Preliminary Investigation

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```
set.seed(110920)
# 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
```

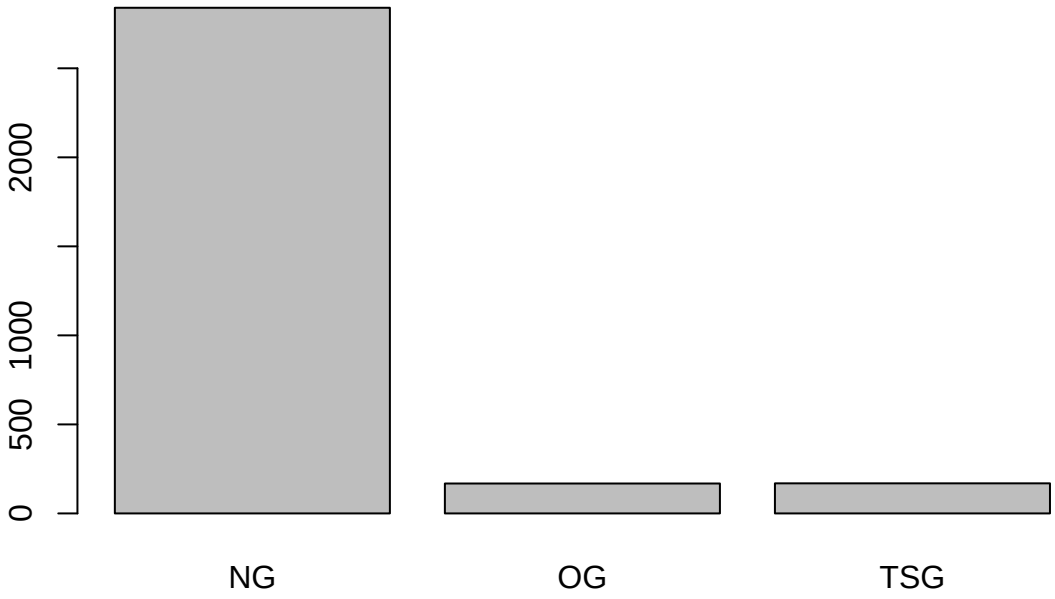
```
training$class <- factor(training$class)
levels(training$class) <- c("NG", "OG", "TSG")
dim(training)
```

```
[1] 3177   99
```

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

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

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



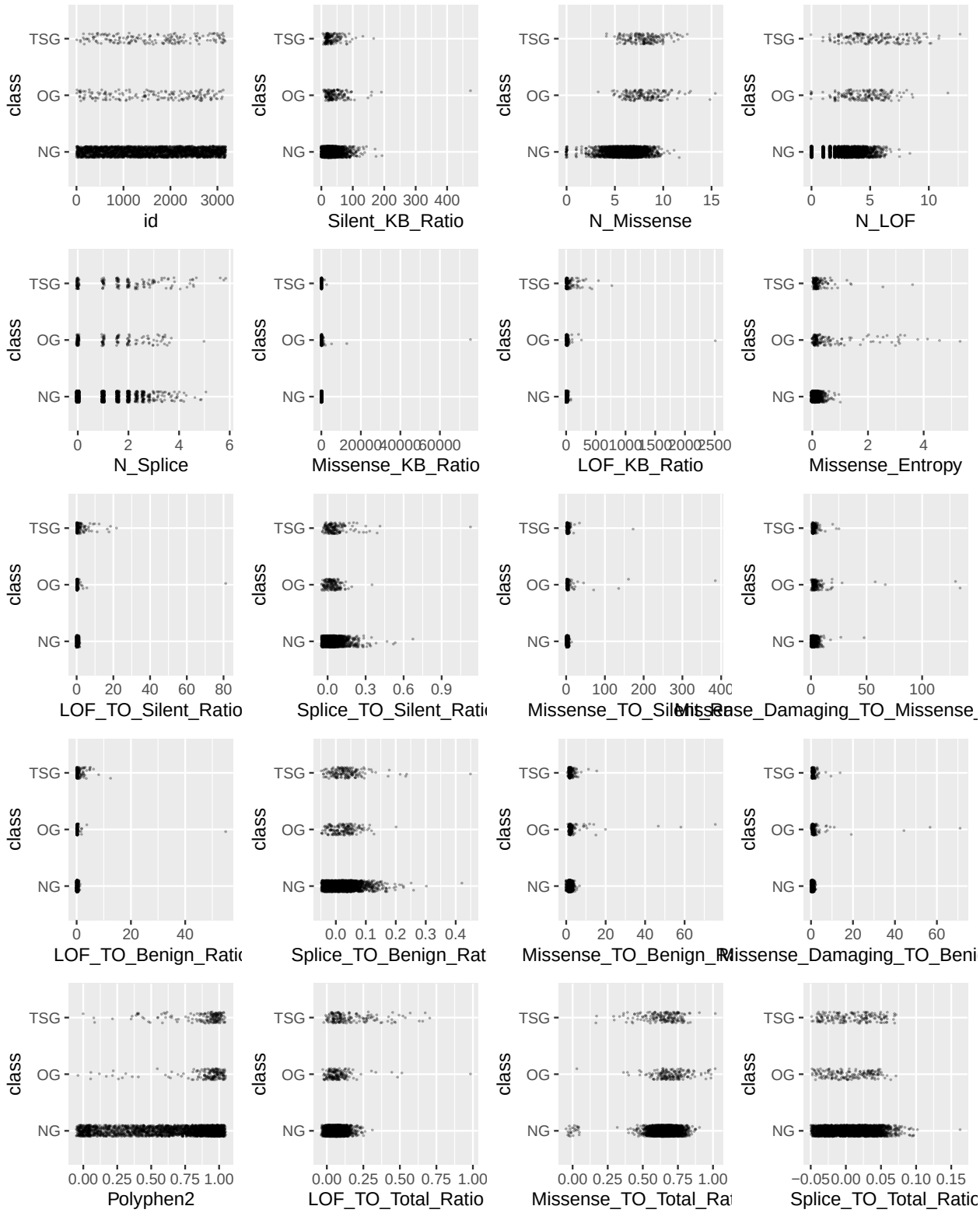

```
table(training$class) / nrow(training)
```

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

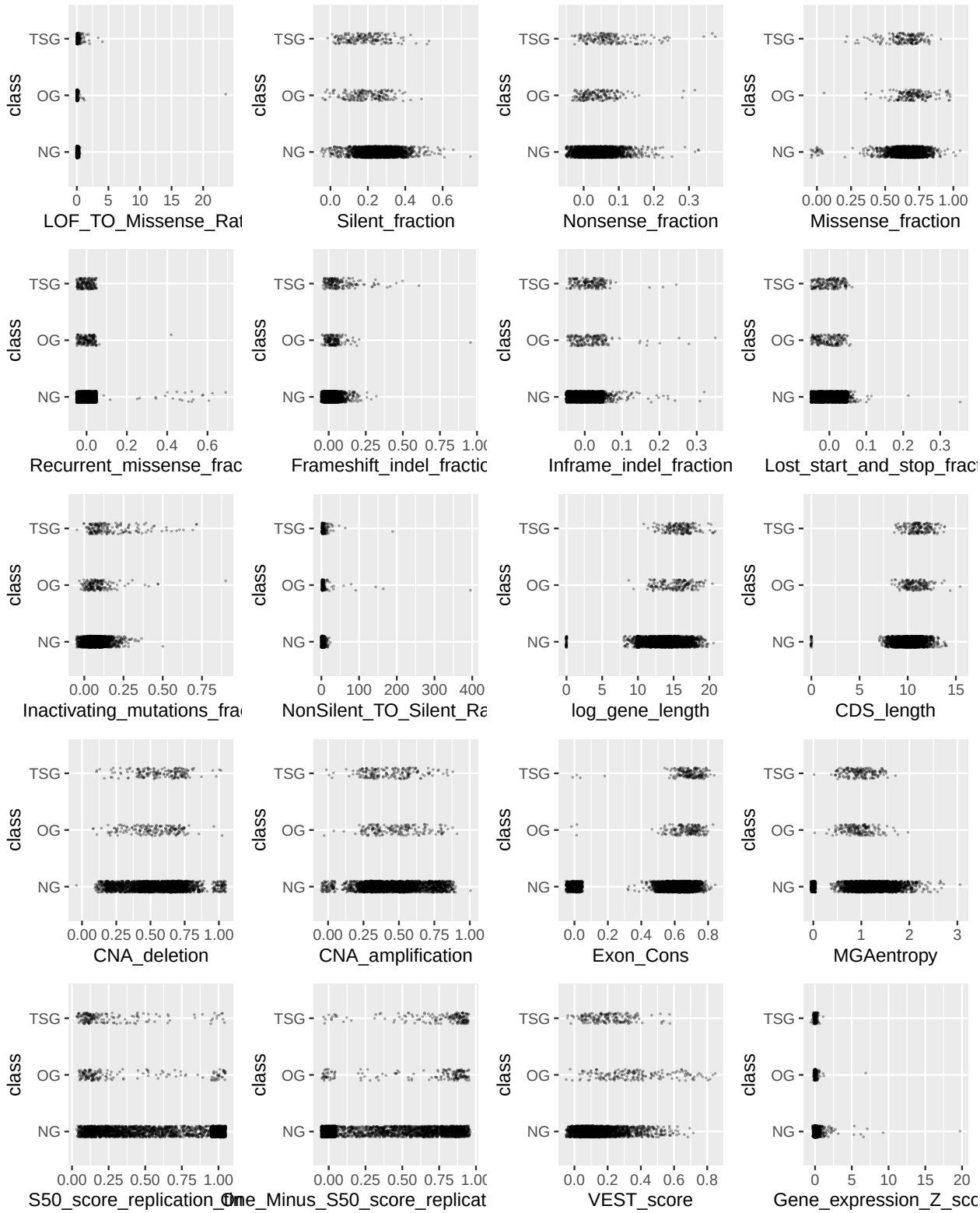
```
any(is.na(training))
```

```
[1] FALSE
```

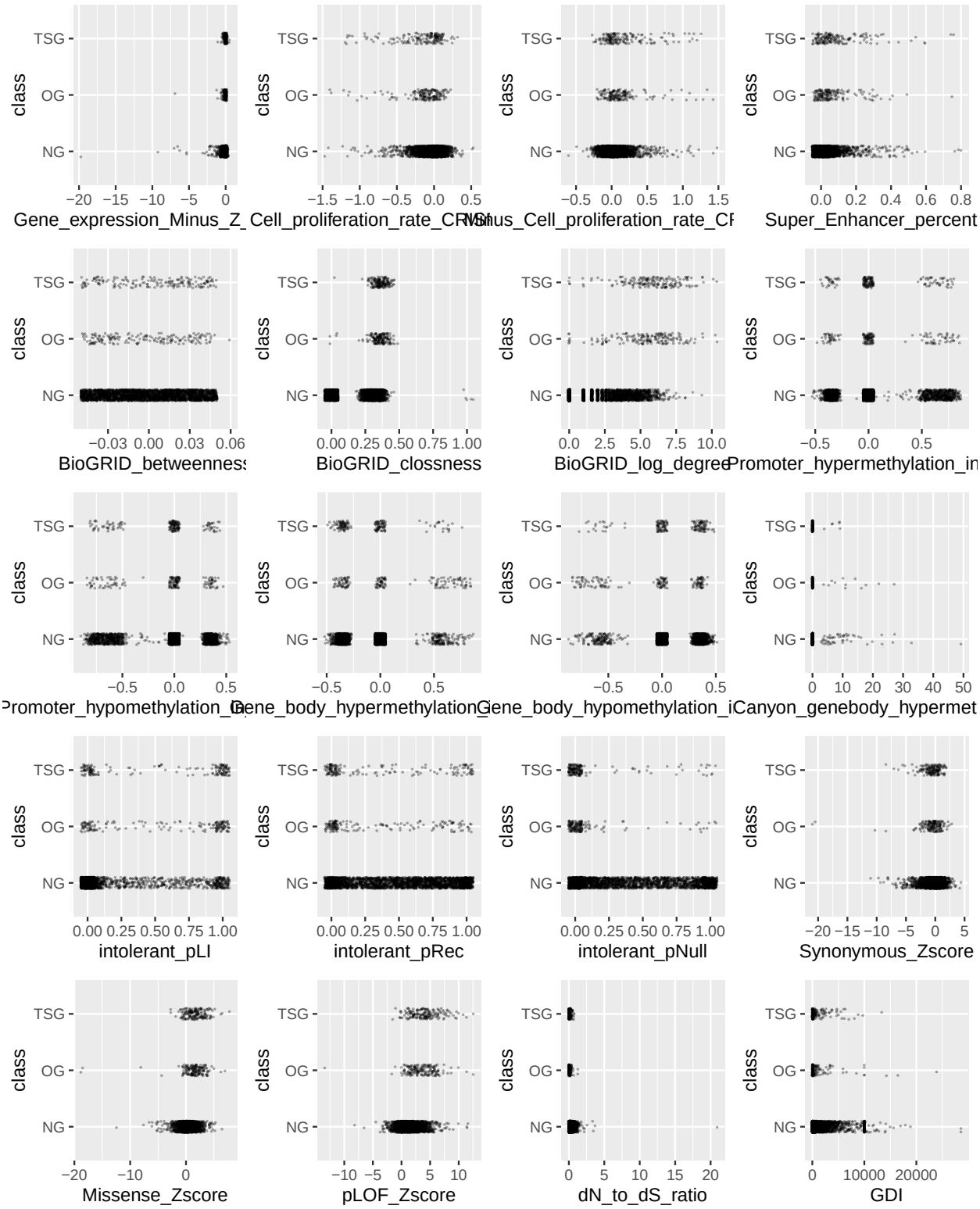
```
library(ggplot2)
scatter <- function(var) {
  ggplot(training, aes_string(var, "class")) +
    geom_jitter(width = 0.05, height = 0.1, size = 0.1,
                colour = rgb(0, 0, 0, alpha = 1 / 3))
}
scat_plot <- lapply(names(training)[-99], scatter)
library(gridExtra)
grid.arrange(grobs = scat_plot[1:20],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



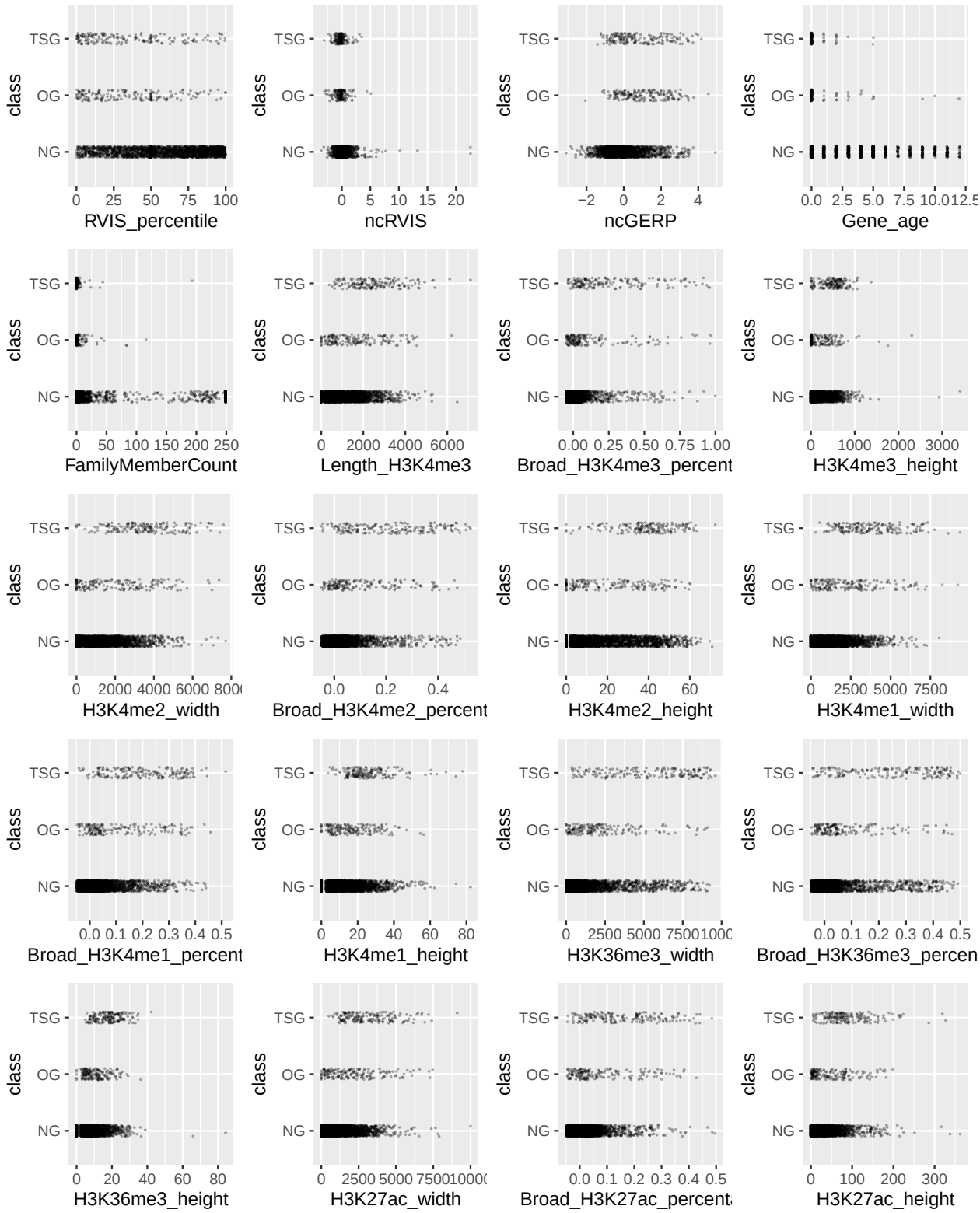

```
grid.arrange(grobs = scat_plot[21:40], ncol = 4)
```



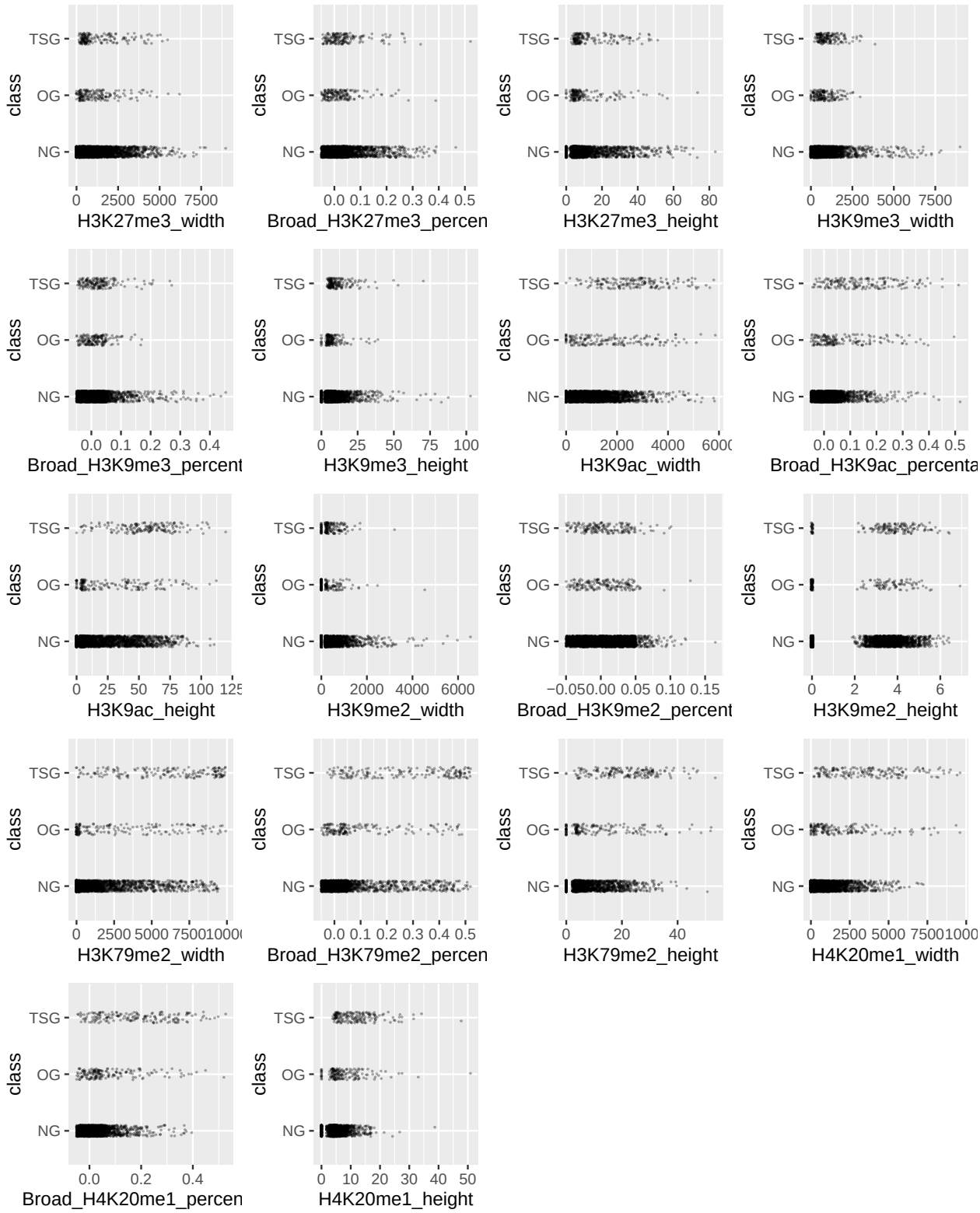

```
grid.arrange(grobs = scat_plot[41:60], ncol = 4)
```




```
grid.arrange(grobs = scat_plot[61:80], ncol = 4)
```




```
grid.arrange(grobs = scat_plot[81:98], ncol = 4)
```




```
sig <- logical(98)
names(sig) <- names(training)[-99]
k <- 1
diffs <- logical(98)
```

```r
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
}
sort(sig[diffs])
```

```
Broad_H4K20me1_percentage
             2.605382e-232
  Broad_H3K9ac_percentage
             8.993961e-184
           H4K20me1_width
             3.222855e-181
          H3K79me2_height
             4.253756e-176
           H3K79me2_width
             2.449130e-175
 Broad_H3K4me2_percentage
             4.311054e-174
Broad_H3K79me2_percentage
             1.188924e-168
 Broad_H3K27ac_percentage
             2.345807e-168
          H4K20me1_height
             1.791736e-164
 Broad_H3K4me1_percentage
             1.065370e-163
Broad_H3K36me3_percentage
             4.471080e-154
           H3K36me3_width
             2.142472e-147
               pLOF_Zscore
             5.366468e-145
 Broad_H3K4me3_percentage
             2.017738e-143
           H3K4me1_width
             5.760242e-141
                VEST_score
             8.594619e-138
                      N_LOF
             2.985376e-137
         Missense_Entropy
             2.153653e-134
           H3K4me2_width
             3.996102e-127
            H3K9ac_width
             8.106205e-120
          H3K36me3_height
             3.589138e-112
           H3K27ac_width
             1.075439e-109
       LOF_TO_Total_Ratio
             1.795563e-106
```

```
                            Length_H3K4me3
                              5.345828e-104
                            H3K27ac_height
                              2.296798e-103
                             H3K9ac_height
                              1.404194e-101
          Inactivating_mutations_fraction
                              3.210725e-84
                            H3K4me3_height
                              6.912938e-81
                                  N_Splice
                              2.765822e-77
                Frameshift_indel_fraction
                              4.847595e-77
                            H3K4me2_height
                              4.174575e-71
                            H3K4me1_height
                              1.800505e-62
Missense_Damaging_TO_Missense_Benign_Ratio
                              1.778682e-49
    One_Minus_S50_score_replication_timing
                              4.727754e-44
             S50_score_replication_timing
                              4.727754e-44
                 Missense_TO_Benign_Ratio
                              2.805142e-43
         Missense_Damaging_TO_Benign_Ratio
                              1.057841e-41
                Super_Enhancer_percentage
                              1.637695e-38
                              LOF_KB_Ratio
                              2.566176e-37
                     LOF_TO_Silent_Ratio
                              3.416804e-35
                NonSilent_TO_Silent_Ratio
                              2.030973e-33
                                CDS_length
                              3.970782e-32
                 Missense_TO_Silent_Ratio
                              2.841077e-24
                   Inframe_indel_fraction
                              5.669973e-16
                  Missense_TO_Total_Ratio
                              1.973442e-09
                        Missense_fraction
                              1.031541e-08
```

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

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
}
```

```
library(dplyr)
```

```
Attaching package: 'dplyr'
```

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

    combine
```

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

    filter, lag
```

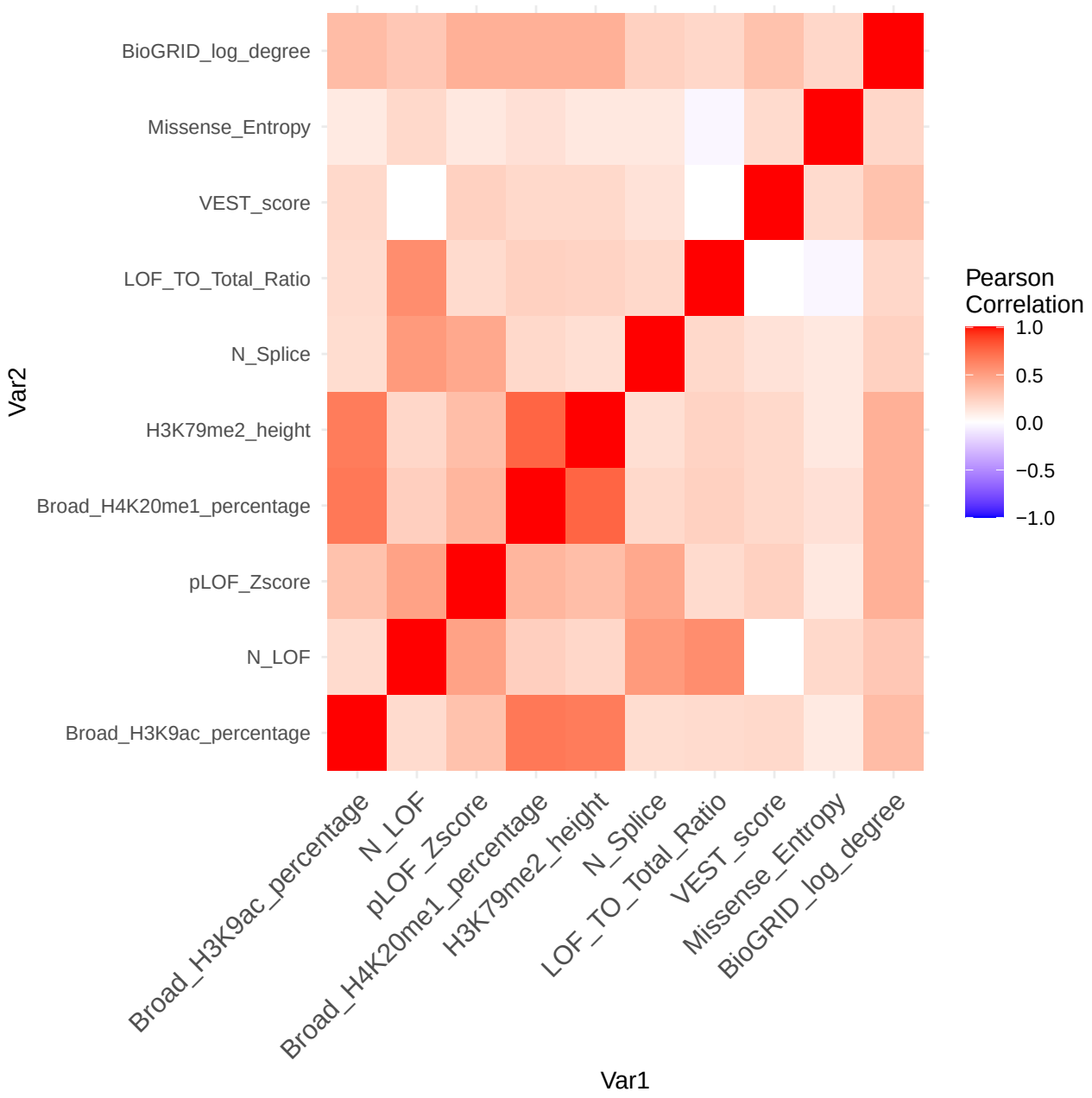
```
The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

```
vars <- training %>% 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_deg
vars$class <- factor(vars$class)
levels(vars$class) <- c("NG", "OG", "TSG")
cor_mtx = round(cor(vars[, names(vars) != "class"]), 2)
library(reshape2)
#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 =
theme_minimal() +
theme(axis.text.x = element_text(angle = 45, vjust = 1, size = 12, hjust = 1))

cor_heatmap
```




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

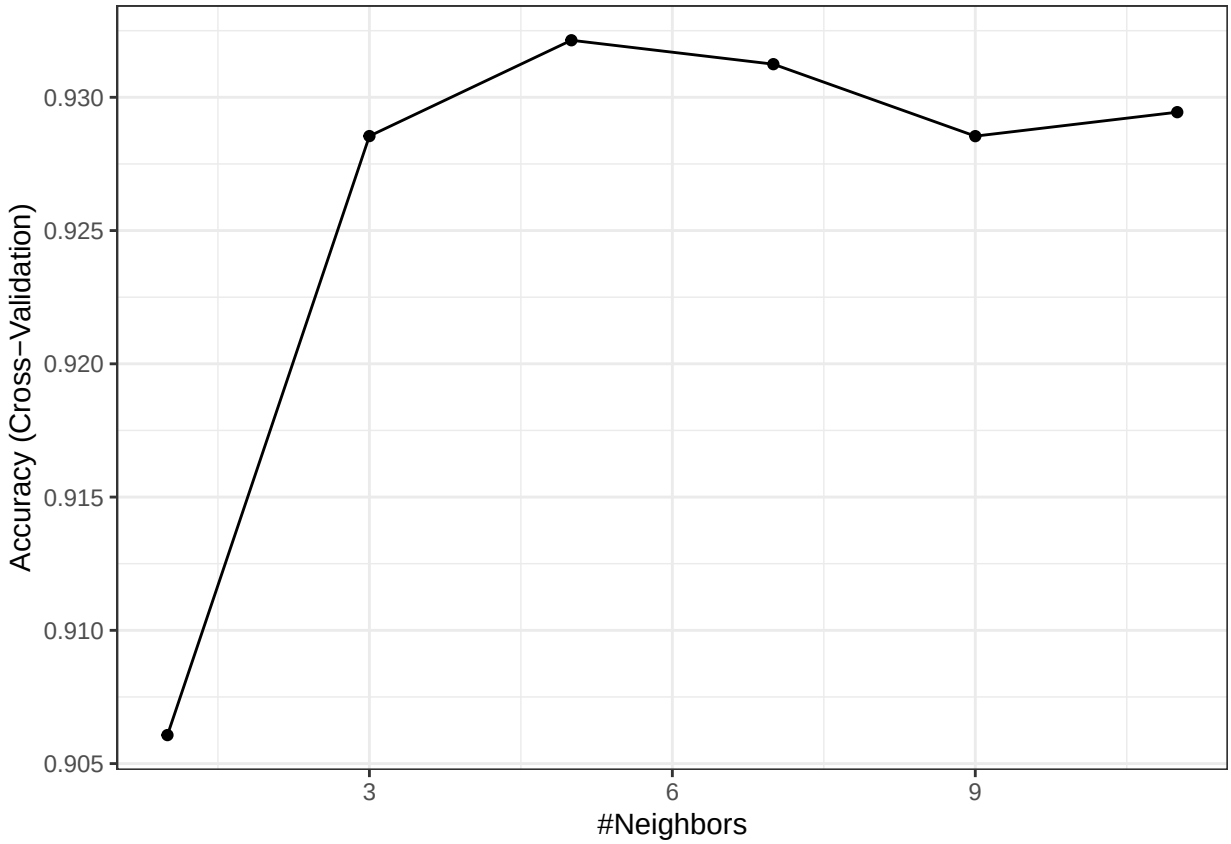
```
Loading required package: lattice
```

```
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 = 5, classProbs = TRUE, savePredictions = TRUE)


knn_ft <- 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(knn_ft) + theme_bw()
```




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

```
[1] 2148
[1] 2008
[1] 2068
[1] 2108
[1] 2068
[1] 2048
```

```
train_cont <- trainControl(method = "cv", number = 5, classProbs = TRUE, savePredictions = TRUE)
qda_ft <- train(class ~ ., data = vars_train, method = "qda", preProc = c("center", "scale"),
                trControl = train_cont)
preds <- predict(qda_ft, 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
```

```
train_cont <- trainControl(method = "cv", number = 5, classProbs = TRUE, savePredictions = TRUE)
lda_ft <- train(class ~ ., data = vars_train, method = "lda", preProc = c("center", "scale"),
                trControl = train_cont)
preds <- predict(lda_ft, 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
```

```
library(MLeval)
```

```
Attaching package: 'MLeval'
```

```
The following object is masked _by_ '.GlobalEnv':

    preds
```

```
res <- evalm(list(knn_ft, qda_ft, lda_ft),gnames=c('KNN',
                                                   'LDA', 'QDA'))
```

```
***MLeval: Machine Learning Model Evaluation***
```

```
Input: caret train function object
```

```
Not averaging probs.
```

```
Group 1 type: cv
```

```
Group 2 type: cv
```

```
Group 3 type: cv
```

```
Observations: 6675
```

```
Number of groups: 3
```

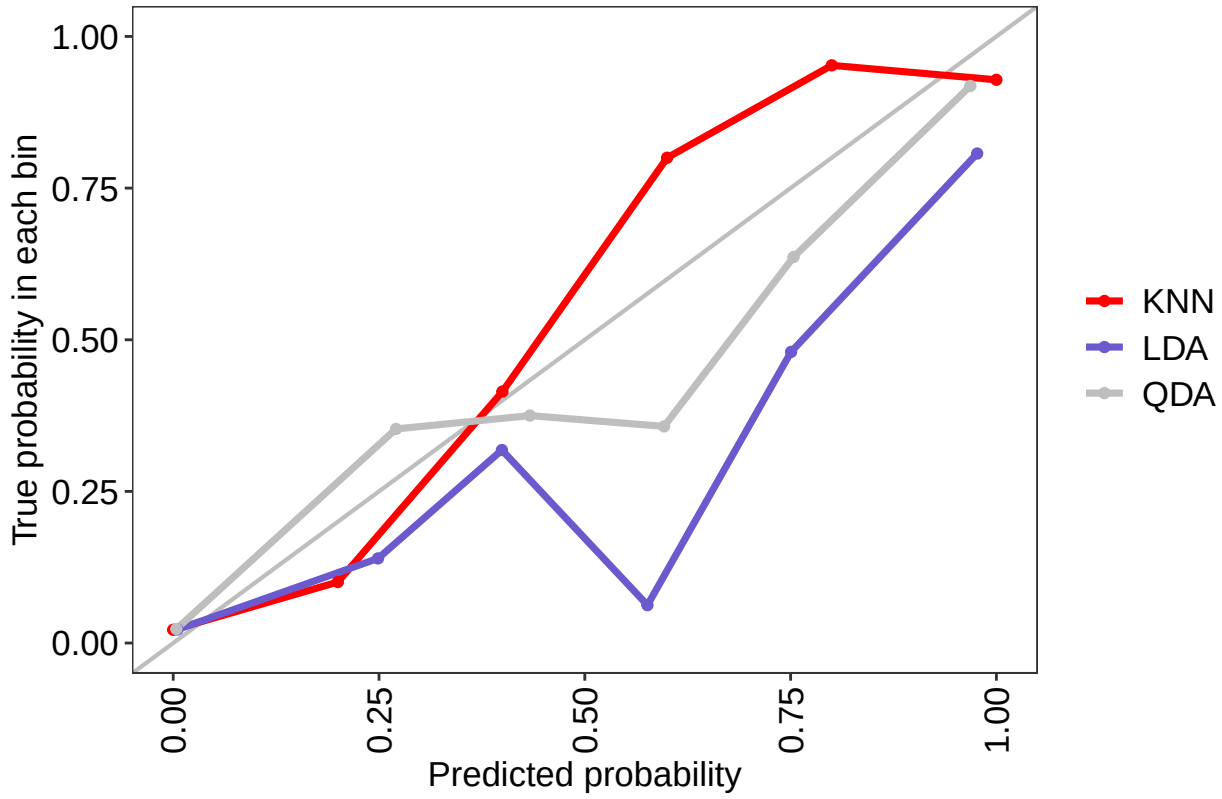
```
Observations per group: 2225
```

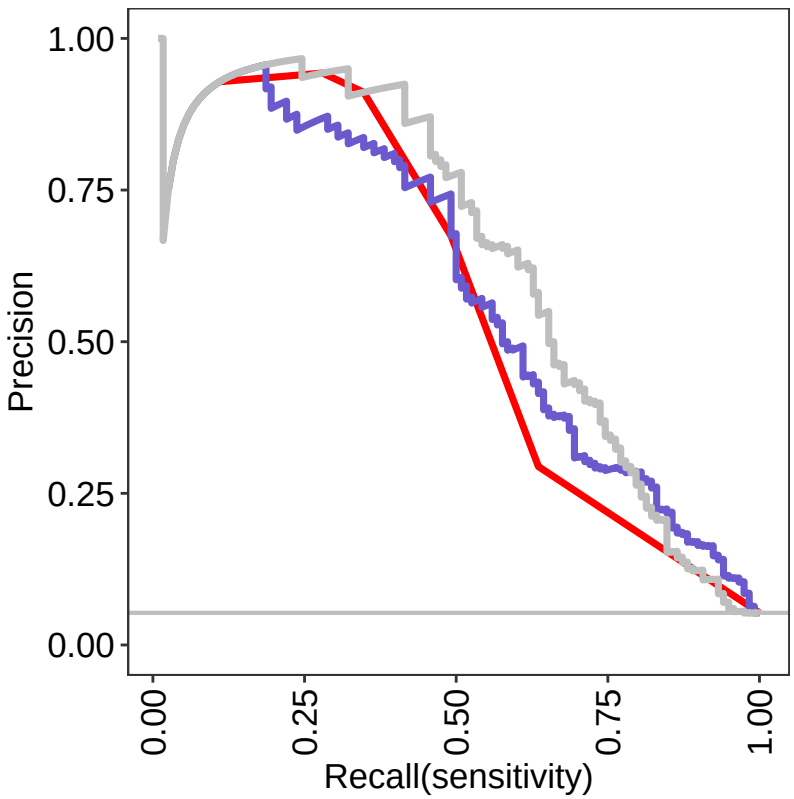
```
Positive: OG
```

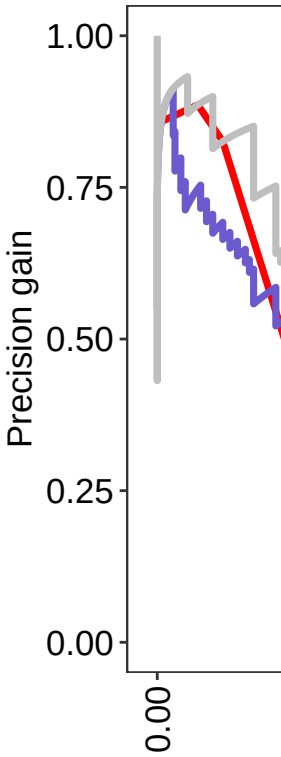
```
Negative: NG
```

```
Group: KNN
```

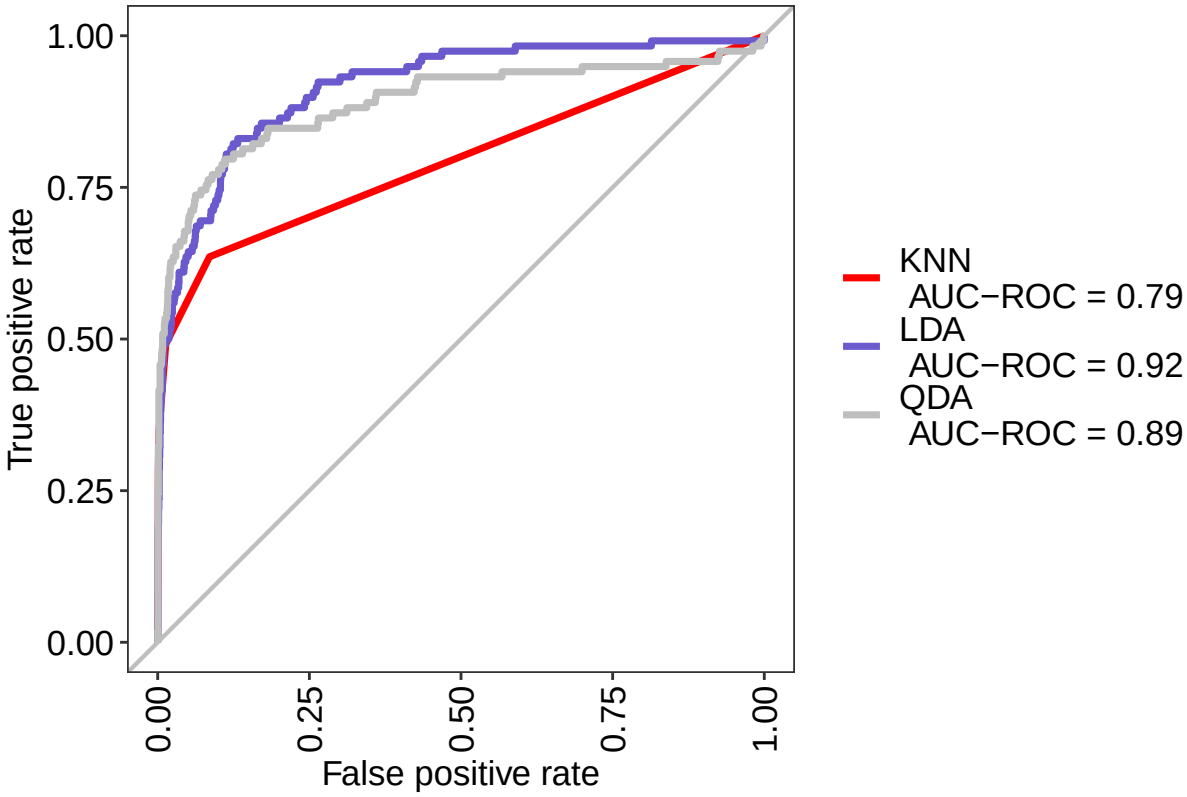
```
Positive: 118
Negative: 1988
Group: LDA
Positive: 118
Negative: 1988
Group: QDA
Positive: 118
Negative: 1988
***Performance Metrics***
```



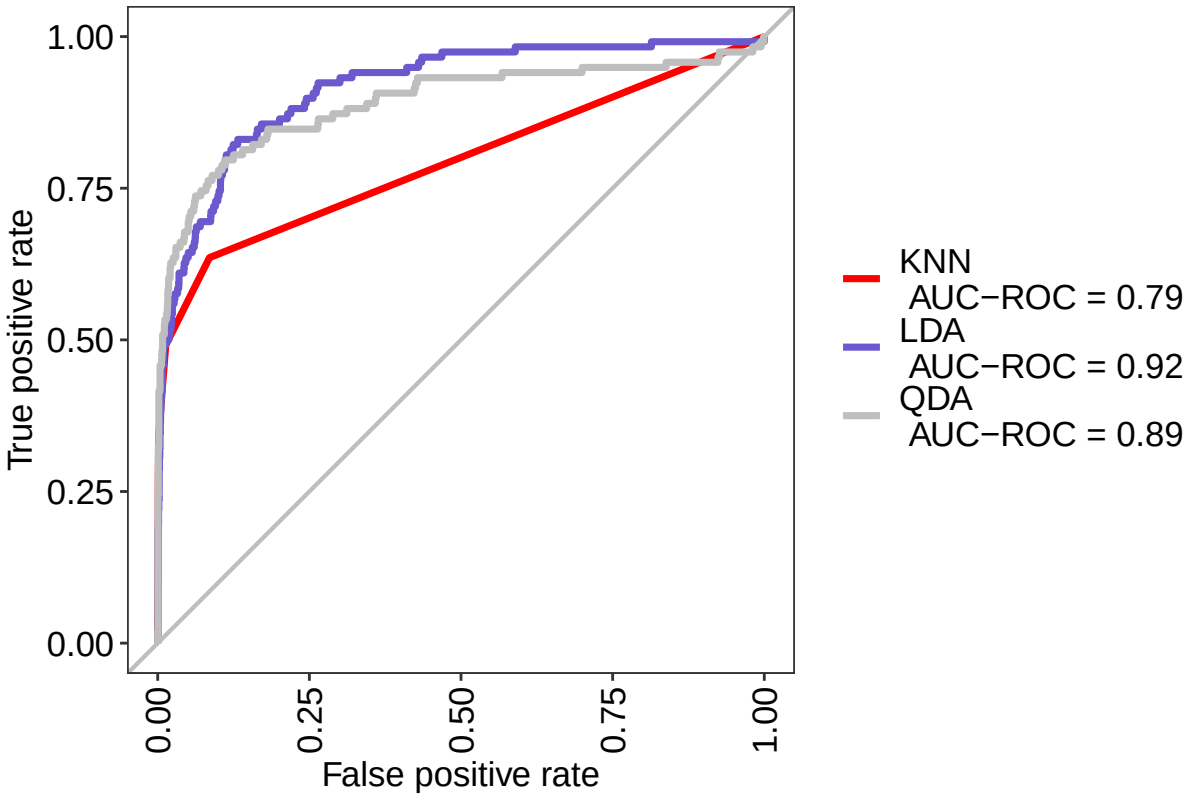





```
KNN Optimal Informedness = 0.550163699693516
LDA Optimal Informedness = 0.698567326023827
QDA Optimal Informedness = 0.685077184204387
KNN AUC-ROC = 0.79
LDA AUC-ROC = 0.92
QDA AUC-ROC = 0.89
```


1.00
0.75
0.50
0.25
0.00
True positive rate
0.00
0.25
0.50
0.75
1.00
False positive rate
KNN
AUC−ROC = 0.79
LDA
AUC−ROC = 0.92
QDA
AUC−ROC = 0.89

```
res$roc
```


1.00
0.75
0.50
0.25
0.00
True positive rate
0.00
0.25
0.50
0.75
1.00
False positive rate
KNN
AUC−ROC = 0.79
LDA
AUC−ROC = 0.92
QDA
AUC−ROC = 0.89

```
library(leaps)
best_subset <- regsubsets(class ~ ., data = training, nbest = 1, nvmax = 20,
                          intercept = TRUE, method = "forward",
                          really.big = TRUE)
```

```
Warning in leaps.setup(x, y, wt = wt, nbest = nbest, nvmax = nvmax, force.in =
force.in, : 5 linear dependencies found
```

```
Reordering variables and trying again:
```

```
sumBS <- summary(best_subset)
plot(best_subset)
```