

Final Model

Eduardo Yuki Yada

Imports

```
library(tidyverse)
library(yaml)
library(tidymodels)
library(usemodels)
library(vip)
```

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
```

Filtering eligible patients

```
df = df %>%
  filter(disch_outcomes_t0 == 0)

df %>% dim
```

```
## [1] 15766 239
```

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_pre_t0_count', # com admission_t0
  '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)
}

length(features)

## [1] 118
print(features)

## [1] "sex" "age" "race"
## [4] "education_level" "patient_state" "underlying_heart_disease"
## [7] "heart_disease" "nyha_basal" "hypertension"
## [10] "prior_mi" "heart_failure" "af"
## [13] "cardiac_arrest" "transplant" "valvopathy"
## [16] "endocardites" "diabetes" "renal_failure"
## [19] "hemodialysis" "stroke" "copd"
## [22] "cancer" "comorbidities_count" "procedure_type_1"
## [25] "reop_type_1" "procedure_type_new" "cied_final_1"
## [28] "cied_final_group_1" "admission_t0" "admission_pre_t0_180d"
## [31] "year_adm_t0" "icu_t0" "dialysis_t0"
## [34] "disch_outcomes_t0" "n_procedure_t0" "admission_t0_emergency"
## [37] "aco" "antiarritmico" "antihipertensivo"
## [40] "betabloqueador" "ieca_bra" "dva"
## [43] "digoxina" "estatina" "diuretico"
## [46] "vasodilatador" "insuf_cardiaca" "espirolactona"
## [49] "bloq_calcio" "trombolitico" "antiplaquetario_vo"
## [52] "antiplaquetario_ev" "insulina" "hipoglicemiante"
## [55] "hormonio_tireoidiano" "broncodilatador" "anticonvulsivante"
## [58] "psicofarmacos" "antifungico" "antiviral"
## [61] "antiretroviral" "classe_meds_qtde" "meds_cardiovasc_qtde"
## [64] "meds_antimicrobianos" "vni" "ventilacao_mecanica"
## [67] "cec" "cir_cardiovascular" "transplante_cardiaco"
## [70] "cir_toracica" "outros_proced_cirurgicos" "traqueostomia"
## [73] "icp" "intervencao_cv" "stent"
## [76] "angioplastia" "cateterismo" "eletrofisiologia"
## [79] "cateter_venoso_central" "drenagem_torax" "proced_invasivos_qtde"
## [82] "cve_desf" "transfusao" "interconsulta"
## [85] "equipe_multiprof" "ecg" "holter"
## [88] "teste_esforco" "espiro_ergoespiro" "tilt_teste"
## [91] "polissonografia" "metodos_graficos_qtde" "laboratorio"
## [94] "cultura" "analises_clinicas_qtde" "citologia"
## [97] "biopsia" "histopatologia_qtde" "angio_rm"
## [100] "angio_tc" "angiografia" "aortografia"
## [103] "arteriografia" "cavografia" "cintilografia"
## [106] "ecocardiograma" "endoscopia" "flebografia"
## [109] "pet_ct" "ultrassom" "tomografia"
## [112] "radiografia" "ressonancia" "exames_imagem_qtde"
## [115] "dieta_enteral" "dieta_parenteral" "bic"
## [118] "mpp"

```

Train test split (70%/30%)

```

set.seed(42)

df[columns_list$outcome_columns] <- lapply(df[columns_list$outcome_columns], factor)
df <- mutate(df, across(where(is.character), as.factor))

df_split <- initial_split(df %>% dplyr::select(all_of(c(features, outcome_column))),

```

```

      prop = .7, strata = all_of(outcome_column))
df_train <- training(df_split)
df_test <- testing(df_split)

dim(df_train)[1] / dim(df)[1]

## [1] 0.6999873
dim(df_test)[1] / dim(df)[1]

## [1] 0.3000127

```

Global parameters

```

k = 4 # Number of folds for cross validation
grid_size = 20 # 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))

```

Functions

```

validation = function(model_fit, new_data) {
  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,
    smoothed = TRUE,
    # arguments for ci
    ci = TRUE,
    ci.alpha = 0.9,
    stratified = FALSE,
    # arguments for plot
    plot = TRUE,
    auc.polygon = TRUE,
    max.auc.polygon = TRUE,
    grid = TRUE,
    print.auc = TRUE,
    show.thres = TRUE
  )

  sens.ci <- ci.se(pROC_obj)
  plot(sens.ci, type = "shape", col = "lightblue")
  plot(sens.ci, type = "bars")

  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]])

```

```

  confusionMatrix(conf_matrix) %>% print

  return(pROC_obj)
}

```

Boosted Tree (XGBoost)

```

xgboost_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())

xgboost_spec <- boost_tree(
  trees = 200,
  tree_depth = tune(),
  min_n = tune(),
  loss_reduction = tune(),
  sample_size = tune(),
  mtry = tune(),
  learn_rate = tune()
) %>%
  set_engine("xgboost") %>%
  set_mode("classification")

xgboost_grid <- grid_latin_hypercube(
  tree_depth(),
  min_n(),
  loss_reduction(),
  sample_size = sample_prop(),
  finalize(mtry(), df_train),
  learn_rate(),
  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")

```

```

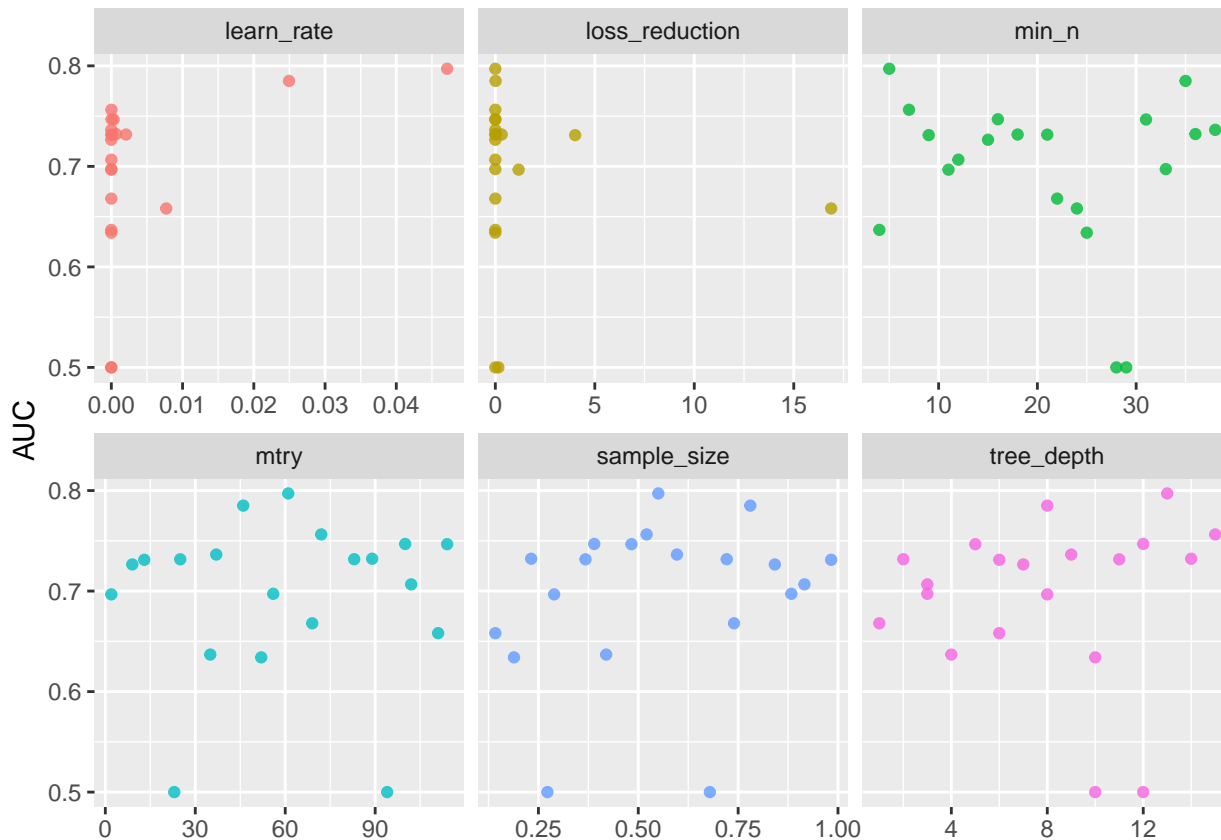
## # A tibble: 5 x 12
##   mtry min_n tree_depth learn_r~1 loss_r~2 sampl~3 .metric .esti~4 mean      n std_err .config
##   <int> <int>      <int>      <dbl>      <dbl>      <dbl> <chr>   <chr>    <dbl> <int>    <dbl> <chr>
## 1     61     5         13 0.0471      2.66e-10  0.550 roc_auc binary  0.797     4 0.00828 Prepro~
## 2     46    35          8 0.0249      1.27e- 2  0.781 roc_auc binary  0.785     4 0.00554 Prepro~
## 3     72     7         15 0.0000196 9.25e- 6  0.521 roc_auc binary  0.756     4 0.00336 Prepro~
## 4    100    16         12 0.0000354 6.51e- 5  0.390 roc_auc binary  0.747     4 0.00443 Prepro~
## 5    114    31          5 0.000325  3.77e- 6  0.483 roc_auc binary  0.747     4 0.00545 Prepro~
## # ... with abbreviated variable names 1: learn_rate, 2: loss_reduction, 3: sample_size,

```

```
## # 4: .estimator
```

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

```
xgboost_tune %>%
  collect_metrics() %>%
  filter(.metric == "roc_auc") %>%
  select(mean, mtry:sample_size) %>%
  pivot_longer(mtry:sample_size,
               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")
```

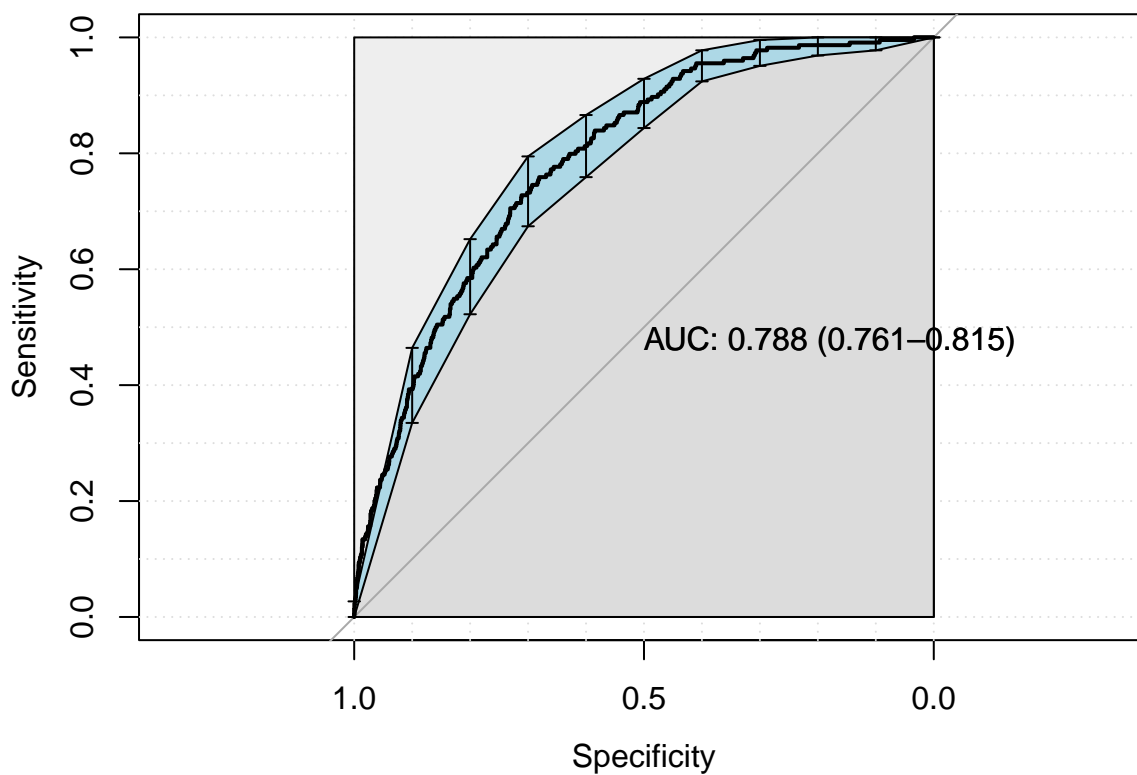


```
final_xgboost_workflow <-
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)

last_xgboost_fit <-
  final_xgboost_workflow %>%
  last_fit(df_split)

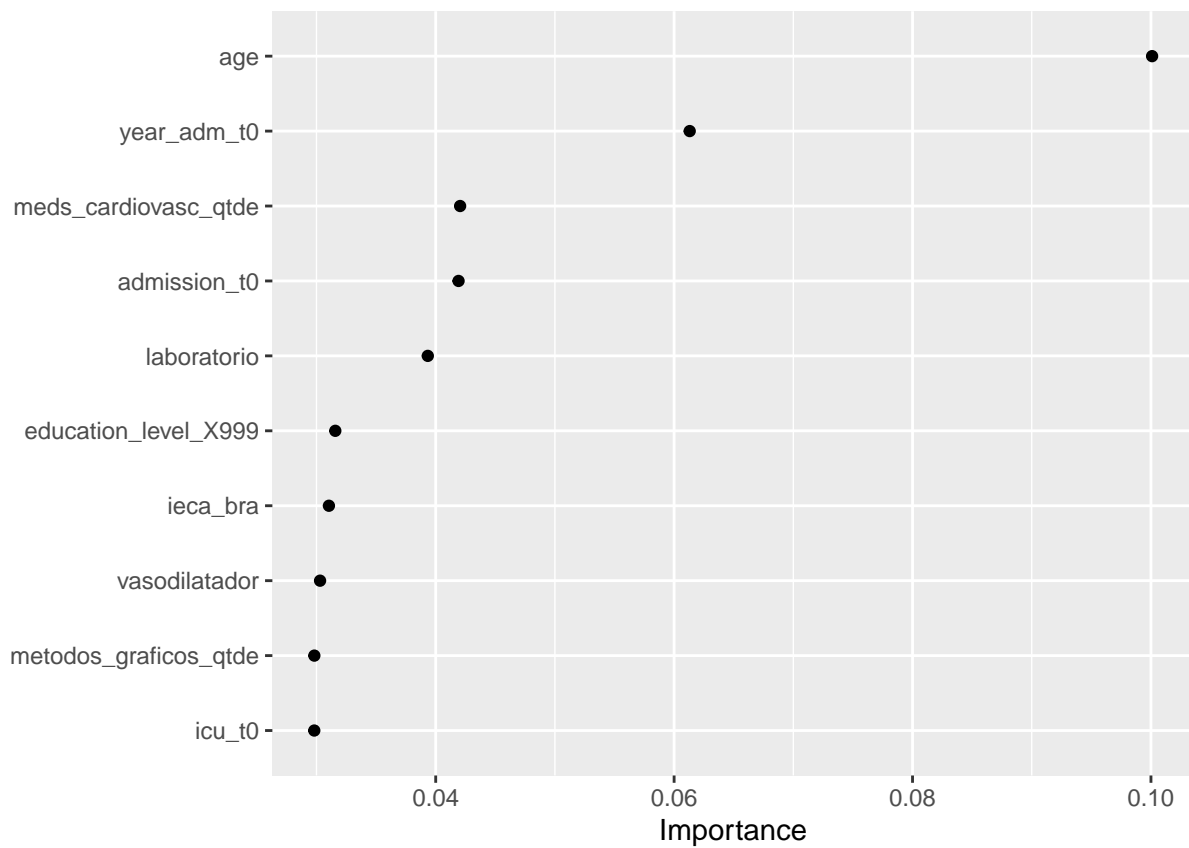
final_xgboost_fit <- extract_workflow(last_xgboost_fit)

xgboost_auc = validation(final_xgboost_fit, df_test)
```



```
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                0 4501  218
##                1    5    6
##
##                Accuracy : 0.9529
##                95% CI : (0.9464, 0.9587)
##      No Information Rate : 0.9526
##      P-Value [Acc > NIR] : 0.4905
##
##                Kappa : 0.0468
##
##  McNemar's Test P-Value : <2e-16
##
##                Sensitivity : 0.99889
##                Specificity : 0.02679
##      Pos Pred Value : 0.95380
##      Neg Pred Value : 0.54545
##      Prevalence : 0.95264
##      Detection Rate : 0.95159
##      Detection Prevalence : 0.99767
##      Balanced Accuracy : 0.51284
##
##      'Positive' Class : 0
##
```

```
final_xgboost_fit %>%
  fit(data = df_train) %>%
  extract_fit_parsnip() %>%
  vip(geom = "point")
```



```
library(SHAPforxgboost)
library(xgboost)
library(Matrix)
library(mltools)

xgb_model <- parsnip::extract_fit_engine(last_xgboost_fit)

trained_rec <- prep(xgboost_recipe, training = df_train)

df_test_baked <- bake(trained_rec, new_data = df_test)

matrix_test <- as.matrix(df_test_baked %>% select(-all_of(outcome_column)))

shap.plot.summary.wrap1(model = xgb_model, X = matrix_test, top_n = 10, dilute = T)
```

