Final Model - readmission_180d

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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. patient_state
5. underlying_heart_disease
6. heart_disease
7. nyha_basal
8. prior_mi
9. heart_failure
10. af
11. cardiac_arrest
12. transplant
13. valvopathy
14. endocardites
15. diabetes
16. renal_failure
17. hemodialysis
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. icu_t0
28. dialysis_t0
29. n_procedure_t0
30. admission_t0_emergency
31. aco
32. antiarritmico
33. betabloqueador
34. ieca_bra
35. dva
36. digoxina
37. estatina
38. diuretico
39. vasodilatador
40. insuf_cardiaca
41. espironolactona
42. bloq_calcio
43. antiplaquetario_ev
44. insulina
45. anticonvulsivante
46. psicofarmacos
47. antifungico
48. antiviral
49. antiretroviral
50. classe_meds_qtde
51. meds_cardiovasc_qtde

52. meds_antimicrobianos
53. vni
54. cec
55. transplante_cardiaco
56. cir_toracica
57. outros_proced_cirurgicos
58. icp
59. intervencao_cv
60. angioplastia
61. cateterismo
62. eletrofisiologia
63. cateter_venoso_central
64. proced_invasivos_qtde
65. cve_desf
66. transfusao
67. interconsulta
68. equipe_multiprof
69. ecg
70. holter
71. teste_esforco
72. espiro_ergoespiro
73. tilt_teste
74. metodos_graficos_qtde
75. laboratorio
76. cultura
77. analises_clinicas_qtde
78. citologia
79. biopsia
80. histopatologia_qtde
81. angio_rm
82. angio_tc
83. arteriografia
84. cintilografia
85. ecocardiograma
86. endoscopia
87. flebografia
88. pet_ct
89. ultrassom
90. tomografia
91. radiografia
92. ressonancia
93. exames_imagem_qtde
94. bic
95. mpp

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: 0.711"
```

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

```
## [1] "Full Model Test AUC: 0.692"
```

Features with zero importance on the initial model:

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

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

1. transplant
2. endocardites
3. renal_failure
4. hemodialysis
5. dialysis_t0
6. n_procedure_t0
7. antiretroviral
8. vni
9. transplante_cardiaco
10. cir_toracica
11. intervencao_cv
12. angioplastia
13. transfusao
14. espiro_ergoespiro
15. tilt_teste
16. angio_rm
17. arteriografia

```
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: 0.710"
```

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

```
## [1] "Trimmed Model Test AUC: 0.693"
```

```
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
95	0.0000	pet_ct
78	0.0015	valvopathy
77	0.0022	flebografia
76	0.0008	heart_disease
75	0.0015	teste_esforco
74	0.0023	insulina
73	0.0012	angio_tc
72	0.0029	antiviral
71	0.0011	underlying_heart_disease
70	0.0010	antiplaquetario_ev
69	0.0032	icp
68	0.0022	antifungico
67	0.0023	cec
66	0.0022	citologia
65	0.0035	cateter_venoso_central
64	0.0023	mpp
63	0.0021	cve_desf
62	0.0033	prior_mi
61	0.0034	cardiac_arrest
60	0.0043	heart_failure
59	0.0028	eletrofisiologia
58	0.0037	endoscopia
57	0.0033	copd
56	0.0051	pet_ct
55	0.0048	nyha_basal
54	0.0049	interconsulta
53	0.0057	holter
52	0.0057	education_level
51	0.0074	digoxina
50	0.0055	tomografia
49	0.0061	ultrassom
48	0.0074	diabetes
47	0.0074	af
46	0.0070	cateterismo
45	0.0072	cintilografia
44	0.0088	ressonancia
43	0.0086	anticonvulsivante
42	0.0099	cultura

Table 1: *(continued)*

Number of Features	AUC Loss	Least Important Feature
41	0.0089	admission_t0_emergency
40	0.0103	betabloqueador

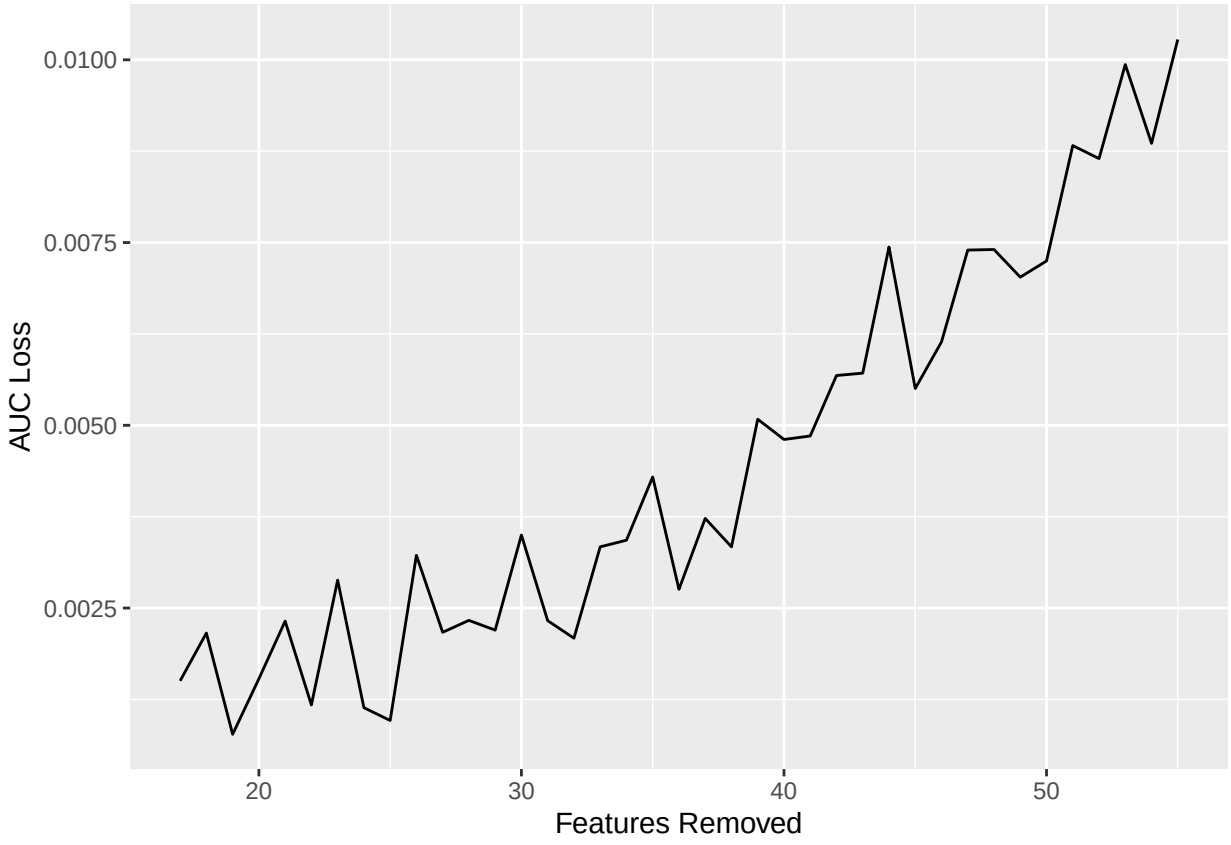
```
if (exists('last_feature_dropped')) {
  selected_features <- c(current_features, last_feature_droped)
} else {
  selected_features <- current_features
}

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: 0.701"
```

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

```
## [1] "Trimmed Model Test AUC: 0.686"
```

```
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. meds_cardiovasc_qtde
2. laboratorio
3. admission_pre_t0_count
4. analises_clinicas_qtde
5. vasodilatador
6. icu_t0
7. classe_meds_qtde
8. diuretico
9. antiarritmico
10. histopatologia_qtde
11. admission_pre_t0_180d
12. equipe_multiprof
13. age
14. cied_final_1
15. psicofarmacos
16. ecg
17. reop_type_1
18. bloq_calcio
19. exames_imagem_qtde
20. espironolactona
21. ecocardiograma
22. metodos_graficos_qtde
23. procedure_type_1
24. biopsia
25. insuf_cardiaca
26. dva
27. ieca_bra
28. meds_antimicrobianos
29. estatina
30. procedure_type_new
31. proced_invasivos_qtde
32. radiografia
33. cied_final_group_1
34. betabloqueador
35. comorbidities_count
36. aco
37. bic
38. outros_proced_cirurgicos
39. patient_state
40. sex

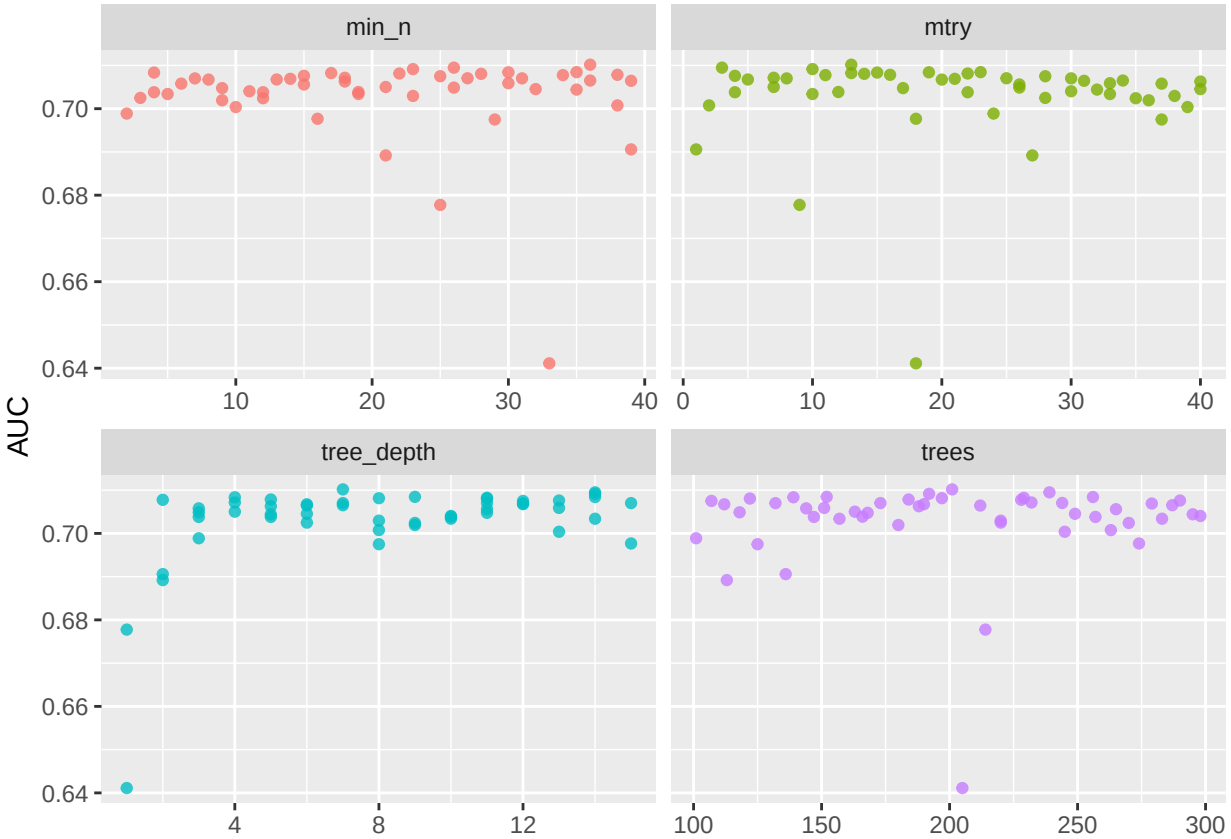
```
lightgbm_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train %>% dplyr::select(all_of(c(selected_features, outcome_column)))) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(),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

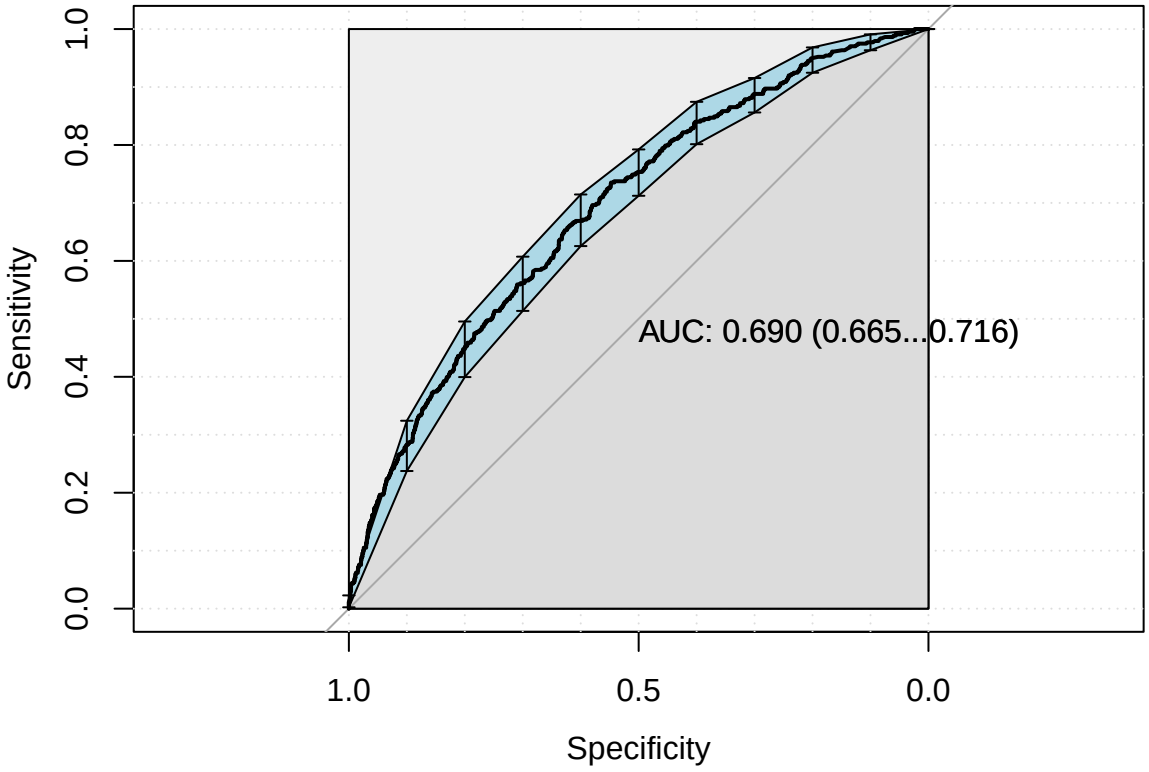
Table 2:

mtry	trees	min_n	tree_depth	learn_rate	loss_reduction	.metric	.estimator	mean	n	std_err	.config
13	201	36	7	0.00001	3e-05	roc_auc	binary	0.71017	4	0.00960	Preprocessor1_
3	239	26	14	0.01074	0e+00	roc_auc	binary	0.70949	4	0.01020	Preprocessor1_
10	192	23	14	0.00000	0e+00	roc_auc	binary	0.70915	4	0.01194	Preprocessor1_
23	152	35	9	0.00000	0e+00	roc_auc	binary	0.70845	4	0.01088	Preprocessor1_
19	256	30	14	0.00000	0e+00	roc_auc	binary	0.70841	4	0.01046	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)
```



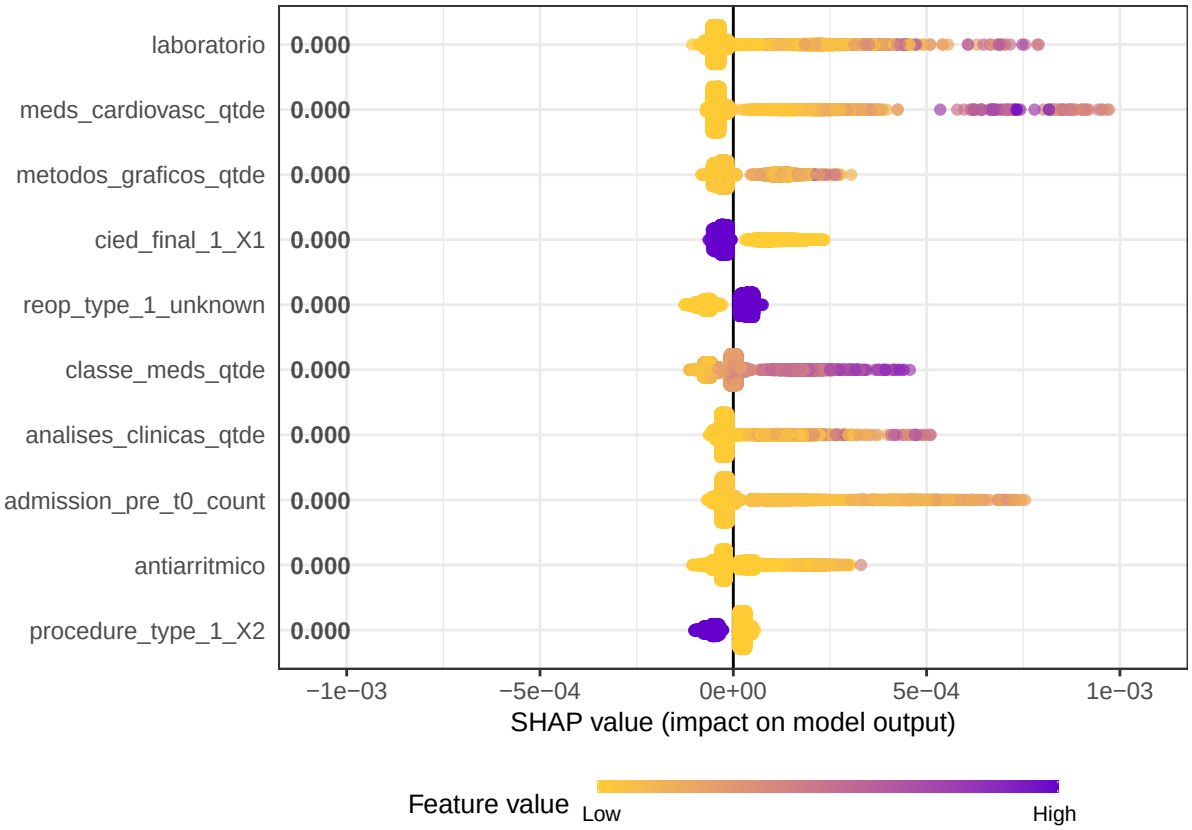

```
##   |
## Confusion Matrix and Statistics
##
##
## test_predictions_class    0    1
##                      0 4292  438
##                      1    0    0
##
##                Accuracy : 0.9074
##                  95% CI : (0.8988, 0.9155)
##     No Information Rate : 0.9074
##     P-Value [Acc > NIR] : 0.5127
##
##                   Kappa : 0
##
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 1.0000
##             Specificity : 0.0000
##          Pos Pred Value : 0.9074
##          Neg Pred Value :    NaN
##              Prevalence : 0.9074
##          Detection Rate : 0.9074
##    Detection Prevalence : 1.0000
##       Balanced Accuracy : 0.5000
##
##        '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

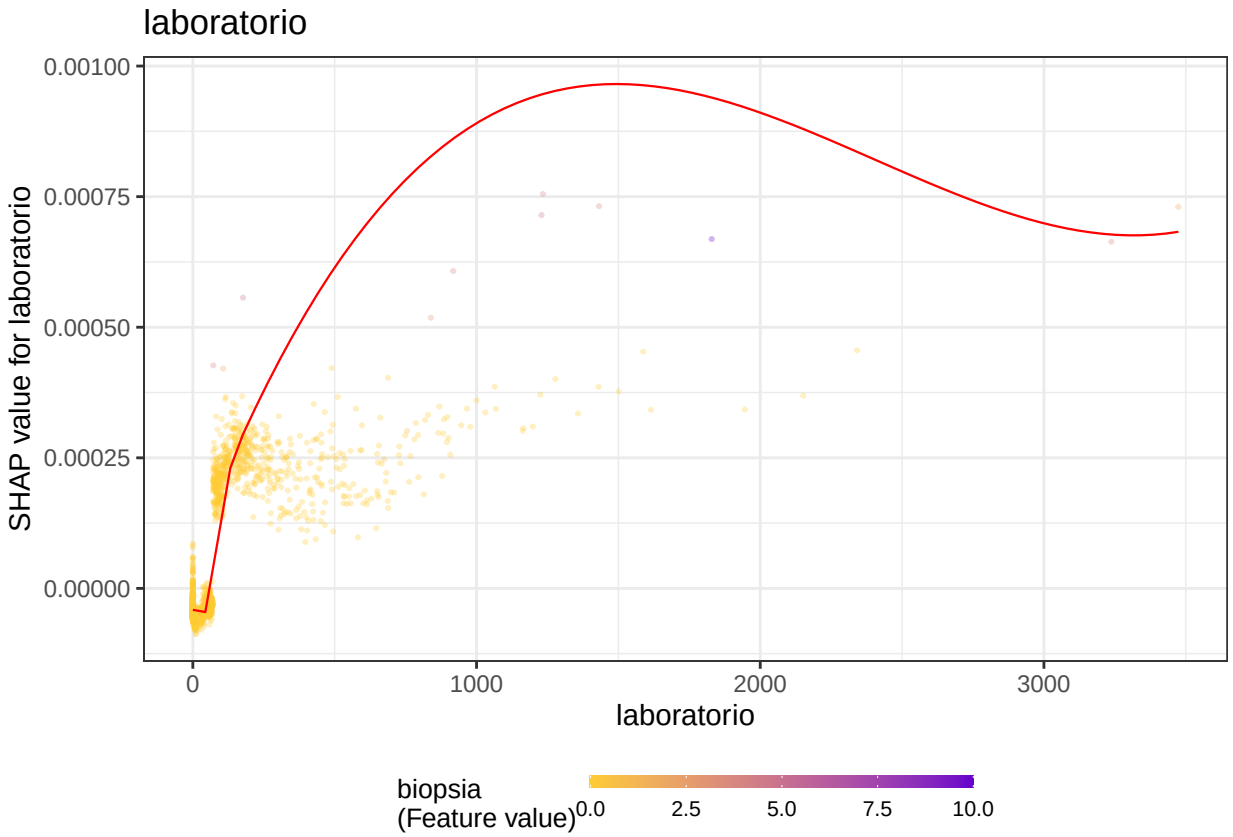
```
lightgbm_model <- parsnip::extract_fit_engine(final_lightgbm_fit)

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)
```



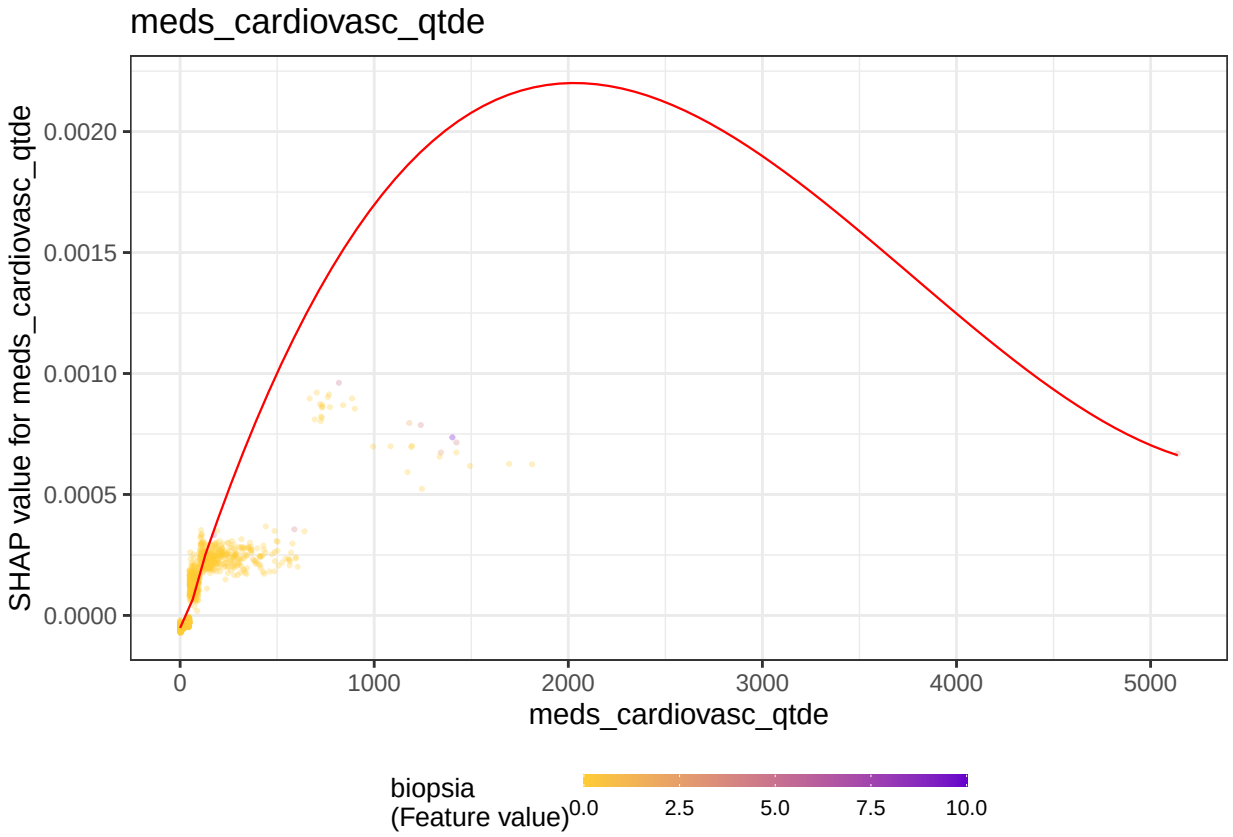

```
# Crunch SHAP values
shap <- shap.prep(lightgbm_model, X_train = matrix_test)

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)
```

```
}
```

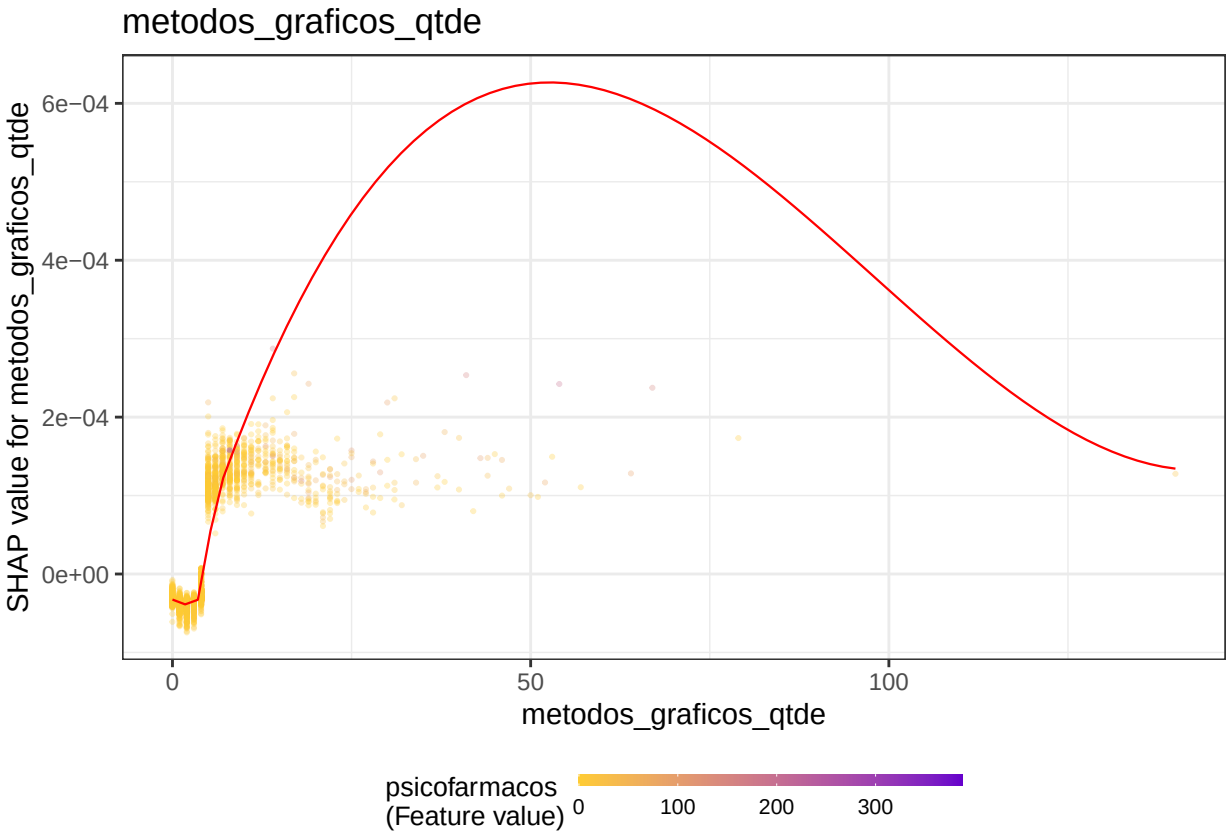
```
## `geom_smooth()` using formula 'y ~ x'
```



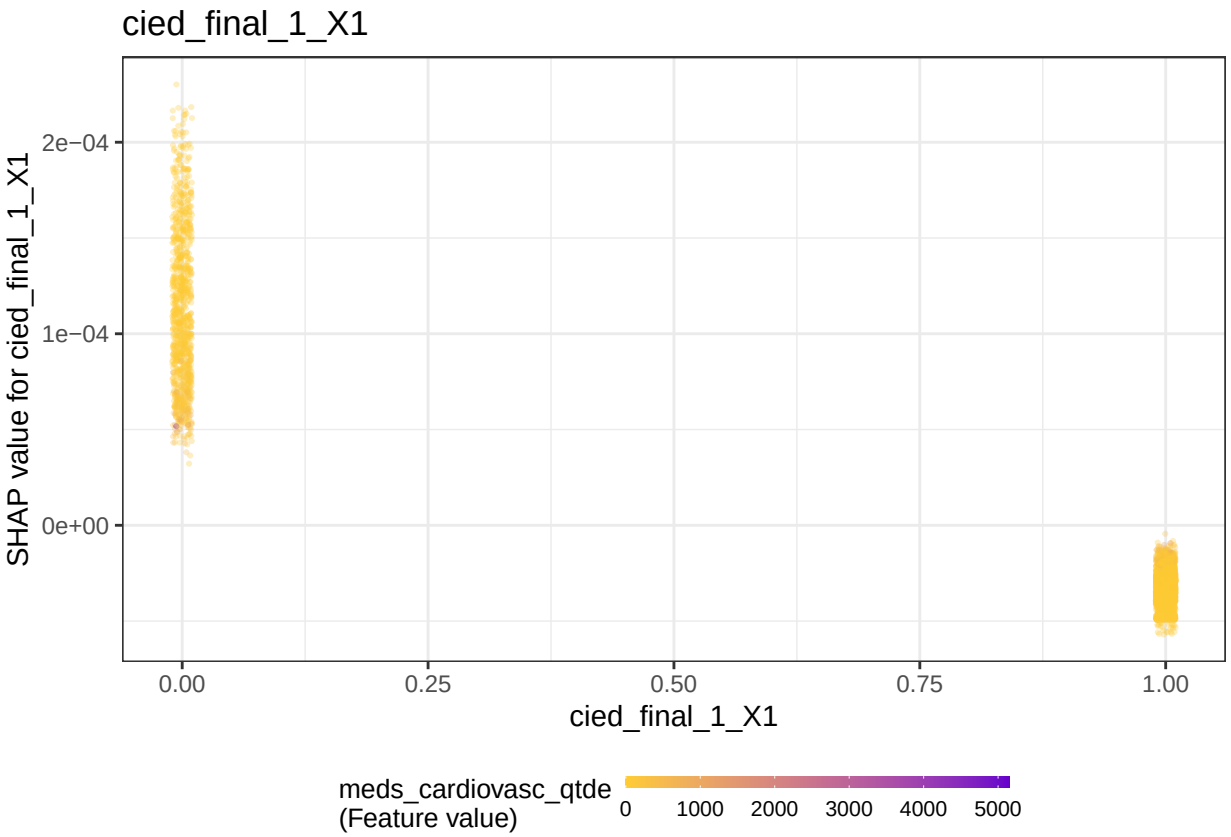

```
## `geom_smooth()` using formula 'y ~ x'
```



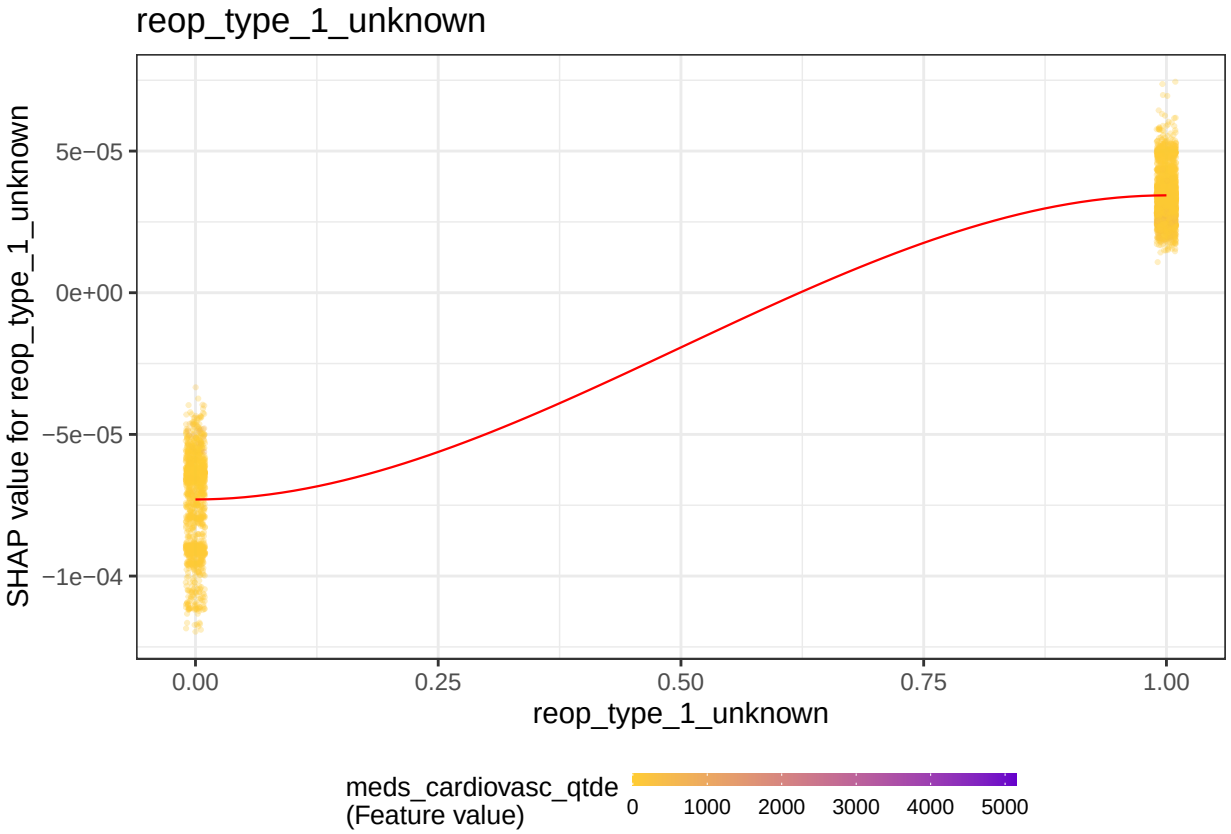

```
## `geom_smooth()` using formula 'y ~ x'
```




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

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

## 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, : at 1.005

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : radius 2.5e-05

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : all data on boundary of nei
## make span bigger

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : There are other near singul
## well. 2.5e-05

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : zero-width neighborhood. ma
## bigger

## Warning: Computation failed in `stat_smooth()`:
## NA/NaN/Inf em chamada de função externa (argumento 5)
```

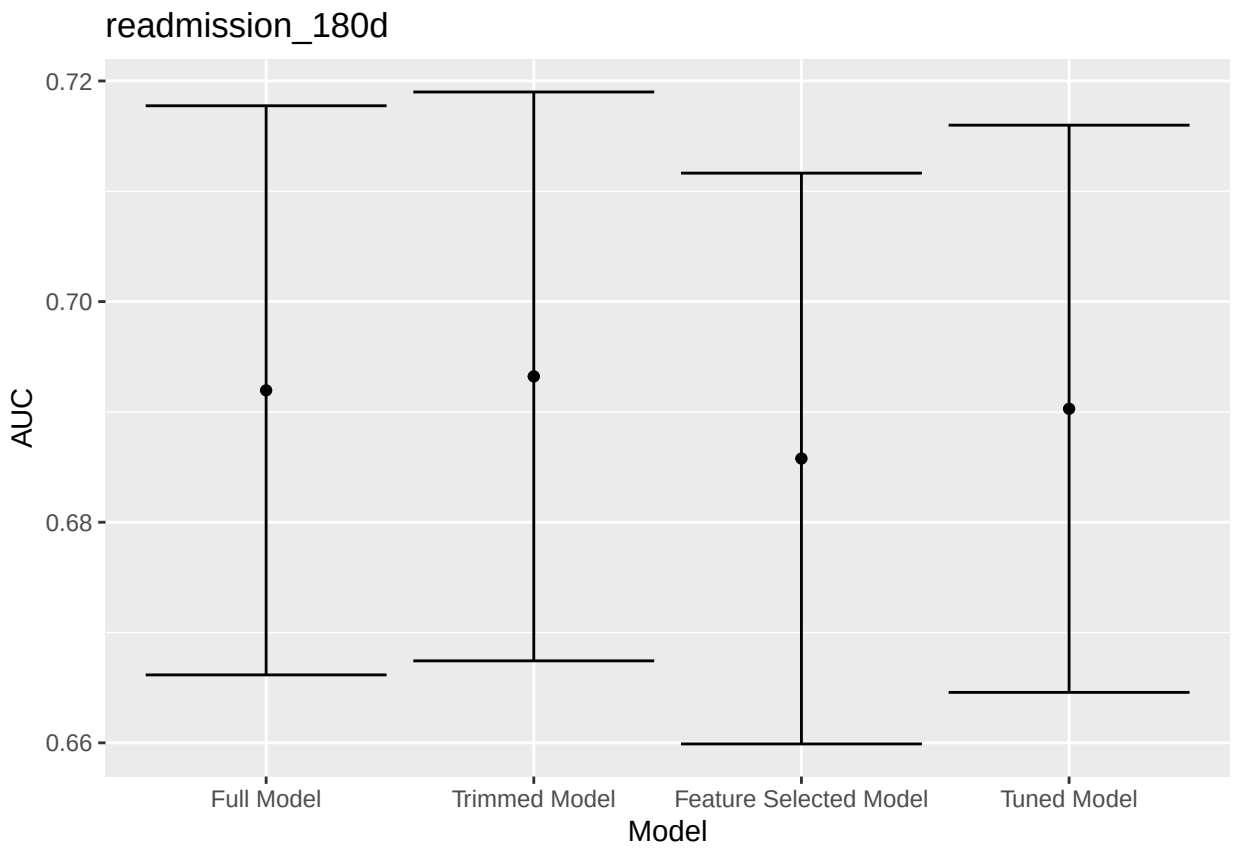



```
## `geom_smooth()` using formula 'y ~ x'
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : pseudoinverse used at -0.00
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric = parametric, : neighborhood radius 1.005
## Warning in simpleLoess(y, x, 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
```



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))
```