

BST 263 Final Project: XGBoost model

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Libraries and functions

```
library(tidyverse)

## -- Attaching packages ----- tidyverse 1.3.2 --
## v ggplot2 3.4.0      v purrr  1.0.1
## v tibble  3.1.8      v dplyr  1.0.10
## v tidyr   1.2.1      v stringr 1.5.0
## v readr   2.1.3      v forcats 0.5.2
## -- Conflicts ----- tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()

library(dplyr)
library(janitor)

##
## Attaching package: 'janitor'
##
## The following objects are masked from 'package:stats':
##
##   chisq.test, fisher.test

library(xgboost)

##
## Attaching package: 'xgboost'
##
## The following object is masked from 'package:dplyr':
##
##   slice

library(glmnet)

## Loading required package: Matrix
##
## Attaching package: 'Matrix'
##
## The following objects are masked from 'package:tidyr':
##
##   expand, pack, unpack
##
## Loaded glmnet 4.1-6
```

```
library(dplyr)
library(class)
library(caret)
```

```
## Loading required package: lattice
##
## Attaching package: 'caret'
##
## The following object is masked from 'package:purrr':
##
##     lift
```

```
library(e1071)
library(caret)
library(ROCR)
```

Load in the data, imputation, and train/test split

```
dat <- read.csv('brfss_final.csv')
outcome <- data.frame(dat$X, dat$MICH, dat$CVDINFR4, dat$CVDCHD4)
outcome %>% group_by(dat.MICH) %>% summarise(count=n())
```

```
## # A tibble: 2 x 2
##   dat.MICH count
##   <int> <int>
## 1     1  14580
## 2     2  14580
```

```
outcome %>% group_by(dat.CVDINFR4) %>% summarise(count=n())
```

```
## # A tibble: 4 x 2
##   dat.CVDINFR4 count
##   <int> <int>
## 1         1  9188
## 2         2 19802
## 3         7   160
## 4         9    10
```

```
outcome %>% group_by(dat.CVDCHD4) %>% summarise(count=n())
```

```
## # A tibble: 4 x 2
##   dat.CVDCHD4 count
##   <int> <int>
## 1         1  9729
## 2         2 18874
## 3         7   550
## 4         9    7
```

```
## remove the ones that responded don't know & not sure in CVDINFR4 & CVDCHD4
```

```
dat <- dat[-which(dat$CVDINFR4 == 7 | dat$CVDINFR4 == 9),]
dat <- dat[-which(dat$CVDCHD4 == 7 | dat$CVDCHD4 == 9),]
```

```
# remove columns that has only 1 value for all rows
```

```
dat <- dat[, -which(names(dat) %in% c("MEDSHEPB", "TOLDCFS", "HAVECFS", "WORKCFS"))]
```

Drop columns with more than 5% data missing, impute the rest using KNN

```
# convert outcome variables
dat$MICHHD <- factor(2-dat$MICHHD)
dat$CVDINFR4 <- factor(2-dat$CVDINFR4)
dat$CVDCRHD4 <- factor(2-dat$CVDCRHD4)

# i believe X is the index column, not needed
# remove weights
dat <- dat[, !colnames(dat) %in% c('X', 'LLCPWT2', 'LLCPWT', 'CLLCPWT', 'STRWT', 'WT2RAKE')]
threshold <- .05
ncol(dat) # 190
```

```
## [1] 190
```

```
###
### Missing data
na_count <- data.frame(na = sapply(dat, function(y) sum(length(which(is.na(y))))))

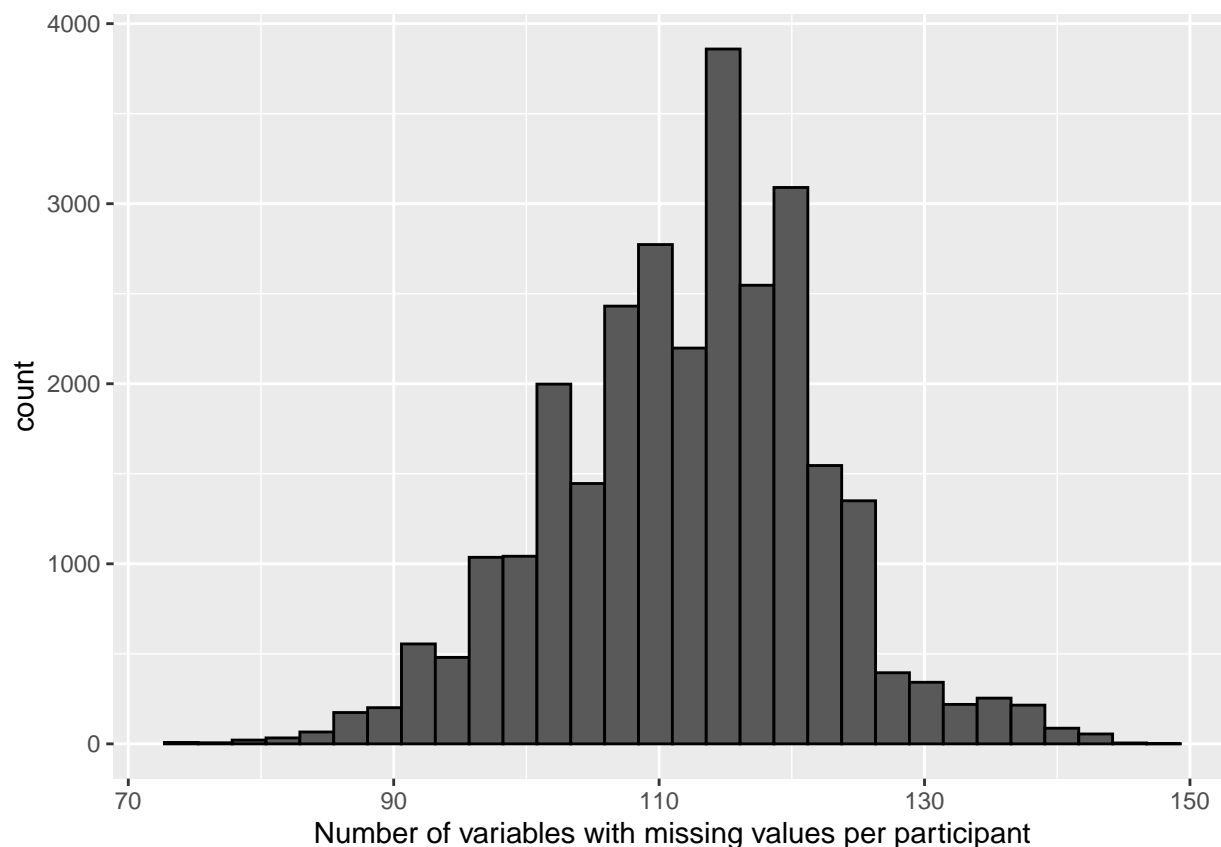
na_count$variable <- rownames(na_count)
rownames(na_count) <- NULL

na_count %>%
  as_tibble() %>%
  select(variable, na) %>%
  filter(na != 0) %>%
  mutate(na_percent = na/28433) %>%
  arrange(desc(na))
```

```
## # A tibble: 153 x 3
##   variable    na na_percent
##   <chr>    <int>     <dbl>
## 1 HAVEHEPC 28430      1.00
## 2 SIGMTES1 28427      1.00
## 3 TRETHERPC 28426      1.00
## 4 PRIRHEPC 28424      1.00
## 5 VCLNTES1 28423      1.00
## 6 HPVADSHT 28413      0.999
## 7 SDNATES1 28406      0.999
## 8 BLDSTFIT 28396      0.999
## 9 CSRVCTL2 28355      0.997
## 10 PSATIME1 28340      0.997
## # ... with 143 more rows
```

```
dat %>%
  mutate(na_rowise = rowSums(is.na(.))) %>%
  ggplot(aes(na_rowise)) + geom_histogram(color = "black") +
  labs(x="Number of variables with missing values per participant")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
###
```

```
dat <- dat[, colMeans(is.na(dat)) <= threshold]
ncol(dat) # 52 columns left
```

```
## [1] 52
```

```
columns_to_impute <- colnames(dat)[colSums(is.na(dat)) > 0]
columns_to_impute
```

```
## [1] "CPDEMO1B" "VETERAN3" "EMPLOY1" "INCOME3" "DEAF" "BLIND"
## [7] "DECIDE" "DIFFWALK" "DIFFDRES" "DIFFALON" "USENOW3" "METSTAT"
## [13] "URBSTAT" "MSCODE" "DRDXAR3"
```

```
str(dat[,columns_to_impute])
```

```
## 'data.frame': 28433 obs. of 15 variables:
## $ CPDEMO1B: int 1 1 8 1 1 8 8 1 1 2 ...
## $ VETERAN3: int 2 2 2 2 1 2 1 2 2 2 ...
## $ EMPLOY1 : int 8 7 2 7 7 7 7 8 7 7 ...
## $ INCOME3 : int 77 3 99 77 7 99 5 77 5 10 ...
## $ DEAF : int 2 2 2 2 2 2 1 2 2 2 ...
## $ BLIND : int 1 2 2 2 2 2 2 2 2 2 ...
## $ DECIDE : int 1 2 1 2 1 2 2 2 2 2 ...
## $ DIFFWALK: int 1 2 2 2 2 1 1 1 2 2 ...
## $ DIFFDRES: int 2 2 2 2 2 1 2 2 2 2 ...
## $ DIFFALON: int 1 2 2 2 2 1 1 2 2 2 ...
## $ USENOW3 : int 3 3 3 3 3 3 3 3 3 3 ...
```

```
## $ METSTAT : int 1 1 1 1 1 2 1 2 1 1 ...
## $ URBSTAT : int 1 1 1 1 1 1 1 1 1 1 ...
## $ MSCODE : int 2 1 3 1 3 2 2 5 2 3 ...
## $ DRDXAR3 : int 1 2 1 1 2 1 1 2 1 1 ...

complete_columns <- colnames(dat)[colSums(is.na(dat)) == 0 &
                                !colnames(dat) %in% c('MICHHD', 'CVDINFR4', 'CVDCRHD4')]

for (c in columns_to_impute) {
  col <- dat[[c]]
  scaled <- scale(dat[, complete_columns])
  knn <- knn(
    train = scaled[!is.na(col), complete_columns],
    test = scaled[is.na(col), complete_columns],
    cl = dat[!is.na(col), c]
  )

  dat[is.na(col), c] = knn
}

colSums(is.na(dat))

## GENHLTH PHYSHLTH MENTHLTH PRIMINSR PERSDOC3 MEDCOST1 CHECKUP1 CVDINFR4
## 0 0 0 0 0 0 0 0
## CVDCRHD4 CVDSTRK3 CHCSCNCR CHCOCNCR CHCCOPD3 ADDEPEV3 CHCKDNY2 DIABETE4
## 0 0 0 0 0 0 0 0
## MARITAL RENTHOM1 NUMHHOL3 CPDEMO1B VETERAN3 EMPLOY1 INCOME3 DEAF
## 0 0 0 0 0 0 0 0
## BLIND DECIDE DIFFWALK DIFFDRES DIFFALON USENOW3 QSTVER QSTLANG
## 0 0 0 0 0 0 0 0
## METSTAT URBSTAT MSCODE STSTR RAWRAKE DUALUSE TOTINDA RFHYPE6
## 0 0 0 0 0 0 0 0
## CHOLCH3 MICHHD ASTHMS1 DRDXAR3 RACE SEX AGE80 CHLDCNT
## 0 0 0 0 0 0 0 0
## EDUCAG SMOKER3 CURECI1 DROCDY3_
## 0 0 0 0

set.seed(263)
train_index <- createDataPartition(dat$MICHHD, p = 0.8, list = FALSE)
train <- dat[train_index, ]
test <- dat[-train_index, ]
```

XGBoost

In summary: 49 variables, 3 possible outcomes (MICHHD, CVDINFR4, CVDCRHD4). N = 22,747 in training data, N = 5,686 in test data.

```
train_variables <- train %>%
  select(-MICHHD, -CVDINFR4, -CVDCRHD4)

train_variables_matrix <- train_variables %>%
  data.matrix()

#train_outcomes <- train %>%
# select(MICHHD, CVDINFR4, CVDCRHD4) %>%
# mutate(across(c(MICHHD, CVDINFR4, CVDCRHD4), as.factor))
```

```

train_outcomes <- train %>%
  pull(MICHHD) %>%
  as.character() %>%
  as.numeric()

test_variables <- test %>%
  select(-MICHHD, -CVDINFR4, -CVDCRHD4)

test_variables_matrix <- test_variables%>%
  data.matrix()

test_outcomes <- test %>%
  pull(MICHHD) %>%
  as.character() %>%
  as.numeric()

```

XGBoost model with all 49 variables

```

set.seed(43)

grid_tune <- expand.grid(
  nrounds = c(500,1000,1500), # Number of boosting rounds
  max_depth = c(1,3,5), # Max depth of tree
  eta = c(0.01, 0.1, 0.3), # Step size shrinkage to prevent overfitting
  gamma = 0, # Minimum loss reduction required to make a further partition on a leaf node of the tree
  colsample_bytree = 1,
  min_child_weight = 1,
  subsample = 1
)

train_control <- trainControl(method = "cv", # Cross validation
  number=3, # 3 folds
  verboseIter = TRUE,
  allowParallel = TRUE)

xgb_tune <- train(x = train_variables,
  y = as.factor(train_outcomes),
  trControl = train_control,
  tuneGrid = grid_tune,
  method= "xgbTree",
  verbose = TRUE)

## + Fold1: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:15:11] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:15:11] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:15:27] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:15:27] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:15:54] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead

```



```

## + Fold2: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:19:33] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:19:33] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold2: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold2: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:19:59] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:19:59] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold2: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:20:06] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:20:06] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:20:22] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:20:22] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:20:49] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:20:49] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:20:55] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:20:55] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:21:12] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:21:12] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.10, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:21:39] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:21:39] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.30, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:21:46] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:21:46] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:22:02] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:22:02] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:22:29] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:22:29] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## Aggregating results
## Selecting tuning parameters
## Fitting nrounds = 500, max_depth = 5, eta = 0.01, gamma = 0, colsample_bytree = 1, min_child_weight = 1
xgb_tune

## eXtreme Gradient Boosting
##
## 22747 samples
## 49 predictor
## 2 classes: '0', '1'

```



```
##
## No pre-processing
## Resampling: Cross-Validated (3 fold)
## Summary of sample sizes: 15164, 15165, 15165
## Resampling results across tuning parameters:
##
##   eta   max_depth nrounds  Accuracy   Kappa
##   0.01   1         500     0.7051480  0.4099337
##   0.01   1        1000     0.7147317  0.4291049
##   0.01   1        1500     0.7164020  0.4324790
##   0.01   3         500     0.7193914  0.4391762
##   0.01   3        1000     0.7218533  0.4440565
##   0.01   3        1500     0.7214576  0.4432469
##   0.01   5         500     0.7218973  0.4442941
##   0.01   5        1000     0.7206224  0.4416680
##   0.01   5        1500     0.7194355  0.4392701
##   0.10   1         500     0.7187319  0.4371864
##   0.10   1        1000     0.7189957  0.4377392
##   0.10   1        1500     0.7193034  0.4383588
##   0.10   3         500     0.7186881  0.4376126
##   0.10   3        1000     0.7148195  0.4297398
##   0.10   3        1500     0.7095441  0.4191234
##   0.10   5         500     0.7087089  0.4176114
##   0.10   5        1000     0.7003122  0.4007361
##   0.10   5        1500     0.6956524  0.3913083
##   0.30   1         500     0.7208860  0.4415254
##   0.30   1        1000     0.7198310  0.4394442
##   0.30   1        1500     0.7193035  0.4383763
##   0.30   3         500     0.7064227  0.4129112
##   0.30   3        1000     0.6993449  0.3986811
##   0.30   3        1500     0.6906404  0.3812383
##   0.30   5         500     0.6923111  0.3846152
##   0.30   5        1000     0.6840903  0.3680191
##   0.30   5        1500     0.6818482  0.3635456
##
## Tuning parameter 'gamma' was held constant at a value of 0
## Tuning
##
## Tuning parameter 'min_child_weight' was held constant at a value of 1
##
## Tuning parameter 'subsample' was held constant at a value of 1
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were nrounds = 500, max_depth = 5, eta
## = 0.01, gamma = 0, colsample_bytree = 1, min_child_weight = 1 and subsample
## = 1.
```

```
xgb_best <- xgb_tune$bestTune

train_control <- trainControl(method = "none",
                              verboseIter = TRUE,
                              allowParallel = TRUE)

final_grid <- expand.grid(nrounds = xgb_best$nrounds,
                          eta = xgb_best$eta,
```

```

        max_depth = xgb_best$max_depth,
        gamma = xgb_best$gamma,
        colsample_bytree = xgb_best$colsample_bytree,
        min_child_weight = xgb_best$min_child_weight,
        subsample = xgb_best$subsample)
xgb_model <- train(x = train_variables,
                  y = as.factor(train_outcomes),
                  trControl = train_control,
                  tuneGrid = final_grid,
                  method = "xgbTree",
                  verbose = TRUE)

## Fitting nrounds = 500, eta = 0.01, max_depth = 5, gamma = 0, colsample_bytree = 1, min_child_weight =
xgb_pred <- predict(xgb_model, test_variables)

#' Confusion Matrix
confusionMatrix(as.factor((xgb_pred)),
                as.factor(test_outcomes))

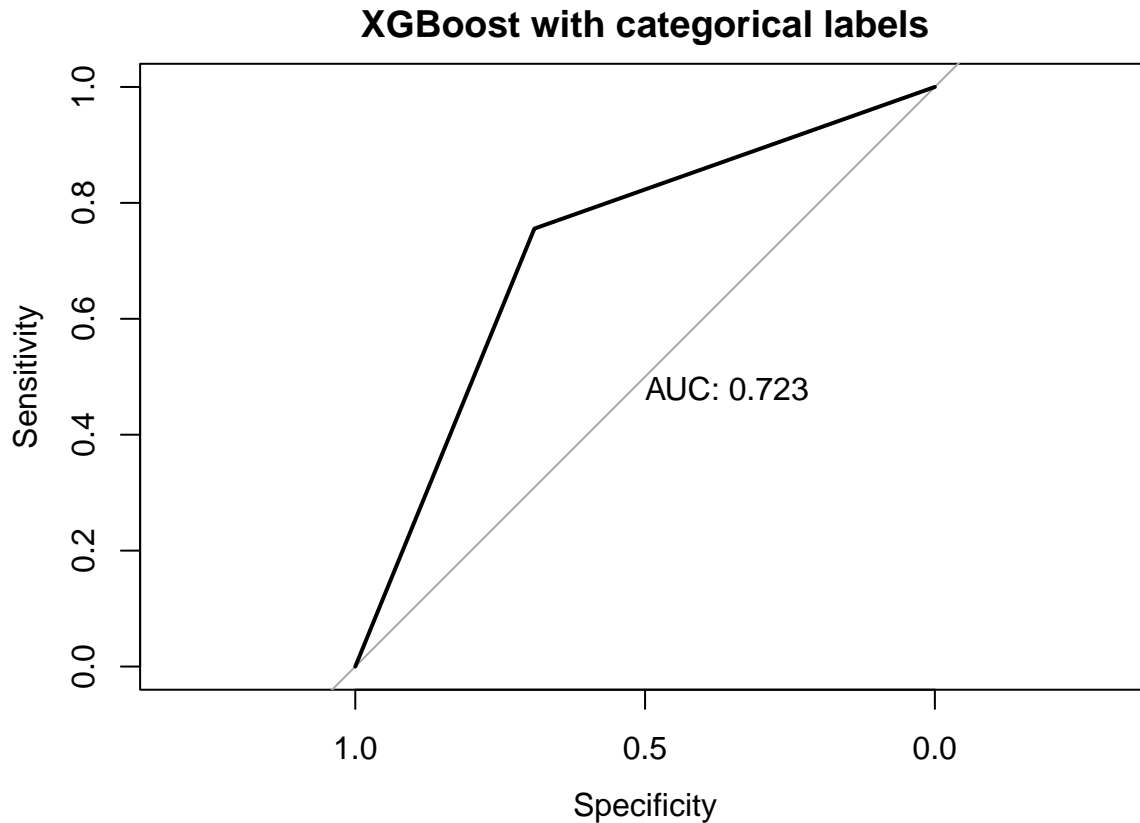
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##           0 2015  677
##           1  901 2093
##
##           Accuracy : 0.7225
##           95% CI : (0.7106, 0.7341)
##           No Information Rate : 0.5128
##           P-Value [Acc > NIR] : < 2.2e-16
##
##           Kappa : 0.4457
##
## Mcnemar's Test P-Value : 1.98e-08
##
##           Sensitivity : 0.6910
##           Specificity : 0.7556
##           Pos Pred Value : 0.7485
##           Neg Pred Value : 0.6991
##           Prevalence : 0.5128
##           Detection Rate : 0.3544
##           Detection Prevalence : 0.4734
##           Balanced Accuracy : 0.7233
##
##           'Positive' Class : 0
##
library(pROC)

## Type 'citation("pROC")' for a citation.
##
## Attaching package: 'pROC'
## The following objects are masked from 'package:stats':

```

```
##
##      cov, smooth, var
roc_score <- roc(test_outcomes, as.numeric(xgb_pred))

## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
plot(roc_score, print.auc = T, main = "XGBoost with categorical labels")
```



XGBoost with One-Hot encoding

49 variables become 220.

Variables to remove: QSTVER, STSTR, RAWRAKE

```
train_variables_2 <- train_variables %>%
  mutate(across(c(-PHYSHLTH, -MENTHLTH, -CPDEMO1B, -STSTR, -RAWRAKE, -AGE80, -DROCDY3_), as.character))

test_variables_2 <- test_variables %>%
  mutate(across(c(-PHYSHLTH, -MENTHLTH, -CPDEMO1B, -STSTR, -RAWRAKE, -AGE80, -DROCDY3_), as.character))

# Make one-hot encoded variables in the training set
dummy <- dummyVars(" ~ .", data=train_variables_2)
train_variables_3 <- data.frame(predict(dummy, newdata = train_variables_2)) %>%
  select(-PRIMINSR6, -CHCCOPD39, -VETERAN33, -DEAF3, -BLIND3, -DIFFWALK3) # Remove 6 one hot encoded va

# Make one-hot encoded variables in the test set
```

```

dummy <- dummyVars(" ~ .", data=test_variables_2)
test_variables_3 <- data.frame(predict(dummy, newdata = test_variables_2))

anti_join(as_tibble(colnames(train_variables_3)), as_tibble(colnames(test_variables_3)))

## Joining, by = "value"
## # A tibble: 0 x 1
## # ... with 1 variable: value <chr>

set.seed(54)

grid_tune <- expand.grid(
  nrounds = c(500,1000,1500), # Number of boosting rounds
  max_depth = c(1,3,5), # Max depth of tree
  eta = c(0.01, 0.1, 0.3), # Step size shrinkage to prevent overfitting
  gamma = 0, # Minimum loss reduction required to make a further partition on a leaf node of the tree
  colsample_bytree = 1,
  min_child_weight = 1,
  subsample = 1
)

train_control <- trainControl(method = "cv", # Cross validation
                             number=3, # 3 folds
                             verboseIter = TRUE,
                             allowParallel = TRUE)

xgb_tune_2 <- train(x = train_variables_3,
                  y = as.factor(train_outcomes),
                  trControl = train_control,
                  tuneGrid = grid_tune,
                  method= "xgbTree",
                  verbose = TRUE)

## + Fold1: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:23:27] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:23:27] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:24:35] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:24:35] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:26:24] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:26:25] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:26:51] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:26:51] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold1: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:28:00] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:28:00] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold1: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500

```



```

## [14:43:45] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## [14:44:52] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:44:52] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## + Fold3: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:46:41] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:46:41] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.01, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold3: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:47:08] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:47:08] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## [14:48:15] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:48:15] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## + Fold3: eta=0.10, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:50:04] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:50:04] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.10, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## + Fold3: eta=0.30, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## [14:50:31] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:50:31] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=1, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=500
## + Fold3: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## [14:51:38] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:51:38] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=3, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1000
## + Fold3: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## [14:53:28] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## [14:53:28] WARNING: src/c_api/c_api.cc:935: `ntree_limit` is deprecated, use `iteration_range` instead
## - Fold3: eta=0.30, max_depth=5, gamma=0, colsample_bytree=1, min_child_weight=1, subsample=1, nrounds=1500
## Aggregating results
## Selecting tuning parameters
## Fitting nrounds = 1000, max_depth = 5, eta = 0.01, gamma = 0, colsample_bytree = 1, min_child_weight
xgb_tune_2

```

```

## eXtreme Gradient Boosting
##
## 22747 samples
## 220 predictor
## 2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (3 fold)
## Summary of sample sizes: 15165, 15164, 15165
## Resampling results across tuning parameters:
##
##  eta  max_depth  nrounds  Accuracy  Kappa
##  0.01  1          500      0.7080055  0.4154891
##  0.01  1          1000     0.7156108  0.4307983
##  0.01  1          1500     0.7179408  0.4354636

```

```
## 0.01 3 500 0.7209302 0.4421745
## 0.01 3 1000 0.7210622 0.4424029
## 0.01 3 1500 0.7204028 0.4410177
## 0.01 5 500 0.7207545 0.4420623
## 0.01 5 1000 0.7213699 0.4432245
## 0.01 5 1500 0.7207104 0.4418455
## 0.10 1 500 0.7185123 0.4366778
## 0.10 1 1000 0.7179408 0.4355307
## 0.10 1 1500 0.7180288 0.4357295
## 0.10 3 500 0.7159625 0.4320790
## 0.10 3 1000 0.7136327 0.4273460
## 0.10 3 1500 0.7110830 0.4221284
## 0.10 5 500 0.7120501 0.4242057
## 0.10 5 1000 0.7072584 0.4145671
## 0.10 5 1500 0.7007520 0.4014728
## 0.30 1 500 0.7170616 0.4337889
## 0.30 1 1000 0.7158747 0.4314583
## 0.30 1 1500 0.7160506 0.4317770
## 0.30 3 500 0.7102476 0.4204758
## 0.30 3 1000 0.6985539 0.3970129
## 0.30 3 1500 0.6926189 0.3850744
## 0.30 5 500 0.6960040 0.3919000
## 0.30 5 1000 0.6885746 0.3771149
## 0.30 5 1500 0.6839585 0.3678674
##
## Tuning parameter 'gamma' was held constant at a value of 0
## Tuning
##
## Tuning parameter 'min_child_weight' was held constant at a value of 1
##
## Tuning parameter 'subsample' was held constant at a value of 1
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were nrounds = 1000, max_depth = 5, eta
## = 0.01, gamma = 0, colsample_bytree = 1, min_child_weight = 1 and subsample
## = 1.
```

```
xgb_best_2 <- xgb_tune_2$bestTune
#Fitting nrounds = 1000, eta = 0.01, max_depth = 5, gamma = 0, colsample_bytree = 1, min_child_weight =

train_control <- trainControl(method = "none",
                              verboseIter = TRUE,
                              allowParallel = TRUE)

final_grid_2 <- expand.grid(nrounds = xgb_best_2$nrounds,
                           eta = xgb_best_2$eta,
                           max_depth = xgb_best_2$max_depth,
                           gamma = xgb_best_2$gamma,
                           colsample_bytree = xgb_best_2$colsample_bytree,
                           min_child_weight = xgb_best_2$min_child_weight,
                           subsample = xgb_best_2$subsample)

xgb_model_2 <- train(x = train_variables_3,
                    y = as.factor(train_outcomes),
                    trControl = train_control,
```

```

        tuneGrid = final_grid_2,
        method = "xgbTree",
        verbose = TRUE)

## Fitting nrounds = 1000, eta = 0.01, max_depth = 5, gamma = 0, colsample_bytree = 1, min_child_weight
xgb_pred_2 <- predict(xgb_model_2, test_variables_3)

confusionMatrix(as.factor((xgb_pred_2)),
                as.factor(test_outcomes))

## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##           0 2014  682
##           1  902 2088
##
##           Accuracy : 0.7214
##           95% CI : (0.7096, 0.733)
##       No Information Rate : 0.5128
##       P-Value [Acc > NIR] : < 2.2e-16
##
##           Kappa : 0.4436
##
##  McNemar's Test P-Value : 3.743e-08
##
##           Sensitivity : 0.6907
##           Specificity : 0.7538
##           Pos Pred Value : 0.7470
##           Neg Pred Value : 0.6983
##           Prevalence : 0.5128
##           Detection Rate : 0.3542
##       Detection Prevalence : 0.4741
##           Balanced Accuracy : 0.7222
##
##       'Positive' Class : 0
##
roc_score_2 <- roc(test_outcomes, as.numeric(xgb_pred_2))

## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
plot(roc_score_2, print.auc = T, main = "XGBoost with one-hot encoding")

```