SDS385 Fall '16: Statistical Models For Big Data
Exercises 01 - Generalized linear models

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A)

The negative log-likelihood can be rewritten like this:

$$
\begin{aligned}
l(\beta) &= -\log\left\{\prod_{i=1}^{N} p(y_i|\beta)\right\} \\
&= -\log\left[\prod_{i=1}^{N}\binom{m_i}{y_i} w_i^{y_i}(1-w_i)^{m_i-y_i}\right] \\
&= c - \sum_{i=1}^{N} y_i \log(w_i) - \sum_{i=1}^{N} m_i \log(1-w_i) + \sum_{i=1}^{N} y_i \log(1-w_i) \\
&= c - \sum_{i=1}^{N} y_i \log\left(\frac{w_i}{1-w_i}\right) - \sum_{i=1}^{N} m_i \log(1-w_i) \\
&= c - \sum_{i=1}^{N} y_i \log\left(\frac{1}{e^{-x_i^T\beta}}\right) - \sum_{i=1}^{N} m_i \log\left(\frac{e^{-x_i^T\beta}}{1+e^{-x_i^T\beta}}\right) \\
&= c - \sum_{i=1}^{N} y_i x_i^T\beta + \sum_{i=1}^{N} m_i x_i^T\beta + \sum_{i=1}^{N} m_i \log(1+e^{-x_i^T\beta}) \\
&\approx \sum_{i=1}^{N}(m_i - y_i)x_i^T\beta + \sum_{i=1}^{N} m_i \log(1+e^{-x_i^T\beta})
\end{aligned}
$$

Its gradient is:

$$\begin{aligned}
\nabla l(\beta) &= \nabla \left(\sum_{i=1}^{N} (m_i - y_i) x_i^T \beta + \sum_{i=1}^{N} m_i \log(1 + e^{-x_i^T \beta}) \right) \\
&= \sum_{i=1}^{N} (m_i - y_i) x_i + \sum_{i=1}^{N} m_i w_i e^{-x_i^T \beta} (-x_i) \\
&= \sum_{i=1}^{N} m_i x_i - \sum_{i=1}^{N} y_i x_i - \sum_{i=1}^{N} m_i (1 - w_i) x_i \\
&= - \sum_{i=1}^{N} y_i x_i + \sum_{i=1}^{N} m_i w_i x_i \\
&= \sum_{i=1}^{N} (m_i w_i - y_i) x_i = \sum_{i=1}^{N} (\hat{y} - y_i) x_i = X^T S
\end{aligned}$$

where S is a vector with i-th element $m_i w_i - y_i$.

B)

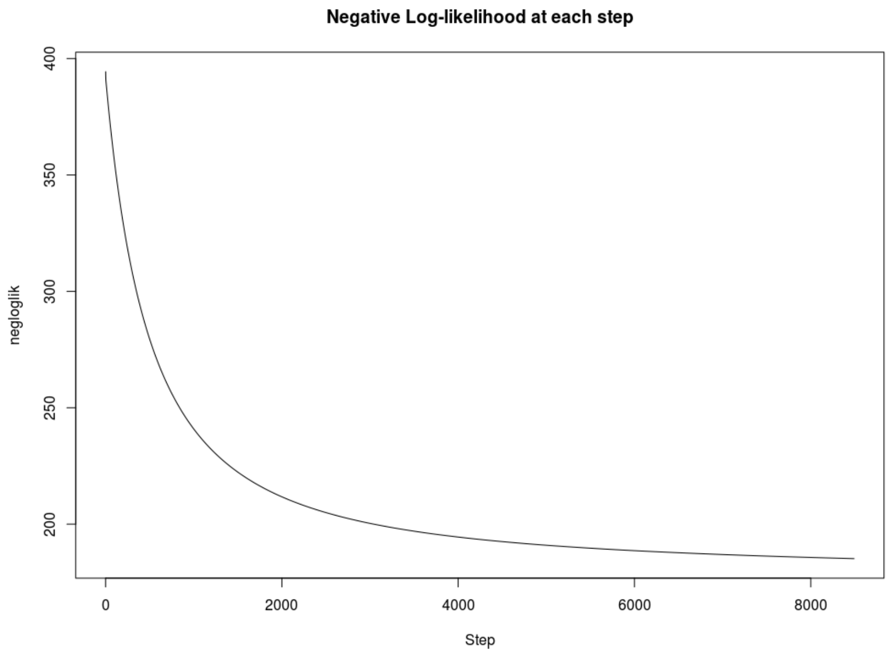
The gradient descent updates at each step the values of our estimated β using this formula:

$$\beta_{t+1} = \beta_t - a \nabla l(\beta_t)$$

with a being the step size. Running the code in appendix, we can obtain the following $\hat{\beta}$:

c	-0.0033014219
V3	-0.0231821340
V4	-0.0174151223
V5	-0.1233097211
V6	0.0182791149
V7	-0.0001358173
V8	0.0004527453
V9	0.0008734747
V10	0.0003869764
V11	-0.0002857808
V12	-0.0001459426

The following graph of the objective function shows us that indeed it's being decreased at each step.



C)

The Hessian is:

$$
\begin{aligned}
\nabla^2 l(\beta) &= \nabla\left(-\sum_{i=1}^{N} y_i x_i + \sum_{i=1}^{N} m_i w_i x_i\right) \\
&= \nabla\left(c + \sum_{i=1}^{N} m_i x_{i1} \frac{1}{1+e^{-x_i^T\beta}} \ , \ \dots \ , \ c + \sum_{i=1}^{N} m_i x_{iP} \frac{1}{1+e^{-x_i^T\beta}}\right) \\
&= \begin{bmatrix}
\sum_{i=1}^{N} m_i x_{i1} \frac{-e^{-x_i^T\beta}}{\left(1+e^{-x_i^T\beta}\right)^2}(-x_{i1}) & \cdots & \sum_{i=1}^{N} m_i x_{i1} \frac{-e^{-x_i^T\beta}}{\left(1+e^{-x_i^T\beta}\right)^2}(-x_{iP}) \\
\vdots & \ddots & \vdots \\
\sum_{i=1}^{N} m_i x_{iP} \frac{-e^{-x_i^T\beta}}{\left(1+e^{-x_i^T\beta}\right)^2}(-x_{i1}) & \cdots & \sum_{i=1}^{N} m_i x_{iP} \frac{-e^{-x_i^T\beta}}{\left(1+e^{-x_i^T\beta}\right)^2}(-x_{iP})
\end{bmatrix} \\
&= \begin{bmatrix}
\sum_{i=1}^{N} m_i x_{i1} x_{i1} w_i(1-w_i) & \cdots & \sum_{i=1}^{N} m_i x_{i1} x_{iP} w_i(1-w_i) \\
\vdots & \ddots & \vdots \\
\sum_{i=1}^{N} m_i x_{iP} x_{i1} w_i(1-w_i) & \cdots & \sum_{i=1}^{N} m_i x_{iP} x_{iP} w_i(1-w_i)
\end{bmatrix} = X^T D X
\end{aligned}
$$

where D is a diagonal matrix with ii-th element $m_i w_i(1-w_i)$. Notice that all the values on the diagonal are positive: this means that the Hessian is defined positive and that our objective function is convex. Then, considering that we can ignore the constant values adding and subtracting them as we need, we can obtain the requested result like this:

$$
\begin{aligned}
q_l(\beta, \beta_0) &= l(\beta_0) + \nabla(\beta_0)^T(\beta - \beta_0) + \frac{1}{2}(\beta - \beta_0)^t \nabla^2(\beta_0)(\beta - \beta_0) \\
&= c + S^T X(\beta - \beta_0) + \frac{1}{2}(\beta - \beta_0)^T X^T D X(\beta - \beta_0) \\
&= c + S^T X\beta + \frac{1}{2}\beta^T X^T D X\beta - \frac{1}{2}\beta^T X^T D X\beta_0 - \frac{1}{2}\beta_0^T X^T D X\beta_0 \\
&= c - (\beta_0^T X^T D - S^T)X\beta + \frac{1}{2}\beta^T X^T D X\beta \\
&= c - (\beta_0^T X^T D - S^T)D^{-1} D X\beta + \frac{1}{2}\beta^T X^T D X\beta \\
&\quad + \frac{1}{2}(\beta_0^T X^T D - S^T)D^{-1} D D^{-1}(\beta_0^T X^T D - S^T)^T \\
&= c + \frac{1}{2}[D^{-1}(\beta_0^T X^T D - S^T)^T - X\beta]^T D[(D^{-1}(\beta_0^T X^T D - S^T)^T - X\beta] \\
&= c + \frac{1}{2}[(X\beta_0 - D^{-1}S) - X\beta]^T D[(X\beta_0 - D^{-1}S) - X\beta] \\
&= c + \frac{1}{2}[Z - X\beta]^T W[Z - X\beta]
\end{aligned}
$$

where Z is the vector $X\beta_0 - D^{-1}S$ and where W is the matrix D.

D)

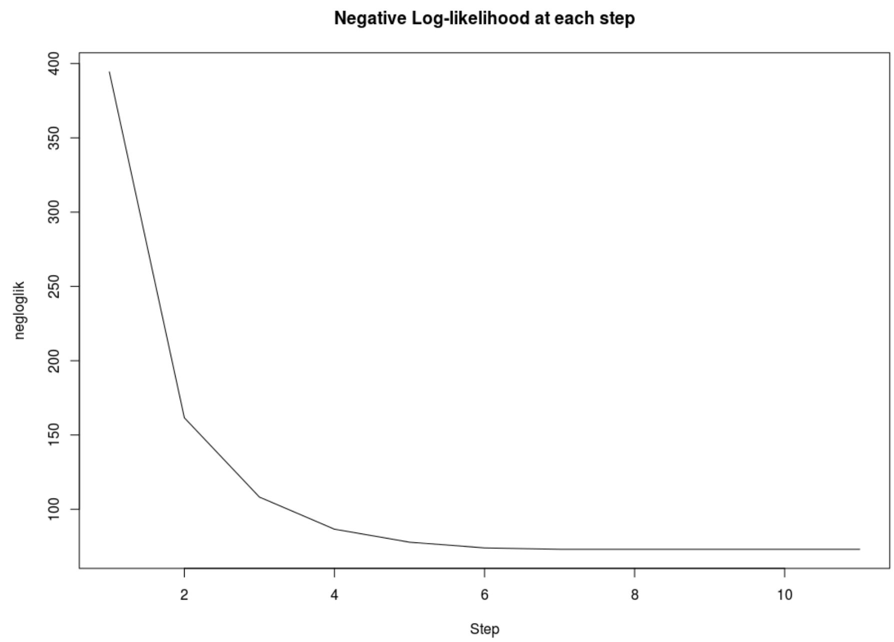
The newton's method updates at each step the values of our estimated β using this formula:

$$\beta_{t+1} = \beta_t - [\nabla^2 l(\beta_t)]^{-1} \nabla l(\beta_t)$$

Running the code in appendix, we can obtain the following $\hat{\beta}$:

c	-7.35951761
V3	-2.04930490
V4	0.38473434
V5	-0.07151042
V6	0.03979620
V7	76.43227376
V8	-1.46242225
V9	8.46869976
V10	66.82175685
V11	16.27824232
V12	-68.33702689

The following graph of the objective function shows us that indeed it's being decreased at each step.



CODE)

```
library(Matrix)

negloglikelihood<-function(m,y,X,beta){
  total<-0
  N<-length(y)
  for(i in 1:N) total<-total+(m[i]-y[i])*t(X[i,])%*%beta+m[i]*log(1+exp(-t(X[i,])%*%beta))
  return(total)
}

gradient_negloglik<-function(m,y,X,beta){
  w<-1/(1+exp(-X%*%beta))
  S<-m*w-y
  grad<-t(X)%*%S
  return(grad)
}

gradient_descent<-function(m,y,X,beta0,stepsize,maxstepnumber,
                           accuracy_obj_fun,accuracy_beta_val){
  negloglik<-numeric(maxstepnumber)
  negloglik[1]<-negloglikelihood(m,y,X,beta0)
```

```
  gradient<-gradient_negloglik(m,y,X,beta0)
  diff_beta_val<-accuracy_beta_val+1
  diff_obj_fun<-accuracy_obj_fun+1
  i<-1
  while(!(i==maxstepnumber)&&
        ((accuracy_beta_val<diff_beta_val)||
        (accuracy_obj_fun<diff_obj_fun))){
    i<-i+1
    beta1<-beta0-stepsize*gradient
    diff_beta_val<-sum(abs(beta0-beta1))
    beta0<-beta1
    negloglik[i]<-negloglikelihood(m,y,X,beta0)
    diff_obj_fun<-negloglik[i-1]-negloglik[i]
    gradient<-gradient_negloglik(m,y,X,beta0)
  }
  return(list(betahat=beta0,negloglik=negloglik,step=i))
}

data_wdbc<-read.csv("./wdbc.csv", header=FALSE)
X<-as.matrix(cbind(rep(1,569),data_wdbc[,3:12]))
y<-data_wdbc[,2]
y<-as.numeric(y=="M")
m<-rep(1,569)

beta0<-rep(0,11)
stepsize<-2/10^8
maxstepnumber<-10000
accuracy_obj_fun<-0.001
accuracy_beta_val<-0.00001
result_grad_desc<-gradient_descent(m,y,X,beta0,stepsize,maxstepnumber,
                                   accuracy_obj_fun,accuracy_beta_val)

result_grad_desc$betahat
plot(result_grad_desc$negloglik[1:result_grad_desc$step],
     main = "Negative Log-likelihood at each step",
     xlab="Step",ylab="negloglik",type="l")

hessian_negloglik<-function(m,y,X,beta){
  w<-as.vector(1/(1+exp(-X%*%beta)))
  D<-diag(m*w*(1-w))
  hes<-t(X)%*%D%*%X
  return(hes)
}

newton_descent<-function(m,y,X,beta0,maxstepnumber,
                         accuracy_obj_fun,accuracy_beta_val){
  negloglik<-numeric(maxstepnumber)
  negloglik[1]<-negloglikelihood(m,y,X,beta0)
  gradient<-gradient_negloglik(m,y,X,beta0)
  hessian<-hessian_negloglik(m,y,X,beta0)
```

```
  diff_beta_val<-accuracy_beta_val+1
  diff_obj_fun<-accuracy_obj_fun+1
  i<-1
  while(!(i==maxstepnumber)&&
        ((accuracy_beta_val<diff_beta_val)||
        (accuracy_obj_fun<diff_obj_fun))){
    i<-i+1
    beta1<-beta0-solve(hessian,gradient)
    diff_beta_val<-sum(abs(beta0-beta1))
    beta0<-beta1
    negloglik[i]<-negloglikelihood(m,y,X,beta0)
    diff_obj_fun<-negloglik[i-1]-negloglik[i]
    gradient<-gradient_negloglik(m,y,X,beta0)
    hessian<-hessian_negloglik(m,y,X,beta0)
  }
  return(list(betahat=beta0,negloglik=negloglik,step=i))
}

result_newton_desc<-newton_descent(m,y,X,beta0,maxstepnumber,
                                   accuracy_obj_fun,accuracy_beta_val)

result_newton_desc$betahat
plot(result_newton_desc$negloglik[1:result_newton_desc$step],
     main = "Negative Log-likelihood at each step",
     xlab="Step",ylab="negloglik",type="l")
```