Lab: Neural Networks

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Lab: Neural networks

Objective: In this lab we will illustrate the applications of neural networks in prediction of a numerical variable and classification via simulations. We will start with the simulation of the regression setting and build a neural network model to predict numerical response. Then we will simulate the classification setting and learn how neural networks can be applied to predict qualitative variable.

Prediction of a numerical outcome

To visualize and understand simulated data, we will limit ourselves to one response and two explanatory variable regression setting. It is recommended to standardize data before fitting neural networks.

1. Simulate uniformly distributed variables x and z and relate them to response y via the following formula:

$$y_i = \cos(3\pi x_i) + \sin(3\pi z_i) + \varepsilon_i$$

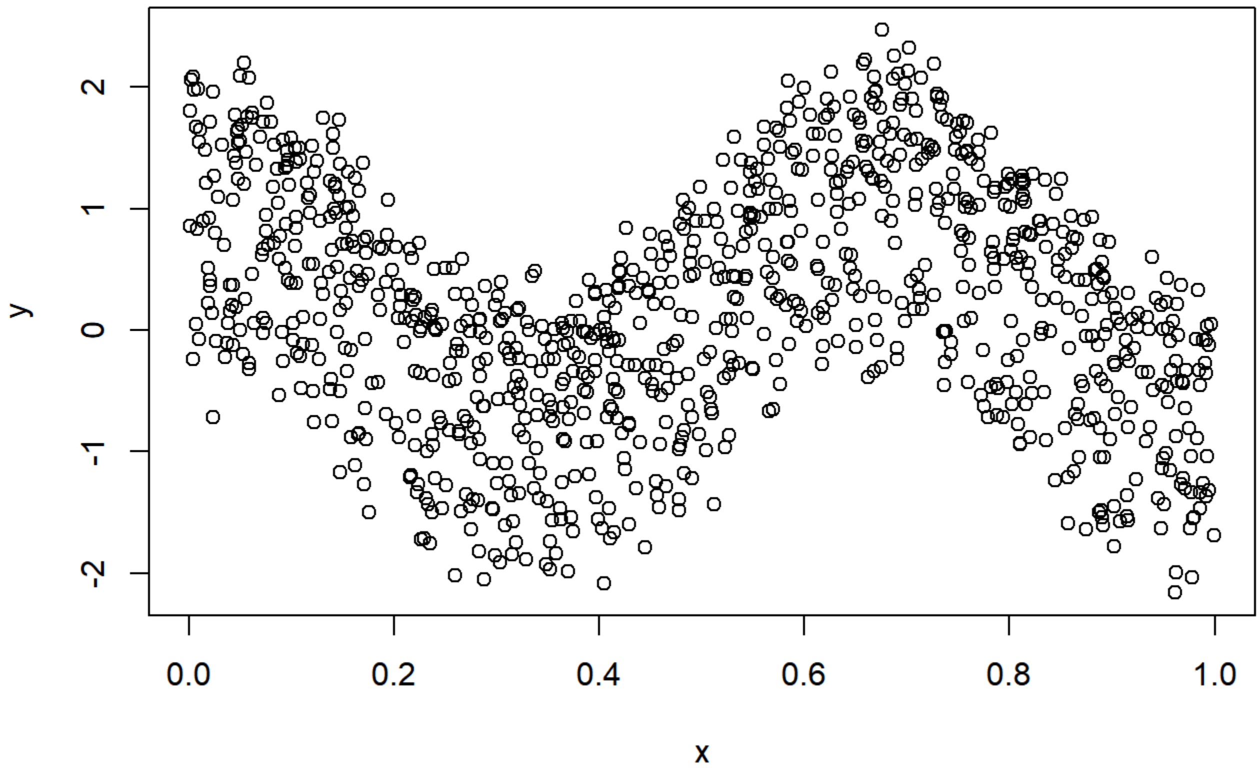
where $\varepsilon \sim \mathcal{N}(0, 0.25^2)$ and $x, z \sim U[0,1]$.

```
set.seed(123)
x=runif(1000)
z=runif(1000)
y=cos(3*pi*x) + sin(3*pi*z) + rnorm(n=1000,mean=0,sd=0.25) #rnorm(1000,sd=0.25)
```

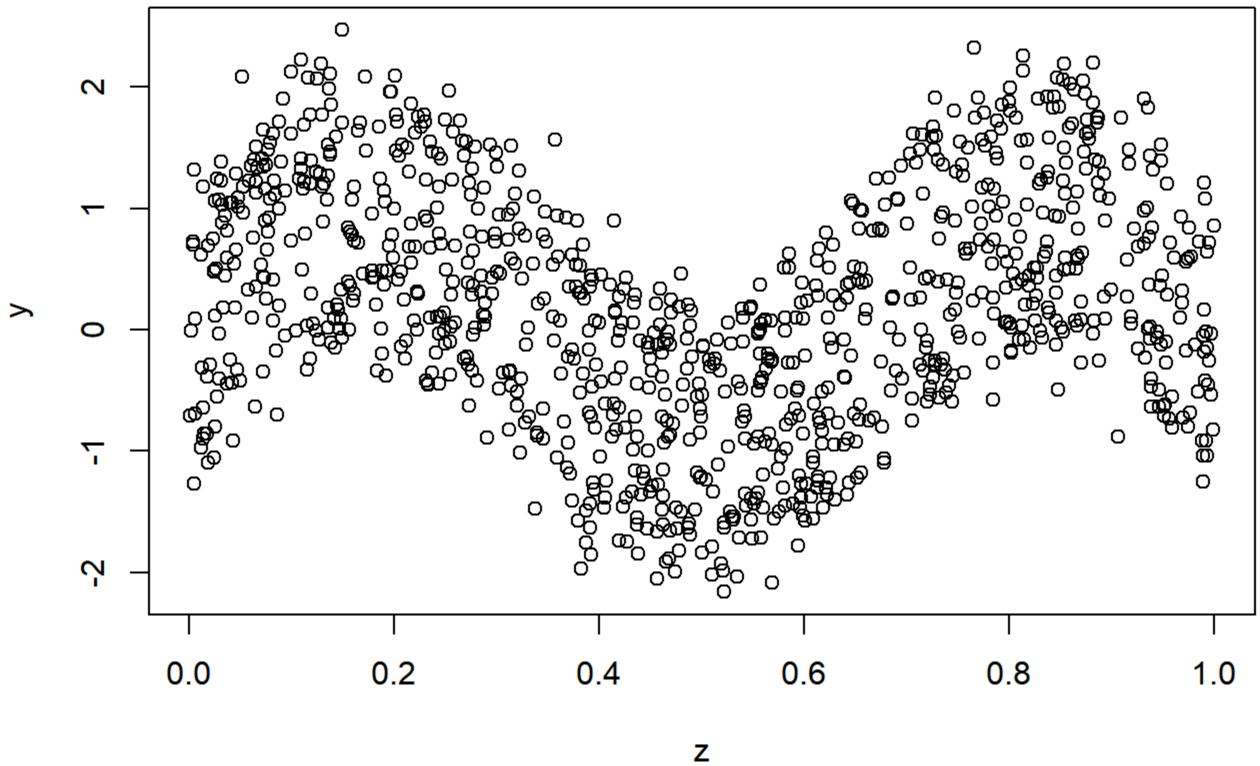
Remark: x and z are explanatory variables, while y is a target variable.

2. Visualize the relationship between y and the independent variables.

```
plot(y~x) # same as plot(x,y)
```




```
plot(z,y) # same as plot(y~z)
```



3. Create a data frame (table) by combining x, y and z.

```
dat=data.frame(x,y,z)
head(dat)
```

```
##           x          y         z
## 1 0.2875775 -0.6238766 0.2736227
## 2 0.7883051 -0.4817732 0.5938669
## 3 0.4089769  0.2371869 0.1601848
## 4 0.8830174  0.4977365 0.8534302
## 5 0.9404673 -0.4932181 0.8477392
## 6 0.0455565  0.1910150 0.4778868
```

4. Install and load neuralnet library.

```
library(neuralnet)
```

5. Build a neural network model and call output object, nn.

```
nn=neuralnet(y~x+z,dat,lifesign = "full")
```

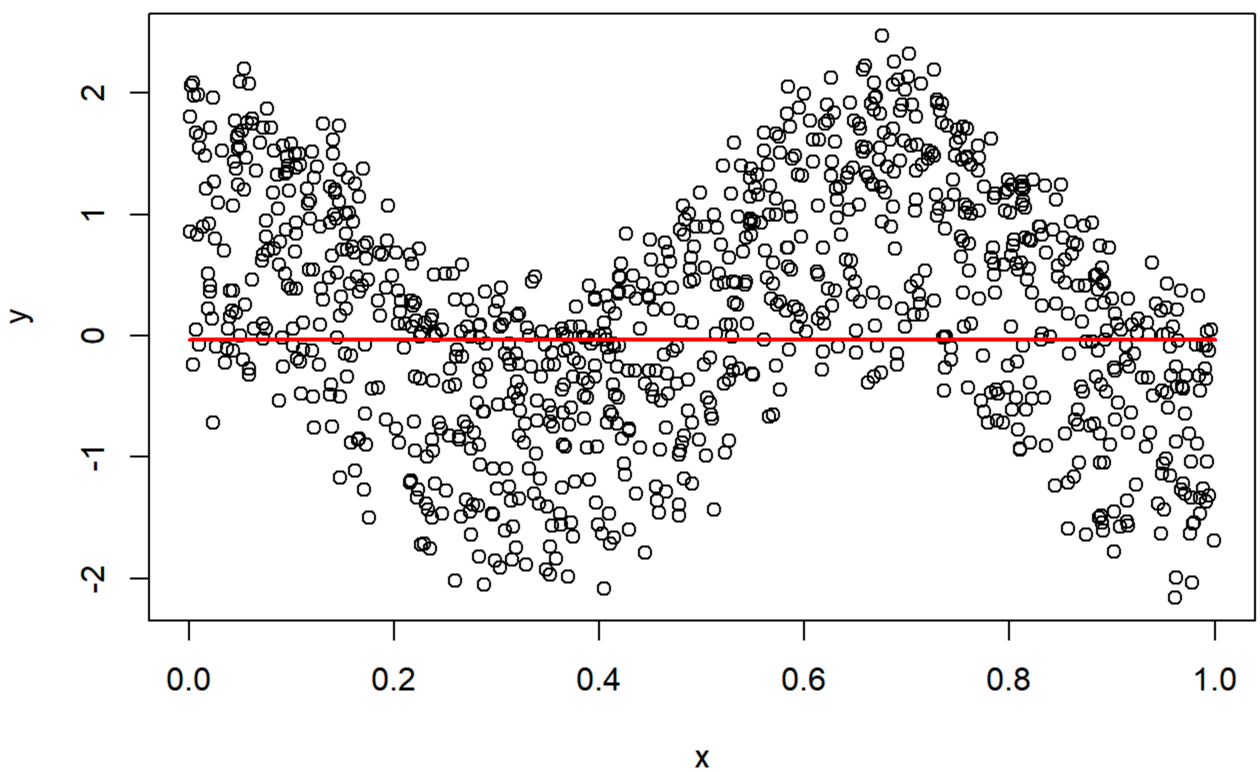
```
## hidden: 1    thresh: 0.01    rep: 1/1    steps:    1000  min thresh: 0.0888017296470194
##                                                    2000  min thresh: 0.0224812735600251
##                                                    2538  error: 426.76371    time: 0.3 secs
```

6. Plot nn.

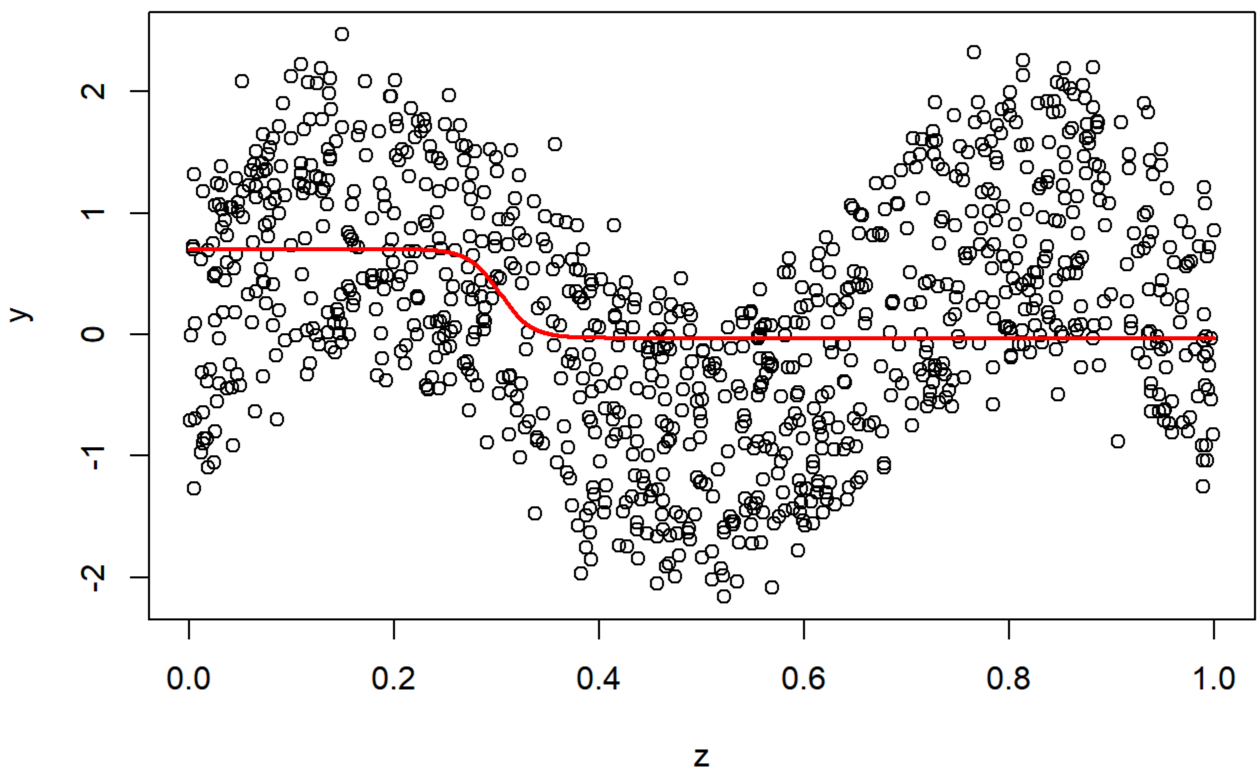
```
plot(nn)
```

7. To evaluate how well the neural network fits data, visualize the relationship between y and the independent variables individually. Does the model fit data well?

```
par(mfrow=c(1,1))   # one graph per page
# z is constant
x.test = seq(0,1,by=0.001)
z.const = rep(0.5,length(x.test))
new.data=data.frame(x=x.test,z=z.const)
y.fit = predict(nn,newdata=new.data)
plot(y~x)
lines(y.fit~x.test,type="l",col="red",lwd=2)
```




```
# x is constant
z.test = seq(0,1,by=0.001)
x.const = rep(0.5,length(x.test))
new.data=data.frame(x=x.const,z=z.test)
y.fit = predict(nn,newdata=new.data)
plot(y~z)
lines(y.fit~z.test,type="l",col="red",lwd=2)
```



8. Play with parameters and see if you can improve the fit.

```
## hidden: 10    thresh: 0.02    rep: 1/1    steps:    1000 min thresh: 1.13873031025351
##                                                     2000 min thresh: 0.654959912174367
##                                                     3000 min thresh: 0.654959912174367
##                                                     4000 min thresh: 0.654959912174367
##                                                     5000 min thresh: 0.654959912174367
##                                                     6000 min thresh: 0.654959912174367
##                                                     7000 min thresh: 0.654959912174367
##                                                     8000 min thresh: 0.649005786023745
##                                                     9000 min thresh: 0.475344114848811
##                                                    10000 min thresh: 0.401600176431921
##                                                    11000 min thresh: 0.27772240535126
##                                                    12000 min thresh: 0.267340666160447
##                                                    13000 min thresh: 0.199588639353924
##                                                    14000 min thresh: 0.182500684121413
##                                                    15000 min thresh: 0.163933685187828
##                                                    16000 min thresh: 0.148383549317606
##                                                    17000 min thresh: 0.139532960632404
##                                                    18000 min thresh: 0.133518041777579
##                                                    19000 min thresh: 0.133518041777579
##                                                    20000 min thresh: 0.133518041777579
##                                                    21000 min thresh: 0.133518041777579
##                                                    22000 min thresh: 0.133518041777579
##                                                    23000 min thresh: 0.109932468546218
##                                                    24000 min thresh: 0.0975334931437044
##                                                    25000 min thresh: 0.0975334931437044
##                                                    26000 min thresh: 0.0973396249843215
##                                                    27000 min thresh: 0.0841686858486113
##                                                    28000 min thresh: 0.072691239539679
##                                                    29000 min thresh: 0.072691239539679
##                                                    30000 min thresh: 0.0670714413418058
##                                                    31000 min thresh: 0.0665960007426352
##                                                    32000 min thresh: 0.0622821863781083
##                                                    33000 min thresh: 0.0618499857725966
##                                                    34000 min thresh: 0.0525346990358695
##                                                    35000 min thresh: 0.0525346990358695
##                                                    36000 min thresh: 0.0510783151975419
##                                                    37000 min thresh: 0.0495295269264467
##                                                    38000 min thresh: 0.0484691901251354
##                                                    39000 min thresh: 0.0484691901251354
##                                                    40000 min thresh: 0.0484691901251354
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##                                                    42000 min thresh: 0.0484691901251354
##                                                    43000 min thresh: 0.0480991981782021
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```
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##                                                     168000 min thresh: 0.0457330054582723
##                                                     169000 min thresh: 0.0457330054582723
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##                                                     171000 min thresh: 0.0457330054582723
##                                                     172000 min thresh: 0.0457330054582723
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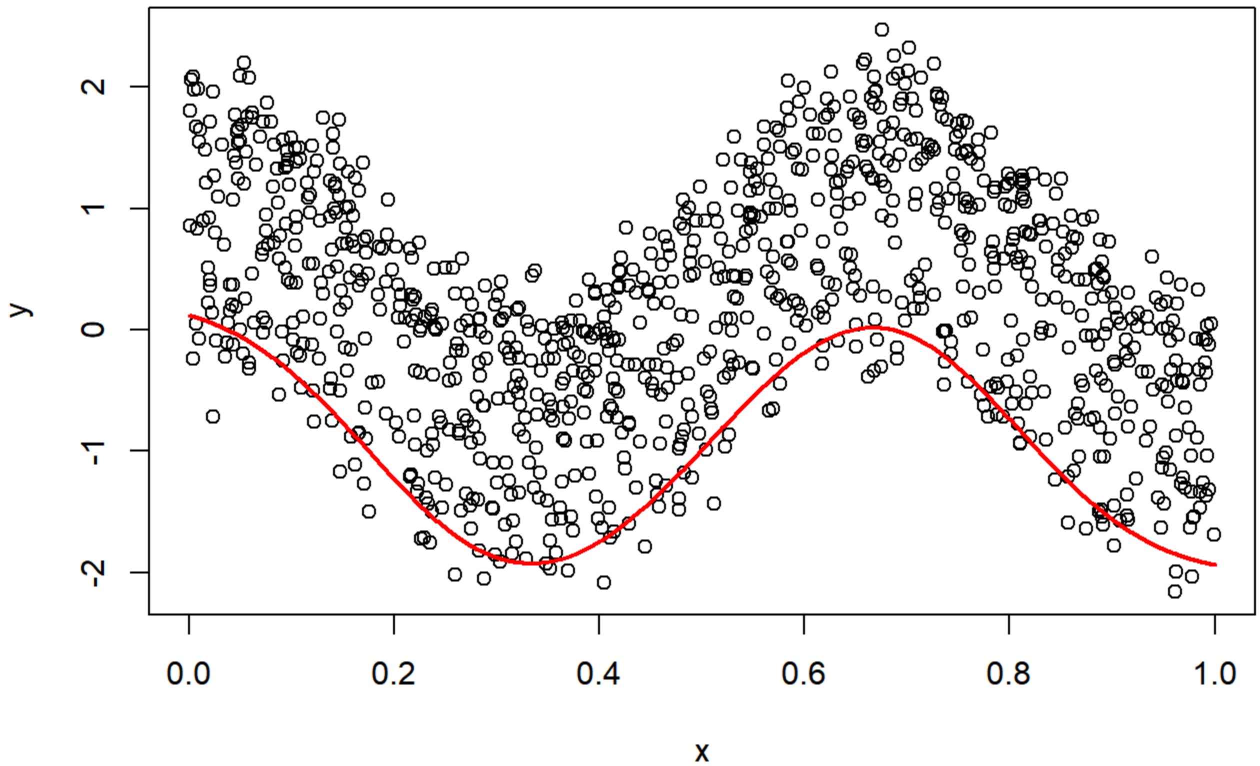
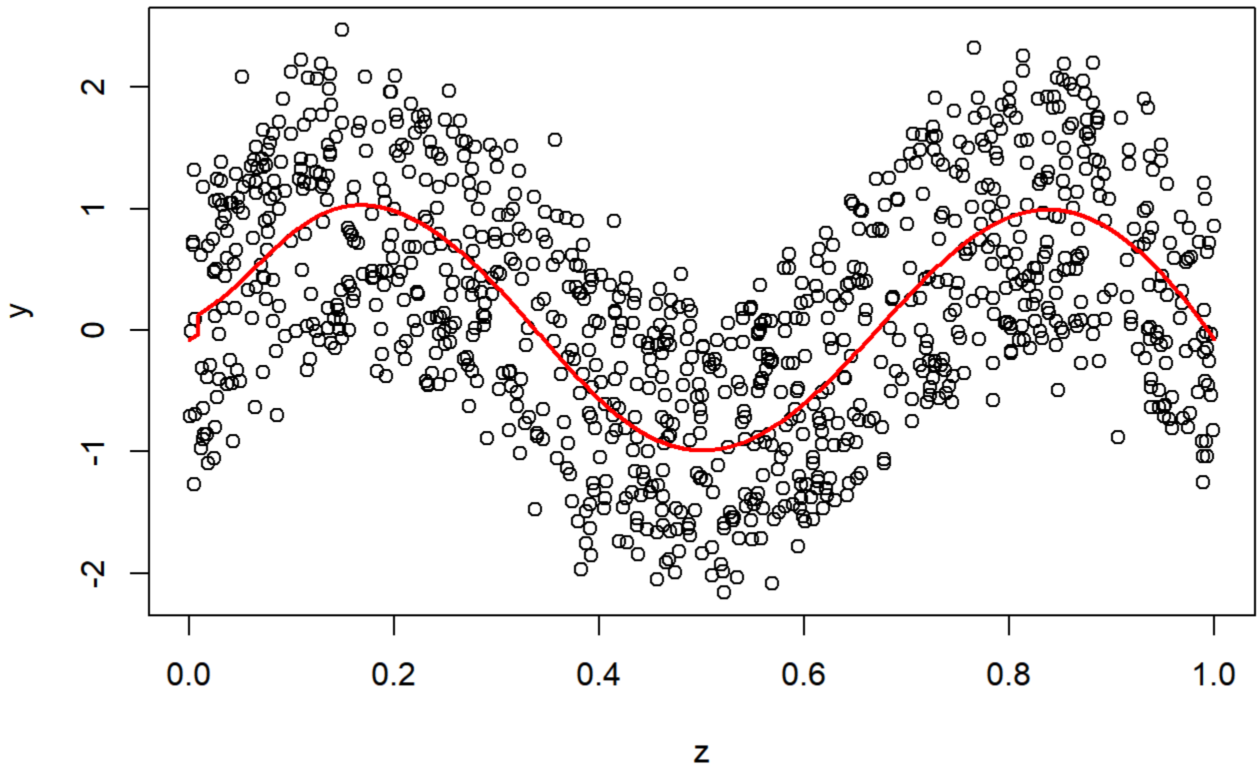
##                                                     174000 min thresh: 0.0457330054582723
##                                                     175000 min thresh: 0.0440154046246972
##                                                     176000 min thresh: 0.0432520726163966
##                                                     177000 min thresh: 0.038335051936843
##                                                     178000 min thresh: 0.0370389357177593
##                                                     179000 min thresh: 0.0345938639812086
##                                                     180000 min thresh: 0.0337330621299765
##                                                     181000 min thresh: 0.031783298390332
##                                                     182000 min thresh: 0.0288415900513552
##                                                     183000 min thresh: 0.0271979067323895
##                                                     184000 min thresh: 0.0249126656893411
##                                                     185000 min thresh: 0.0238520821918045
##                                                     186000 min thresh: 0.0212255028320159
##                                                     187000 min thresh: 0.0211669907892056
##                                                     188000 min thresh: 0.0201869225523252
##                                                     188359 error: 30.86721 time: 1.71 mins
```

```
plot(nn)
```

```
# z is constant
x.test = seq(0,1,by=0.001)
z.const = rep(0.5,length(x.test))
new.data=data.frame(x=x.test,z=z.const)
y.fit = predict(nn,newdata=new.data)
plot(y~x)
lines(y.fit~x.test,type="l",col="red",lwd=2)
```




```
# x is constant
z.test = seq(0,1,by=0.001)
x.const = rep(0.5,length(z.test))
new.data=data.frame(x=x.const,z=z.test)
y.fit = predict(nn,newdata=new.data)
plot(y~z)
lines(y.fit~z.test,type="l",col="red",lwd=2)
```



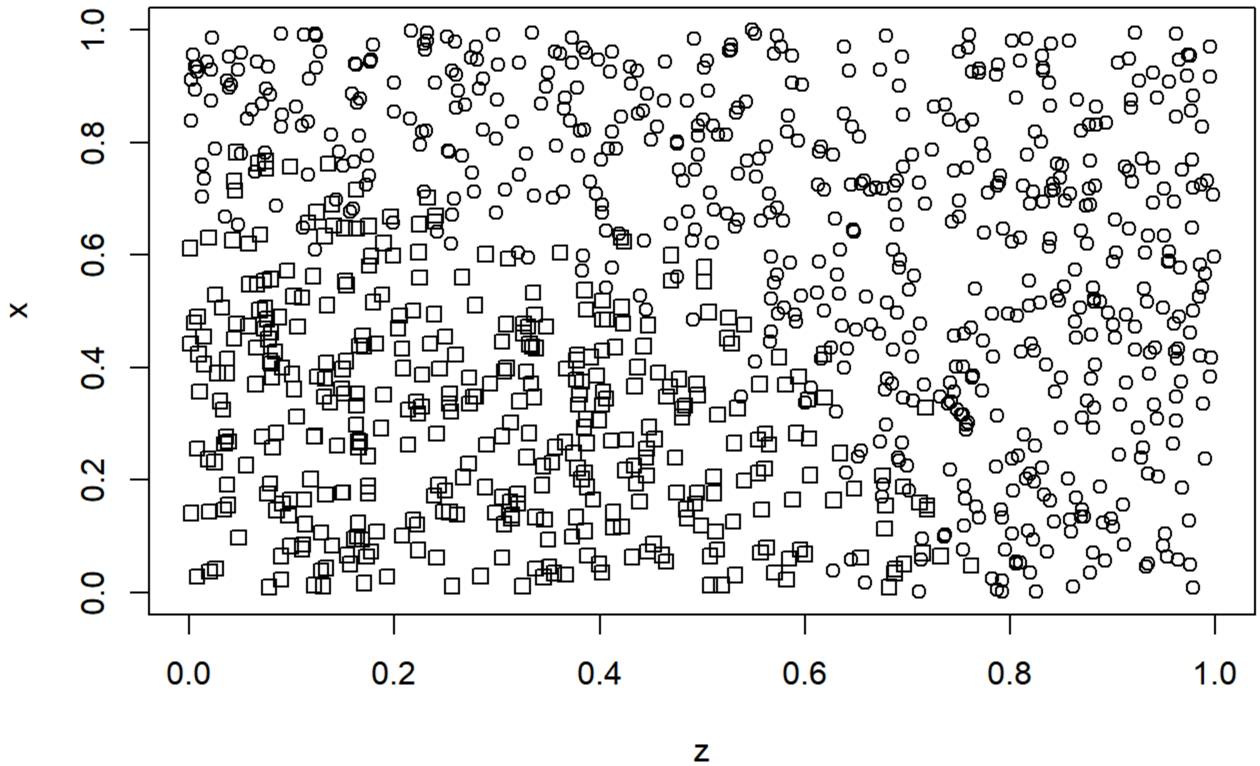
Classification

9. Now we will divide a square [0, 1] × [0, 1] of points whose components are uniformly distributed random variables into two classes: points that lie inside the circle belong to class 1, while points outside the circle, belong to class 2.

```
set.seed(1)
x=runif(1000)
z=runif(1000)
o=order(z) #from largest to smallest
# gernerate target variable which a categorical variable with classes 0 and 1
# and add some noise(uniformly distributed variables from interval-0.15,0.15)
# using rnuif() near the boundary
y=ifelse(x^2+z^2+runif(1000, min=-0.15, max=0.15)>0.5, 1, 0)
```

10. Plot the data.

```
plot(x~z, pch=y)
```




```
# pch parameter is for the shape of the dots on the graph
# we use target variable which either takes 0 or 1 to indicate which class
# each observations falls into
```

11. Create a data frame.

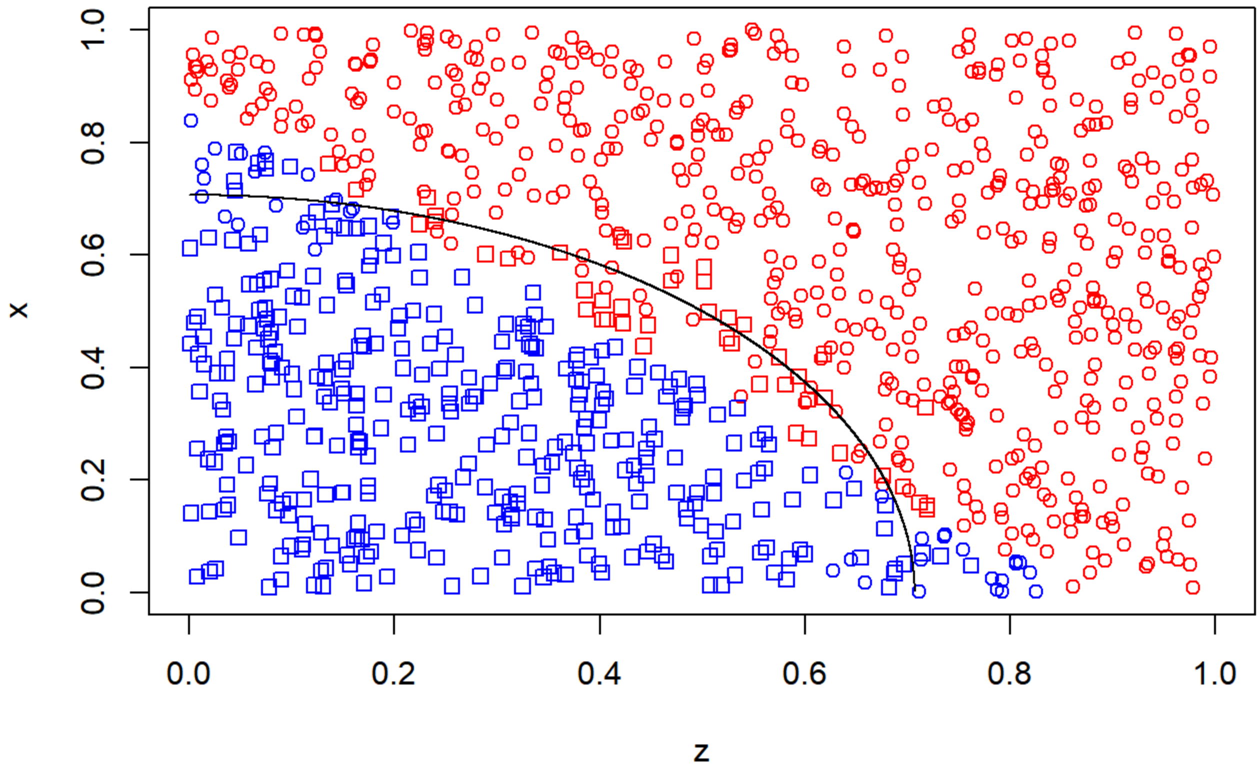
```
dat=data.frame(x,z,y) # a table with three columns x, y, and z
```

12. Build a logistic regression model. Use glm function to build a model, predict function to generate likelihoods, and ifelse function to perform classification.

```
glm.mod=glm(y~x+z, family=binomial) # logist regression is a generalized lm (thus glm)
# let's use threshold of 0.5 for classification of predicted probabilities
glm.class=ifelse(predict(glm.mod, type="response")>0.5, "red", "blue")
```

13. Plot data, logistic regression classifier and overlay the true classification boundary.

```
plot(x~z, pch=y, col=glm.class) # style shows true class, color predicted
z.plot=seq(from=0, to=sqrt(0.5), by=0.0001)
lines(sqrt(0.5-z.plot^2)~z.plot)
```



The logistic

model draws a linear boundary calssifier. It is possible to create a nonlinear boundry classifier with logistic regression model, but we will see that neural network with one hidden layer will solve this problem:

14. Fit neural network with one hidden layer.

```
# I did not specify in the question how many neurons to use in the hidden layer
# I chose 5 to start with
nn=neuralnet(factor(y)~x+z, data=dat, linear.output=FALSE,err.fct = 'ce', hidden=2, lifesign="full",likelih
ood = TRUE)
```

```
## hidden: 2    thresh: 0.01    rep: 1/1    steps:    1000  min thresh: 0.351568215742833
##                                                    2000  min thresh: 0.351568215742833
##                                                    3000  min thresh: 0.34348782700136
##                                                    4000  min thresh: 0.247442748339532
##                                                    5000  min thresh: 0.189832366581837
##                                                    6000  min thresh: 0.142197943124195
##                                                    7000  min thresh: 0.115942352723432
##                                                    8000  min thresh: 0.0961304987632295
##                                                    9000  min thresh: 0.0773203327127489
##                                                   10000  min thresh: 0.0661663508205158
##                                                   11000  min thresh: 0.057996059687797
##                                                   12000  min thresh: 0.0548970357408292
##                                                   13000  min thresh: 0.0499942185600567
##                                                   14000  min thresh: 0.0458102066635456
##                                                   15000  min thresh: 0.0458102066635456
##                                                   16000  min thresh: 0.0451102531697499
##                                                   17000  min thresh: 0.0354205391089424
##                                                   18000  min thresh: 0.0354205391089424
##                                                   19000  min thresh: 0.0354205391089424
##                                                   20000  min thresh: 0.0339548977179044
##                                                   21000  min thresh: 0.0339548977179044
##                                                   22000  min thresh: 0.0339548977179044
##                                                   23000  min thresh: 0.0330060332796814
##                                                   24000  min thresh: 0.0280730435647373
##                                                   25000  min thresh: 0.0280730435647373
##                                                   26000  min thresh: 0.0278107420770805
##                                                   27000  min thresh: 0.0263599669118729
##                                                   28000  min thresh: 0.0250385711654691
##                                                   29000  min thresh: 0.0224725372527359
##                                                   30000  min thresh: 0.0224725372527359
##                                                   31000  min thresh: 0.0224725372527359
##                                                   32000  min thresh: 0.0210243090515935
##                                                   33000  min thresh: 0.0200363909472427
##                                                   34000  min thresh: 0.0198505048893302
##                                                   35000  min thresh: 0.0184466368024244
##                                                   36000  min thresh: 0.0184466368024244
##                                                   37000  min thresh: 0.0184466368024244
##                                                   38000  min thresh: 0.0152058980741429
##                                                   39000  min thresh: 0.0152058980741429
##                                                   40000  min thresh: 0.0152058980741429
##                                                   41000  min thresh: 0.0152058980741429
##                                                   42000  min thresh: 0.0146908819741202
##                                                   43000  min thresh: 0.0146908819741202
##                                                   44000  min thresh: 0.0134206825551871
##                                                   45000  min thresh: 0.0130640776605731
##                                                   46000  min thresh: 0.0130640776605731
##                                                   47000  min thresh: 0.0127537430878616
##                                                   48000  min thresh: 0.0125113043885643
##                                                   49000  min thresh: 0.0116916581149704
##                                                   50000  min thresh: 0.0116916581149704
##                                                   51000  min thresh: 0.0116916581149704
##                                                   52000  min thresh: 0.0109298353357926
##                                                   53000  min thresh: 0.0109298353357926
##                                                   54000  min thresh: 0.0100839254360358
##                                                   55000  min thresh: 0.0100839254360358
```

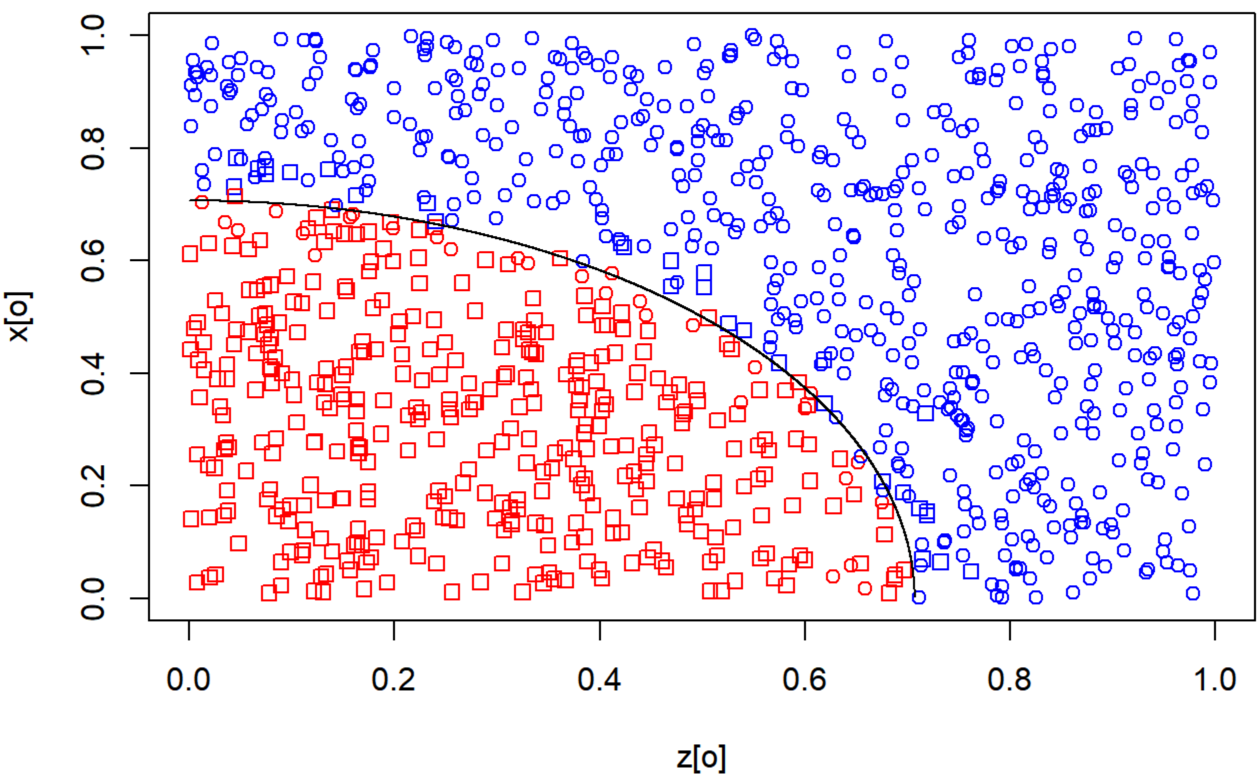
```
##                                                     56000  min thresh: 0.0100839254360358
##                                                     56766  error: 235.97027    aic: 495.94055   bic: 554.83
361  time: 15.19 secs
```

15. Perform classification based on predicted probabilities using 0.5 threshold.

```
y.classification = ifelse(predict(nn,newdata=dat)>0.5, "red", "blue")
```

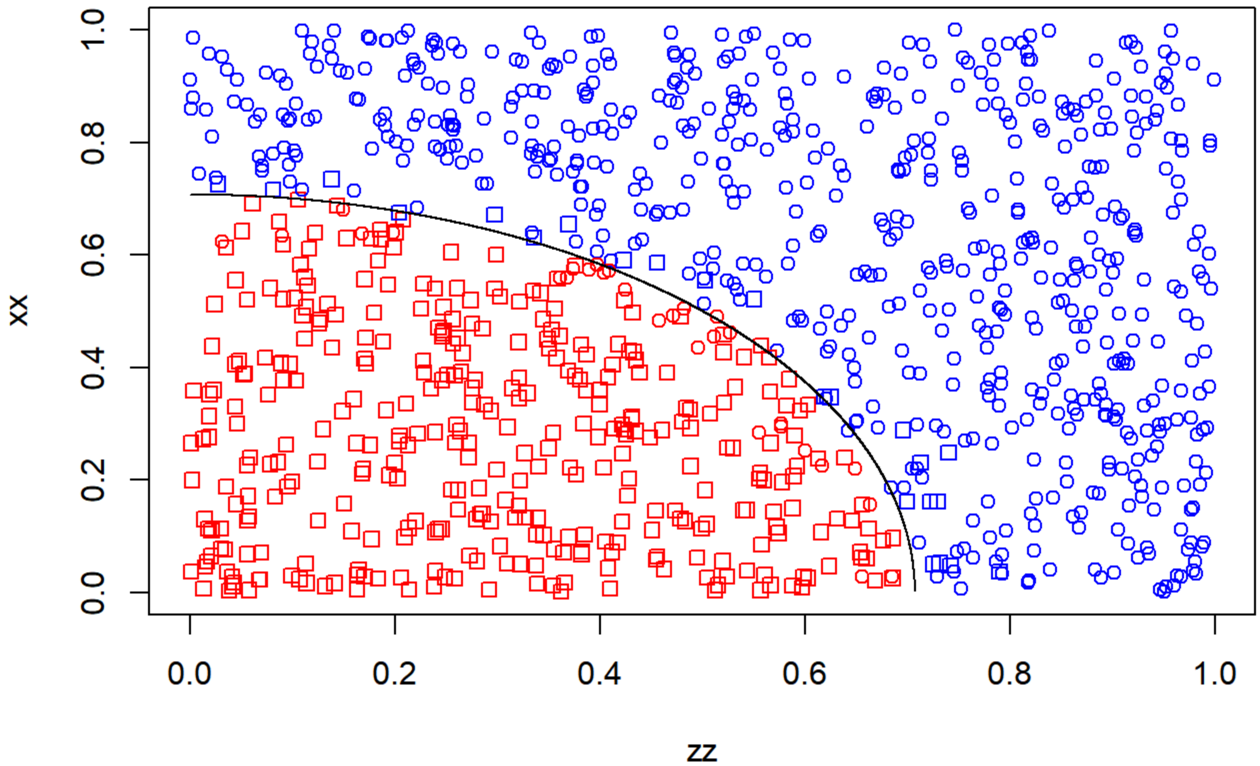
16. Plot the data and the NN classifier.

```
plot(x[o]~z[o], pch=y[o], col=y.classification[o])
z.plot=seq(from=0, to=sqrt(0.5), by=0.0001)
lines(sqrt(0.5-z.plot^2)~z.plot)
```



17. Does the model overfit the date? Apply the validation approach to answer this question.

```
xx=runif(1000)
zz=runif(1000)
yy=ifelse(xx^2+zz^2+runif(1000, min=-0.15, max=0.15)>0.5, 1, 0)
nn.class.p=ifelse(predict(nn, newdata =data.frame(x=xx, z=zz))>0.5, "red","blue")
plot(xx~zz, pch=yy, col=nn.class.p)
z.plot=seq(from=0, to=sqrt(0.5), by=0.0001)
lines(sqrt(0.5-z.plot^2)~z.plot)
```



xx
zz
0.0
0.2
0.4
0.6
0.8
1.0