# Exercise 2

Collin Real

### Import Libraries/Data

```
library(mlbench)
library(dplyr)
library(e1071)
library(kernlab)
library(AppliedPredictiveModeling)
library(caret)
library(ggplot2)
library(tidyverse)
library(corrplot)
data(Glass)
```

### Data Structure

```
str(Glass)
```

```
'data.frame':   214 obs. of  10 variables:
 $ RI  : num  1.52 1.52 1.52 1.52 1.52 ...
 $ Na  : num  13.6 13.9 13.5 13.2 13.3 ...
 $ Mg  : num  4.49 3.6 3.55 3.69 3.62 3.61 3.6 3.61 3.58 3.6 ...
 $ Al  : num  1.1 1.36 1.54 1.29 1.24 1.62 1.14 1.05 1.37 1.36 ...
 $ Si  : num  71.8 72.7 73 72.6 73.1 ...
 $ K   : num  0.06 0.48 0.39 0.57 0.55 0.64 0.58 0.57 0.56 0.57 ...
 $ Ca  : num  8.75 7.83 7.78 8.22 8.07 8.07 8.17 8.24 8.3 8.4 ...
 $ Ba  : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Fe  : num  0 0 0 0 0 0.26 0 0 0 0.11 ...
 $ Type: Factor w/ 6 levels "1","2","3","5",..: 1 1 1 1 1 1 1 1 1 1 ...
```

### Descriptive Statistics

```r
summary(Glass)
```

```
       RI               Na              Mg              Al       
 Min.   :1.511   Min.   :10.73   Min.   :0.000   Min.   :0.290  
 1st Qu.:1.517   1st Qu.:12.91   1st Qu.:2.115   1st Qu.:1.190  
 Median :1.518   Median :13.30   Median :3.480   Median :1.360  
 Mean   :1.518   Mean   :13.41   Mean   :2.685   Mean   :1.445  
 3rd Qu.:1.519   3rd Qu.:13.82   3rd Qu.:3.600   3rd Qu.:1.630  
 Max.   :1.534   Max.   :17.38   Max.   :4.490   Max.   :3.500  
       Si              K                Ca               Ba       
 Min.   :69.81   Min.   :0.0000   Min.   : 5.430   Min.   :0.000  
 1st Qu.:72.28   1st Qu.:0.1225   1st Qu.: 8.240   1st Qu.:0.000  
 Median :72.79   Median :0.5550   Median : 8.600   Median :0.000  
 Mean   :72.65   Mean   :0.4971   Mean   : 8.957   Mean   :0.175  
 3rd Qu.:73.09   3rd Qu.:0.6100   3rd Qu.: 9.172   3rd Qu.:0.000  
 Max.   :75.41   Max.   :6.2100   Max.   :16.190   Max.   :3.150  
       Fe            Type  
 Min.   :0.00000   1:70  
 1st Qu.:0.00000   2:76  
 Median :0.00000   3:17  
 Mean   :0.05701   5:13  
 3rd Qu.:0.10000   6: 9  
 Max.   :0.51000   7:29  
```

### Variable Skewness - Calculated

```
# Skewness between -1 amd 1 is excellent, between -2 and 2 is acceptable, values beyond -2
RI_ = Glass$RI
Na_ = Glass$Na
Mg_ = Glass$Mg
Al_ = Glass$Al
Si_ = Glass$Si
K_ = Glass$K
Ca_ = Glass$Ca
Ba_ = Glass$Ba
Fe_ = Glass$Fe

paste0('RI: ', skewness(RI_))
```

```
[1] "RI: 1.60271508274373"
```

```
paste0('Na: ', skewness(Na_))
```

```
[1] "Na: 0.447834258917133"
```

```
paste0('Mg: ', skewness(Mg_))
```

```
[1] "Mg: -1.13645227846653"
```

```
paste0('Al: ', skewness(Al_))
```

```
[1] "Al: 0.89461041611312"
```

```
paste0('Si: ', skewness(Si_))
```

```
[1] "Si: -0.720239210805621"
```

```
paste0('K: ', skewness(K_))
```

```
[1] "K: 6.46008889572281"
```

```r
paste0('Ca: ', skewness(Ca_))
```

```
[1] "Ca: 2.01844629445302"
```

```r
paste0('Ba: ', skewness(Ba_))
```

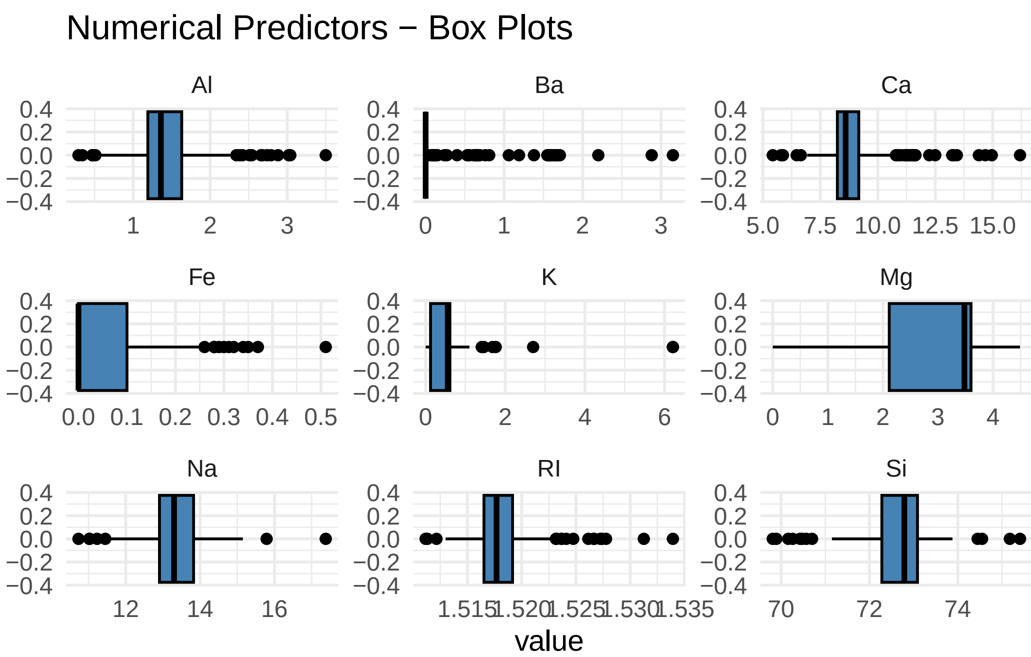
```
[1] "Ba: 3.36867996880571"
```

```r
paste0('Fe: ', skewness(Fe_))
```

```
[1] "Fe: 1.7298107095598"
```

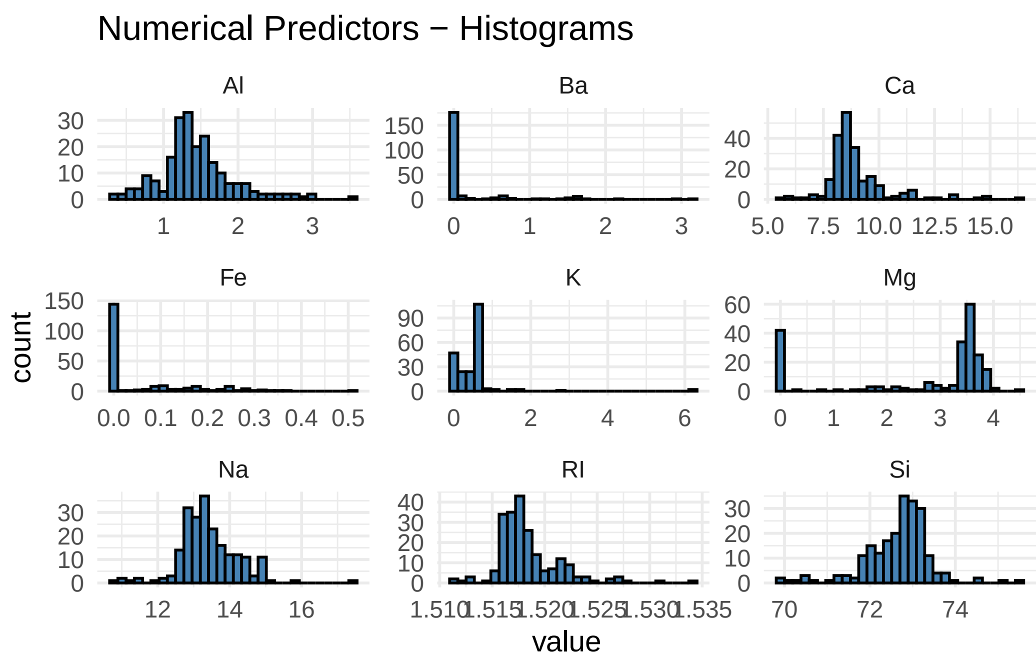
### Box Plots

```
Glass %>%
  select_if(is.numeric) %>%
  gather() %>%
  ggplot(aes(value)) +
  geom_boxplot(color='black', fill='steelblue') +
  facet_wrap(~key, scales = 'free') +
  ggtitle(("Numerical Predictors - Box Plots")) +
  theme_minimal()
```



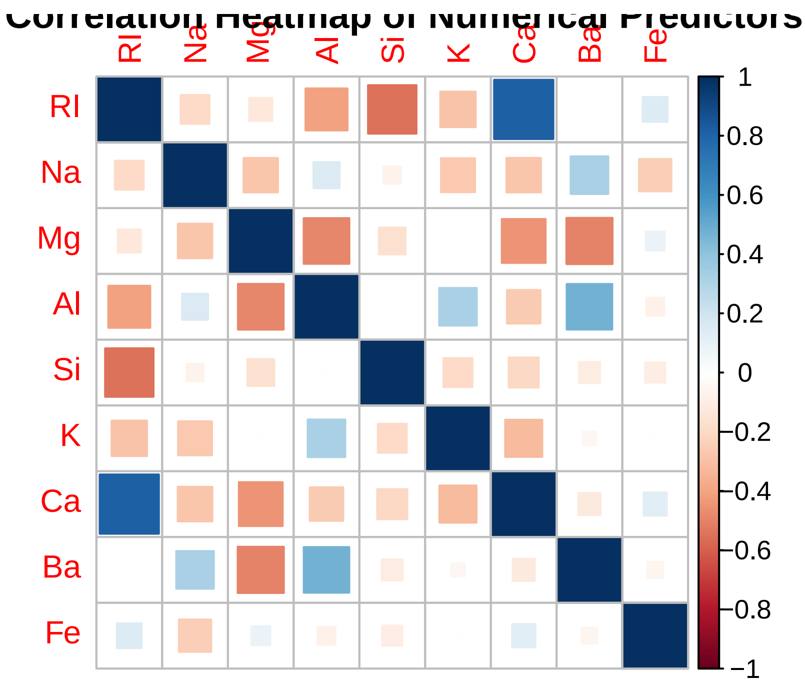
### Histogram Plots

```
Glass %>%
  select_if(is.numeric) %>%
  gather() %>%
  ggplot(aes(value)) +
  geom_histogram(color='black', fill='steelblue') +
  facet_wrap(~key, scales = 'free') +
  ggtitle(("Numerical Predictors - Histograms")) +
  theme_minimal()
```



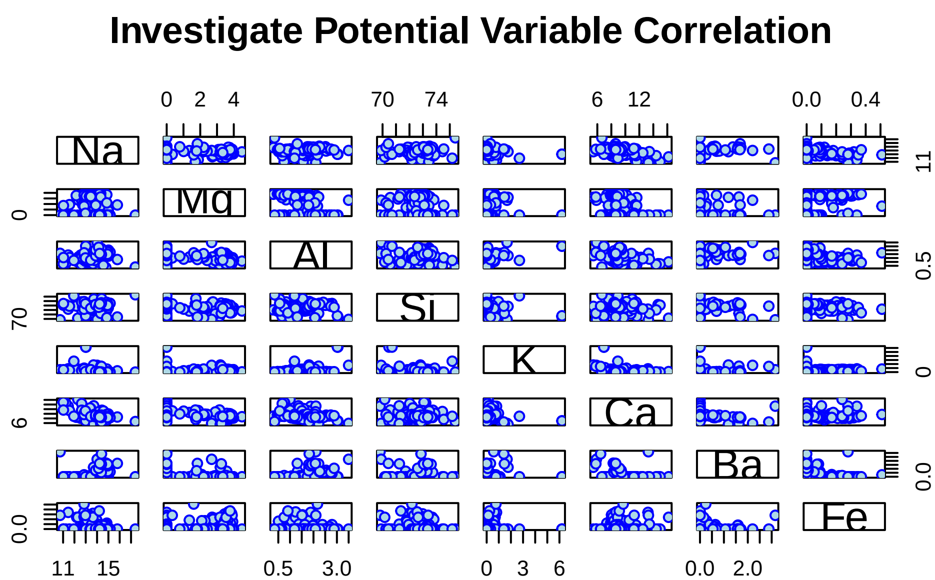
**Heatmap Correlation**

```
Glass %>%
  select_if(is.numeric) %>%
  cor() %>%
  corrplot(method = "square", title = 'Correlation Heatmap of Numerical Predictors')
```



#### Scatterplot Correlation

```
plot(~Na+Mg+Al+Si+K+Ca+Ba+Fe,
     data=Glass,
     main="Investigate Potential Variable Correlation",
     col='blue',
     bg='lightblue',
     pch = 21)
```




#### Question A) & B)

To explore the predictor variables, I created boxplots, histograms, scatterplots, and a heatmap to understand the distributions and relationships among the predictor variables to gain a better understanding. There are outliers in our dataset for variables Ca, Fe, K, and Na. Variables Ba, Ca, Fe, and K are skewed to the right, indicating that we might improve our classification model by applying a transformation.

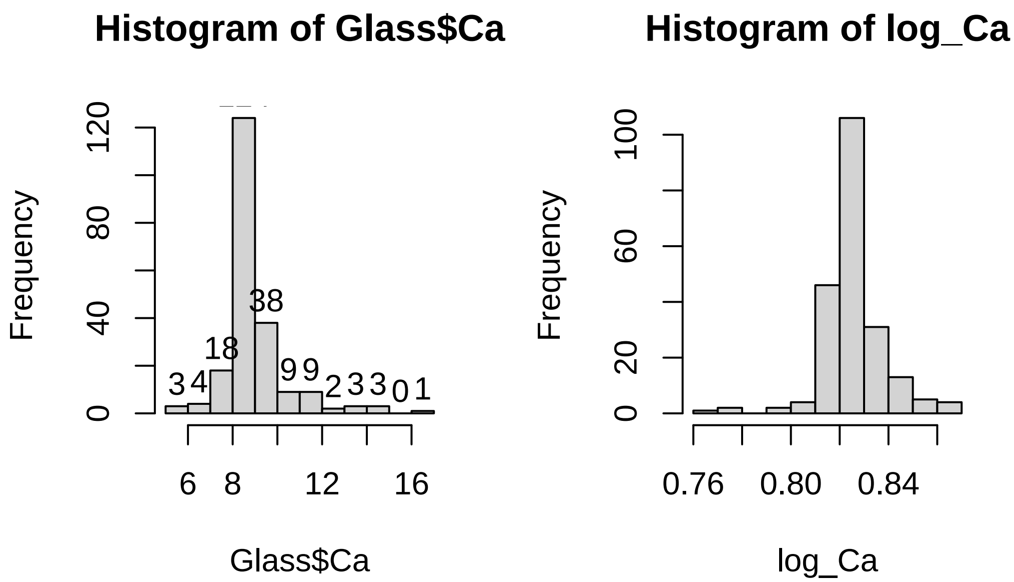
### Question C)

Since we identified skewness in variables Ba, Ca, Fe, and K, we applied a BoxCox transformation to each variable. After reviewing the distribution plots of our transformed variables, we concluded that the transformation was only slightly effective for the Ca variable. See the below outputs comparing the histogram plots between the original and transformed data for each variable.

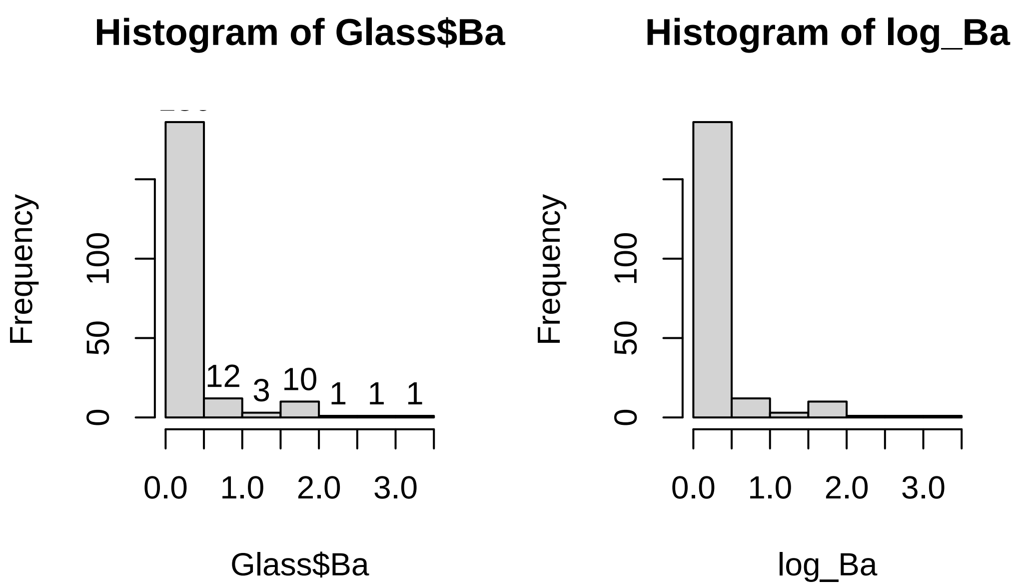
#### Make transformations on 3 skewed variables: K, Ca, and Ba

```
transform_Ca <- BoxCoxTrans(Glass$Ca)
log_Ca <- predict(transform_Ca, Glass$Ca)
#hist(log_Ca)
#log_Ca

transform_Ba <- BoxCoxTrans(Glass$Ba)
log_Ba <- predict(transform_Ba, Glass$Ba)
#hist(log_Ba)
#log_Ba

transform_Fe <- BoxCoxTrans(Glass$Fe)
log_Fe <- predict(transform_Fe, Glass$Fe)
#hist(log_Fe)
#log_Fe

transform_K <- BoxCoxTrans(Glass$K)
log_K <- predict(transform_K, Glass$K)
#hist(log_K)
#log_K
```

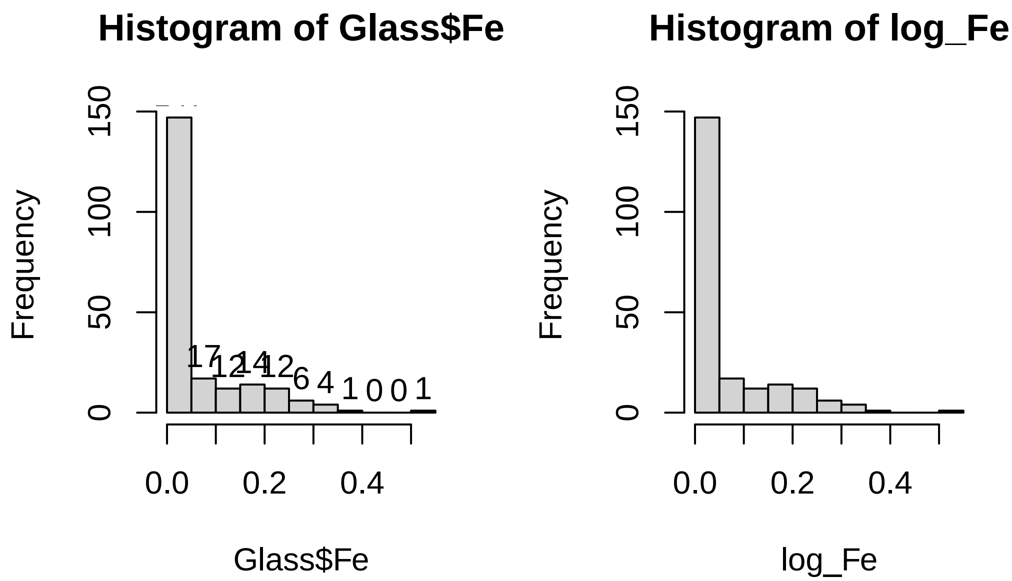
```
par(mfrow = c(1, 2))
ca = hist(Glass$Ca)
text(ca$mids,ca$counts,labels=ca$counts, adj=c(0.5, -0.5))
hist(log_Ca)
```



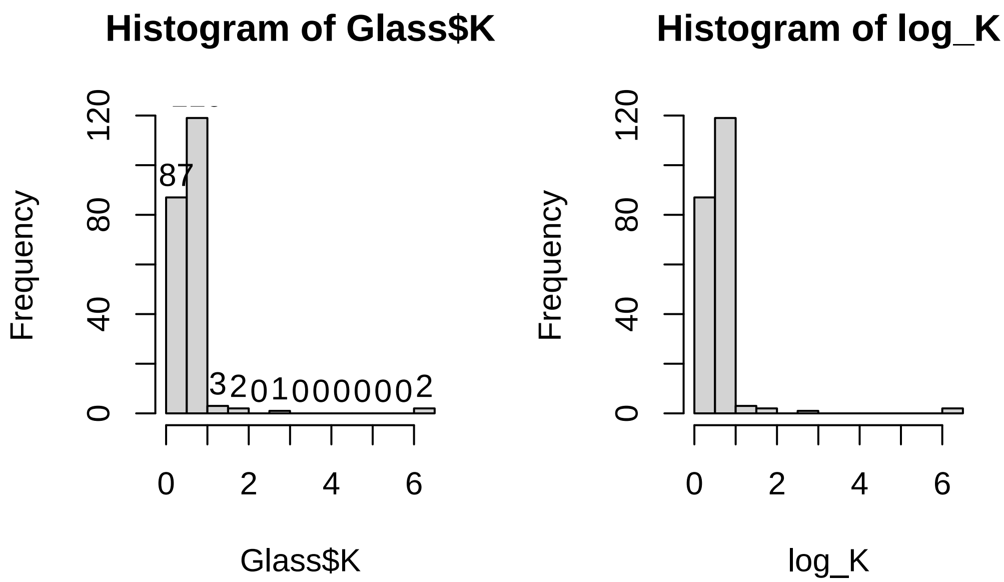

```r
par(mfrow = c(1, 2))
ba = hist(Glass$Ba)
text(ba$mids,ba$counts,labels=ba$counts, adj=c(0.5, -0.5))
hist(log_Ba)
```



```r
par(mfrow = c(1, 2))
fe = hist(Glass$Fe)
text(fe$mids,fe$counts,labels=fe$counts, adj=c(0.5, -0.5))
hist(log_Fe)
```




```r
par(mfrow = c(1, 2))
k = hist(Glass$K)
text(k$mids,k$counts,labels=k$counts, adj=c(0.5, -0.5))
hist(log_K)
```


Histogram of Glass$K
Frequency
0
40
80
120
87
3
2
0
1
0
0
0
0
0
0
2
0
2
4
6
Glass$K
Histogram of log_K
Frequency
0
40
80
120
0
2
4
6
log_K

**Question 4)**

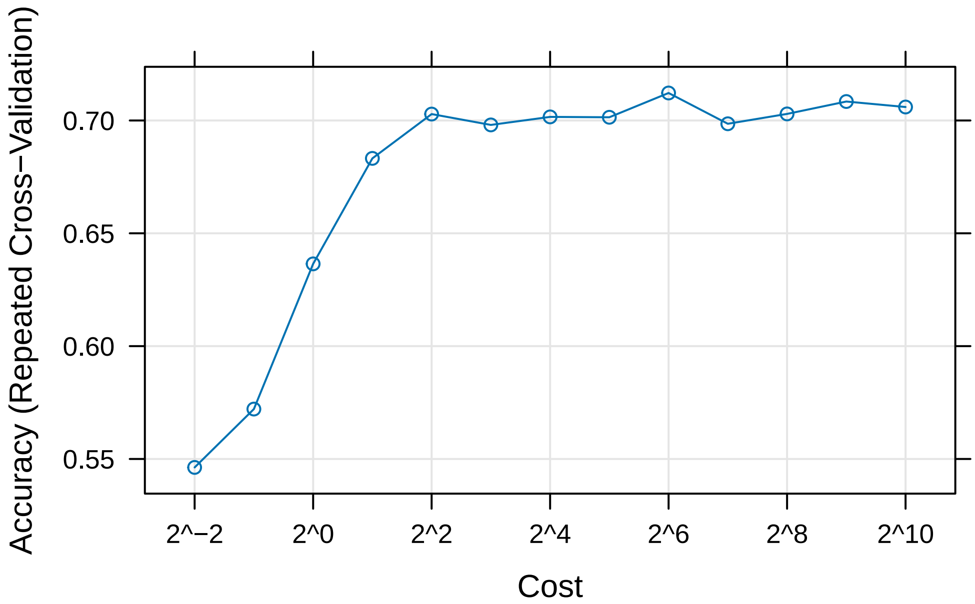
```r
set.seed(231)
sigDist <- sigest(Type~ ., data = Glass, frac = 1)
sigDist
```

```
       90%        50%        10% 
0.03407935 0.11297847 0.62767315 
```

```r
svmTuneGrid <- data.frame(sigma = as.vector(sigDist)[1], C = 2^(-2:10))
svmTuneGrid
```

```
        sigma       C
1  0.03407935    0.25
2  0.03407935    0.50
3  0.03407935    1.00
4  0.03407935    2.00
5  0.03407935    4.00
6  0.03407935    8.00
7  0.03407935   16.00
8  0.03407935   32.00
9  0.03407935   64.00
10 0.03407935  128.00
11 0.03407935  256.00
12 0.03407935  512.00
13 0.03407935 1024.00
```

```r
set.seed(1056)
#It may take a while to run
svmFit <- train(Type~ ., data = Glass, method = "svmRadial",
preProc = c("center", "scale"),tuneGrid = svmTuneGrid,
trControl = trainControl(method = "repeatedcv", repeats = 5))

plot(svmFit, scales = list(x = list(log = 2)))
```


Accuracy (Repeated Cross−Validation)
0.70
0.65
0.60
0.55
2^−2
2^0
2^2
2^4
2^6
2^8
2^10
Cost