

Supplementary file 1. Modeling code.

```
##partition data
```

```
set.seed(107)
```

```
inTrain <- createDataPartition(y = data$class, p = .75, list = FALSE)
```

```
train_set <- data[inTrain,]
```

```
test_set <- data[-inTrain,]
```

```
y_train= train_set [,c (12)]
```

```
train_pred= train_set [,c (2:9)]
```

```
y_test= test_set [,c (12)]
```

```
test_pred= test_set [,c (2:9)]
```

```
##cross-validate
```

```
cvCtrl <- trainControl(method = "repeatedcv", number = 10, repeats = 3)
```

```
##classify
```

```
xgb <- caret::train(train_set, y_train, method = "xgbTree", metric = "Accuracy",  
trControl = cvCtrl)
```

```
##validate
```

```
test_xgb = predict(xgb, newdata = test_pred)
```