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.

Problem 1 continued on next page. . .

Problem1

Paul Mendoza

December 9, 2016

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

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

```
Table1
```

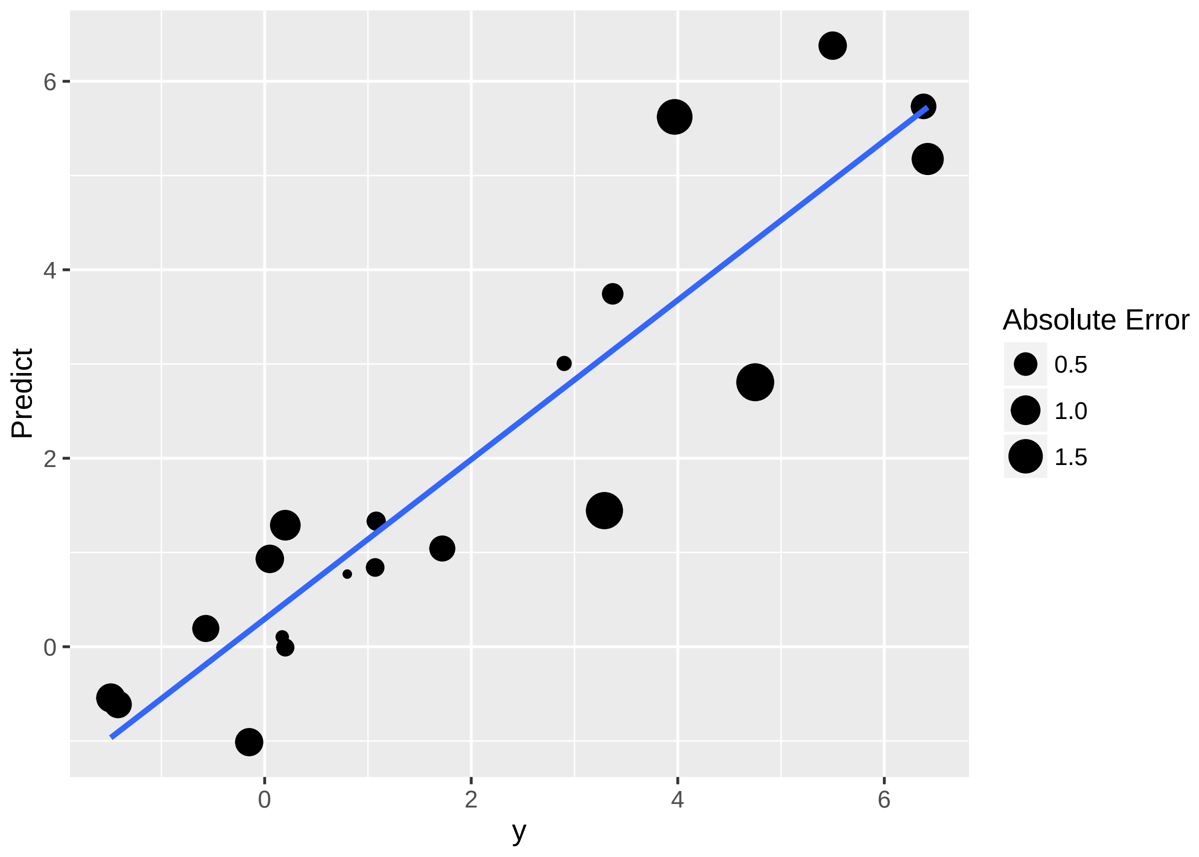
```
##       x1    x2     y
## 1   0.99  0.98  6.42
## 2  -0.75 -0.76  0.20
## 3  -0.50 -0.48  0.80
## 4  -1.08 -1.08 -0.57
## 5   0.09  0.09  4.75
## 6  -1.28 -1.27 -1.42
## 7  -0.79 -0.79  1.07
## 8  -1.17 -1.17  0.20
## 9  -0.57 -0.57  1.08
## 10 -1.62 -1.62 -0.15
## 11  0.34  0.35  2.90
## 12  0.51  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

```
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
```

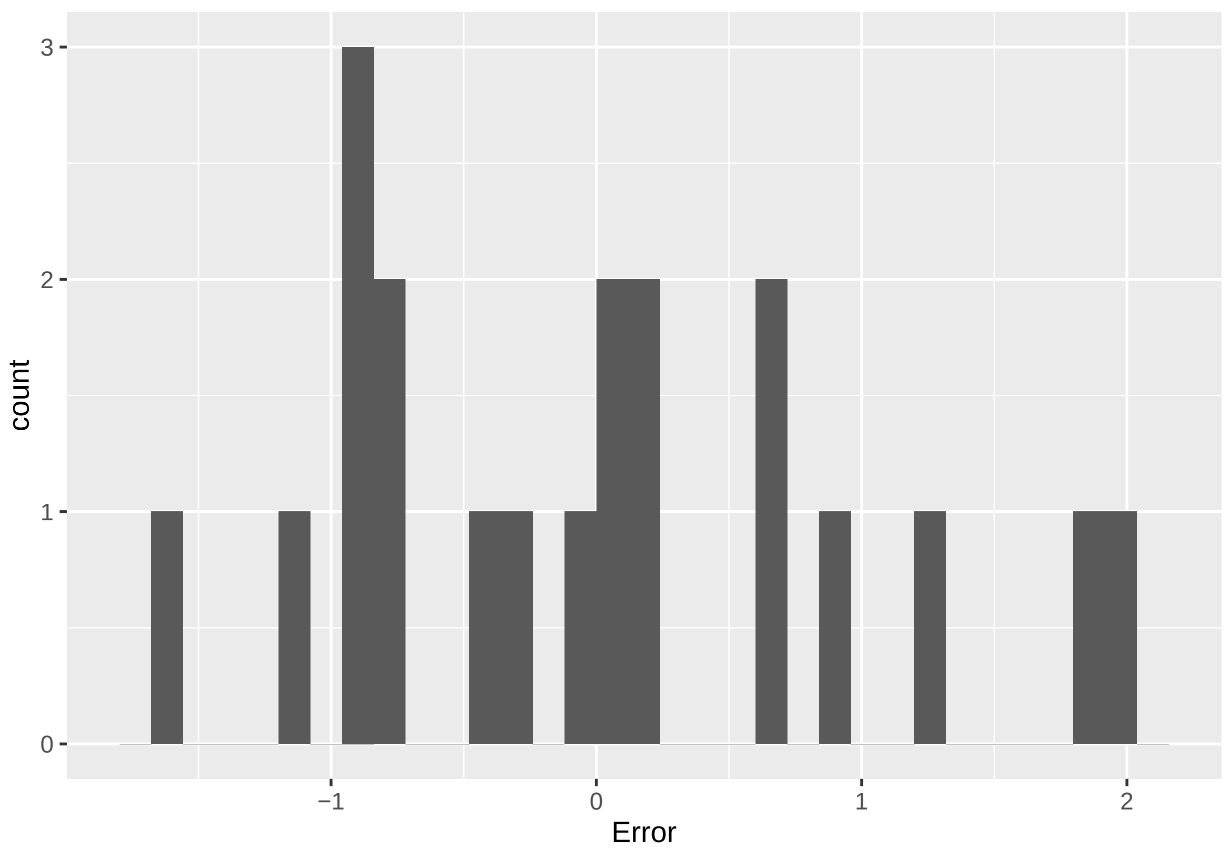
```r
plotDF<-Table1
plotDF[,'Type']<-'Train'
plotDF$Predict<-predict(LeastFit,plotDF[,1:2])
plotDF$Error<-plotDF$y-plotDF$Predict
ggplot(plotDF,aes(x=y,y=Predict,size=abs(Error)))+geom_point()+
  scale_size("Absolute Error")+geom_smooth(method="lm",se=F,size=1)
```



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

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

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

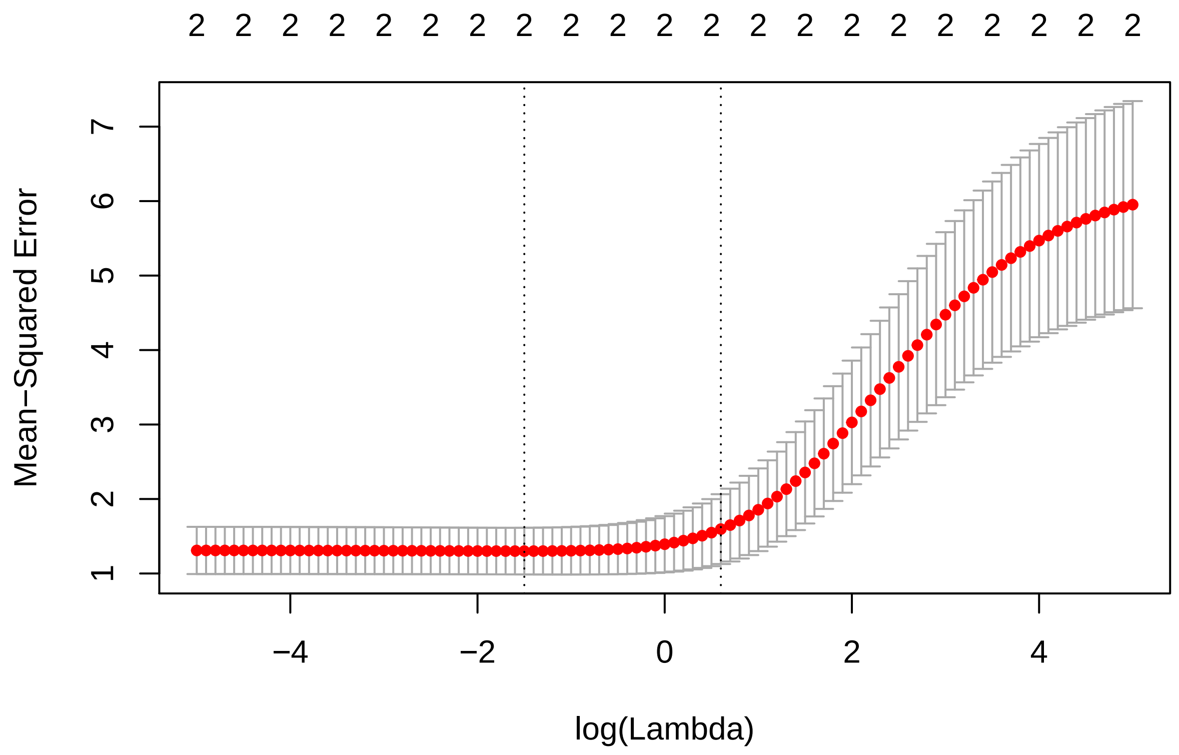


```
sensitivities <- coef(LeastFit)
sensDF <- data.frame(Method = 0, Var = 0, Value=0)
sensDF[1:length(sensitivities),'Method'] <- "Least-Squares"
sensDF[1:length(sensitivities),'Var'] <- names(sensitivities)
sensDF[1:length(sensitivities),'Value'] <- (sensitivities)
rowStart <- length(sensitivities)+1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

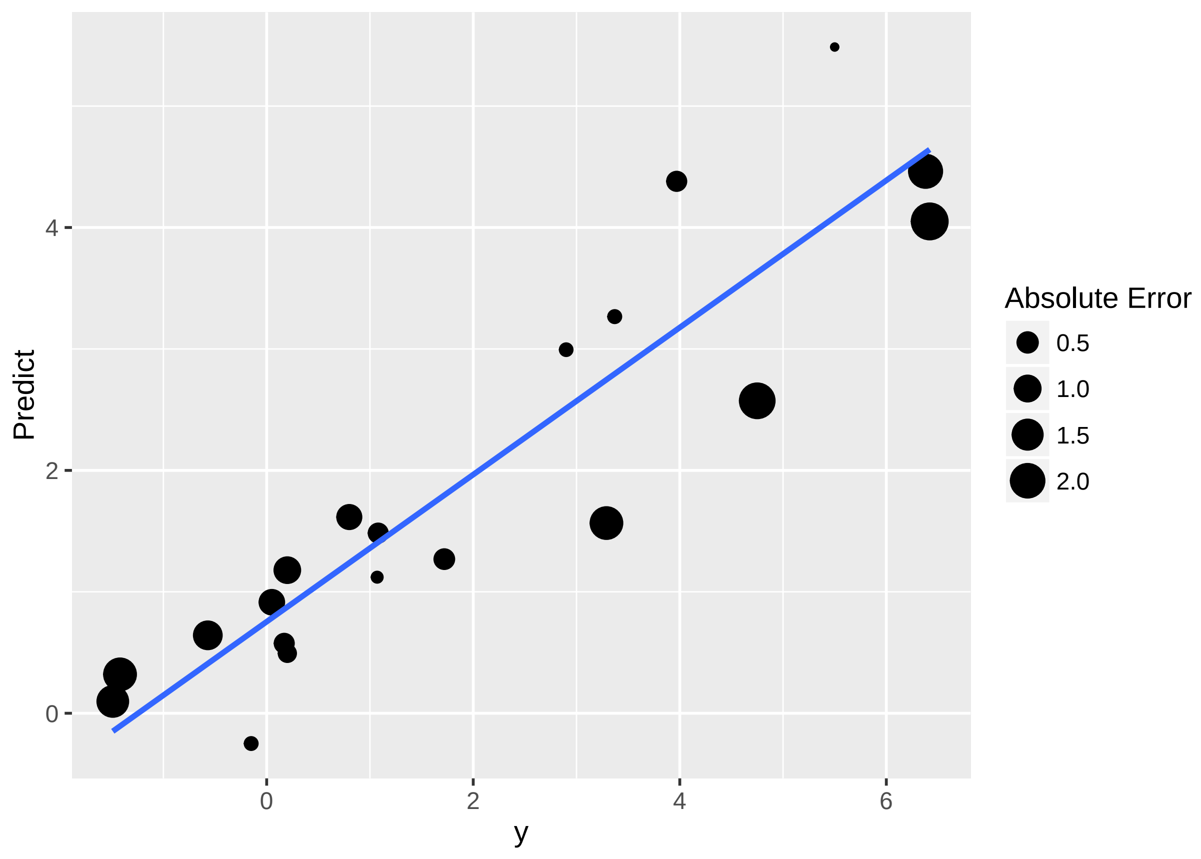
2. Ridge Regression

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)
```



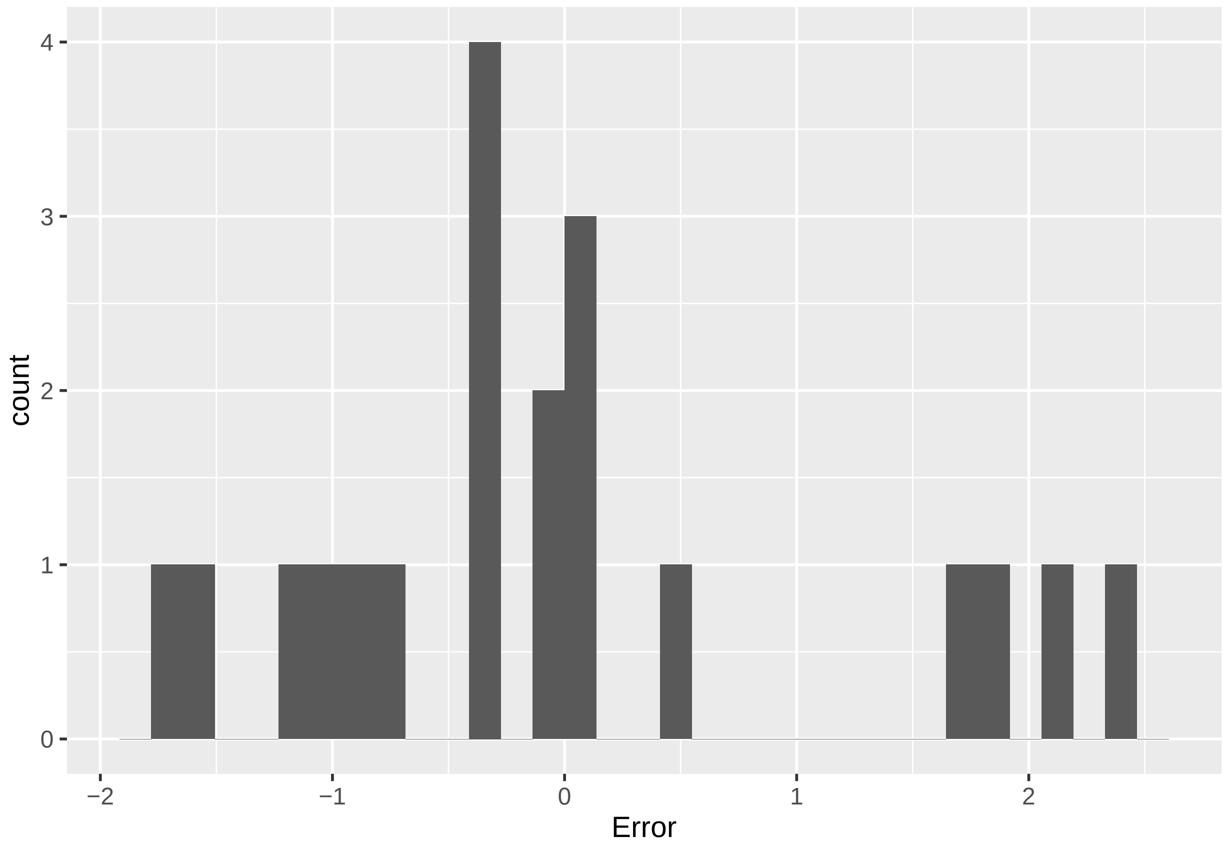
```
lambda <- crossValid$lambda.min
sensitivities <- coef(crossValid)
plotDF <- Table1
plotDF[,'Type'] <- 'Train'
plotDF[,"Predict" ]<- data.frame(Predict=predict(crossValid,as.matrix(plotDF[,1:2]),
                                                 lambda=lambda))
plotDF$Error <- plotDF$y-plotDF$Predict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



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

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

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

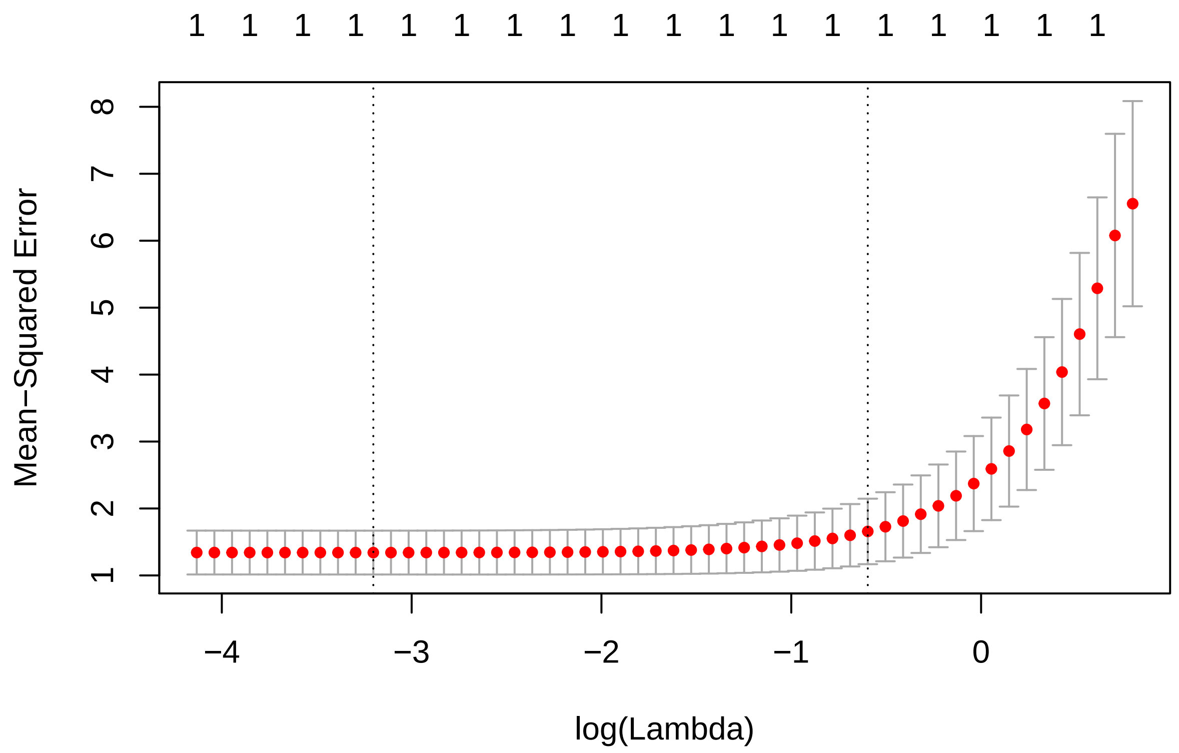


```
sensDF[rowStart:(rowStart + length(sensitivities)-1),'Method'] <- "Ridge"
sensDF[rowStart:(rowStart+length(sensitivities)-1),'Var']<-t(t(rownames(sensitivities)))
sensDF[rowStart:(rowStart +length(sensitivities)-1),'Value']<-as.numeric(sensitivities)
rowStart <- rowStart + length(sensitivities)
```

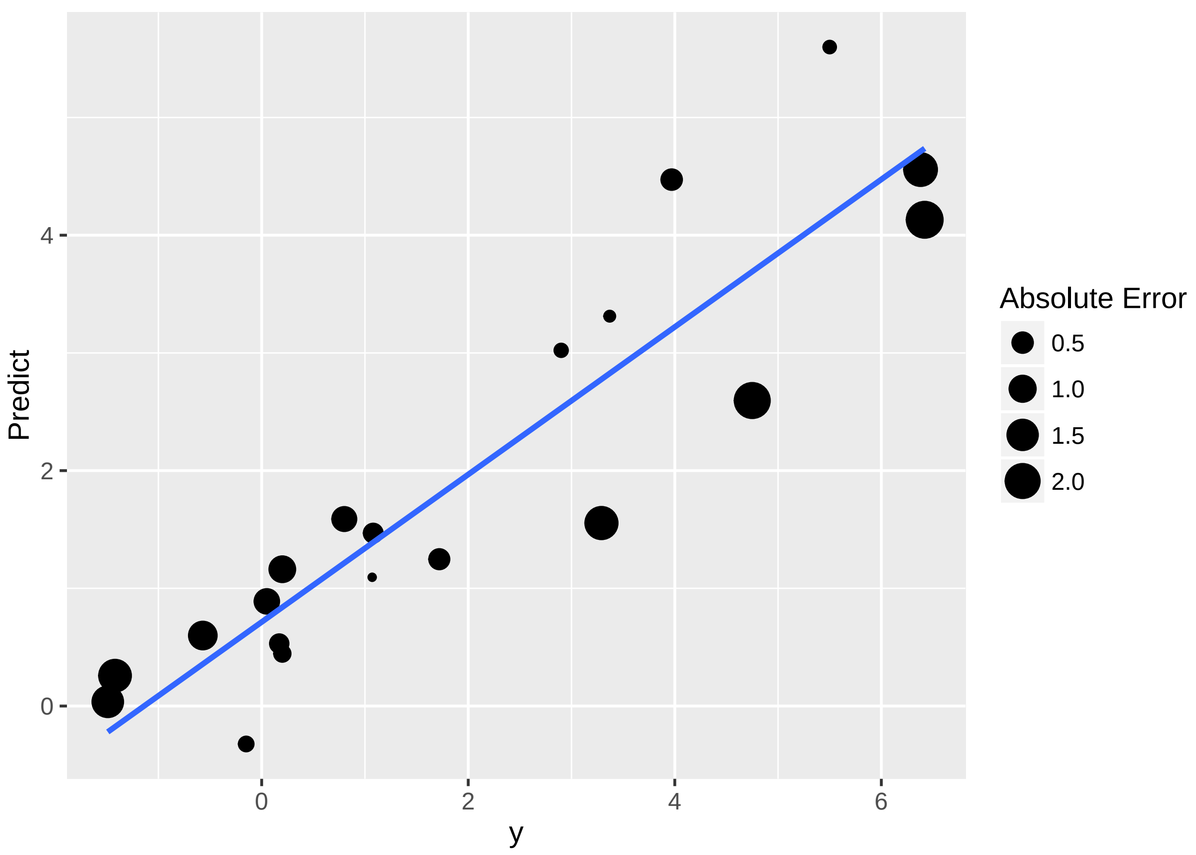
3. Lasso Regression

Lasso regression sets alpha=1

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



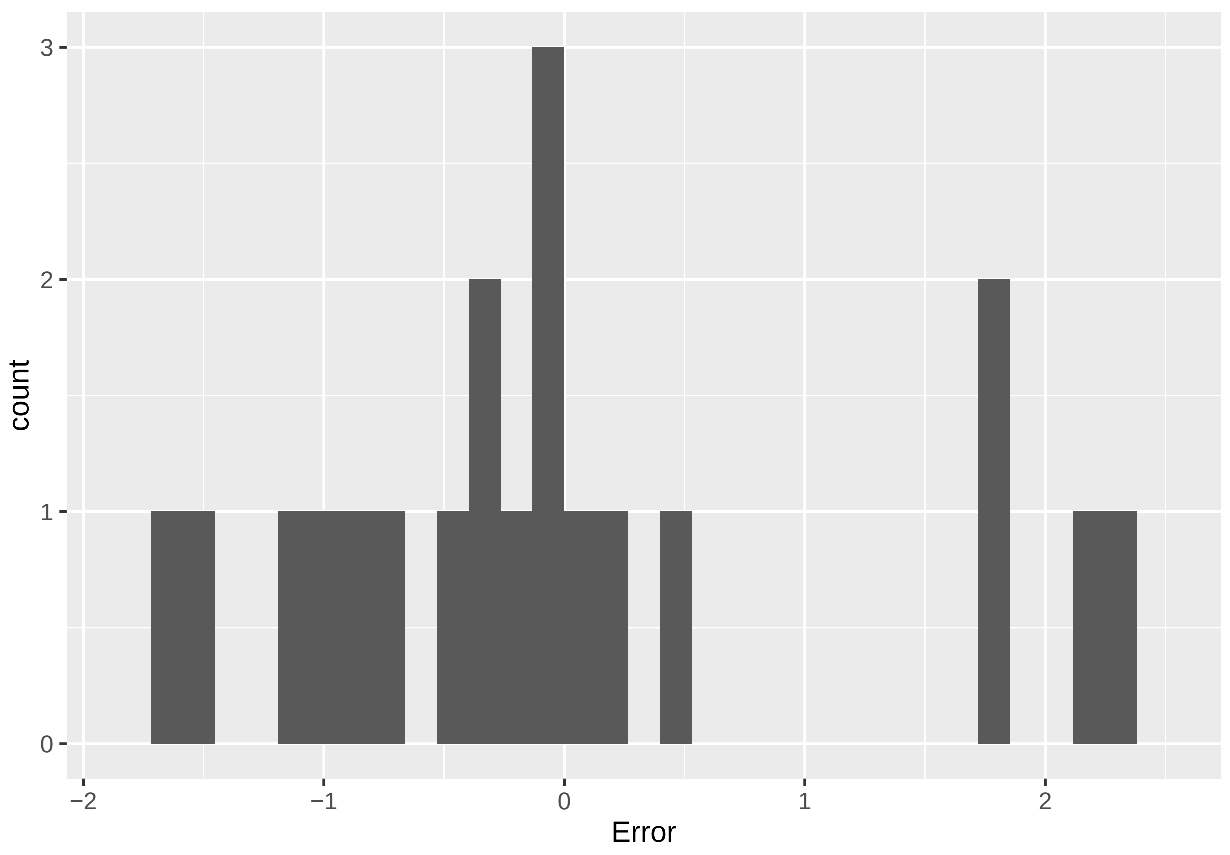
```r
lambda <- crossValid$lambda.min
sensitivities <- coef(crossValid)
plotDF <- Table1
plotDF[,'Type'] <- 'Train'
plotDF[,"Predict" ]<- data.frame(Predict=predict(crossValid,as.matrix(Table1[,1:2]),
                                                 lambda=lambda))

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
```

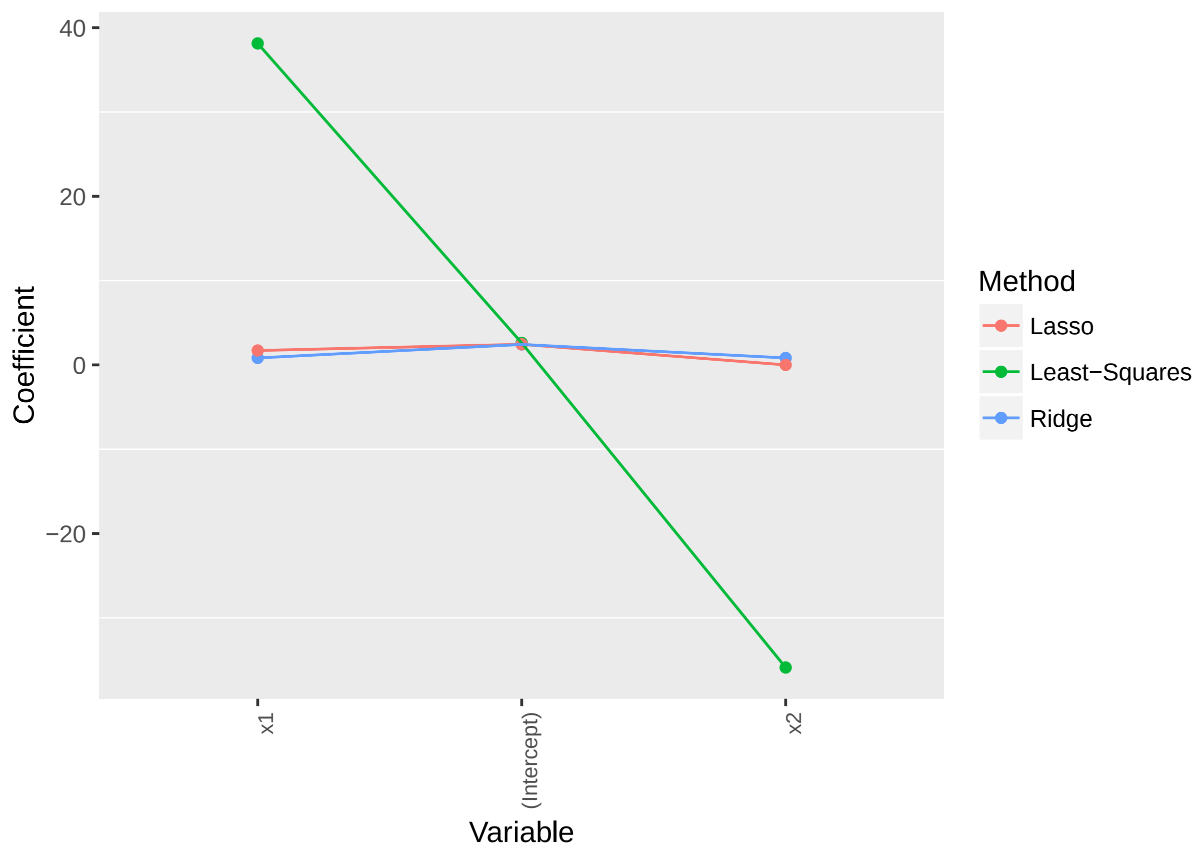
```r
ggplot(plotDF,aes(x=Error)) + geom_histogram()
```



```
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:

$$\int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi^\dagger \bigtriangledown^2 \phi + \phi^\dagger \frac{\phi}{L^2}\right) = \int_0^X dx \int_0^Y dy \int_0^Z dz \left(\phi \bigtriangledown^2 \phi^\dagger + \phi \frac{\phi^\dagger}{L^2}\right) \tag{1}$$

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:

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

Problem 2 continued on next page. . .

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, $v = \phi$, $dv = \frac{\delta\phi}{\delta x}dx$.

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

At the boundaries, both ϕ and $\phi^\dagger$ are a constant, and the derivatives of both at the boundaries are equal, and therefore those terms cancel, leaving

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

which is equal to the x component of the $\bigtriangledown^2$ term of the RHS of equation 1 above.

Compute the sensitivity to the QoI:

I don't know if this is the right way to go about this, but if you modify the first equation listed in this problem to:

$$\phi = L^2 \left[\frac{Q}{D} + \bigtriangledown^2 \phi \right]$$

and use it as a substitution, then we get something like this,

$$\begin{aligned}
\text{QoI} &= \int_0^X dx \int_0^Y dy \int_0^Z dz\ \frac{D}{L^2}\phi \\
&= \int_0^X dx \int_0^Y dy \int_0^Z dz\ \frac{D}{L^2}\left(L^2 \left[\frac{Q}{D} + \bigtriangledown^2 \phi \right] \right) \\
&= \int_0^X dx \int_0^Y dy \int_0^Z dz\ \left[Q + D \bigtriangledown^2 \phi \right]
\end{aligned}$$

If Q and D both are independent of space, then

$$\text{QoI} = QXYZ + D \left[\int_0^Y dy \int_0^Z dz\ \left| \frac{\delta\phi}{\delta x} \right|_{x=0}^{x=X} + \int_0^X dx \int_0^Z dz\ \left| \frac{\delta\phi}{\delta y} \right|_{y=0}^{y=Y} + \int_0^X dx \int_0^Z dz\ \left| \frac{\delta\phi}{\delta z} \right|_{z=0}^{z=Z} \right]$$

I'm not sure how the adjoint helps me though.

Problem 3

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

(a) Simple random sampling

(b) Stratifid sampling

(c) A van der Corput sequence of base 2

(d) A van der Corput sequence of base 3

Simple random sampling samples U(0,1) and plugs this value into the inverse CDF. Stratified sampling separates U(0,1) into equal bins and samples "Randomly" in each bin. Van der Corput sequences divides an interval into a a number of equal subintervals.

For example, the ordinary van der Corput sequence in base 3 is given by 1/3, 2/3, 1/9, 4/9, 7/9, 2/9, 5/9, 8/9, 1/27.

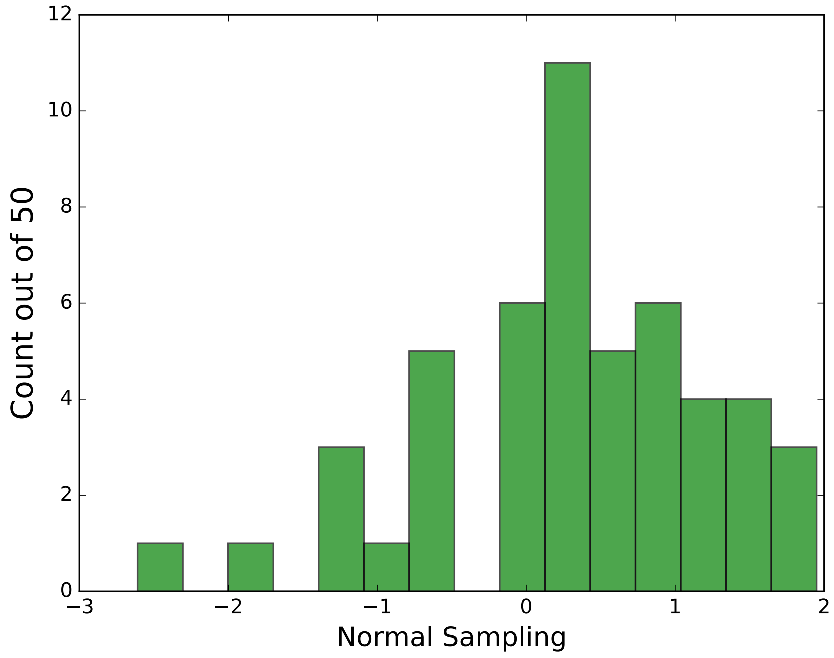
Listing 1: Script for Problem

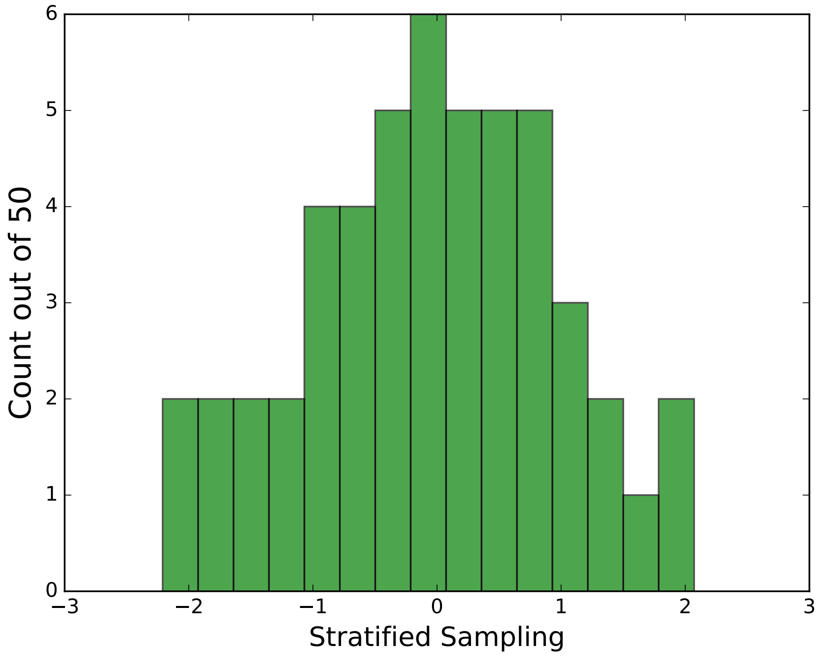
```python
#!/usr/bin/env python3

#################################################################
#################### Import packages ########################
#################################################################

import numpy as np
import matplotlib.pyplot as plt
import time
start_time = time.time()
from scipy.stats import norm

#################################################################
####################### Functions ###########################
#################################################################

#Van der Corput sequence function found online
def vdc(n, base=2):
    vdc, denom = 0,1
    while n:
        denom *= base
        n, remainder = divmod(n, base)
        vdc += remainder / denom
    return vdc

#################################################################
##################### Calculations ##########################
#################################################################

#Make sure Nstrata <= N

N=50  #samples
```

Problem 3 continued on next page. . .

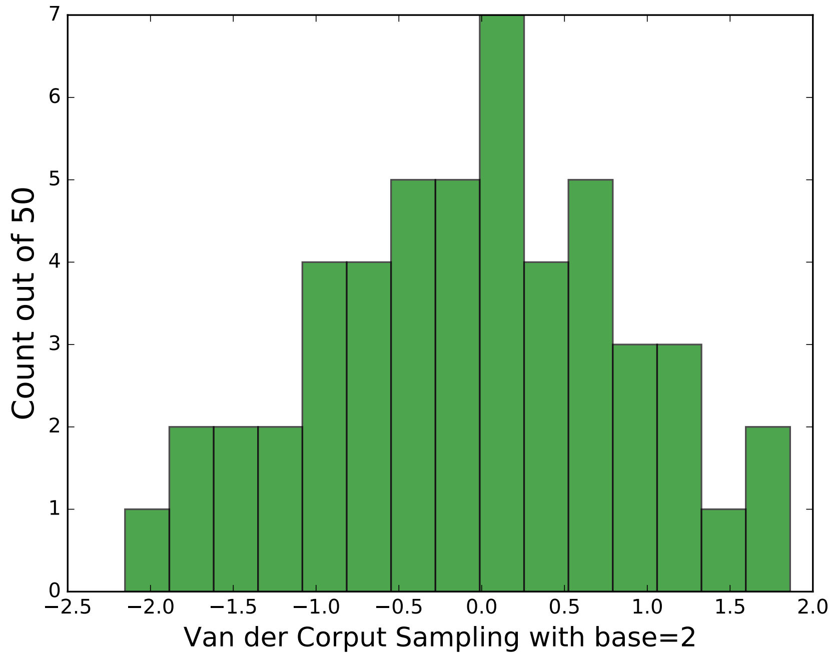
```
Nbins=15  #hist plot
Nstrata=49
filename="V2Norm.pdf"
#Stratified or Normal or Van der Corput
Xlabel="Van der Corput Sampling with base=2"
RandomNumbers=[]
vanBase=2;van=True

#Sampling for normal and stratified
if not van:
    Nloop=int(N/Nstrata)*Nstrata
    for i in range(0,int(N/Nstrata)):
        for j in range(0,Nstrata):
            RandomNumbers.append(np.random.uniform(low=j/Nstrata,
                                high=(j+1)/Nstrata,size=1))
    #If N/Nstrata doesn't divide evenly
    if Nloop<N:
        for j in range(0,N-Nloop):
            RandomNumbers.append(np.random.uniform(low=j/Nstrata,
                            high=(j+1)/Nstrata,size=1))
#Sampling for van
if van:
    for i in range(0,N):
        RandomNumbers.append(vdc(i+1,vanBase))

#Sample the inverse of the CDF of the standard normal
#distribution
Samples=norm.ppf(RandomNumbers)

#Generate histogram
fig=plt.figure()
ax=fig.add_subplot(111)
ax.set_xlabel(Xlabel,fontsize=16)
ax.set_ylabel('Count out of '+str(N),fontsize=18)
ax.hist(Samples,Nbins,color='green',alpha=0.7,edgecolor='black')
#ax.set_xlim(-500,500)
plt.savefig(filename)

##################### Time To execute ################

print("--- %s seconds ---" % (time.time() - start_time))
```

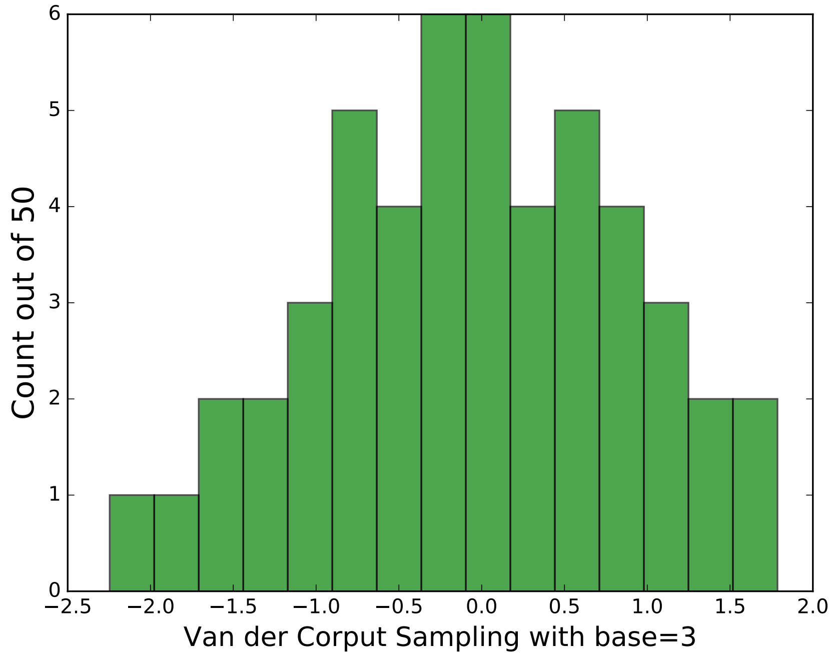
Problem 3 continued on next page. . .





Problem 3 continued on next page. . .


Count out of 50
Van der Corput Sampling with base=2
−2.5 −2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0
0 1 2 3 4 5 6 7


Count out of 50
Van der Corput Sampling with base=3
−2.5 −2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0
0 1 2 3 4 5 6

Problem 4

Consider the Rosenbrock function $f(x,y) = (1-x)^2 + 100(y-x^2)^2$. Assume that $x = 2t-1$, where T $\sim$ $B(3,2)$ and $y = 2s-1$, where S $\sim$ $B(1.1,2)$. Estimate the probability that $f(x,y)$ is less than 10 using:

(a) a first-order second-moment reliability method

(b) Latin hypercube sampling using 50 points

(c) A Halton sequence using 50 points

Compare this with the probability you calculate using 10^5 random samples. (*Hint: Matlab has a built-in function for sampling beta R.V.'s "betard"*).

The answer is simple