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

Matteo Vestrucci

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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)

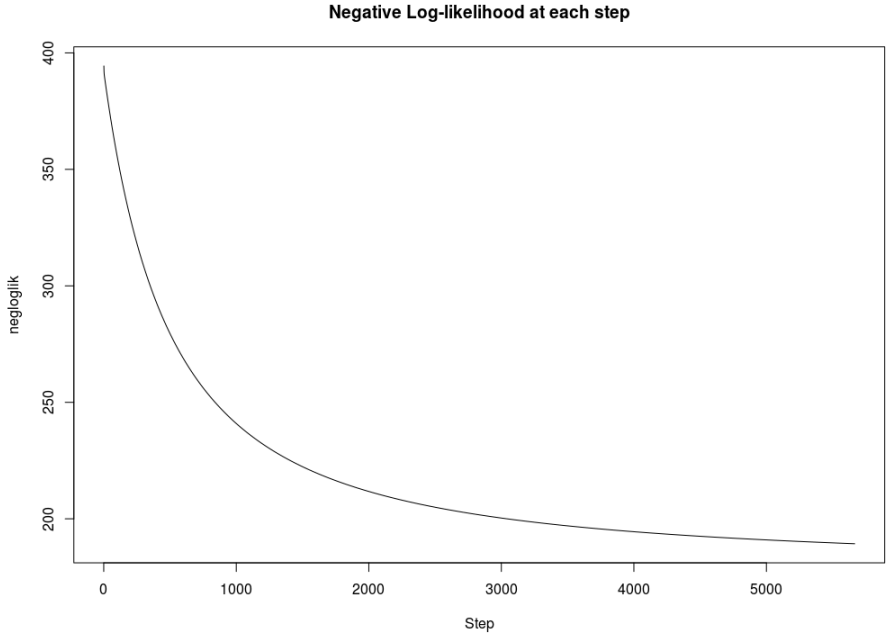
The gradient descent updates at each step the values of our estimated β using this formula:

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

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

c	-0.0035100566
V3	-0.0246244308
V4	-0.0146632623
V5	-0.1287157063
V6	0.0190177752
V7	-0.0001249631
V8	0.0005526005
V9	0.0010221945
V10	0.0004504115
V11	-0.0002718301
V12	-0.0001462899

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 $m_i w_i(1-w_i)$. Then, considering that we can ignore the constant values adding and subtracting them as

we need, we can obtain the requested result like this:

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

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

D)

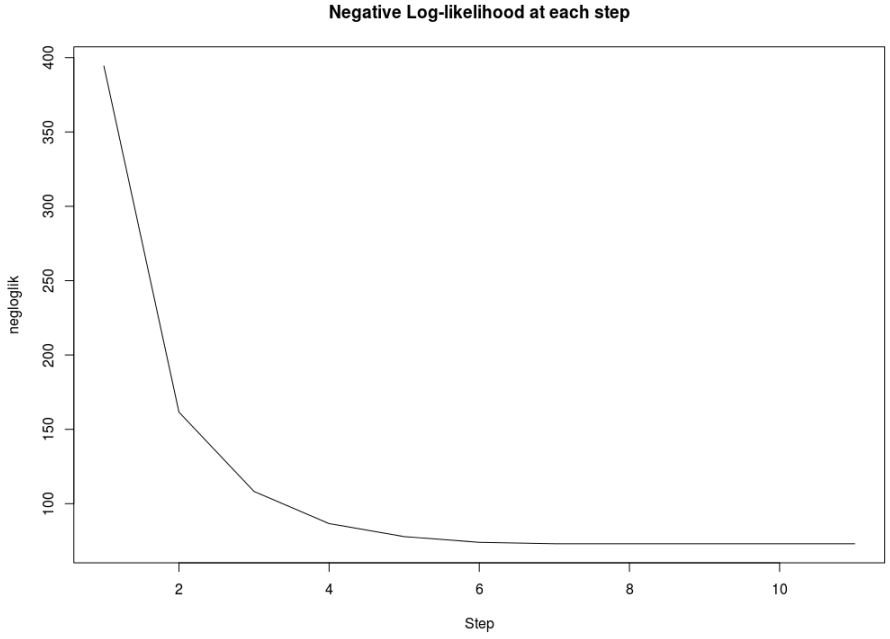
The newton's method updates at each step the values of our estimated β using this formula:

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

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

c	-0.0028183932
V3	-0.0198393341
V4	-0.0213693672
V5	-0.1092486557
V6	0.0162758326
V7	-0.0001475889
V8	0.0002700320
V9	0.0005926614
V10	0.0002666690
V11	-0.0002962445
V12	-0.0001390434

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){
  negloglik<-numeric(maxstepnumber)
  negloglik[1]<-negloglikelihood(m,y,X,beta0)
  gradient<-gradient_negloglik(m,y,X,beta0)
  difference<-accuracy+1
  i<-1
  while(!(i==maxstepnumber)&&(accuracy<difference)){
```

```
    i<-i+1
    beta1<-beta0-stepsize*gradient
    difference<-sum(abs(beta0-beta1))
    beta0<-beta1
    negloglik[i]<-negloglikelihood(m,y,X,beta0)
    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<-0.00001
result_grad_desc<-gradient_descent(m,y,X,beta0,stepsize,maxstepnumber,accuracy)

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){
  negloglik<-numeric(maxstepnumber)
  negloglik[1]<-negloglikelihood(m,y,X,beta0)
  gradient<-gradient_negloglik(m,y,X,beta0)
  hessian<-hessian_negloglik(m,y,X,beta0)
  difference<-accuracy+1
  i<-1
  while(!(i==maxstepnumber)&&(accuracy<difference)){
    i<-i+1
    beta1<-beta0-solve(hessian,gradient)
    difference<-sum(abs(beta0-beta1))
    beta0<-beta1
    negloglik[i]<-negloglikelihood(m,y,X,beta0)
    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)

result_grad_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")
```