Final Model - death_2year

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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)
```

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))
```

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_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)
}
```

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. 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. admission_t0_emergency
30. aco
31. antiarritmico
32. ieca_bra
33. dva
34. digoxina
35. estatina
36. diuretico
37. vasodilatador
38. insuf_cardiaca
39. espironolactona
40. antiplaquetario_ev
41. insulina
42. psicofarmacos
43. antifungico
44. antiviral
45. classe_meds_qtde
46. meds_cardiovasc_qtde
47. meds_antimicrobianos
48. vni
49. outros_proced_cirurgicos
50. icp
51. angioplastia

52. cateterismo
53. cateter_venoso_central
54. proced_invasivos_qtde
55. transfusao
56. interconsulta
57. equipe_multiprof
58. ecg
59. holter
60. teste_esforco
61. tilt_teste
62. metodos_graficos_qtde
63. laboratorio
64. cultura
65. analises_clinicas_qtde
66. citologia
67. histopatologia_qtde
68. angio_tc
69. cintilografia
70. ecocardiograma
71. endoscopia
72. flebografia
73. pet_ct
74. ultrassom
75. tomografia
76. radiografia
77. ressonancia
78. exames_imagem_qtde
79. bic

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)))
```

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
```

Functions

```
niceFormatting = function(df, caption="", digits = 2, font_size = NULL){
  df %>%
    kbl(booktabs = T, longtable = T, caption = caption, digits = digits, format = "latex") %>%
```

```
    kable_styling(font_size = font_size,
                  latex_options = c("striped", "HOLD_position", "repeat_header"))
}
```

```
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)
}
```

Feature Selection

```
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_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]))
}
```

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

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: 0.761"
```

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

```
## [1] "Full Model Test AUC: 0.771"
```

Features with zero importance on the initial model:

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

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

1. heart_disease
2. hemodialysis
3. dialysis_t0
4. antiviral
5. vni
6. icp
7. cateter_venoso_central
8. transfusao
9. teste_esforco
10. citologia

11. angio_tc
12. flebografia
13. pet_ct

```
trimmed_features <- full_model$importance$Feature
hyperparameters$mtry = min(hyperparameters$mtry, length(trimmed_features))
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: 0.757"
```

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

```
## [1] "Trimmed Model Test AUC: 0.768"
```

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

if (full_model$cv_auc - trimmed_model$cv_auc < max_auc_loss) {
  current_features <- trimmed_features
  current_model <- trimmed_model
  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(trimmed_features),
            `AUC Loss` = current_auc_loss,
            `Least Important Feature` = current_least_important)
} else {
  current_features <- features
  current_model <- full_model
  current_least_important <- tail(current_model$importance$Feature, 1)
  current_auc_loss <- 0
}

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(df_train, 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))
}

selection_results %>% niceFormatting(digits = 4)
```

Table 1:

Number of Features	AUC Loss	Least Important Feature
79	0.0000	angioplastia
66	0.0031	underlying_heart_disease
65	0.0050	histopatologia_qtde
64	0.0036	antifungico
63	0.0042	copd
62	0.0050	tilt_teste
61	0.0037	bic
60	0.0035	procedure_type_new
59	0.0048	reop_type_1
58	0.0054	endoscopia
57	0.0065	nyha_basal
56	0.0073	ressonancia
55	0.0080	holter
54	0.0069	insulina
53	0.0082	cardiac_arrest
52	0.0087	procedure_type_1
51	0.0104	tomografia

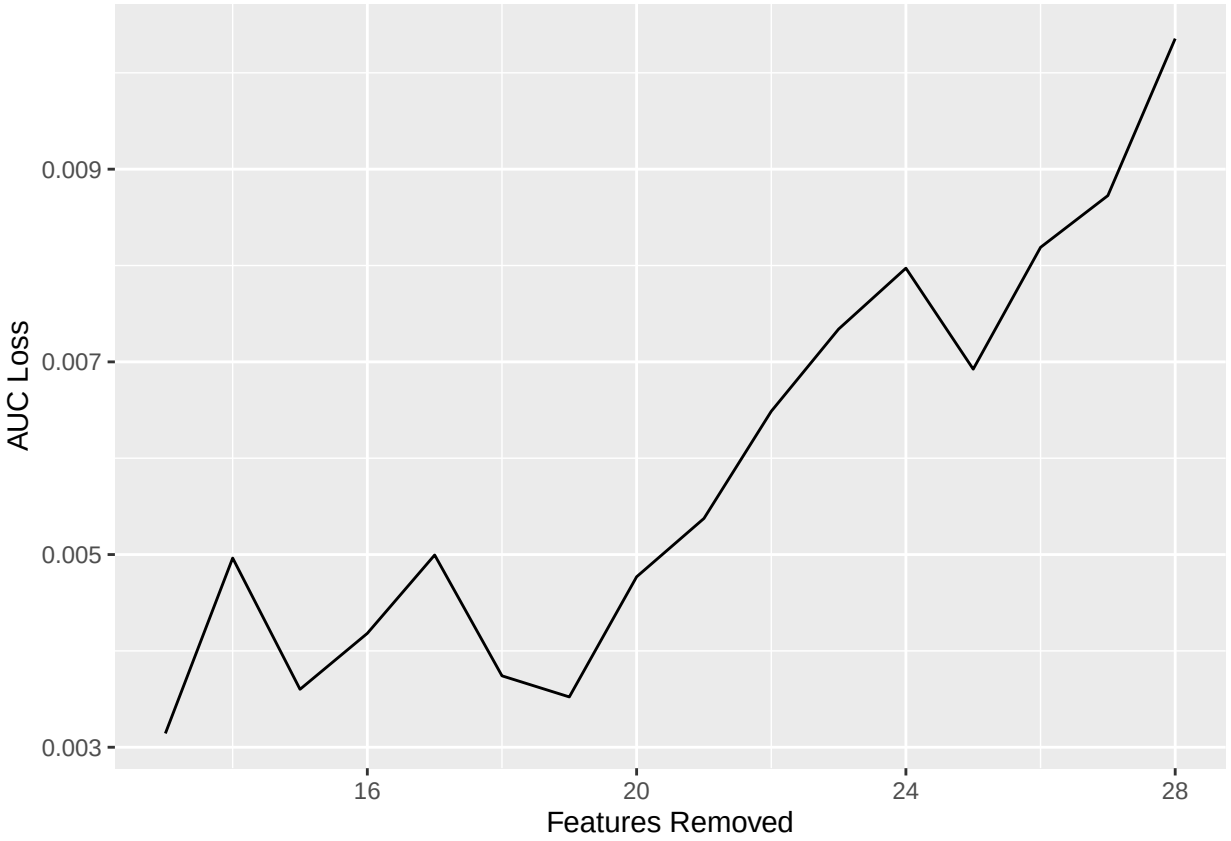
```
if (exists('last_feature_dropped')) {
  selected_features <- c(current_features, last_feature_droped)
} else {
  selected_features <- current_features
}

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

```
## [1] "Trimmed Model CV Train AUC: 0.752"
```

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

```
## [1] "Trimmed Model Test AUC: 0.756"
```

```
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()
```



Hyperparameter tuning

Selected features:

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

1. laboratorio
2. vasodilatador
3. analises_clinicas_qtde
4. admission_pre_t0_count
5. espironolactona
6. age
7. year_adm_t0
8. comorbidities_count
9. meds_cardiovasc_qtde
10. icu_t0
11. cied_final_group_1
12. admission_pre_t0_180d
13. diuretico
14. antiarritmico
15. equipe_multiprof
16. classe_meds_qtde
17. meds_antimicrobianos
18. psicofarmacos
19. metodos_graficos_qtde
20. ecg
21. insuf_cardiaca
22. estatina
23. ieca_bra
24. dva
25. radiografia
26. exames_imagem_qtde
27. ultrassom
28. proced_invasivos_qtde

29. cied_final_1
30. ecocardiograma
31. admission_t0_emergency
32. interconsulta
33. af
34. heart_failure
35. prior_mi
36. cateterismo
37. cintilografia
38. valvopathy
39. digoxina
40. aco
41. hypertension
42. cultura
43. diabetes
44. tomografia
45. education_level
46. renal_failure
47. sex
48. outros_proced_cirurgicos
49. stroke
50. antiplaquetario_ev
51. angioplastia

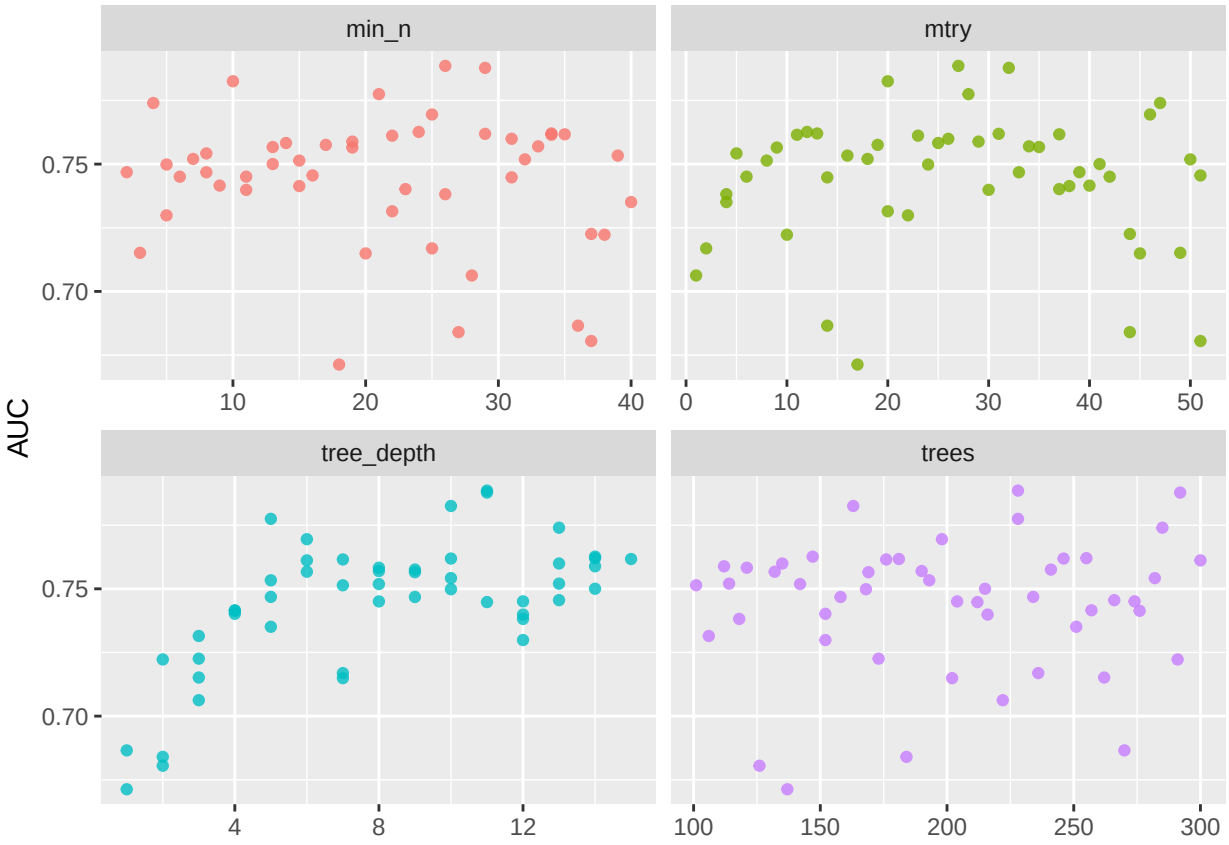
```
lightgbm_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train %>% dplyr::select(all_of(c(selected_features, outcome_column)))) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), 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") %>%
  niceFormatting(digits = 5)
```

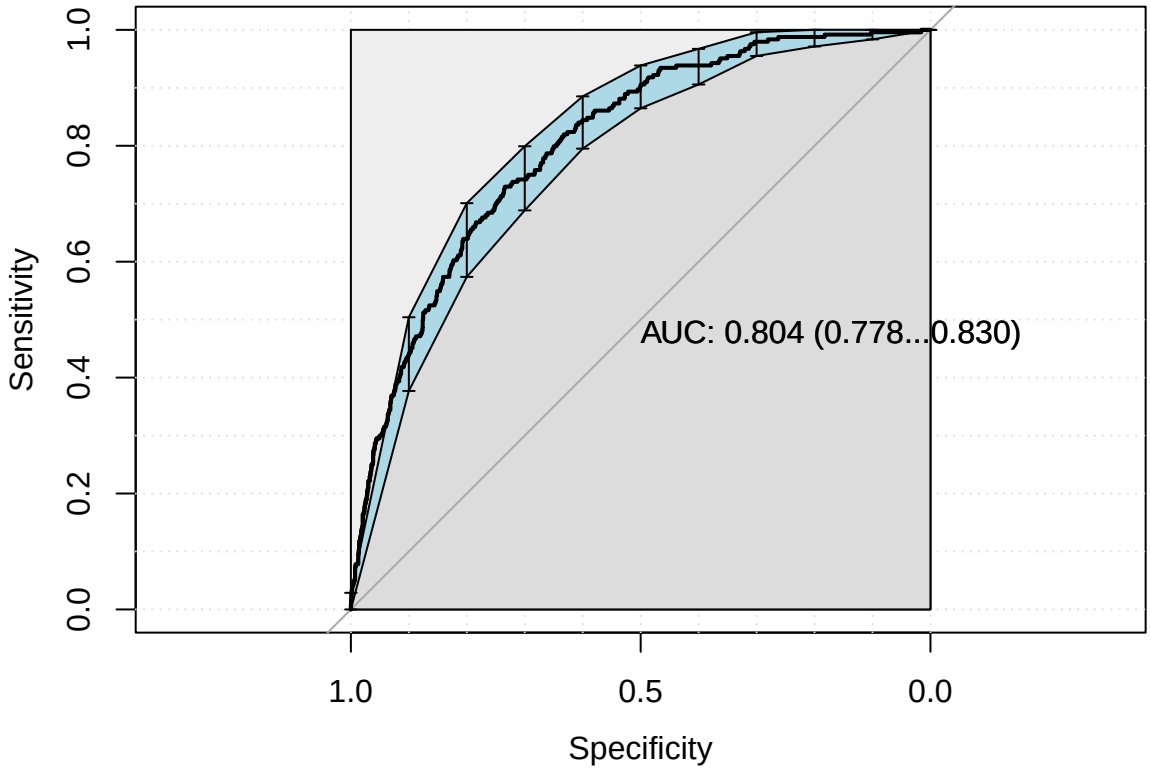
Table 2:

mtry	trees	min_n	tree_depth	learn_rate	loss_reduction	.metric	.estimator	mean	n	std_err	.config
27	228	26	11	0.01592	0.00007	roc_auc	binary	0.78857	4	0.01289	Preprocessor1_
32	292	29	11	0.01002	0.00000	roc_auc	binary	0.78781	4	0.01329	Preprocessor1_
20	163	10	10	0.02782	0.00085	roc_auc	binary	0.78253	4	0.01324	Preprocessor1_
28	228	21	5	0.00597	0.38249	roc_auc	binary	0.77747	4	0.01205	Preprocessor1_
47	285	4	13	0.00487	0.00001	roc_auc	binary	0.77400	4	0.01449	Preprocessor1_

```
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)
```



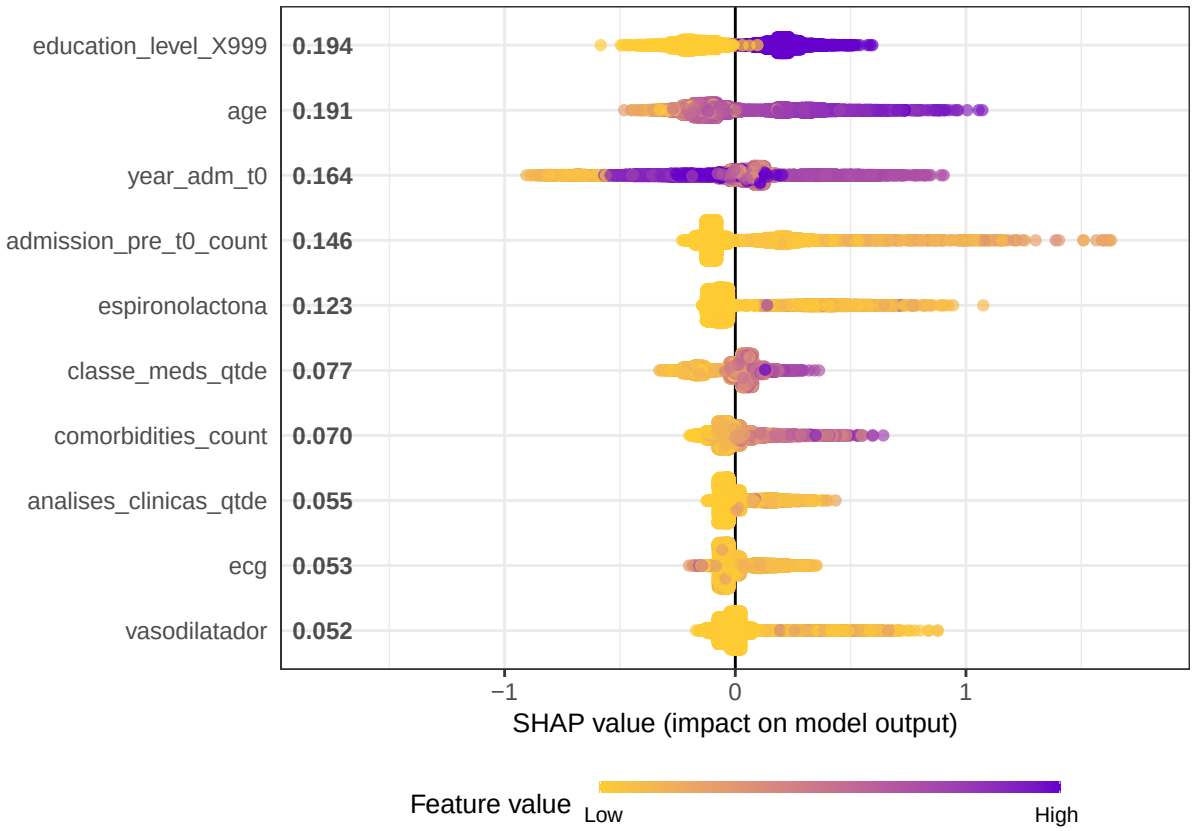

```
##   |
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4485  241
##                      1    1    3
##
##                Accuracy : 0.9488
##                  95% CI : (0.9422, 0.9549)
##     No Information Rate : 0.9484
##     P-Value [Acc > NIR] : 0.4646
##
##                   Kappa : 0.0226
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.9998
##             Specificity : 0.0123
##          Pos Pred Value : 0.9490
##          Neg Pred Value : 0.7500
##              Prevalence : 0.9484
##          Detection Rate : 0.9482
##    Detection Prevalence : 0.9992
```

```
##       Balanced Accuracy : 0.5060
##
##        '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

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)))

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




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

```r
for (x in shap.importance(shap, names_only = TRUE)[1:5]) {
  p <- shap.plot.dependence(
    shap,
    x = x,
    color_feature = "auto",
    smooth = TRUE,
    jitter_width = 0.01,
    alpha = 0.3
  ) +
    labs(title = x)
  print(p)
}
```

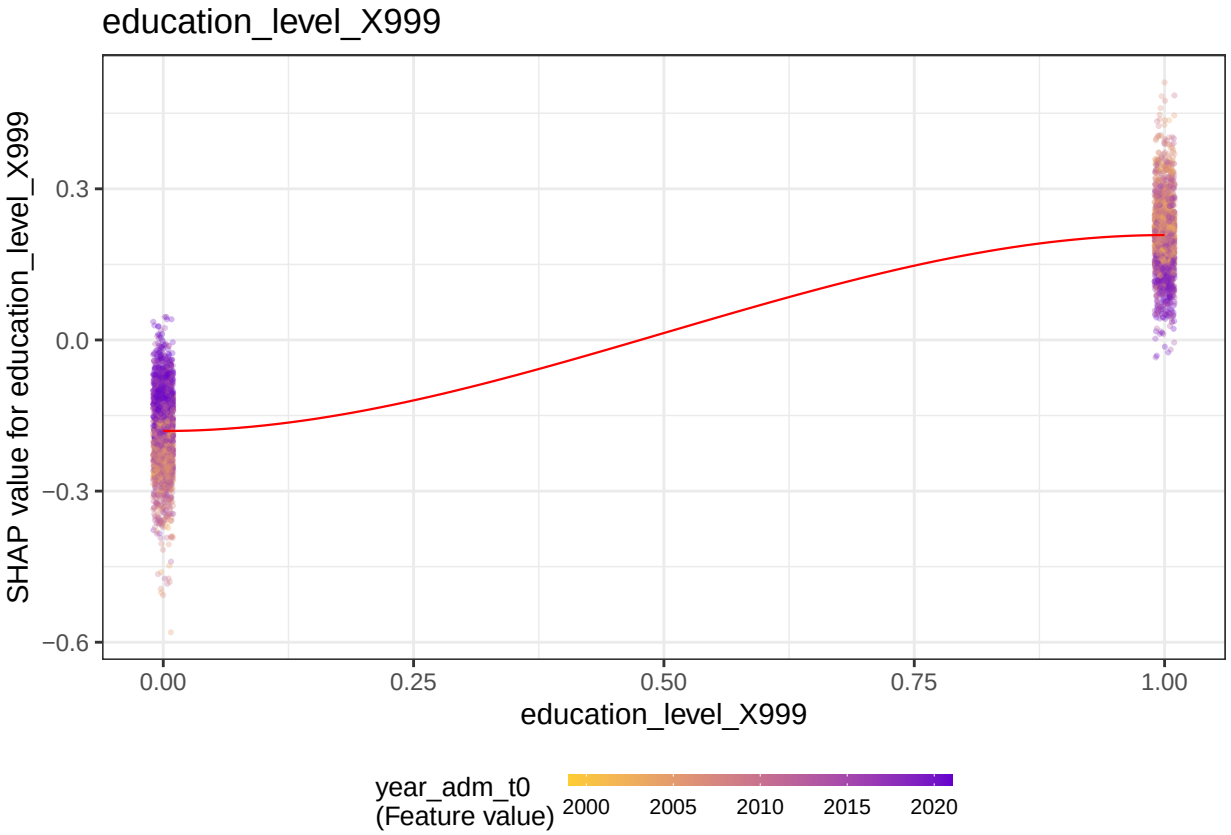
```
## `geom_smooth()` using formula 'y ~ x'
```

```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : pseudoinverse used at -0.00
```

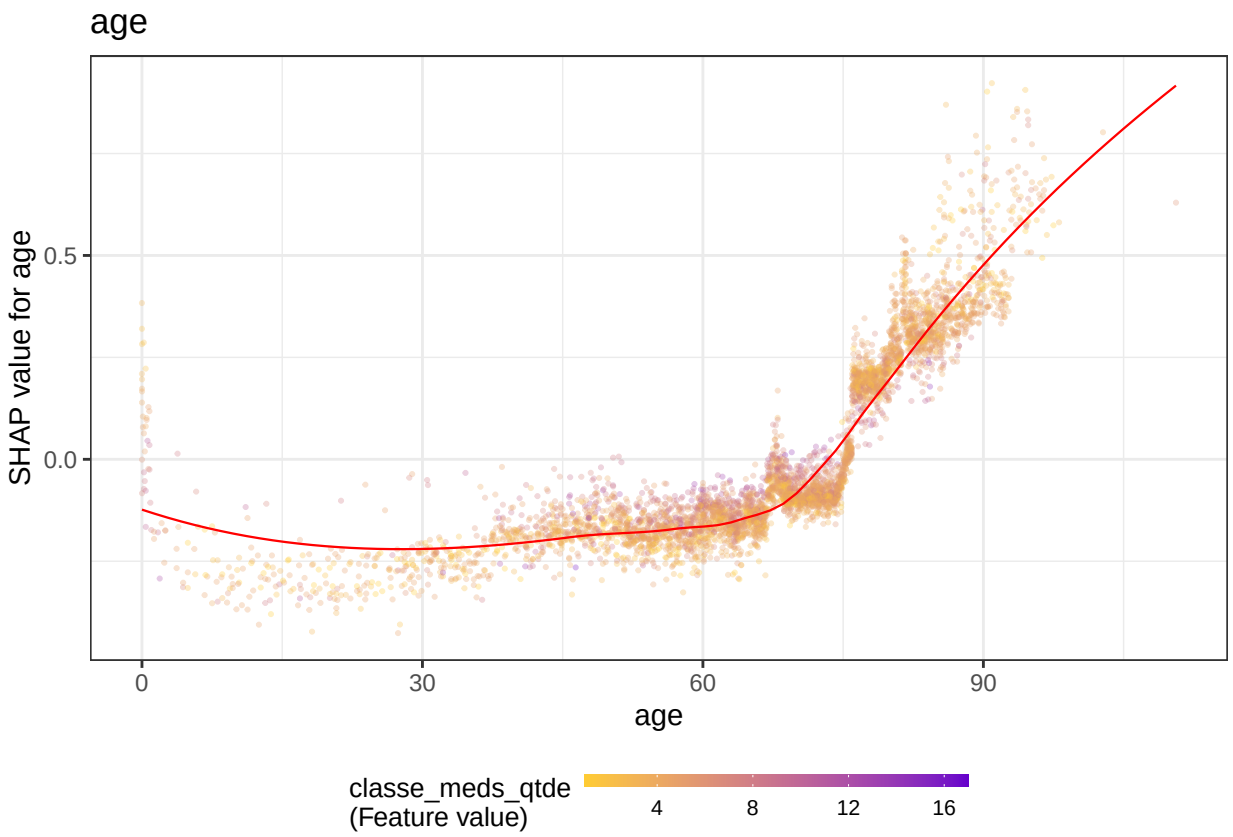
```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : neighborhood radius 1.005
```

```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : reciprocal condition number
```

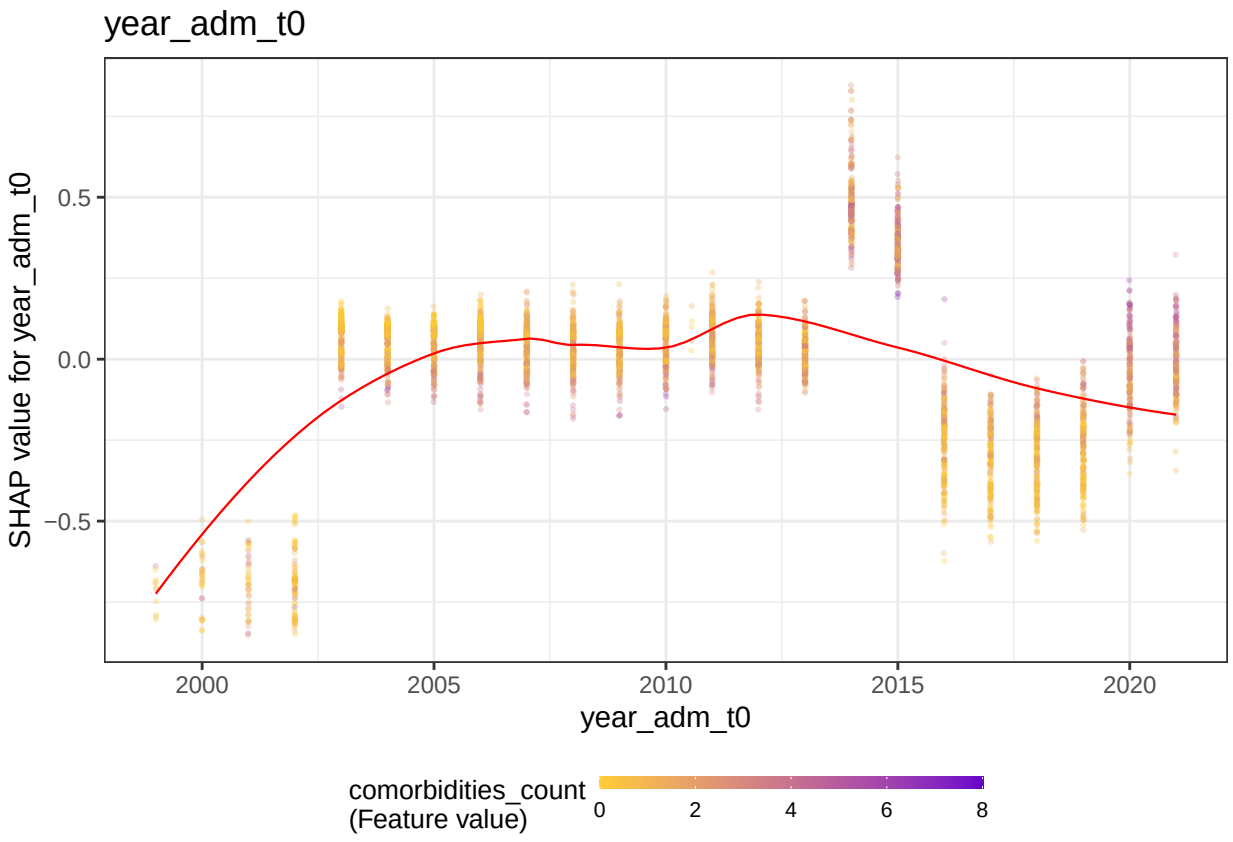
```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : There are other near singul
## well. 1.01
```




```
## `geom_smooth()` using formula 'y ~ x'
```

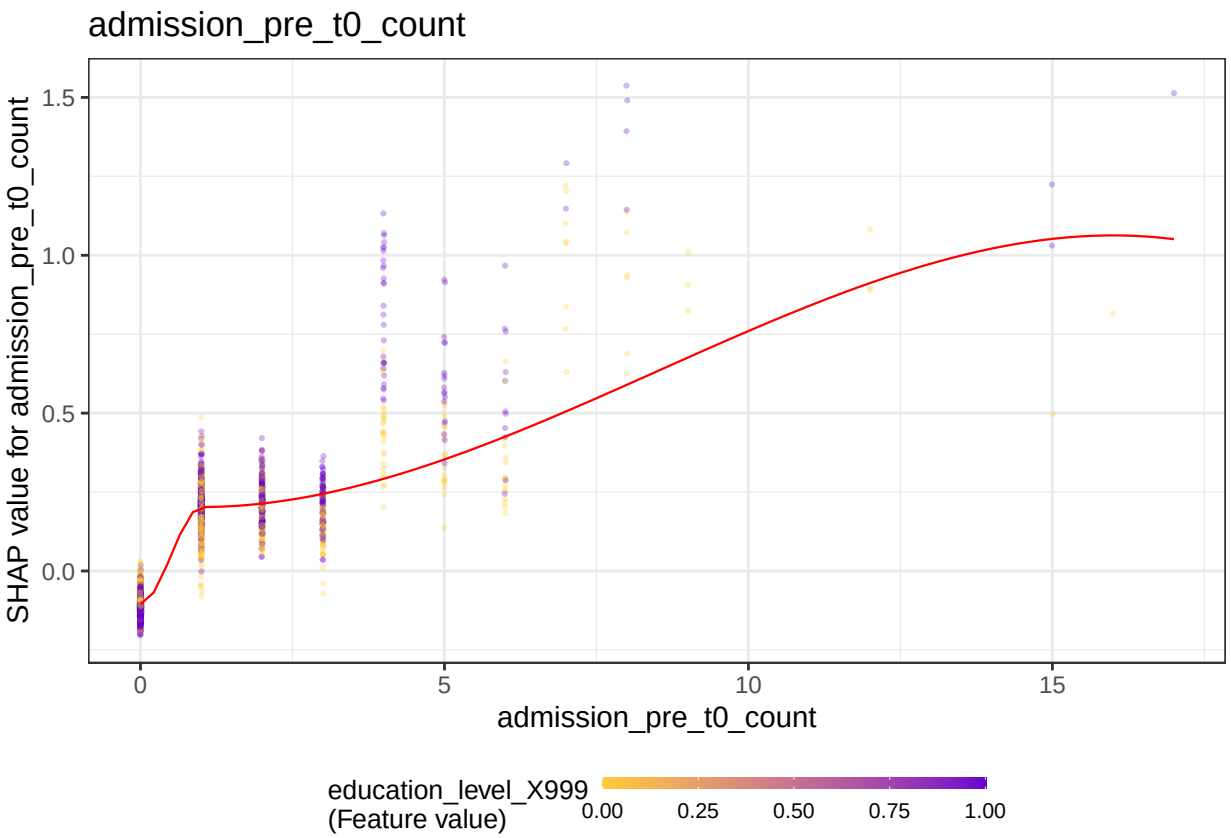



```
## `geom_smooth()` using formula 'y ~ x'
```

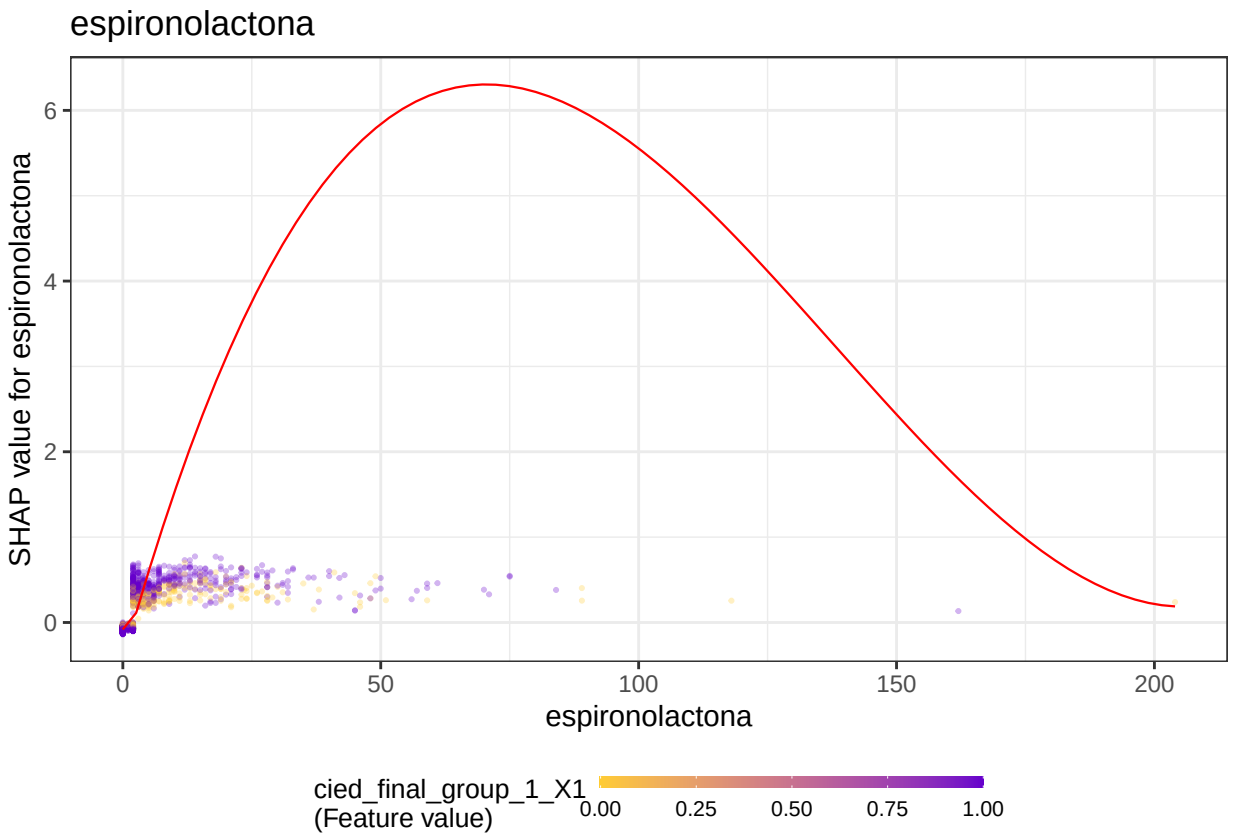



```
## `geom_smooth()` using formula 'y ~ x'
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : pseudoinverse used at -0.08
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : neighborhood radius 1.085
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : reciprocal condition number
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : There are other near singul
```

```
## well. 1
```

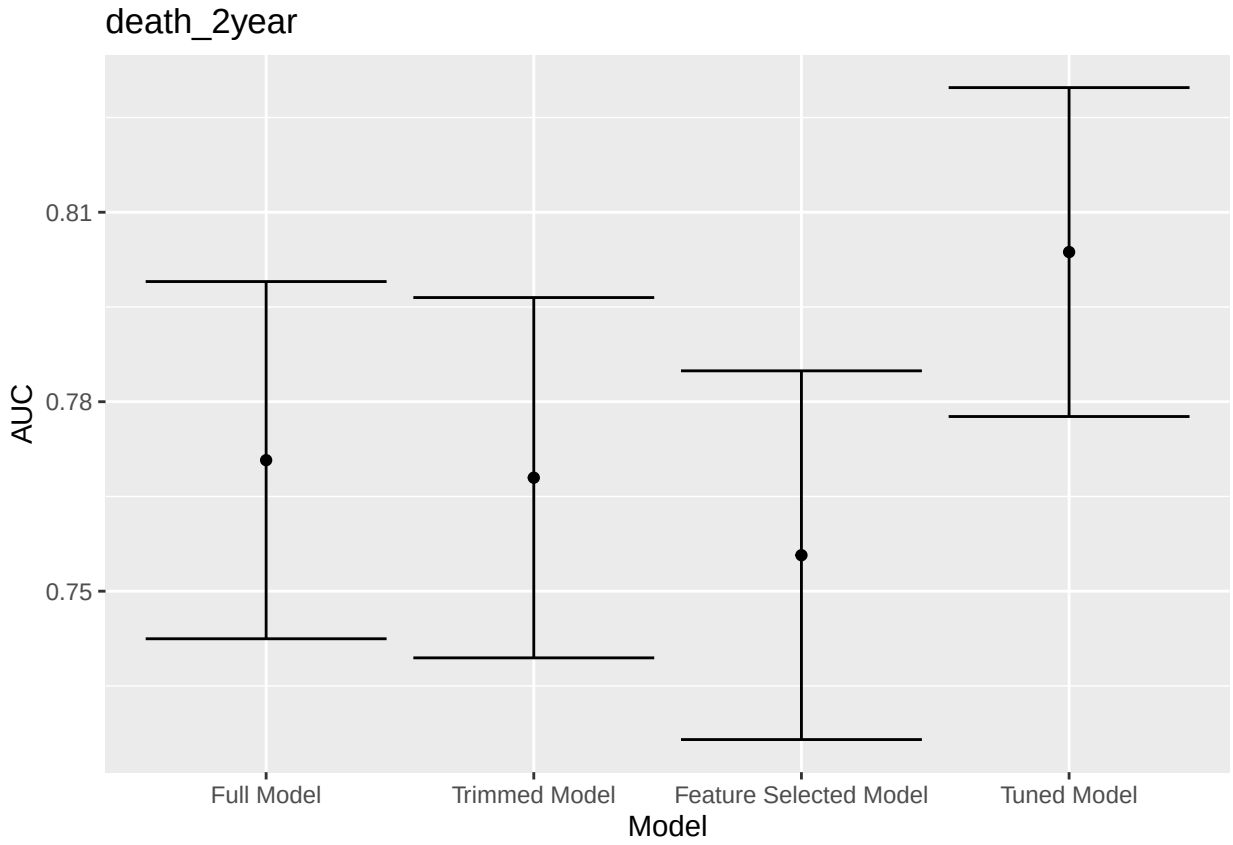



```
## `geom_smooth()` using formula 'y ~ x'
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : pseudoinverse used at -1.02
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : neighborhood radius 2.9806
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : reciprocal condition number
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : There are other near singul
## well. 3.8441
```



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$ci[3],
  # 'Oversampled Model', as.numeric(oversampled_model$auc), oversampled_model$auc_lower, oversampled_model$auc_u
  # 'Undersampled Model', as.numeric(undersampled_model$auc), undersampled_model$auc_lower, undersampled_model$a
) %>%
  mutate(Target = outcome_column,
         Model = factor(Model,
                        levels = c('Full Model', 'Trimmed Model',
                                   'Feature Selected Model', 'Tuned Model',
                                   'Oversampled Model', 'Undersampled Model')))

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




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