

NUEN 647
Uncertainty Quantification for Nuclear Engineering
Homework 3

Due on Saturday, December 10, 2016

Dr. McClarren

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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

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```
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
```

```

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)

```



```

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

```

```

##          Error
## Error 0.04902635

```

```

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

```



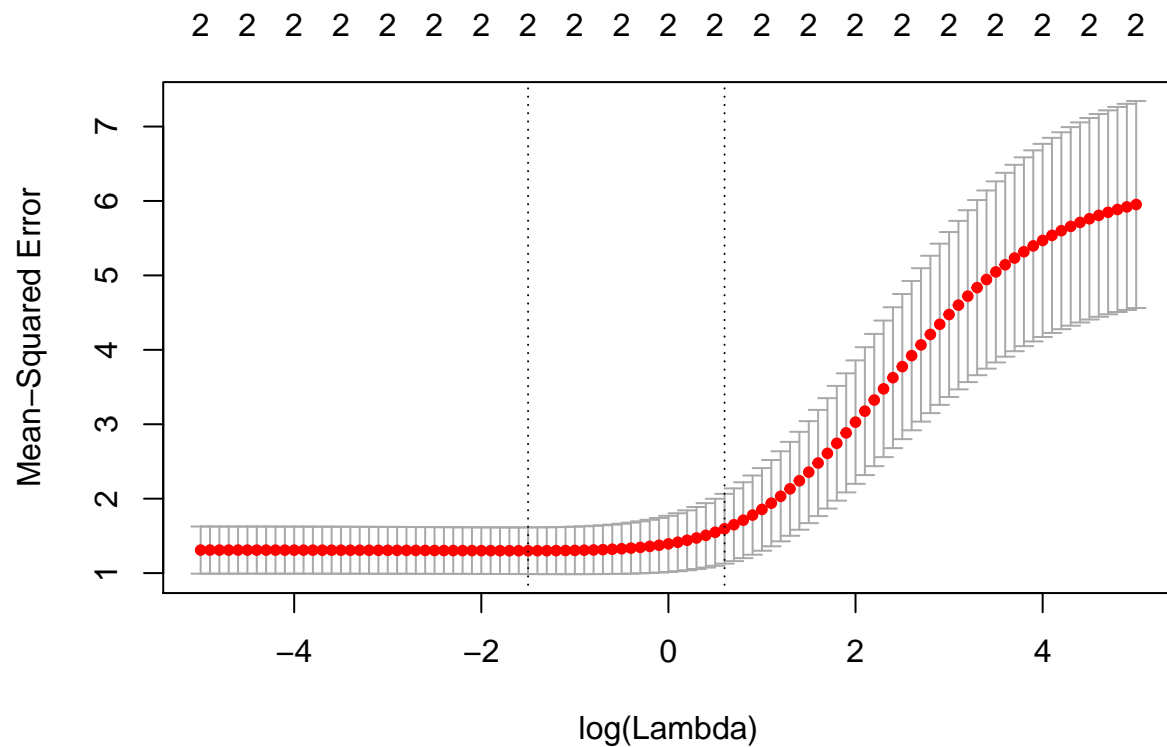
```
sensitivities <- coef(LeastFit)
sensDF <- data.frame(Method = 0, Var = 0, Value=0)
sensDF[1:length(sensitivities), 'Method'] <- "Least-Squares"
sensDF[1:length(sensitivities), 'Var'] <- names(sensitivities)
sensDF[1:length(sensitivities), 'Value'] <- (sensitivities)
rowStart <- length(sensitivities)+1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

2. Ridge Regression

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

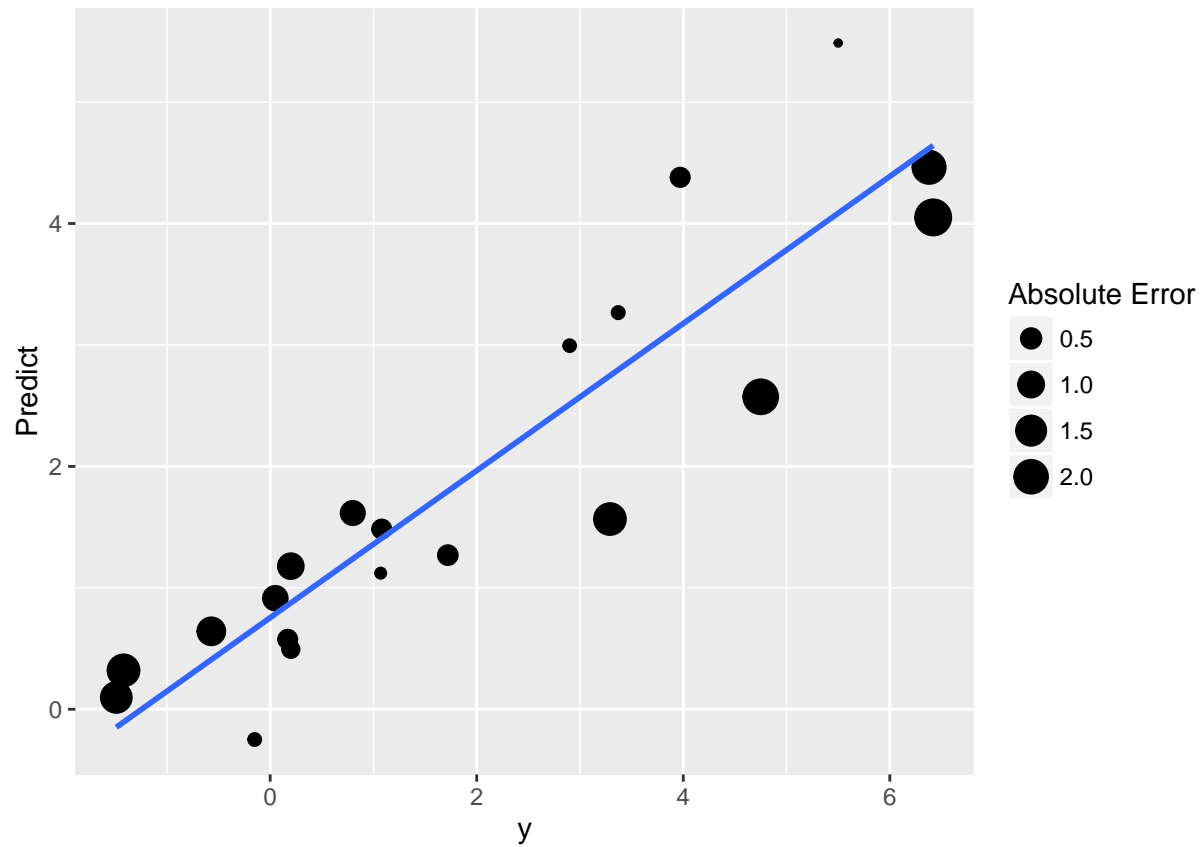
```
crossValid <- cv.glmnet(as.matrix(Table1[,1:2]),
                        as.matrix(Table1$y), alpha = 0,
                        lambda=exp(seq(-5,5,by=0.1)))

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)
```



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

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

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

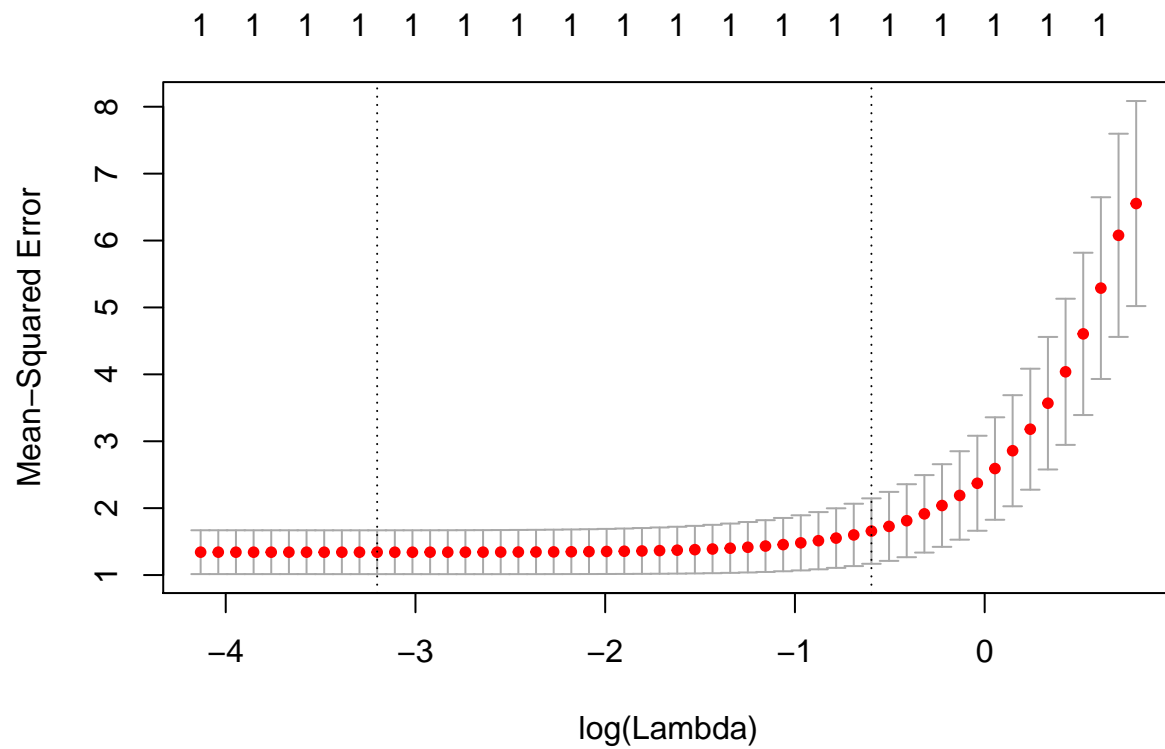



```
sensDF[rowStart:(rowStart + length(sensitivities)-1), 'Method'] <- "Ridge"
sensDF[rowStart:(rowStart+length(sensitivities)-1), 'Var']<-t(t(rownames(sensitivities)))
sensDF[rowStart:(rowStart +length(sensitivities)-1), 'Value']<-as.numeric(sensitivities)
rowStart <- rowStart + length(sensitivities)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

3. Lasso Regression

Lasso regression sets alpha=1

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



```
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)
```



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

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

```
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 coefficients.

Problem 2

Derive the adjoint operator for the equation

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

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

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

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

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

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

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

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 dimensions. 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:

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

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, ∇^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 $v = \frac{\delta\phi}{\delta x}$, $dv = \frac{\delta^2\phi}{\delta x^2} dx$ 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 $u = \frac{\delta\phi^\dagger}{\delta x}$, $du = \frac{\delta^2\phi^\dagger}{\delta x^2} dx$ 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 ϕ^\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 ∇^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:

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

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

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

If Q and D both are independent of space, then

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

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

Problem 3

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

- (a) Simple random sampling
- (b) Stratified 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 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

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

#####
##### Import packages #####
5 #####

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

#####
##### Functions #####
15 #####

#Van der Corput sequence function found online
def vdc(n, base=2):
    vdc, denom = 0,1
20     while n:
        denom *= base
        n, remainder = divmod(n, base)
        vdc += remainder / denom
    return vdc
25

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

30 #Make sure Nstrata <= N

N=50 #samples
```



```

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

40
   #Sampling for normal and stratified
   if not van:
       Nloop=int(N/Nstrata)*Nstrata
       for i in range(0,int(N/Nstrata)):
45           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:
50                   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:
55       for i in range(0,N):
           RandomNumbers.append(vdc(i+1,vanBase))

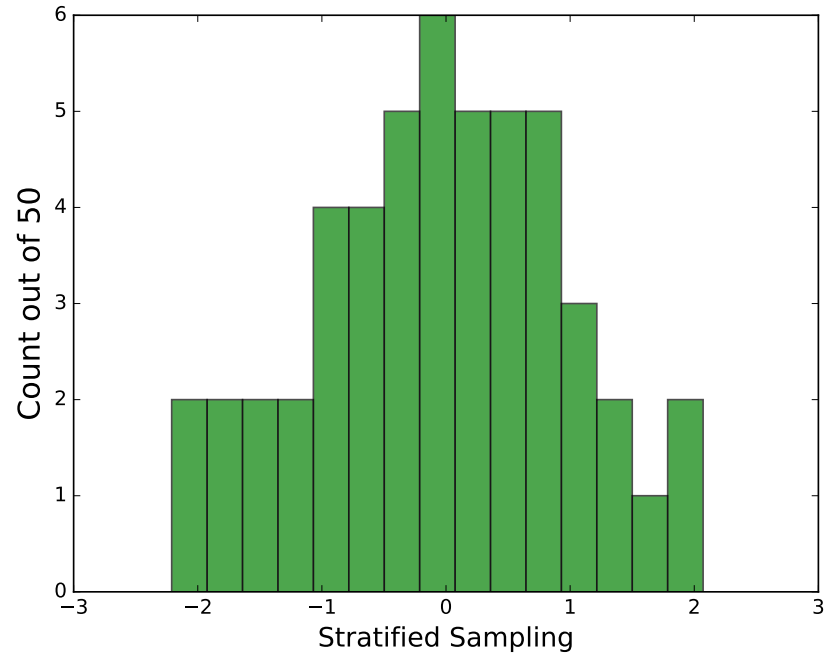
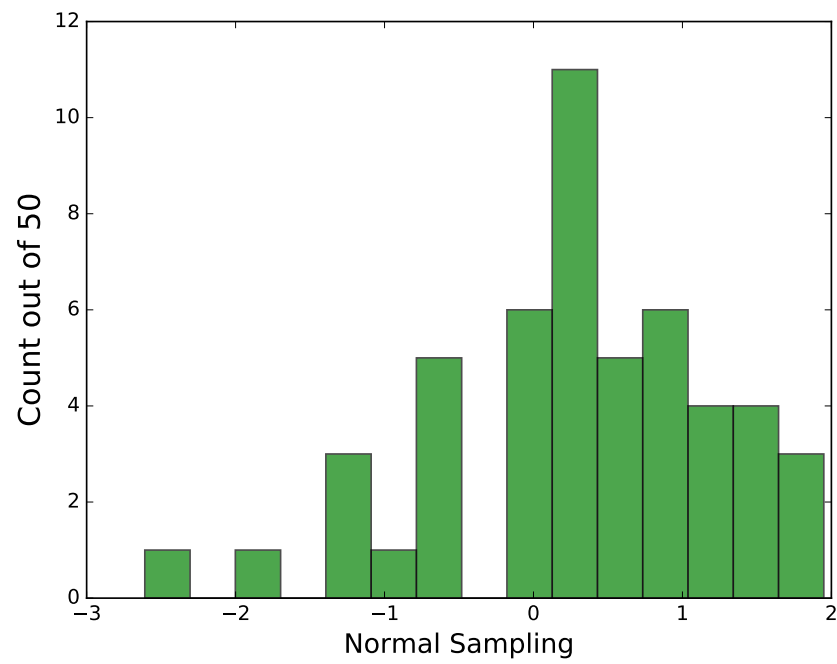
   #Sample the inverse of the CDF of the standard normal
   #distribution
60 Samples=norm.ppf(RandomNumbers)

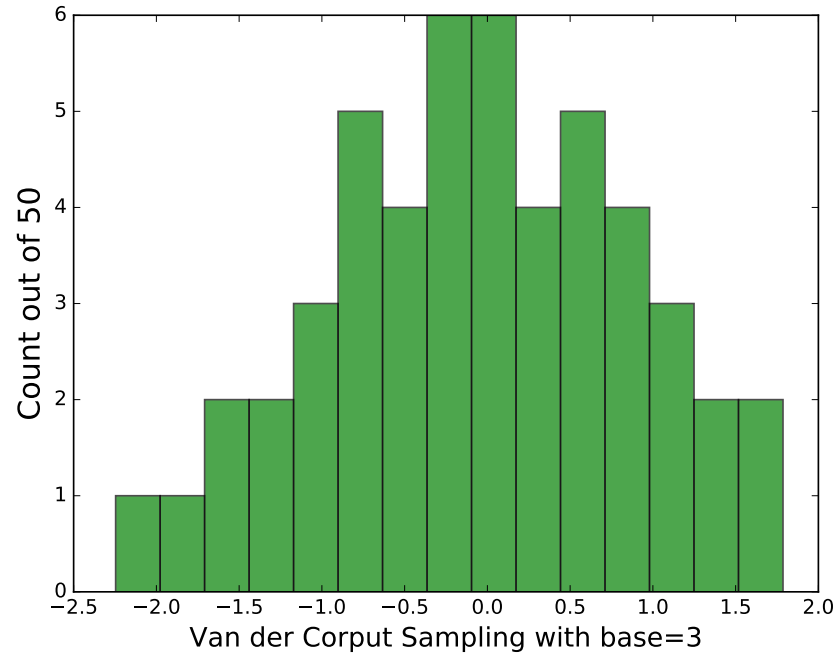
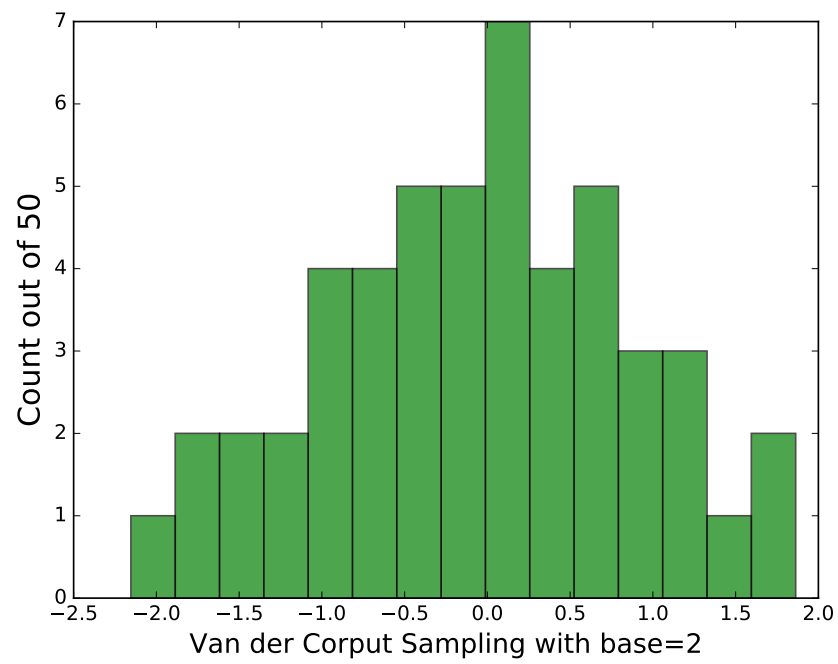
   #Generate histogram
   fig=plt.figure()
   ax=fig.add_subplot(111)
65 ax.set_xlabel(Xlabel,fontsize=16)
   ax.set_ylabel('Count out of '+str(N),fontsize=18)
   ax.hist(Samples,Nbins,color='green',alpha=0.7,edgecolor='black')
   #ax.set_xlim(-500,500)
   plt.savefig(filename)

70
   ##### Time To execute #####

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

```





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"*).

A first-order second-moment reliability method

Will use a gaussian approximation as shown in section 7.3 in the course notes (FORM).

In this method the performance function ($Z(x, y)$) is a function of the random variables x and y , and is defined such that the failure surface is the location where $Z = 0$ (top of page 119 Ch 7) such that $Z < 0$ represents failure and $Z > 0$ represents success. For the case above, this would mean that our performance function is:

$$\begin{aligned} Z &= 10 - f(x, y) \\ &= 10 - (1 - x)^2 + 100(y - x^2)^2 \end{aligned}$$

Next, the probability of failure is defined as:

$$p_{fail} = 1 - \Phi\left(\frac{\mu_Z}{\sigma_Z}\right)$$

Where Φ is the CDF for a standard normal, μ_Z and σ_Z are the mean and standard deviation of Z . As a reminder, if Z were a standard normal, defined such that any part of Z that is less than 0 is failure. Then because $\mu_Z = 0$ there would be a 50% chance of failure. If Z were a non standard normal, then the distance from zero would be normalized (by dividing by σ_Z) to units of σ , and as μ_Z increases, the chance of failure would continue to decrease, which make sense, as the mean of the performance function moves further and further away from the failure point ($Z = 0$), the probability of failure decreases.

I am trying to spell this out for myself, because I was really confused about this. There are two things I would like to point out to future self. First, Z may not be normal, which is why this method is only exact if Z is normal, otherwise its an approximation. Second, if μ_Z were less than 0, then the equation for the probability of failure should (I think) change to

$$p_{fail} = 0.5 + \Phi\left(\frac{|\mu_Z|}{\sigma_Z}\right)$$

Also third, I am not sure if Z has to be a typical PDF or CDF, will let you know after I do some of the math McClarren gave.

The mean for Z was defined as

$$\mu_Z \approx g(\mu_{x,y})$$

where g is the function we defined as Z (first part of the Taylor expansion of Z). The standard deviation of Z was defined as the second part of the Taylor expansion of Z (without covariances because we are going to assume that all random variables are independent), namely

$$\sigma_Z^2 = \left(\left| \frac{\delta g}{\delta x} \right|_{\mu_x} \sigma_x \right)^2 + \left(\left| \frac{\delta g}{\delta y} \right|_{\mu_y} \sigma_y \right)^2$$

$$\frac{\delta g}{\delta x} = -2(x-1) - 400x(x^2 - y)$$

$$\frac{\delta g}{\delta y} = -200(y - x^2)$$

Also for a beta R.V

$$\mu = \frac{a}{a+b}$$

$$\sigma^2 = \frac{ab}{(a+b)^2(a+b+1)}$$

Listing 2: Script for Problem

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

#####
##### Import packages #####
5 #####

import time
start_time = time.time()
import Functions as fun
10

#####
##### Calculations #####
15 #####

N=10000 #Samples
Nbins=200 #Hist Plot
Nstrata=1000
filename="Histf.pdf"
20

Xlabel="Stratified Sampling both samples"
RandomNumbersX=fun.Rstrat(N,Nstrata)
RandomNumbersY=fun.Rstrat(N,Nstrata)

25 Samplest=fun.beta.ppf(RandomNumbersX,3,2)
Sampless=fun.beta.ppf(RandomNumbersY,1.1,2)

ut=fun.betau(3,2)
us=fun.betau(1.1,2)
30 ot=fun.betao(3,2)
```

```
os=fun.betao(1.1,2)
ux=fun.X(ut)
uy=fun.Y(us)

35
print("X mean is "+str(ux))
print("Y mean is "+str(uy))
print("X sig is "+str((ot**0.5)*2))
print("Y sig is "+str((os**0.5)*2))
40 print("Mean Z is "+str(fun.Z()))
quit()

X=fun.X(Samplest)
Y=fun.Y(Samplest)

45
f=fun.Rosen(X,Y)

Xlabel="Rosenbrock Function Histogram"
(I)=fun.HIST(Xlabel,f,Nbins,filename,N)

50
PGreater=sum(i<10 for i in f)/N

print("The probability of being less than 10 is: "+str(PGreater[0]))

55

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

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

The output is 0.3795 probability of being less than 10. Here is a PDF of the function f generated from the code above.

