

Homework 4

4375 Machine Learning with Dr. Mazidi

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This script will run Logistic Regression and Naive Bayes on the BreastCancer data set which is part of package mlbench.

Step 1: Data exploration

- Load package mlbench, installing it at the console if necessary
- Load data(BreastCancer)
- Run str() and head() to look at the data
- Run summary() on the Class column
- Use R code to calculate and output the percentage in each class, with a label using paste()

Comment on the types of predictors available in terms of their data types: There is alot of predictors, most of which relate to the cell or parts of the cell.

```
# your code here
library(mlbench)
data(BreastCancer)
df <- BreastCancer
str(BreastCancer)
```

```
## 'data.frame': 699 obs. of 11 variables:
## $ Id : chr "1000025" "1002945" "1015425" "1016277" ...
## $ Cl.thickness : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 5 5 3 6 4 8 1 2 2 4 ...
## $ Cell.size : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 1 1 2 ...
## $ Cell.shape : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 2 1 1 ...
## $ Marg.adhesion : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 5 1 1 3 8 1 1 1 1 ...
## $ Epith.c.size : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 2 7 2 3 2 7 2 2 2 2 ...
## $ Bare.nuclei : Factor w/ 10 levels "1","2","3","4",...: 1 10 2 4 1 10 10 1 1 1 ...
## $ Bl.cromatin : Factor w/ 10 levels "1","2","3","4",...: 3 3 3 3 3 9 3 3 1 2 ...
## $ Normal.nucleoli: Factor w/ 10 levels "1","2","3","4",...: 1 2 1 7 1 7 1 1 1 1 ...
## $ Mitoses : Factor w/ 9 levels "1","2","3","4",...: 1 1 1 1 1 1 1 1 5 1 ...
## $ Class : Factor w/ 2 levels "benign","malignant": 1 1 1 1 1 2 1 1 1 1 ...
```

```
head(BreastCancer)
```

```
##      Id Cl.thickness Cell.size Cell.shape Marg.adhesion Epith.c.size
## 1 1000025          5         1         1             1           2
## 2 1002945          5         4         4             5           7
```

```
## 3 1015425      3      1      1      1      2
## 4 1016277      6      8      8      1      3
## 5 1017023      4      1      1      3      2
## 6 1017122      8     10     10      8      7
##   Bare.nuclei Bl.cromatin Normal.nucleoli Mitoses   Class
## 1          1          3          1      1   benign
## 2         10          3          2      1   benign
## 3          2          3          1      1   benign
## 4          4          3          7      1   benign
## 5          1          3          1      1   benign
## 6         10          9          7      1 malignant
```

```
summary(BreastCancer[,c(11)])
```

```
##      benign malignant
##      458         241
```

```
total <- 458 + 241
benignAmount <- 458/total * 100
malignantAmount <- 241 / total * 100
print(paste(benignAmount,"% are benign class and ",malignantAmount,"% are malignant."))
```

```
## [1] "65.5221745350501 % are benign class and  34.4778254649499 % are malignant."
```

Step 2: First logistic regression model

- Cell.size and Cell.shape are in one of 10 levels
- Build a logistic regression model called glm0, where Class is predicted by Cell.size and Cell.shape
- Do you get any error or warning messages? Google the message and try to decide what happened
- Run summary on glm0 to confirm that it did build a model
- Write about why you think you got this warning message and what you could possibly do about it. List the source of your information in a simple markdown link.

Your commentary here: Because the dataset is whole and complete and we are not using training data, so the predictors have very higher accuracy leading to a very good model.

```
# your code here
glm0 <- glm(Class~Cell.size+Cell.shape, data = df, family = "binomial")
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
summary(glm0)
```

```
##
## Call:
## glm(formula = Class ~ Cell.size + Cell.shape, family = "binomial",
##      data = df)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
```

```
## -2.6380 -0.0844 -0.0844 0.0000 3.3583
##
## Coefficients:
##          Estimate Std. Error z value Pr(>|z|)
## (Intercept)    7.77977   757.06727   0.010   0.992
## Cell.size.L    10.45177   950.68968   0.011   0.991
## Cell.size.Q     0.04063  1479.65504   0.000   1.000
## Cell.size.C    10.70546   948.84001   0.011   0.991
## Cell.size^4    12.06582  1241.92612   0.010   0.992
## Cell.size^5     0.74199   792.70275   0.001   0.999
## Cell.size^6    -3.08210  1011.79270  -0.003   0.998
## Cell.size^7     7.47104  1044.50458   0.007   0.994
## Cell.size^8     5.60143   830.93455   0.007   0.995
## Cell.size^9   -10.22144  1812.16582  -0.006   0.995
## Cell.shape.L   18.15803  2619.03235   0.007   0.994
## Cell.shape.Q    9.14381  1500.17053   0.006   0.995
## Cell.shape.C    5.50082  1302.51283   0.004   0.997
## Cell.shape^4   -2.23752  2679.86462  -0.001   0.999
## Cell.shape^5   -5.76978  3193.32564  -0.002   0.999
## Cell.shape^6   -5.58415  2713.54558  -0.002   0.998
## Cell.shape^7   -3.94569  1740.80748  -0.002   0.998
## Cell.shape^8   -1.82009   827.39666  -0.002   0.998
## Cell.shape^9   -0.77209   257.90960  -0.003   0.998
##
## (Dispersion parameter for binomial family taken to be 1)
##
##      Null deviance: 900.53  on 698  degrees of freedom
## Residual deviance: 198.66  on 680  degrees of freedom
## AIC: 236.66
##
## Number of Fisher Scoring iterations: 19
```

Step 3: Data Wrangling

Notice in the `summary()` of `glm0` that most of the levels of `Cell.size` and `Cell.shape` became predictors and that they had very high p-values, that is, they are not good predictors. We would need a lot more data to build a good logistic regression model this way. Many examples per factor level are generally required for model building. A better approach might be to just have 2 levels for each variable.

In this step:

- Add two new columns to `BreastCancer` as listed below:
 - a. `Cell.small` which is a binary factor that is 1 if `Cell.size==1` and 0 otherwise
 - b. `Cell.regular` which is a binary factor that is 1 if `Cell.shape==1` and 0 otherwise
- Run `summary()` on `Cell.size` and `Cell.shape` as well as the new columns
- Comment on the distribution of the new columns
- Do you think what we did is a good idea? Why or why not?

Your commentary here: The distribution was good for the new columns having about a 50 50 split. This was probably a good idea since it gives us another predictor which has a balanced distribution.

```
# BreastCancer$Cell.small column
df$Cell.small <- 0
df$Cell.small[df$Cell.size==1] <- 1
df$Cell.small <- factor(df$Cell.small)

df$Cell.regular <- 0
df$Cell.regular[df$Cell.shape==1] <- 1
df$Cell.regular <- factor(df$Cell.regular)

df$Class <- factor(df$Class)

summary(df[,c(3,4,12,13)])
```

```
##      Cell.size      Cell.shape Cell.small Cell.regular
## 1         :384      1         :353      0:315      0:346
## 10        : 67      2         : 59      1:384      1:353
## 3         : 52     10         : 58
## 2         : 45      3         : 56
## 4         : 40      4         : 44
## 5         : 30      5         : 34
## (Other): 81      (Other): 95
```

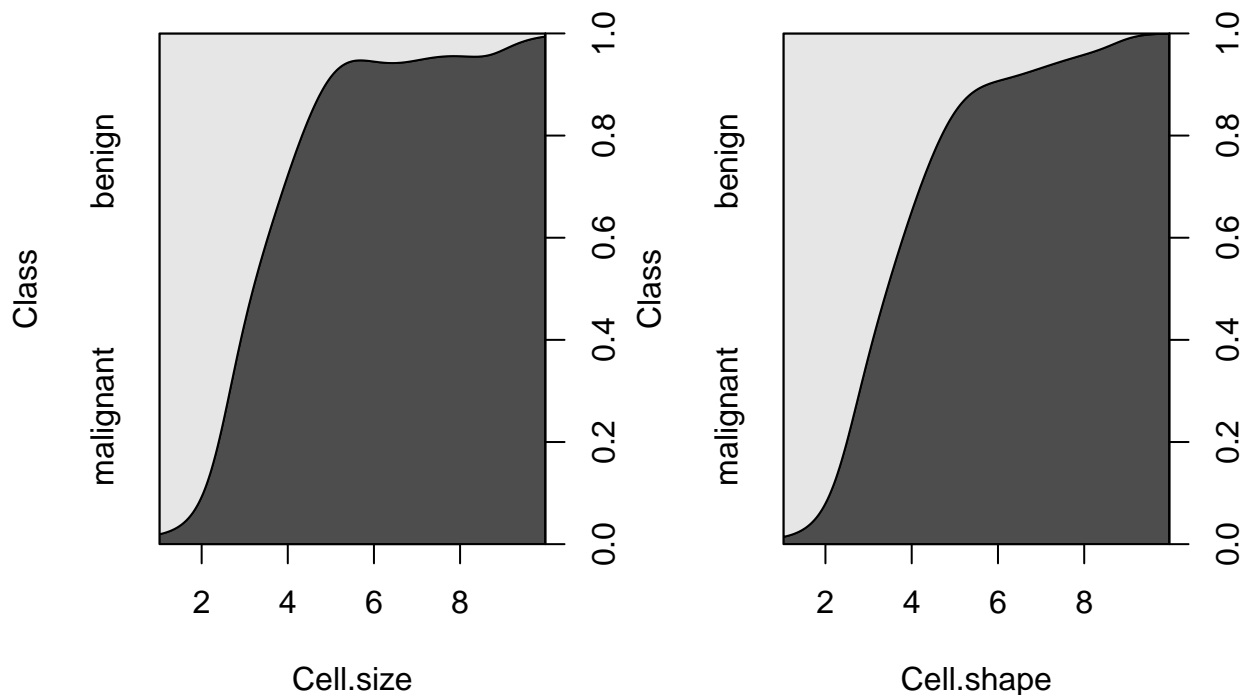
```
# BreastCancer$Cell.regular column
```

Step 4: Examine the relationship of malignancy to Cell.size and Cell.shape

- Create conditional density plots using the original Cell.size and Cell.shape, but first, attach() the data to reduce typing
- Then use par(mfrow=c(1,2)) to set up a 1x2 grid for two cdplot() graphs with Class~Cell.size and Class~Cell.shape
- Observing the plots, write a sentence or two comparing size and malignant, and shape and malignant
- Do you think our cutoff points for size==1 and shape==1 were justified now that you see this graph? Why or why not?

Your commentary here: The smaller cell sizes and non regular sized shapes usually correlated with being malignant. I think our cutoff was justified since the data was relatively balanced.

```
# your code here
attach(df)
par(mfrow=c(1,2))
cdplot(Class~Cell.size)
cdplot(Class~Cell.shape)
```

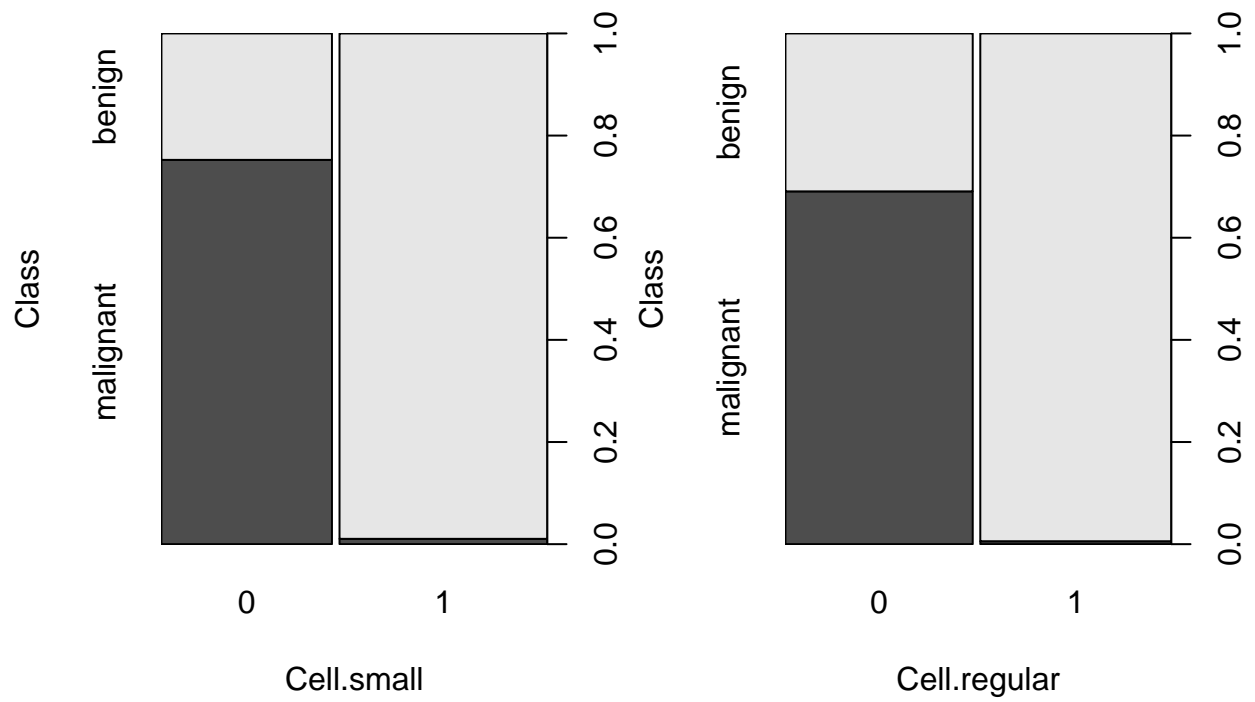


Step 5: Explore the new columns

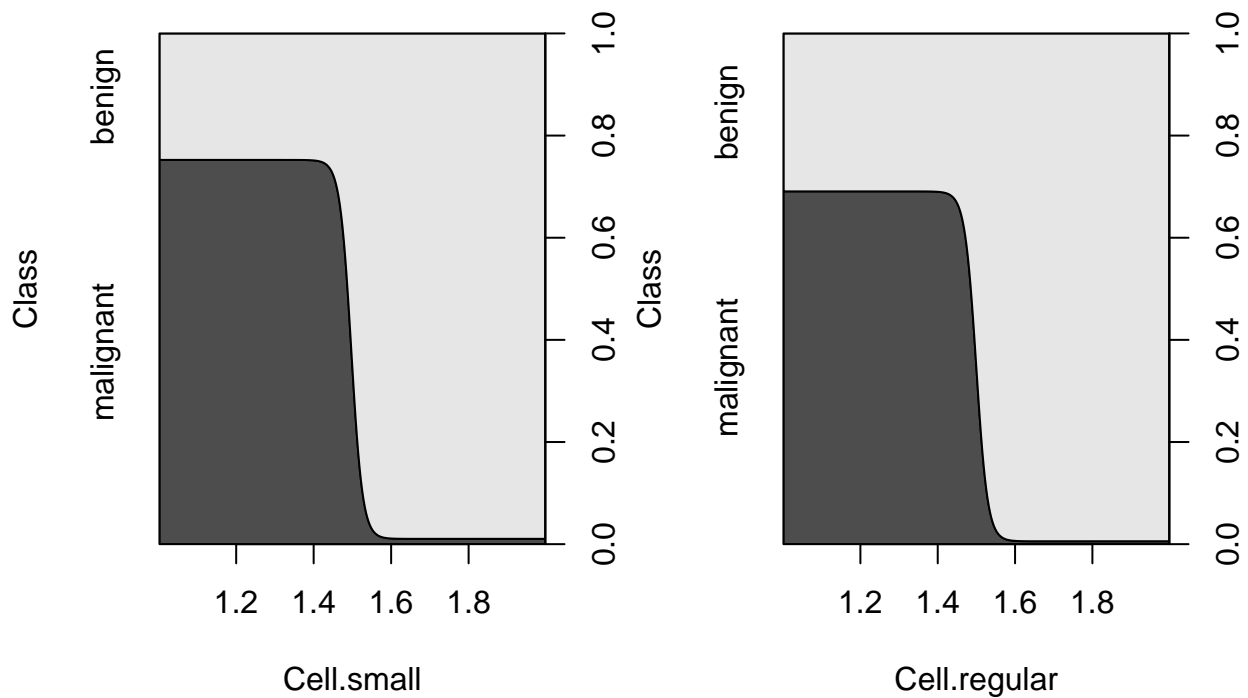
- Create plots (not cdfplots) with the two new columns
- Again, use `par(mfrow=c(1,2))` to set up a 1x2 grid for two `plot()` graphs with `Class~Cell.small` and `Class~Cell.regular`
- Now create two `cdplot()` graphs for the new columns
- Compute and output with labels the following: ((Examples on p. 142 may help)
 - a. calculate the percentage of malignant observations that are small
 - b. calculate the percentage of malignant observations that are small
 - c. calculate the percentage of malignant observations that are regular
 - d. calculate the percentage of malignant observations that are not regular
- Write whether you think small and regular will be good predictors

Your commentary here: Small and regular will probably be good predictors as it shows that most malignant cases have non small cells and irregular cell shapes.

```
# plots here
par(mfrow=c(1,2))
plot(Class~Cell.small,data = df)
plot(Class~Cell.regular,data = df)
```



```
cdplot(Class~Cell.small,data = df)
cdplot(Class~Cell.regular,data = df)
```



```
# calculations and output here
```

```
newList1 <- df[,c(11,12)]
```

```
newList2 <- df[,c(11,13)]
```

```
newList1$mal<- FALSE
```

```
newList1$mal[newList1$Class == "malignant"] <- TRUE
```

```
newList2$mal<- FALSE
```

```
newList2$mal[newList2$Class == "malignant"] <- TRUE
```

```
malSmall1 <- subset(newList1,mal==TRUE)
```

```
summary(malSmall1$Cell.small)
```

```
##    0    1
```

```
## 237    4
```

```
malReg1 <- subset(newList2,mal==TRUE)
```

```
summary(malReg1$Cell.regular)
```

```
##    0    1
```

```
## 239    2
```

```
print(paste("Malignant and Small percentage: ", 4/241 * 100, "%"))
```

```
## [1] "Malignant and Small percentage: 1.6597510373444 %"
```

```
print(paste("Malignant and not Small percentage", 237/241 * 100, "%"))
```

```
## [1] "Malignant and not Small percentage 98.3402489626556 %"
```

```
print(paste("Malignant and Regular percentage: ", 2/241 * 100, "%"))
```

```
## [1] "Malignant and Regular percentage: 0.829875518672199 %"
```

```
print(paste("Malignant and not Regular percentage", 237/241 * 100, "%"))
```

```
## [1] "Malignant and not Regular percentage 98.3402489626556 %"
```

Step 6: Train/test split

- Divide the data into 80/20 train/test sets, using seed 1234

```
# your code here
set.seed(1234)
i <- sample(1:nrow(df), .8*nrow(df), replace=FALSE)
train <- df[i,]
test <- df[-i,]
```

Step 7: Build a logistic regression model

- Build a logistic regression model predicting malignant with two predictors: Cell.small and Cell. regular
- Run summary() on the model
- Which if any of the predictors are good predictors?
- Comment on the model null variance versus residual variance and what it means
- Comment on the AIC score

Your commentary here: The residual deviance is significantly lower than the null deviance which is a good sign. The AIC is a little high but not the highest.

```
# your code here
glm1 <- glm(Class == "malignant" ~ Cell.regular + Cell.small, data = train, family = "binomial")
summary(glm1)
```

```
##
## Call:
## glm(formula = Class == "malignant" ~ Cell.regular + Cell.small,
##      family = "binomial", data = train)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
## -1.8314  -0.0445  -0.0445   0.6433   3.7198
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
```



```
## (Intercept)      1.4701      0.1672      8.791 < 2e-16 ***
## Cell.regular1   -3.7044      0.7603     -4.873 1.10e-06 ***
## Cell.small1     -4.6830      0.7411     -6.319 2.64e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##      Null deviance: 721.78  on 558  degrees of freedom
## Residual deviance: 255.73  on 556  degrees of freedom
## AIC: 261.73
##
## Number of Fisher Scoring iterations: 8
```

Step 8: Evaluate on the test data

- Test the model on the test data
- Compute and output accuracy
- Output the confusion matrix and related stats using the confusionMatrix() function in the caret package
- Were the mis-classifications more false positives or false negatives?

Your commentary here: The misclassifications were more false negatives than false positives.

```
# your code here
library(caret)
```

```
## Loading required package: lattice
```

```
## Loading required package: ggplot2
```

```
pred <- predict(glm1, newdata=test, type = "response")
pr <- ifelse(pred > .5, "malignant", "benign")
pr1 <- ifelse(pred > .5, 2, 1) #if use string for acc doesn't work
acc1 <- mean(pr1==as.integer(test$Class))
print(paste("glm1 accuracy = ", acc1))
```

```
## [1] "glm1 accuracy = 0.885714285714286"
```

```
confusionMatrix(as.factor(pr), test$Class, positive="malignant")
```

```
## Confusion Matrix and Statistics
##
##              Reference
## Prediction  benign malignant
##   benign      79         2
##   malignant   14        45
##
##              Accuracy : 0.8857
##              95% CI : (0.821, 0.9332)
##   No Information Rate : 0.6643
```

```
##      P-Value [Acc > NIR] : 1.386e-09
##
##              Kappa : 0.759
##
## Mcnemar's Test P-Value : 0.00596
##
##      Sensitivity : 0.9574
##      Specificity : 0.8495
##      Pos Pred Value : 0.7627
##      Neg Pred Value : 0.9753
##      Prevalence : 0.3357
##      Detection Rate : 0.3214
##      Detection Prevalence : 0.4214
##      Balanced Accuracy : 0.9035
##
##      'Positive' Class : malignant
##
```

```
#table(pr, test$Class)
```

Step 9: Model coefficients

- The coefficients from the model are in units of logits. Extract and output the coefficient of Cell.small with glm1\$coefficients[]
- Find the estimated probability of malignancy if Cell.small is true using exp(). See the example on p. 107 of the pdf.
- Find the probability of malignancy if Cell.small is true over the whole BreastCancer data set and compare results. Are they close? Why or why not?

Your commentary here: The probability of malignancy was 1.6597510373444 from step 5. It is sort of close to the predicted possibility but a bit lower. However in the 2nd model where I used Cell.regular and Cell.small as predictors the estimated was much closer.

```
# your code here
glm1$coefficients[3]
```

```
## Cell.small1
##      -4.682999
```

```
glmTest <- glm(Class~Cell.regular+Cell.small, data = df, family = "binomial")
glmTest$coefficients[3]
```

```
## Cell.small1
##      -4.040546
```

```
estProb <- exp(glm1$coefficients[3])/(1+exp(glm1$coefficients[3]))
#first probability based off of Cell.shape and Cell.size, 2nd one based off of Cell.regular and Cell.sma
print(paste("The estimated probablity for malignancy based of regular cells is ",estProb * 100,"% (using C
```

```
## [1] "The estimated probablity for malignancy based of regular cells is  0.916643037925551 % (using C
```

```
estProb2 <- exp(glmTest$coefficients[3])/(1+exp(glmTest$coefficients[3]))
print(paste("The estimated probability for malignancy based of regular cells is ",estProb2 * 100,"% (using Ce
```

```
## [1] "The estimated probability for malignancy based of regular cells is 1.72838857161458 % (using Ce
```

Step 10: More logistic regression models

- Build two more models, glm_small using only Cell.small, and glm_regular using Cell.regular as the predictor
- Use anova(glm_small, glm_regular, glm1) to compare all 3 models, using whatever names you used for your models. Analyze the results of the anova().
- Also, compare the 3 AIC scores of the models. Feel free to use the internet to help you interpret AIC scores.

Your commentary here: The comparison shows that the 3rd model has the lowest residual deviation. Its AIC was also the lowest showing that it was the best model.

```
# your code here
glm_small <- glm(Class== "malignant"~Cell.small,data = train, family="binomial")
glm_regular <- glm(Class=="malignant"~Cell.regular, data = train, family="binomial")
anova(glm_small, glm_regular, glm1)
```

```
## Analysis of Deviance Table
##
## Model 1: Class == "malignant" ~ Cell.small
## Model 2: Class == "malignant" ~ Cell.regular
## Model 3: Class == "malignant" ~ Cell.regular + Cell.small
##   Resid. Df Resid. Dev Df Deviance
## 1         557      300.75
## 2         557      370.02  0  -69.268
## 3         556      255.73  1  114.288
```

```
summary(glm_small)
```

```
##
## Call:
## glm(formula = Class == "malignant" ~ Cell.small, family = "binomial",
##      data = train)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
## -1.6942  -0.1143  -0.1143   0.7375   3.1729
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)    1.1632     0.1479   7.864 3.71e-15 ***
## Cell.small1    -6.1903     0.7246  -8.544 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## (Dispersion parameter for binomial family taken to be 1)
##
## Null deviance: 721.78 on 558 degrees of freedom
## Residual deviance: 300.75 on 557 degrees of freedom
## AIC: 304.75
##
## Number of Fisher Scoring iterations: 7
```

```
summary(glm_regular)
```

```
##
## Call:
## glm(formula = Class == "malignant" ~ Cell.regular, family = "binomial",
## data = train)
##
## Deviance Residuals:
## Min 1Q Median 3Q Max
## -1.5266 -0.1197 -0.1197 0.8645 3.1438
##
## Coefficients:
## Estimate Std. Error z value Pr(>|z|)
## (Intercept) 0.7916 0.1292 6.125 9.07e-10 ***
## Cell.regular1 -5.7261 0.7212 -7.939 2.04e-15 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
## Null deviance: 721.78 on 558 degrees of freedom
## Residual deviance: 370.02 on 557 degrees of freedom
## AIC: 374.02
##
## Number of Fisher Scoring iterations: 7
```

```
summary(glm1)
```

```
##
## Call:
## glm(formula = Class == "malignant" ~ Cell.regular + Cell.small,
## family = "binomial", data = train)
##
## Deviance Residuals:
## Min 1Q Median 3Q Max
## -1.8314 -0.0445 -0.0445 0.6433 3.7198
##
## Coefficients:
## Estimate Std. Error z value Pr(>|z|)
## (Intercept) 1.4701 0.1672 8.791 < 2e-16 ***
## Cell.regular1 -3.7044 0.7603 -4.873 1.10e-06 ***
## Cell.small1 -4.6830 0.7411 -6.319 2.64e-10 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## (Dispersion parameter for binomial family taken to be 1)
##
##      Null deviance: 721.78  on 558  degrees of freedom
## Residual deviance: 255.73  on 556  degrees of freedom
## AIC: 261.73
##
## Number of Fisher Scoring iterations: 8
```

Step 11: A Naive Bayes model

- Build a Naive Bayes Model Class ~ Cell.small + Cell.regular on the training data using library e1071
- Output the model parameters
- Answer the following questions:
 - a. What percentage of the training data is benign?
 - b. What is the likelihood that a malignant sample is not small?
 - c. What is the likelihood that a malignant sample is not regular?

Your commentary here: a. 65.29517% is benign b. 98.969072% c. 98.969072%

```
# your code here
library(e1071)
nb1 <- naiveBayes(Class~Cell.small+Cell.regular, data = train)
nb1
```

```
##
## Naive Bayes Classifier for Discrete Predictors
##
## Call:
## naiveBayes.default(x = X, y = Y, laplace = laplace)
##
## A-priori probabilities:
## Y
##      benign malignant
## 0.6529517 0.3470483
##
## Conditional probabilities:
##      Cell.small
## Y      0      1
## benign 0.16438356 0.83561644
## malignant 0.98969072 0.01030928
##
##      Cell.regular
## Y      0      1
## benign 0.23835616 0.76164384
## malignant 0.98969072 0.01030928
```

Step 12: Evaluate the model

- Predict on the test data with Naive Bayes model
- Output the confusion matrix
- Are the results the same or different? Why do you think that is the case?

Your commentary here: The confusion matrix is the same. Its the same because they are both classifying and since the data is well balanced

```
# your code here
predNB <- predict(nb1, newdata=test)
#head(predNB, n=2)
library(caret)
confusionMatrix(predNB, test$Class, positive="malignant")
```

```
## Confusion Matrix and Statistics
##
##              Reference
## Prediction  benign malignant
##   benign      79          2
##   malignant   14         45
##
##              Accuracy : 0.8857
##              95% CI : (0.821, 0.9332)
##   No Information Rate : 0.6643
##   P-Value [Acc > NIR] : 1.386e-09
##
##              Kappa : 0.759
##
##  Mcnemar's Test P-Value : 0.00596
##
##              Sensitivity : 0.9574
##              Specificity : 0.8495
##              Pos Pred Value : 0.7627
##              Neg Pred Value : 0.9753
##              Prevalence : 0.3357
##              Detection Rate : 0.3214
##   Detection Prevalence : 0.4214
##   Balanced Accuracy : 0.9035
##
##   'Positive' Class : malignant
##
```