Model Selection - readmission 180d

Eduardo Yuki Yada

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
repeats <- params$repeats
RUN_ALL_MODELS <- params$RUN_ALL_MODELS
Hmisc::list.tree(params)

## params = list 5 (968 bytes)
## . outcome_column = character 1= readmission_180d
## . k = double 1= 10
## . grid_size = double 1= 20
## . repeats = double 1= 2
## . RUN_ALL_MODELS = logical 1= FALSE
Minutes to run: 0</pre>
```

Imports

```
library(tidyverse)
library(yaml)
library(tidymodels)
library(usemodels)
library(vip)
library(bonsai)
library(lightgbm)
library(caret)
library(pROC)
source("aux_functions.R")
```

Minutes to run: 0

Loading data

recursive = TRUE)

```
dir.create(file.path("./auxiliar/model_selection/performance/"),
           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)
Minutes to run: 0
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))
features = base::intersect(eligible_features, features_list)
gluedown::md_order(features, seq = TRUE, pad = TRUE)
## 01. sex
## 02. age
## 03. education_level
## 04. patient_state
## 05. underlying_heart_disease
## 06. heart_disease
## 07. nyha_basal
## 08. prior_mi
## 09. 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. ventilacao_mecanica
- ## 55. cec
- ## 56. transplante_cardiaco
- ## 57. cir_toracica
- ## 58. outros_proced_cirurgicos
- ## 59. icp
- ## 60. intervencao_cv
- ## 61. angioplastia
- ## 62. cateterismo
- ## 63. eletrofisiologia
- ## 64. cateter_venoso_central
- ## 65. proced_invasivos_qtde
- ## 66. cve_desf
- ## 67. transfusao
- ## 68. interconsulta
- ## 69. equipe_multiprof
- ## 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. ressonancia
## 92. exames_imagem_qtde
## 93. bic
## 94. mpp
## 95. hospital_stay
Minutes to run: 0
```

Train test split (70%/30%)

Minutes to run: 0.001

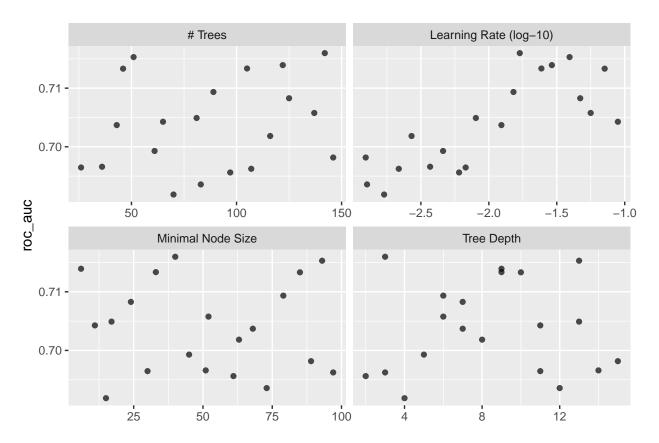
Boosted Tree (XGBoost)

```
xgboost_recipe <-</pre>
 recipe(formula = sprintf("%s ~ .", outcome_column) %% as.formula, data = df_train) %>%
  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())
xgboost_spec <- boost_tree(</pre>
 trees = tune(),
 min_n = tune(),
 tree_depth = tune(),
 learn_rate = tune(),
) %>%
  set_engine("xgboost",
            nthread = 8) \%
  set_mode("classification")
xgboost_grid <- grid_latin_hypercube(</pre>
```

```
trees(range = c(25L, 150L)),
  min_n(range = c(2L, 100L)),
  tree_depth(range = c(2L, 15L)),
  learn_rate(range = c(-3, -1), trans = log10_trans()),
  size = grid_size
xgboost_workflow <-</pre>
  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")
best_xgboost <- xgboost_tune %>%
  select_best("roc_auc")
autoplot(xgboost_tune, metric = "roc_auc")
final_xgboost_workflow <-</pre>
  xgboost_workflow %>%
  finalize_workflow(best_xgboost)
last_xgboost_fit <-</pre>
  final_xgboost_workflow %>%
  last_fit(df_split)
final_xgboost_fit <- extract_workflow(last_xgboost_fit)</pre>
xgboost_auc <- validation(final_xgboost_fit, df_test)</pre>
extract_vip(final_xgboost_fit, pred_wrapper = predict,
            reference_class = "0")
xgboost_parameters <- xgboost_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(trees, min_n, tree_depth, learn_rate, loss_reduction) %>%
  as.list
saveRDS(
  xgboost_parameters,
  file = sprintf(
    "./auxiliar/model_selection/hyperparameters/xgboost_%s.rds",
    outcome_column
  )
)
preds <- predict(final_xgboost_fit, new_data = df_train, type = "prob") %%</pre>
  rename_at(vars(starts_with(".pred_")), ~ str_remove(., ".pred_")) %>%
  .$`1`
hist(preds)
```

Boosted Tree (LightGBM)

```
lightgbm_recipe <-</pre>
  recipe(formula = sprintf("%s ~ .", outcome_column) %% as.formula, data = df_train) %>%
  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 spec <- boost tree(</pre>
  trees = tune(),
 \min_n = tune(),
 tree_depth = tune(),
 learn_rate = tune(),
  sample_size = 1
) %>%
  set_engine("lightgbm",
             nthread = 8) %>%
  set_mode("classification")
lightgbm_grid <- grid_latin_hypercube(</pre>
  trees(range = c(25L, 150L)),
  min_n(range = c(2L, 100L)),
  tree_depth(range = c(2L, 15L)),
  learn_rate(range = c(-3, -1), trans = log10_trans()),
  size = grid_size
lightgbm_workflow <-</pre>
  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 10
     trees min_n tree_depth learn_rate .metric .estimator mean
                                                                    n std_err .config
##
    <int> <int>
                      <int>
                                <dbl> <chr> <chr>
                                                          <dbl> <int> <dbl> <chr>
## 1
     142 40
                        3
                                0.0169 roc_auc binary
                                                          0.716
                                                                   10 0.0100 Preprocessor1_Model08
## 2
             93
                                0.0393 roc_auc binary
                                                                   10 0.0120 Preprocessor1_Model19
       51
                        13
                                                          0.715
## 3
       122
             6
                         9
                                0.0291 roc_auc binary
                                                          0.714
                                                                   10 0.0122 Preprocessor1 Model01
## 4
       105
              33
                         9
                                0.0244 roc_auc binary
                                                          0.713
                                                                   10 0.0119 Preprocessor1_Model07
                         10
                                0.0712 roc_auc binary
                                                          0.713
                                                                   10 0.0130 Preprocessor1_Model17
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)</pre>
```

```
Sensitivity

AUC: 0.693 (0.667–0.719)

1.0 0.5 0.0

Specificity
```

```
Specificity
## [1] "Optimal Threshold: 0.07"
##
  Confusion Matrix and Statistics
##
       reference
##
  data
           0
##
      0 2442
              127
##
      1 1850 311
##
                  Accuracy: 0.582
##
                    95% CI: (0.5678, 0.5961)
##
##
       No Information Rate: 0.9074
       P-Value [Acc > NIR] : 1
##
##
##
                     Kappa : 0.1009
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.5690
##
               Specificity: 0.7100
##
            Pos Pred Value : 0.9506
##
            Neg Pred Value: 0.1439
##
                Prevalence: 0.9074
##
            Detection Rate: 0.5163
##
      Detection Prevalence: 0.5431
##
         Balanced Accuracy : 0.6395
##
##
          'Positive' Class: 0
##
lightgbm_parameters <- lightgbm_tune %>%
  show_best("roc_auc", n = 1) %>%
  select(-.metric, -.estimator, -.config, -mean, -n, -std_err) %>%
  as.list
```

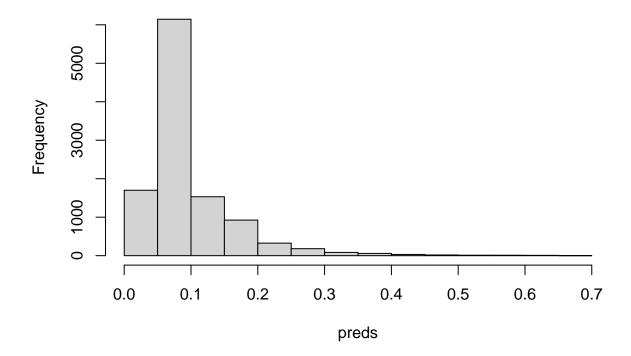
Hmisc::list.tree(lightgbm_parameters)

```
## lightgbm_parameters = list 4 (736 bytes)
## . trees = integer 1= 142
## . min_n = integer 1= 40
## . tree_depth = integer 1= 3
## . learn_rate = double 1= 0.016901

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

Minutes to run: 3.781

Histogram of preds



Minutes to run:

0.006

GLM

```
glmnet_recipe <-
    recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula, data = df_train) %>%
    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()) %>%
    step_zv(all_predictors()) %>%
    step_normalize(all_numeric_predictors())

glmnet_spec <-
    logistic_reg(penalty = 0) %>%
    set_mode("classification") %>%
```

Decision Tree

```
tree_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %% as.formula, data = df_train) %>%
  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()) %>%
  step_zv(all_predictors())
tree_spec <-
  decision_tree(cost_complexity = tune(),
                tree_depth = tune(),
                min_n = tune()) %>%
  set_mode("classification") %>%
  set_engine("rpart")
tree_grid <- grid_latin_hypercube(cost_complexity(),</pre>
                                  tree_depth(),
                                  min_n(),
                                  size = grid_size)
tree_workflow <-
  workflow() %>%
  add_recipe(tree_recipe) %>%
  add_model(tree_spec)
tree_tune <-
  tree_workflow %>%
  tune_grid(resamples = df_folds,
            grid = tree_grid)
tree_tune %>%
  collect_metrics()
autoplot(tree_tune, metric = "roc_auc")
tree_tune %>%
```

```
show_best("roc_auc")
best tree <- tree tune %>%
  select_best("roc_auc")
final_tree_workflow <-
  tree_workflow %>%
  finalize_workflow(best_tree)
last_tree_fit <-</pre>
  final_tree_workflow %>%
  last_fit(df_split)
final_tree_fit <- extract_workflow(last_tree_fit)</pre>
tree_auc <- validation(final_tree_fit, df_test)</pre>
extract_vip(final_tree_fit, pred_wrapper = predict,
            reference_class = "0", use_matrix = FALSE,
            method = 'model')
# extract_vip(final_tree_fit, pred_wrapper = predict,
              reference_class = "1", use_matrix = FALSE,
#
              method = 'permute')
```

Random Forest

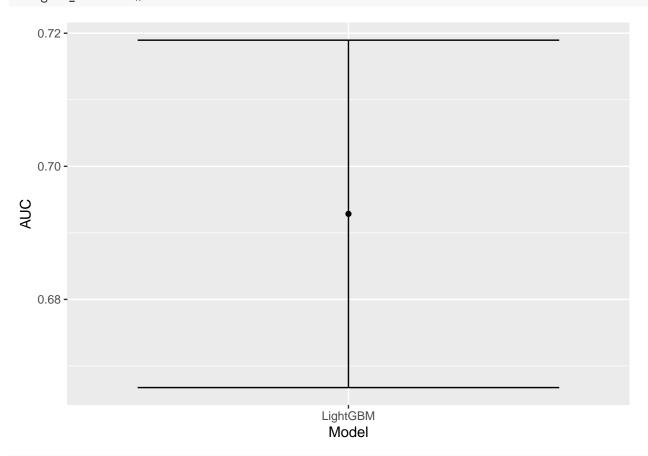
```
rf_recipe <-
  recipe(formula = sprintf("%s ~ .", outcome_column) %>% as.formula,
         data = df_train) %>%
  step_novel(all_nominal_predictors()) %>%
  step_unknown(all_nominal_predictors()) %>%
  step_other(all_nominal_predictors(), threshold = 0.05, other = ".merged") %>%
  step_dummy(all_nominal_predictors()) %>%
  step_zv(all_predictors()) %>%
  step_impute_mean(all_numeric_predictors())
rf spec <-
  rand_forest(mtry = tune(),
              trees = tune(),
              min_n = tune()) \%
  set mode("classification") %>%
  set_engine("randomForest",
             probability = TRUE,
             nthread = 8)
rf_grid <- grid_latin_hypercube(mtry(range = c(1L, 50L)),</pre>
                                 trees(range = c(100L, 300L)),
                                 \min_n(),
                                 size = grid_size)
rf_workflow <-
  workflow() %>%
  add_recipe(rf_recipe) %>%
  add_model(rf_spec)
rf_tune <-
 rf_workflow %>%
```

```
tune_grid(resamples = df_folds,
            grid = rf_grid)
rf_tune %>%
  collect_metrics()
autoplot(rf_tune, metric = "roc_auc")
rf tune %>%
  show_best("roc_auc")
best_rf <- rf_tune %>%
  select_best("roc_auc")
final_rf_workflow <-
  rf_workflow %>%
  finalize_workflow(best_rf)
last_rf_fit <-</pre>
  final rf workflow %>%
  last_fit(df_split)
final_rf_fit <- extract_workflow(last_rf_fit)</pre>
rf_auc <- validation(final_rf_fit, df_test)</pre>
pfun_rf <- function(object, newdata) predict(object, data = newdata)</pre>
extract_vip(final_rf_fit, pred_wrapper = predict,
            reference_class = "1", use_matrix = FALSE,
            method = 'model')
# extract_vip(final_rf_fit, pred_wrapper = predict,
               reference_class = "1", use_matrix = FALSE,
               method = 'permute')
```

Models Comparison

```
if (RUN_ALL_MODELS) {
  df_auc <- tibble::tribble(</pre>
    ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
    'XGBoost', as.numeric(xgboost_auc$auc), xgboost_auc$ci[1], xgboost_auc$ci[3],
    'LightGBM', as.numeric(lightgbm_auc$auc), lightgbm_auc$ci[1], lightgbm_auc$ci[3],
    'GLM', as.numeric(glmnet_auc$auc), glmnet_auc$ci[1], glmnet_auc$ci[3],
    'Decision Tree', as.numeric(tree_auc$auc), tree_auc$ci[1], tree_auc$ci[3],
    'Random Forest', as.numeric(rf_auc$auc), rf_auc$ci[1], rf_auc$ci[3]
  ) %>%
   mutate(Target = outcome_column)
} else {
  df_auc <- tibble::tribble(</pre>
    ~Model, ~`AUC`, ~`Lower Limit`, ~`Upper Limit`,
    'LightGBM', as.numeric(lightgbm_auc$auc), lightgbm_auc$ci[1], lightgbm_auc$ci[3]
 ) %>%
   mutate(Target = outcome_column)
}
df_auc %>%
  ggplot(aes(x = Model, y = AUC, ymin = `Lower Limit`, ymax = `Upper Limit`)) +
```

geom_point() +
geom_errorbar()



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

Minutes to run: 0.002