

Model #6

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Transforming and Cleaning the Data

```
training <- read.csv("training.csv", stringsAsFactors = TRUE)
training$class <- factor(training$class)
levels(training$class) <- c("NG", "OG", "TSG")
outlier <- function(data) {
  low <- mean(data) - 3 * sd(data)
  high <- mean(data) + 3 * sd(data)
  which(data < low | data > high)
}
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)
outlier_index <- sort(table(unlist(lapply(training[, -99], outlier))), decreasing = TRUE)
outlier_index[1:100]
```

| | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 915 | 1280 | 2918 | 517 | 1914 | 2182 | 3052 | 1173 | 2215 | 3049 | 259 | 740 | 1749 | 1979 | 2998 | 417 |
| 24 | 24 | 24 | 22 | 22 | 22 | 20 | 19 | 19 | 19 | 18 | 18 | 18 | 18 | 18 | 17 |
| 441 | 806 | 2297 | 422 | 635 | 1258 | 1570 | 2278 | 2518 | 2729 | 80 | 150 | 2694 | 169 | 276 | 341 |
| 17 | 17 | 17 | 16 | 16 | 16 | 16 | 16 | 16 | 16 | 15 | 15 | 15 | 14 | 14 | 14 |
| 1528 | 1556 | 1726 | 1809 | 1911 | 1955 | 2071 | 2624 | 2641 | 3120 | 3142 | 73 | 277 | 364 | 751 | 1244 |
| 14 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 13 | 13 | 13 | 13 | 13 |
| 1330 | 2329 | 2787 | 343 | 1138 | 1171 | 1188 | 1372 | 1460 | 2031 | 2251 | 2968 | 2983 | 3166 | 352 | 634 |
| 13 | 13 | 13 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 11 | 11 |
| 907 | 923 | 1096 | 1858 | 2636 | 588 | 1137 | 1317 | 1463 | 1561 | 1740 | 1991 | 2487 | 2540 | 2555 | 2621 |
| 11 | 11 | 11 | 11 | 11 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 2815 | 3029 | 74 | 144 | 657 | 789 | 857 | 1267 | 1610 | 1932 | 2022 | 2093 | 2142 | 2534 | 2666 | 2721 |
| 10 | 10 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 |
| 2848 | 2900 | 3027 | 155 | | | | | | | | | | | | |
| 9 | 9 | 9 | 8 | | | | | | | | | | | | |

```

training <- training[-as.numeric(names(outlier_index)[1:50]),]
sort(training$Missense_TO_Silent_Ratio, decreasing = TRUE)[1:10]

[1] 384.98658 172.91420 135.59623 71.09712 23.21809 21.81193 20.37791
[8] 19.42402 19.38769 15.84808

training <- training[-which(training$Missense_TO_Silent_Ratio > 100), ]
sort(training$Missense_KB_Ratio, decreasing = TRUE)[1:10]

[1] 2063.9413 1296.6625 1060.0601 952.3810 931.4227 726.8519 594.7603
[8] 593.3610 581.5085 516.8084

training <- training[-which(training$Missense_KB_Ratio > 2000), ]
sort(training$LOF_TO_Silent_Ratio, decreasing = TRUE)[1:10]

[1] 81.177835 9.030120 6.470238 5.582840 4.741460 4.558252 4.176630
[8] 4.058140 4.039062 4.021930

training <- training[-which(training$LOF_TO_Silent_Ratio > 5), ]
sort(training$Gene_expression_Z_score, decreasing = TRUE)[1:10]

[1] 19.720 9.210 7.080 6.883 6.590 6.280 5.321 5.316 3.161 2.767

training <- training[-which(training$Gene_expression_Z_score > 4), ]
sort(training$dN_to_dS_ratio, decreasing = TRUE)[1:10]

[1] 20.950 3.649 3.446 3.372 2.574 2.194 2.183 2.102 1.921 1.744

training <- training[-which(training$dN_to_dS_ratio > 5),]
sort(training$Silent_KB_Ratio, decreasing = TRUE)[1:10]

[1] 474.4745 193.1684 174.0558 171.0362 166.4971 160.2273 158.7697 148.5800
[9] 143.6782 135.2657

training <- training[-which(training$Silent_KB_Ratio > 200), ]
sort(training$Lost_start_and_stop_fraction, decreasing = TRUE)[1:10]

[1] 0.333 0.167 0.118 0.087 0.074 0.071 0.071 0.068 0.067 0.067

training <- training[-which(training$Lost_start_and_stop_fraction > 0.2),]
sort(training$Synonymous_Zscore, decreasing = FALSE)[1:10]

[1] -20.5110 -10.9780 -10.2960 -9.7346 -9.3720 -8.8090 -8.4062 -8.3918
[9] -8.1076 -8.1076

training <- training[-which(training$Synonymous_Zscore < -15), ]
numeric_training <- training[,-99]

n_zeroes <- rep(NA, nrow(numeric_training))

for(i in seq_len(nrow(numeric_training))){
  row_i_zeroes <- 0
  for(j in seq_len(ncol(numeric_training))){
    if(round(numeric_training[i,j], digits = 5) == 0){
      row_i_zeroes <- row_i_zeroes + 1
    }
  }
  n_zeroes[i] <- row_i_zeroes
}

```

```
training <- training[n_zeroes <= 50, ]
```

```
library(dplyr)
```

Attaching package: 'dplyr'

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

combine

The following objects are masked from 'package:stats':

filter, lag

The following objects are masked from 'package:base':

intersect, setdiff, setequal, union

#function to calculate wca

```
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)))  
}
```

Set new threshold to account for unbalanced data

```
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)  
    }  
  } else {  
    output <- 0  
  }  
  output  
}
```

Multinom (Logistic Regression)

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

Loading required package: lattice

```
set.seed(12)
vars <- training %>% select(Broad_H3K9ac_percentage, N_LOF, pLOF_Zscore,
                           Missense_Entropy,
                           N_Splice, LOF_T0_Total_Ratio, VEST_score,
                           BioGRID_log_degree,
                           Broad_H3K79me2_percentage, FamilyMemberCount,
                           S50_score_replication_timing, Gene_expression_Z_score,
                           Polyphen2, Broad_H3K36me3_percentage, class)
vars_test <- createDataPartition(vars$class, p = 0.76,
                                  list = FALSE)
vars_train <- vars[vars_test, ]
vars_test <- vars[-vars_test, ]

mn <- nnet::multinom(class ~ ., data = vars_train, model = TRUE)

# weights: 48 (30 variable)
initial value 2529.005489
iter 10 value 1107.105807
iter 20 value 691.259918
iter 30 value 488.541584
iter 40 value 360.054663
iter 50 value 357.690644
final value 357.690368
converged

tidymn <- broom::tidy(mn) %>% arrange(p.value)
terms <- tidymn$term[-(1:2)]
terms <- unique(terms)

vars_mn <- training %>% select("VEST_score", "BioGRID_log_degree",
                              "Missense_Entropy",
                              "Broad_H3K9ac_percentage",
                              "N_LOF", "Broad_H3K36me3_percentage",
                              "pLOF_Zscore", "N_Splice", "LOF_T0_Total_Ratio",
                              "FamilyMemberCount", "Polyphen2",
                              "Broad_H3K79me2_percentage", "Gene_expression_Z_score",
                              "S50_score_replication_timing"
                              ) # these are just the predictors it liked

tests <- read.csv("test.csv")
preds <- predict(mn, newdata = vars_test, type = "prob")
predclass <- apply(preds, 1, classify)
tbl <- table(predclass, vars_test$class)
score(tbl)

[1] 1634
[1] 0.8252525
tbl
```

| predclass | NG | OG | TSG |
|-----------|-----|----|-----|
| 0 | 574 | 2 | 4 |
| 1 | 54 | 31 | 5 |
| 2 | 32 | 2 | 22 |