Final Model

Eduardo Yuki Yada

Imports

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

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

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
```

Minutes to run: 0.002

Filtering eligible pacients

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

df %>% dim
```

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

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')
```

```r
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. 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. disch_outcomes_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. classe_meds_qtde
## 45. meds_cardiovasc_qtde
## 46. meds_antimicrobianos
## 47. outros_proced_cirurgicos
## 48. icp
## 49. angioplastia
## 50. cateterismo
## 51. eletrofisiologia
## 52. cateter_venoso_central
## 53. proced_invasivos_qtde
## 54. transfusao
## 55. equipe_multiprof
## 56. ecg
## 57. holter
## 58. teste_esforco
## 59. tilt_teste
## 60. metodos_graficos_qtde
## 61. laboratorio
## 62. cultura
## 63. analises_clinicas_qtde
## 64. citologia
## 65. histopatologia_qtde
## 66. angio_tc
## 67. angiografia
## 68. cintilografia
## 69. ecocardiograma
## 70. endoscopia
## 71. flebografia
## 72. pet_ct
## 73. ultrassom
## 74. tomografia
## 75. radiografia
## 76. ressonancia
## 77. exames_imagem_qtde
## 78. bic
```

Minutes to run: 0

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
```

Minutes to run: 0.004

Global parameters

```
k <- 4 # Number of folds for cross validation
grid_size <- 50 # 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))

max_auc_loss <- 0.01
```

Minutes to run: 0

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

Feature Selection

```
model_fit_wf <- function(features, outcome_column, hyperparameters){
  model_recipe <-
    recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
           data = df_train %>% select(all_of(c(features, outcome_column)))) %>%
    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())

  model_spec <-
    do.call(boost_tree, hyperparameters) %>%
    set_engine("lightgbm") %>%
    set_mode("classification")

  model_workflow <-
    workflow() %>%
    add_recipe(model_recipe) %>%
    add_model(model_spec)

  model_fit_rs <- model_workflow %>%
    fit_resamples(df_folds)

  model_fit <- model_workflow %>%
    fit(df_train)

  model_auc <- validation(model_fit, df_test, plot=F)

  raw_model <- parsnip::extract_fit_engine(model_fit)

  feature_importance <- lgb.importance(raw_model, percentage = TRUE)

  return(list(cv_auc = collect_metrics(model_fit_rs) %>% filter(.metric == 'roc_auc') %>% .$mean,
              importance = feature_importance,
              auc = as.numeric(model_auc$auc),
              auc_lower = model_auc$ci[1],
              auc_upper = model_auc$ci[3]))
}
```

Minutes to run: 0

```
hyperparameters <- readRDS(
  sprintf(
    "../EDA/auxiliar/hyperparameters/model_selection/lightgbm_parameters_%s.rds",
    outcome_column
  )
)

full_model <- model_fit_wf(features, outcome_column, hyperparameters)

sprintf('Full Model CV Train AUC: %.3f' ,full_model$cv_auc)
```

```
## [1] "Full Model CV Train AUC: 0.772"
```

```
sprintf('Full Model Test AUC: %.3f' ,full_model$auc)
```

```
## [1] "Full Model Test AUC: 0.794"
```

Minutes to run: 0.085

Features with zero importance on the initial model:

```
unimportant_features <- setdiff(features, full_model$importance$Feature)

unimportant_features %>%
  gluedown::md_order()
```

```
## 01. heart_disease
## 02. hemodialysis
## 03. disch_outcomes_t0
## 04. insulina
## 05. icp
## 06. angioplastia
## 07. eletrofisiologia
## 08. holter
## 09. tilt_teste
## 10. angio_tc
## 11. angiografia
## 12. cintilografia
## 13. endoscopia
## 14. pet_ct
## 15. tomografia
```

Minutes to run: 0

```
trimmed_features <- full_model$importance$Feature
hyperparameters$mtry = min(hyperparameters$mtry, length(trimmed_features))
trimmed_model <- model_fit_wf(trimmed_features,
                              outcome_column, hyperparameters)

sprintf('Trimmed Model CV Train AUC: %.3f' ,trimmed_model$cv_auc)
```

```
## [1] "Trimmed Model CV Train AUC: 0.774"
```

```
sprintf('Trimmed Model Test AUC: %.3f' ,trimmed_model$auc)
```

```
## [1] "Trimmed Model Test AUC: 0.792"
```

Minutes to run: 0.077

```
current_features <- trimmed_features
current_model <- trimmed_model
current_least_important <- tail(trimmed_model$importance$Feature, 1)
current_auc_loss <- full_model$cv_auc - trimmed_model$cv_auc

selection_results <- tibble::tribble(
  ~`Number of Features`, ~`AUC Loss`, ~`Least Important Feature`,
  length(features), 0, tail(full_model$importance$Feature, 1),
  length(trimmed_features), current_auc_loss, tail(trimmed_model$importance$Feature, 1)
)

while (current_auc_loss < max_auc_loss){
  last_feature_droped <- current_least_important

  current_features <- setdiff(current_features, current_least_important)
  hyperparameters$mtry = min(hyperparameters$mtry, length(current_features))
  current_model <- model_fit_wf(current_features, outcome_column, hyperparameters)
  current_least_important <- tail(current_model$importance$Feature, 1)

  current_auc_loss <- full_model$cv_auc - current_model$cv_auc

  selection_results <- selection_results %>%
    add_row(`Number of Features` = length(current_features),
            `AUC Loss` = current_auc_loss,
            `Least Important Feature` = current_least_important)
```

```
  print(c(length(current_features), current_auc_loss))
}
```

```
## [1] 62.000000000 -0.001922938
## [1] 61.00000000 -0.00169378
## [1] 60.00000000 -0.00437528
## [1] 59.000000000 -0.003673008
## [1] 58.000000000 -0.001887603
## [1] 57.000000000 -0.002405554
## [1] 56.000000000 -0.002198867
## [1] 55.00000000 -0.00331345
## [1] 54.000000000 -0.001830387
## [1] 53.000000000 -0.002012769
## [1] 52.000000000 -0.003655927
## [1] 51.000000000 -0.002333093
## [1] 50.000000000 -0.004839169
## [1] 49.000000000 -0.002007191
## [1] 48.00000000 -0.00459511
## [1] 47.000000000 -0.002154702
## [1] 46.00000000 -0.00361575
## [1] 45.000000000 -0.003631562
## [1] 44.000000000 -0.003124298
## [1] 43.000000000 -0.003648686
## [1] 42.000000000 -0.003342892
## [1] 41.000000000 -0.001720201
## [1] 40.0000000 -0.0025675
## [1] 39.000000000 -0.002663349
## [1] 38.000000000 -0.002467878
## [1] 37.000000000 -0.003886223
## [1] 36.000000000 -0.004142356
## [1] 35.000000000 -0.004799504
## [1] 34.00000000 -0.00451158
## [1] 33.000000000 -0.004653525
## [1] 32.000000000 -0.005641003
## [1] 31.000000000 -0.005935382
## [1] 30.000000000 -0.003988177
## [1] 29.000000000 -0.006513056
## [1] 28.000000000 -0.005778275
## [1] 27.000000000 -0.006364936
## [1] 26.000000000 -0.006178642
## [1] 25.000000000 -0.006196591
## [1] 24.000000000 -0.006634212
## [1] 23.000000000 -0.005965601
## [1] 22.000000000 -0.005247426
## [1] 21.00000000 -0.00457134
## [1] 20.00000000 -0.00419719
## [1] 19.000000000 -0.004119863
## [1] 18.000000000 -0.004177408
## [1] 17.000000000 -0.002756282
## [1] 16.000000000 -0.002585998
## [1] 15.000000000 -0.002492944
## [1] 14.000000000 -0.001817881
## [1] 13.0000000000 -0.0009201005
## [1] 12.000000000  0.004246546
## [1] 11.000000000  0.003293567
## [1] 10.000000000  0.007233306
## [1] 9.00000000 0.01451922
```

```
selection_results
```

```
## # A tibble: 56 x 3
##    `Number of Features` `AUC Loss` `Least Important Feature`
```

```
##                    <int>      <dbl> <chr>
##  1                    78    0       ressonancia
##  2                    63   -0.00272 cardiac_arrest
##  3                    62   -0.00192 aco
##  4                    61   -0.00169 ressonancia
##  5                    60   -0.00438 sex
##  6                    59   -0.00367 teste_esforco
##  7                    58   -0.00189 ultrassom
##  8                    57   -0.00241 flebografia
##  9                    56   -0.00220 citologia
## 10                    55   -0.00331 dialysis_t0
## # ... with 46 more rows
```

Minutes to run: 3.38

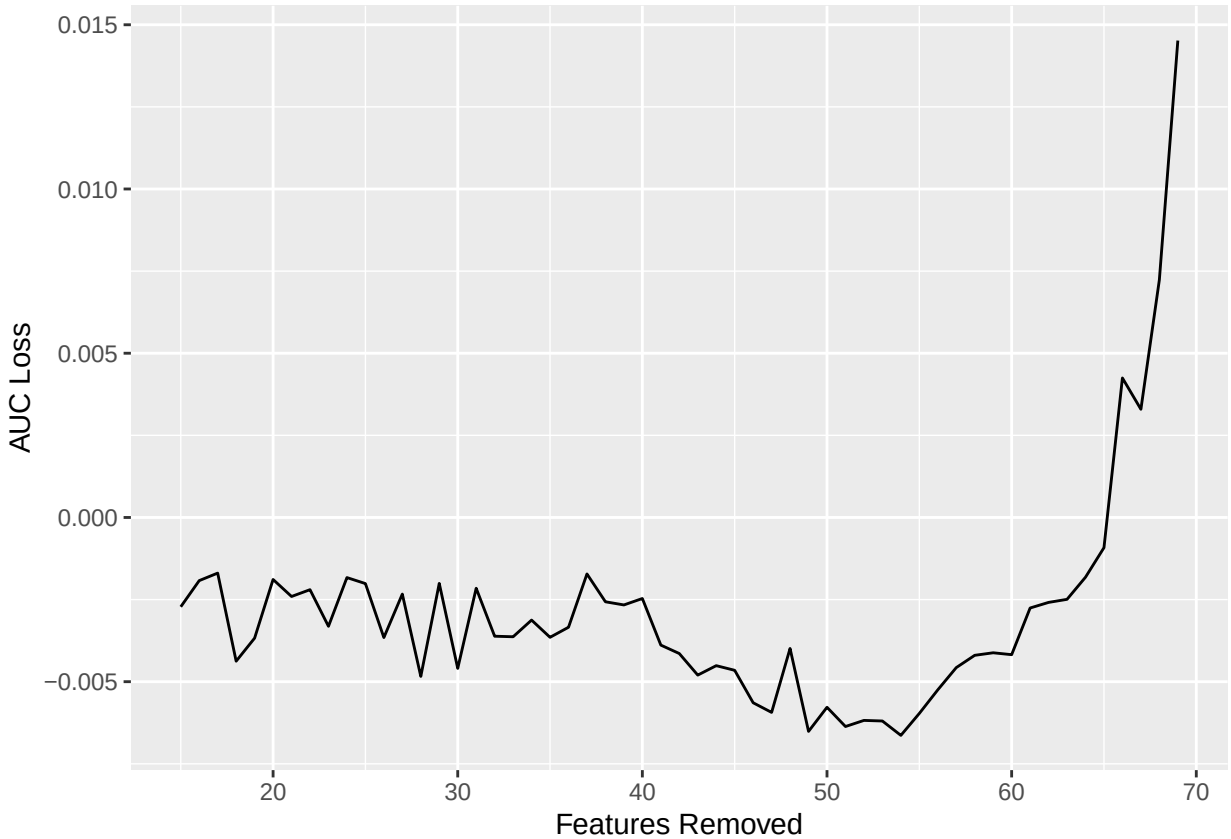
```
selected_features <- c(current_features, last_feature_droped)

feature_selected_model <- model_fit_wf(selected_features,
                                       outcome_column, hyperparameters)

sprintf('Trimmed Model CV Train AUC: %.3f', feature_selected_model$cv_auc)
```

```
## [1] "Trimmed Model CV Train AUC: 0.765"
```

```
sprintf('Trimmed Model Test AUC: %.3f', feature_selected_model$auc)
```

```
## [1] "Trimmed Model Test AUC: 0.783"
```

```
selection_results %>%
  filter(`Number of Features` < length(features)) %>%
  mutate(`Features Removed` = length(features) - `Number of Features`) %>%
  ggplot(aes(x = `Features Removed`, y = `AUC Loss`)) +
  geom_line()
```



Minutes to run: 0.046

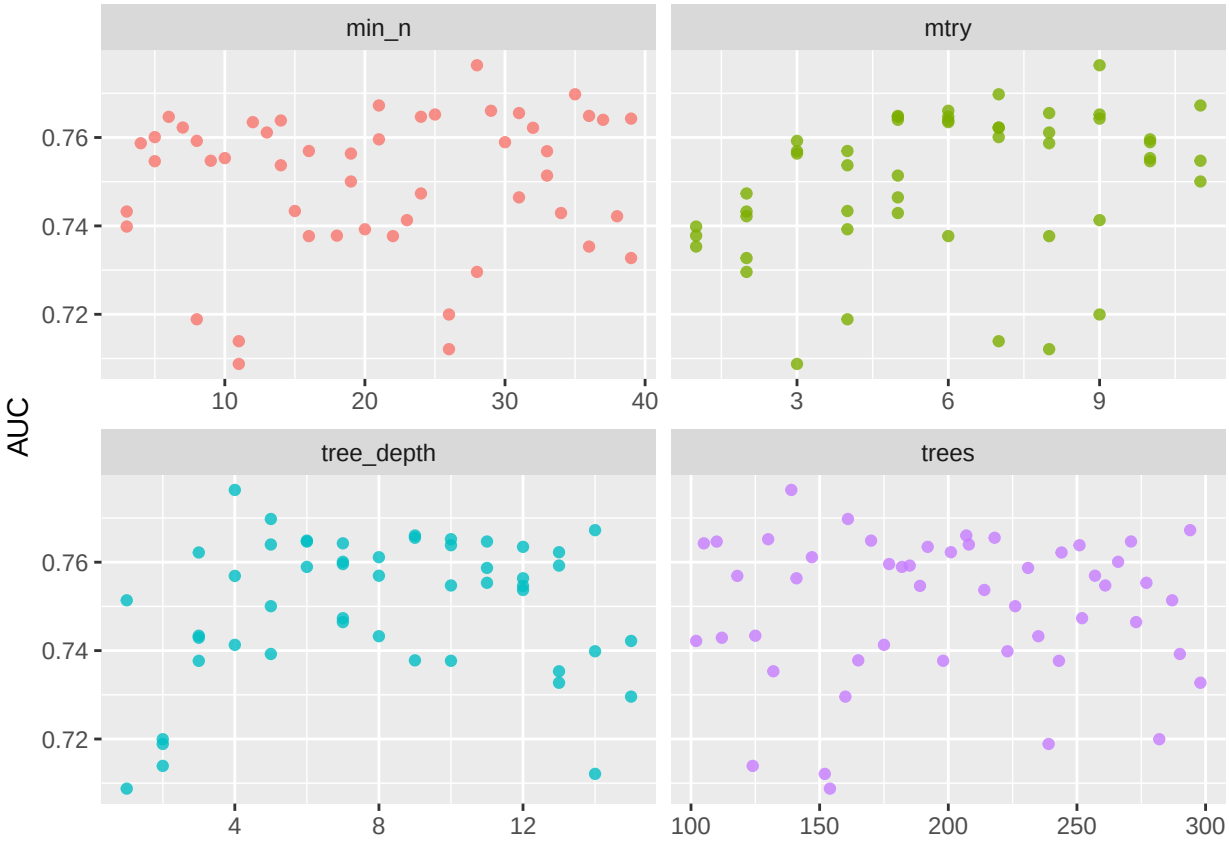
Hyperparameter tuning

```
lightgbm_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train %>% dplyr::select(all_of(c(selected_features, outcome_column)))) %>%
  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_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()
) %>%
  set_engine("lightgbm") %>%
  set_mode("classification")

lightgbm_grid <- grid_latin_hypercube(
  finalize(mtry(),
           df_train %>% dplyr::select(all_of(c(selected_features, outcome_column)))),
  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")
```

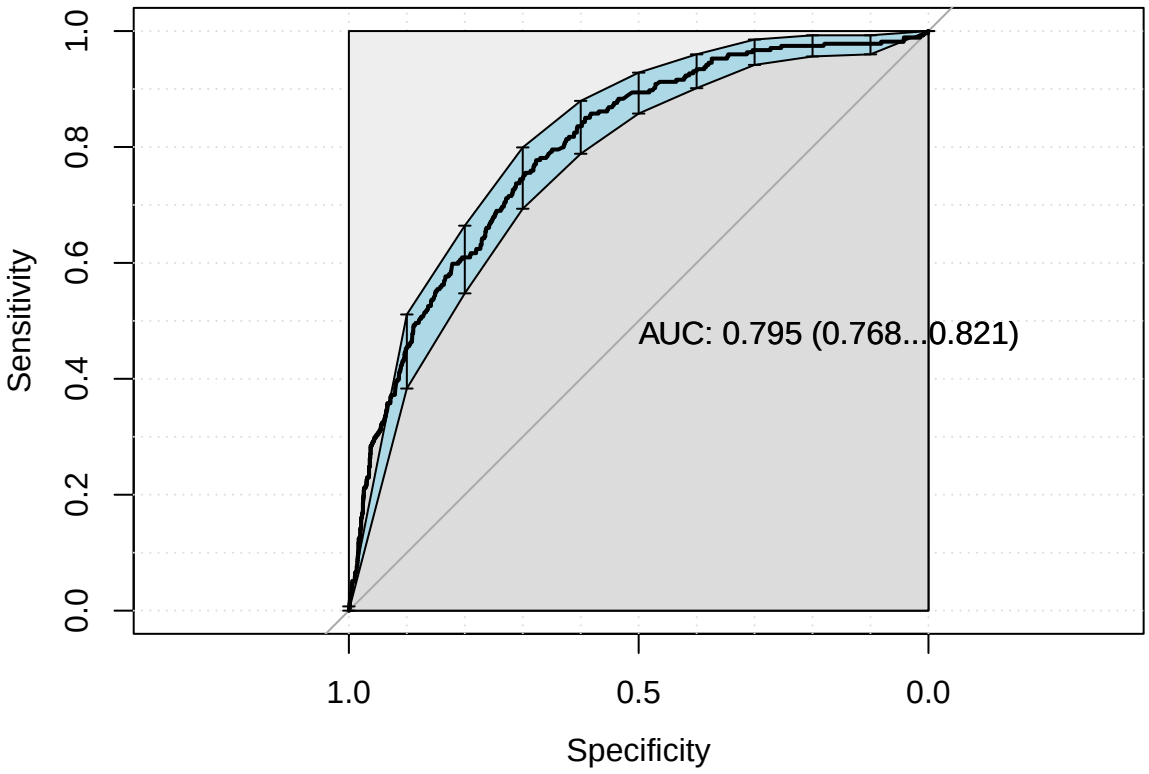
```
## # A tibble: 5 x 12
##    mtry trees min_n tree_depth  learn_rate loss_reduction .metric .estimator  mean     n std_err .config
##   <int> <int> <int>      <int>       <dbl>          <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1     9   139    28          4 0.0240           9.36e- 2 roc_auc binary     0.776     4  0.0144 Preprocessor
## 2     7   161    35          5 0.00462          2.96e- 5 roc_auc binary     0.770     4  0.0194 Preprocessor
## 3    11   294    21         14 0.0152           2.69e-10 roc_auc binary     0.767     4  0.0138 Preprocessor
## 4     6   207    29          9 0.00000827       3.38e- 2 roc_auc binary     0.766     4  0.0196 Preprocessor
## 5     8   218    31          9 0.000000277      3.19e- 9 roc_auc binary     0.766     4  0.0196 Preprocessor
```

```
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)
```



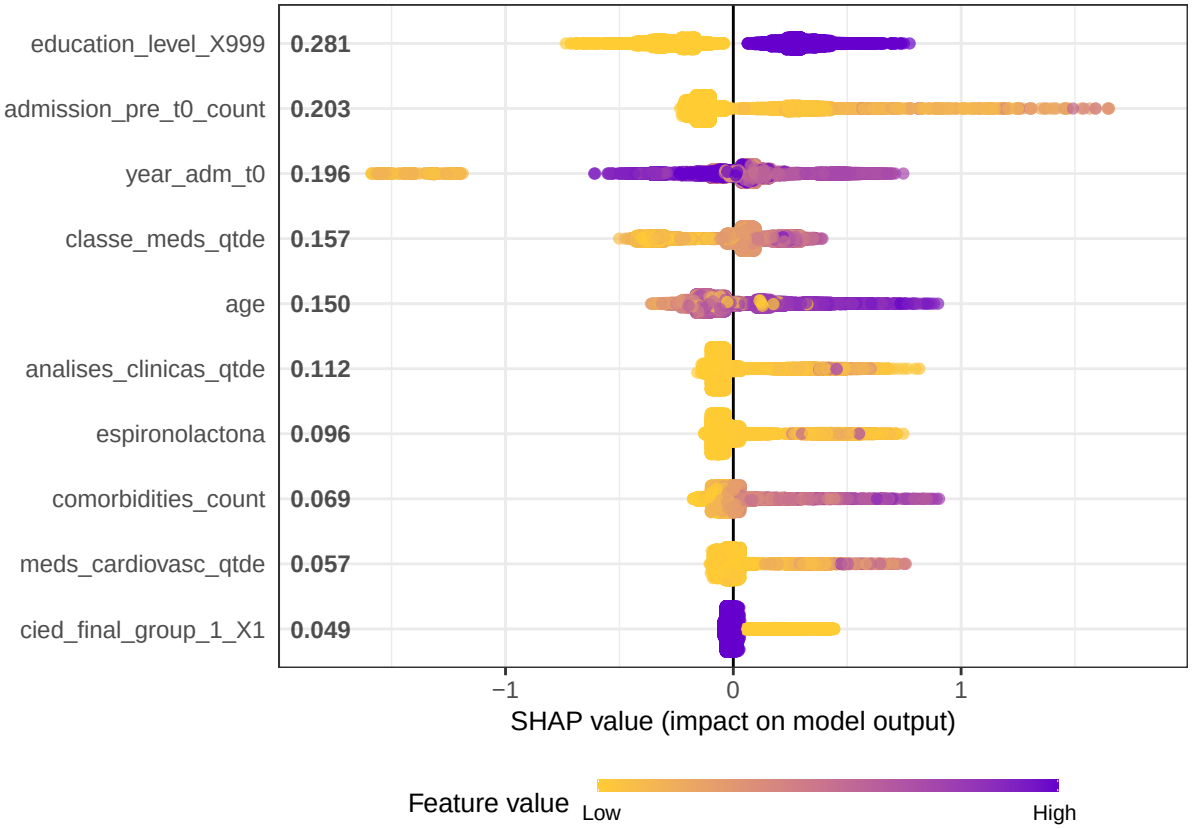

```
##   |
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4455  274
##                      1    1    0
##
##                Accuracy : 0.9419
##                  95% CI : (0.9348, 0.9484)
##     No Information Rate : 0.9421
##     P-Value [Acc > NIR] : 0.5408
##
##                   Kappa : -4e-04
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.9998
##             Specificity : 0.0000
##          Pos Pred Value : 0.9421
##          Neg Pred Value : 0.0000
##              Prevalence : 0.9421
##          Detection Rate : 0.9419
##    Detection Prevalence : 0.9998
##       Balanced Accuracy : 0.4999
##
##        '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
```

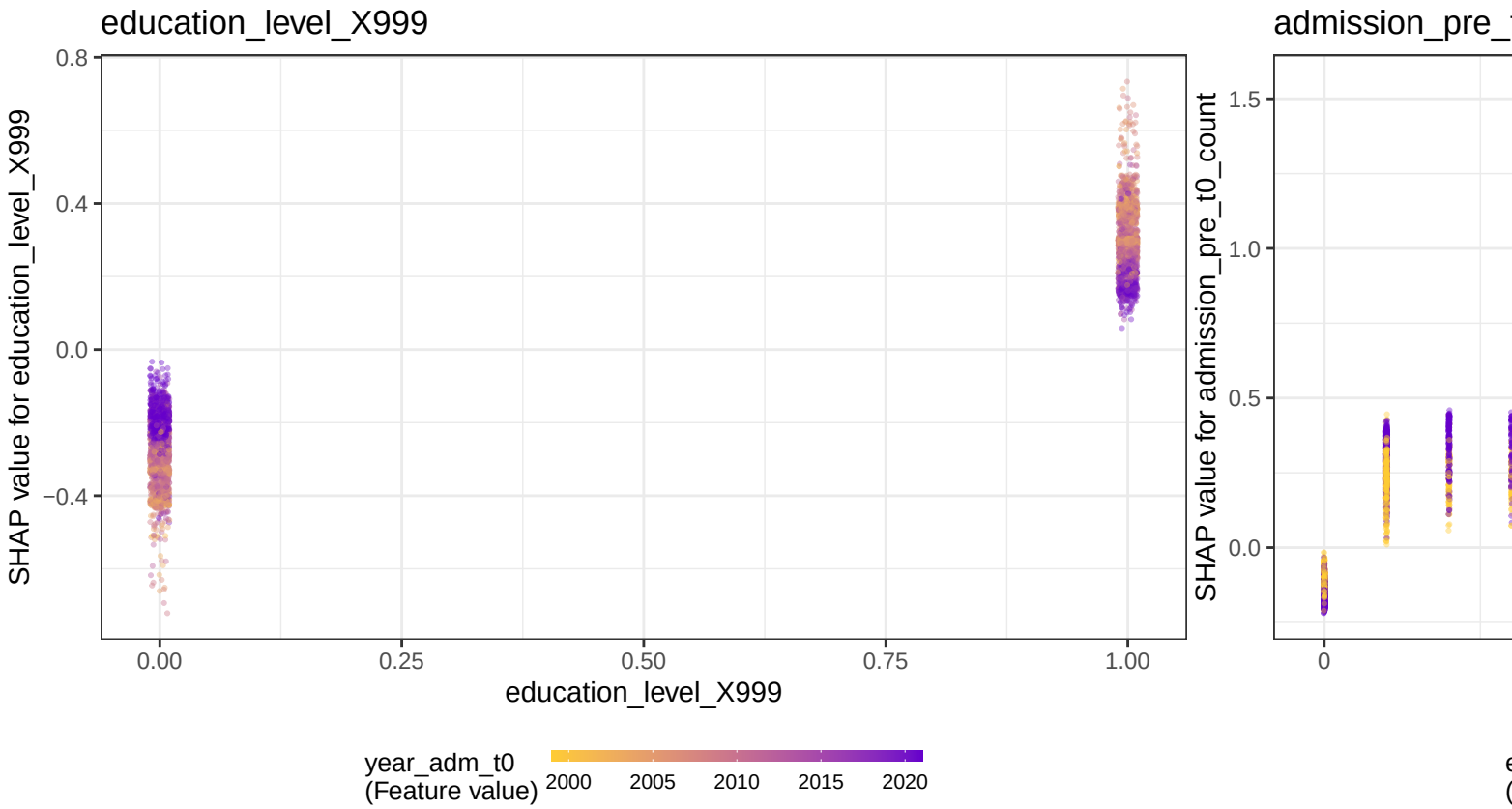
Minutes to run: 1.435

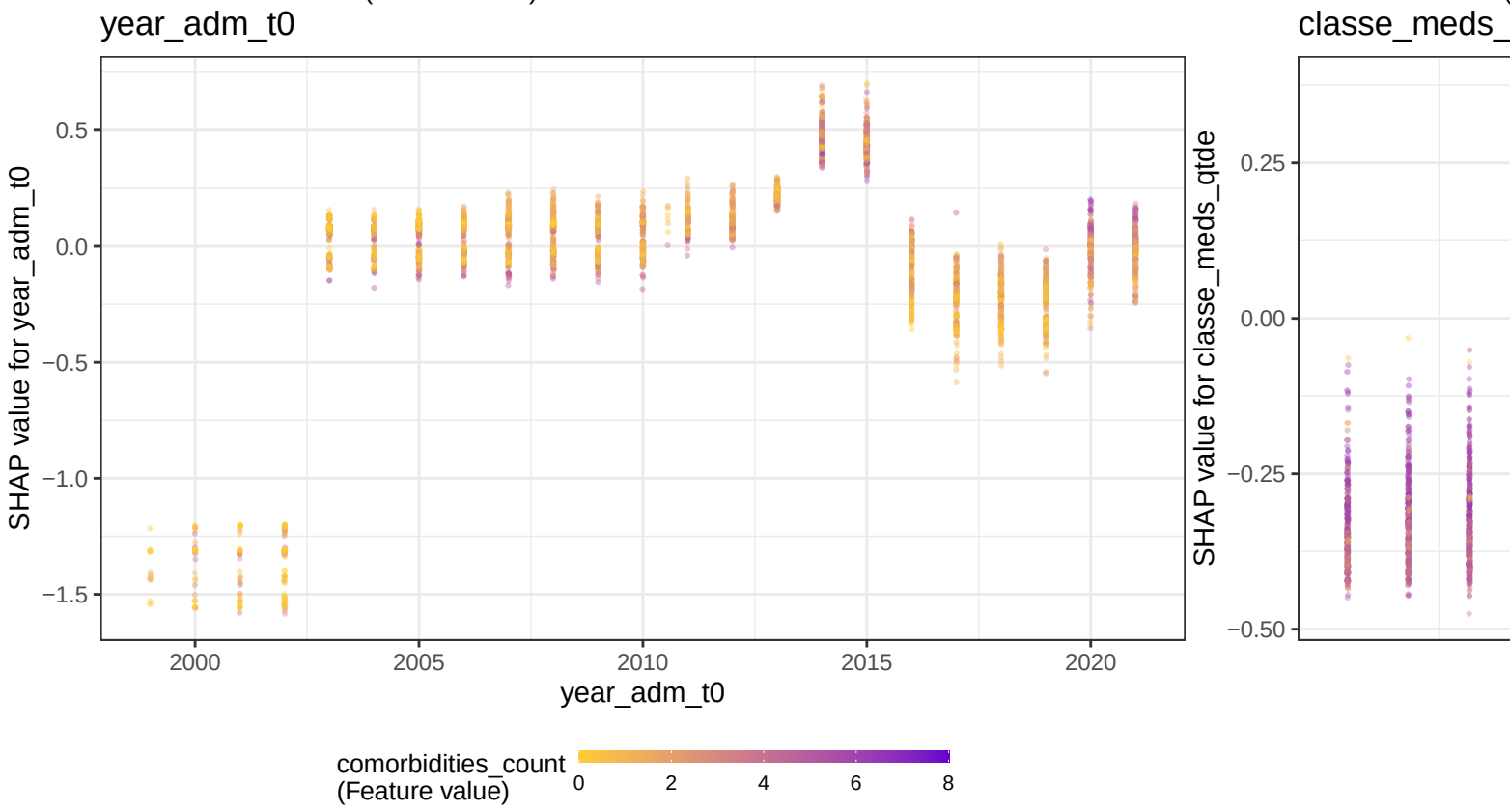
```
lightgbm_model <- parsnip::extract_fit_engine(final_lightgbm_fit)
```

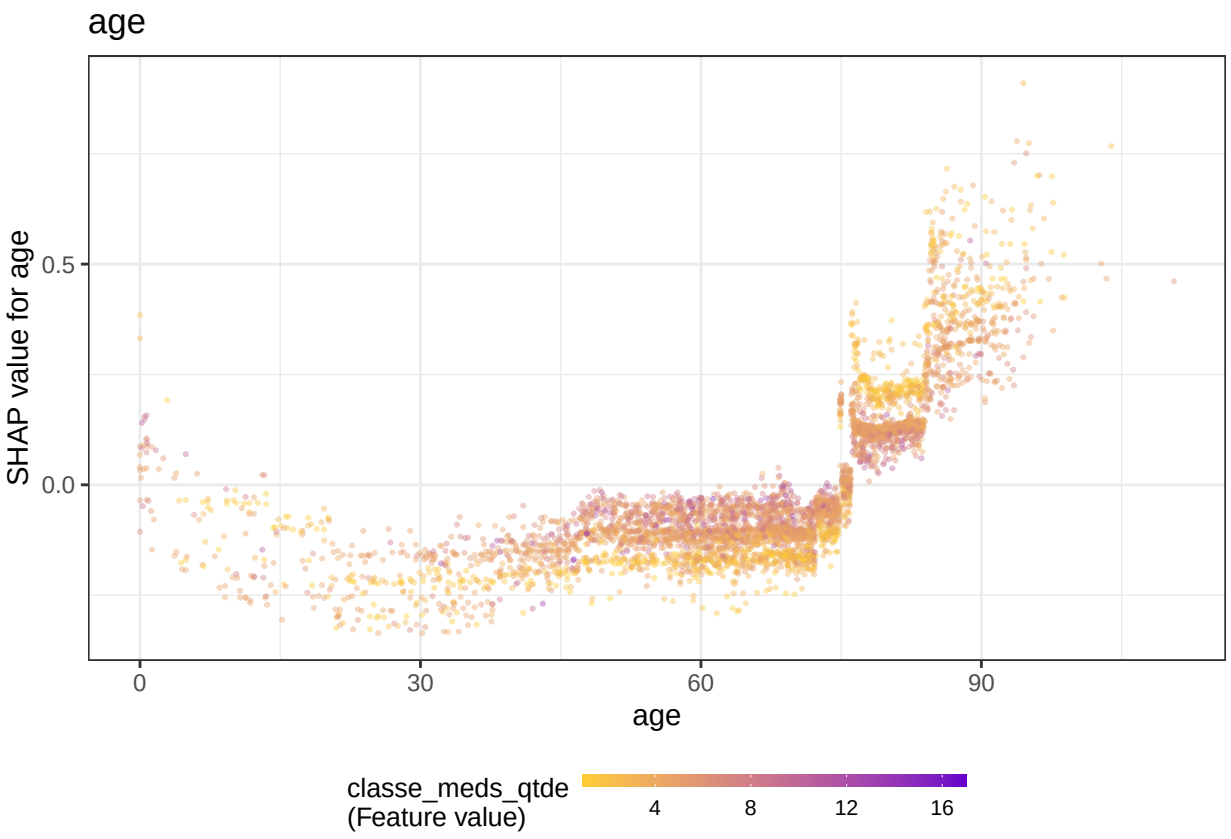
```r
trained_rec <- prep(lightgbm_recipe, training = df_train)

df_train_baked <- bake(trained_rec, new_data = df_train)
df_test_baked <- bake(trained_rec, new_data = df_test)

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

shap.plot.summary.wrap1(model = lightgbm_model, X = matrix_train, top_n = 10, dilute = F)
```




```r
# Crunch SHAP values
shap <- shap.prep(lightgbm_model, X_train = matrix_test)

for (x in shap.importance(shap, names_only = TRUE)[1:5]) {
  p <- shap.plot.dependence(
    shap,
    x = x,
    color_feature = "auto",
    smooth = FALSE,
    jitter_width = 0.01,
    alpha = 0.4
    ) +
  ggtitle(x)
  print(p)
}
```


education_level_X999
SHAP value for education_level_X999
0.8
0.4
0.0
−0.4
0.00
0.25
0.50
0.75
1.00
education_level_X999
admission_pre_
SHAP value for admission_pre_t0_count
1.5
1.0
0.5
0.0
0
year_adm_t0
(Feature value)
2000
2005
2010
2015
2020


year_adm_t0
SHAP value for year_adm_t0
0.5
0.0
−0.5
−1.0
−1.5
2000
2005
2010
2015
2020
year_adm_t0
classe_meds_
SHAP value for classe_meds_qtde
0.25
0.00
−0.25
−0.50
comorbidities_count
(Feature value)
0
2
4
6
8

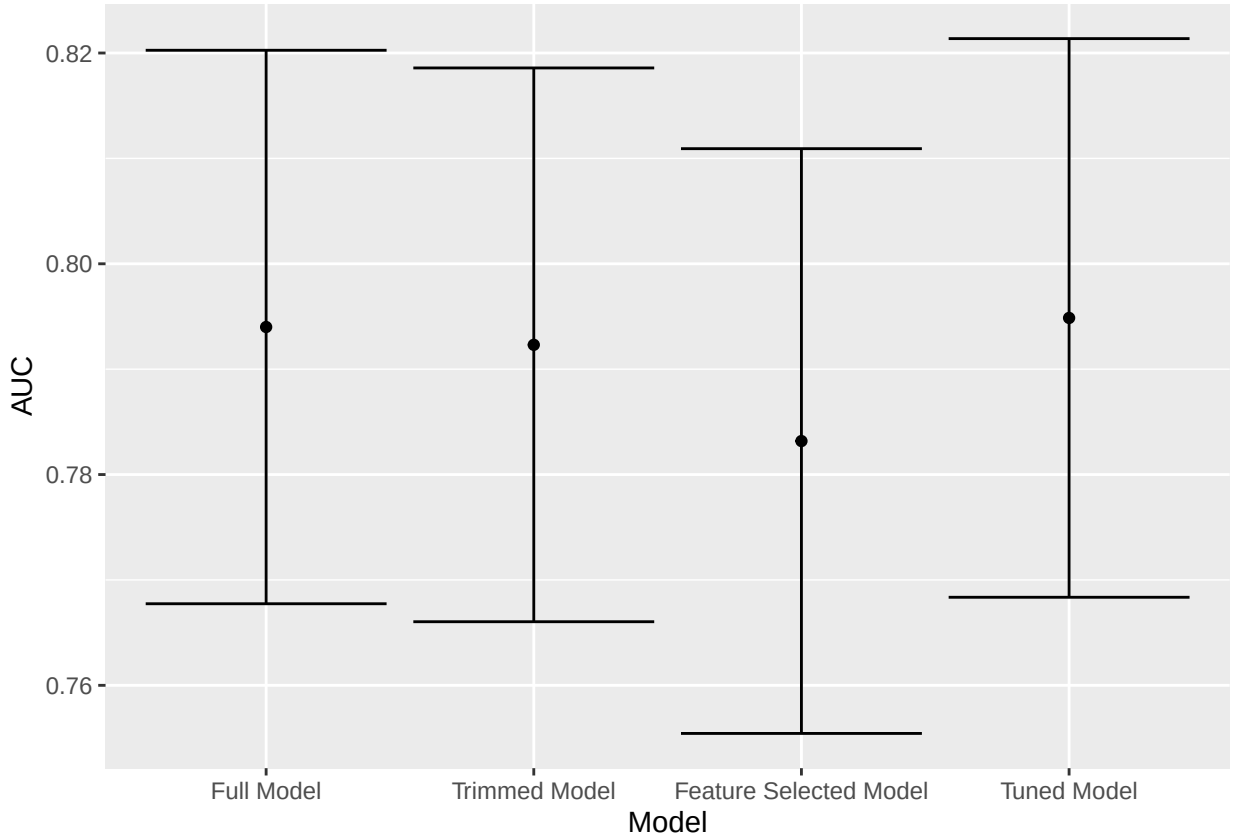


Minutes to run: 0.1

Minutes to run: 0

Models Comparison

```
df_auc <- tibble::tribble(
  ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
  'Full Model', full_model$auc, full_model$auc_lower, full_model$auc_upper,
  'Trimmed Model', trimmed_model$auc, trimmed_model$auc_lower, trimmed_model$auc_upper,
  'Feature Selected Model', feature_selected_model$auc, feature_selected_model$auc_lower, feature_selected_model
  'Tuned Model', as.numeric(lightgbm_auc$auc), lightgbm_auc$ci[1], lightgbm_auc$ci[3]
) %>%
  mutate(Target = outcome_column,
         Model = factor(Model,
                        levels = c('Full Model', 'Trimmed Model',
                                   'Feature Selected Model', 'Tuned Model')))

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




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

# Save the final model
saveRDS(final_lightgbm_fit, sprintf("../EDA/results/%s/final_model.RData", outcome_column))
```

Minutes to run: 0.005