Final Model - death_1year

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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
max_auc_loss <- params$max_auc_loss # Max accepted loss of AUC for reducing num of features
repeats <- params$repeats
```

Imports

```
library(tidyverse)
library(yaml)
library(tidymodels)
library(usemodels)
library(vip)
library(kableExtra)
library(SHAPforxgboost)
library(xgboost)
library(Matrix)
library(mltools)
library(bonsai)
library(lightgbm)
library(pROC)
library(caret)
library(themis)

source("aux_functions.R")

select <- dplyr::select
```

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

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

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

```
            recursive = TRUE)

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

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)
```

```
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)
}
```

Starting features:

```
gluedown::md_order(features, seq = TRUE, pad = TRUE)
```

1. sex
2. age
3. education_level
4. underlying_heart_disease
5. heart_disease
6. nyha_basal
7. hypertension
8. prior_mi
9. 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. antiviral
46. classe_meds_qtde
47. meds_cardiovasc_qtde
48. meds_antimicrobianos
49. vni
50. ventilacao_mecanica
51. transplante_cardiaco
52. cir_toracica
53. outros_proced_cirurgicos
54. icp
55. cateterismo
56. cateter_venoso_central
57. proced_invasivos_qtde
58. transfusao
59. interconsulta
60. equipe_multiprof
61. holter
62. teste_esforco
63. tilt_teste
64. metodos_graficos_qtde
65. laboratorio
66. cultura
67. analises_clinicas_qtde
68. citologia
69. histopatologia_qtde
70. angio_tc
71. angiografia
72. aortografia

73. cintilografia
74. ecocardiograma
75. endoscopia
76. flebografia
77. pet_ct
78. ultrassom
79. tomografia
80. ressonancia
81. exames_imagem_qtde
82. bic
83. hospital_stay

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) %>% select(all_of(c(features, outcome_column)))
df_test <- testing(df_split) %>% select(all_of(c(features, outcome_column)))

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

Feature Selection

```
custom_dummy_names <- function(var, lvl, ordinal = FALSE) {
  dummy_names(var, lvl, ordinal = FALSE, sep = "__")
}

model_fit_wf <- function(df_train, 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_dummy(all_nominal_predictors(), naming = custom_dummy_names)

  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) %>%
    separate(Feature, c("Feature","value"), "__", fill = 'right') %>%
    group_by(Feature) %>%
    summarise(Gain = sum(Gain),
              Cover = sum(Cover),
              Frequency = sum(Frequency))

  cv_results <- collect_metrics(model_fit_rs) %>% filter(.metric == 'roc_auc')

  return(
    list(
      cv_auc =  cv_results$mean,
      cv_auc_std_err = cv_results$std_err,
      importance = feature_importance,
      auc = as.numeric(model_auc$auc),
      auc_lower = model_auc$ci[1],
      auc_upper = model_auc$ci[3]
    )
  )
}
```

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

hyperparameters$sample_size <- 1

full_model <- model_fit_wf(df_train, features, outcome_column, hyperparameters)

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

```
## [1] "Full Model CV Train AUC: 0.809"
```

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

```
## [1] "Full Model Test AUC: 0.798"
```

```
# full_model$importance %>%
#   filter(str_detect(Feature, 'education'))
#
# full_model$importance %>%
#   filter(str_detect(Feature, 'education')) %>%
#   summarise(across(where(is.numeric), ~ sum(.x, na.rm = TRUE)))
#
# full_model$importance %>%
#   separate(Feature, c("Feature","value"), "__") %>%
#   group_by(Feature) %>%
#   summarise(Gain = sum(Gain),
#             Cover = sum(Cover),
#             Frequency = sum(Frequency))
```

Features with zero importance on the initial model:

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

unimportant_features %>%
```

```
  gluedown::md_order()
```

1. underlying_heart_disease
2. heart_disease
3. hypertension
4. prior_mi
5. heart_failure
6. af
7. cardiac_arrest
8. renal_failure
9. stroke
10. copd
11. cancer
12. procedure_type_1
13. reop_type_1
14. cied_final_1
15. admission_pre_t0_180d
16. dialysis_t0
17. admission_t0_emergency
18. digoxina
19. antiplaquetario_ev
20. insulina
21. antiviral
22. vni
23. ventilacao_mecanica
24. transplante_cardiaco
25. cir_toracica
26. icp
27. transfusao
28. holter
29. tilt_teste
30. laboratorio
31. cultura
32. histopatologia_qtde
33. angio_tc
34. angiografia
35. aortografia
36. cintilografia
37. pet_ct
38. tomografia
39. ressonancia
40. bic

```
trimmed_features <- full_model$importance$Feature
trimmed_model <- model_fit_wf(df_train, trimmed_features,
                              outcome_column, hyperparameters)

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

```
## [1] "Trimmed Model CV Train AUC: 0.814"
```

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

```
## [1] "Trimmed Model Test AUC: 0.798"
```

```
selection_results <- tibble::tribble(
  ~`Tested Feature`, ~`Dropped`, ~`Number of Features`, ~`CV AUC`, ~`CV AUC Std Error`, ~`Total AUC Loss`, ~`Ins
  'None', TRUE, length(features), full_model$cv_auc, full_model$cv_auc_std_err, 0, 0
)

whitelist <- c()

if (full_model$cv_auc - trimmed_model$cv_auc < max_auc_loss) {
```

```
  current_features <- trimmed_features
  current_model <- trimmed_model
  current_auc_loss <- full_model$cv_auc - current_model$cv_auc
  instant_auc_loss <- full_model$cv_auc - current_model$cv_auc

  selection_results <- selection_results %>%
    add_row(`Tested Feature` = 'All unimportant',
            `Dropped` = TRUE,
            `Number of Features` = length(trimmed_features),
            `CV AUC` = current_model$cv_auc,
            `CV AUC Std Error` = current_model$cv_auc_std_err,
            `Total AUC Loss` = current_auc_loss,
            `Instant AUC Loss` = instant_auc_loss)
} else {
  current_features <- features
  current_model <- full_model
  current_auc_loss <- 0
}

while (current_auc_loss < max_auc_loss & mean(current_features %in% whitelist) < 1) {
  zero_importance_features <- setdiff(current_features, current_model$importance$Feature) %>%
    setdiff(whitelist)
  if (length(zero_importance_features) > 0) {
    current_least_important <- zero_importance_features[1]
  } else {
    current_least_important <-
      tail(setdiff(current_model$importance$Feature, whitelist), 1)
  }
  test_features <-
    setdiff(current_features, current_least_important)
  current_model <-
    model_fit_wf(df_train, test_features, outcome_column, hyperparameters)
  instant_auc_loss <-
    tail(selection_results %>% filter(Dropped) %>% .$`CV AUC`, n = 1) - current_model$cv_auc
  current_auc_loss <- full_model$cv_auc - current_model$cv_auc

  if (instant_auc_loss < max_auc_loss / 5 &
      current_auc_loss < max_auc_loss) {
    dropped <- TRUE
    current_features <- test_features
  } else {
    dropped <- FALSE
    whitelist <- c(whitelist, current_least_important)
  }

  selection_results <- selection_results %>%
    add_row(
      `Tested Feature` = current_least_important,
      `Dropped` = dropped,
      `Number of Features` = length(test_features),
      `CV AUC` = current_model$cv_auc,
      `CV AUC Std Error` = current_model$cv_auc_std_err,
      `Total AUC Loss` = current_auc_loss,
      `Instant AUC Loss` = instant_auc_loss
    )

  print(c(
    length(current_features),
    round(current_auc_loss, 4),
    round(instant_auc_loss, 4),
    current_least_important
```

```
  ))
}
```

```
## [1] "43"          "0.0186"      "0.0237"      "year_adm_t0"
```

```
selection_results %>%
  rename(Features = `Number of Features`) %>%
  niceFormatting(digits = 4, label = 1)
```

Table 1:

Tested Feature	Dropped	Features	CV AUC	CV AUC Std Error	Total AUC Loss	Instant AUC Loss
None	TRUE	83	0.8088	0.0072	0.0000	0.0000
All unimportant	TRUE	43	0.8139	0.0055	-0.0051	-0.0051
year_adm_t0	FALSE	42	0.7902	0.0058	0.0186	0.0237

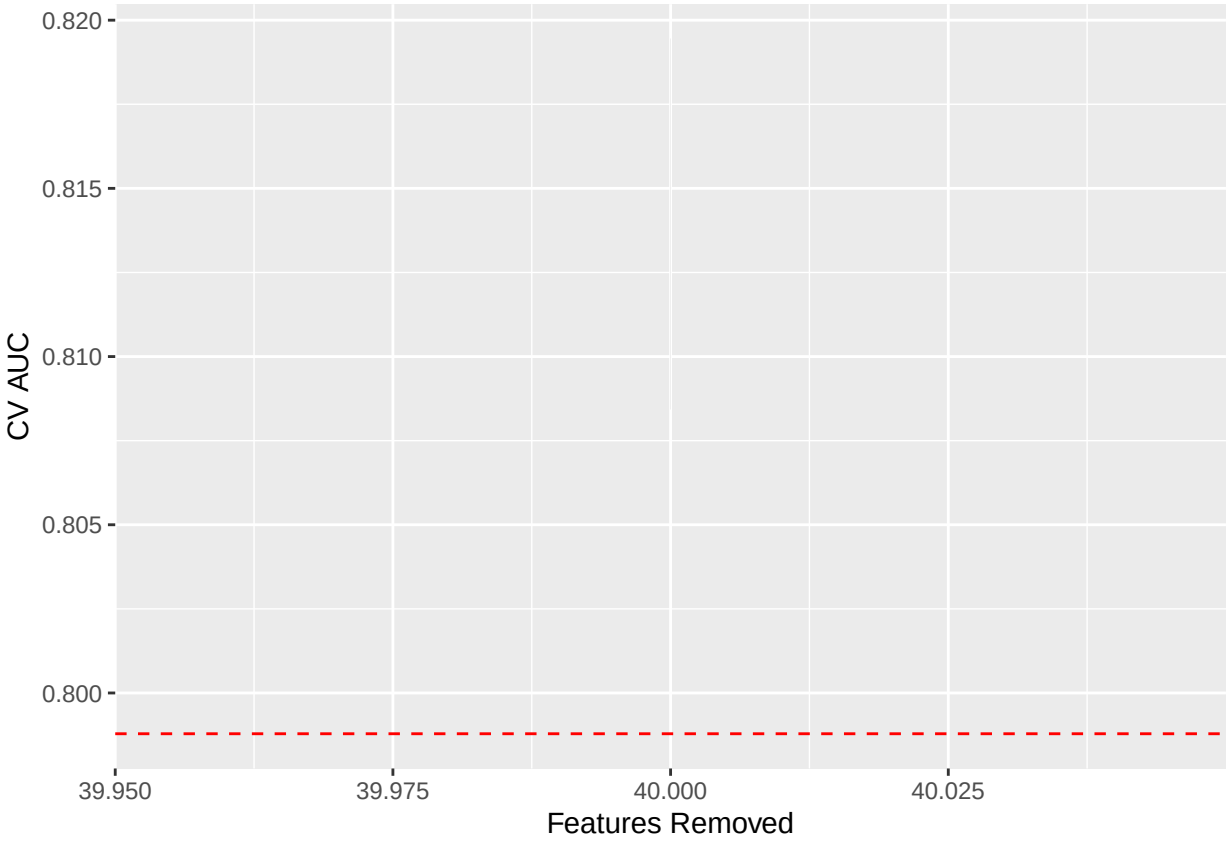
```
if (exists('last_feature_dropped')) {
  selected_features <- c(current_features, last_feature_droped)
} else {
  selected_features <- current_features
}

con <- file(sprintf('./auxiliar/final_model/selected_features/%s.yaml', outcome_column), "w")
write_yaml(selected_features, con)
close(con)

feature_selected_model <- model_fit_wf(df_train, selected_features,
                                       outcome_column, hyperparameters)

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

```
## [1] "Selected Model CV Train AUC: 0.814"
```

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

```
## [1] "Selected Model Test AUC: 0.798"
```

```
 selection_results <- selection_results %>%
  filter(`Number of Features` < length(features)) %>%
  mutate(`Features Removed` = length(features) - `Number of Features`,
         `CV AUC Low` = `CV AUC` - `CV AUC Std Error`,
         `CV AUC High` = `CV AUC` + `CV AUC Std Error`)

selection_results %>%
  filter(Dropped) %>%
  ggplot(aes(x = `Features Removed`, y = `CV AUC`,
             ymin = `CV AUC Low`, ymax = `CV AUC High`)) +
  geom_line() +
  geom_ribbon(alpha = .3) +
  geom_hline(yintercept = full_model$cv_auc - max_auc_loss,
             linetype = "dashed", color = "red")
```



Hyperparameter tuning

Selected features:

```
gluedown::md_order(selected_features, seq = TRUE, pad = TRUE)
```

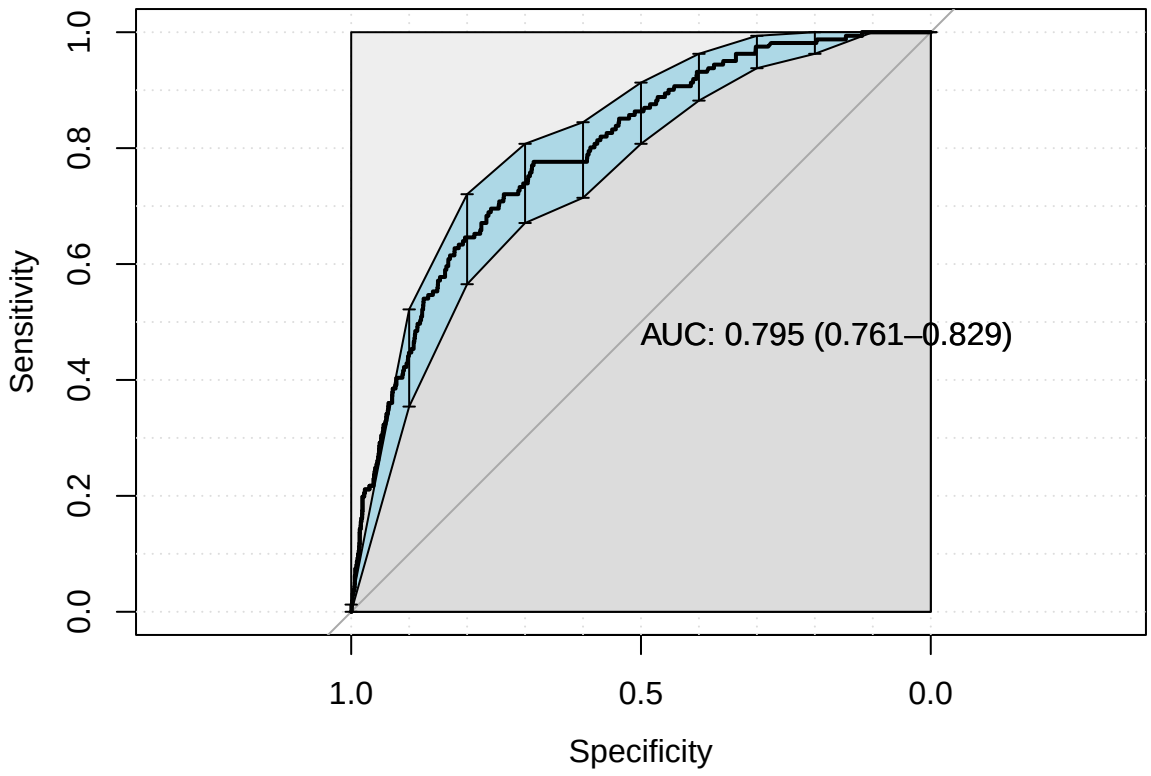
1. aco
2. admission_pre_t0_count
3. age
4. analises_clinicas_qtde
5. antiarritmico
6. antifungico
7. cateter_venoso_central
8. cateterismo
9. cied_final_group_1
10. citologia
11. classe_meds_qtde
12. comorbidities_count
13. diabetes
14. diuretico
15. dva
16. ecocardiograma
17. education_level
18. endoscopia
19. equipe_multiprof
20. espironolactona
21. estatina
22. exames_imagem_qtde
23. flebografia
24. hemodialysis
25. hospital_stay
26. icu_t0
27. ieca_bra

28. insuf_cardiaca
29. interconsulta
30. meds_antimicrobianos
31. meds_cardiovasc_qtde
32. metodos_graficos_qtde
33. nyha_basal
34. outros_proced_cirurgicos
35. proced_invasivos_qtde
36. procedure_type_new
37. psicofarmacos
38. sex
39. teste_esforco
40. ultrassom
41. valvopathy
42. vasodilatador
43. year_adm_t0

Standard

```
lightgbm_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train %>% 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())

lightgbm_tuning <- function(recipe) {

  lightgbm_spec <- boost_tree(
    trees = tune(),
    min_n = tune(),
    tree_depth = tune(),
    learn_rate = tune(),
    loss_reduction = tune(),
    sample_size = 1.0
  ) %>%
    set_engine("lightgbm") %>%
    set_mode("classification")

  lightgbm_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(),
    size = grid_size
  )

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

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

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

```
    niceFormatting(digits = 5, label = 4)

  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)

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

  return(list(auc = as.numeric(lightgbm_auc$auc),
              auc_lower = lightgbm_auc$ci[1],
              auc_upper = lightgbm_auc$ci[3],
              parameters = lightgbm_parameters,
              fit = final_lightgbm_fit))
}

standard_results <- lightgbm_tuning(lightgbm_recipe)
```

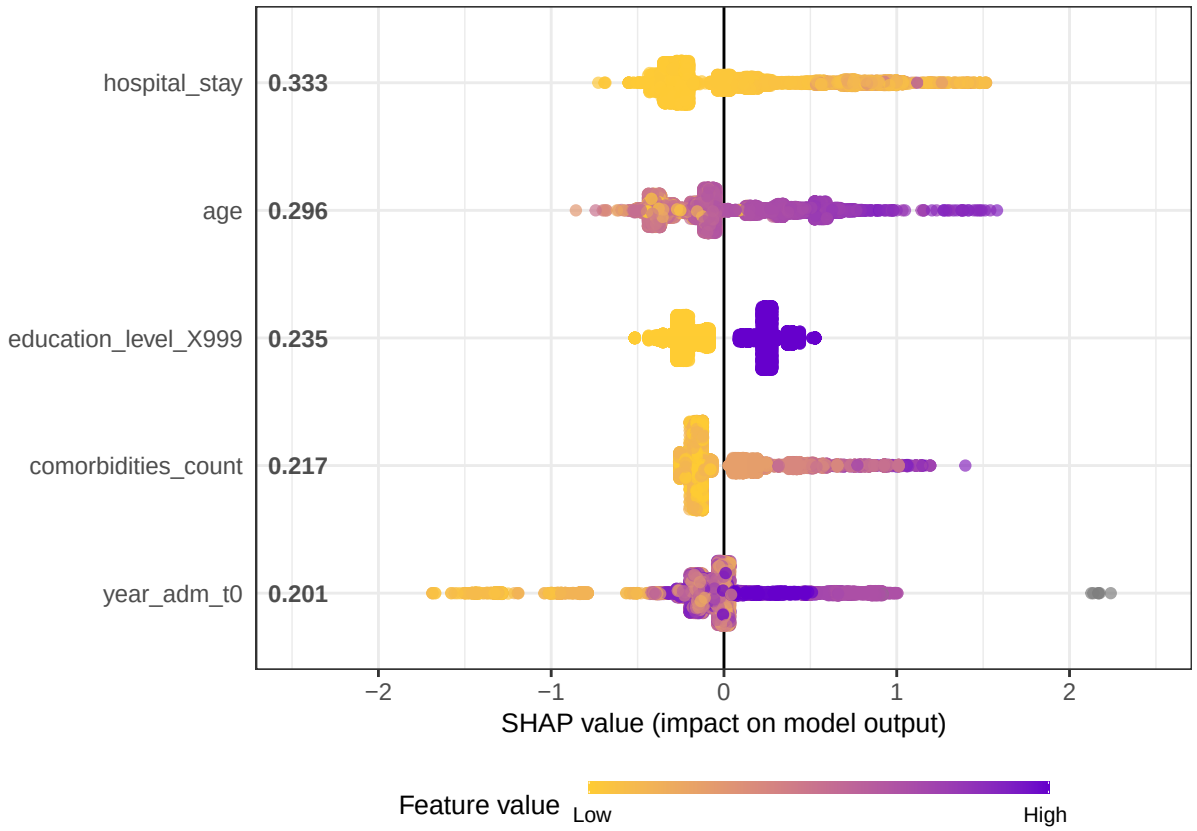


```
## [1] "Optimal Threshold: 0.02"
## Confusion Matrix and Statistics
##
##     reference
## data    0    1
##    0 3131   36
##    1 1438  125
##
##                Accuracy : 0.6884
##                  95% CI : (0.675, 0.7016)
##     No Information Rate : 0.966
##     P-Value [Acc > NIR] : 1
##
##                   Kappa : 0.0888
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.68527
##             Specificity : 0.77640
##          Pos Pred Value : 0.98863
##          Neg Pred Value : 0.07997
##              Prevalence : 0.96596
##          Detection Rate : 0.66195
##    Detection Prevalence : 0.66956
##       Balanced Accuracy : 0.73083
##
##        'Positive' Class : 0
##
```

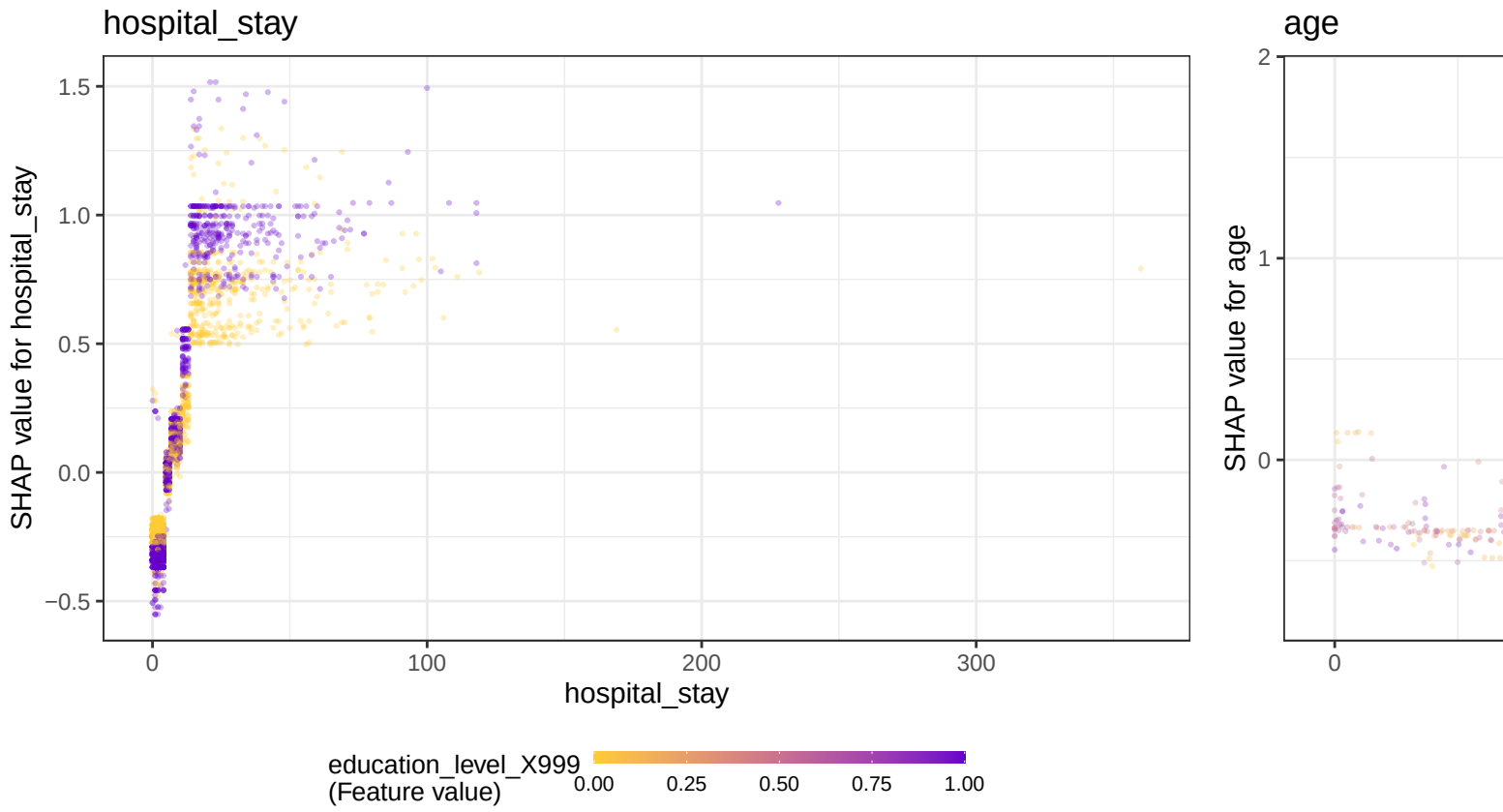
```
final_lightgbm_fit <- standard_results$fit
lightgbm_parameters <- standard_results$parameters

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

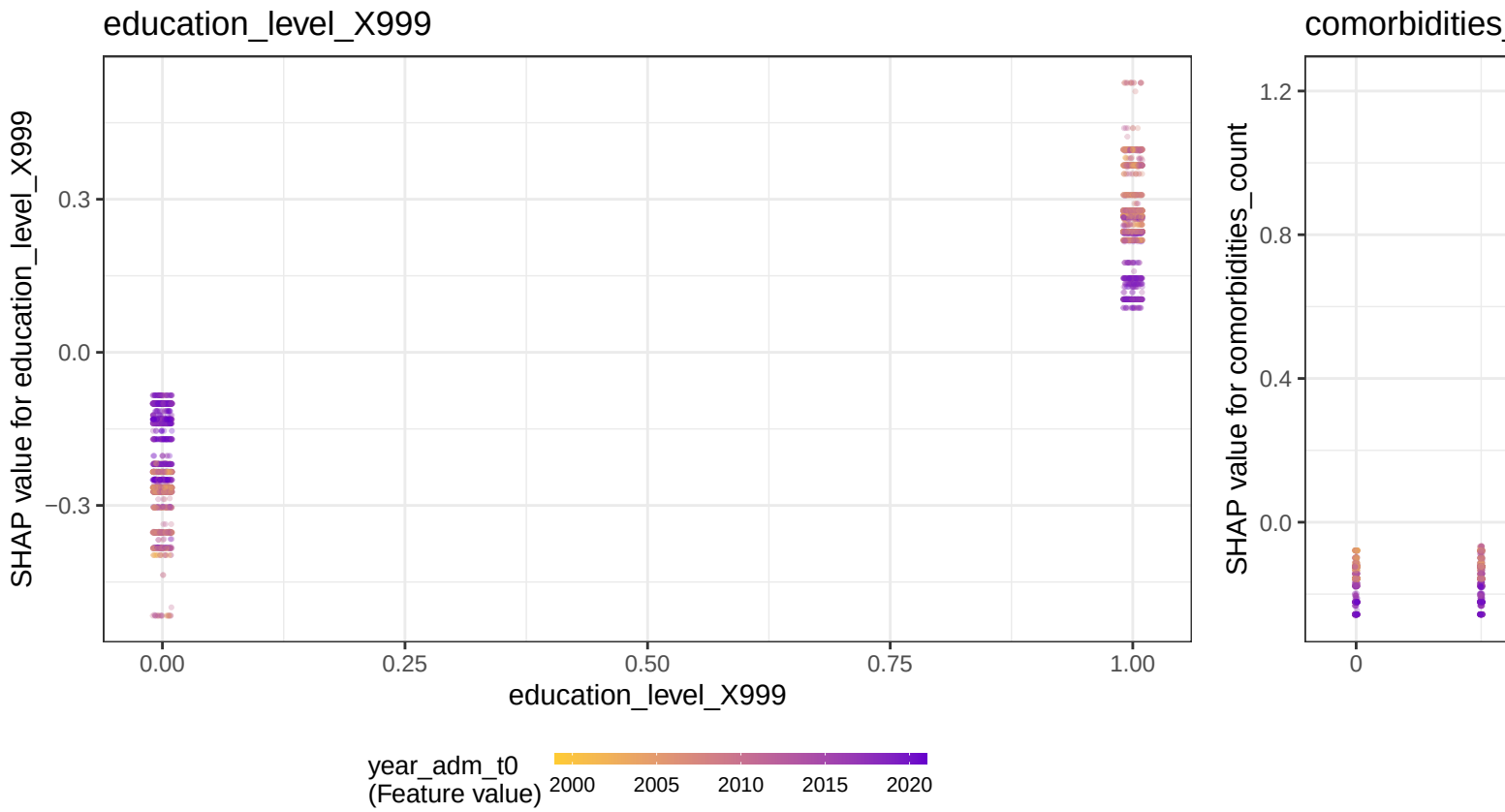
SHAP values

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

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)))

n_plots <- min(5, length(selected_features))

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

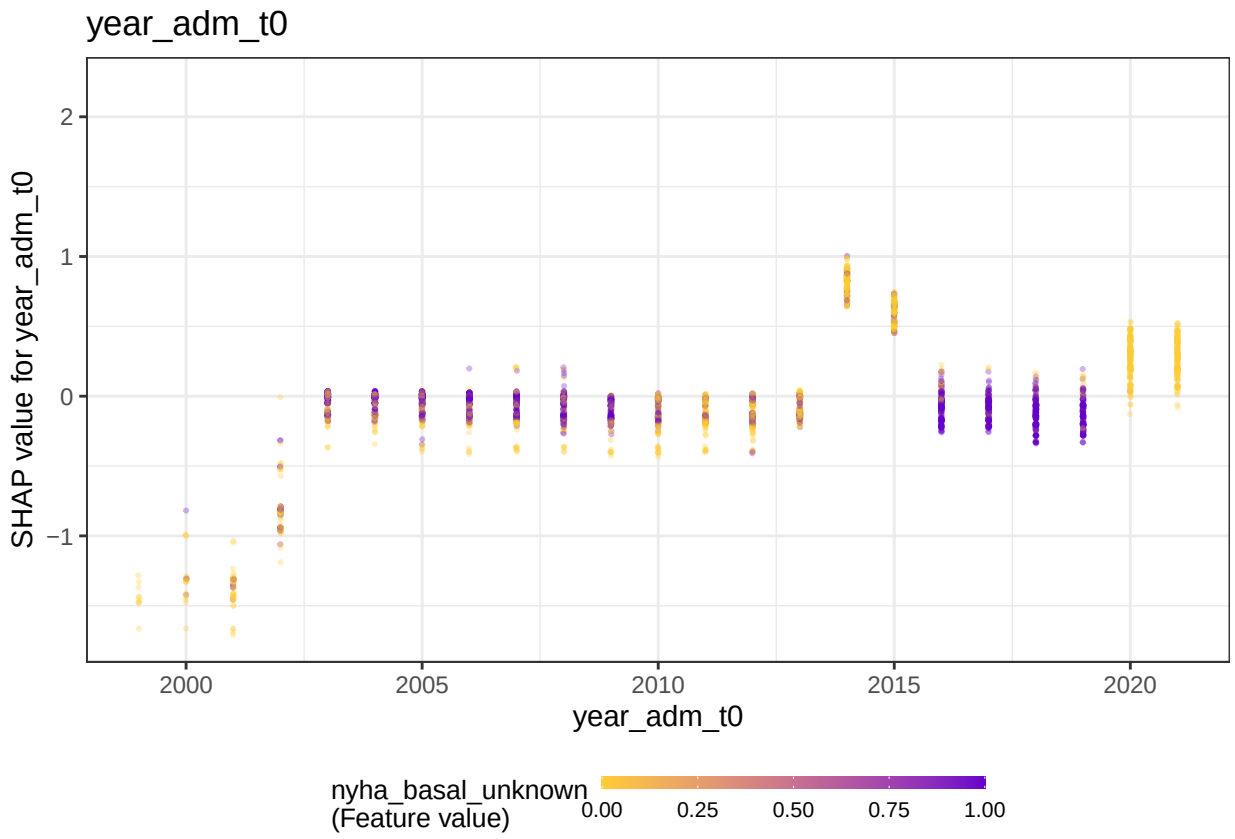



```
shap <- shap.prep(lightgbm_model, X_train = matrix_test)

for (x in shap.importance(shap, names_only = TRUE)[1:n_plots]) {
  p <- shap.plot.dependence(
    shap,
    x = x,
    color_feature = "auto",
    smooth = FALSE,
    jitter_width = 0.01,
    alpha = 0.3
  ) +
    labs(title = x)
  print(p)
}
```






```
## Warning: Removed 10 rows containing missing values (geom_point).
```

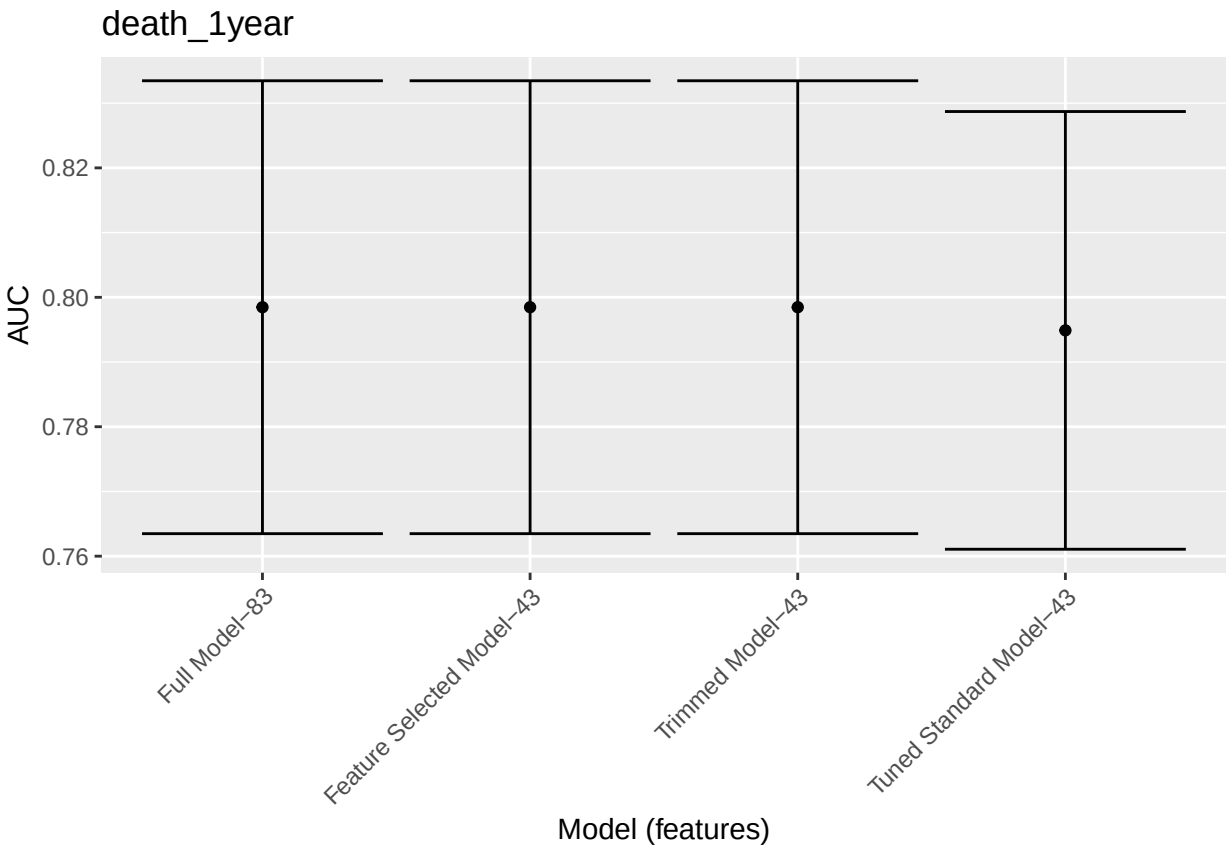



```
## $num_iterations
## [1] 63
##
## $learning_rate
## [1] 0.2356244
##
## $max_depth
## [1] 2
##
## $feature_fraction
## [1] 1
##
## $min_data_in_leaf
## [1] 4
##
## $min_gain_to_split
## [1] 2.100208e-08
##
## $bagging_fraction
## [1] 1
##
## $num_class
## [1] 1
##
## $objective
## [1] "binary"
##
## $num_threads
## $num_threads$num_threads
## [1] 0
##
##
## $seed
```

```
## [1] 29668
##
## $deterministic
## [1] TRUE
##
## $verbose
## [1] -1
##
## $metric
## list()
##
## $interaction_constraints
## list()
##
## $feature_pre_filter
## [1] FALSE
```

Models Comparison

```
df_auc <- tibble::tribble(
  ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`, ~`Features`,
  'Full Model', full_model$auc, full_model$auc_lower, full_model$auc_upper, length(features),
  'Trimmed Model', trimmed_model$auc, trimmed_model$auc_lower, trimmed_model$auc_upper, length(trimmed_features)
  'Feature Selected Model', feature_selected_model$auc, feature_selected_model$auc_lower, feature_selected_model
  'Tuned Standard Model', standard_results$auc, standard_results$auc_lower, standard_results$auc_upper, length(s
) %>%
  mutate(Target = outcome_column,
         `Model (features)` = fct_reorder(paste0(Model, "-", Features), -Features))

df_auc %>%
  ggplot(aes(
    x = `Model (features)`,
    y = AUC,
    ymin = `Lower Limit`,
    ymax = `Upper Limit`
  )) +
  geom_point() +
  geom_errorbar() +
  labs(title = outcome_column) +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))
```




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