Homework 3

M1399.000100, Seoul National University, Spring 2023

Due 23:00 Wed, 2024-05-22

Append your answer below each question. Submit the modified version of this Rmd file and the output pdf file, together with other necessary files such as images and R source code. The submitted version of this Rmd file should be knit ted to an pdf file ideally identical to the submitted one.

When writing your own R code, do NOT use R packages that implement the functions you are asked to write. i.e., you must write your own code from scratch.

No late submission is accepted.

Q1. Iterative method

1. Write an R function jacobi implementing Jacobi's method for solving linear equation Ax = b, with interface

```
library(Matrix)
jacobi <- function(A, b, x0, maxit=100, tol=1.0e-6, history=FALSE, verbose=FALSE) {
    nbrows <- ncol(A)
    x <- x0
    numit <- 0
    nrmdx <- Inf
    converged <- FALSE
   xhist <- NULL
    if (history) {
        xhist <- vector("list", maxit)</pre>
    while (numit < maxit) {
        numit <- numit + 1
        x_t <- x
        deltax <- b - A%*%x
        for (i in 1:nbrows){
          deltax[i] = deltax[i]/A[i, i]
        x <- x + deltax
        nrmdx <- norm(deltax, "m")</pre>
        if (verbose) {
            print(norm(x-x_t, "2"))
        if (history) xhist[[numit]] <- x
        if (nrmdx < tol) {
            converged <- TRUE
            break
    if (history) xhist <- xhist[seq_len(numit)]</pre>
    ret <- list(sol = x, iter = numit, hist = xhist, converged = converged)
    ret
```

where x0 is the initial iterate, maxit is the maximum number of iteration to run, to I is the tolerance for convergence test, and history and verbose are debugging flags; if history == TRUE, then your function should store each iterate x (excluding x0) in a list; if verbose == TRUE, then your function should print the error between the current and previous iterates as mesuared by the Euclidean norm.

The return value should be a list having four fields:

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- sol: numeric object of length ncol(A) containing the last iterate of the method.
- iter: number of iterations ran
- hist: if history == TRUE, list of length iter containing all the iterates; otherwise NULL
- converged: logical variable indicating whether the final error is below to l

Assume that \mathbf{A} is square and its diagonal elements are nonzero. Vectorize (https://bookdown.org/rdpeng/rprogdatascience/vectorized-operations.html) your code as much as possible.

Using the get2DPoissonMatrix() function defined in the Lecture Note on Iterative Methods for Solving Linear Equations (also provided below), generate the coefficient matrix as follows.

```
get1DPoissonMatrix <- function(n) {</pre>
 Matrix::bandSparse(n, n, #dimensions
                    (-1):1, #band, diagonal is number 0
                    list(rep(-1, n-1),
                    rep(4, n).
                    rep(-1, n-1))
# Generate 2-dimensional discrete Poisson matrix
#' @param n Grid size. Output will be a n^2 by n^2 matrix.
get2DPoissonMatrix <- function(n) { # n^n by n^n</pre>
   T <- get1DPoissonMatrix(n)
    eye <- Matrix::Diagonal(n)
    N \leftarrow n * n \# dimension of the final square matrix
    ## construct two block diagonal matrices
    D <- bdiag(rep.int(list(T), n))
    0 <- bdiag(rep.int(list(-eye), n - 1))</pre>
    ## augment 0 and add them together with D
    rbind(cbind(Matrix(0, nrow(0), n), 0), Matrix(0, n, N)) +
     cbind(rbind(Matrix(0, n, ncol(0)), 0), Matrix(0, N, n))
n <- 50
A <- get2DPoissonMatrix(n)
set.seed(456) # seed
b \leftarrow rnorm(n^2)
```

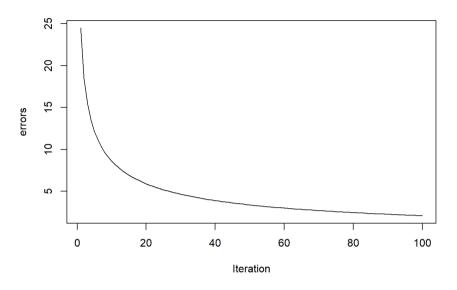
Then find the solution to A ** x = b using your jacobi() function. In doing this, use the hist field of your return object to produce a convergence plot like the following.



```
x0 = rep(0, 50^2)
result <- jacobi(A, b, x0, history = TRUE, maxit = 100)

errors <- sapply(result$hist, function(x) norm(b - A %*% x, "2"))

plot(errors, type = "1", xlab = "Iteration")</pre>
```



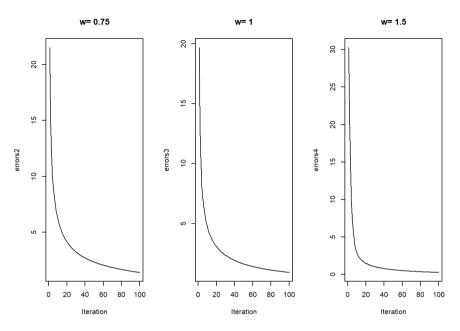
2. Repeat the above for the successive over-relaxation (SOR) method, with interface

```
sor <- function(A, b, x0, w=1.1, maxit=100, tol=1.0e-6, history=FALSE, verbose=FALSE) {
   nbrows <- ncol(A)
   x <- x0
   numit <- 0
   xhist <- NULL
   converged = FALSE
   if (history) {
   xhist <- vector("list", maxit)</pre>
   while (numit < maxit) {
       numit <- numit + 1
       x_t <- x
       for (i in 1:nbrows) {
       sumj \leftarrow sum(A[i,] * x) - A[i, i] * x[i]
       x[i] \leftarrow (1 - w) * x[i] + (w / A[i,i]) * (b[i] - sumj)
       error = norm(x-x_t, "2")
       if (verbose) {
           print(error)
       if (history) xhist[[numit]] <- x
       if (error < tol) {
            converged <- TRUE
           break
   if (history) xhist <- xhist[seq_len(numit)]</pre>
   ret <- list(sol = x, iter = numit, hist = xhist, converged = converged)
   ret
 }
```

Experiment with various values of the relaxation parameter w.

```
result2 <- sor(A, b, x0, w = 0.75, history = TRUE, maxit = 100)
result3 <- sor(A, b, x0, w = 1, history = TRUE, maxit = 100)
result4 <- sor(A, b, x0, w = 1.5, history = TRUE, maxit = 100)

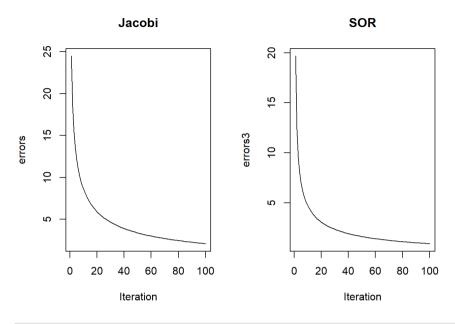
errors2 <- sapply(result2$hist, function(x) norm(b - A **% x, "2"))
errors3 <- sapply(result3$hist, function(x) norm(b - A **% x, "2"))
errors4 <- sapply(result4$hist, function(x) norm(b - A **% x, "2"))
par(mfrow=c(1,3))
plot(errors2, type = "l", xlab = "lteration", main = "w= 0.75")
plot(errors3, type = "l", xlab = "lteration", main = "w= 1")
plot(errors4, type = "l", xlab = "lteration", main = "w= 1.5")
```



w가 클수록 수렴속도가 빠르다.

Discuss the difference between Jacobi's method and SOR (which includes the Gauss-Seidel) in terms of number of iterations to converge, [wall-clock time](https://en.wikipedia.org/wiki/Elapsed_real_time) of your code, etc. What do you think is the main reasons for the differences?

```
par(mfrow=c(1,2))
plot(errors, type = "I", xlab = "Iteration", main = "Jacobi")
plot(errors3, type = "I", xlab = "Iteration", main = "SOR")
```



```
library("microbenchmark")
benchmark_results <- microbenchmark(
    jacobi = jacobi(A, b, x0, history = FALSE, verbose = FALSE),
    sor = sor(A, b, x0, w = 1.0, history = FALSE, verbose = FALSE), times = 1
)</pre>
```

print(benchmark_results)

```
## Unit: seconds
## expr min |q mean median uq max neval
## jacobi 31.67939 31.67939 31.67939 31.67939 1
## sor 55.93251 55.93251 55.93251 55.93251 55.93251 1
```

오차가 줄어드는 정도가 SOR이 더 빠르다. 반복에 걸리는 시간은 Jacobi가 더 빠르다. Jacobi에서는 각 반복에 대한 업데이트가 이전 반복의 값만을 기반으로 하므로 수렴 속도가 느리다. SOR에서는 현재 반복 내에서 가장 최근의 값을 활용하기 때문에 방법을 더 빠르게 수렴한다.

- 3. (PageRank) Now let us implement the PageRank algorithm using the SOR method. The Wikipedia Vote Network dataset, available at https://snap.stanford.edu/data/wiki-Vote.html (https://snap.stanford.edu/data/wiki-Vote.html), describes the voting network among the administrators of Wikipedia. The compressed text file Wiki-Vote.txt.gz in the SNAP website encodes this network in an edgelist format. The number of edges is 103689.
- a. Convert the edgelist into an adjacency matrix. This matrix should be a sparse dgCMatrix provided in the Matrix package. Use the readr::read_tsv() function to read the edgelist into a tbl , a tidyverse dataframe. Then convert it into an igraph graph structure by using

```
df <- readr::read_tsv("wiki-Vote.txt.gz", comment = "#", col_names = FALSE)
```

Rows: 103689 Columns: 2 ## — Column specification — ## Delimiter: "Wt" ## dbl (2): X1, X2 ## ## i Use `spec()` to retrieve the full column specification for this data. ## i Specify the column types or set `show_col_types = FALSE` to quiet this message.

```
vote <- igraph∷graph_from_edgelist(as.matrix(df), directed=TRUE)
```

where `df` is the `tbl` for the imported edgelist. Finally,

A2 <- igraph::as_adjacency_matrix(vote, sparse=TRUE)

will give you the desired adjacency matrix. The resulting matrix should have a dimension 8297 by 8297.

b. Implement the PageRank algorithm using SOR. Since the A matrix is sparse and large, your code in Problem 2 is likely very inefficient. Recall that we need to solve

$$(\mathbf{I} - \mathbf{P}^T)\mathbf{x} = \mathbf{0}$$

where $\mathbf{P}=(p_{ij})$ with

$$p_{ij} = egin{cases} (1-p)/n + p a_{ij}/r_i, & r_i > 0, \ 1/n, & r_i = 0; \end{cases}$$

 r_i is the out-degree of node i, $A=(a_{ij})$, and p is the probability of surfing from node i to j. Directly constructing the coefficient matrix from A, e.g.,

```
 \{r \ B \leftarrow Matrix:: Diagonal(n) \ for \ (i \ in \ which(outdeg > 0)) \ \{ \qquad for \ (j \ in \ seq\_len(ncol(A))) \ \{ \qquad if \ (A[i,j] > 0) \ B[i,j] \leftarrow B[i,j] - (1-p) \ / \ n-p \ \star A[i,j] \ / \ outdeg[i,j] \ \}
```

won't terminate easily in most of laptops. (This is because modifying a sparse matrix is not efficient.) Instead, you should implement multiplication of each row of $\mathbf{I} - \mathbf{P}^T$ with \mathbf{x} within the SOR loop, by using only A and p.

Write an R function pagerank with interface

```
pagerank <- function(A, x0, p=0.85, w=1.5, maxit=100, tol=1.0e-6, history=FALSE, verbose=FALSE) {
    nbrows <- ncol(A)
    r <- applv(A, 1, sum)
    dangling \leftarrow which(r == 0) # dangling nodes
    x <- x0
    numit <- 0
    xhist <- NULL
    converged = FALSE
    if (history) {
    xhist <- vector("list", maxit)</pre>
    while (numit < maxit) {
        numit <- numit + 1
        x_t <- x
        for (i in 1:nbrows) {
          if (r[i]>0){
            sumi \leftarrow sum(p * A[i, ] * x / r[i])
            x[i] \leftarrow (1 - w) * x[i] + w * (sumj + (1 - p) / nbrows)
            x[i] \leftarrow (1 - w) * x[i] + w * (1 - p) / nbrows
        error = norm(x-x_t, "2")
        if (verbose) {
            print(error)
        if (history) xhist[[numit]] <- x</pre>
        if (error < tol) {
            converged <- TRUE
            break
    if (history) xhist <- xhist[seq_len(numit)]</pre>
    if (any(x < 0)) {
    warning("Method converged but the solution has negative elements.")
    ret <- list(sol = x, iter = numit, hist = xhist, converged = converged)
    ret
```

implementing this idea. Your return object should be the same as sor() above, but should additionally check nonnegativity of your solution to generate a warning "Method converged but the solution has negative elements." Write your function by completing the skeleton code above.

Apply your pagerank() to the Wikipedia Vote Network dataset with p=0.85, convert your solution to probability, and report the top 10 nodes in terms of the PageRank score.

```
n2 <- nrow(A2)
x02 <- rep(1/n2, n2)
resultp <- pagerank(A2, x02)
```

```
score <- resultp$sol / sum(resultp$sol)
top10 <- order(score, decreasing = TRUE)[1:10]
top10</pre>
```

[1] 2748 2749 301 6985 349 612 2179 2180 6533 6534

Q2. Contraction map

Recall that function F:[a,b] o [a,b] is *contractive* if there exists a nonnegative constant L < 1 such that

$$|F(x) - F(y)| \le L|x - y| \tag{Lip}$$

for all $x,y\in [a,b]$.

1. Show that if F is differentiable on [a,b], then condtion (Lip) is equivalent to

for all $x \in [a,b]$.

Now suppose we want to find a root of a differentiable function f(x) on (a,b). Consider the following iteration

$$x^{(t+1)} = x^{(t)} + \alpha f(x^{(t)}) \quad (\alpha \neq 0).$$
 (Iter)

- 2. When does iteration (Iter) converge?
- 3. Discuss the advantage of introducing the α .
- 4. Relate iteration (Iter) with the gradient descent method for minimization of a twice differentiable function.

 $\begin{array}{lll} \mathbb{Q}_{2}. \\ 1.0 \left| F(n) - F(u) \left(\leq L(n_{2}) \right) \right| \Rightarrow & F(n) \leq L \\ \mathbb{Z}_{1} \mathcal{L}_{2} \mathcal{L}_{2} \mathcal{L}_{3} \mathbb{Z}_{3} \mathbb{Z}_{3} \mathbb{Z}_{4} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathcal{L}_{5} \mathcal{L}_{2} \mathcal{L}_{3} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb{Z}_{5} \mathbb{Z}_{5} \\ \mathbb$

- 2. $\chi^{(t+1)} = F(\chi^{(t)}) z_1 z_2 + g$, $F(\chi^{(t)}) = \chi^{(t)} + \alpha f(\chi^{(t)}) \cdot |^{\alpha_1}$. $\chi^{(t+1)} = F(\chi^{(t)}) z_1 z_2 + g$, $F(\chi^{(t)}) = \chi^{(t+1)} e[\alpha_1 \beta_1] e[\alpha_1 \beta_1] = \chi^{(t+1)} e[\alpha_1 \beta_1] e[\alpha_1 \beta_1]$

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Q3. Poisson regression

1. In the lecture note on optimization, we used step-halving in the Fisher scoring of the Poisson regression analysis of the quarterly count data of AIDS deaths in Australia. Repeat this using the **Armijo rule**. Use the interface

```
poissonreg <- function(x, y, maxiter=10000, tol=1e-6, alpha=.2, gamma=.6) {
    beta0 <- matrix(0, nrow = 2, ncol=1)
    betaold <- beta0
    stop <- FALSE
    iter <- 1
    beta <- beta0
    inneriter <- rep(0. maxiter)
    lik <- function(bet) {eta <- bet[1] + bet[2]*x; sum(y*eta - exp(eta))}
    likold <- lik(betaold)
    while ((!stop) && (iter < maxiter)) {
       eta <- beta[1] + x * beta[2]
       w <- exp(eta) # lambda
       grad <- as.matrix(c(sum(y-w), sum((y-w)*x)))
       # line search by Armijo rule
       s <- 1.0
       while (TRUE && (inneriter[iter] < 10)) {
           beta <- beta + s * grad /sum((x^2*w))
           curlik <- lik(beta)
           likold <- likold + alpha*s*sum(grad/sum((x^2*w)))</pre>
           if (curlik > likold) break
           s <- s * gamma
           inneriter[iter] <- inneriter[iter] +1</pre>
       #print(c(as.numeric(beta), inneriter[iter], curlik, likold))
       betadiff <- beta - betaold
       if (norm(betadiff, "F") < tol) stop <- TRUE
       betaold <- beta
       likold <- curlik
       iter <- iter + 1
    return(list(val=as.numeric(beta), iter=iter, inneriter=inneriter[1:iter]))
```

where alpha and gamma corresponds to the Armijo rule parameters α and β , respectively. Also, execute the following code.

Test code deaths <- c(0, 1, 2, 3, 1, 4, 9, 18, 23, 31, 20, 25, 37, 45) quarters <- seq_along(deaths) poissonreg(quarters, deaths)\$val

[1] 0.3382443 0.2566411

2. In the same lecture note, it is stated that Poisson regression has the objective function $f(\beta) = -\sum_{i=1}^n \left[y_i \mathbf{x}_i^T \beta - \exp(\mathbf{x}_i^T \beta) - \log(y_i!) \right]$ and its gradient

$$egin{aligned}
abla f(eta) &= -\sum_{i=1}^n ig(y_i \mathbf{x}_i - \exp(\mathbf{x}_i^T eta) \mathbf{x}_iig) \ &= -\sum_{i=1}^n (y_i - \lambda_i) \mathbf{x}_i = -\mathbf{X}^T (\mathbf{y} - oldsymbol{\lambda}) \end{aligned}$$

where ${f X}$ is the design matrix, ${f y}$ is the response

is not Lipschitz continuous. Show this.

$(0.3.2) \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	
$\forall f(\beta_1) = -X^T(\gamma - \lambda_1)$, $\nabla f(\beta_2) = -X^T(\gamma - \lambda_2)$	
$ abla f(\beta_1) - \mathcal{T} f(\beta_2) = \chi^{T} (\mathcal{D}_1 - \mathcal{D}_2) $	
(xt/1-7) = xtexs, - ex32) > (xt(01-02) (+ xiting now onether	
10A(B1) - V A(B2) = 1xT (21-22) 1 > XT (B1 -B2)	
=> 1 of (u) - Of (v) 1 < L (u-v) 01 L2 Ezyobbl 104 = 12.	

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Q4. Gradient descent

1. In K-class logistic regression, we observe n independent categorical variables with K>2 categories, each associated with covariates. Let \mathbf{y}_i be the ith observation and $\mathbf{x}_i \in \mathbf{R}^p$ be the associated covariate vector. We use a dummy variable encoding for the response so that \mathbf{y}_i is a K-dimensional binary vector with only one component being 1. Let p_k be the probability of the kth category. We want to model the logit transform of p_k as a linear function of the covariate \mathbf{x}_i . Due to the constraint $\sum_{k=1}^K p_k = 1$, we set

$$\log rac{p_k}{p_K} = \mathbf{x}_i^T oldsymbol{eta}_k, \quad k=1,\ldots,K-1$$

and $oldsymbol{eta}_K=0.$

- a. Express the log likelihood of the data in terms of the matrices $\mathbf{Y}=(y_{ik})\in\mathbb{R}^{n\times K}$ and $\mathbf{X}=[\mathbf{x}_1,\ldots,\mathbf{x}_n]^T$ or their components. You may ignore terms irrelevant to $\boldsymbol{\beta}_k$.
- b. Write down a gradient ascent step for estimating coefficients $\mathbf{B} = [m{eta}_1, \dots, m{eta}_{K-1}]$.

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Q4. P (y=n 1x)= extpon					
f (ym px) = Px (+ px) +ym					
= e ym 18 px + (1-ym)18 (1-bx) =	exp (ym 1g Pm	+ lg (1-pn)			
la) = = [YTUBAN+ (HIM) lg (HAN)					
= Z[u, x] n - 101 (HPXTA)					
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Buttle But + XIAN L(M)					
Vl(An) = = [ynx: - ertan					
= E (yTK-PW) XT					
,					

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Q5. IRLS

1. A researcher is interested in how variables, such as GRE (Graduate Record Exam scores), GPA (grade point average) and prestige of the undergraduate institution, effect admission into graduate school. The response variable, admit/don't admit, is a binary variable. The data is available at https://stats.idre.ucla.edu/stat/data/binary.csv (https://stats.idre.ucla.edu/stat/data/binary.csv). How to analyze these data can be found in the website https://stats.idre.ucla.edu/r/dae/logit-regression/ (https://stats.idre.ucla.edu/r/dae/logit-regression/). You can use the following code to load the data.

mydata <- read.csv("binary.csv")</pre>

Implement the iteratively reweighted least squares (IRLS) algorithm for fitting a logistic regression model, and apply your algorithm to the admission data above. Use the interface below.

```
logistic <- function(y, X, beta0=NULL, maxiter=500, tol=1e-8) {
   beta0 \leftarrow rep(0, ncol(X))
   betaold <- beta0
   stop <- FALSE
   iter <- 1
   inneriter <- rep(0, maxiter)
   beta <- beta0
   lik <- function(bet) {eta <- X%*%bet ; sum(y*eta - log(1+exp(eta)))}
   likold <- lik(betaold)
   while ((!stop) && (iter < maxiter)) {
       eta <- X %*% betaold
       w < -1/(1+exp(-eta))
       s<- 1.0
       for (i in 1:length(inneriter)){
         z < -eta + s * (v/w-1)
         m \leftarrow Im(z\sim X - 1, weights = w)
         beta <- as.matrix(coef(m))
         beta[is.na(beta)] = 0
         curlik <- lik(beta)
         if (curlik > likold) break
         s < -s * 0.5
         inneriter[iter] <- inneriter[iter] + 1</pre>
     betadiff <- beta - betaold
     if (norm(betadiff, "F") < tol) stop <- TRUE
     likold <- curlik
     betaold <- beta
     iter <- iter+1
   return(list(coef = as.numeric(beta), iter = iter))
```

The return object should be a list comprised of <code>coef</code> , containing the fitted regression coefficient, and <code>iter</code> , the number of iterations ran. Note that the variable <code>rank</code> is categorical data.

Compare your result with glm() function in R. You can use the following code.

```
mydata$rank <- as.factor(mydata$rank)
X <- data.frame(cbind(1, mydata$gre, mydata$rank))
X[, 4] <- as.factor(X[, 4])
X2 <- model.matrix(~1+X[, 4])
X <- as.matrix(cbind(X[, 1:3], X2[,2:4]))
head(X)</pre>
```

```
## X1 X2 X3 X[, 4]2 X[, 4]3 X[, 4]4
## 1 1 380 3.61
## 2 1 660 3.67
                  0
                                 0
## 3 1 800 4.00
                  0
                         0
                                0
## 4 1 640 3.19
## 5 1 520 2.93
                                1
                  0
                         0
## 6 1 760 3.00
                                0
```

결과가 같다.