Final Project Code

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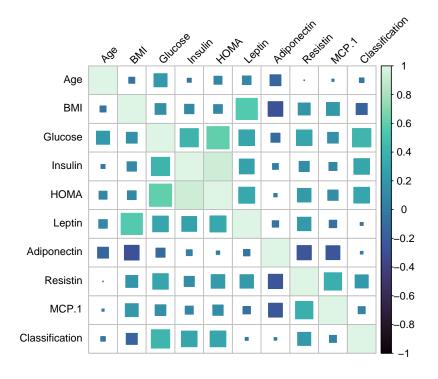
Libraries & Data Pre-processing

```
library(rio) ## importing data
library(tidyverse) ## data wrangling
library(corrplot) ## correlation plot
library(boot) ## bootstrap
library(gridExtra) ## grid visualization
library(glmnet) ## glm models
library(caret) ## various ML tools & models
library(ROCR) ## ROC-AUC score
library(leaps) ## model selection
library(bestglm) ## extended model selection
#library(GGally) ## optional: full features visualization
dt <- import('breastR2.xlsx') ## Make sure the data set file is in the working directory
head(dt[,1:9]) ## excluding the response variable
##
    Age
             BMI Glucose Insulin
                                      HOMA Leptin Adiponectin Resistin
## 1 48 23.50000
                      70
                          2.707 0.4674087 8.8071
                                                      9.702400 7.99585 417.114
## 2 83 20.69049
                                                      5.429285 4.06405 468.786
                      92
                          3.115 0.7068973 8.8438
## 3 82 23.12467
                      91
                          4.498 1.0096511 17.9393
                                                     22.432040 9.27715 554.697
## 4 68 21.36752
                      77
                           3.226 0.6127249 9.8827
                                                      7.169560 12.76600 928.220
## 5 86 21.11111
                      92
                           3.549 0.8053864 6.6994
                                                      4.819240 10.57635 773.920
                           3.226 0.7320869 6.8317
## 6 49 22.85446
                      92
                                                     13.679750 10.31760 530.410
## The positive response (diagnosed with BC) is coded as 1
dt$Classification <- ifelse(dt$Classification==1, 0,1)</pre>
table(dt$Classification)
##
## 0 1
## 52 64
str(dt) ## All the features are continuous numerical variables
## 'data.frame':
                   116 obs. of 10 variables:
                   : num 48 83 82 68 86 49 89 76 73 75 ...
## $ Age
                          23.5 20.7 23.1 21.4 21.1 ...
## $ BMI
                   : num
                          70 92 91 77 92 92 77 118 97 83 ...
## $ Glucose
                   : num
## $ Insulin
                   : num
                          2.71 3.12 4.5 3.23 3.55 ...
## $ HOMA
                          0.467 0.707 1.01 0.613 0.805
                   : num
##
   $ Leptin
                          8.81 8.84 17.94 9.88 6.7 ...
                   : num
## $ Adiponectin : num
                          9.7 5.43 22.43 7.17 4.82 ...
## $ Resistin
                   : num 8 4.06 9.28 12.77 10.58 ...
## $ MCP.1
                   : num 417 469 555 928 774 ...
```

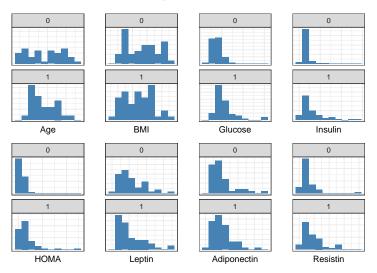
```
## $ Classification: num 0 0 0 0 0 0 0 0 0 ...
summary(dt)
                                   Glucose
                                                   Insulin
##
        Age
                      BMI
  Min.
         :24.0
                 Min.
                      :18.37
                                Min.
                                       : 60.00
                                                Min. : 2.432
##
   1st Qu.:45.0
                 1st Qu.:22.97
                                1st Qu.: 85.75
                                                1st Qu.: 4.359
## Median :56.0
                 Median :27.66
                                Median : 92.00
                                                Median : 5.925
## Mean :57.3
                 Mean :27.58 Mean : 97.79
                                                Mean
                                                      :10.012
  3rd Qu.:71.0
                 3rd Qu.:31.24 3rd Qu.:102.00
                                                3rd Qu.:11.189
##
## Max.
        :89.0
                 Max. :38.58 Max.
                                      :201.00
                                                Max.
                                                       :58.460
##
       AMOH
                        Leptin
                                     Adiponectin
                                                       Resistin
## Min. : 0.4674
                  Min. : 4.311
                                    Min.
                                         : 1.656
                                                   Min.
                                                           : 3.210
## 1st Qu.: 0.9180
                   1st Qu.:12.314
                                    1st Qu.: 5.474
                                                   1st Qu.: 6.882
## Median : 1.3809
                   Median :20.271
                                    Median : 8.353
                                                    Median :10.828
## Mean : 2.6950 Mean :26.615
                                    Mean
                                         :10.181
                                                    Mean :14.726
## 3rd Qu.: 2.8578
                    3rd Qu.:37.378
                                    3rd Qu.:11.816
                                                    3rd Qu.:17.755
## Max. :25.0503
                  Max. :90.280
                                    Max. :38.040 Max. :82.100
##
       MCP.1
                    Classification
## Min. : 45.84
                  Min. :0.0000
## 1st Qu.: 269.98
                   1st Qu.:0.0000
## Median : 471.32
                   Median :1.0000
## Mean : 534.65
                   Mean :0.5517
## 3rd Qu.: 700.09
                    3rd Qu.:1.0000
## Max.
         :1698.44
                    Max.
                         :1.0000
set.seed(123) ## for replication
## Setting aside the validation holdout set (15% of the data)
train_test <- createDataPartition(dt$Classification, times = 1, p = 0.15, list = F)
holdout set <- dt[train test,]
dt <- dt[-train_test,]</pre>
## Number of instances in the training set:
nrow(dt)
## [1] 98
## The training set is fairly split between the two classes of response
table(dt$Classification)
##
## 0 1
## 44 54
table(holdout_set$Classification)
##
## 0 1
## 8 10
```

Exploratory Data Analysis (EDA)

Correlation between features and the response

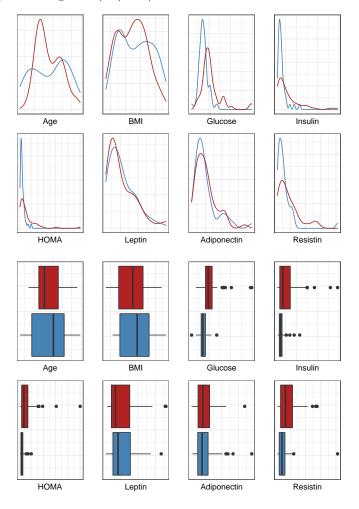


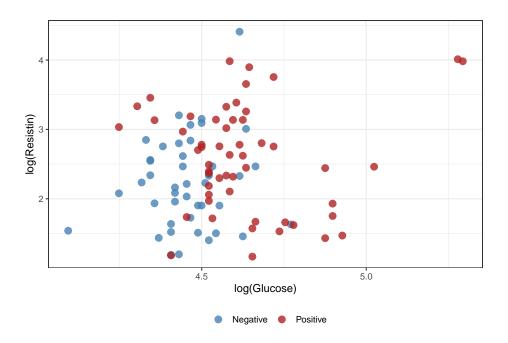
Distribution of Instances for each Feature by Class



Frequency & Range of Instances for each Feature by Class

Red: Positive (w/ BC) | Blue: Negative (wo/ BC)





Data Preparation

Log & Scale Transformation

```
dt_old <- dt ## backup of train data set before transformations
#dt <- dt_old

log_trans <- function (x) {sapply(x, log)}
scale_trans <- function(x){sapply(x, scale)}

dt[,3:9] <- log_trans(dt[,3:9])
dt[,1:9] <- data.frame(scale_trans(dt[,1:9]))

holdout_old <- holdout_set ## backup of test data set before transformations
#holdout_set<- holdout_old

holdout_set[,3:9] <- log_trans(holdout_set[,3:9])
holdout_set[,1:9] <- data.frame(scale_trans(holdout_set[,1:9]))</pre>
```

Setting Up Feature Matrix & Dataframe

Classification Models

Linear Logistic Models

Logistic Model w/ & Wo/ Bootstrap

```
## Simple Logistic Model
mdl.log.simp <- glm(Classification ~ ., family = 'binomial', data = train_dat)
coef.simp <- coef(mdl.log.simp)</pre>
#summary(mdl.log.simp)
exp(coef(mdl.log.simp))
## (Intercept)
                                    BMI
                                            Glucose
                                                        Insulin
                                                                        HOMA
                       Age
##
     3.6636467
                 0.5248574
                             0.1995530
                                          0.0000000
                                                      0.0000000
                                                                         Tnf
                                                                  `I(BMI^2)`
##
        Leptin Adiponectin
                              Resistin
                                              MCP.1
                                                      `I(Age^2)`
     1.5915139
                1.7569791
                             2.2827981
                                          1.2534737
                                                      0.2128077
                                                                   0.6976718
## Testing for models' fit (reduced (without Age^2 & BMI^2) vs. full)
mdl.log.red <- glm(Classification ~ ., family = 'binomial', data = train_dat[,c(-10,-11)])
#summary(mdl.log.red)
anova(mdl.log.red, mdl.log.simp, test = 'F')
## Analysis of Deviance Table
## Model 1: Classification ~ Age + BMI + Glucose + Insulin + HOMA + Leptin +
       Adiponectin + Resistin + MCP.1
## Model 2: Classification ~ Age + BMI + Glucose + Insulin + HOMA + Leptin +
       Adiponectin + Resistin + MCP.1 + `I(Age^2)` + `I(BMI^2)`
    Resid. Df Resid. Dev Df Deviance
                                            F Pr(>F)
            88
                   81.000
## 1
## 2
            86
                   62.696 2 18.303 9.1517 0.000106 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
# Pseudo R-Squared values
DescTools::PseudoR2(mdl.log.simp,which = c('CoxSnell', 'McFadden'))
## CoxSnell McFadden
## 0.5210244 0.5350134
## Bootstrap Logistic Model
## Setting up Bootstrap function
set.seed(123)
fn_est <- function(data, idx){</pre>
 mdl.boot <- glm(Classification ~ ., family = 'binomial', data = data[idx,])</pre>
  coefs <- mdl.boot$coefficients</pre>
 return(coefs)
}
L <- 1000 ## bootstrap samples = 1000
bts_est <- boot(data = train_dat, statistic = fn_est, R=L)</pre>
## storing bootstrap results in a matrix
boot.mat <- matrix(0, nrow = L, ncol=length(colnames(mdl.mat)))</pre>
for (i in 1:L) boot.mat[i,] <- bts_est$t[i,]</pre>
boot.mat <- apply(boot.mat, MARGIN = 2, median, na.rm = T) ## Median of bootstraped coefficients
```

```
names(boot.mat) <- colnames(mdl.mat)</pre>
## setting up a function to calculate prob. score out of logit score
logit.pred <- function(data, coefs, thresh=0.5){</pre>
  factor(ifelse(1/(1+exp(-(data %*% coefs)))>=thresh, 1,0))
y_prd_simp <- logit.pred(mdl.mat, coef.simp) ## prediction of simple logistic model
y_prd_boot <- logit.pred(mdl.mat, boot.mat) ## prediction of logit bootstrap model</pre>
## setting up a function to calculate classification metrics
metrics <- function(y_true, y_hat){</pre>
  tr_accu <- mean(y_true == y_hat)</pre>
  tr_sens <- sensitivity(y_true, y_hat, positive = '1')</pre>
  tr_spc <- specificity(y_true, y_hat, negative = '0')</pre>
  tr_f1 <- F_meas(y_true, y_hat)</pre>
  prd <- prediction(as.numeric(y_hat),labels = y_true)</pre>
  tr_auc <- as.numeric(performance(prd,measure="auc")@y.values)</pre>
  data.frame(Accuracy = tr_accu, Recall=tr_sens, Specificity=tr_spc, F1=tr_f1, AUC=tr_auc)
}
## this data frame store our models' prediction metrics on the training set
model.perf <- data.frame(Model="Logistic",</pre>
                          round(metrics(train_dat$Classification, y_prd_simp),2))
model.perf <- rbind(model.perf, data.frame(Model="Logistic (Boot)",</pre>
                          round(metrics(train_dat$Classification, y_prd_boot),2)))
```

Lasso CV Models

```
## Lasso LOOV
set.seed(123)
mdl.loigtLOOV <- cv.glmnet(x = mdl.mat[,-1], y = train_dat$Classification,
                           family=binomial, nfolds = nrow(train dat))
## Coefficients (LOOV Lasso)
Lasso_LV_Coefs <- predict(mdl.loigtLOOV, newx = mdl.mat[,-1], type='coefficient')
coef_lass_LV <- data.frame(Var = c('Intercept',</pre>
                                    Lasso_LV_Coefs@Dimnames[[1]][-1])[c(Lasso_LV_Coefs@i+1)],
           `Lasso LOOV` = round(Lasso_LV_Coefs@x, 3))
coef_lass_LV_ac <- rbind(coef_lass_LV,</pre>
                         data.frame(Var = colnames(mdl.mat)[-1][c(!((colnames(mdl.mat)[-1])%in% coef_la
## Performance on the training set
y_prd_lgL00V <- factor(ifelse(predict(mdl.loigtL00V, newx = mdl.mat[,-1],</pre>
                                       type='response')>0.5, 1,0))
## Lasso K-fold(10)
set.seed(123)
mdl.loigtKfold <- cv.glmnet(x = mdl.mat[,-1], y = train_dat$Classification,
                             family=binomial, nfolds = 10)
#Coefficients (k-fold Lasso) [uncomment to run]
```

```
Lasso_K10_Coefs <- predict(mdl.loigtKfold, newx = mdl.mat[,-1],type='coefficient')</pre>
coef_lass_k10 <- data.frame(Var = c('Intercept',</pre>
                                      Lasso_K10_Coefs@Dimnames[[1]][-1])[c(Lasso_K10_Coefs@i+1)],
           `Lasso K-fold` = round(Lasso_K10_Coefs@x, 3))
coef_lass_k10_ac <- rbind(coef_lass_k10,</pre>
                           data.frame(Var = colnames(mdl.mat)[-1][c(!((colnames(mdl.mat)[-1])%in% coef l.
## Performance on the training set
y_prd_lgKfold <- factor(ifelse(predict(mdl.loigtKfold, newx = mdl.mat[,-1],</pre>
                                        type='response')>0.5, 1,0))
## coefficients of the Lasso models:
coefs_lasso_final <- merge(coef_lass_k10_ac, coef_lass_LV_ac, by='Var')</pre>
## storing the models' performance in the metrics data frame
model.perf <- rbind(model.perf, data.frame(</pre>
            Model='Logistic (LOOV)',round(metrics(train_dat$Classification,
                                                    y_prd_lgL00V),2)))
model.perf <- rbind(model.perf, data.frame(</pre>
            Model='Logistic (Kfold=10)', round(metrics(train_dat$Classification,
                                                         y_prd_lgKfold),2)))
```

Logit Subset Models

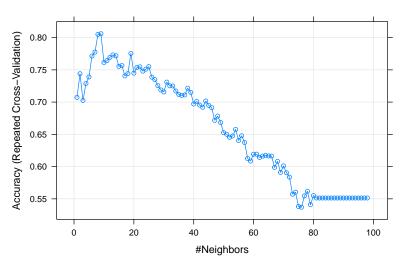
```
## Subset Criteria (BestGLM)
set.seed(123)
lgs_subs <- function(data, ctn='AIC', meth='exhaustive'){</pre>
  mdl.bglm <- bestglm(data, family = binomial, IC=ctn, method = meth)</pre>
  tmp_names <- names(mdl.bglm$BestModel$coefficients)</pre>
  tmp names <- case when(
                 tmp_names == "`I(Age^2)`" ~ "I(Age^2)",
                 tmp names == "`I(BMI^2)`" ~ "I(BMI^2)",
                 TRUE ~ as.character(tmp_names)
  coefs <- mdl.bglm$BestModel$coefficients</pre>
  names(coefs) <- tmp_names</pre>
  return(coefs)
coefs_ex_AIC <- lgs_subs(data=train_dat)</pre>
coefs_ex_BIC <- lgs_subs(data=train_dat,ctn='BIC')</pre>
coefs_fw_AIC <- lgs_subs(data=train_dat,meth = 'forward')</pre>
coefs_fw_BIC <- lgs_subs(data=train_dat,ctn = 'BIC', meth = 'forward')</pre>
coefs_bw_AIC <- lgs_subs(data=train_dat,meth = 'backward')</pre>
coefs_bw_BIC <- lgs_subs(data=train_dat,ctn = 'BIC', meth = 'backward')</pre>
y_prd_ex_AIC <- logit.pred(mdl.mat[,names(coefs_ex_AIC)],</pre>
                              coefs ex AIC)
y_prd_ex_BIC <- logit.pred(mdl.mat[,names(coefs_ex_BIC)],</pre>
                             coefs_ex_BIC)
y_prd_fw_AIC <- logit.pred(mdl.mat[,names(coefs_fw_AIC)],</pre>
                             coefs_fw_AIC)
```

```
y_prd_fw_BIC <- logit.pred(mdl.mat[,names(coefs_fw_BIC)],</pre>
                            coefs_fw_BIC)
y_prd_bw_AIC <- logit.pred(mdl.mat[,names(coefs_bw_AIC)],</pre>
                            coefs_bw_AIC)
y_prd_bw_BIC <- logit.pred(mdl.mat[,names(coefs_bw_BIC)],</pre>
                            coefs_bw_BIC)
## Metrics of All Subset Models
cbind(Model=c('Best subset - AIC', 'Best subset - BIC', 'Forward - AIC',
                'Forward - BIC', 'Backward - AIC', 'Backward - BIC'),
      round(rbind(metrics(train_dat$Classification, y_prd_ex_AIC ),
            metrics(train_dat$Classification, y_prd_ex_BIC ),
            metrics(train_dat$Classification, y_prd_fw_AIC ),
            metrics(train dat$Classification, y prd fw BIC ),
            metrics(train_dat$Classification, y_prd_bw_AIC ),
            metrics(train_dat$Classification, y_prd_bw_BIC )),2))
                 Model Accuracy Recall Specificity F1 AUC
## 1 Best subset - AIC
                            0.87
                                   0.87
                                               0.86 0.85 0.86
                            0.84
## 2 Best subset - BIC
                                   0.84
                                               0.83 0.81 0.83
                                               0.86 0.85 0.86
         Forward - AIC
                            0.87
                                   0.87
## 4
         Forward - BIC
                            0.84
                                   0.84
                                               0.83 0.81 0.83
        Backward - AIC
## 5
                            0.87
                                   0.87
                                               0.86 0.85 0.86
## 6
        Backward - BIC
                            0.84
                                   0.84
                                               0.83 0.81 0.83
## Coefficients of all selected logistic models
coefs all logit <- merge(data.frame(Var = c('Intercept',colnames(mdl.mat)[-1]),</pre>
                                     Simple.Logit = round(exp(coef.simp),3),
                                     row.names = NULL, check.names = F),
      merge (coefs_lasso_final,
             data.frame(Var = c('Intercept', names(coefs fw AIC)[-1]),
                        Subset = round(exp(coefs_fw_AIC),3), row.names = NULL),
             by='Var', all.x = T, all.y = T, ),
      all.x = T, all.y = T, by='Var')
coefs_all_logit[is.na(coefs_all_logit)] <-0</pre>
coefs_all_logit[rank(c('Intercept',colnames(mdl.mat)[-1])),] %>%
 data.frame(row.names = NULL)
##
              Var Simple.Logit Lasso.K.fold Lasso.LOOV Subset
## 1
        Intercept
                         3.664
                                       0.734
                                                  0.786 2.059
## 2
                         0.525
                                       0.000
                                                  0.000 0.000
              Age
## 3
              BMI
                         0.200
                                      -0.245
                                                 -0.293 0.267
## 4
          Glucose
                         0.000
                                       0.739
                                                  0.783 0.000
## 5
          Insulin
                                       0.000
                                                  0.000 0.000
                         0.000
## 6
             AMOH
                            Inf
                                       0.149
                                                  0.176
## 7
           Leptin
                         1.592
                                       0.000
                                                  0.000 0.000
## 8 Adiponectin
                         1.757
                                       0.000
                                                  0.000 1.810
                                                  0.256 2.670
## 9
         Resistin
                         2.283
                                       0.218
## 10
            MCP.1
                         1.253
                                       0.000
                                                  0.000 0.000
         I(Age^2)
## 11
                         0.213
                                      -0.490
                                                 -0.526 0.236
## 12
         I(BMI^2)
                         0.698
                                       0.000
                                                 -0.010 0.000
model.perf <- rbind(model.perf, data.frame(</pre>
Model='Logistic (Fwd Sel.)', round(metrics(train_dat$Classification, y_prd_fw_AIC ),2)))
```

Non-Parametric Models

k-NN

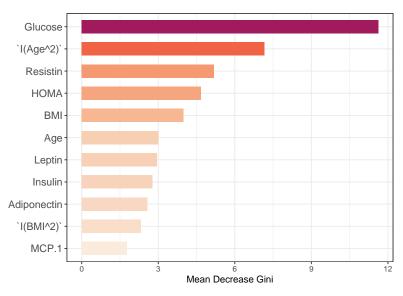
K-NN Fine-Tuning



```
y_prd_knn <- predict(clf_knn, newdata = train_dat, type='raw')
model.perf <- rbind(model.perf, data.frame(
    Model='K-NN', round(metrics(train_dat$Classification, y_prd_knn),2)))</pre>
```

Random Forest

```
Accuracy = max(clf_rf$results$Accuracy)))
## result of grid search for RF models
rf_res
##
     N_Trees mtry Accuracy
## 1
         500
              10 0.7394949
## 2
        1000
                6 0.7398653
## 3
        1500
                6 0.7361616
## 4
        2000
               6 0.7324579
## 5
        2500
                6 0.7394949
## 6
       3000
                6 0.7321549
## so we use mtry = 6 and ntree=1000
clf_rf <- train(Classification ~. , data = train_dat, method = 'rf',</pre>
                tuneGrid = expand.grid(.mtry = 6), ntree=1000)
rf_feats <- clf_rf$finalModel$importance[,1]</pre>
ggplot() +
  geom_col(aes(y=reorder(names(rf_feats), rf_feats), x= rf_feats, fill=rf_feats), width = 0.6) +
  scale_fill_viridis(option = 'rocket', direction = -1, begin=0.4, end=1) +
  labs(x='Mean Decrease Gini', y='') +
  theme(legend.position = 'none', axis.text.y = element_text(size=12))
```



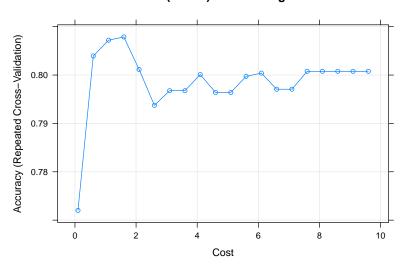
```
y_pred_rf <- predict(clf_rf, newdata = train_dat, type = 'raw')
model.perf <- rbind(model.perf, data.frame(
    Model='RF', round(metrics(train_dat$Classification, clf_rf$finalModel$predicted),2)))</pre>
```

SVM (Linear & Radial Kernel)

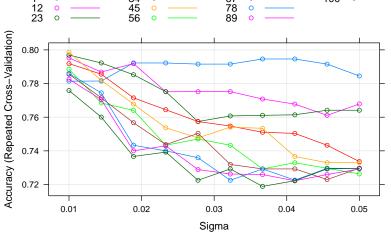
```
### SVM Linear
set.seed(123)

clf_svm_1 <- train(Classification~., data = train_dat,</pre>
```

SVM (Linear) Fine-Tuning







```
y_pred_svm_r <- predict(clf_svm_r, newdata = train_dat, type = 'raw')
model.perf <- rbind(model.perf, data.frame(
    Model='SVM (Radial)', round(metrics(train_dat$Classification, y_pred_svm_r),2)))
model.perf</pre>
```

```
##
                    Model Accuracy Recall Specificity
                                                         F1 AUC
## 1
                              0.87
                                     0.87
                                                  0.86 0.85 0.86
                Logistic
## 2
         Logistic (Boot)
                              0.64
                                     0.73
                                                  0.58 0.65 0.65
         Logistic (LOOV)
## 3
                              0.83
                                     0.80
                                                  0.86 0.79 0.82
## 4 Logistic (Kfold=10)
                              0.82
                                     0.79
                                                  0.86 0.78 0.81
                              0.87
## 5 Logistic (Fwd Sel.)
                                     0.87
                                                  0.86 0.85 0.86
                    K-NN
                              0.86
                                     0.87
                                                  0.84 0.84 0.86
                              0.76
## 7
                      RF
                                     0.75
                                                  0.76 0.71 0.75
## 8
            SVM (Linear)
                              0.88
                                     0.86
                                                  0.90 0.86 0.87
## 9
            SVM (Radial)
                              0.94
                                     0.93
                                                  0.95 0.93 0.94
```

Applying on the Validation/Holdout Set

```
type='response')>0.5, 1,0))
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='Lasso (LOOV)', round(metrics(test_dat$Classification, test_lgLOOV),2)))
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='Lasso (K-fold)', round(metrics(test_dat$Classification, test_lgKfold),2)))
test_fw_AIC <- logit.pred(mdl.tst[,names(coefs_fw_AIC)],</pre>
                            coefs fw AIC)
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='Logistic (Fwd Sel.)', round(metrics(test_dat$Classification, test_fw_AIC ),2)))
## K-NN
test_knn <- predict(clf_knn, newdata = test_dat, type='raw')</pre>
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='K-NN', round(metrics(test_dat$Classification, test_knn),2)))
## RF
test_rf <- predict(clf_rf, newdata = test_dat, type = 'raw')</pre>
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='RF', round(metrics(test_dat$Classification, test_rf),2)))
## SVM Linear
test_svm_l <- predict(clf_svm_l, newdata = test_dat, type = 'raw')</pre>
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='SVM (Linear)', round(metrics(test_dat$Classification, test_svm_1),2)))
## SVM Radial
test_svm_r <- predict(clf_svm_r, newdata = test_dat, type = 'raw')</pre>
tst.perf <- rbind(tst.perf, data.frame(</pre>
 Model='SVM (Radial)', round(metrics(test_dat$Classification, test_svm_r),2)))
tst.perf
##
                   Model Accuracy Recall Specificity
                                                         F1 AUC
## 1
         Logistic (Base)
                              0.50
                                     0.55
                                                  0.43 0.40 0.49
## 2
         Logistic (Boot)
                              0.44
                                     0.50
                                                  0.33 0.29 0.42
## 3
            Lasso (LOOV)
                              0.67
                                     0.67
                                                  0.67 0.57 0.65
## 4
          Lasso (K-fold)
                              0.67
                                     0.67
                                                  0.67 0.57 0.65
## 5 Logistic (Fwd Sel.)
                              0.50
                                     0.55
                                                  0.43 0.40 0.49
## 6
                    K-NN
                              0.83
                                     0.82
                                                  0.86 0.80 0.82
## 7
                      RF
                              0.72
                                     0.86
                                                  0.64 0.74 0.74
            SVM (Linear)
                              0.72
## 8
                                     0.73
                                                  0.71 0.67 0.71
## 9
            SVM (Radial)
                              0.89
                                     1.00
                                                  0.80 0.89 0.90
```