Preliminary Investigation

Ethan Allavarpu with Andy's Edits

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Setup

```
set.seed(110920)
library(tidyverse)
```

```
-- Attaching packages ---------------------------------------------------------------------------------
```

```
v ggplot2 3.3.2     v purrr   0.3.4
v tibble  3.0.3     v dplyr   1.0.2
v tidyr   1.1.2     v stringr 1.4.0
v readr   1.3.1     v forcats 0.5.0
```

```
-- Conflicts ------------------------------------------------------------------------------------------ t
x dplyr::filter() masks stats::filter()
x dplyr::lag()    masks stats::lag()
```

```
# sample <- read.csv("sample.csv", stringsAsFactors = TRUE)
# sample
```

```
training <- read.csv("training.csv", stringsAsFactors = TRUE)
sort(abs(cor(training)["class", ]), decreasing = TRUE)[2:19]
```

```
Broad_H4K20me1_percentage   Broad_H3K9ac_percentage            H4K20me1_width
                0.5309561                0.4810581                 0.4789003
       BioGRID_log_degree           H3K79me2_height            H3K79me2_width
                0.4764364                0.4719210                 0.4709266
 Broad_H3K4me2_percentage  Broad_H3K27ac_percentage           H4K20me1_height
                0.4693101                0.4641367                 0.4595187
 Broad_H3K4me1_percentage Broad_H3K79me2_percentage  Broad_H3K4me3_percentage
                0.4580446                0.4571273                 0.4315878
Broad_H3K36me3_percentage             H3K4me1_width            H3K36me3_width
                0.4306293                0.4287817                 0.4275987
              pLOF_Zscore                    N_LOF             H3K4me2_width
                0.4227907                0.4212450                 0.4080466
```

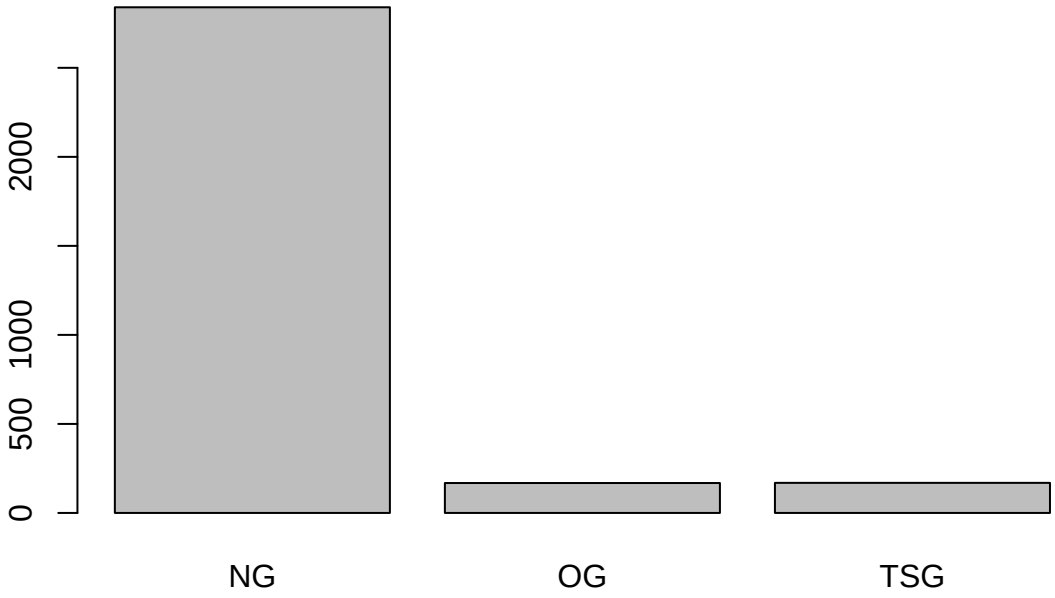
```
training$class <- factor(training$class)
levels(training$class) <- c("NG", "OG", "TSG")
dim(training)
```

```
[1] 3177   99
```

```
names(training)[c(1, 99)]
```

```
[1] "id"    "class"
```

```r
barplot(table(training$class))
```




```r
table(training$class) / nrow(training)
```

```
        NG         OG        TSG
0.89392509 0.05288008 0.05319484
```

```r
any(is.na(training))
```

```
[1] FALSE
```

```r
# library(ggplot2)
# scatter <- function(var) {
#   ggplot(training, aes_string(var, "class")) +
#     geom_jitter(width = 0.05, height = 0.1, size = 0.1,
#                 colour = rgb(0, 0, 0, alpha = 1 / 3))
# }
# scat_plot <- lapply(names(training)[-99], scatter)
# library(gridExtra)
# grid.arrange(grobs = scat_plot[1:20], ncol = 4)
# grid.arrange(grobs = scat_plot[21:40], ncol = 4)
# grid.arrange(grobs = scat_plot[41:60], ncol = 4)
# grid.arrange(grobs = scat_plot[61:80], ncol = 4)
# grid.arrange(grobs = scat_plot[81:98], ncol = 4)
```

```r
sig <- logical(98)
names(sig) <- names(training)[-99]
k <- 1
diffs <- logical(98)
for (var in names(training)[-99]) {
  model <- aov(training[[var]] ~ factor(training$class))
  sig[k] <- summary(model)[[1]][1, 5]
  diffs[k] <- all(TukeyHSD(model)$`factor(training$class)`[, 4] < 0.05)
  k <- k + 1
}
```

```r
head(sort(sig[diffs]), 15)
```

```
Broad_H4K20me1_percentage   Broad_H3K9ac_percentage            H4K20me1_width
             2.605382e-232             8.993961e-184             3.222855e-181
          H3K79me2_height            H3K79me2_width  Broad_H3K4me2_percentage
             4.253756e-176             2.449130e-175             4.311054e-174
Broad_H3K79me2_percentage  Broad_H3K27ac_percentage           H4K20me1_height
             1.188924e-168             2.345807e-168             1.791736e-164
 Broad_H3K4me1_percentage Broad_H3K36me3_percentage            H3K36me3_width
             1.065370e-163             4.471080e-154             2.142472e-147
               pLOF_Zscore  Broad_H3K4me3_percentage             H3K4me1_width
             5.366468e-145             2.017738e-143             5.760242e-141
```

```r
score <- function (conf_mat) {
  print(sum(diag(conf_mat) * c(1, 20, 20)))
  print(sum(diag(conf_mat) * c(1, 20, 20)) / sum(apply(conf_mat, 2, sum) * c(1, 20, 20)))
} #weighted scoring algorithm

classify <- function(probs) {
  if (any(probs[2:3] > 0.05)) {
    subset <- probs[2:3]
    output <- which(subset == max(subset))
    if (length(output) > 1) {
      output <- sample(1:2, 1)
      # if OG and TSG both have equal probabilities, pick one randomly
    }
  } else {
    output <- 0
  }
  output
}
```

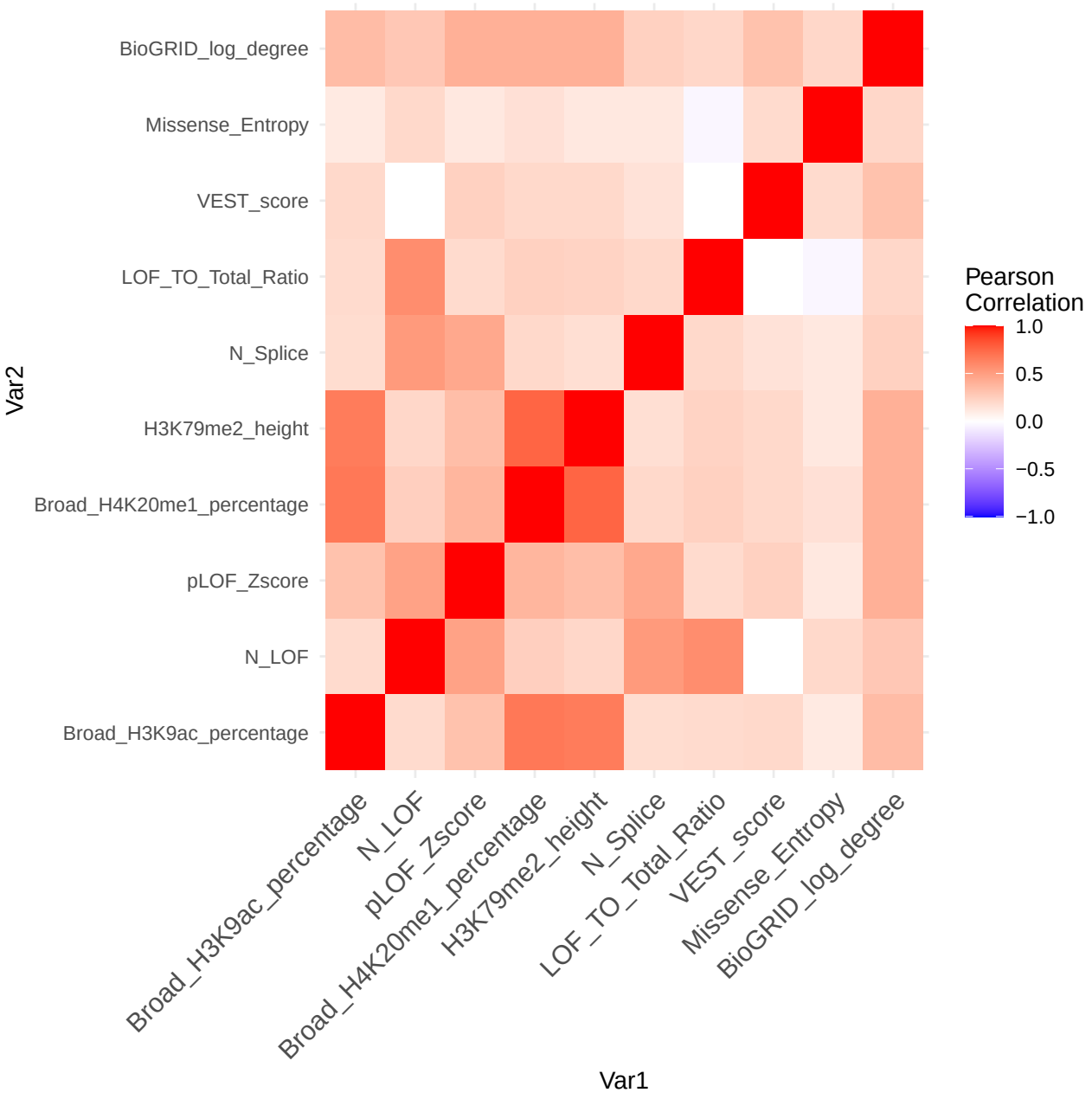
```r
# Selection of Predictors
vars <- training %>% dplyr::select(
  Broad_H3K9ac_percentage, N_LOF, pLOF_Zscore, Broad_H4K20me1_percentage,
  H3K79me2_height, N_Splice, LOF_TO_Total_Ratio, VEST_score,
  Missense_Entropy, BioGRID_log_degree, class
)
vars$class <- factor(vars$class)
levels(vars$class) <- c("NG", "OG", "TSG")


cor_mtx = round(cor(vars[, names(vars) != "class"]), 2)
library(reshape2)
```

```
Attaching package: 'reshape2'
```

```
The following object is masked from 'package:tidyr':

    smiths
```

```r
#reshape it
melted_cor_mtx <- melt(cor_mtx)

#draw the heatmap
```

```
cor_heatmap = ggplot(data = melted_cor_mtx, aes(x=Var1, y=Var2, fill=value)) +
  geom_tile()
cor_heatmap = cor_heatmap +
scale_fill_gradient2(
  low = "blue", high = "red", mid = "white", midpoint = 0, limit = c(-1,1),
  space = "Lab", name="Pearson\nCorrelation"
) +
theme_minimal() +
theme(axis.text.x = element_text(angle = 45, vjust = 1, size = 12, hjust = 1))

cor_heatmap
```



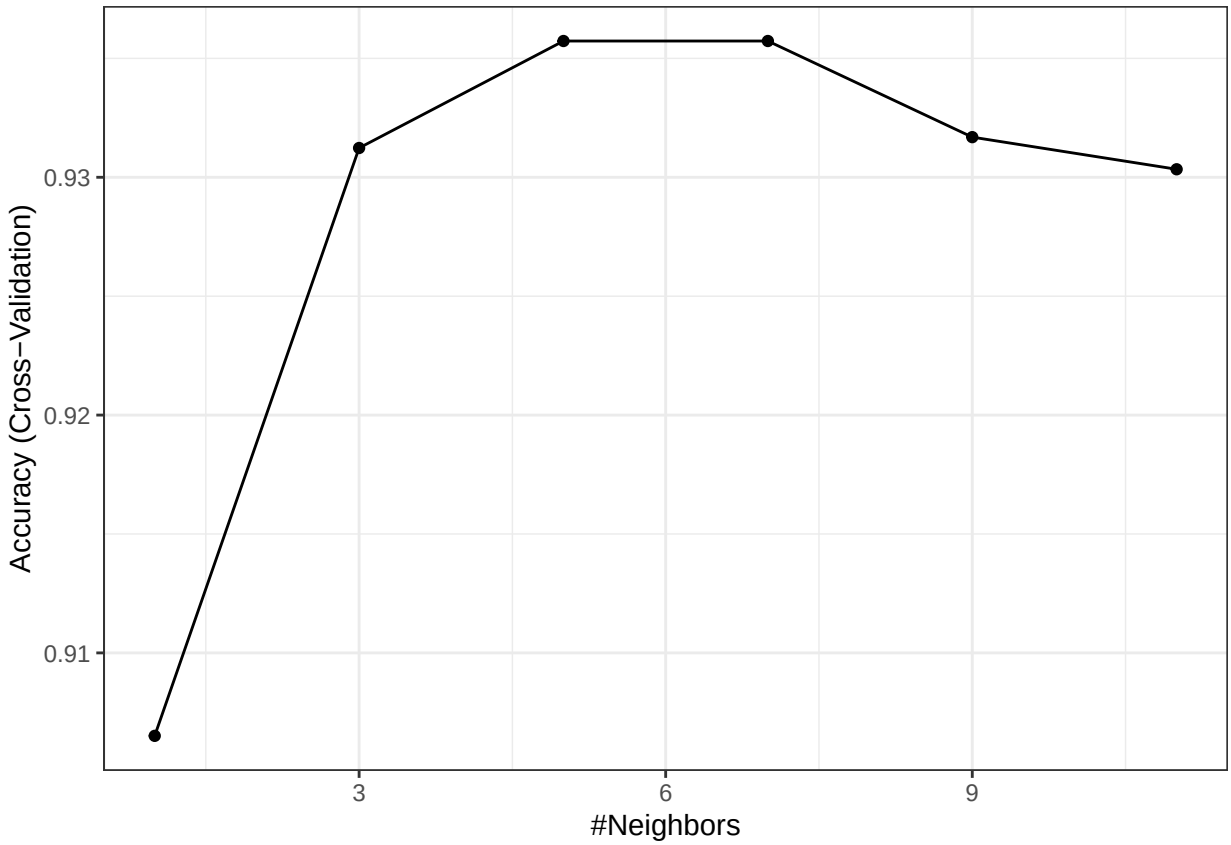
Techniques

KNN

```
set.seed(nrow(training) +421314)
library(caret)
```

```
Loading required package: lattice


Attaching package: 'caret'

The following object is masked from 'package:purrr':

    lift
```

```
vars_test <- createDataPartition(vars$class, p = 0.7,
                                 list = FALSE)
vars_train <- vars[vars_test, ]
vars_test <- vars[-vars_test, ]

train_cont <- trainControl(method = "cv", number = 10, classProbs = TRUE,
                           savePredictions = TRUE
                           )
mod <- train(class ~ ., data = vars_train, method = "knn",
                preProc = c("center", "scale"),
                trControl = train_cont,
                tuneGrid = expand.grid(k = seq(from = 1, to = 11, by = 2))
                )

ggplot(mod) + theme_bw()
```




```
for (k in seq(from = 1, to = 11, by = 2)) {
  preds <- predict(mod, newdata = vars_test, type = "prob")
  knn_mod <- table("pred" = unlist(apply(preds, 1, classify)), "obs" = vars_test$class)
  knn_mod
  score(knn_mod)
}
```

```
[1] 2063
[1] 0.723352
[1] 2083
[1] 0.7303647
[1] 2103
[1] 0.7373773
[1] 2103
[1] 0.7373773
[1] 2083
[1] 0.7303647
[1] 2083
[1] 0.7303647
```

QDA

```
train_cont <- trainControl(method = "cv", number = 10, classProbs = TRUE,
                           savePredictions = TRUE
                           )
mod <- train(class ~ ., data = vars_train, method = "qda",
                preProc = c("center", "scale"),
                trControl = train_cont)
preds <- predict(mod, newdata = vars_test, type = "prob")

qda_mod <- table("pred" = apply(preds, 1, classify), "obs" = vars_test$class)
qda_mod
```

```
    obs
pred  NG  OG TSG
   0 768   9   8
   1  16  28   3
   2  68  13  39
```

```
score(qda_mod)
```

```
[1] 2108
[1] 0.7391304
```

LDA

```
train_cont <- trainControl(
  method = "cv", number = 10, classProbs = TRUE, savePredictions = TRUE
)
mod <- train(class ~ ., data = vars_train, method = "lda",
                preProc = c("center", "scale"),
                trControl = train_cont
                )
preds <- predict(mod, newdata = vars_test, type = "prob")

lda_mod <- table("pred"=apply(preds, 1, classify), "obs" = vars_test$class)
lda_mod
```

```
    obs
pred  NG  OG TSG
   0 804   9   6
   1  19  30   7
   2  29  11  37
```

```
score(lda_mod)
```

```
[1] 2144
[1] 0.7517532
```