Report code

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This markdown file contains the code used to produce all plots and conduct all statistical analysis contained within the report.

Setup

First load the important packages.

```
library(tidyverse)
library(reshape2)
library(ggplot2)
library(glmnet)
library(ROCR)
library(caret)
library(cvms)
library(tibble)
library(pROC)
library(checkmate)
library(BBmisc)
library(testit)
library(devtools)
library(mlr)
```

Next, install and load the `higgsboson` package.

```
install_github("https://github.com/hsansford1/higgsboson")
```

```
##
##      checking for file ‘/tmp/Rtmpc2FceE/remotes13c25ad9f575/hsansford1-higgsboson-5b77e2b/DESCRIPTIO
##   -  preparing ‘higgsboson’:
##    checking DESCRIPTION meta-information ...  v  checking DESCRIPTION meta-information
##   -  checking for LF line-endings in source and make files and shell scripts
##   -  checking for empty or unneeded directories
## -  looking to see if a ‘data/datalist’ file should be added
##        NB: this package now depends on R (>= 3.5.0)
##        WARNING: Added dependency on R >= 3.5.0 because serialized objects in  serialize/load version
## -  building 'higgsboson_0.1.0.tar.gz'
##
##
```

```
library(higgsboson)
```

Access the data included in the package. First load the data used to train the models.

```
train <- higgsboson::training
```

Put the data in the format required for training:

```
df_train <- train[,2:33] #remove eventid
df_train <- df_train[,-31] #remove weights

df_train$Label <- ifelse(df_train$Label=="s",1,0) #encode "s" and "b" to 1 - 0 (resp.)
df_train$Label <- as.factor(df_train$Label) #need this as factor for caret package
```

Use the `reweight` function to normalise the weights (use `??reweight` to see function help). `Ns()` and `Nb()` are hardcoded values of N_s and N_b for the higgsboson dataset (see 'Problem Formulation' section of report for explanation of these values).

```
weights <- reweight(train$Weight, df_train$Label, Ns(), Nb())
```

Set all missing values equal to zero.

```
df_train[df_train==-999] <- 0
```

To get a standardised data set `st_train`, run the following.

```
st_train <- df_train
st_train <- as.data.frame(scale(df_train[,1:30]))
st_train["Label"] <- df_train$Label
```

Weighted Logistic Regression with custom AMS metric

The `mlr` package allows the use of custom metrics. First, define the classification task and make the logistic learner

```
trainTask <- makeClassifTask(data = st_train,
                             target = "Label",
                             positive = 1,
                             weights = weights
                             )

logistic.learner <- makeLearner("classif.logreg", predict.type = "response")
```

Use the custom AMS measure created in the `higgsboson` package `AMS_measure()` to conduct cross-validation on fitting the weighted logistic regression (WLR). This gives us an idea of the AMS we can expect to get from a test set.

```
set.seed(22)
AMS_mlr <- AMS_measure()
cv.logistic <- crossval(learner = logistic.learner, task = trainTask, iters = 5,
                        stratify = TRUE,
                        measures = AMS_mlr,
                        show.info = F, models=TRUE)
cv.logistic$aggr
```

```
## AMS_weighted.test.mean
##              0.2326592
```

```
cv.logistic$measures.test
```

```
##   iter AMS_weighted
## 1    1    0.4093149
## 2    2    0.1659211
## 3    3    0.2190233
## 4    4    0.2178583
## 5    5    0.1511781
```

Now, we fit a WLR model using the whole training data set and check how it performs on the test data.

```
train_control <- trainControl(method = "cv", number = 10)

fmodel <- caret::train(Label ~ .,
                       data = st_train,
                       trControl = train_control,
                       method = "glm",
                       weights = weights,
                       family=binomial()
)

test <- higgsboson::test

df_test <- test[,2:33] #remove eventid
df_test <- df_test[,-31] #remove weights
df_test$Label <- ifelse(df_test$Label=="s",1,0) #encode "s" and "b" to 1 - 0 (resp.) for logistic regre
df_test$Label <- as.factor(df_test$Label) #need this as factor for caret
# set misssing values to 0 and standardise data
df_test[df_test==-999] <- 0
st_test <- as.data.frame(scale(df_test[,1:30]))
st_test$Label <- df_test$Label

weights_test <- reweight(test$Weight, st_test$Label, Ns(), Nb()) # extract weights

truth <- st_test$Label
response <- predict(fmodel, newdata = st_test[,-length(st_test)])

AMS_weighted(truth, response, weights_test)
```

```
## [1] 0.1818793
```

Two-stage maximisation

Below is the code for conducting the two-stage maximisation of the AMS.

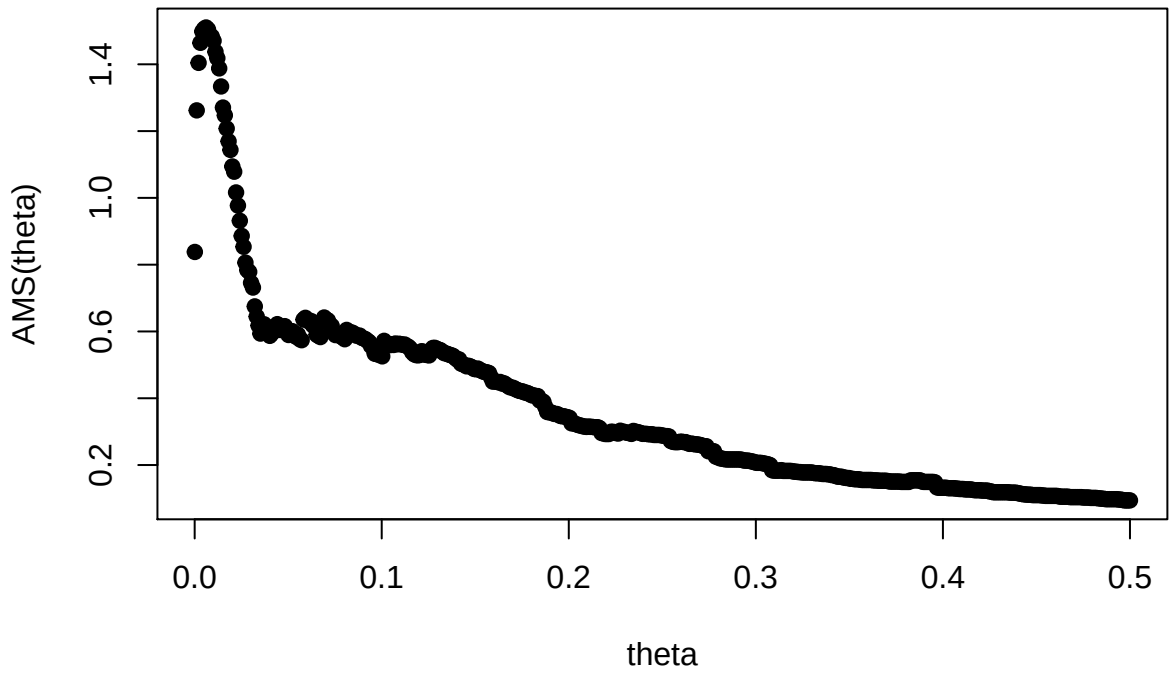
First we create a training/validation split of the training data that preserves the overall class distribution.

```
trainIndex <- createDataPartition(st_train$Label, p = .8, list = FALSE, times = 1)

Train <- st_train[ trainIndex,]
Valid  <- st_train[-trainIndex,]
```

We then fit a WLR model using the new training set `Train`, before visualising how the AMS varies with threshold `theta`. This informs the users decision of how to set the parameters `theta_0` and `theta_1` in the function `threshold_CV` in the `higgsboson` package (use `??threshold_CV` for help on this function). We can see that the peak definitely occurs in the range 0 to 0.1.

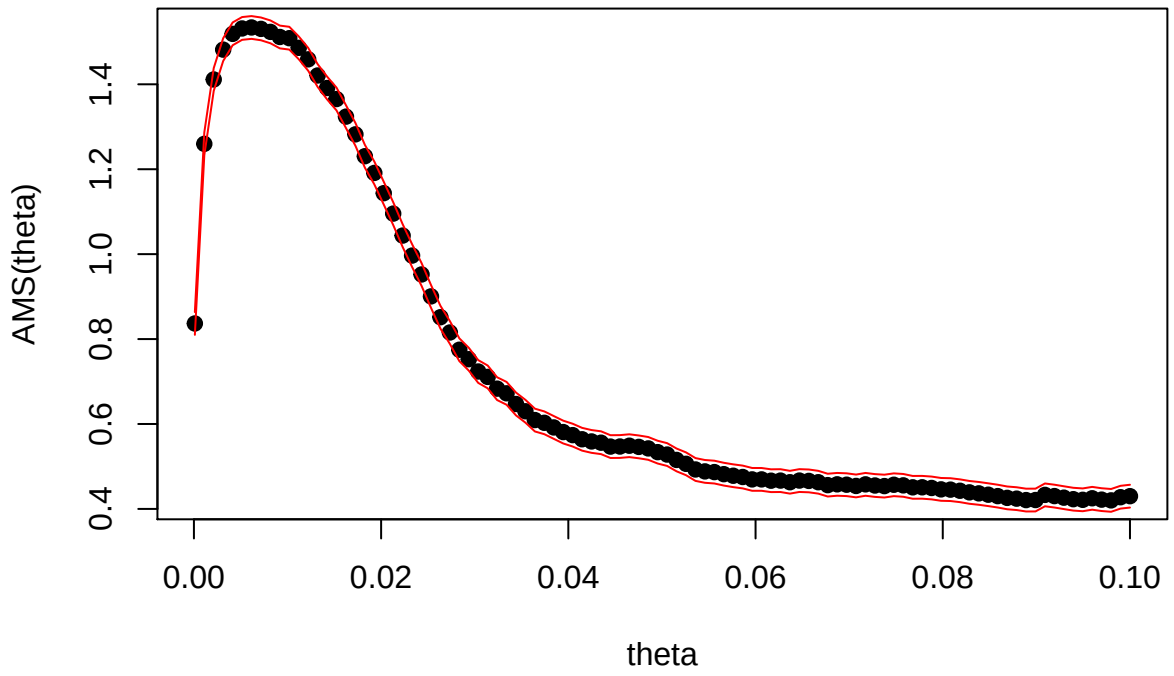
```
weights_Train <- reweight(weights[trainIndex], Train$Label, Ns(), Nb())
weights_Valid <- reweight(weights[-trainIndex], Valid$Label, Ns(), Nb())

logreg_weighted2 <- caret::train(Label ~ .,
                       data = Train,
                       method = "glm",
                       weights = weights_Train,
                       family=binomial()
```

```
)


#Plot AMS for different values of threshold theta
theta_vals <- as.data.frame(seq(0.0001, 0.5, length.out=500)) # generate small sample thresholds theta
AMS_vals <- apply(theta_vals, 1, AMS(logreg_weighted2,Valid[,1:30],Valid[31], weights_Valid)) #compute
plot(as.array(unlist(theta_vals)), AMS_vals, xlab="theta", ylab="AMS(theta)", pch=19) #plot it
```



Now, using the plot above, we can set `theta_0 = 0.0001` and `theta_1=0.1` in the `threshold_CV` function.

```
theta_CV <- threshold_CV(st_train, st_train$Label, weights, theta_0=0.0001, theta_1=0.1, n=100)
```



```
theta_CV
```

```
## $max_theta
## [1] 0.006154545
##
## $max_AMS
## [1] 1.533845
##
## $mean_AMS_sd
## [1] 0.0268266
##
## $max_thetas
## [1] 0.007163636 0.007163636 0.005145455 0.006154545 0.005145455
```

We can now use the threshold found in the cross-validation to find our predictions on the test set and the resulting AMS.

```
theta <- theta_CV$max_theta

probabilities <- predict(logreg_weighted2$finalModel, st_test[,1:30], type = "response")

predicted.classes <- ifelse(probabilities > theta, 1, 0)

Label_valid <-  as.array(unlist(st_test[,31]))
Label_valid <- as.numeric(levels(Label_valid))[Label_valid] #convert from factor to numeric

AMS_weighted(Label_valid, predicted.classes, weights_test)
```

```
## [1] 1.526392
```

Principal-Component Analysis

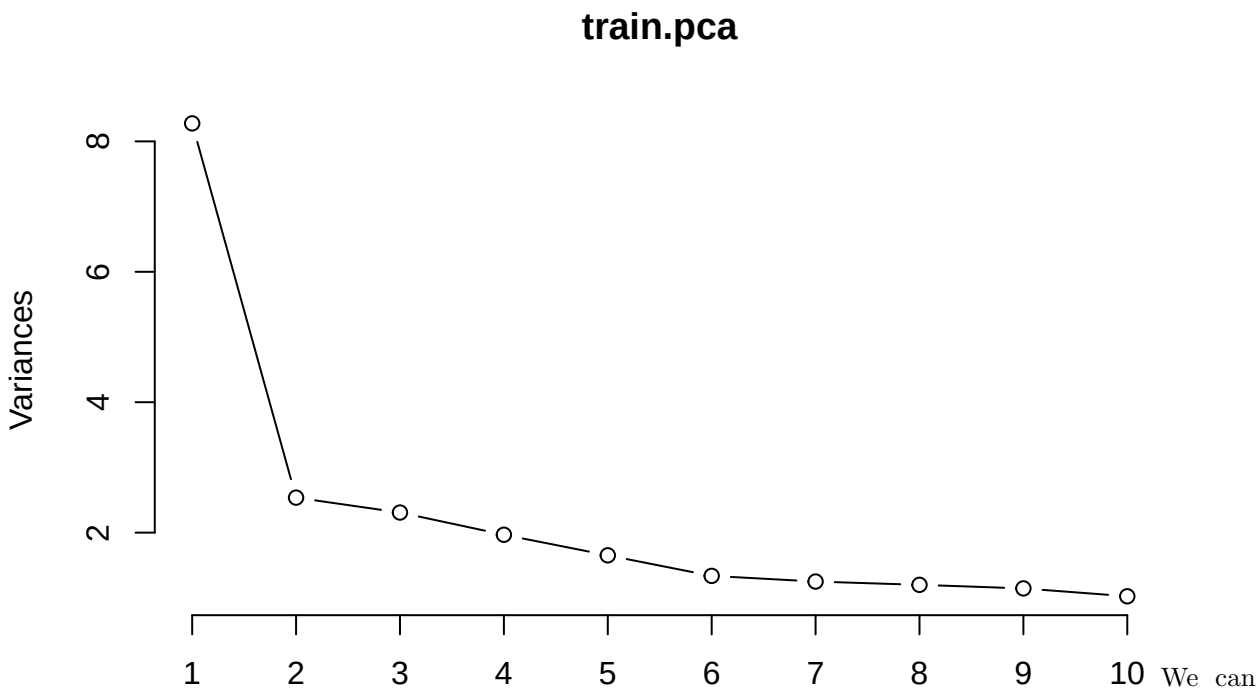
Alternatively, we can perform PCA on the data set before fitting a model and tuning the threshold. This will reduce the dimension of the data set, improving the speed of the function and, hopefully, reduce any overfitting of the more complicated model.

```
train.pca <- prcomp(st_train[,1:30])
summary(train.pca)
```

```
## Importance of components:
##                            PC1     PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     2.8768 1.59275 1.51937 1.40279 1.28531 1.15624 1.11806
## Proportion of Variance 0.2759 0.08456 0.07695 0.06559 0.05507 0.04456 0.04167
## Cumulative Proportion  0.2759 0.36042 0.43737 0.50296 0.55803 0.60259 0.64426
##                            PC8     PC9    PC10    PC11    PC12    PC13    PC14
## Standard deviation     1.09531 1.07001 1.01201 1.00306 0.93818 0.87197 0.86820
## Proportion of Variance 0.03999 0.03816 0.03414 0.03354 0.02934 0.02534 0.02513
## Cumulative Proportion  0.68425 0.72242 0.75656 0.79009 0.81943 0.84478 0.86990
##                           PC15    PC16    PC17    PC18    PC19   PC20    PC21
## Standard deviation     0.80557 0.74824 0.71231 0.66525 0.60098 0.5198 0.48412
## Proportion of Variance 0.02163 0.01866 0.01691 0.01475 0.01204 0.0090 0.00781
## Cumulative Proportion  0.89153 0.91020 0.92711 0.94186 0.95390 0.9629 0.97072
##                           PC22    PC23    PC24    PC25    PC26    PC27    PC28
## Standard deviation     0.46176 0.39368 0.37755 0.35851 0.30716 0.25633 0.24541
## Proportion of Variance 0.00711 0.00517 0.00475 0.00428 0.00314 0.00219 0.00201
## Cumulative Proportion  0.97782 0.98299 0.98774 0.99203 0.99517 0.99736 0.99937
```

```
##                             PC29      PC30
## Standard deviation     0.13754 3.534e-06
## Proportion of Variance 0.00063 0.000e+00
## Cumulative Proportion  1.00000 1.000e+00
```

```
screeplot(train.pca, type="lines")
```



We can see that the first two PCA's account for the majority of the vaiance, but we shall keep the first three as a precaution.

```
st_train_dimred <- data.frame("PCA1"=train.pca$x[,1],"PCA2"=train.pca$x[,2],"PCA3"=train.pca$x[,3])
st_train_dimred["Label"] <- st_train$Label
```

Now, we can perform the first stage of the two-stage procedure as above.

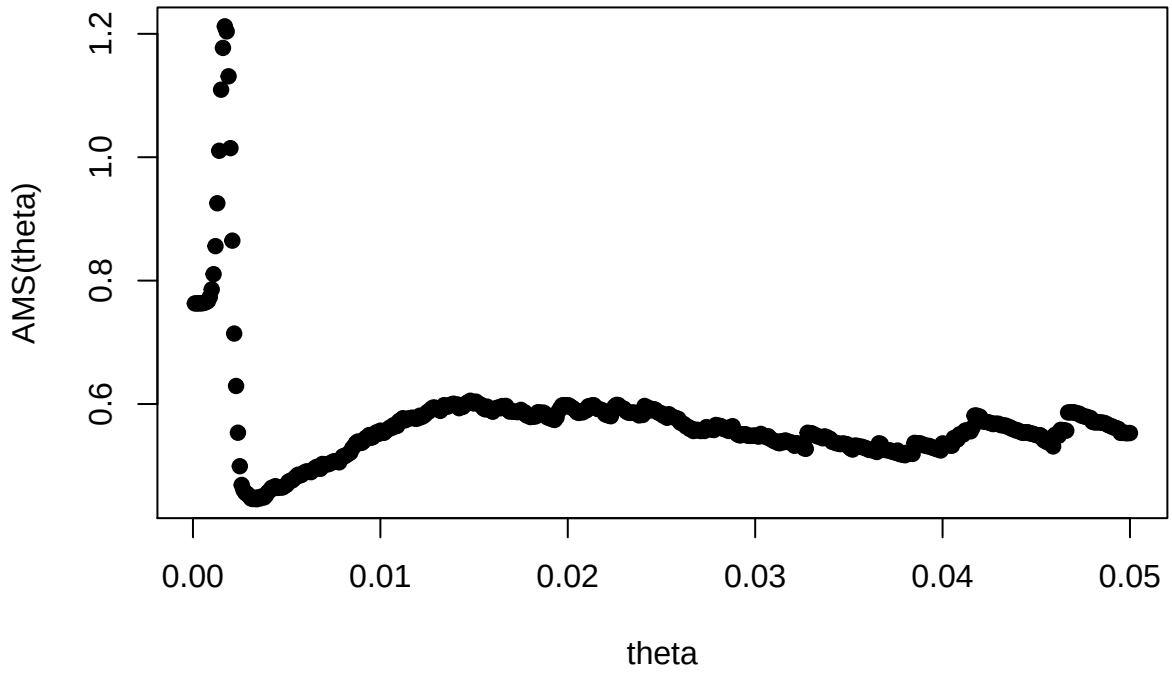
```
trainIndex <- createDataPartition(st_train_dimred$Label, p = .8,
                                  list = FALSE,
                                  times = 1)

Train <- st_train_dimred[ trainIndex,]
Valid  <- st_train_dimred[-trainIndex,]


weights_Train <- reweight(weights[trainIndex], Train$Label, Ns(), Nb())
weights_Valid <- reweight(weights[-trainIndex], Valid$Label, Ns(), Nb())

logreg_weighted_pca <- caret::train(Label ~ .,
                                    data = Train,
                                    method = "glm",
                                    weights = weights_Train,
                                    family=binomial()
)
print(logreg_weighted_pca)
```

```
## Generalized Linear Model
```

```
##
## 200001 samples
##      3 predictor
##      2 classes: '0', '1'
##
## No pre-processing
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 200001, 200001, 200001, 200001, 200001, 200001, ...
## Resampling results:
##
##   Accuracy   Kappa
##   0.6580688  0.0006967816
```

Now we can plot the AMS for varying values of the threshold theta.

```
theta_vals <- as.data.frame(seq(0.0001, 0.05, length.out=500)) # generate small sample thresholds theta
AMS_vals <- apply(theta_vals, 1, AMS(logreg_weighted_pca,Valid[,1:3],Valid[4], weights_Valid)) #compute
plot(as.array(unlist(theta_vals)), AMS_vals, xlab="theta", ylab="AMS(theta)", pch=19) #plot it
```




```
max_theta <- theta_vals[which.max(AMS_vals),1]
max_theta
```

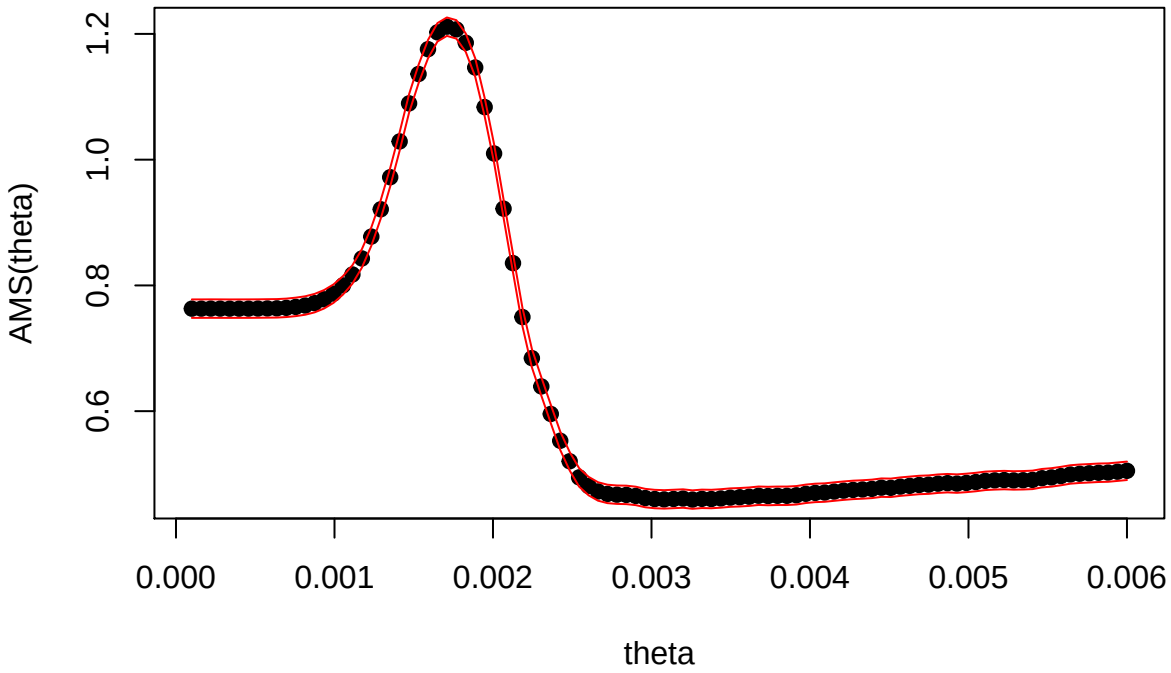
```
## [1] 0.0017
```

```
max_AMS <- AMS_vals[which.max(AMS_vals)]
max_AMS
```

```
## [1] 1.212122
```

We can see that the peak occurs between very small values of theta, hence we try `theta_0=0.0001` and `theta_1=0.006` in the `threshold_CV` function.

```
theta_CV <- threshold_CV(st_train_dimred[,1:3], st_train_dimred$Label, weights=weights, theta_0=0.0001,
```




```
theta_CV  #less variance, both of theta and of AMS
```

```
## $max_theta
## [1] 0.001709091
##
## $max_AMS
## [1] 1.211464
##
## $mean_AMS_sd
## [1] 0.01466137
##
## $max_thetas
## [1] 0.001709091 0.001709091 0.001709091 0.001709091 0.001709091
```

Finally, we can now use the threshold found in the cross-validation to find our predictions on the test set and the resulting AMS.

```
theta <- theta_CV$max_theta

probabilities <- predict(logreg_weighted2$finalModel, st_test[,1:30], type = "response")

predicted.classes <- ifelse(probabilities > theta, 1, 0)

Label_valid <-  as.array(unlist(st_test[,31]))
Label_valid <- as.numeric(levels(Label_valid))[Label_valid] #convert from factor to numeric

AMS_weighted(Label_valid, predicted.classes, weights_test)
```

```
## [1] 1.370724
```