NUEN 647
Uncertainty Quantification for Nuclear Engineering
Homework 3

Due on Saturday, December 10, 2016

Dr. McClarren

Paul Mendoza

Contents

Problem 1

Fit the data in Table 1 to a linear model using

(a) Least squares

(b) Ridge Regression

(c) Lasso Regression

Table 1: Data to fit linear model $y = a + bx_1 + cx_2$

	x_1	x_2	y
1	0.99	0.98	6.42
2	-0.75	-0.76	0.20
3	-0.50	-0.48	0.80
4	-1.08	-1.08	-0.57
5	0.09	0.09	4.75
6	-1.28	-1.27	-1.42
7	-0.79	-0.79	1.07
8	-1.17	-1.17	0.20
9	-0.57	-0.57	1.08
10	-1.62	-1.62	-0.15
11	0.34	0.35	2.90
12	0.51	0.51	3.37
13	-0.91	-0.92	0.05
14	1.85	1.86	5.50
15	-1.12	-1.12	0.17
16	-0.70	-0.70	1.72
17	1.19	1.18	3.97
18	1.24	1.23	6.38
19	-0.52	-0.52	3.29
20	-1.41	-1.41	-1.49

Be sure to do cross-validation for each fit, and for each method present your best estimate of the model.

Did this problem in R, and appended the PDF on the following pages.

Problem1

Paul Mendoza

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```r
require(magrittr)
require(dplyr)
require(ggplot2)
require(glmnet)
```

Fit the data in Table 1 to a linear model using:

```r
Table1
```

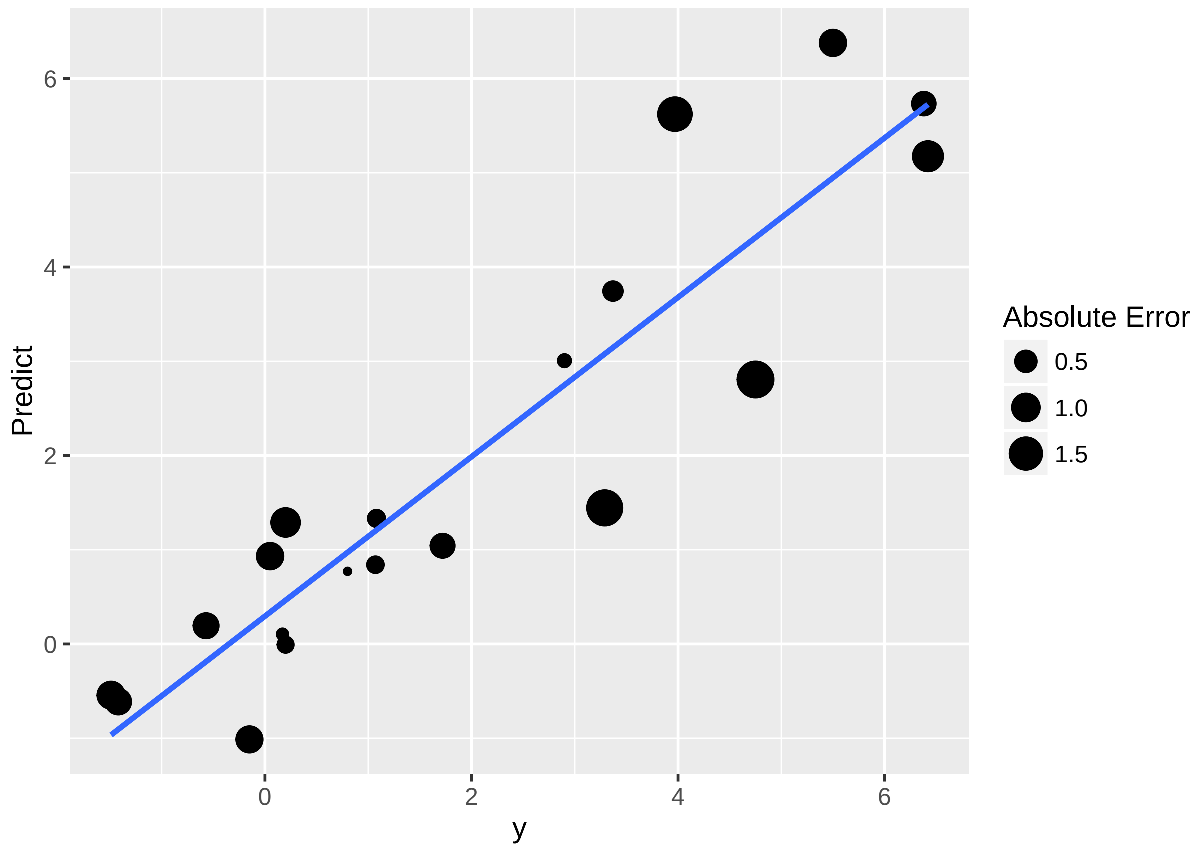
```
##       x1    x2     y
## 1   0.99  0.98  6.42
## 2  -0.75 -0.76  0.20
## 3  -0.50 -0.48  0.80
## 4  -1.08 -1.08 -0.57
## 5   0.09  0.09  4.75
## 6  -1.28 -1.27 -1.42
## 7  -0.79 -0.79  1.07
## 8  -1.17 -1.17  0.20
## 9  -0.57 -0.57  1.08
## 10 -1.62 -1.62 -0.15
## 11  0.34  0.35  2.90
## 12  0.51  0.51  3.37
## 13 -0.91 -0.92  0.05
## 14  1.85  1.86  5.50
## 15 -1.12 -1.12  0.17
## 16 -0.70 -0.70  1.72
## 17  1.19  1.18  3.97
## 18  1.24  1.23  6.38
## 19 -0.52 -0.52  3.29
## 20 -1.41 -1.41 -1.49
```

1. Least Squares

```r
LeastFit<-lm(formula = y~x1+x2,data=Table1)
LeastFit
```

```
##
## Call:
## lm(formula = y ~ x1 + x2, data = Table1)
##
## Coefficients:
## (Intercept)           x1           x2
##       2.606       38.133      -35.900
```

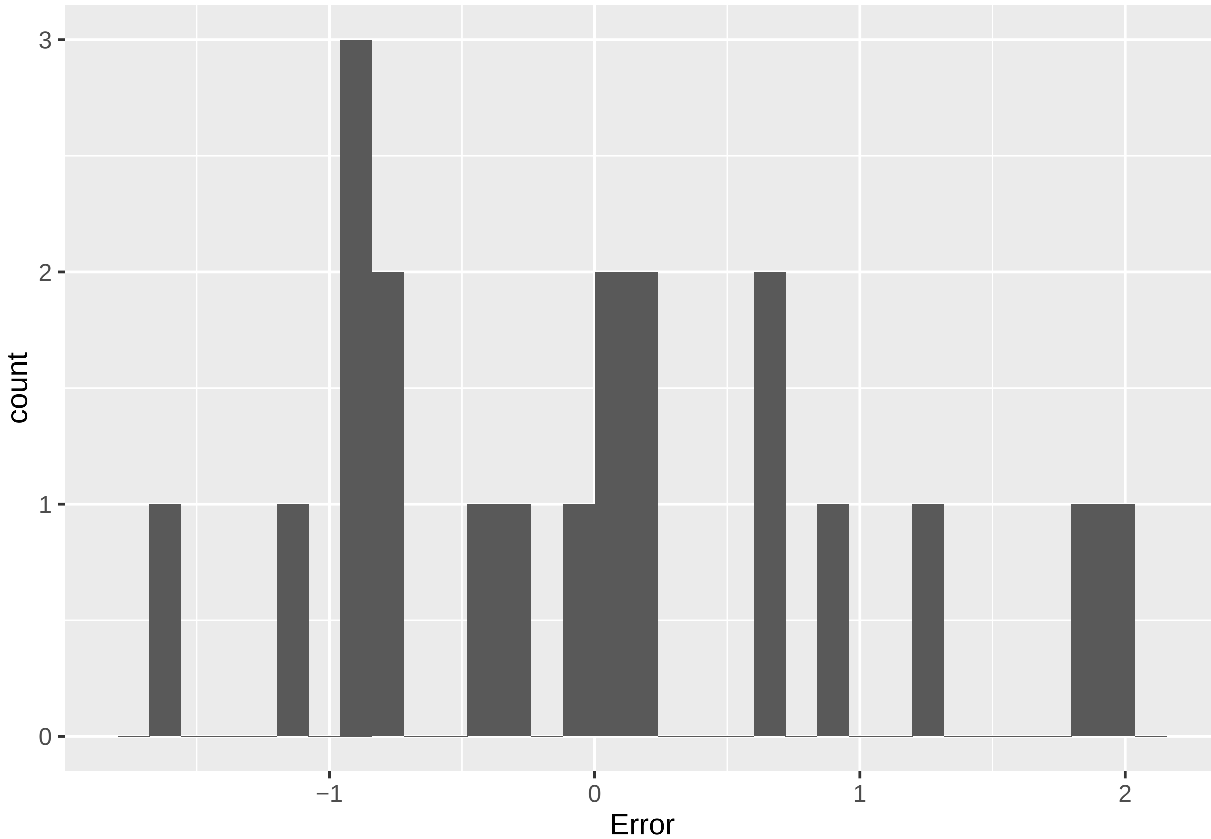
```r
plotDF<-Table1
plotDF[,'Type']<-'Train'
plotDF$Predict<-predict(LeastFit,plotDF[,1:2])
plotDF$Error<-plotDF$y-plotDF$Predict
ggplot(plotDF,aes(x=y,y=Predict,size=abs(Error)))+geom_point()+
  scale_size("Absolute Error")+geom_smooth(method="lm",se=F,size=1)
```




```r
sqrt(var(data.frame(plotDF %>% filter(Type=="Train") %>% select(Error))))/20
```

```
##             Error
## Error 0.04902635
```

```r
ggplot(plotDF,aes(x=Error)) + geom_histogram()
```

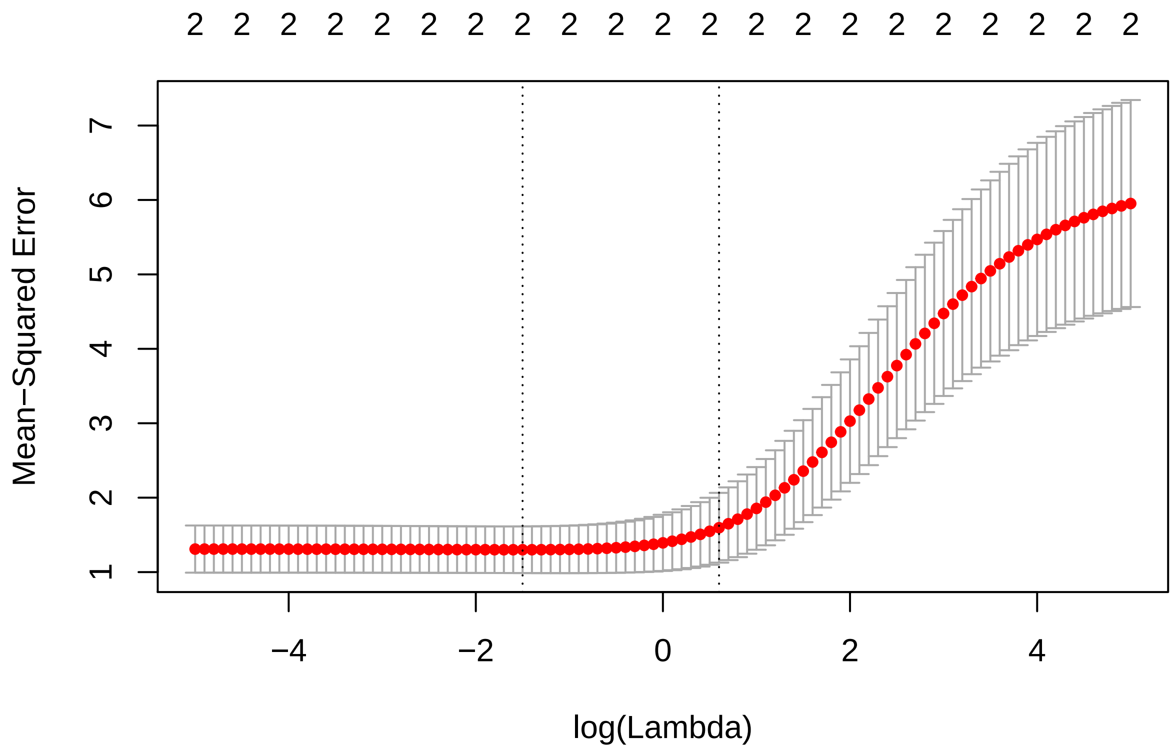



```
sensitivities <- coef(LeastFit)
sensDF <- data.frame(Method = 0, Var = 0, Value=0)
sensDF[1:length(sensitivities),'Method'] <- "Least-Squares"
sensDF[1:length(sensitivities),'Var'] <- names(sensitivities)
sensDF[1:length(sensitivities),'Value'] <- (sensitivities)
rowStart <- length(sensitivities)+1
```

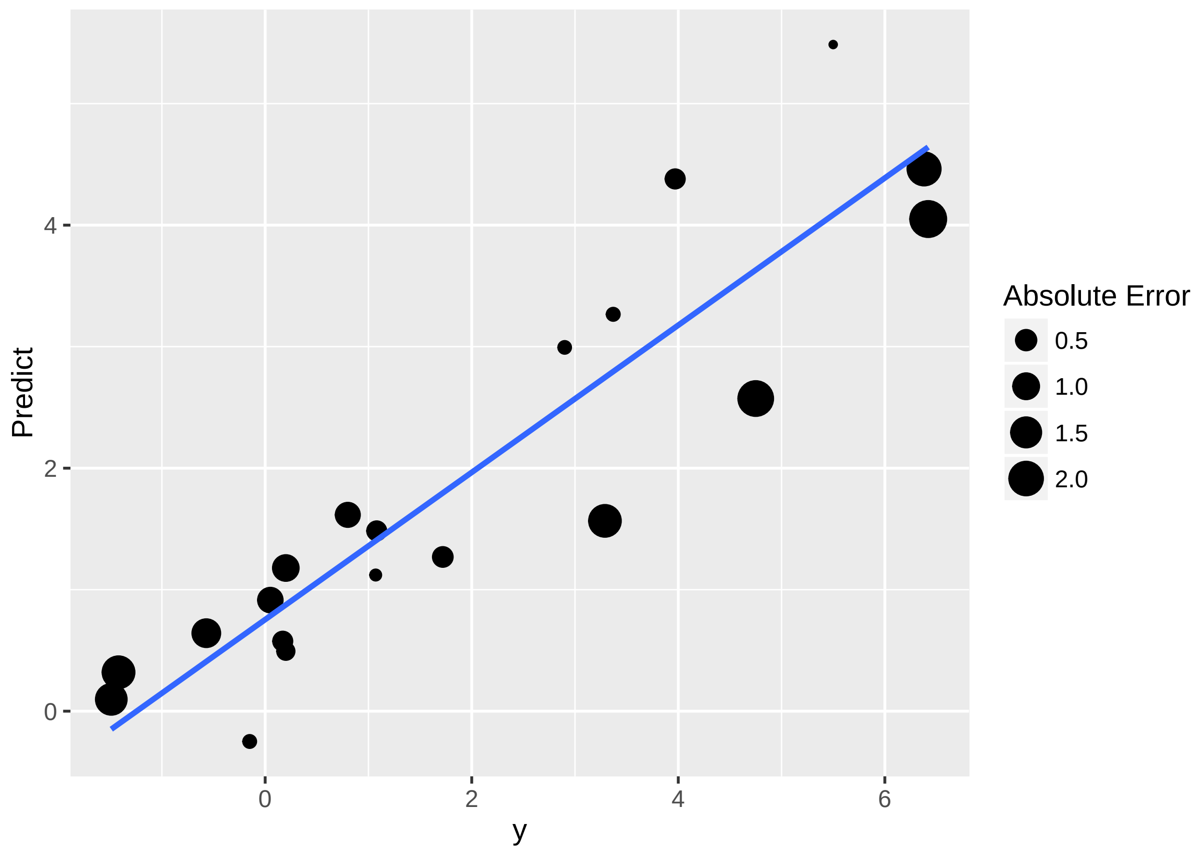
2. Ridge Regression

Ridge regression sets alpha=0, which adds damping to the coefficients

```
crossValid <- cv.glmnet(as.matrix(Table1[,1:2]),
                        as.matrix(Table1$y),alpha = 0,
                        lambda=exp(seq(-5,5,by=0.1)))

plot(crossValid)
```



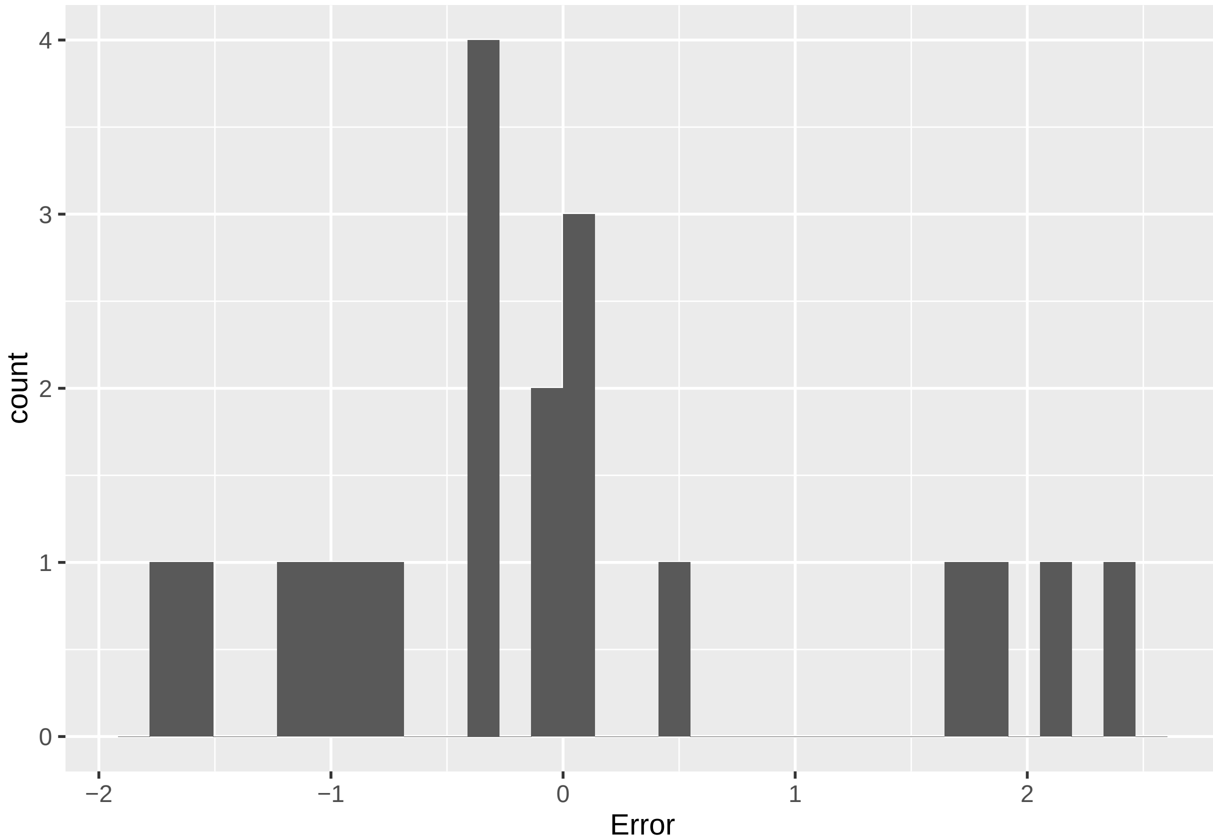

```
lambda <- crossValid$lambda.min
sensitivities <- coef(crossValid)
plotDF <- Table1
plotDF[,'Type'] <- 'Train'
plotDF[,"Predict" ]<- data.frame(Predict=predict(crossValid,as.matrix(plotDF[,1:2]),
                                              lambda=lambda))
plotDF$Error <- plotDF$y-plotDF$Predict
ggplot(plotDF,aes(x=y,y=Predict,size=abs(Error))) + geom_point() +
scale_size("Absolute Error") + geom_smooth(method="lm",se=F,size=1)
```




```r
sqrt(var(data.frame(plotDF %>% filter(Type=="Train") %>% select(Error))))/20
```

```
##             Error
## Error 0.05982956
```

```r
ggplot(plotDF,aes(x=Error)) + geom_histogram()
```

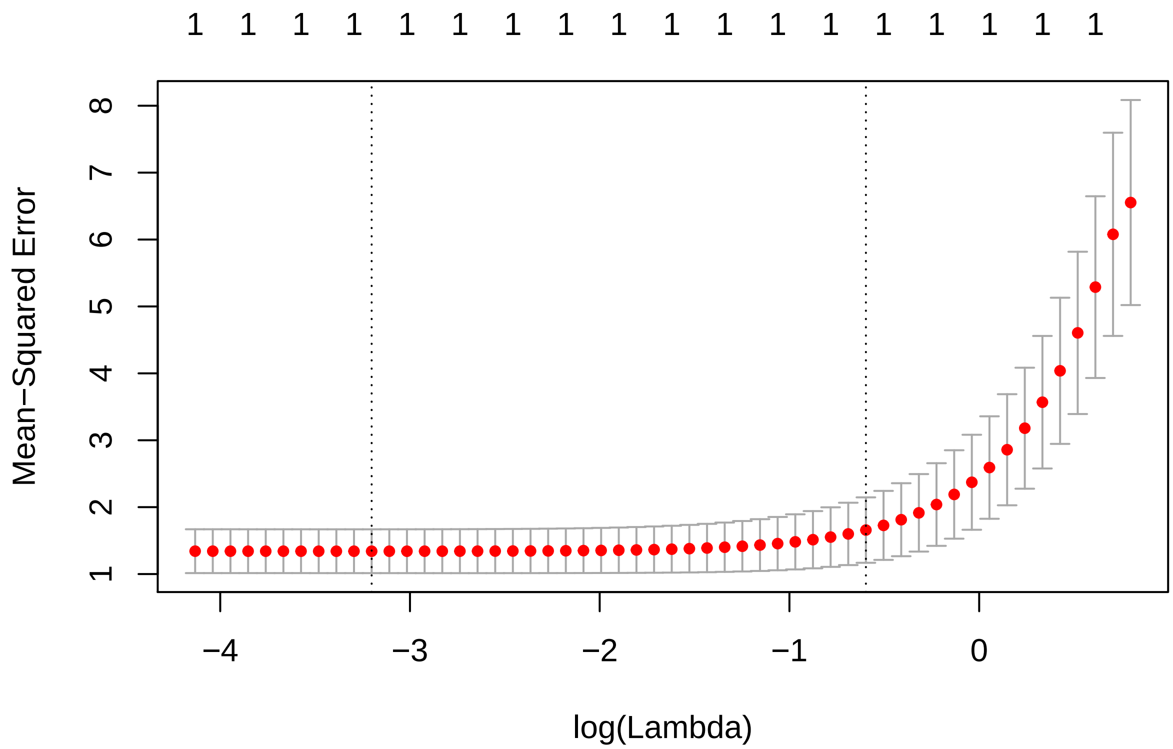



```
sensDF[rowStart:(rowStart + length(sensitivities)-1),'Method'] <- "Ridge"
sensDF[rowStart:(rowStart+length(sensitivities)-1),'Var']<-t(t(rownames(sensitivities)))
sensDF[rowStart:(rowStart +length(sensitivities)-1),'Value']<-as.numeric(sensitivities)
rowStart <- rowStart + length(sensitivities)
```

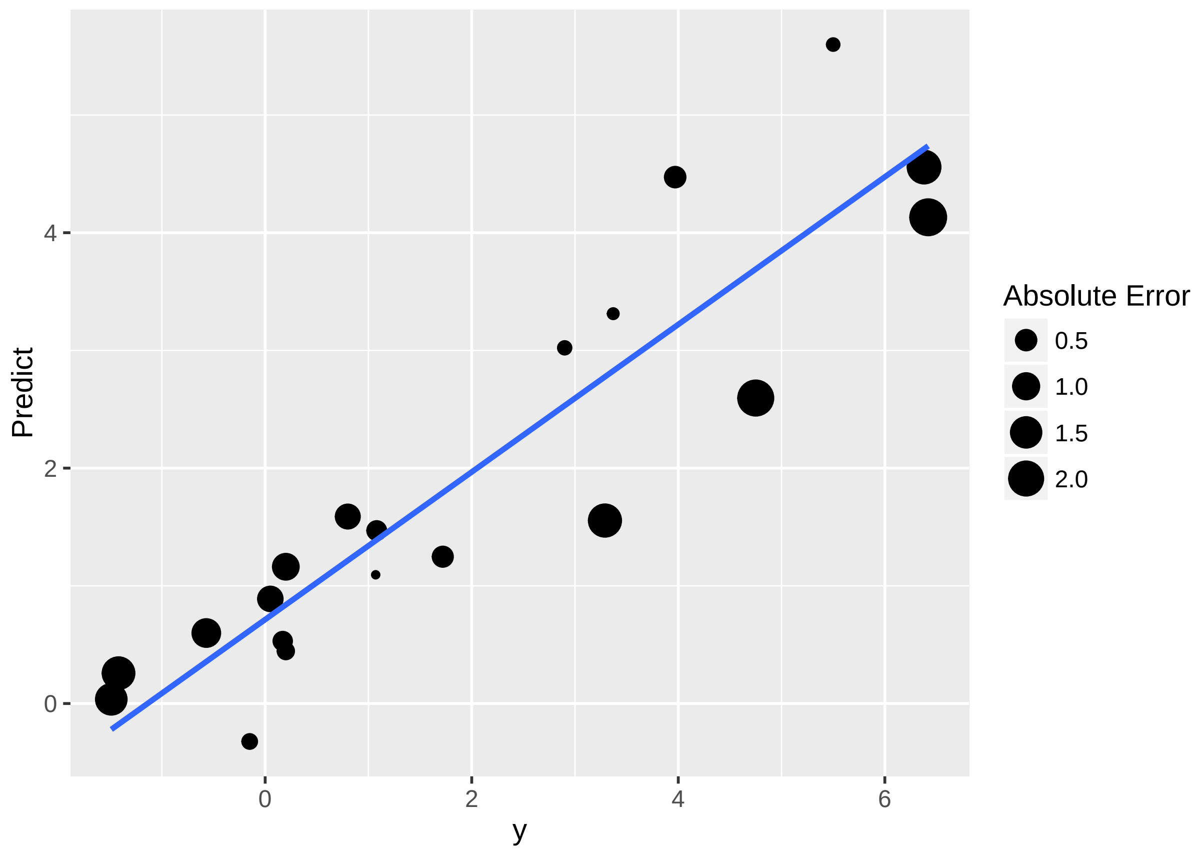
3. Lasso Regression

Lasso regression sets alpha=1

```
crossValid <- cv.glmnet(as.matrix(Table1[,1:2]),as.matrix(Table1$y),alpha = 1)
plot(crossValid)
```



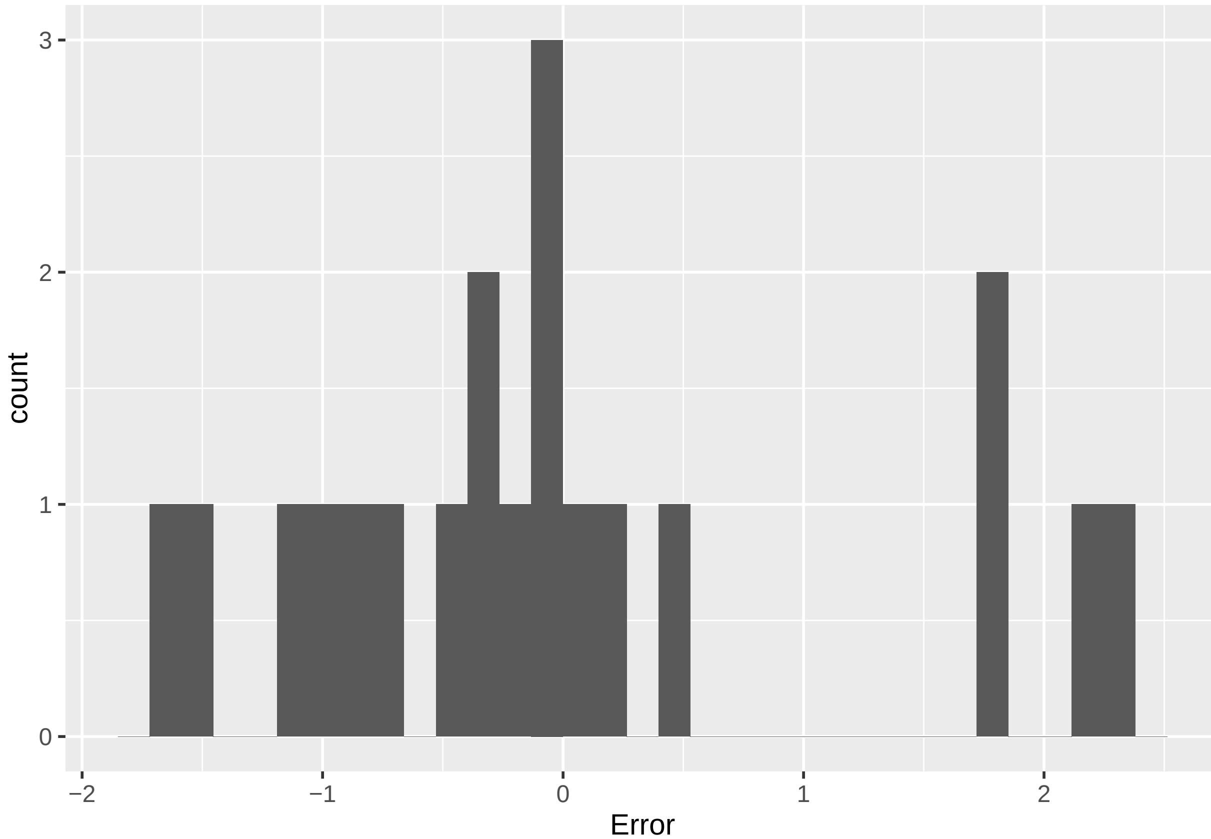

```r
lambda <- crossValid$lambda.min
sensitivities <- coef(crossValid)
plotDF <- Table1
plotDF[,'Type'] <- 'Train'
plotDF[,"Predict" ]<- data.frame(Predict=predict(crossValid,as.matrix(Table1[,1:2]),
                                               lambda=lambda))

plotDF$Error <- plotDF$y-plotDF$Predict
ggplot(plotDF,aes(x=y,y=Predict,size=abs(Error))) + geom_point() +
scale_size("Absolute Error") + geom_smooth(method="lm",se=F,size=1)
```




```r
sqrt(var(data.frame(plotDF %>% filter(Type=="Train") %>% select(Error))))/20
```

```
##              Error
## Error 0.05832321
```

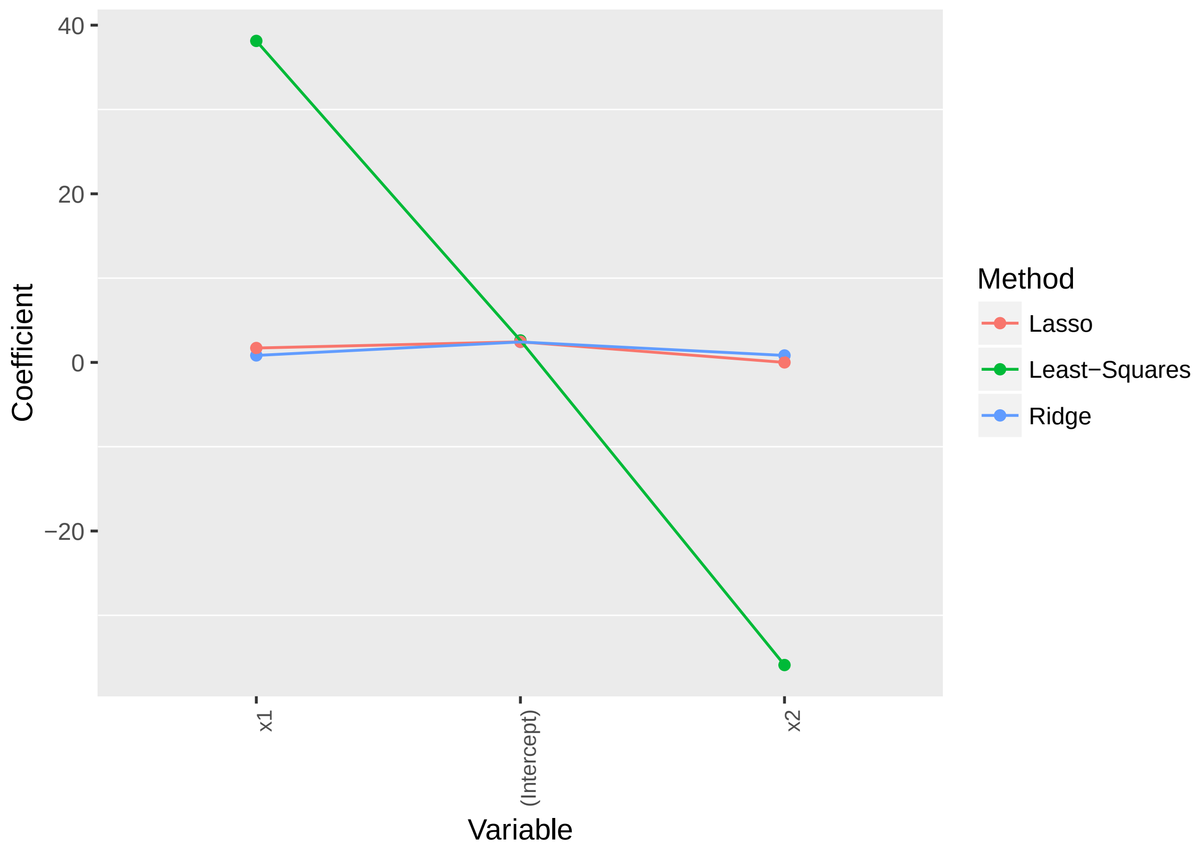
```r
ggplot(plotDF,aes(x=Error)) + geom_histogram()
```




```
sensDF[rowStart:(rowStart + length(sensitivities)-1),'Method'] <- "Lasso"
sensDF[rowStart:(rowStart+length(sensitivities)-1),'Var']<-t(t(rownames(sensitivities)))
sensDF[rowStart:(rowStart +length(sensitivities)-1),'Value']<-as.numeric(sensitivities)
rowStart <- rowStart + length(sensitivities)
```

Compare Methods

```
ggplot(sensDF,aes(x=reorder(Var,-Value),y=Value,color=Method,group=Method)) +
  geom_point() + geom_line() +
  theme(panel.grid.major = element_blank(),
        axis.text.x = element_text(angle = 90, hjust = 1, size=8))+
  scale_x_discrete("Variable") + scale_y_continuous("Coefficient")
```



The Lasso and Ridge are both more bounded in their coefficents.

Problem 2

Derive the adjoint operator for the equation

$$-\bigtriangledown^2 \phi(x,y,z) + \frac{1}{L^2}\phi(x,y,z) = \frac{Q}{D}$$

$$\phi(0,y,z) = \phi(x,0,z) = \phi(x,y,0) = \phi(X,y,z) = \phi(x,Y,z) = \phi(x,y,Z) = C$$

Compute the sensitivity to the QOI:

$$QoI = \int_0^X dx \int_0^Y dy \int_0^Z dz \frac{D}{L^2}\phi(x,y,z)$$

for X,Y,Z,L,, and Q.

Derive the adjoint operator

Define the operator $\mathcal{L}$ as

$$\mathcal{L} = \bigtriangledown^2 + \frac{1}{L^2}$$

and the adjoint $\mathcal{L}^\dagger$ as

$$\mathcal{L}^\dagger = \bigtriangledown^2 + \frac{1}{L^2}$$

$$\phi^\dagger(0,y,z) = \phi^\dagger(x,0,z) = \phi^\dagger(x,y,0) = \phi^\dagger(X,y,z) = \phi^\dagger(x,Y,z) = \phi^\dagger(x,y,Z) = C$$

Setting:

$$\left|\frac{\delta\phi^\dagger}{\delta x}\right|_{x=0} = \left|\frac{\delta\phi}{\delta x}\right|_{x=0}$$

and

$$\left|\frac{\delta\phi^\dagger}{\delta x}\right|_{x=X} = \left|\frac{\delta\phi}{\delta x}\right|_{x=X}$$

and similar for the other two dimentions. Also define the inner product as:

$$(u,v) = \int_0^X dx \int_0^Y dy \int_0^Z dz\ uv$$

Proof, in order to prove that this is an adjoint operator for the above equation, it needs to be shown that $(\mathcal{L}\phi, \phi^\dagger) = (\phi, \mathcal{L}^\dagger\phi^\dagger)$.

Equivalent to:

$$\int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi^\dagger \bigtriangledown^2 \phi + \phi^\dagger \frac{\phi}{L^2}\right) = \int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi \bigtriangledown^2 \phi^\dagger + \phi\frac{\phi^\dagger}{L^2}\right)$$

The terms

$$\int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi^\dagger \frac{\phi}{L^2}\right) = \int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi\frac{\phi^\dagger}{L^2}\right)$$

are equal. For the other term with, $\bigtriangledown^2$, we can expand to:

$$\int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi^\dagger \left[\frac{\delta^2\phi}{\delta x^2} + \frac{\delta^2\phi}{\delta y^2} + \frac{\delta^2\phi}{\delta z^2}\right]\right)$$

Focusing on the x terms, noting that y and z will have the same derivation. Integration by parts, with $u = \phi^\dagger$, $du = \frac{\delta\phi^\dagger}{\delta x}dx$, and $v = \frac{\delta\phi}{dx}$, $dv = \frac{\delta^2\phi}{\delta x^2}dx$ yields.

$$\int_0^Y dy \int_0^Z dz \left(\int_0^X dx\ \phi^\dagger \frac{\delta^2\phi}{\delta x^2}\right) = \int_0^Y dy \int_0^Z dz \left(\left|\phi^\dagger \frac{\delta\phi}{\delta x}\right|_{x=0}^{x=X} - \int_0^X dx\ \frac{\delta\phi}{\delta\ x}\frac{\delta\phi^\dagger}{\delta x}dx\right)$$

Performing another integration by parts, with $u = \frac{\delta\phi^\dagger}{\delta x}$, $du = \frac{\delta^2\phi^dag}{\delta x}dx$ and, $v = \phi$, $dv = \frac{\delta\phi}{\delta x}dx$.

$$k$$

Problem 3

For the random variable X $\sim$ N(0,1) draw fifty samples and generate histograms using the following sampling techniques

(a) Simple random sampling

(b) Stratifid sampling