DATA621 HW2

Misha Kollontai, Matthew Baker, Erinda Budo, Subhalaxmi Rout, Don Padmaperuma

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Libraries

```
library(dplyr)
library(ggplot2)
library(reshape2)
library(kableExtra)
library(DT)
```

---

1. Downloading the Data

```
df <- read.csv("https://raw.githubusercontent.com/mkollontai/DATA621_GroupWork/master/HW2/classification-output-data.csv")
df_hw2 <- df[,c('class', 'scored.class','scored.probability')]
```

We have pulled the data and simplified our dataframe into just the 3 columns in question:

- class
- scored.class
- scored.probability

---

2. Simple Confusion Matrix

```
table(df_hw2$class, df_hw2$scored.class)
```

```
##
##       0   1
##   0 119   5
##   1  30  27
```

This confusion matrix shows us the number of entries of each class against what they were predicted to be. In this table the row indicates the actual class, whereas the column signifies the predicted value (scored.class). We can therefore deduce that of the 57 total cases of class '1', 27 were predicted to be class '1' correctly. The other 30 were mistakenly predicted to be of class '0'. For the actual class '0' cases, 5 were mistakenly predicted to be class '1', whereas 119 were correctly identified.

In order to calculate all of the following evaluations of the predictions made within this dataframe we need to identify the number of:

- True Positives - Correctly identified class '1' cases
- False Positives - Class '0' cases incorrectly identified as class '1'
- True Negatives - Correctly identified class '0' cases
- False Negatives - Class '1' cases incorrectly identified as class '0'

In order to avoid repeating code required to identify these outcomes, let's crate a function that calculates the number associated with each of these four outcomes.

```
outcomes <- function(df){
  outs <- aggregate(df, by = list(df[,1], df[,2]), FUN=length) %>%
    select(1:3) %>%
    `colnames<-` (c('class','prediction','count'))
  return(outs)
  #Within this df, in the 'count' column:
  #the first row is our True Negative (TN),
  #the second row is False Negatives (FN),
  #third row is False Positives (FP) and
  #final row is the True Positives (TP).
}

outcomes(df_hw2) %>%
  kable() %>%
  kable_paper('hover', full_width = F)
```

class	prediction	count
0	0	119
1	0	30
0	1	5
1	1	27

---

3. Accuracy Calculation

To calculate accuracy we must use the formula

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

```
acc <- function(df){
  outs <- outcomes(df)
  TN <- outs$count[1]
  FN <- outs$count[2]
  TP <- outs$count[4]
  FP <- outs$count[3]
  acc <- (TP+TN)/(TP+FP+TN+FN)
  return(acc)
}
acc(df_hw2)
```

```
## [1] 0.8066298
```

---

4. Classification Error Rate Calculation

To calculate classification error we must use the formula

$$ClassificationErrorRate = \frac{FP + FN}{TP + FP + TN + FN}$$

```
cer <- function(df){
  outs <- outcomes(df)
  TN <- outs$count[1]
  FN <- outs$count[2]
  TP <- outs$count[4]
  FP <- outs$count[3]
  cer <- (FP+FN)/(TP+FP+TN+FN)
  return(cer)
}
cer(df_hw2)
```

```
## [1] 0.1933702
```

The calculations for these two measures are such that summing the two should yield 1:

```
acc(df_hw2) + cer(df_hw2)
```

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

---

5. Precision Calculation

To calculate precision we must use the formula

$$Precision = \frac{TP}{TP + FP}$$

```
prec <- function(df){
  outs <- outcomes(df)
  TP <- outs$count[4]
  FP <- outs$count[3]
  prec <- (TP)/(TP+FP)
  return(prec)
}
prec(df_hw2)
```

```
## [1] 0.84375
```

---

6. Sensitivity Calculation

To calculate sensitivity we must use the formula

$$Sensitivity = \frac{TP}{TP + FN}$$

```
sens <- function(df){
  FN <- sum(df$class == 1 & df$scored.class ==0)
  TP <- sum(df$class == 1 & df$scored.class ==1)
  sens <- (TP)/(TP+FN)
  return(sens)
}
sens(df_hw2)
```

```
## [1] 0.4736842
```

---

7. Specificity Calculation

To calculate specficity we must use the formula

$$Specificity = \frac{TN}{TN + FP}$$

```
spec <- function(df){
  TN <- sum(df$class == 0 & df$scored.class ==0)
  FP <- sum(df$class == 0 & df$scored.class ==1)
  spec <- (TN)/(TN+FP)
  return(spec)
}
spec(df_hw2)
```

```
## [1] 0.9596774
```

---

8. F1 Calculation

To calculate F1 we must use the formula

$$F1 = \frac{2 * Precision * Sensitivity}{Precision + Sensitivity}$$

```
f1 <- function(df){
  prec <- prec(df)
  sens <- sens(df)
  f1 <- (2*prec*sens)/(prec+sens)
  return(f1)
}
f1(df_hw2)
```

```
## [1] 0.6067416
```

---

9. Bounds of F1

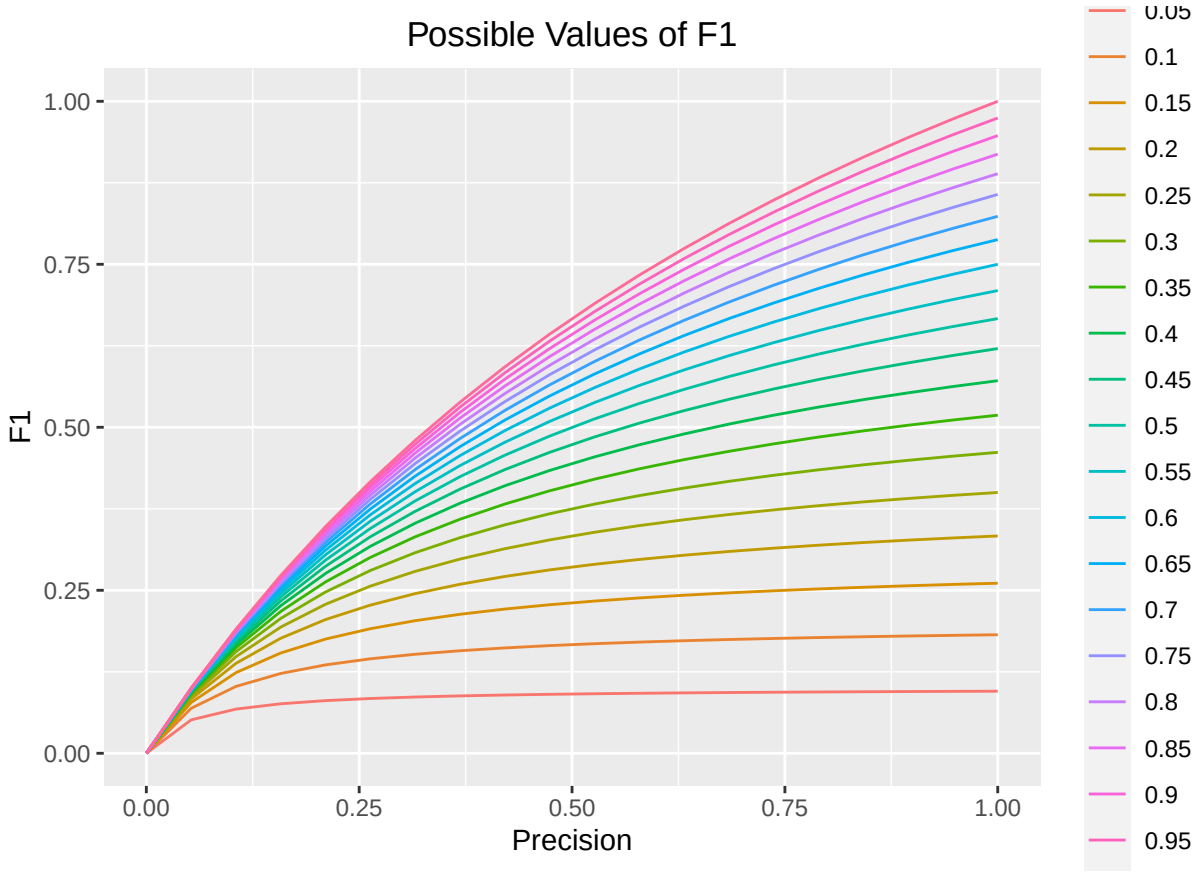
To show the bounds of F1, let's simplify the euation to a more manageable form:

$$F1 = \frac{2ps}{p + s}$$

The following code generates 'l' evenly-spaced values between 0 and 1 for the Precision. It then uses a loop to generate the calculated F1 values through the same range of Sensitivity values corresponding to each of the Precision values. The plot below shows calculated F1 on the y-axis, with each line corresponding to the calculation associated with a particular Sensitivity value.

```
#Partially used approach from (https://stackoverflow.com/questions/14704742/use-for-loop-to-plot-multiple-lines-in-single-plot-u
l <- 20
p <- seq(0,1, length.out = l)
df <- NULL
for(i in 1:l){
  j <- i/l
  temp_df <- data.frame(x = p, y = (2*p*j)/(p+j), col = rep(j:j,each = l))
  df <- rbind(df, temp_df)
```

```
}
ggplot(df,aes(x=x,y=y,group=col,color=factor(col))) +
  geom_line() +
  ggtitle('Possible Values of F1') +
  theme(plot.title = element_text(hjust = 0.5)) +
  ylab('F1') +
  xlab('Precision') +
  ylim(0,1)
```



As we can clearly see, **the range of possible values for F1 is between 0 and 1**, as it was for both the Precision and the Sensitivity. We can clearly see that higher values of both Precision and Sensitivity result in higher F-1 values, with the highest value of 1 resulting from both Precision and Sensitivity being 1.

---

10. Function for ROC curve

Write a function that generates an ROC curve from a data set with a true classification column (class in our example) and a probability column (scored.probability in our example). Your function should return a list that includes the plot of the ROC curve and a vector that contains the calculated area under the curve (AUC). Note that I recommend using a sequence of thresholds ranging from 0 to 1 at 0.01 intervals.

The ROC curve shows the trade-off between sensitivity and specificity. It is plotted with True Positive Rate and False Positive Rate at all possible pairings of those values (from 0 to 1)

True Positive Rate = Sensitivity

False positive Rate = 1 - Specificity

```
roc <- function(df){

for (threshold in seq(0,1,0.01))
  {
  #create dataset for each threshold
  temp1 <- data.frame(class = df[,1], scored.class = if_else(df[,3] >= threshold,1,0),
                      scored.probability = df[,3])

  #create vectors to store TPR & FPR for all datasets
  if(!exists('TPR') & !exists('FPR'))
    {
    TPR <- sens(temp1)
    FPR <- 1- spec(temp1)
  }
  else
    {
    TPR <- c(TPR,sens(temp1))
    FPR <- c(FPR, 1- spec(temp1))
  }
}

roc_df1 <- data.frame(TPR, FPR) %>% arrange(FPR)


# AUC calculation
```

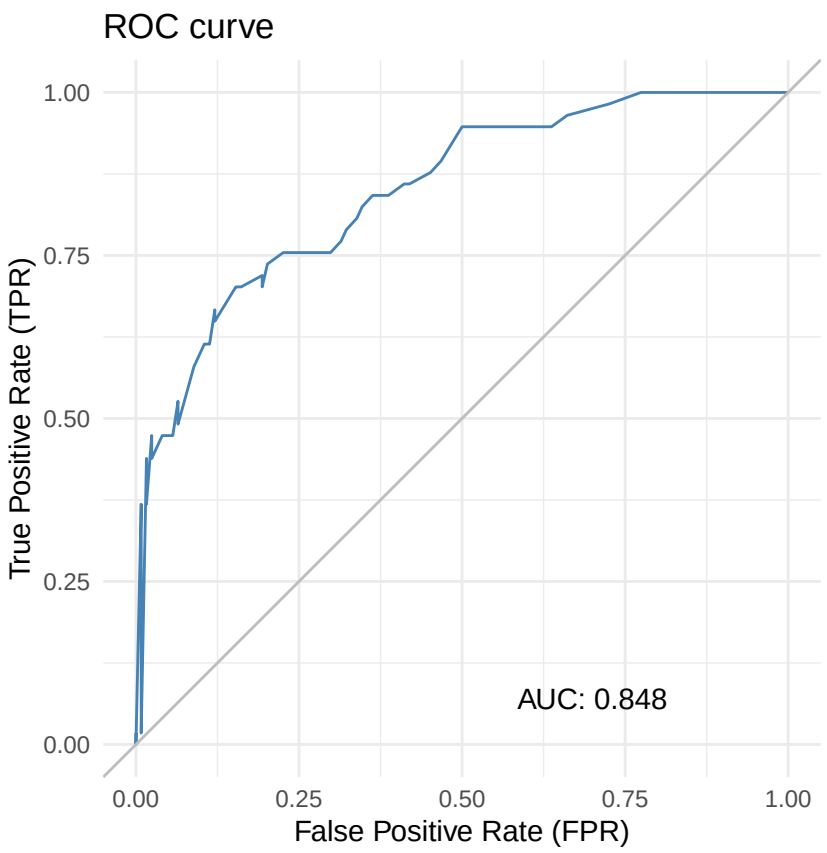
```
  diff_FPR <- c(diff(roc_df1$FPR), 0)
  diff_TPR <- c(diff(roc_df1$TPR), 0)
  AUC <- round(sum(roc_df1$TPR * diff_FPR) + sum(diff_TPR * diff_FPR)/2, 3)


  #Create plot
  plot <- ggplot(roc_df1) +
    geom_line(aes(FPR, TPR), color = "steel blue") +
    ggtitle("ROC curve") +
    theme(plot.title = element_text(hjust = 0.5)) +
    xlab("False Positive Rate (FPR)") +
    ylab("True Positive Rate (TPR)") +
    theme_minimal() +
    annotate(geom = "text", x = 0.7, y = 0.07,label = paste("AUC:", round(AUC, 3))) +
    geom_abline(intercept = 0, slope = 1, linetype = "solid", col = "gray") +
    coord_equal(ratio = 1)

  q10_list <- list(plot,AUC)
  return(q10_list)
}

q10 <- roc(df_hw2)
```

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



---

11. Use your created R functions and the provided classification output data set to produce all of the classification metrics discussed above.

```
df_detail <- c(acc(df_hw2), cer(df_hw2), f1(df_hw2), prec(df_hw2), sens(df_hw2), spec(df_hw2))
names(df_detail) <- c("Accuracy", "Classification Error Rate", "F1-Score",
                      "Percision", "Sensitivity", "Specificity")
kable(df_detail, col.names = "Values") %>%
  kable_paper('hover', full_width = F)
```

	Values
Accuracy	0.8066298
Classification Error Rate	0.1933702
F1-Score	0.6067416
Percision	0.8437500
Sensitivity	0.4736842
Specificity	0.9596774

---

12. Investigate the caret package. In particular, consider the functions confusionMatrix, sensitivity, and specificity. Apply the functions to the data set. How do the results compare with your own functions?

```
library(caret)
library(e1071)

cf<- confusionMatrix(as.factor(df_hw2$scored.class), as.factor(df_hw2$class), positive = '1')
print(cf)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 119  30
##          1   5  27
##
##                Accuracy : 0.8066
##                  95% CI : (0.7415, 0.8615)
##     No Information Rate : 0.6851
##     P-Value [Acc > NIR] : 0.0001712
##
##                   Kappa : 0.4916
##
##  Mcnemar's Test P-Value : 4.976e-05
##
##             Sensitivity : 0.4737
##             Specificity : 0.9597
##          Pos Pred Value : 0.8438
##          Neg Pred Value : 0.7987
##              Prevalence : 0.3149
##          Detection Rate : 0.1492
##    Detection Prevalence : 0.1768
##       Balanced Accuracy : 0.7167
##
##        'Positive' Class : 1
##
```

```
# caret package confusion matrix
cf$table
```

```
##           Reference
## Prediction   0   1
##          0 119  30
##          1   5  27
```

```
# created function for confusion matrix
df_hw2 %>% select(scored.class, class) %>% table()
```

```
##             class
## scored.class   0   1
##            0 119  30
##            1   5  27
```

```
caret_fn <- c(cf$byClass["Sensitivity"], cf$byClass["Specificity"])
user_fn <- c(sens(df_hw2), spec(df_hw2))
tble <- cbind(caret_fn, user_fn)
kable(tble) %>%
  kable_paper('hover', full_width = F)
```

	caret_fn	user_fn
Sensitivity	0.4736842	0.4736842
Specificity	0.9596774	0.9596774

The *caret* package yields the same confusion matrix as the $confusionMatrix$ function. We can also see that it yields the same values for **sensitivity** and **specificity** as were generated by our custom functions.

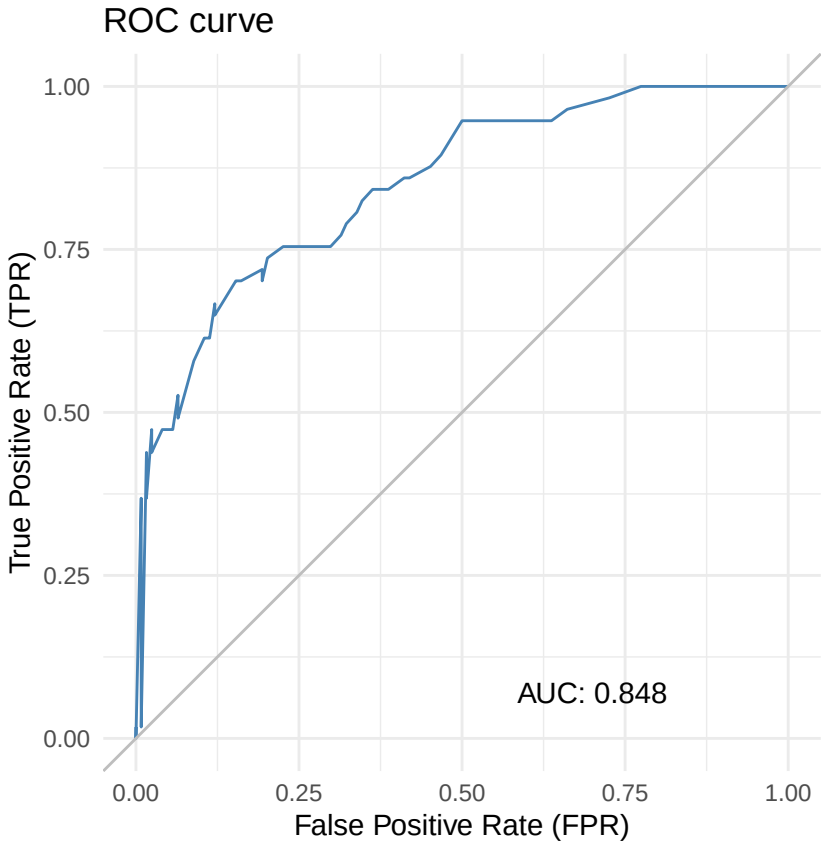
---

13. Investigate the pROC package. Use it to generate an ROC curve for the data set. How do the results compare with your own functions?

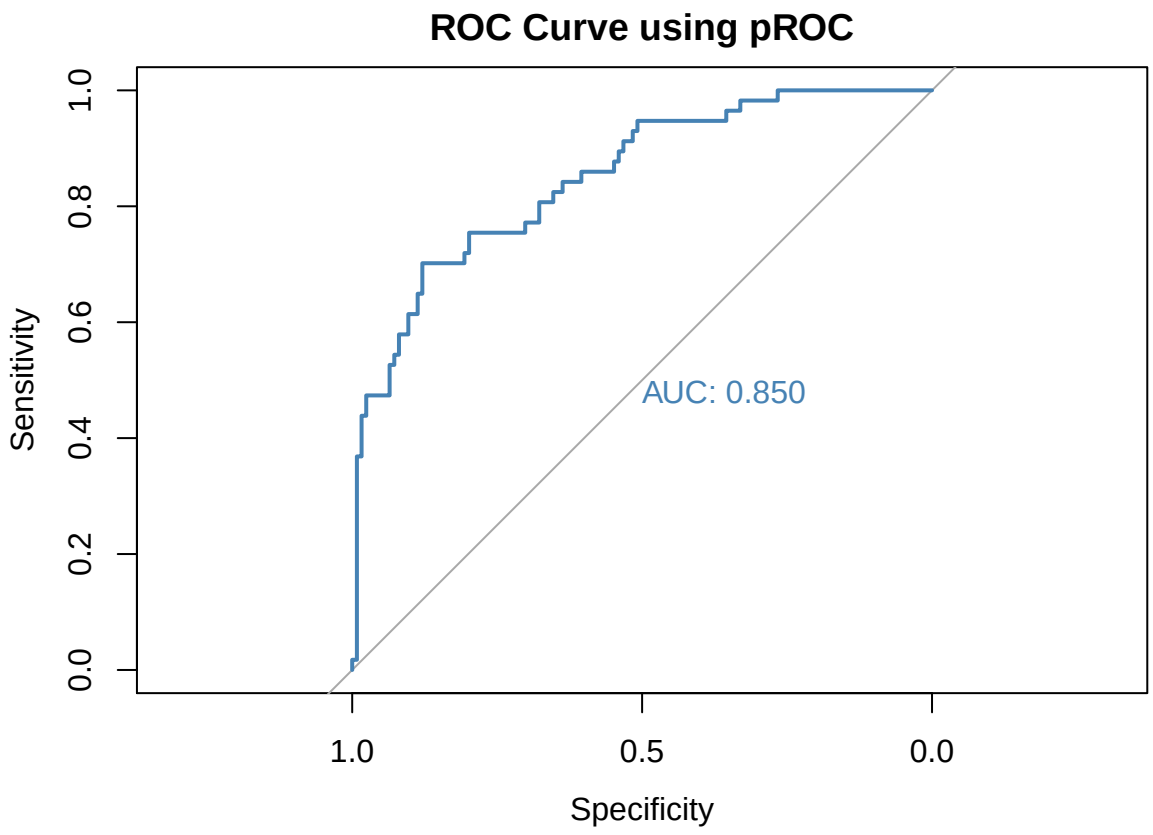
```
require(pROC)

q10[1]
```

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




```
pROC::roc(response = df_hw2$class,
    predictor = df_hw2$scored.probability,
    plot = TRUE,
    print.auc = TRUE,
    col="steel blue",
    bg="grey",
    main = "ROC Curve using pROC")
```




```
##
## Call:
## roc.default(response = df_hw2$class, predictor = df_hw2$scored.probability,     plot = TRUE, print.auc = TRUE, col = "steel blu
##
## Data: df_hw2$scored.probability in 124 controls (df_hw2$class 0) < 57 cases (df_hw2$class 1).
## Area under the curve: 0.8503
```

The two plots above show that results are very similiar in the `pROc` package and our custom *roc* function for both the curve and AUC calculation.