SDS 385: Exercises 1 - Preliminaries

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Problem 1

(A)

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^{N} \frac{w_i}{2} \left(y_i - x_i^T \beta\right)^2 \tag{1}$$

$$= \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2}(Y - X\beta)^T W (Y - X\beta) \tag{2}$$

$$\frac{1}{2}(Y - X\beta)^T W (Y - X\beta) = \frac{1}{2}(Y^T - \beta^T X^T) W (Y - X\beta) \tag{3}$$

$$= \frac{1}{2}(Y^T W - \beta^T X^T W)(Y - X\beta) \tag{4}$$

$$= \frac{1}{2}(Y^T W Y - \beta^T X^T W Y - Y^T W X \beta + \beta^T X^T W X \beta) \tag{5}$$

$$= \frac{1}{2}(Y^T W Y - 2(X\beta)^T W Y + \beta^T X^T W X \beta) \tag{6}$$

$$= \frac{1}{2} Y^T W Y - (X\beta)^T W Y + \frac{1}{2}\beta^T X^T W X \beta, \tag{7}$$

because

$$\beta^T X^T W Y = (X\beta)^T W Y, \tag{8}$$

and

$$Y^T W X \beta = (Y^T W X \beta)^T \because Y^T W X \beta \in \mathbb{R}^1 \tag{9}$$

$$(Y^T W X \beta)^T = (W X \beta)^T Y = (X\beta)^T W^T Y = (X\beta)^T W Y. \tag{10}$$

We want to minimize the objective function from Eqn. (7), so we take the gradient with respect to β and set it equal to zero. For each of the three terms, their are respective gradients with respect to β are

(i)

$$\frac{\partial}{\partial \beta} \frac{1}{2} Y^T W Y = 0 \tag{11}$$

(ii)

$$\frac{\partial}{\partial \beta} - (X\beta)^T W Y = -X^T W Y \tag{12}$$

(iii)

$$\frac{\partial}{\partial \beta} \frac{1}{2} \beta^T X^T W X \beta = \frac{1}{2} \beta^T (X^T W X + (X^T W X)^T) \tag{13}$$

$$= X^T W X \beta. \tag{14}$$

Summing these terms and equaling them to zero yields

$$X^T W X \beta - X^T W Y = 0 \therefore \tag{15}$$

$$(X^T W X)\hat{\beta} = X^T W Y \tag{16}$$

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(B) The brute force method of solving Eqn. (16) is the *inversion method*, i.e.

$$\hat{\beta} = (X^T W X)^{-1} X^T W y. \tag{17}$$

However, this method is computationally expensive. Therefore I propose an alternative methods to solving this matrix equation using the Cholesky decomposition. **Cholesky Decomposition**
Let

$$C = X^T W X, \;\; D = X^T W y \tag{18}$$

so

$$C\hat{\beta} = D. \tag{19}$$

We decompose matrix C into a product of a lower-triangular matrix and an upper-triangular matrix, such that $U = L^T$ so

$$C = LU = LL^T \therefore \tag{20}$$

$$LL^T\hat{\beta} = D. \tag{21}$$

Furthermore we define matrix $A = L^T\hat{\beta}$. Thus we are left with two matrix equations to solve.

$$LA = D \tag{22}$$

$$L^T\hat{\beta} = A \tag{23}$$

This method will be much less computationally intensive than the inversion method because R can leverage the fact that the two left-matrices L and $U = L^T$ are triangular. We still must invert L and L^T but this is simpler than taking an inverse of a more complicated matrix $X^T W X$. This is similar to an LU decomposition, with the exception that we necessarily have two triangular matrices that are transposes of one another. Therefore, this method gains a computational advantage over LU decomposition from symmetric exploitation.

(C) Code for implementing this method is shown in the appendix to this paper. Below are results from benchmarking these two methods, the inversion method and the method of Cholesky decomposition. The Cholesky method consistently outperforms the inversion method in computing efficiency; however, its edge over the inversion method drops off with increasing N keeping P constant, while its edge improves with increasing P keeping N constant.

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ times = 5, unit = "ms") # N = 2000, P = 500
Unit: milliseconds
                expr      min       lq     mean   median       uq      max
 Inv.method(X, W, y) 768.6836 774.2118 785.1086 789.9117 793.2050 799.5309
 Cho.decomp(X, W, y) 479.4100 480.9378 507.0890 508.4939 522.5065 544.0970
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ times = 5, unit = "ms") # N = 4000, P = 500
Unit: milliseconds
                expr       min       lq      mean    median        uq       max
 Inv.method(X, W, y) 1219.0058 1230.432 1241.7503 1235.6394 1253.5155 1270.1589
 Cho.decomp(X, W, y)  952.4912  956.046  964.0765  958.8309  976.0884  976.9259
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ times = 5, unit = "ms") # N = 2000, P = 1000
Unit: milliseconds
                expr      min       lq     mean  median       uq      max neval
 Inv.method(X, W, y) 4347.542 4377.584 4394.977 4394.56 4409.392 4445.806     5
 Cho.decomp(X, W, y) 2012.607 2014.392 2041.574 2017.97 2050.955 2111.945     5
    > microbenchmark(
    + Inv.method(X, W, y),
    + Cho.decomp(X, W, y),
    + times = 5, unit = "ms") # N = 4000, P = 1000
    Unit: milliseconds
                  expr      min       lq     mean   median       uq      max
     Inv.method(X, W, y) 6365.297 6704.451 7394.312 7143.601 8085.007 8673.203
     Cho.decomp(X, W, y) 3887.150 4073.163 4274.318 4351.933 4352.873 4706.470
```

Figure 1: Benchmarking the inversion and Cholesky method for different N and P

(D) The `Matrix` package in R is suited to handle sparse matrices. We do this by redefining X as `X <- Matrix(X, sparse = TRUE)`. By doing this, R streamlines its handling of the X matrix and subsequent matrix products incorporating X by storing X as a coordinate list of non-zero entries as opposed to a

matrix with many zeros within it. For the sparse method, we again use the Cholesky decomposition after converting X to a sparse matrix. In the benchmarks below, we see the computational advantage gained by handling X in this fashion. Here, α represents the density of X, i.e., the proportion of entries which are non-zero. The increase in efficiency is more noticeable with higher sparsity, although even for $\alpha = 0.25$ the effect is still quite dramatic.

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 500, alpha = 0.02
Unit: milliseconds
                      expr      min       lq      mean    median        uq
       Inv.method(X, W, y) 737.2686 759.2310 777.88289 777.13764 788.57304
       Cho.decomp(X, W, y) 477.1558 487.8474 495.89320 501.13615 505.09096
 Cho.decompSPARSE(X, W, y)  86.5331  94.7683  96.63769  95.98655  98.72639
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 1000, alpha = 0.02
Unit: milliseconds
                      expr       min        lq      mean   median        uq
       Inv.method(X, W, y) 4710.3185 4931.8045 5188.5055 5157.074 5237.1337
       Cho.decomp(X, W, y) 2364.0034 2426.9523 2660.8243 2668.589 2793.3968
 Cho.decompSPARSE(X, W, y)  527.0455  591.6044  602.6213  603.253  645.1521
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 500, alpha = 0.05
Unit: milliseconds
                      expr      min       lq     mean    median        uq
       Inv.method(X, W, y) 911.9994 998.2114 991.7138 1002.9189 1013.9052
       Cho.decomp(X, W, y) 629.7340 633.9266 673.3554  690.7624  700.1041
 Cho.decompSPARSE(X, W, y) 159.6571 162.6814 178.2505  180.8469  185.6584
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 1000, alpha = 0.05
Unit: milliseconds
                      expr       min        lq      mean    median        uq
       Inv.method(X, W, y) 4965.8643 4978.5698 5093.2457 5007.6897 5237.9068
       Cho.decomp(X, W, y) 2251.6841 2330.9450 2397.7684 2420.4825 2446.5866
 Cho.decompSPARSE(X, W, y)  720.0268  755.9948  793.4475  772.5409  841.1671
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 500, alpha = 0.25
Unit: milliseconds
                      expr      min       lq     mean   median       uq
       Inv.method(X, W, y) 836.1431 839.0217 857.1903 852.6260 857.0857
       Cho.decomp(X, W, y) 542.3195 543.8558 569.7348 561.1348 562.7806
 Cho.decompSPARSE(X, W, y) 250.6403 272.0944 275.7578 277.0591 284.7214
```

```
> microbenchmark(
+ Inv.method(X, W, y),
+ Cho.decomp(X, W, y),
+ Cho.decompSPARSE(X, W, y),
+ times=5, unit = "ms") # N = 2000, P = 1000, alpha = 0.25
Unit: milliseconds
                      expr      min       lq     mean   median       uq
       Inv.method(X, W, y) 4926.726 4951.693 5025.735 5029.666 5047.827
       Cho.decomp(X, W, y) 2375.101 2419.114 2465.391 2502.977 2506.080
 Cho.decompSPARSE(X, W, y) 1165.509 1172.599 1255.190 1260.516 1277.994
```

Figure 2: Benchmarking for various values of N, P, and density level α

Problem 2

(A) We have $y_i \sim \text{Binomial}(m_i, w_i)$, where

$$w_i = \frac{1}{1+\exp(-x_i^T\beta)}, \;\; 1 - w_i = \frac{\exp(-x_i^T\beta)}{1+\exp(-x_i^T\beta)}, \tag{24}$$

so the negative log likelihood is

$$\ell(\beta) = -\log\left\{\prod_{i=1}^N p(y_i|\beta)\right\} \tag{25}$$

$$= -\log\left\{\prod_{i=1}^N \binom{m_i}{y_i}(w_i)^{y_i}(1-w_i)^{m_i-y_i}\right\} \tag{26}$$

$$= -\left\{\sum_{i=1}^N \left(\log\binom{m_i}{y_i} + y_i\log(w_i) + (m_i - y_i)\log(1-w_i)\right)\right\} \tag{27}$$

$$= -\left\{\sum_{i=1}^N \left(\log\binom{m_i}{y_i} + y_i\log\left(\frac{1}{1+\exp(-x_i^T\beta)}\right) + (m_i-y_i)\log\left(\frac{\exp(-x_i^T\beta)}{1+\exp(-x_i^T\beta)}\right)\right)\right\} \tag{28}$$

$$= -\left\{\sum_{i=1}^N \left(\log\binom{m_i}{y_i} - y_i\log(1+\exp(-x_i^T\beta)) - (m_i-y_i)x_i^T\beta - m_i\log(1+\exp(-x_i^T\beta)) + y_i\log(1+\exp(-x_i^T\beta))\right)\right. \tag{29}$$

$$= -\left\{\sum_{i=1}^N \left(\log\binom{m_i}{y_i} - (m_i-y_i)x_i^T\beta - m_i\log(1+\exp(-x_i^T\beta))\right)\right\} \tag{30}$$

$$= \sum_{i=1}^N \left((m_i-y_i)x_i^T\beta + m_i\log(1+\exp(-x_i^T\beta)) - \log\binom{m_i}{y_i}\right) \tag{31}$$

$$\tag{32}$$

The gradient for this expression is,

$$\nabla\ell(\beta) = \sum_{i=1}^N \left((m_i-y_i)x_i - m_i\frac{\exp(-x_i^T\beta)}{1+\exp(-x_i^T\beta)}x_i\right) \tag{33}$$

$$= \sum_{i=1}^N \left((m_i-y_i)x_i - m_i(1-w_i)x_i\right) \tag{34}$$

$$= \sum_{i=1}^N (m_iw_i - y_i)x_i \tag{35}$$

$$= -X^T(y - mw) \tag{36}$$

where y is the $n \times 1$ vector of responses and mw is the element-wise product of the two $n \times 1$ vectors m and w.

(B) Code for implementing the gradient descent method is shown in the appendix. Note that we normalize the values in the X matrix and add a column of 1's to make an intercept term. We start by having an initial arbitrary guess for β, which we define as β_0. Then we use an iterative process to converge upon the true value of β based on the calculated gradient of the log likelihood at $\hat{\beta}_t$ and an arbitrary step size, α, as follows:

$$\hat{\beta}_{t+1} = \hat{\beta}_t - \alpha \times \nabla\ell(\hat{\beta}_t) \tag{37}$$

Problem 2 continued on next page...

	Grad descent	R: `glm`
$\hat{\beta}_1$	0.48553	0.48702
$\hat{\beta}_2$	-7.14618	-7.22185
$\hat{\beta}_3$	1.65481	1.65476
$\hat{\beta}_4$	-1.80713	-1.73763
$\hat{\beta}_5$	13.99290	14.00485
$\hat{\beta}_6$	1.07426	1.07495
$\hat{\beta}_7$	-0.07319	-0.07723
$\hat{\beta}_8$	0.67573	0.67512
$\hat{\beta}_9$	2.59383	2.59287
$\hat{\beta}_{10}$	0.44615	0.44626
$\hat{\beta}_{11}$	-0.48276	-0.48248

Table 1: Comparison of results from gradient descent and `glm`

We use an intial guess of $\beta_0 = 0$, a step size of $\alpha = 0.025$, and 50,000 iterations and reach convergence in optimizing the log likelihood, as shown in the trace plot below. Our final estimations of β are reported below along with estimations from R's native `glm` function. The two sets of estimates are in close agreement with one another.

(C) We need to calculate the Hessian matrix of the log likelihood function, $\nabla^2 \ell(\beta)$. The Hessian will be a $P \times P$ matrix, with the element in row i and column j being[1]

$$\frac{\partial^2}{\partial\beta_i \partial\beta_j}\ell(\beta) = \frac{\partial}{\partial\beta_i}\left(\frac{\partial}{\partial\beta_j}\ell(\beta)\right) \tag{38}$$

$$= \frac{\partial}{\partial\beta_i}\left(\frac{\partial}{\partial\beta_j}\sum_{k=1}^{N}(\dots)\right) \tag{39}$$

$$= \frac{\partial}{\partial\beta_i}\left(\sum_{k=1}^{N}(m_k w_k - y_k)x_{kj}\right) \tag{40}$$

$$= \sum_{k=1}^{N} x_{ki}x_{kj}m_k w_k(1-w_k) \tag{41}$$

Note:

$$\frac{\partial}{\partial\beta_i}w_k = x_{ki}\frac{\exp(-x_k^T\beta)}{(1+\exp(-x_k^T\beta))^2} \tag{42}$$

$$= x_{ki}w_k(1-w_k) \tag{43}$$

This matrix is equivalent to $X^T W X$ where $W = \text{diag}(m_1 w_1(1-w_1), \dots, m_N w_N(1-w_N))$

Let $a = (y - mw)$. We have already shown that $\nabla\ell(\beta) = -X^T(y-mw) = -X^T a$ and $\nabla^2\ell(\beta) = X^T W X$.

[1] Notice the reindexing shown below for summations.

Problem 2 continued on next page...

The second-order Taylor approximation for $\ell(\beta)$ around the point β_0 is,[2]

$$\hat{\ell}(\beta) = \ell(\beta_0) + (\nabla\ell(\beta))^T(\beta - \beta_0) + \frac{1}{2}(\beta - \beta_0)^T\nabla^2\ell(\beta)(\beta - \beta_0) \tag{44}$$

$$= \ell(\beta_0) + (-X^Ta)^T(\beta - \beta_0) + \frac{1}{2}(\beta - \beta_0)^TX^TWX(\beta - \beta_0) \tag{45}$$

$$= \frac{1}{2}([\beta - \beta_0] - (X^TWX)^{-1}X^Ta)^TX^TWX([\beta - \beta_0] - (X^TWX)^{-1}X^Ta) + c \tag{46}$$

$$= \frac{1}{2}(\beta - \beta_0 + X^{-1}W^{-1}(X^T)^{-1}X^Ta)^TX^TWX(\beta - \beta_0 + X^{-1}W^{-1}(X^T)^{-1}X^Ta) + c \tag{47}$$

$$= \frac{1}{2}(\beta - \beta_0 + X^{-1}W^{-1}a)^TX^TWX(\beta - \beta_0X^{-1}W^{-1}a) + c \tag{48}$$

$$= \frac{1}{2}(X\beta - X\beta_0 + XX^{-1}W^{-1}a)^TW(X\beta - X\beta_0 + XX^{-1}W^{-1}a) + c \tag{49}$$

$$= \frac{1}{2}(X\beta - X\beta_0 + W^{-1}a)^TW(X\beta - X\beta_0 + W^{-1}a) + \dots \tag{50}$$

$$= \frac{1}{2}(z - X\beta)^TW(z - X\beta) + c, \tag{51}$$

where c is some constant, $z = X\beta_0 + W^{-1}a = X\beta_0 + W^{-1}(y - mw)$

(D) Now we use Newton's to estimate β. This is also an iterative process, though now we need far fewer iterations to achieve convergence because we are taking the curvature of our objective function ($\ell(\beta)$) into account. In fact, we only use 10 iterations and achieve estimates $\hat{\beta}$ which are *exactly* in line with estimates from `glm`.

Newton's Method:

$$\hat{\beta}_{t+1} = \hat{\beta}_t - (\nabla^2\ell(\hat{\beta}_t))^{-1}\nabla\ell(\hat{\beta}_t) \tag{52}$$

	N.'s method	R: `glm`
$\hat{\beta}_1$	0.48702	0.48702
$\hat{\beta}_2$	-7.22185	-7.22185
$\hat{\beta}_3$	1.65476	1.65476
$\hat{\beta}_4$	-1.73763	-1.73763
$\hat{\beta}_5$	14.00485	14.00485
$\hat{\beta}_6$	1.07495	1.07495
$\hat{\beta}_7$	-0.07723	-0.07723
$\hat{\beta}_8$	0.67512	0.67512
$\hat{\beta}_9$	2.59287	2.59287
$\hat{\beta}_{10}$	0.44626	0.44626
$\hat{\beta}_{11}$	-0.48248	-0.48248

Figure 3: Comparison of results from Newton's method and `glm`

(E) Gradient descent requires many iterations, and there is no simple way to know what step size is wise. In contrast, Newton's method converges upon the MLE with far fewer iterations. However, for Newton's

[2]Help with completing the square obtained from: `https://justindomke.wordpress.com/completing-the-square-in-n-dimensions/`

Problem 2 continued on next page...

method we must invert the Hessian matrix, is computationally intensive for large matrices and will be impossible if the Hessian is singular.

```
############################################################
######### Created by Spencer Woody on 24 Aug 2016 #########
############################################################

library(Matrix)
library(microbenchmark)

### No. 1 pt C

# Set N, P, X, W, and y

N <- 4000
P <- 1000

X <- matrix(rnorm(N * P), nrow = N)
y <- matrix(rnorm(N), nrow = N)
W <- diag(rep(1, N))

# Inversion method

Inv.method <- function(X.Inv, W.Inv, y.Inv) {
    XtWX <- (t(X.Inv)*diag(W.Inv)) %*% X.Inv
    XtWY <- (t(X.Inv)*diag(W.Inv)) %*% y.Inv
    bhat.Inv <- solve(XtWX) %*% XtWY
    return(bhat.Inv)
}

Cho.decomp <- function(X.Cho, W.Cho, y.Cho) {
    D.Cho <- (t(X.Cho)*diag(W.Cho)) %*% y.Cho
    C.Cho <- (t(X.Cho)*diag(W.Cho)) %*% X.Cho

    U.Cho <- chol(C.Cho)
    L.Cho <- t(U.Cho)

    u <- forwardsolve(L.Cho, D.Cho)
    bhat.Cho <- backsolve(U.Cho, u)

    return(bhat.Cho)
}

microbenchmark(
    Inv.method(X, W, y),
    Cho.decomp(X, W, y),
    times = 5, unit = "ms") # N = 4000, P = 1000


### No. 1 pt D

N <- 2000
P <- 1000

# Sparsity measure # 0.01, 0.05, 0.25
alpha <- 0.25
```

```r
X <- matrix(rnorm(N * P), nrow = N)
mask <- matrix(rbinom(N * P, 1, alpha), nrow = N)
X <- mask * X
W <- diag(rep(1, N))


Cho.decompSPARSE <- function(X.Cho, W.Cho, y.Cho) {
    X.Cho <- Matrix(X.Cho, sparse = T)
    D.Cho <- (t(X.Cho)*diag(W.Cho)) %*% y.Cho
    C.Cho <- (t(X.Cho)*diag(W.Cho)) %*% X.Cho

    U.Cho <- chol(C.Cho)
    L.Cho <- t(U.Cho)

    u <- forwardsolve(L.Cho, D.Cho)
    bhat.Cho <- backsolve(U.Cho, u)

    return(bhat.Cho)
}



microbenchmark(
    Inv.method(X, W, y),
    Cho.decomp(X, W, y),
    Cho.decompSPARSE(X, W, y),
    times=5, unit = "ms") # N = 2000, P = 1000, alpha = 0.25

# END
```

```
#############################################################
######### Created by Spencer Woody on 24 Aug 2016 #########
#############################################################

# Read in data file, standardize X

wdbc <- read.csv("wdbc.csv", header = FALSE)

X <- as.matrix(wdbc[, 3:12])
X <- scale(X)
X <- cbind(rep(1, nrow(X)), X)

y <- wdbc[, 2]
y <- y == "M"
beta <- as.matrix(rep(0, ncol(X)))
mi <- 1

# Function for computing w.i

comp.wi <- function (X, beta) {
    wi <- 1 / (1 + exp(-X %*% beta))
    return(wi)
}

# Function for computing likelihood

loglik <- function(beta, y, X, mi) {
    loglik <- apply((mi - y) * (X %*% beta)+ mi*log(1 + exp(-X %*% beta)), 2, sum)
    return(loglik)
}
# Function for computing gradient for likelihood

grad.loglik <- function(beta, y, X, mi){
  grad <- array(NA, dim = length(beta))
  wi <- comp.wi(X, beta)
  grad <- apply(X*as.numeric(mi * wi - y), 2, sum)
  return(grad)
}

###
### Gradient descent
###

stepfactor <- 0.025
n.steps <- 50000
log.lik <- NULL

for (step in 1:n.steps) {
    log.lik[step] <- loglik(beta, y, X, mi)
    beta <- beta - stepfactor * grad.loglik(beta, y, X, mi)
}

# Create trace plot of likelihood, check for convergence
```

```r
png("beta_trace1.png")
plot(log.lik,
     main = "Trace Plot for log likelihood(beta)",
     xlab = "Step",
     ylab = "log likelihood(beta)")
dev.off()

# Compare results to R's glm function

mymodel <- glm(y ~ X[, c(-1)], family = "binomial")
summary(mymodel)

print(beta)

###
### Newton's method
###

beta.N <- as.matrix(rep(0, ncol(X)))

n.steps <- 10
log.lik2 <- NULL

for (step in 1:n.steps) {
    log.lik2[step] <- loglik(beta, y, X, mi)
    w.i <- as.numeric(comp.wi(X, beta.N))
    W <- diag(w.i*(1-w.i))
    Hessian <- t(X) %*% W %*% X
    beta.N <- beta.N - solve(Hessian) %*% grad.loglik(beta.N, y, X, mi)
}

# Show estimates from Newton's method

round(as.matrix(coef(mymodel)) - beta.N, 8)
```