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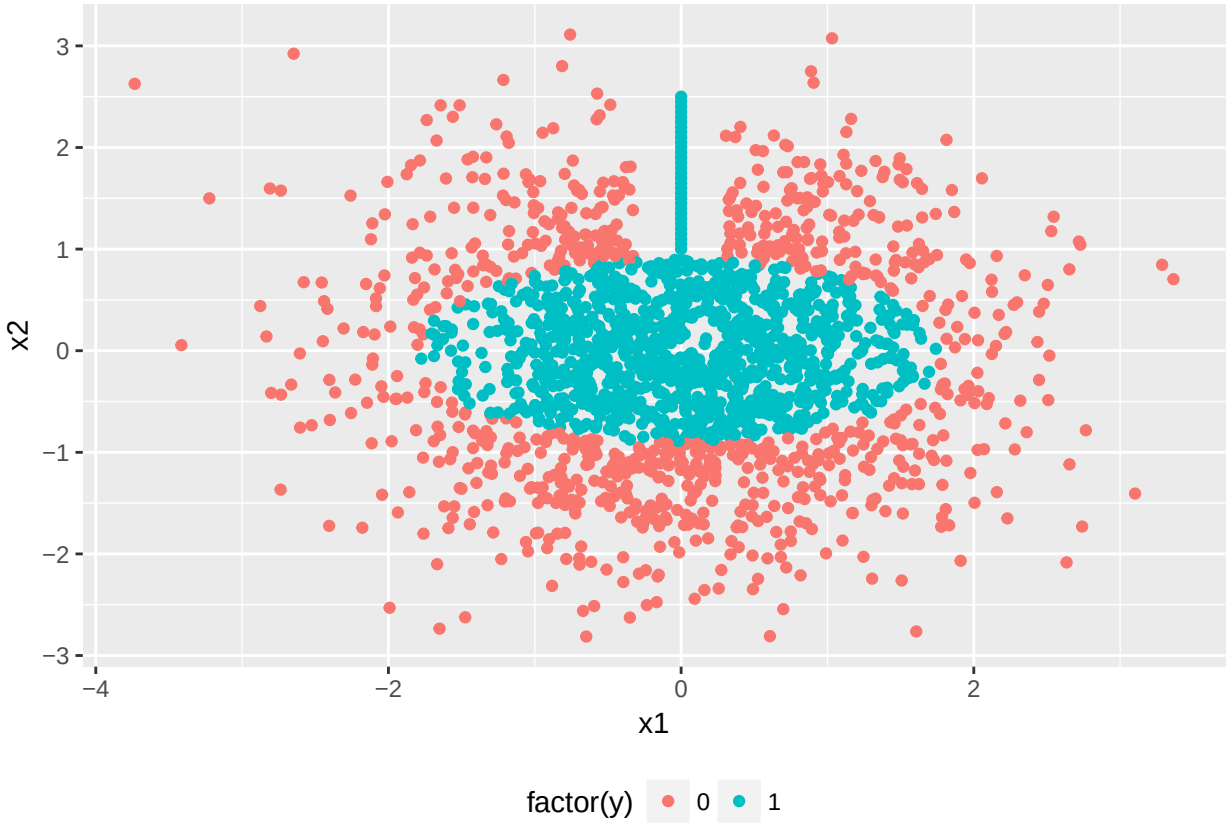
Math 504

Homework 12

2. In this problem you will implement a neural network to solve a classification problem. To keep things simple - since time is limited - the data will consist of covariates $x^{(i)} \in \mathbb{R}^2$ and a response $y_i \in \{0, 1\}$ for $i = 1, 2, \ldots, N$ (notice y takes on only two possible values). The classification problem involves fitting the model $y \sim f(x)$ over functions $f(x)$ that can be parameterized by our neural net, which is described below. The attached file `nn.txt` contains the samples. Each sample, corresponding to a row in the file, gives the three values $(x_1^{(i)}, x_2^{(i)}, y_i)$.

(a) Visualize the dataset by plotting it with different colors for the two classes of y.

```
setwd("G:\\math\\504");require(ggplot2,quietly=T)
nn<-read.table("nn.txt",header=T)
p <- ggplot(nn, aes(x1, x2)) + geom_point(aes(colour = factor(y))) +
  theme(legend.position="bottom");p
```



(b) Let η be the parameters of the neural net (i.e. all the α's and β's). What is the dimension of η in terms of m?

$$\dim(\eta) = m \cdot (2+3) + 2$$

(c) Write a function $NN(x, \eta, m)$ which takes a sample $x \in \mathbb{R}^2$ and a choice for η and returns the values of Y_1 and Y_2. (Hint: It may be helpful to write functions such as `get_alpha(eta, i)`, which given η and i returns $\alpha^{(i)}$, and `get_alpha_0(eta, i)`, which given η and i returns $\alpha_0^{(i)}$. Using such functions will greatly simplify your code.)

```
sigmoid<-function(a,w){ (1+exp(-a[1]-apply(w,1, function(w)  t(a[-1])%*%w ) ))^(-1)}

NN<-function(x,eta,m){

    X<-as.matrix(x)

    Alpha<-matrix(eta[1:prod( c(dim(X)[2] + 1, m ) )], dim(X)[2] + 1 , m)
    Z<-apply(Alpha,2, function(v) sigmoid(v,X))

    Beta<-matrix( eta[(prod(dim(Alpha))+1):length(eta) ], dim(Z)[2]+1, 2)

    T<-apply(Beta,2, function(v) sigmoid(v,Z))
    Y<- apply(T,2, function(x) exp(x))
    Y<-Y/rowSums(Y)
    return(Y)
}

head( NN(nn[,-3],  runif(22,-1,1) , 4) )
```

```
##           [,1]      [,2]
## [1,] 0.6075932 0.3924068
## [2,] 0.5824194 0.4175806
## [3,] 0.6133456 0.3866544
## [4,] 0.5936146 0.4063854
## [5,] 0.5994467 0.4005533
## [6,] 0.6097807 0.3902193
```

(d) Explain why the log likelihood function $\log L(\eta)$ for the neural net is given by

$$\log L(\eta) = \sum_{i=1}^{N} (1 - y_i) \log(Y_1) + y_i \log(Y_2). \tag{1}$$

(In class, when I wrote the log likelihood, I forgot the log on the Y_1 and Y_2!) Write a function that computes $\log L(\eta)$ (you will need to pass the data to the function). Write a function that uses finite difference to compute the gradient of $\log L(\eta)$.

We are trying to classify each data point by a function that approximates $P(Y|X)$. This is similar to logistic (or other binary regression) because we have two classes and we can derive the likelihood in the same way. Let $\pi = P(y = 1|x)$.

$$\mathcal{L}(\eta) = \prod_{i=1}^{N} pi_i^{y_i}(1-pi_i)^{1-y_i}$$
$$\ell(\eta) = \sum_{i=1}^{N} y_i \log(\pi_i) + (1-y_i)\log(1-\pi_i)$$

For our neural net, we know our $Y_1 \sim P(y=0|x)$ and $Y_2 \sim P(y=1|x)$, so:

$$\begin{aligned}\ell(\eta) &= \sum_{i=1}^{N}(1-y_i)\log(1-\pi_i) + y_i\log(\pi_i) \\ &= \sum_{i=1}^{N}(1-y_i)\log(Y_1) + y_i\log(Y_2).\end{aligned}$$

```
gradL<-function(eta,x,y,m ){

    y<-as.matrix(y)
    dimeta<-m*(dim(x)[2]+1)+2*(1+m)
    gradf<-rep(NA,dimeta)

    Y<-NN(x,eta,m)
    ETA<-eta

    logl<-sum( (1-y)*log(Y[,1]) + ( y)*log(Y[,2])  )
    for( i in 1:dimeta){

        ETA[i]<-eta[i]+(10^-6)

        Yp<-NN(x,ETA,m)

        gradf[i]<-(sum( (1-y)*log(Yp[,1]) + ( y)*log(Yp[,2])  ) - logl  ) / (10^-6) }

    return(gradf)
}

gradL(runif(22,-1,1),nn[,-3],nn[,3],4)
```

```
##  [1]  -1.264570  -1.097999  -1.571286  -6.280004  -5.606430  -4.035833
##  [7]   3.967688   1.454933   6.608245   6.557200   6.862346   6.640199
## [13] -15.389007 -32.084048 -38.248082 -45.026807 -63.683950 -42.982801
## [19] -27.934155 -22.452417 -15.535959   2.081133
```

(e) Set $m = 4$ and train your neural net by maximizing the $\log L(\eta)$ using steepest ascent. (It took me roughly 45 minutes of run time to get a good fit, roughly 3000 iterations. Your results may vary from this depending on implemenation and hardware.)

```
logL<-function(x,y,eta,m){
    Y<-NN(x,eta,m)
    return( sum( (1-y)*log(Y[,1]) + ( y)*log(Y[,2])  ) )    }

j=1;current_grad <- gradL(Alpha , X , nn[,3] , 4 )

for(i in j:(3000)) {

    d <- current_grad/Norm(current_grad)

    s <- 1
    current_logL <- logL(X,nn[,3],Alpha,4)

    while(logL(X,nn[,3],Alpha+s*d,4)  < current_logL)
         s <- s/2

  Alpha <- Alpha + s*d
  current_grad <-  gradL(Alpha , X , nn[,3] , 4 ) }
```

```
#Alpha is eta (alphas and betas)
Alpha
```

```
##  [1]  -3.7748365   2.1178734   0.3139542  -5.5415006  -0.5958018
##  [6]   5.8168459  11.0561352   0.2074085  14.0207743  25.2868297
## [11]  16.0428078   3.8300725  15.9792114  23.4815794  23.2210775
## [16] -13.5097426 -12.2073593 -18.6510642 -27.0546378 -27.4979835
## [21]  15.2350215  14.7081561
```

(f) Remember that a classifier in this case is a function $F(x) : \mathbb{R}^2 \to \{0, 1\}$, where $x \in \mathbb{R}^2$. Once you choose η by by computing the maximum likelihood in (e), choose a cutoff $p \in [0, 1]$. Set F by

$$F(x) = \begin{cases} 0 & \text{if } Y_1(x, \eta) < p \\ 1 & \text{if } Y_1(x, \eta) \geq p \end{cases} \tag{2}$$

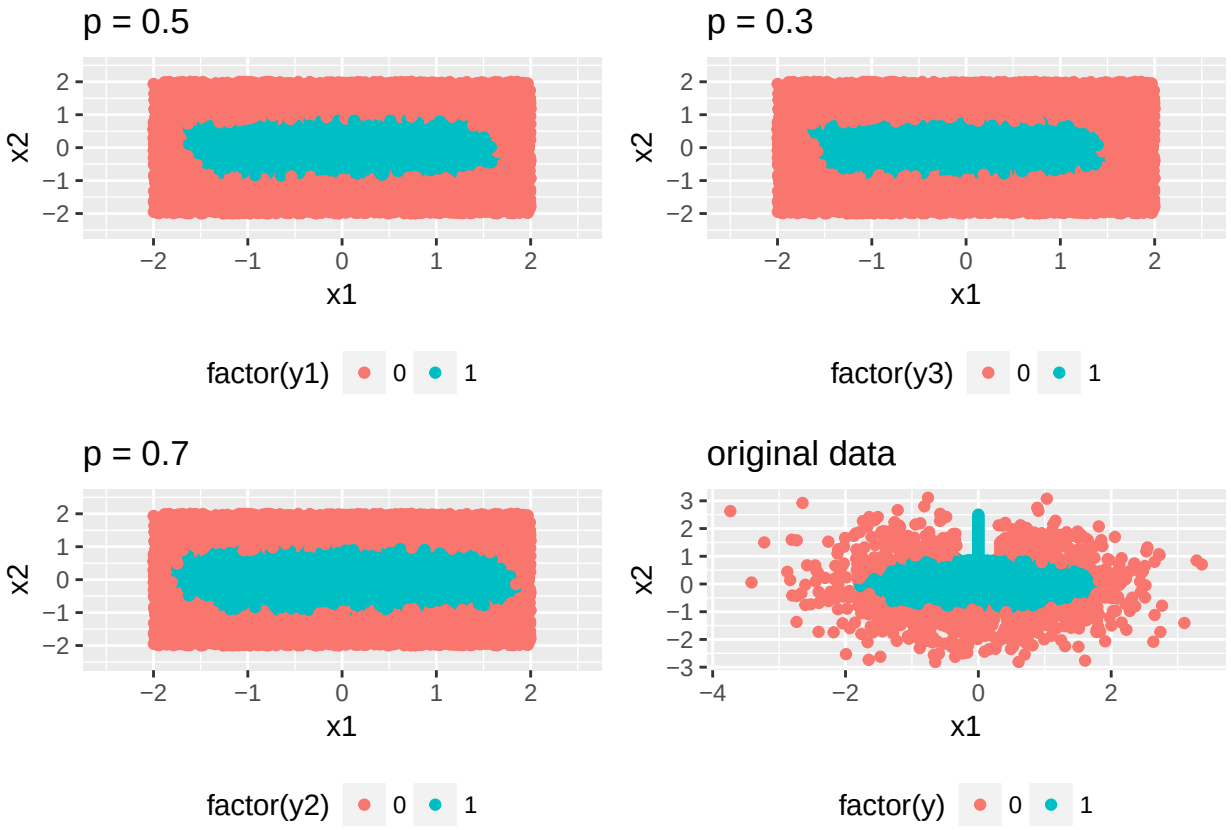
Try different value of p and for each p, visualize your classifier. You can do this in any way you like, but here is one way. Generate many points in $\mathbb{R}^2$, determine the predicted class of each using your classifier, and then plot as in part (a). You can generate random coordinates within $[-2, 2]$, which is roughly where all the data points lie, using

```
x1 <- 4*runif(10000) - 2
x2 <- 4*runif(10000) - 2
```

`runif(10000)` generates 10000 numbers uniformly distributed on $[0, 1]$.

```
x1<-matrix(4*runif(20000 )-2, 10000,2)
test<-as.data.frame((NN(x1,Alpha ,4)))
test<-cbind(test,x1)
test$y1<- ifelse( test[,1]>.5 , 0,1)
test$y2<- ifelse( test[,1]>.7 , 0,1)
test$y3<- ifelse( test[,1]>.3 , 0,1)
names(test)[3:4]<-c("x1","x2")

p1 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y1))) +
```

```
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.5") +
  theme(legend.position="bottom")
p2 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y2))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.7") +
  theme(legend.position="bottom")
p3 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y3))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.3") +
  theme(legend.position="bottom")
p<- p + ggtitle("original data")
multiplot(p1, p2, p3,p,  cols=2)
```



(g) Now repeat (e) and (f), but in your log likelihood, include a penalty term of the form,

$$\rho\left(\sum_{i=1}^{m}\|\alpha^{(i)}\|^2+\sum_{j=1}^{2}\|\beta^{(j)}\|^2\right). \tag{3}$$

Given that we are maximizing, explain why you should subtract the penalty term rather than add it onto the log-likelihood in (d). Train your net with several values of ρ, visualize the resulting classifier for differnt p, and compare your results.

We wish to maximize the likelihood (or alternatively the log-likelihood) so in order to impose a penalty we will reduce the likelihood. This is done by subtracting the penalty term rather than adding it.

```
PlogL<-function(x,y,eta,m,rho){
    X<-as.matrix(x)
    ALPHA<-matrix(eta[1:prod( c(dim(X)[2] + 1, m ) )], dim(X)[2] + 1 , m)
    Beta<-matrix(eta[(prod( c(dim(X)[2] + 1, m ) )+1):length(eta)],
        m+1,2)
    ALPHA<-as.vector(t(ALPHA[-1 ,])) ;Beta<-as.vector(t(Beta[-1 ,]))
  Norm <- function(w){  sqrt(sum(w^2))}

    Y<-NN(x,eta,m)
    return( sum( (1-y)*log(Y[,1]) + ( y)*log(Y[,2])  ) -
        rho*(sum(Norm(ALPHA)^2)+sum(Norm(Beta)^2) )
    )   }
```

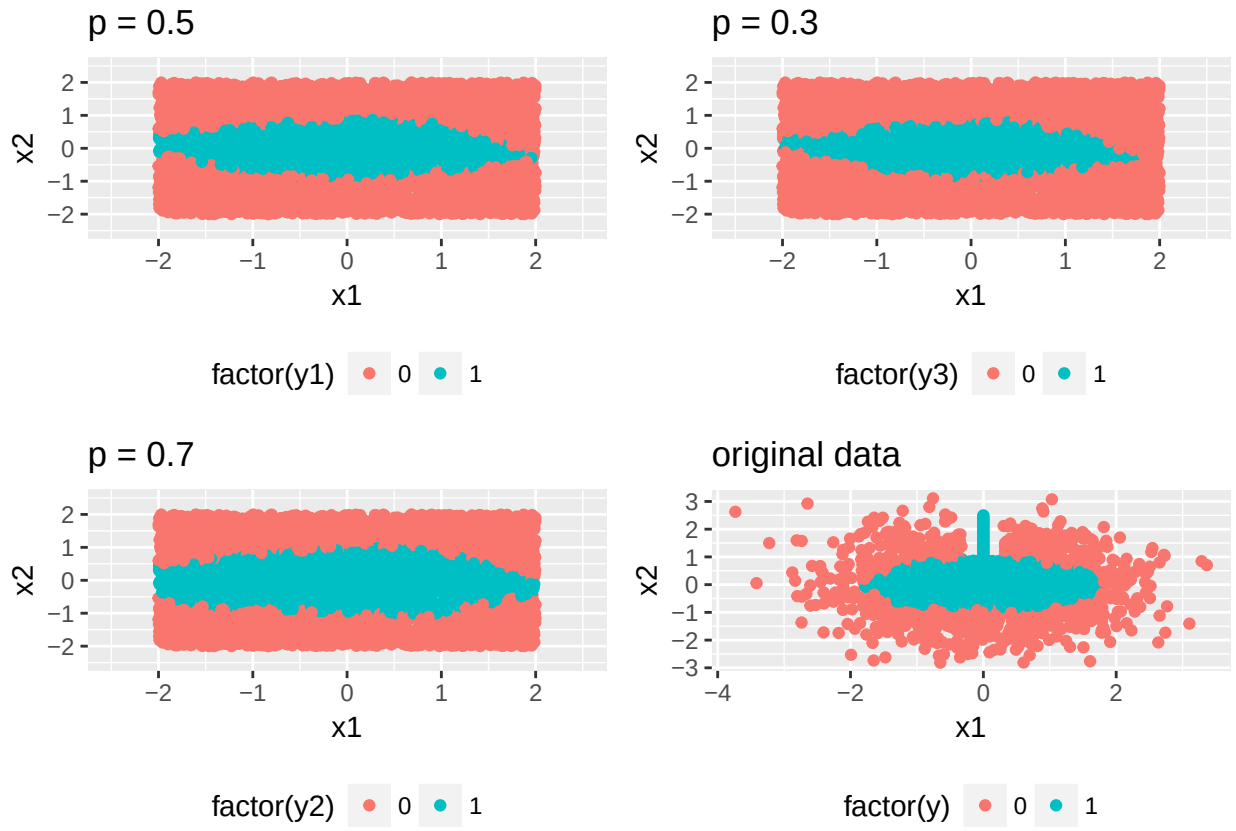
$\rho = 0.1$

```
j=1;current_grad <- gradL(Alpha , X , nn[,3] , 4 )
system.time(
 for(i in j:(2000)) {
    #iter <- iter + 1

    d <- current_grad/Norm(current_grad)

    s <- 1
    #current_logL <- logL(X,nn[,3],Alpha,4)
    current_logL <- PlogL(X,nn[,3],Alpha,4,100)

    while(logL(X,nn[,3],Alpha+s*d,4)  < current_logL)
         s <- s/2

    # update
    Alpha <- Alpha + s*d
    current_grad <-  gradL(Alpha , X , nn[,3] , 4 ) } )


j=i
```

```
##  [1]  -4.217173   2.129696   2.291096  -5.749465  -1.505578   5.422963
##  [7]  10.917247  -2.730573  12.886107  10.326642   5.094741   9.110171
## [13]  13.503592  21.919573  22.305991 -10.991376 -10.851156 -14.688772
## [19] -23.092542 -24.351591  12.003044  12.654236
```

```
x1<-matrix(4*runif(10000 )-2, 5000,2)
test<-as.data.frame((NN(x1,Alpha ,4)))
test<-cbind(test,x1)
test$y1<- ifelse( test[,1]>.5 , 0,1)
test$y2<- ifelse( test[,1]>.7 , 0,1)
test$y3<- ifelse( test[,1]>.3 , 0,1)
```

```r
names(test)[3:4]<-c("x1","x2")

p1 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y1))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.5") +
  theme(legend.position="bottom")
p2 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y2))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.7") +
  theme(legend.position="bottom")
p3 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y3))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.3") +
  theme(legend.position="bottom")

multiplot(p1, p2, p3,  p,cols=2)
```



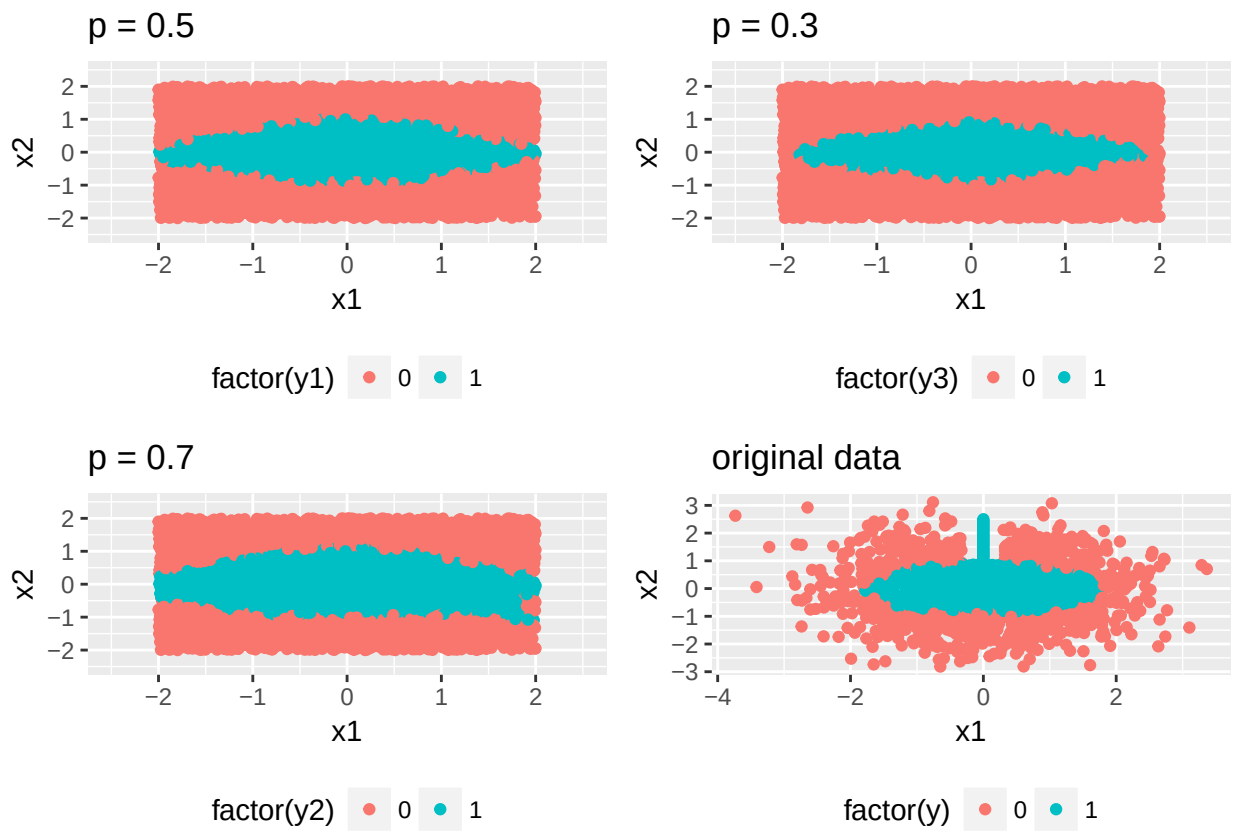
$\rho = 1$

```r
j=1;current_grad <- gradL(Alpha , X , nn[,3] , 4 )
system.time(
 for(i in j:(2000)) {
    #iter <- iter + 1

    d <- current_grad/Norm(current_grad)
```

```
    s <- 1
    current_logL <- PlogL(X,nn[,3],Alpha,4,1)

    while(logL(X,nn[,3],Alpha+s*d,4)  < current_logL)
         s <- s/2

    Alpha <- Alpha + s*d
    current_grad <-  gradL(Alpha , X , nn[,3] , 4 ) } )


j=i
```

```
##  [1]  -5.012726   2.095720   3.540725  -5.324588  -2.108554   3.957979
##  [7]   9.760088  -4.196175   9.938802   6.688340   2.643233   7.210336
## [13]  15.743670  24.279396  24.855088 -12.204780 -14.039753 -18.199320
## [19] -26.719915 -28.098740  13.621660  15.881839
```

```
x1<-matrix(4*runif(10000 )-2, 5000,2)
test<-as.data.frame((NN(x1,Alpha ,4)))
test<-cbind(test,x1)
test$y1<- ifelse( test[,1]>.5 , 0,1)
test$y2<- ifelse( test[,1]>.7 , 0,1)
test$y3<- ifelse( test[,1]>.3 , 0,1)
names(test)[3:4]<-c("x1","x2")

p1 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y1))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.5") +
  theme(legend.position="bottom")
p2 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y2))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.7") +
  theme(legend.position="bottom")
p3 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y3))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.3") +
  theme(legend.position="bottom")

multiplot(p1, p2, p3,  p, cols=2)
```



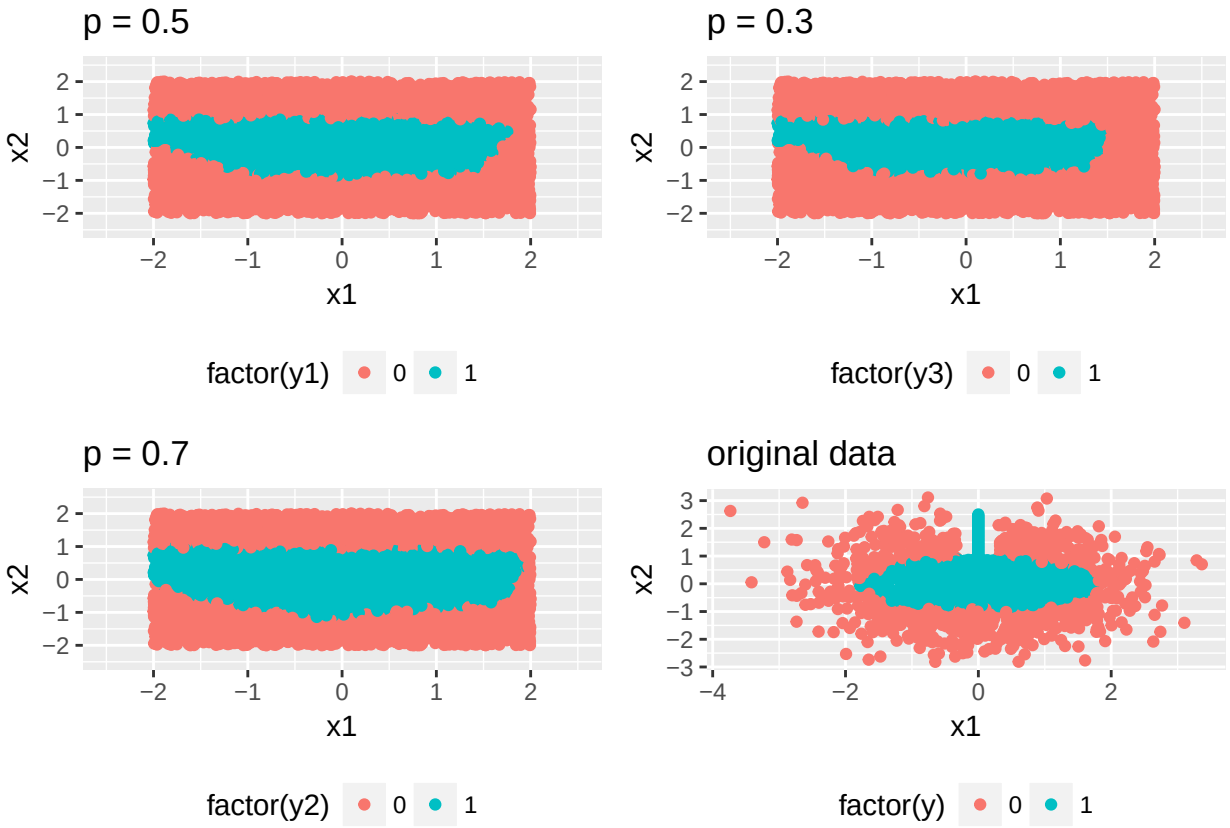
$\rho = 100$

```
j=1;current_grad <- gradL(Alpha , X , nn[,3] , 4 )
system.time(
 for(i in j:(2000)) {

    d <- current_grad/Norm(current_grad)

    s <- 1
    current_logL <- PlogL(X,nn[,3],Alpha,4,100)

    while(logL(X,nn[,3],Alpha+s*d,4)  < current_logL)
         s <- s/2

    Alpha <- Alpha + s*d
    current_grad <-  gradL(Alpha , X , nn[,3] , 4 ) } )


j=i
```

```
##  [1]  -4.80870303   2.51425207  -0.70430171  -8.39809328   0.07027287
##  [6]   8.89975250  13.39129423   0.16705617  16.70429985  19.56583078
## [11]  10.80716806  10.69527465  12.34268115  20.81992539  21.16594983
## [16]  -9.72328246 -10.27706135 -12.66218131 -21.14339824 -22.67591064
```

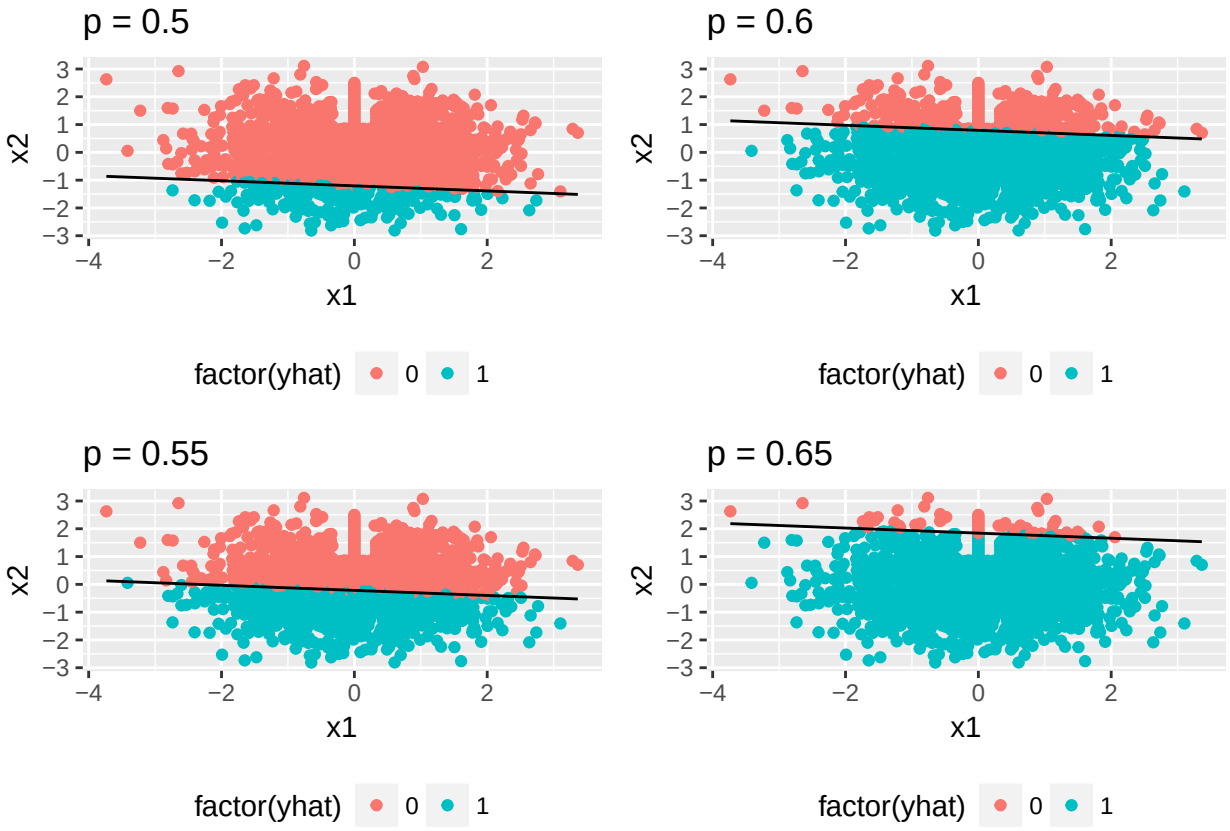
```
## [21]   9.49389847  10.38622987
```

```
x1<-matrix(4*runif(10000 )-2, 5000,2)
test<-as.data.frame((NN(x1,Alpha ,4)))
test<-cbind(test,x1)
test$y1<- ifelse( test[,1]>.5 , 0,1)
test$y2<- ifelse( test[,1]>.7 , 0,1)
test$y3<- ifelse( test[,1]>.3 , 0,1)
names(test)[3:4]<-c("x1","x2")

p1 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y1))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.5") +
  theme(legend.position="bottom")
p2 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y2))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.7") +
  theme(legend.position="bottom")
p3 <- ggplot(test, aes(x1, x2)) + geom_point(aes(colour = factor(y3))) +
  ylim(-2.5, 2.5) + xlim( -2.5,2.5 ) + ggtitle("p = 0.3") +
  theme(legend.position="bottom")

multiplot(p1, p2, p3, p,  cols=2)
```



3. Repeat problem 2, but now use a logistic regression to build your classifier. How does the logistic regression classifier compare to the neural net classifier?

```
nn.fit<-glm(y~.,data = nn, family = "binomial")
logclass<-cbind(nn,predict(nn.fit,type="response"))

logclass$yhat<-ifelse( logclass[,4]> .5 , 0,1)
p1 <- ggplot(logclass, aes(x1, x2)) + geom_point(aes(colour = factor(yhat))) +
    stat_function(fun=function(x){ -(0.2447 /0.2031 ) -(0.0186*x/0.2031 ) -
    (log((1/.5)-1) /0.2031 ) }, geom="line" , color = "black") + ggtitle("p = 0.5")+
  theme(legend.position="bottom")

logclass$yhat<-ifelse( logclass[,4]> .55 , 0,1)
p2 <- ggplot(logclass, aes(x1, x2)) + geom_point(aes(colour = factor(yhat))) +
    stat_function(fun=function(x){ -(0.2447 /0.2031 ) -(0.0186*x/0.2031 ) -
    (log((1/.55)-1) /0.2031 ) },    geom="line" , color = "black") + ggtitle("p = 0.55")+
  theme(legend.position="bottom")

logclass$yhat<-ifelse( logclass[,4]> .6 , 0,1)
p3<- ggplot(logclass, aes(x1, x2)) + geom_point(aes(colour = factor(yhat))) +
    stat_function(fun=function(x){ -(0.2447 /0.2031 ) -(0.0186*x/0.2031 ) -
    (log((1/.6)-1) /0.2031 ) }, geom="line" , color = "black") + ggtitle("p = 0.6")+
  theme(legend.position="bottom")

logclass$yhat<-ifelse( logclass[,4]> .65 , 0,1)
p4 <- ggplot(logclass, aes(x1, x2)) + geom_point(aes(colour = factor(yhat))) +
    stat_function(fun=function(x){ -(0.2447 /0.2031 ) -(0.0186*x/0.2031 ) -
    (log((1/.65)-1) /0.2031 ) },    geom="line" , color = "black") + ggtitle("p = 0.65")+
  theme(legend.position="bottom")

multiplot(p1, p2, p3, p4,  cols=2)
```


p = 0.5
p = 0.6
p = 0.55
p = 0.65
x1
x2
factor(yhat)
0
1