

SDS 385: Exercises 1 - Preliminaries

August 23, 2016

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Problem 1

(A)

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

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

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

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

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

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

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

because

$$\beta^T X^T W Y = (X\beta)^T W Y, \quad (8)$$

and

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

$$(Y^T W X \beta)^T = (W X \beta)^T Y = (X\beta)^T W^T Y = (X\beta)^T W Y. \quad (10)$$

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)

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

(ii)

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

(iii)

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

$$= X^T W X \beta. \quad (14)$$

Summing these terms and equaling them to zero yields

$$X^T W X \beta - X^T W Y = 0 \therefore \quad (15)$$

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

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

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

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

$$C = X^T W X, \quad D = X^T W y \quad (18)$$

so

$$C \hat{\beta} = D. \quad (19)$$

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

$$C = LU = LL^T \therefore \quad (20)$$

$$LL^T \hat{\beta} = D. \quad (21)$$

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

$$LA = D \quad (22)$$

$$L^T \hat{\beta} = A \quad (23)$$

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 793.2858 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 958.0309 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) 3087.150 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 857.0057
Cho.decomp(X, W, y) 542.3195 543.8550 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

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

so the negative log likelihood is

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

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

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

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

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

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

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

$$(32)$$

The gradient for this expression is,

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

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

$$= \sum_{i=1}^N (m_i w_i - y_i) x_i \quad (35)$$

$$= -X^T (y - mw) \quad (36)$$

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

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

	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 initial 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 being¹

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

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

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

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

Note:

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

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

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 $\nabla^2 \ell(\beta) = X^T W X$.

¹Notice the reindexing shown below for summations.

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

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

$$= \ell(\beta_0) + (-X^T a)^T (\beta - \beta_0) + \frac{1}{2} (\beta - \beta_0)^T X^T W X (\beta - \beta_0) \quad (45)$$

$$= \frac{1}{2} ([\beta - \beta_0] - (X^T W X)^{-1} X^T a)^T X^T W X ([\beta - \beta_0] - (X^T W X)^{-1} X^T a) + c \quad (46)$$

$$= \frac{1}{2} (\beta - \beta_0 + X^{-1} W^{-1} (X^T)^{-1} X^T a)^T X^T W X (\beta - \beta_0 + X^{-1} W^{-1} (X^T)^{-1} X^T a) + c \quad (47)$$

$$= \frac{1}{2} (\beta - \beta_0 + X^{-1} W^{-1} a)^T X^T W X (\beta - \beta_0 + X^{-1} W^{-1} a) + c \quad (48)$$

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

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

$$= \frac{1}{2} (z - X\beta)^T W (z - X\beta) + c, \quad (51)$$

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:

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

	N.'s method	R: <code>glm</code>
$\hat{\beta}_1$	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 while Newton's method must invert a matrix, which may either be impossible and is computationally intensive for large matrices.

²Help with completing the square obtained from: <https://justindomke.wordpress.com/completing-the-square-in-n-dimensions/>

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

5 library(Matrix)
  library(microbenchmark)

  ### No. 1 pt C

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

  N <- 4000
  P <- 1000

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

  # Inversion method

20 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
25   return(bhat.Inv)
}

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

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

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

  return(bhat.Cho)
}

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

45

  ### No. 1 pt D

  N <- 2000
50 P <- 1000

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



```

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

60 # Inv.methodSPARSE <- function(X.Inv, W.Inv, y.Inv) {
#   X <- Matrix(X, sparse = T)
#   XtWX <- (t(X.Inv)*diag(W.Inv)) %*% X.Inv
#   XtWY <- (t(X.Inv)*diag(W.Inv)) %*% y.Inv
#   bhat.Inv = solve(XtWX, XtWY)
65 #   return(bhat.Inv)
# }

Cho.decompSPARSE <- function(X.Cho, W.Cho, y.Cho) {
  X.Cho <- Matrix(X.Cho, sparse = T)
70 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)
75
  u <- forwardsolve(L.Cho, D.Cho)
  bhat.Cho <- backsolve(U.Cho, u)

  return(bhat.Cho)
80 }

microbenchmark(
85   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
90 # END

```

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

5 # Read in data file, standardize X

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

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

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

# Function for computing w.i

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

25 # 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)
30 }

# Function for computing gradient for likelihood

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

40 ###
### Gradient descent
###

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

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

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

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

   # Compare results to R's glm function

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

print(beta)

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

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

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

for (step in 1:n.steps) {
   log.lik2[step] <- loglik(beta, y, X, mi)
80   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)
}
85

   # Show estimates from Newton's method

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