Measuring Performance: Evaluating SMOTE

Spiro Stilianoudakis

Contents

Loading Packages

```
library(caret)
```

```
## Warning: package 'caret' was built under R version 3.4.4
## Loading required package: lattice
## Loading required package: ggplot2
## Warning: package 'ggplot2' was built under R version 3.4.4
```

```
#library(data.table)
library(gbm)
```

```
## Loading required package: survival
##
## Attaching package: 'survival'
## The following object is masked from 'package:caret':
##
##     cluster
## Loading required package: splines
## Loading required package: parallel
## Loaded gbm 2.1.3
```

```
library(pROC)
```

```
## Warning: package 'pROC' was built under R version 3.4.4
## Type 'citation("pROC")' for a citation.
##
## Attaching package: 'pROC'
## The following objects are masked from 'package:stats':
##
##     cov, smooth, var
```

```r
library(plyr)
library(dplyr)
```

```
## Warning: package 'dplyr' was built under R version 3.4.4
```

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

```
## The following objects are masked from 'package:plyr':
##
##     arrange, count, desc, failwith, id, mutate, rename, summarise,
##     summarize
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```r
library(DMwR)
```

```
## Loading required package: grid
```

```
##
## Attaching package: 'DMwR'
```

```
## The following object is masked from 'package:plyr':
##
##     join
```

```r
library(gridExtra)
```

```
##
## Attaching package: 'gridExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

```r
library(ggplot2)
library(leaps)
#library(DT)
library(knitr)
```

```
## Warning: package 'knitr' was built under R version 3.4.4
```

Setting Working directory

```r
setwd("C:/Users/Spiro Stilianoudakis/Documents/TAD_data/RData/GM12878/testing_SMOTE")
```

Testing SMOTE

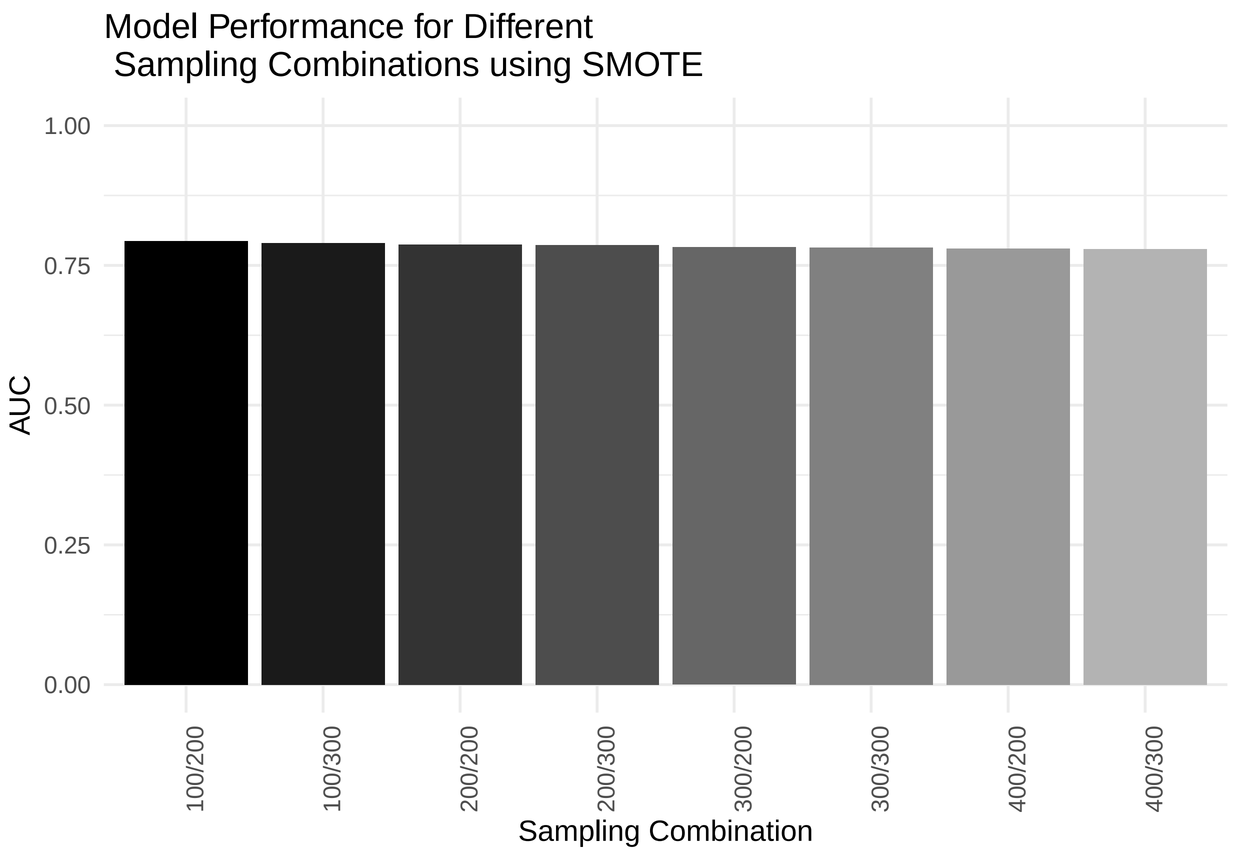
```r
enetlst_sm <- readRDS("C:/Users/Spiro Stilianoudakis/Documents/TAD_data/RData/GM12878/testing_SMOTE/ene

#Plotting Performance
auc.sm <- data.frame(Combination=c("100/200","200/200","300/200","400/200",
                                   "100/300","200/300","300/300","400/300"),
                       AUC=c(enetlst_sm[[3]][1],enetlst_sm[[3]][2],enetlst_sm[[3]][3],
                             enetlst_sm[[3]][4],enetlst_sm[[3]][5],enetlst_sm[[3]][6],
                             enetlst_sm[[3]][7],enetlst_sm[[3]][8]))

auc.sm <- auc.sm[order(auc.sm$AUC, decreasing=TRUE),]

auc.sm$Combination <- factor(auc.sm$Combination, levels=auc.sm$Combination)

auc.sm
```

```
##   Combination       AUC
## 1     100/200 0.7936148
## 5     100/300 0.7898228
## 2     200/200 0.7872268
## 6     200/300 0.7864398
## 3     300/200 0.7824853
## 7     300/300 0.7820608
## 4     400/200 0.7802347
## 8     400/300 0.7790618
```

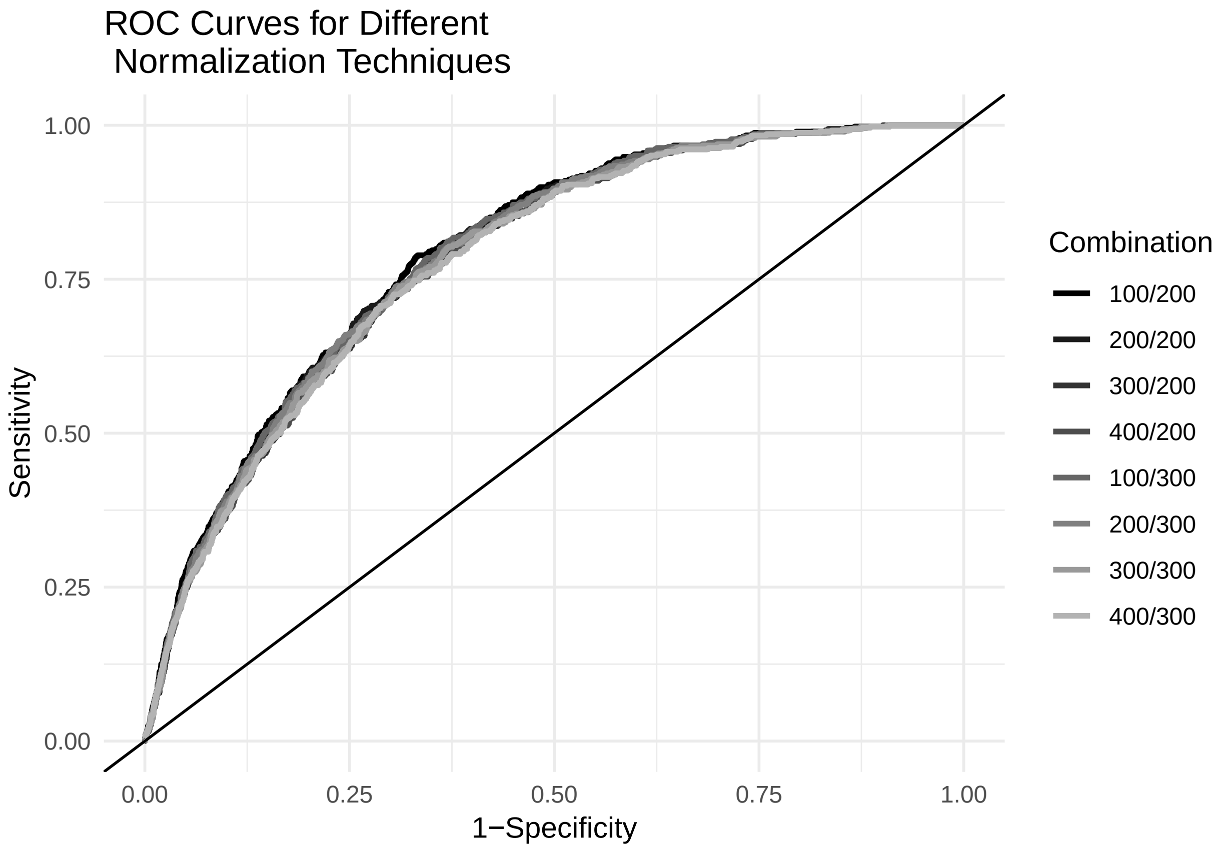
```r
#datatable(auc.sm)
kable(auc.sm)
```

	Combination	AUC
1	100/200	0.7936148
5	100/300	0.7898228
2	200/200	0.7872268
6	200/300	0.7864398
3	300/200	0.7824853
7	300/300	0.7820608
4	400/200	0.7802347
8	400/300	0.7790618

```r
p<-ggplot(data=auc.sm, aes(x=Combination, y=AUC, fill=Combination)) +
  xlab("Sampling Combination") + ylab("AUC") +
  geom_bar(stat="identity") + ylim(0,1) +
  scale_fill_manual(values=gray(seq(0,.7,.1)), guide=FALSE) +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +
  ggtitle("Model Performance for Different \n Sampling Combinations using SMOTE")
p
```



```
onetwo <- data.frame(fpr=enetlst_sm[[2]][,1],tpr=enetlst_sm[[1]][,1], Combo = "100/200");
twotwo <- data.frame(fpr=enetlst_sm[[2]][,2],tpr=enetlst_sm[[1]][,2], Combo = "200/200");
threetwo <- data.frame(fpr=enetlst_sm[[2]][,3],tpr=enetlst_sm[[1]][,3], Combo = "300/200");
fourtwo <- data.frame(fpr=enetlst_sm[[2]][,4],tpr=enetlst_sm[[1]][,4], Combo = "400/200");
onethree <- data.frame(fpr=enetlst_sm[[2]][,5],tpr=enetlst_sm[[1]][,5], Combo = "100/300");
twothree <- data.frame(fpr=enetlst_sm[[2]][,6],tpr=enetlst_sm[[1]][,6], Combo = "200/300");
threethree <- data.frame(fpr=enetlst_sm[[2]][,7],tpr=enetlst_sm[[1]][,7], Combo = "300/300");
fourthree <- data.frame(fpr=enetlst_sm[[2]][,8],tpr=enetlst_sm[[1]][,8], Combo = "400/300")

allrocdat <- rbind.data.frame(onetwo,
                              twotwo,
                              threetwo,
                              fourtwo,
                              onethree,
                              twothree,
                              threethree,
                              fourthree)

ggplot(data=allrocdat, aes(x=fpr, y=tpr, color=Combo)) +
  geom_line(size=1) +
  scale_colour_manual(name="Combination",
    labels=c("100/200",
             "200/200",
             "300/200",
             "400/200",
             "100/300",
             "200/300",
             "300/300",
             "400/300"),
    values=gray(seq(0,.7,.1))) +
  xlab("1-Specificity") +
  ylab("Sensitivity") +
  xlim(0, 1) +
  ylim(0, 1) +
  geom_abline(intercept=0, slope=1) +
  theme_minimal() +
  ggtitle("ROC Curves for Different \n Normalization Techniques")
```



Bootstrap

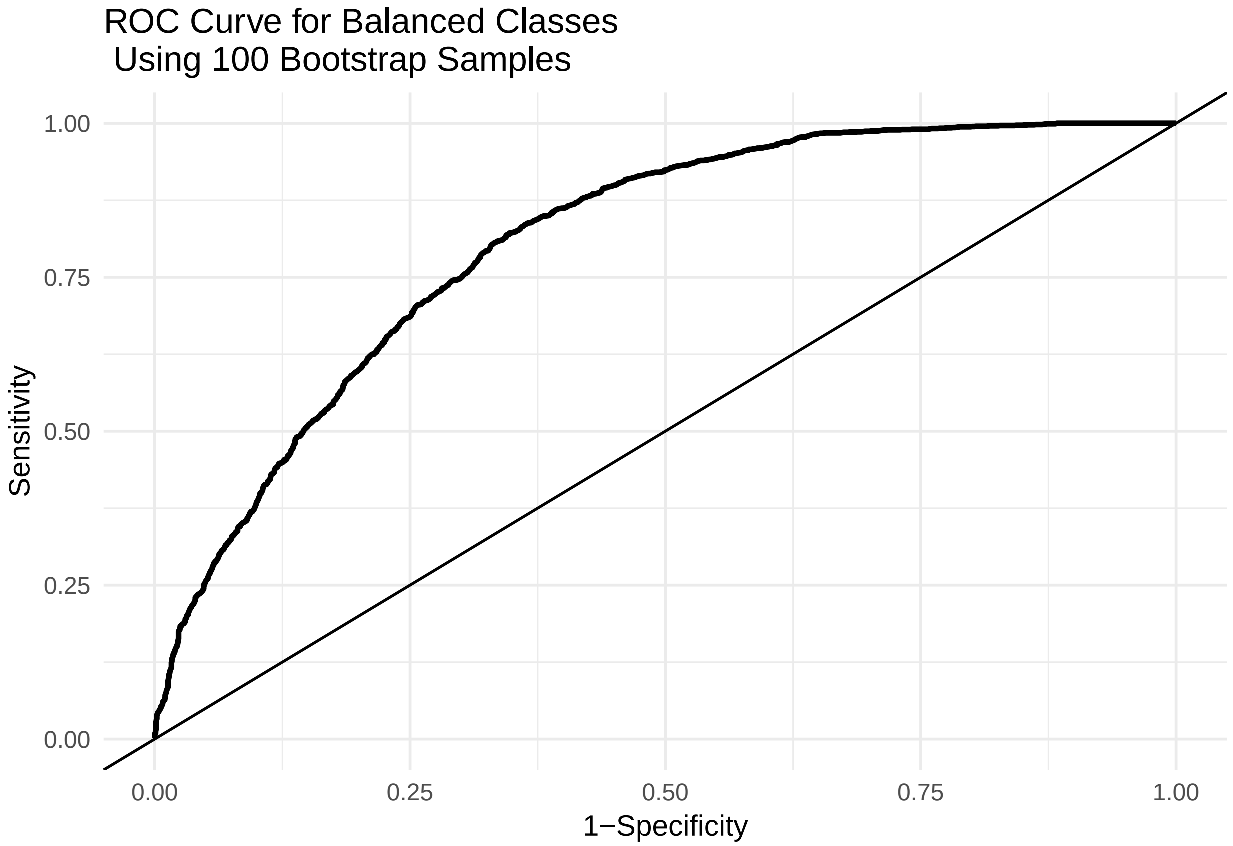
```
enetlst_bs <- readRDS("C:/Users/Spiro Stilianoudakis/Documents/TAD_data/RData/GM12878/testing_SMOTE/ene

#Mean AUC across 100 bootstrap samples
enetlst_bs[[3]]
```

```
## [1] 0.8150594 0.8014177 0.8032703 0.8138675 0.7917615
```

```
auc.bs <- round(mean(enetlst_bs[[3]]),3)
auc.bs
```

```
## [1] 0.805
```

```
#roc curve
fpr.bs <- rowMeans(enetlst_bs[[2]])
tpr.bs <- rowMeans(enetlst_bs[[1]])
rocdat.bs <- data.frame(fpr=fpr.bs, tpr=tpr.bs)
ggplot(rocdat.bs, aes(x=fpr, y=tpr)) +
  geom_line(size=1, color="black") +
  xlab("1-Specificity") +
  ylab("Sensitivity") +
  xlim(0, 1) +
  ylim(0, 1) +
  geom_abline(intercept=0, slope=1) +
  theme_minimal() +
  ggtitle("ROC Curve for Balanced Classes \n Using 100 Bootstrap Samples")
```



Comparing additional performance metrics across all methods

```
options(scipen = 999)

enetperf_sm <- readRDS("C:/Users/Spiro Stilianoudakis/Documents/TAD_data/RData/GM12878/testing_SMOTE/en
enetperf_b <- readRDS("C:/Users/Spiro Stilianoudakis/Documents/TAD_data/RData/GM12878/testing_SMOTE/enet

round(enetperf_sm,2)
```

```
##                   [,1]     [,2]     [,3]     [,4]     [,5]     [,6]     [,7]
## TN          57722.00 62345.00 64076.00 65046.00 62720.00 65803.00 66564.00
## FN            190.00   246.00   271.00   289.00   239.00   287.00   305.00
## FP          16078.00 11455.00  9724.00  8754.00 11080.00  7997.00  7236.00
## TP            298.00   242.00   217.00   199.00   249.00   201.00   183.00
## Total       74288.00 74288.00 74288.00 74288.00 74288.00 74288.00 74288.00
## Sensitivity     0.61     0.50     0.44     0.41     0.51     0.41     0.38
## Specificity     0.78     0.84     0.87     0.88     0.85     0.89     0.90
## Kappa           0.02     0.03     0.03     0.03     0.03     0.03     0.03
## Accuracy        0.78     0.84     0.87     0.88     0.85     0.89     0.90
## Precision       0.02     0.02     0.02     0.02     0.02     0.02     0.02
## FPR             0.22     0.16     0.13     0.12     0.15     0.11     0.10
## FNR             0.39     0.50     0.56     0.59     0.49     0.59     0.62
## FOR             0.00     0.00     0.00     0.00     0.00     0.00     0.00
## NPV             1.00     1.00     1.00     1.00     1.00     1.00     1.00
## MCC             0.08     0.08     0.07     0.07     0.08     0.08     0.07
## F1              0.76     0.66     0.62     0.58     0.68     0.58     0.55
##                 [,8]
## TN          67192.00
## FN            314.00
## FP           6608.00
## TP            174.00
## Total       74288.00
## Sensitivity     0.36
## Specificity     0.91
## Kappa           0.04
## Accuracy        0.91
## Precision       0.03
## FPR             0.09
## FNR             0.64
## FOR             0.00
## NPV             1.00
## MCC             0.07
## F1              0.53
```

```
round(as.matrix(rowMeans(enetperf_b)),2)
```

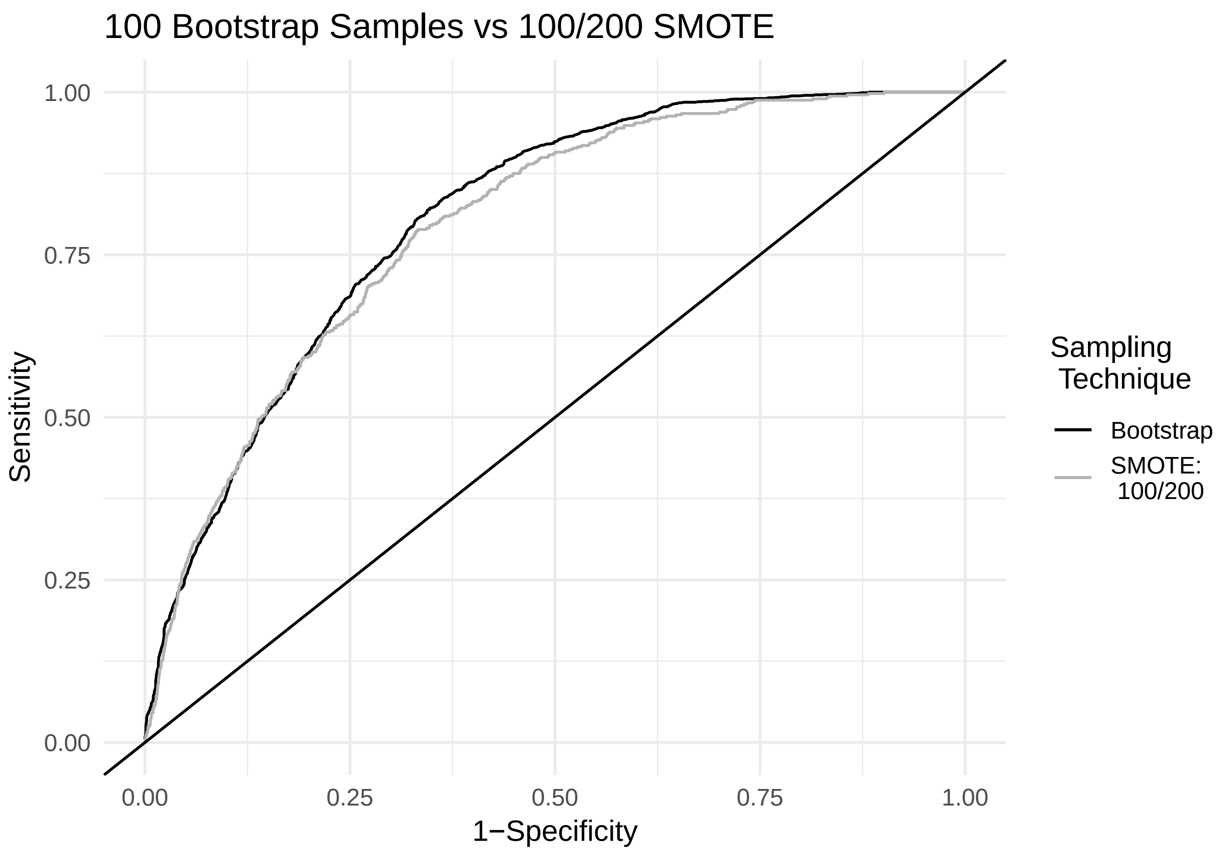
```
##               [,1]
## TN          333.00
## FN          109.40
## FP          155.00
## TP          380.60
## Total       978.00
## Sensitivity   0.78
## Specificity   0.68
## Kappa         0.46
## Accuracy      0.73
## Precision     0.71
## FPR           0.32
## FNR           0.22
## FOR           0.25
## NPV           0.75
## MCC           0.46
## F1            0.87
```

```r
perfdat <- cbind.data.frame(rownames(enetperf_b),
                            round(enetperf_sm,2),
                            round(as.matrix(rowMeans(enetperf_b)),2))
rownames(perfdat) <- NULL
colnames(perfdat) <- c("Metric","100/200", "200/200", "200/200", "200/200",
                       "100/300", "200/300", "300/300", "400/300",
                       "Bootstraps")

kable(perfdat)
```

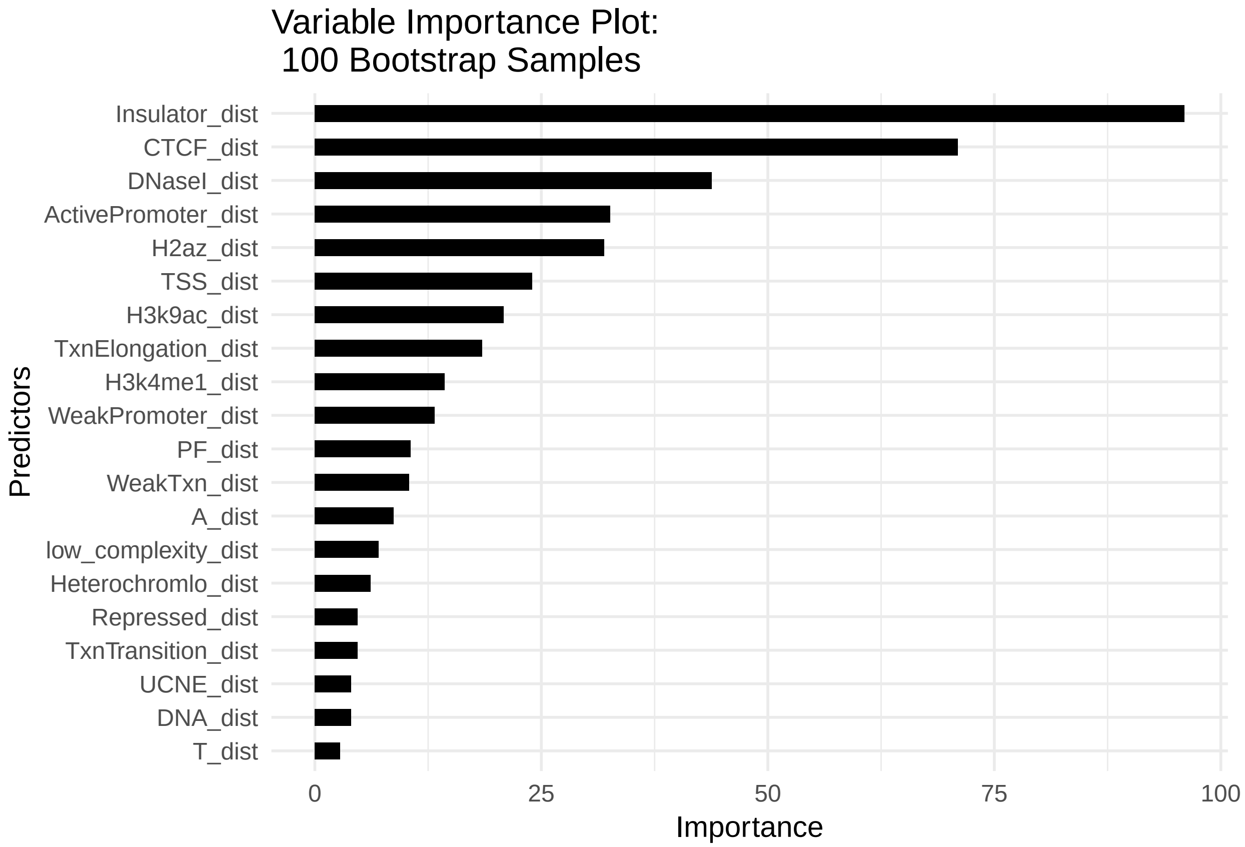
Metric	100/200	200/200	200/200	200/200	100/300	200/300	300/300	400/300	Bootstraps
TN	57722.00	62345.00	64076.00	65046.00	62720.00	65803.00	66564.00	67192.00	333.00
FN	190.00	246.00	271.00	289.00	239.00	287.00	305.00	314.00	109.40
FP	16078.00	11455.00	9724.00	8754.00	11080.00	7997.00	7236.00	6608.00	155.00
TP	298.00	242.00	217.00	199.00	249.00	201.00	183.00	174.00	380.60
Total	74288.00	74288.00	74288.00	74288.00	74288.00	74288.00	74288.00	74288.00	978.00
Sensitivity	0.61	0.50	0.44	0.41	0.51	0.41	0.38	0.36	0.78
Specificity	0.78	0.84	0.87	0.88	0.85	0.89	0.90	0.91	0.68
Kappa	0.02	0.03	0.03	0.03	0.03	0.03	0.03	0.04	0.46
Accuracy	0.78	0.84	0.87	0.88	0.85	0.89	0.90	0.91	0.73
Precision	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.71
FPR	0.22	0.16	0.13	0.12	0.15	0.11	0.10	0.09	0.32
FNR	0.39	0.50	0.56	0.59	0.49	0.59	0.62	0.64	0.22
FOR	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.25
NPV	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.75
MCC	0.08	0.08	0.07	0.07	0.08	0.08	0.07	0.07	0.46
F1	0.76	0.66	0.62	0.58	0.68	0.58	0.55	0.53	0.87

Comparing 100/200 SMOTE with Bootstrapped model

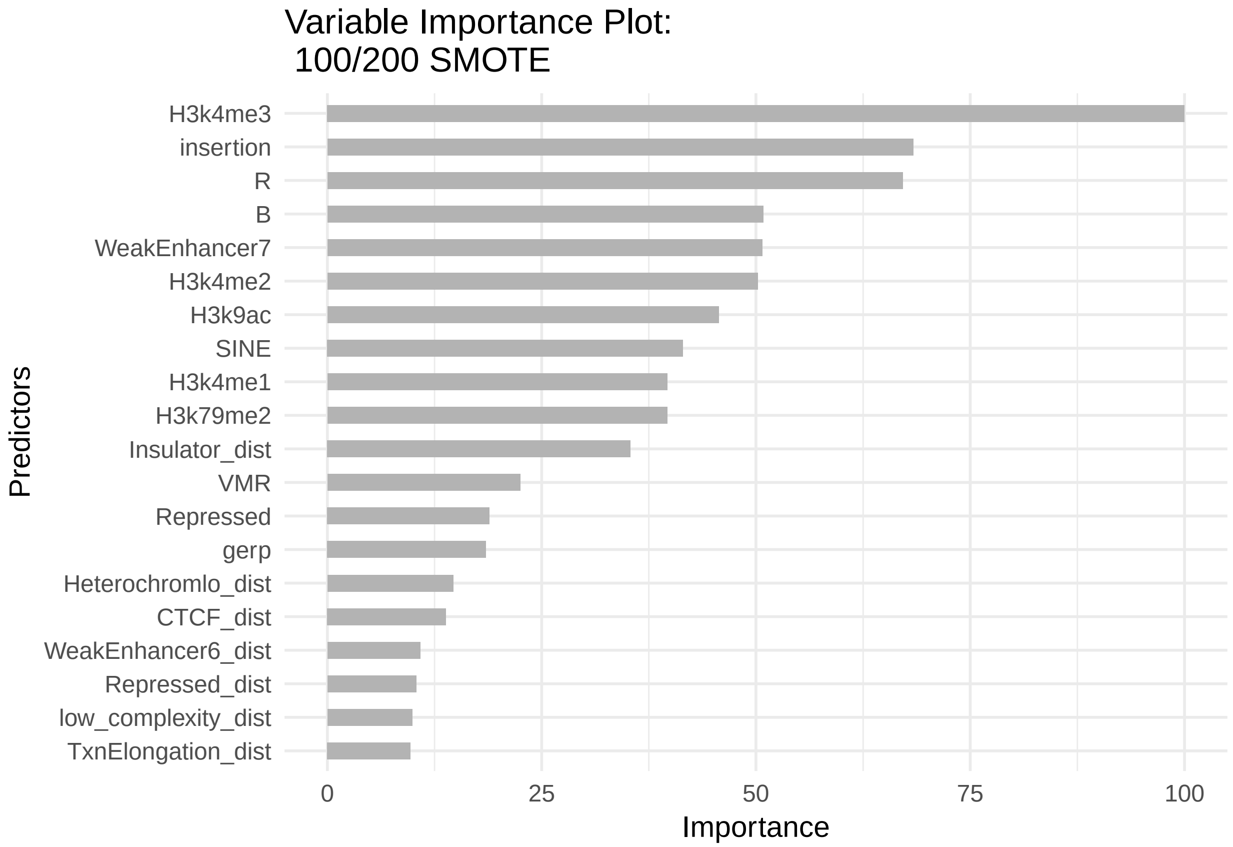
```r
ggplot() +
  geom_line(aes(fpr, tpr, colour=gray(.7)[1]), rocdat.bs) +
  geom_line(aes(fpr, tpr, colour="black"), onetwo) +
  scale_colour_manual(name="Sampling \n Technique",
    labels=c("Bootstrap","SMOTE: \n 100/200"),
    values=c("black",gray(.7))) +
  xlab("1-Specificity") +
  ylab("Sensitivity") +
  xlim(0, 1) +
  ylim(0, 1) +
  geom_abline(intercept=0, slope=1) +
  theme_minimal() +
  ggtitle("100 Bootstrap Samples vs 100/200 SMOTE")
```



```
varimp.bs <- as.vector(rowMeans(enetlst_bs[[4]]))
Labels <- rownames(enetlst_bs[[4]])
Labels[grep("Gm12878_", Labels)] <- gsub("Gm12878_","",Labels[grep("Gm12878_", Labels)])
varimp.bs.df <- data.frame(Feature=Labels,
                                 Importance=varimp.bs)
varimp.bs.df <- varimp.bs.df[order(varimp.bs.df$Importance),]
varimp.bs.df <- varimp.bs.df[(dim(varimp.bs.df)[1]-19):dim(varimp.bs.df)[1],]
varimp.bs.df$Feature <- factor(varimp.bs.df$Feature,
                                     levels=varimp.bs.df$Feature)
p.bs <- ggplot(varimp.bs.df, aes(x=Feature, y=Importance)) +
  xlab("Predictors") +
  ylab("Importance") +
  #ggtitle("Importance Plot for Gradient Boosting Machine") +
  geom_bar(stat="identity",
           width=.5,
           position="dodge",
           fill="black") +
  coord_flip() +
  theme_minimal() +
  ggtitle("Variable Importance Plot: \n 100 Bootstrap Samples")
p.bs
```



```
varimp.sm <- as.vector(enetlst_sm[[4]][,1])
Labels <- names(enetlst_sm[[4]][,1])
Labels[grep("Gm12878_", Labels)] <- gsub("Gm12878_","",Labels[grep("Gm12878_", Labels)])
varimp.sm.df <- data.frame(Feature=Labels,
                                 Importance=varimp.sm)
varimp.sm.df <- varimp.sm.df[order(varimp.sm.df$Importance),]
varimp.sm.df <- varimp.sm.df[(dim(varimp.sm.df)[1]-19):dim(varimp.sm.df)[1],]
varimp.sm.df$Feature <- factor(varimp.sm.df$Feature,
                                     levels=varimp.sm.df$Feature)
p.sm <- ggplot(varimp.sm.df, aes(x=Feature, y=Importance)) +
  xlab("Predictors") +
  ylab("Importance") +
  #ggtitle("Importance Plot for Gradient Boosting Machine") +
  geom_bar(stat="identity",
           width=.5,
           position="dodge",
           fill=gray(.7)) +
  coord_flip() +
  theme_minimal() +
  ggtitle("Variable Importance Plot: \n 100/200 SMOTE")
p.sm
```


Variable Importance Plot:
100/200 SMOTE
Predictors
H3k4me3
insertion
R
B
WeakEnhancer7
H3k4me2
H3k9ac
SINE
H3k4me1
H3k79me2
Insulator_dist
VMR
Repressed
gerp
Heterochromlo_dist
CTCF_dist
WeakEnhancer6_dist
Repressed_dist
low_complexity_dist
TxnElongation_dist
0
25
50
75
100
Importance