

Model Selection - death_3year

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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_3year
## . k = double 1= 10
## . grid_size = double 1= 30
## . repeats = double 1= 2
## . RUN_ALL_MODELS = logical 1= TRUE
```

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: 0.007

```
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))

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. underlying_heart_disease
```

06. heart_disease
07. nyha_basal
08. hypertension
09. prior_mi
10. heart_failure
11. af
12. cardiac_arrest
13. valvopathy
14. diabetes
15. renal_failure
16. hemodialysis
17. stroke
18. copd
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. espirolactona
41. antiplaquetario_ev
42. insulina
43. anticonvulsivante
44. psicofarmacos
45. antifungico
46. classe_meds_qtde
47. meds_cardiovasc_qtde
48. meds_antimicrobianos
49. ventilacao_mecanica
50. transplante_cardiaco
51. outros_proced_cirurgicos
52. icp
53. angioplastia
54. cateterismo
55. eletrofisiologia
56. cateter_venoso_central
57. proced_invasivos_qtde
58. transfusao
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. angiografia
## 71. cintilografia
## 72. ecocardiograma
## 73. endoscopia
## 74. flebografia
## 75. pet_ct
## 76. ultrassom
## 77. tomografia
## 78. ressonancia
## 79. exames_imagem_qtde
## 80. bic
## 81. 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 <- rsample::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, 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 <-
  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_size .metric .estimator mean    n std_err .config
##   <int> <int>    <int>      <dbl>      <dbl>      <dbl> <chr>   <chr>    <dbl> <int>  <dbl> <chr>
## 1    89    20      12      0.0900    0.0000556      0.488 roc_auc binary  0.807   10 0.0107 Preproc
## 2   189    14       4      0.0518    0.00000481     0.446 roc_auc binary  0.806   10 0.00962 Preproc
## 3   191    19       3      0.103     0.0000000481    0.934 roc_auc binary  0.804   10 0.00917 Preproc
## 4    50    17       5      0.152     0.00000235     0.738 roc_auc binary  0.803   10 0.0105 Preproc
## 5   196    36      12      0.139     0.0844         0.388 roc_auc binary  0.801   10 0.0107 Preproc

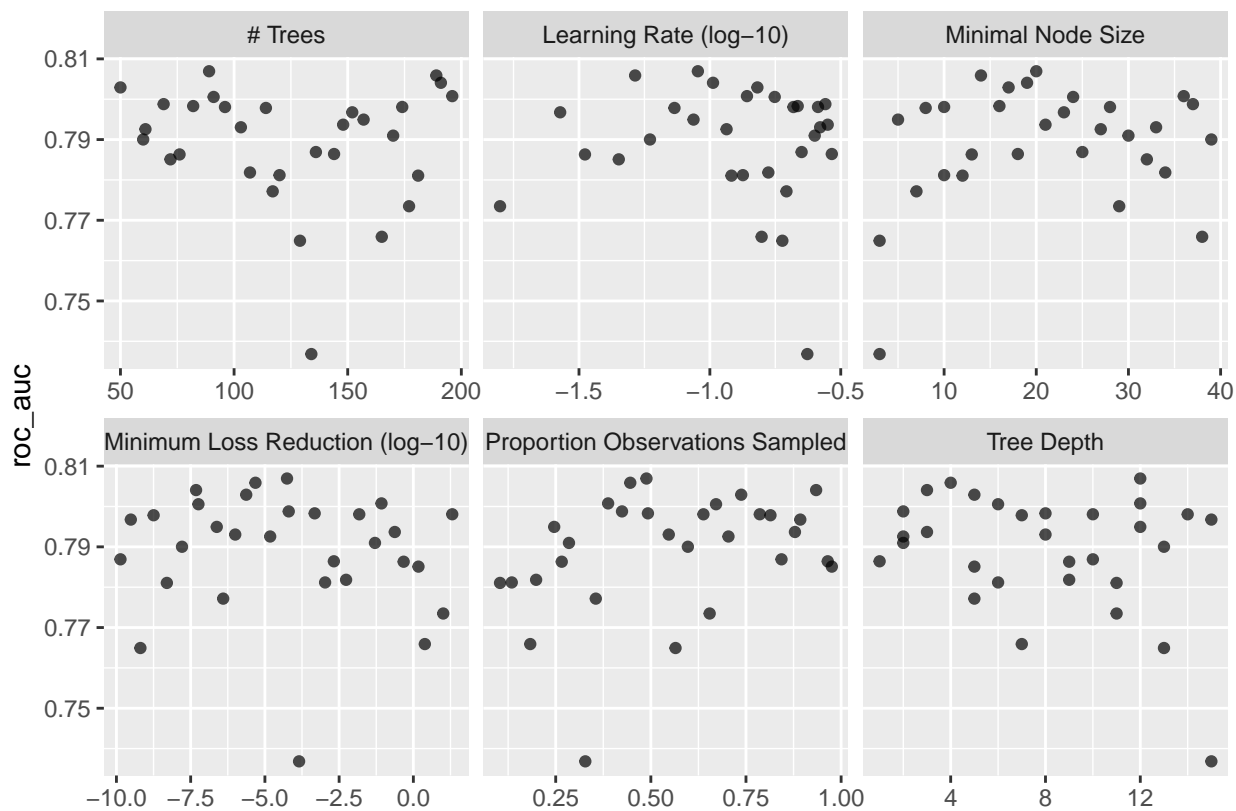
```

```

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

autoplot(xgboost_tune, metric = "roc_auc")

```

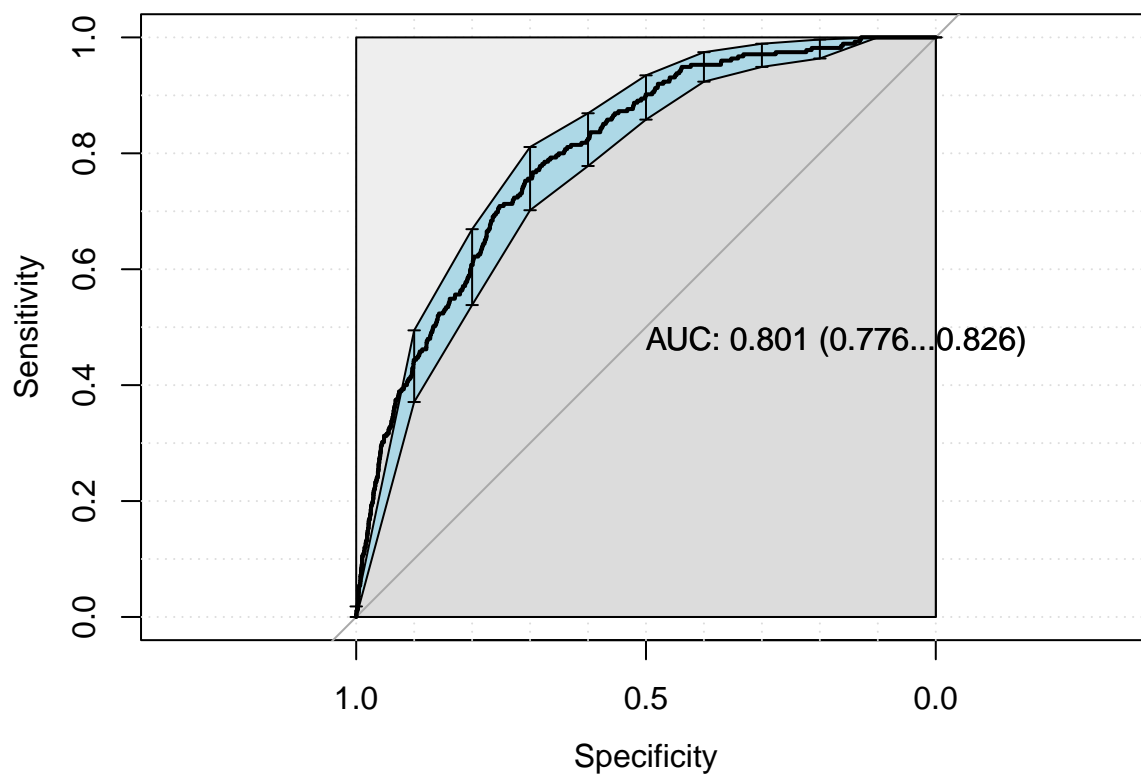


```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

last_xgboost_fit <-
  final_xgboost_workflow %>%
  last_fit(df_split)

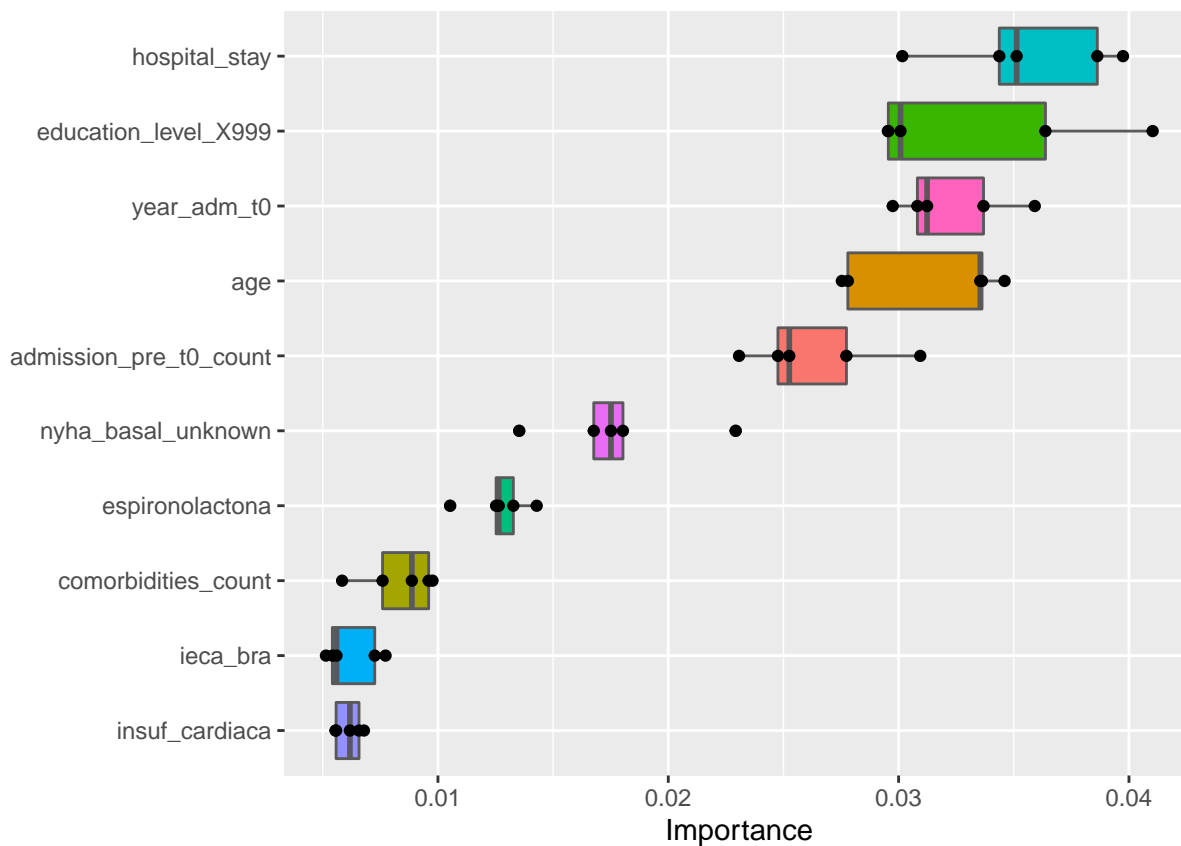
final_xgboost_fit <- extract_workflow(last_xgboost_fit)

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



|

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



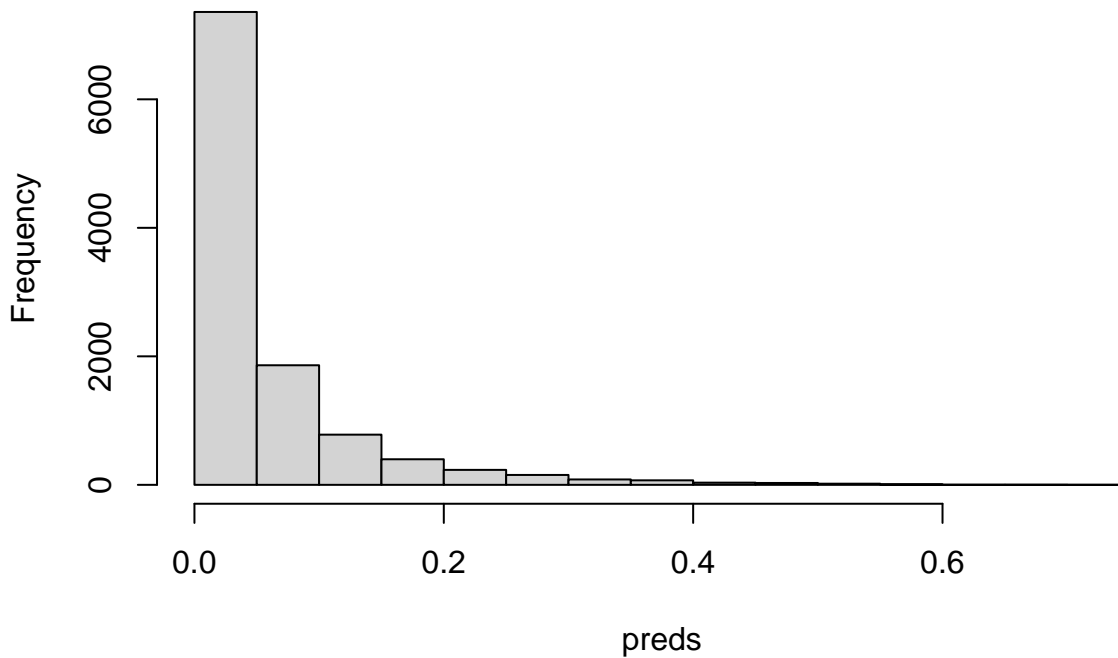
```
xgboost_parameters <- xgboost_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(trees, min_n, tree_depth, learn_rate, loss_reduction) %>%
  as.list

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

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:

12.624

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(),  
  sample_size = 1  
) %>%  
  set_engine("lightgbm",  
    nthread = 8) %>%  
  set_mode("classification")  
  
lightgbm_grid <- grid_latin_hypercube(  
  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 <-
```

```

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   108    37      11    0.0353 roc_auc binary  0.797    10  0.0100 Preprocessor1_Model11
## 2    49    83      15    0.0697 roc_auc binary  0.797    10  0.0110 Preprocessor1_Model25
## 3   139    76       7    0.0204 roc_auc binary  0.796    10  0.0100 Preprocessor1_Model23
## 4    93    50      13    0.0241 roc_auc binary  0.795    10  0.0102 Preprocessor1_Model15
## 5    63    56      14    0.0410 roc_auc binary  0.795    10  0.0101 Preprocessor1_Model17

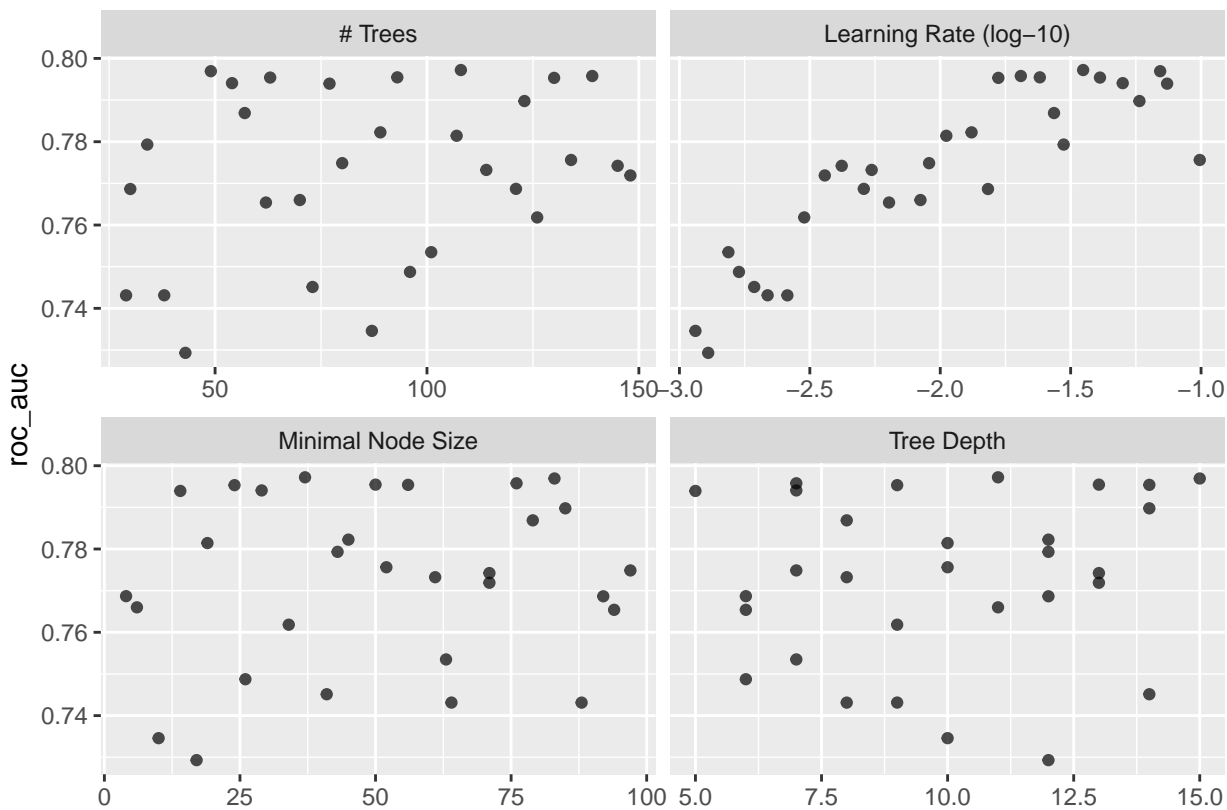
```

```

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

autoplot(lightgbm_tune, metric = "roc_auc")

```



```

final_lightgbm_workflow <-
  lightgbm_workflow %>%
  finalize_workflow(best_lightgbm)

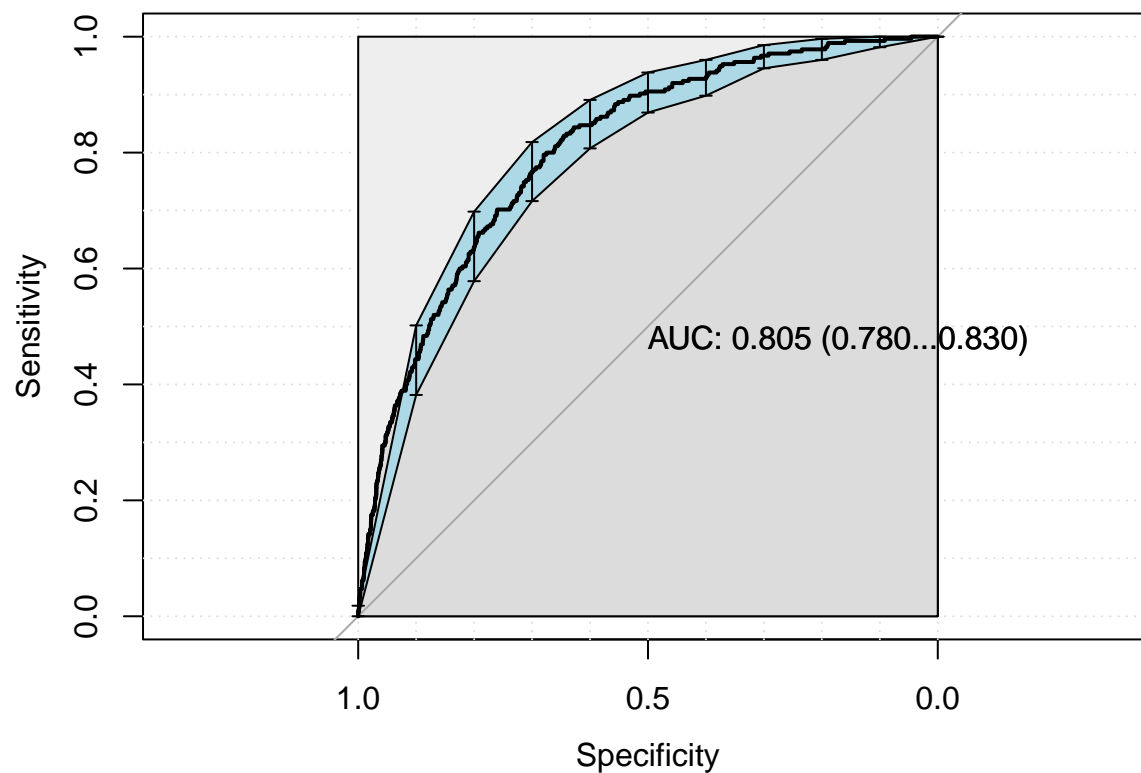
last_lightgbm_fit <-
  final_lightgbm_workflow %>%

```

```
last_fit(df_split)

final_lightgbm_fit <- extract_workflow(last_lightgbm_fit)

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



|

```
##
##           'Positive' Class : 0
##

lightgbm_parameters <- lightgbm_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(-.metric, -.estimator, -.config, -mean, -n, -std_err) %>%
  as.list

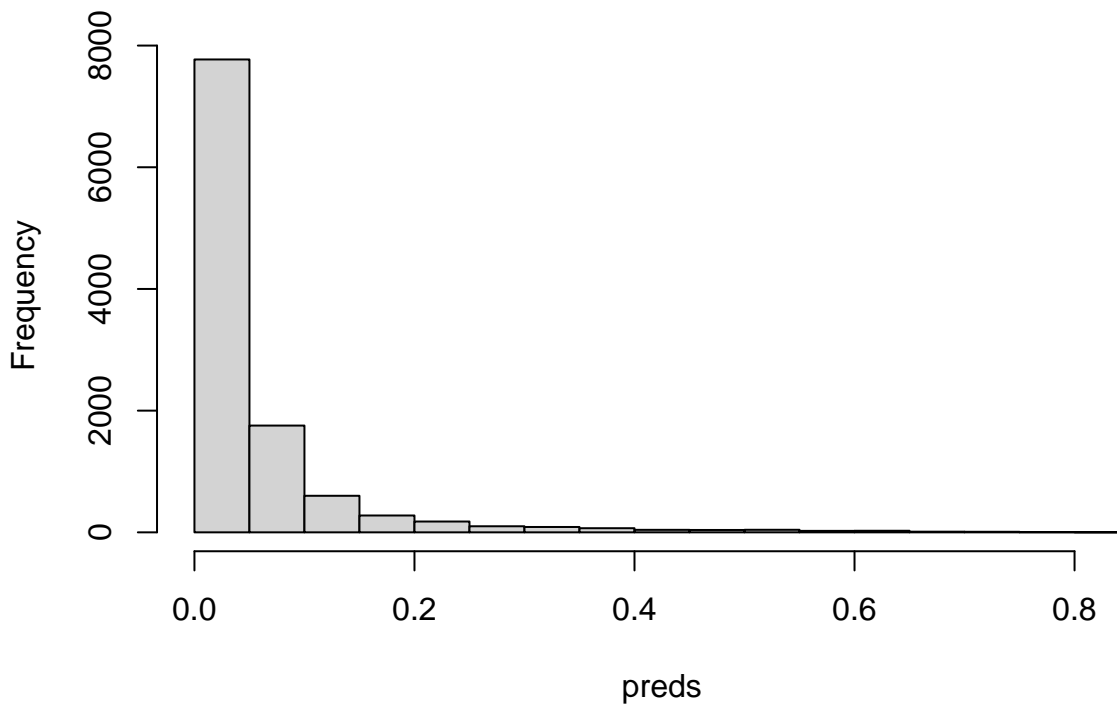
Hmisc::list.tree(lightgbm_parameters)
```

```
## lightgbm_parameters = list 4 (736 bytes)
## . trees = integer 1= 108
## . min_n = integer 1= 37
## . tree_depth = integer 1= 11
## . learn_rate = double 1= 0.035312
```

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

Minutes to run: 3.682

Histogram of preds



0.005

Minutes to run:

GLM

```

glmnet_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()) %>%
  step_zv(all_predictors()) %>%
  step_normalize(all_numeric_predictors())

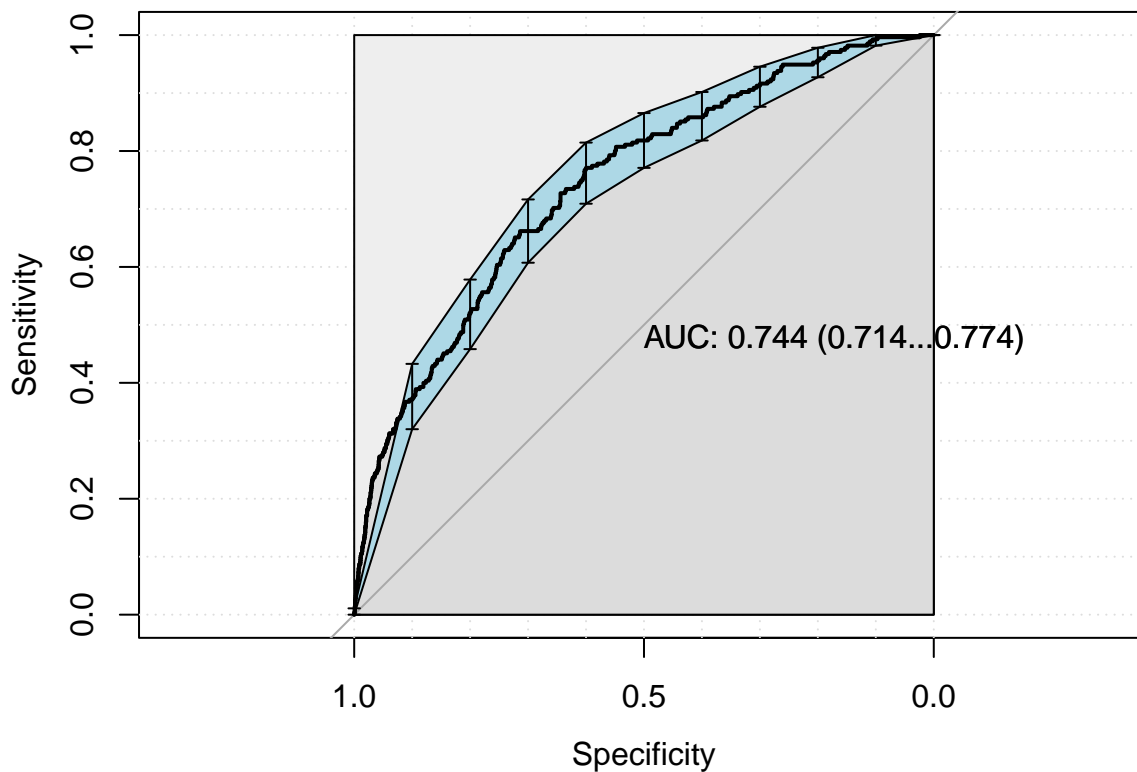
glmnet_spec <-
  logistic_reg(penalty = 0) %>%
  set_mode("classification") %>%
  set_engine("glmnet")

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)

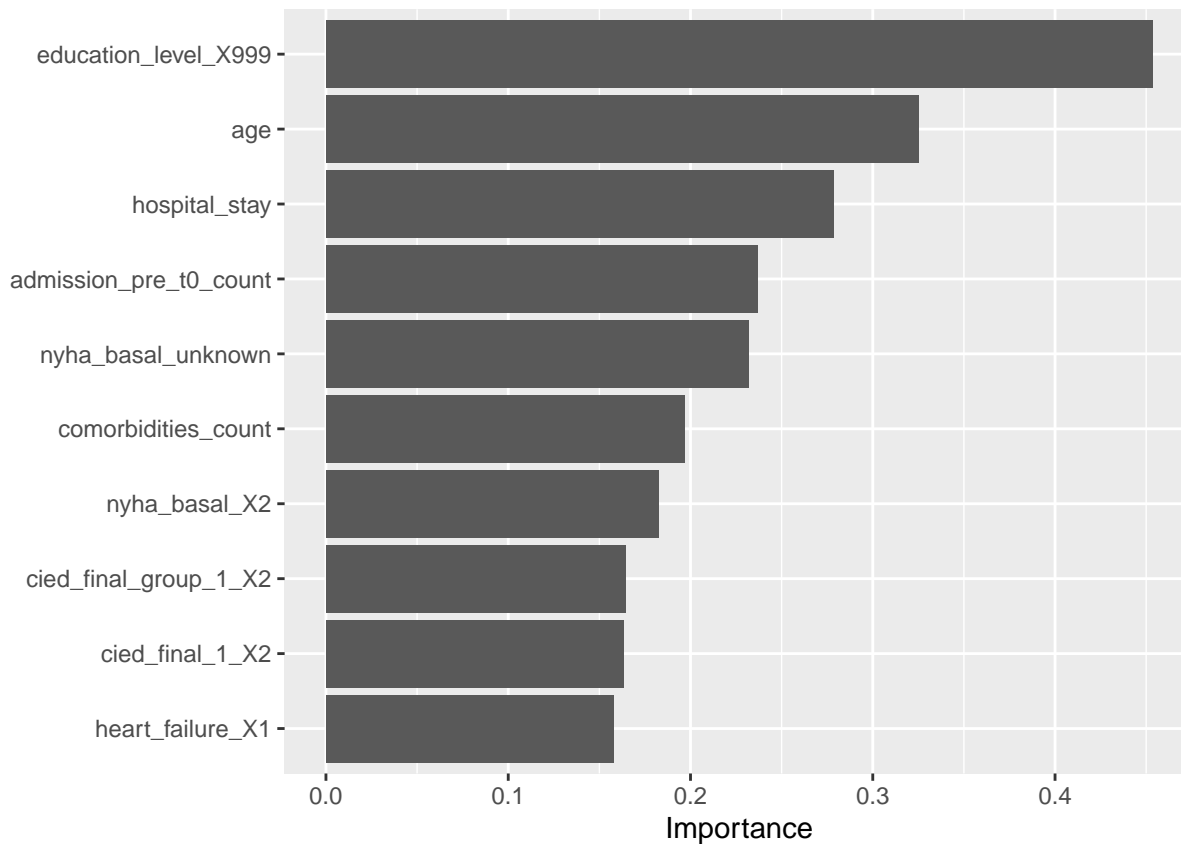
```



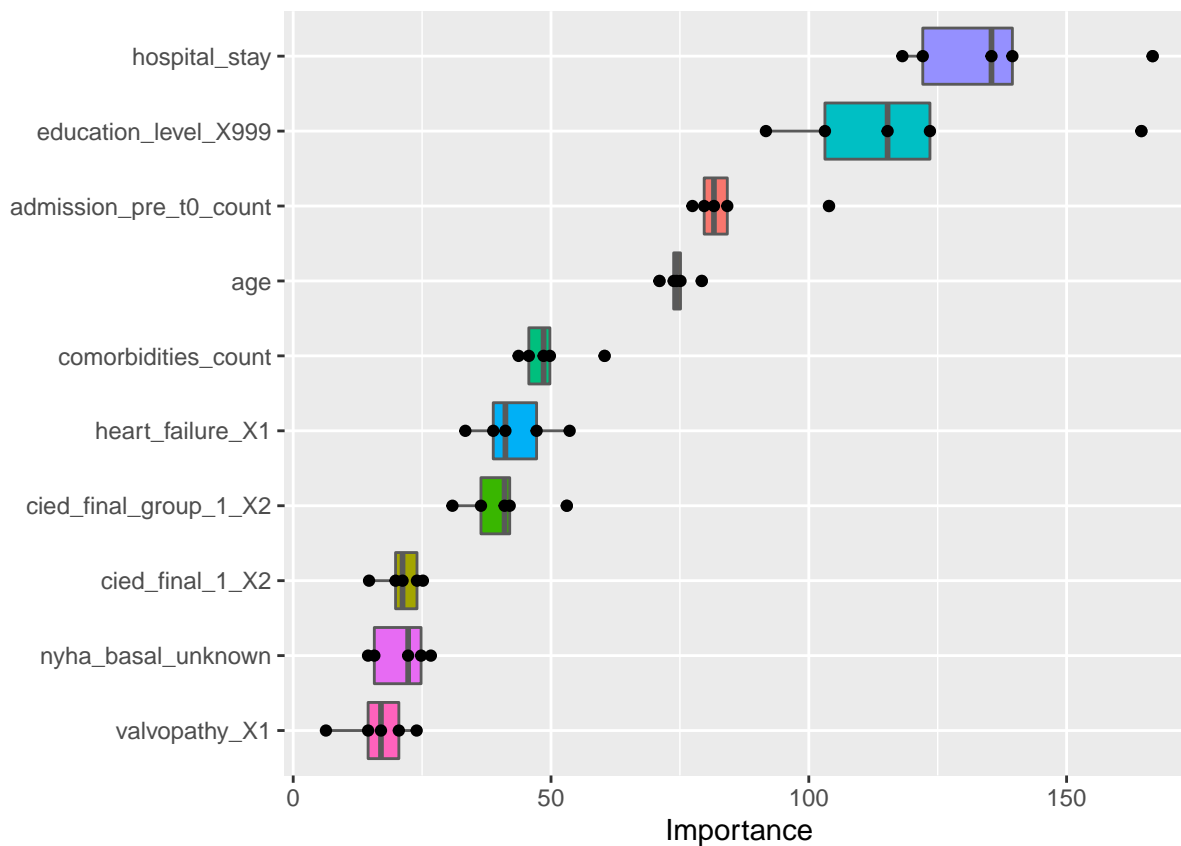
```
##
##           Accuracy : 0.7108
##           95% CI : (0.6976, 0.7237)
## No Information Rate : 0.9419
## P-Value [Acc > NIR] : 1
##
##           Kappa : 0.1245
##
## Mcnemar's Test P-Value : <2e-16
##
##           Sensitivity : 0.7138
##           Specificity : 0.6618
##           Pos Pred Value : 0.9716
##           Neg Pred Value : 0.1249
##           Prevalence : 0.9419
##           Detection Rate : 0.6723
##           Detection Prevalence : 0.6920
##           Balanced Accuracy : 0.6878
##
##           '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:

2.725

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)

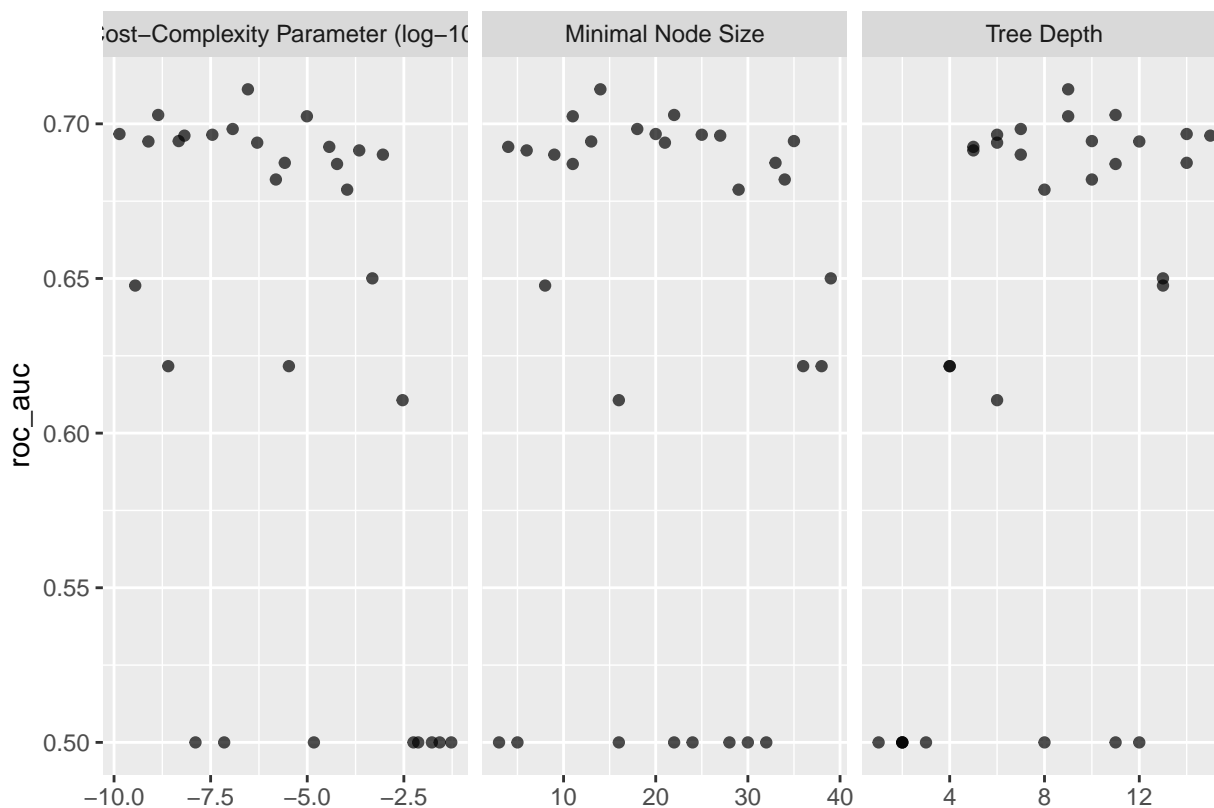
tree_tune <-
  tree_workflow %>%
```

```
tune_grid(resamples = df_folds,
          grid = tree_grid)
```

```
tree_tune %>%
  collect_metrics()
```

```
## # A tibble: 60 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      2.21e- 4         5      6 accuracy binary    0.939    10 0.00229 Preprocessor1_Model101
## 2      2.21e- 4         5      6 roc_auc  binary    0.691    10 0.0148  Preprocessor1_Model101
## 3      2.67e- 2         8     32 accuracy binary    0.942    10 0.00259 Preprocessor1_Model102
## 4      2.67e- 2         8     32 roc_auc  binary    0.5      10 0      Preprocessor1_Model102
## 5      2.63e- 6        14     33 accuracy binary    0.936    10 0.00303 Preprocessor1_Model103
## 6      2.63e- 6        14     33 roc_auc  binary    0.687    10 0.0181  Preprocessor1_Model103
## 7      7.44e- 3         3     30 accuracy binary    0.942    10 0.00259 Preprocessor1_Model104
## 8      7.44e- 3         3     30 roc_auc  binary    0.5      10 0      Preprocessor1_Model104
## 9      7.76e-10        12     13 accuracy binary    0.926    10 0.00256 Preprocessor1_Model105
## 10     7.76e-10        12     13 roc_auc  binary    0.694    10 0.0128  Preprocessor1_Model105
## # ... 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      2.91e- 7         9     14 roc_auc binary    0.711    10 0.0135  Preprocessor1_Model125
## 2      1.39e- 9        11     22 roc_auc binary    0.703    10 0.0145  Preprocessor1_Model118
```


## 3	9.79e- 6	9	11	roc_auc	binary	0.702	10	0.0136	Preprocessor1_Model17
## 4	1.18e- 7	7	18	roc_auc	binary	0.698	10	0.0156	Preprocessor1_Model16
## 5	1.38e-10	14	20	roc_auc	binary	0.697	10	0.0109	Preprocessor1_Model29

```

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

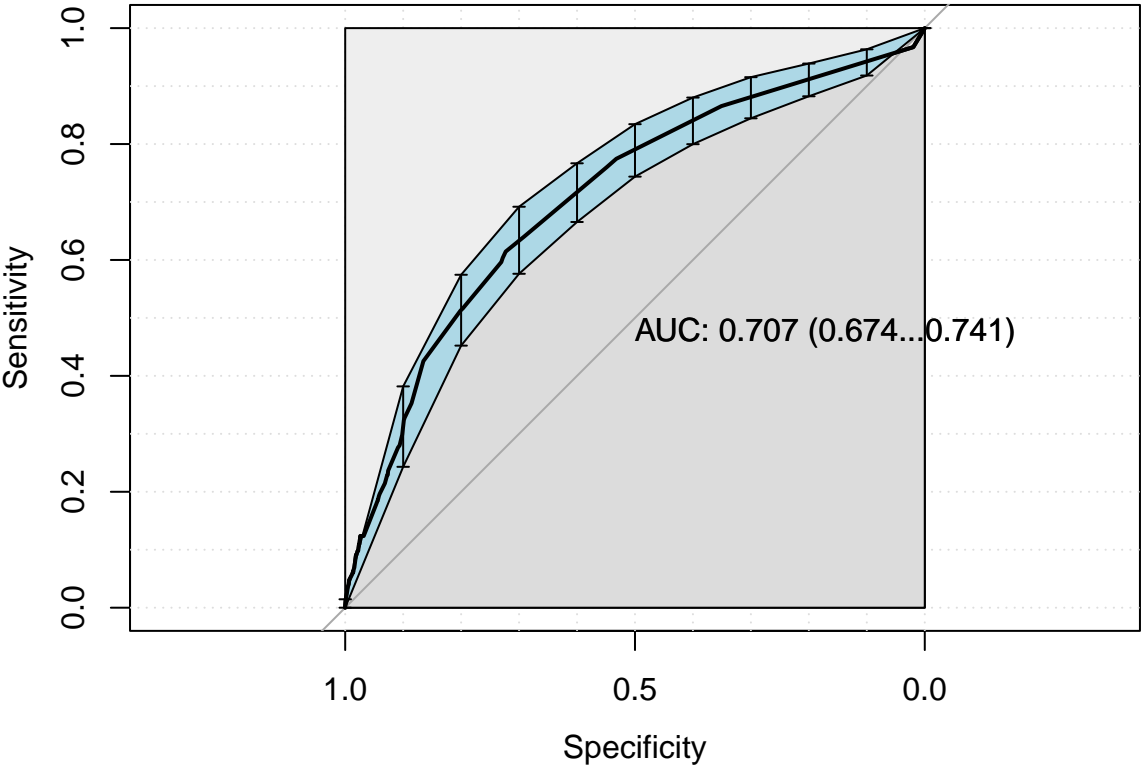
final_tree_workflow <-
  tree_workflow %>%
  finalize_workflow(best_tree)

last_tree_fit <-
  final_tree_workflow %>%
  last_fit(df_split)

final_tree_fit <- extract_workflow(last_tree_fit)

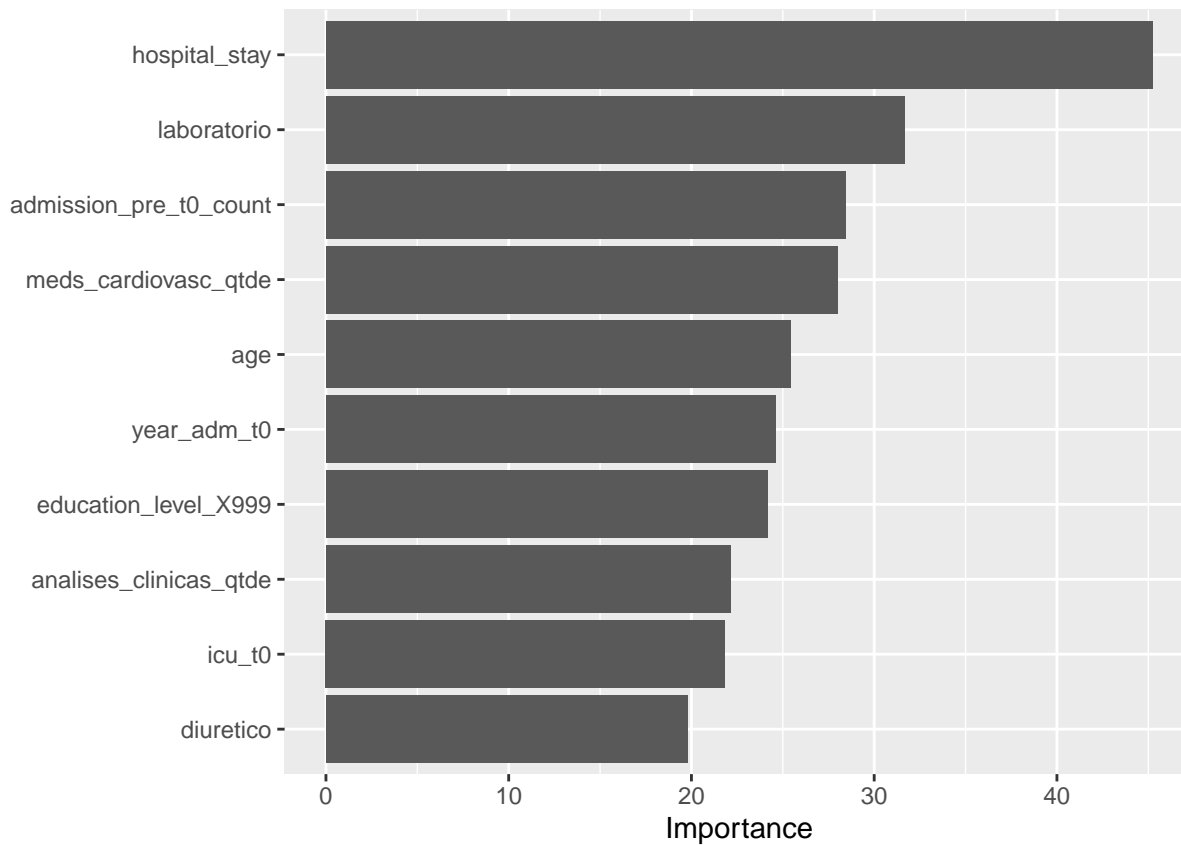
tree_auc <- validation(final_tree_fit, df_test)

```



```
##          Kappa : 0.1154
##
##  McNemar's Test P-Value : <2e-16
##
##          Sensitivity : 0.7230
##          Specificity : 0.6145
##          Pos Pred Value : 0.9681
##          Neg Pred Value : 0.1205
##          Prevalence : 0.9419
##          Detection Rate : 0.6810
##          Detection Prevalence : 0.7034
##          Balanced Accuracy : 0.6688
##
##          'Positive' Class : 0
##
```

```
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: 10.365

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()

```

```

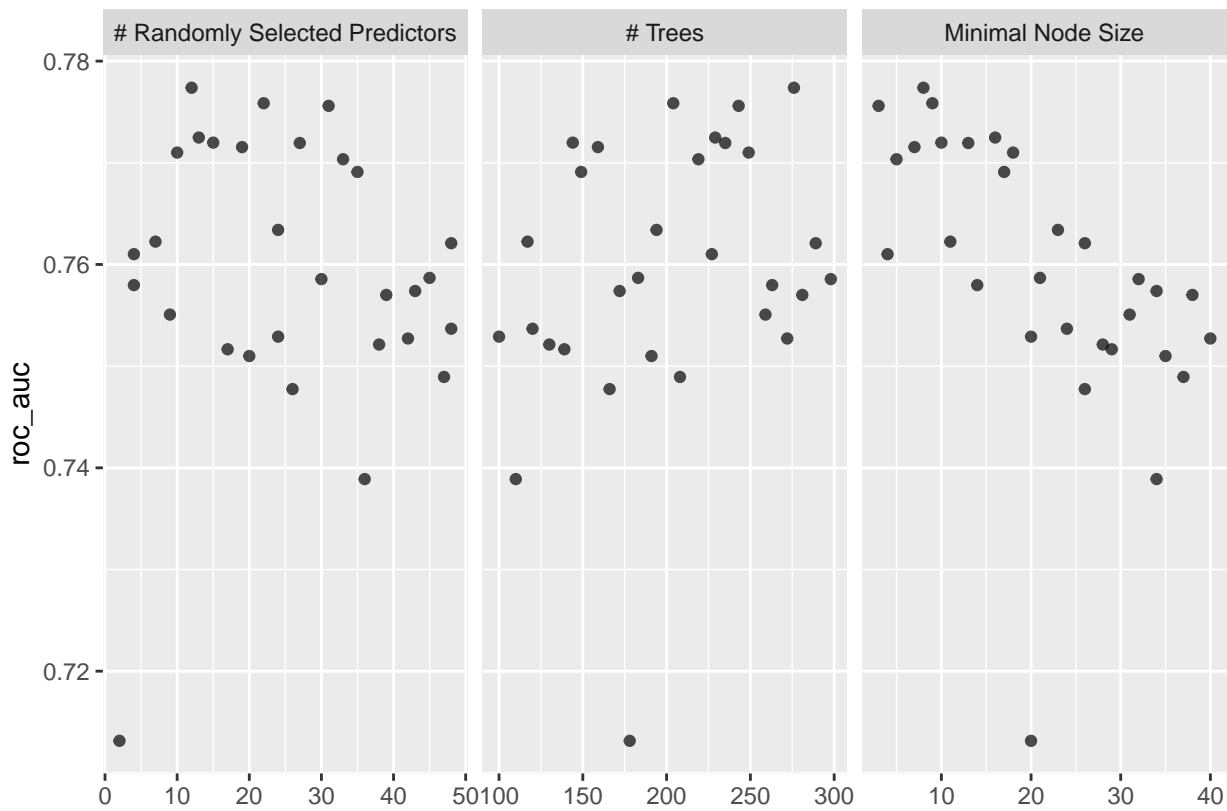
## # A tibble: 60 x 9
##   mtry trees min_n .metric .estimator mean      n std_err .config
##   <int> <int> <int> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1     24   194    23 accuracy binary    0.942    10 0.00249 Preprocessor1_Model01
## 2     24   194    23 roc_auc  binary    0.763    10 0.0118  Preprocessor1_Model01
## 3     19   159     7 accuracy binary    0.942    10 0.00254 Preprocessor1_Model02
## 4     19   159     7 roc_auc  binary    0.772    10 0.0109  Preprocessor1_Model02
## 5     24   100    20 accuracy binary    0.942    10 0.00268 Preprocessor1_Model03
## 6     24   100    20 roc_auc  binary    0.753    10 0.0135  Preprocessor1_Model03
## 7     39   281    38 accuracy binary    0.942    10 0.00269 Preprocessor1_Model04
## 8     39   281    38 roc_auc  binary    0.757    10 0.00947 Preprocessor1_Model04
## 9     15   144    10 accuracy binary    0.942    10 0.00270 Preprocessor1_Model05
## 10    15   144    10 roc_auc  binary    0.772    10 0.0108  Preprocessor1_Model05
## # ... with 50 more rows

```

```

autoplot(rf_tune, metric = "roc_auc")

```



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

```
## # A tibble: 5 x 9
##   mtry trees min_n .metric .estimator mean      n std_err .config
##   <int> <int> <int> <chr>   <chr>   <dbl> <int>   <dbl> <chr>
## 1    12   276     8 roc_auc binary  0.777    10 0.0108 Preprocessor1_Model16
## 2    22   204     9 roc_auc binary  0.776    10 0.00969 Preprocessor1_Model23
## 3    31   243     3 roc_auc binary  0.776    10 0.0114 Preprocessor1_Model20
## 4    13   229    16 roc_auc binary  0.772    10 0.0122 Preprocessor1_Model25
## 5     5    15    10 roc_auc binary  0.772    10 0.0108 Preprocessor1_Model05
```

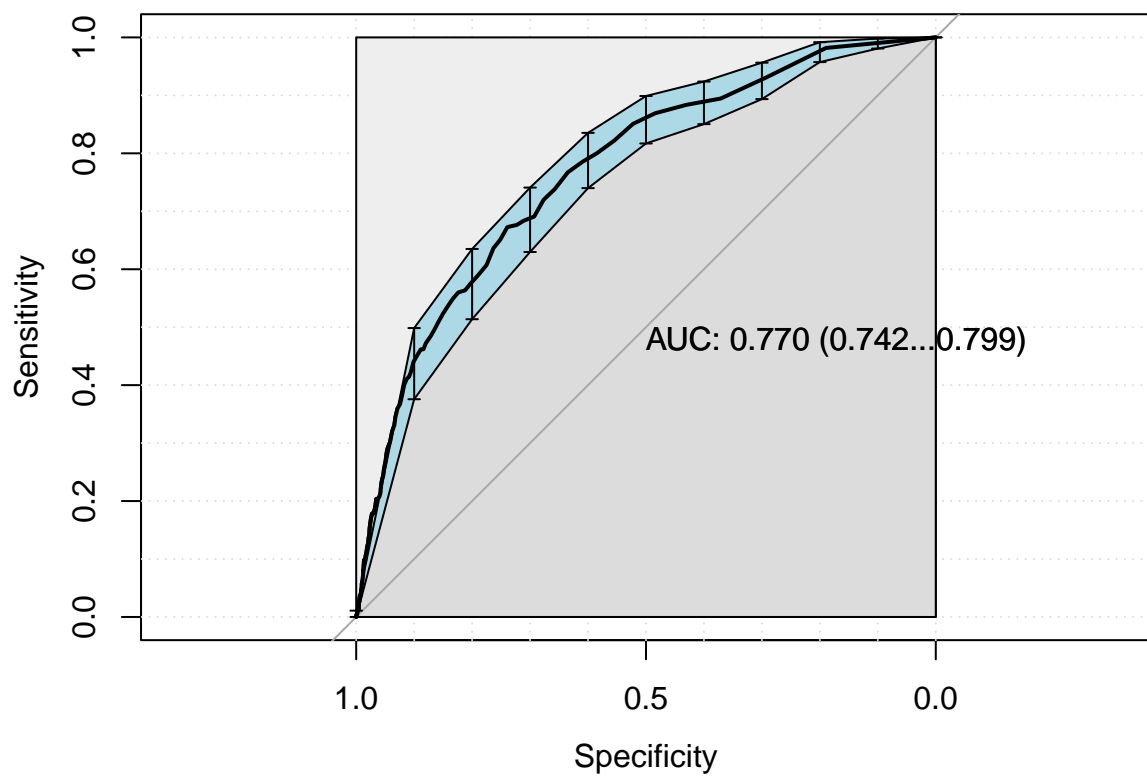
```
best_rf <- rf_tune %>%
  select_best("roc_auc")

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)

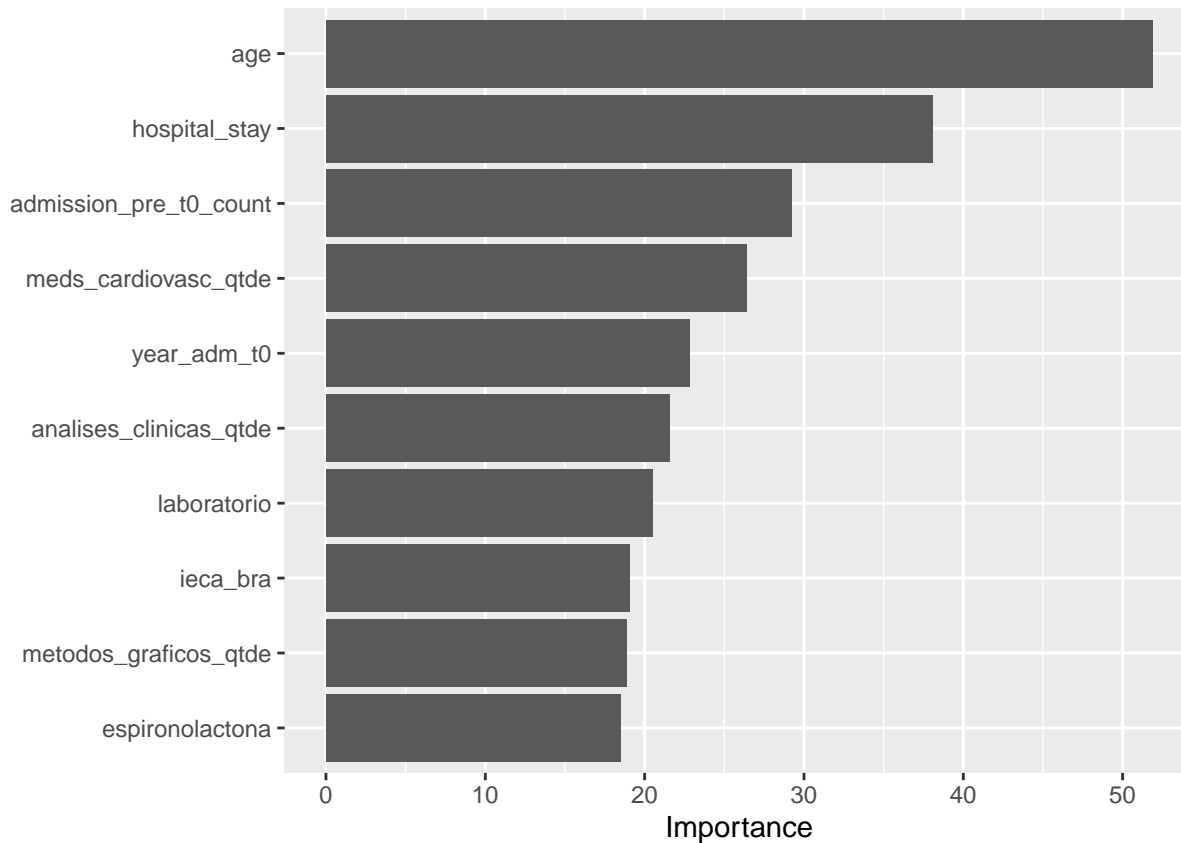
rf_auc <- validation(final_rf_fit, df_test)
```



|

```
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')
```



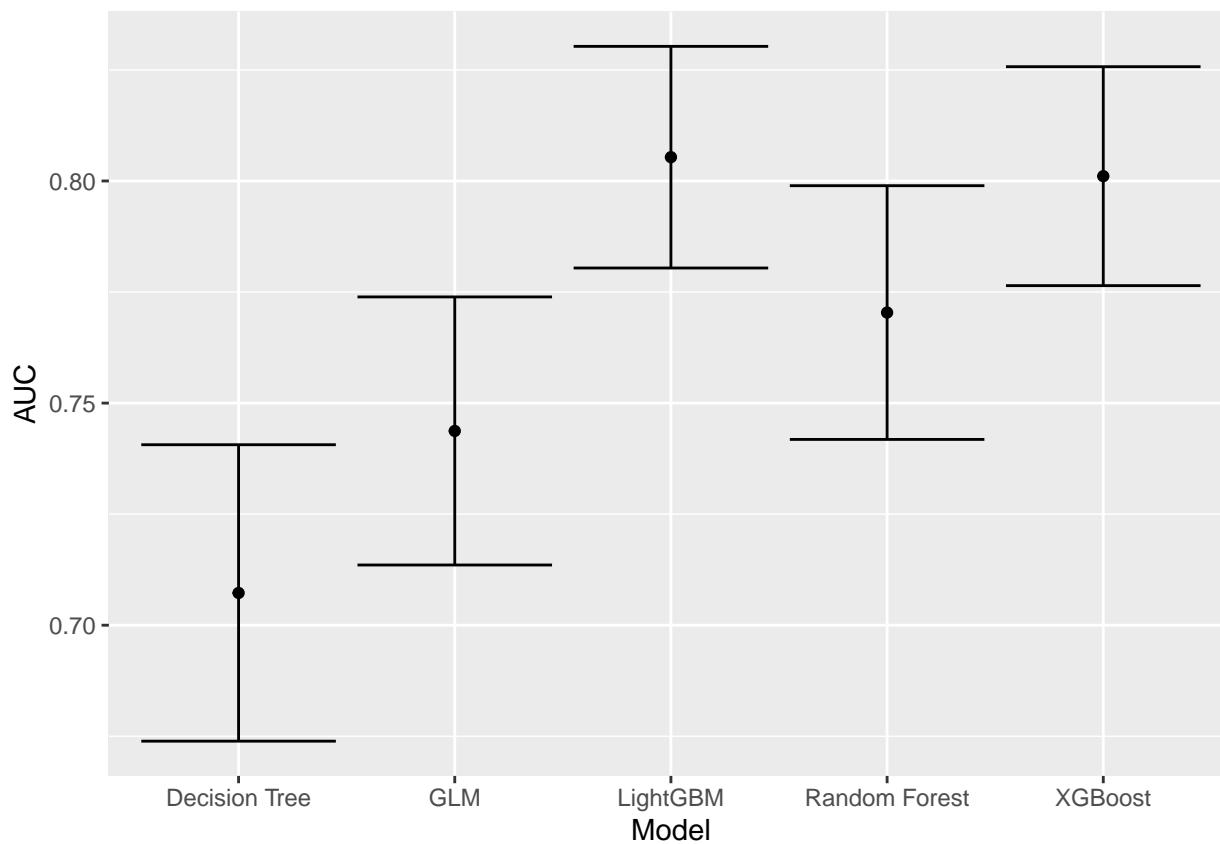
```
# extract_vip(final_rf_fit, pred_wrapper = predict,
#             reference_class = "1", use_matrix = FALSE,
#             method = 'permute')
```

Minutes to run: 132.569

Models Comparison

```
if (RUN_ALL_MODELS) {
  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$ci[3]
  ) %>%
    mutate(Target = outcome_column)
} else {
  df_auc <- tibble::tribble(
    ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
    'LightGBM', as.numeric(lightgbm_auc$auc), lightgbm_auc$ci[1], lightgbm_auc$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: 0.002