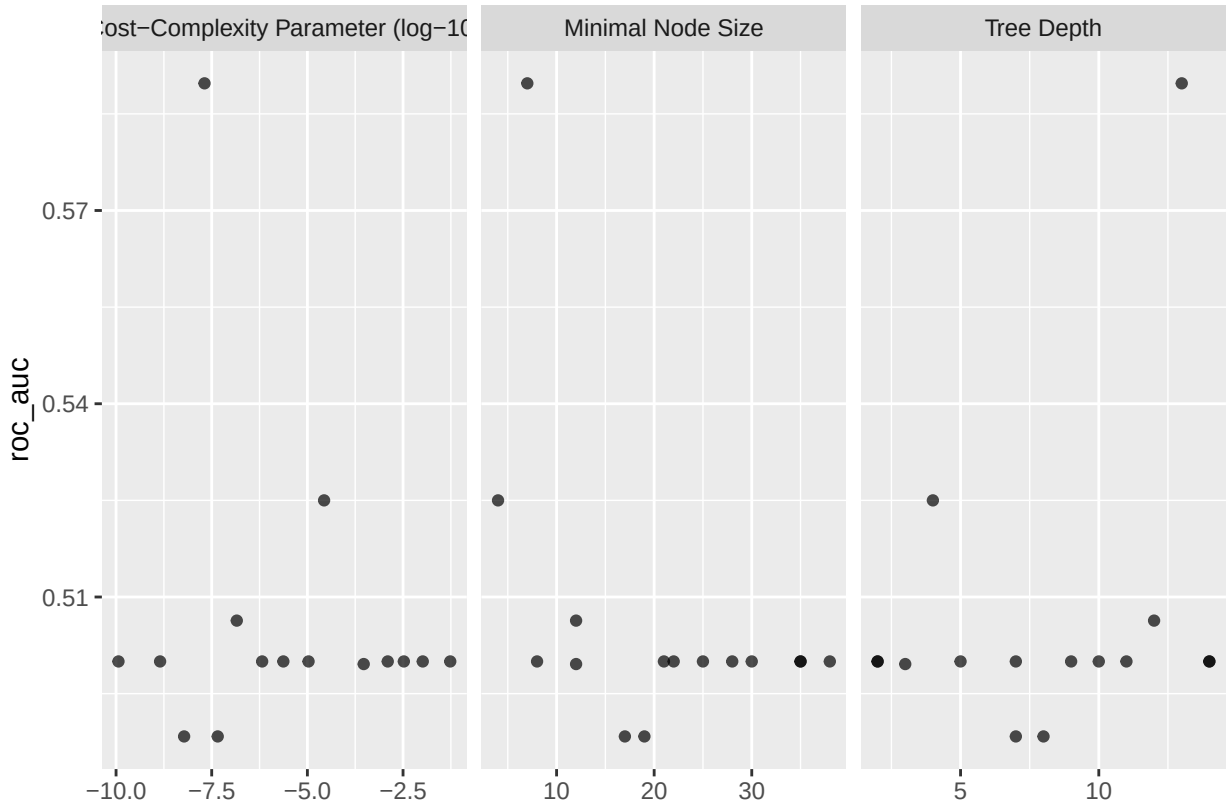


Minutes to run: 1.525

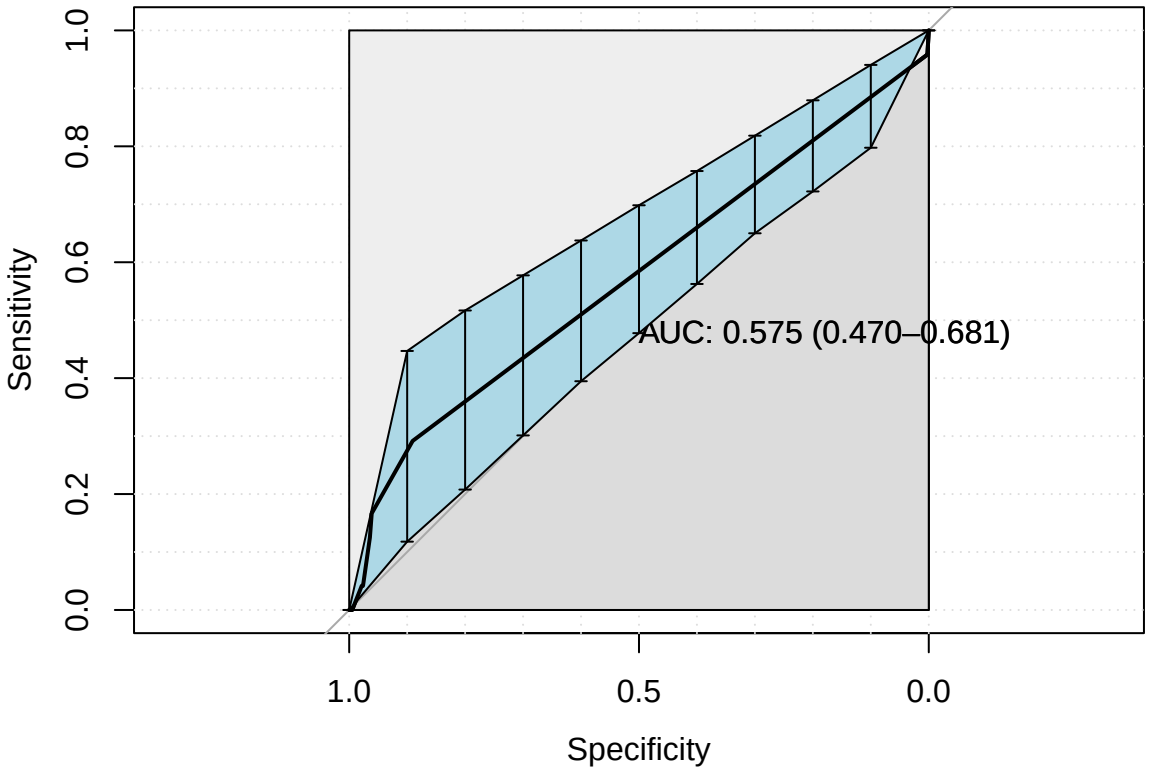
Decision Tree

```
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()) %>%
  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(),
                                  tree_depth(),
                                  min_n(),
                                  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)
```

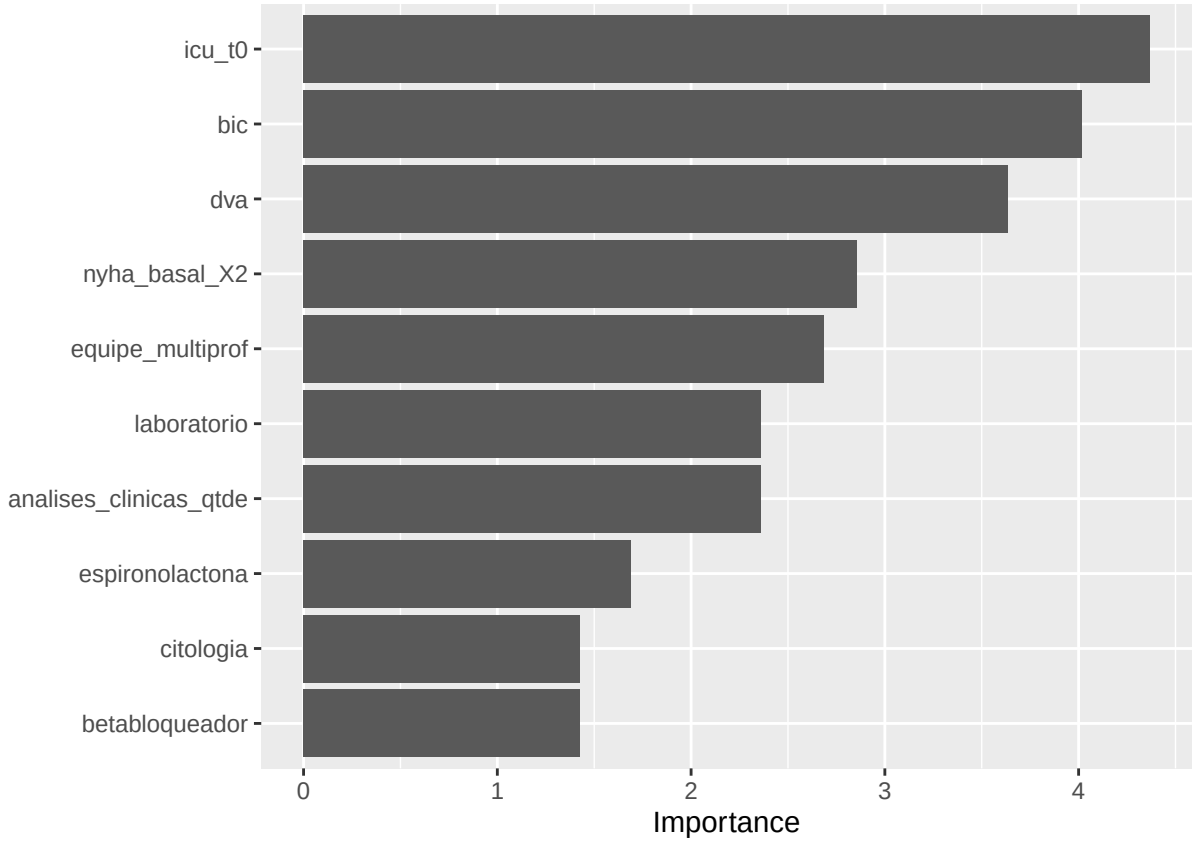
```
tree_tune %>%
  collect_metrics()

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)
```




```
extract_vip(final_tree_fit, pred_wrapper = predict,
            reference_class = "0", use_matrix = FALSE,
            method = 'model')
```



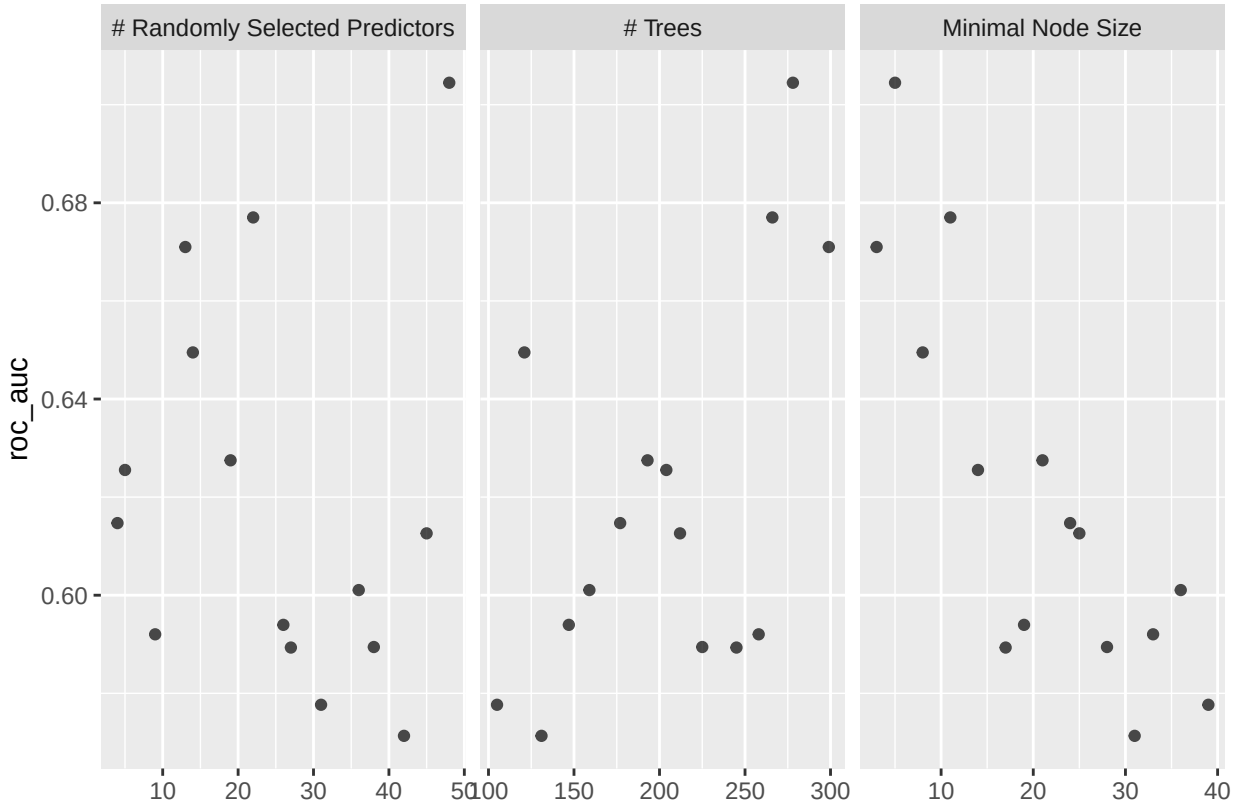

```
# extract_vip(final_tree_fit, pred_wrapper = predict,
#             reference_class = "1", use_matrix = FALSE,
```

```
#             method = 'permute')
```

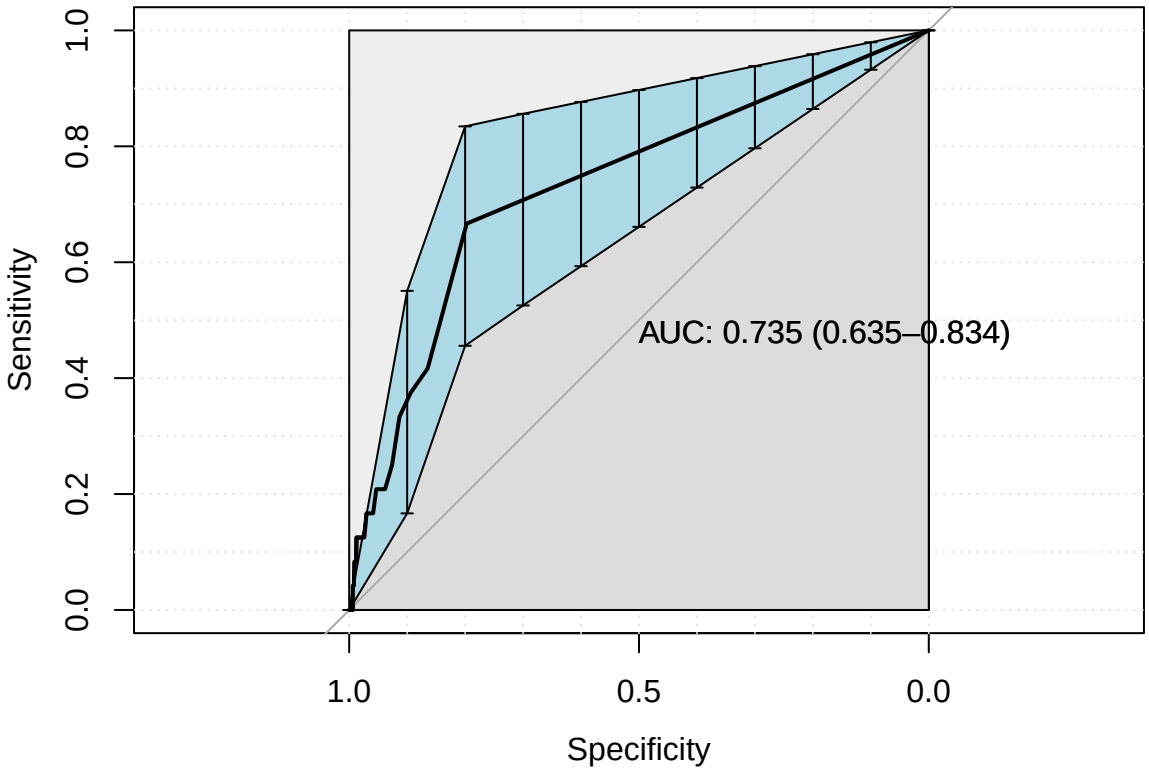
Minutes to run: 0.876

Random Forest

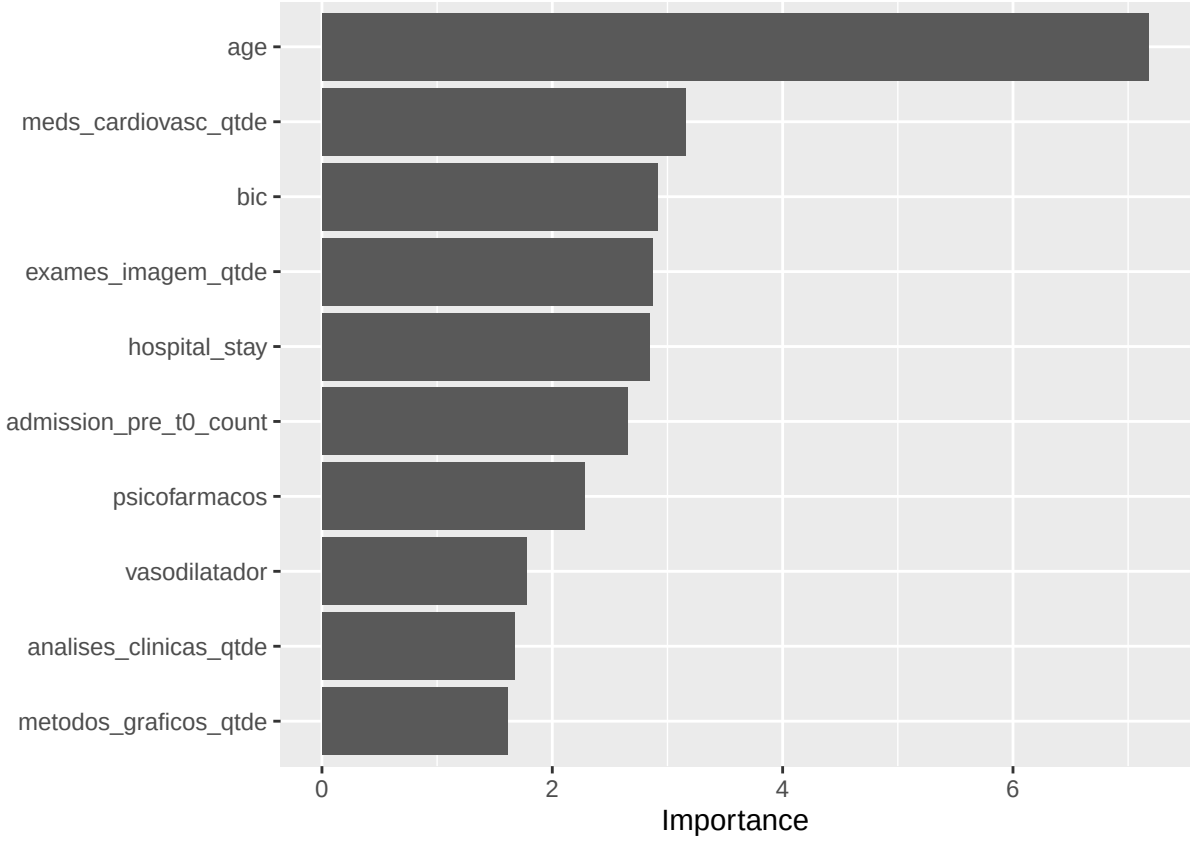
```
rf_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other = ".merged") %>%
  step_dummy(all_nominal_predictors()) %>%
  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()

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)
```




```
pfun_rf <- function(object, newdata) predict(object, data = newdata)

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

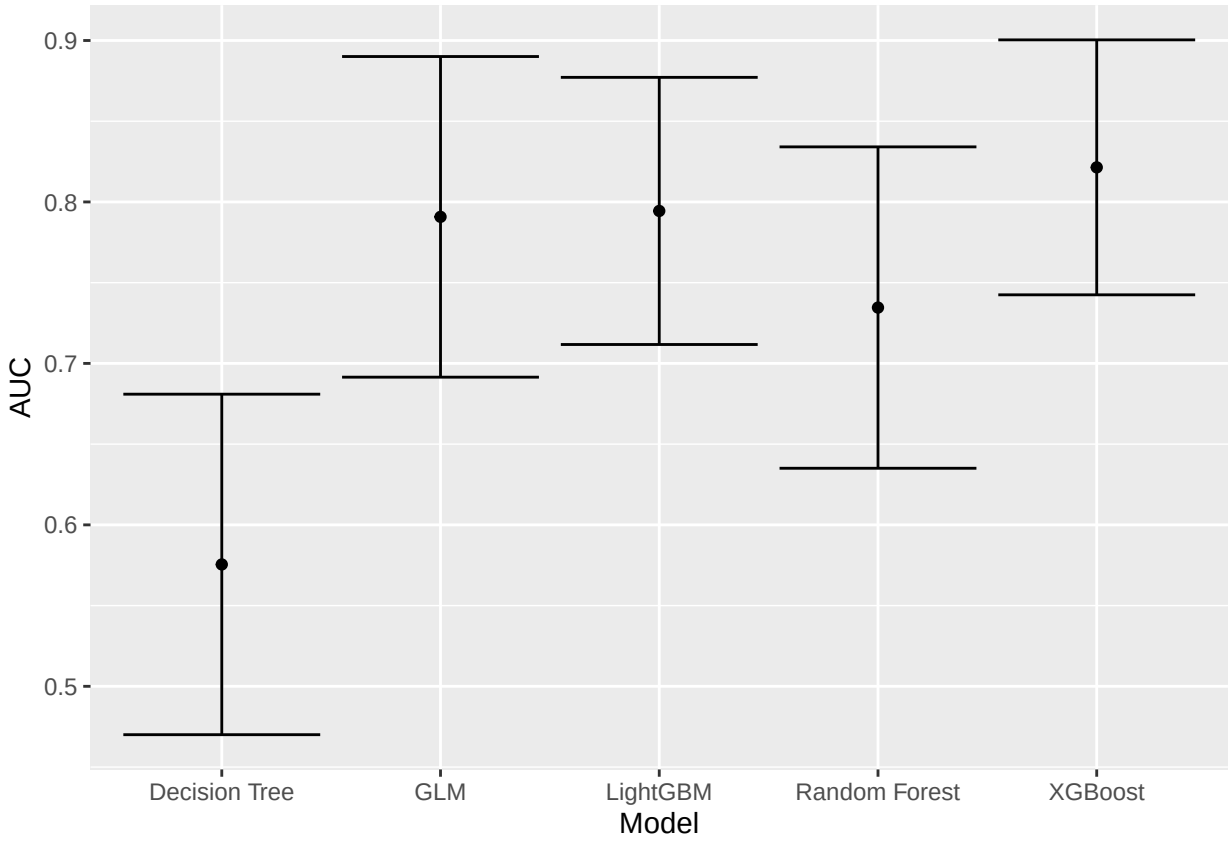


```
# extract_vip(final_rf_fit, pred_wrapper = predict,
#             reference_class = "1", use_matrix = FALSE,
#             method = 'permute')
```

Minutes to run: 13.084

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(glmnet_auc$auc), glmnet_auc$ci[1], glmnet_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("./auxiliar/model_selection/performance/%s.RData", outcome_column))
```

Minutes to run: 0.01