Homework 2

M1399.000100, Seoul National University, Spring 2024

Due 23:00 Sunday, 2024-04-28

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Note

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 a 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.

You can modify the code chunks below to include your solution.

No late submission is accepted.

Q1. LU decomposition

1. Let $A \in \mathbb{R}^{n \times n}$ be nonsingular. Show that A has an LU decomposition if and only if for each k with $1 \le k \le n$, the upper left $k \times k$ block A[1:k,1:k] is nonsingular. Prove that this LU decomposition is unique.

_
Q1.1.
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image1

2. Write the R function LUdecomp below that computes the LU decomposition of a given matrix with the following interface:

```
LUdecomp <- function(LUobj, tol=1e-8) {
n <- nrow(LUobj$A) # assume square matrix
ipiv <- seq_len(n) # array of the permutation indexes of the rows
info <- 0
                   # indicator of success
for (k in seq_len(n-1)) {
    # partial pivoting
    pivot <- k
    curmax <- abs(LUobj$A[k, k])</pre>
    for (i in k + seq_len(max(n-k, 0))) {
      if (abs(LUobj$A[i,k]) > curmax) {
        curmax <- abs(LUobj$A[i,k])</pre>
        pivot <- i
      }
    }
    if (pivot != k) {
    # swap permutation indexes
      temp <- ipiv[k]</pre>
      ipiv[k] <- ipiv[pivot]</pre>
      ipiv[pivot] <- temp</pre>
    # swap rows
    for (j in seq_len(n)) {
      temp <- LUobj$A[k, j]
      LUobj$A[k, j] <- LUobj$A[pivot, j]
      LUobj$A[pivot, j] <- temp
    }
    # singularity test
    if (abs(LUobj\$A[k,k]) < tol){}
      info <- k
      break
    }
    else{
      info <- 0
    # Gaussian Elimination
    for (i in k + seq_len(max(n-k, 0))) {
      num <- LUobj$A[i,k] / LUobj$A[k,k]</pre>
    for (j in k + seq\_len(max(n-k, 0))) {
      LUobj$A[i,j] <- LUobj$A[i,j] - num*LUobj$A[k, j]
    }
    }
return(list(ipiv = ipiv, info = info))
```

The decomposition **must** be done *in place*. That is, if $A = LU \in \mathbb{R}^{n \times n}$, the U should overwrite the upper triangular part of the input matrix A, and the strictly lower triangular part of A should be overwritten by the same part of the L matrix computed. (Where does the diagonal part of L go?) Since R does not allow in-place modification of atomic objects, you are recommended to use a Reference Class (http://adv-r.had.co.nz/R5.html) (RC) object.

The RC for this homework can be declared by

```
setRefClass("LUclass",
  fields = list(
    A = "matrix", # n * n matrix
    b = "vector" # vector of length n
)
)
```

A RC object can be created, for instance, by

```
A <- matrix(c(1.0, 0.667, 0.5, 0.333), nrow=2)
b <- c(1.5, 1.0)
LUobj <- new("LUclass", A=A, b=b)
```

```
LUob i
```

```
## Reference class object of class "LUclass"

## Field "A":

## [1,1] [,2]

## [1,] 1.000 0.500

## [2,] 0.667 0.333

## Field "b":

## [1] 1.5 1.0
```

```
LUdecomp(LUobj)$LUobj
```

```
## NULL
```

Matrix A stored in LUobj can be referenced by LUobj\$A, and vector b can be by LUobj\$b (field b is reserved for the next question).

You must also implement partial pivoting: function LUdecomp must return a list that consists of two elements:

The first element <code>ipiv</code> of the list is the array of the permutation indexes of the rows, and the second element <code>info</code> is the indicator of success: if A is (numerically) singular, the function must return the row index where singularity occurs (where may a singularity occur in the LU decomposition?) as the second return value; otherwise return <code>0</code>. Use <code>tol</code> to determine the singularity.

3. Using the LUdecomp function written above, write function LUsolve0 that solves the linear equation Ax = b with interface

```
LUsolveO <- function(LUobj) {
# test if square
n <- nrow(LUobj$A)</pre>
if (ncol(LUobj$A) != n)
    stop("Matrix is not square.")
# do LU decomposition
lu <- LUdecomp(LUobj)</pre>
# test singularity of A
if (lu$info != 0)
 stop()
# in-place permutation of b
for (i in seq_len(n)) {
  temp <- LUobj$b[i]</pre>
 LUobj$b[i] <- LUobj$b[lu$ipiv[i]]
 LUobj$b[lu$ipiv[i]] <- temp
# forward substitution
for (i in seq_len(n)) {
    for (j in seq_len(i-1)) {
      LUobj$b[i] <- LUobj$b[i] - LUobj$A[i, j] * LUobj$b[j]
    }
    LUobj$b[i] <- LUobj$b[i] / LUobj$A[i, i]
# backsolve
for (i in rev(seq_len(n))) {
    for (j in i + seq\_len(max(n-i, 0))) {
      LUobj$b[i] \leftarrow LUobj$b[i] - LUobj$A[i, j] * LUobj$b[j]
     }
    LUobj$b[i] \leftarrow LUobj$b[i] / LUobj$A[i, i]
return(LUobj$b)
```

```
LUsolveO(LUobj)
```

```
## [1] 1.502241027 -0.004482054
```

again in place. That is, in addition to LUobjA overwritten by LUdecomp, vector LUobjb should be overwritten by the solution $A^{-1}b$. Your code should check if LUobjA is singular and generate an error.

4. Finally, write a wrapper function (https://en.wikipedia.org/wiki/Wrapper function) LUsolve with interface

```
LUsolve <- function(A, b) {
  LUobj <- new("LUclass", A = A, b = b)
  solution = LUsolveO(LUobj)
  return(solution)
}</pre>
```

which does **not** alter neither A nor b but solves Ax = b by calling LUsolve0 . Compare your results with the R expression solve(A, b).

5. Use your LUsolve to solve Ax = b with A and b given below.

```
library(Matrix)
A <- t(matrix(c(2.0, -4.0, 2.0, 4.0, -9.0, 7.0, 2.0, 1.0, 3.0), ncol=3))
b <- c(6.0, 20.0, 14.0)
```

```
LUsolve(A, b)
```

```
## [1] -10.494318 1.051136 7.562500
```

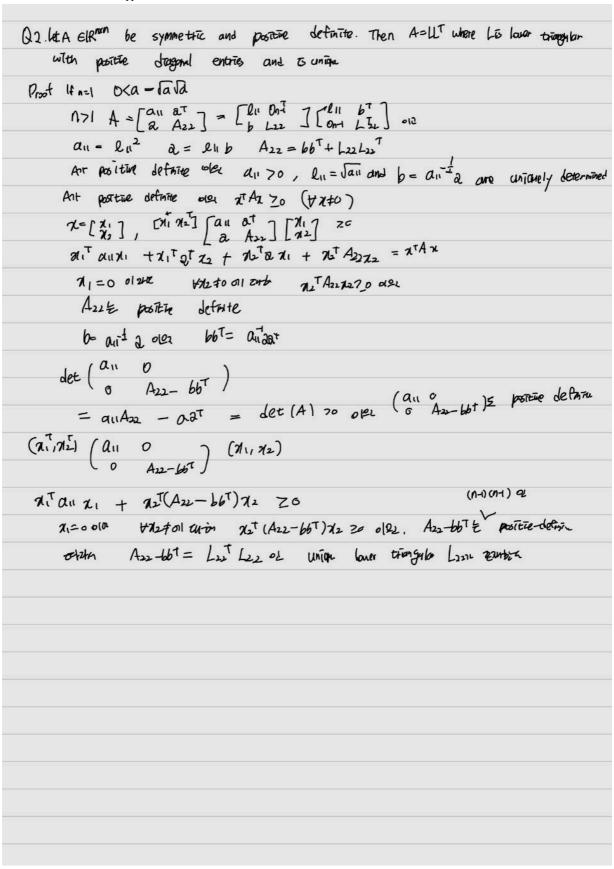
```
solve(A, b)
```

```
## [1] 2 1 3
```

Q2. Cholesky decomposition

- 1. Complete the *proof of the Cholesky decomposition* in lecture note 3 on Cholesky decomposition by showing that
 - A₂₂ is positive definite, and

• $\mathbf{A}_{22} - \mathbf{b}\mathbf{b}^T = \mathbf{A}_{22} - a_{11}^{-1}\mathbf{a}\mathbf{a}^T$ is positive definite of size $(n-1) \times (n-1)$.



Q3. QR decomposition

- 2. From the *lecture note 4 on QR decomposition*, explain why classical Gram-Schmidt (cgs()) fails with the given matrix A.
- 3. From the same lecture note, explain why the modified Gram-Schmidt (mgs()) fails with the given matrix B . Will the classical Gram-Schmidt succeed?

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3. Implement the Householder QR decomposition in R.

• The algorithm should be in-place: let the R matrix occupy the upper triangular part of the input X ∈ R^{n×p}. Below the diagonal place the vectors u_k that define the Householder transformation matrix H_k = I − 2u_ku_k^T/u_k^Tu_k. By setting the first element of u_k to 1, you can fit in these vectors in X. The algorithm should fill an additional vector storing the values of 2/u_k^Tu_k. This is how the LAPACK routine geqr f (https://netlib.org/lapack/explore-html/df/dc5/group_variants_g_ecomputational_ga3766ea903391b5cf9008132f7440ec7b.html) is designed. Note that Q can be recovered from u₁, u₂, ..., u_p.

- The algorithm should simultaneously compute the right-hand side of the equation that is reduced from the normal equation $\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^T\mathbf{v}$.
- · Stop your algorithm if the input matrix is not full column rank.
- · The function interface should be

```
householder <- function(QRobj, tol=1e-16) {
  n <- dim(QRobj$qr)[1] # additional variable
  p <- dim(QRobj$qr)[2] # additional variable
  if (n < p)
      stop("Column rank is deficient.")
  for (j in seq_len(min(n-1,p))) { # no transform for a number if n = p
    # compute R_jj
      R_{jj} \leftarrow sqrt(sum(QRobj qr[j:n, j]^2))
      # set the 1st element of u_j to 1 and compute rest of (unnormalized) u_j
      u_{j} \leftarrow c(1, QRobj\$qr[(j+1):n, j])
      if (abs(u_i) < tol) {
      stop("Column rank is deficient.")
      ## YOUR CODE HERE
      # compute scale
      scale \leftarrow sum(u_j^2)
      # update X[j:n, (j+1):p] with householder matrix generated by u_j
      for (i in j + seq_len(max(p-j, 0))) {
      QRobj\$qr[j:n, i] \leftarrow QRobj\$qr[j:n, i] - 2 * (u_j %*% t(u_j)/scale)
      # update RHS
      QRobj$pivot[j] <- j</pre>
      if (j < p) {
       QRobj qr[(j+1):n, j] \leftarrow u_j[-1]
  return(QRobj)
```

taking a Reference Class (RC) object

```
setRefClass("QRclass",
  fields = list(
  qr = "matrix", # n * p matrix, n >= p.
  scale = "vector", # Householder scalar, length p
  y = "vector" # RHS for least squares, length n
  )
)
```

You may initialize a QRclass object by setting scale=vector("numeric", p) and y=vector("numeric", n), for example.

· Write a separate routine

```
recoverQ <- function(QRobj) {
    # Q = H_1 H_2 ... H_{p-1} |
    n <- dim(QRobj$qr)[1]
    p <- dim(QRobj$qr)[2]
    Q <- diag(n)
    for (j in rev(seq_len(min(n-1,p)))) {
        u_j <- c(1, QRobj$qr[(j+1):n, j])
        scale <- sum(u_j^2)
        Q[j:n, j:n] <- Q[j:n, j:n] - 2 * (crossprod(u_j, Q[j:n, j:n]) / scale) %*% u_j %
    *% t(u_j)
     }
    Q
}</pre>
```

that recovers Q.

- Using your function, compute the QR decomposition of the matrices A and B of the previous question. Compare the orthogonality of the computed Q matrix.
- 4. Use your householder() and recoverQ() functions to estimate the regression coefficients and variance estimate $\hat{\sigma}^2$ of the following covariates $\mathbf{x}_1, \mathbf{x}_2$ and the response variable \mathbf{y} .

```
x1 \leftarrow c(1, 2, 3, 5, 5, 7)

x2 \leftarrow c(1, 3, 3, 4, 4, 5)

y \leftarrow c(2, 4, 5, 8, 8, 9)
```

Q4. Least squares

The Longley (https://www.itl.nist.gov/div898/strd/lls/data/Longley.shtml) data set of labor statistics was one of the first used to test accuracy of least squares computations. This data set is built in R and is available by calling data(datasets::longley). The Longley data set consists of one response variable (number of people employed) and six predictor variables (GNP implicit price deflator, Gross National Product, number of unemployed, number of people in the armed forces, 'noninstitutionalized' population \geq 14 years of age, year) observed yearly from 1947 to 1962.

- 1. Load the data set into R and construct a data matrix X for linear model $y = X\beta + \varepsilon$. Include an intercept in your model.
 - Using the R command svd(), list up the 7 singular values of X. What is the condition number of X?

• Construct the Gram matrix $G = X^T X$. List up the 7 singular values of G. What is the condition number of G?

```
library(datasets)
X <- as.matrix(cbind(Intercept = 1, datasets::longley[, -ncol(longley)]))
singular.X <- svd(X)$d
(condition <- max(singular.X) / min(singular.X))</pre>
```

[1] 23845862

```
G<-t(X) %*% X
singular.g <- svd(G)$d
(condition <- max(singular.g) / min(singular.g))
```

```
## [1] 5.685684e+14
```

- 2. Using householder() and recoverQ() functions you wrote for Q3, compute the regression coefficients $\hat{\beta}$, their standard errors, and variance estimate $\hat{\sigma}^2$. Verify your results using the R function Im().
- 3. Using the Cholesky decomposition of \mathbf{G} , compute the regression coefficients $\hat{\boldsymbol{\beta}}$, their standard errors, and variance estimate $\hat{\sigma}^2$. Compare the results with the values of the above question.

Q5. Iterative method

- 1. Show that the norm $\|\mathbf{x}\|_{\delta}$ in the *lecture note 5 on iterative methods* is indeed a vector norm.
- 2. A $n \times n$ matrix \mathbf{A} is strictly column diagonally dominant if $|a_{ii}| > \sum_{j \neq i} |a_{ji}|$ for all $i = 1, \dots, n$. Can strictly column diagonally dominance of a matrix \mathbf{A} guarantee the convergence of the Jacobi method and Gauss-Seidel methods to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$?
- 3. Consider solving the linear system of equations Ax = b using the Jacobi's method, where

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

Note the eigenvalues of A are analytically given by

$$\lambda_i = 2 - 2\cos\frac{i\pi}{n+1}, \quad i = 1, 2, ..., n.$$

a. Find the spectral radius of R, when the Jacobi iteration is written as

$$\mathbf{x}^{(k+1)} = \mathbf{R}\mathbf{x}^{(k)} + \mathbf{c}.$$

Will the iterative algorithm converge?

b. Let the eigenvector of A associated with the eigenvalue λ_i be $v_i \in \mathbb{R}^n$. Then we can express the error of the iteration as

$$\boldsymbol{\varepsilon}^{(k)} := \mathbf{x}^{(k)} - \mathbf{x}^* = a_1^{(k)} \mathbf{v}_1 + a_2^{(k)} \mathbf{v}_2 + \dots + a_n^{(k)} \mathbf{v}_n,$$

for some scalars $a_1^{(k)},...,a_n^{(k)}$;

 \mathbf{x}^* is the true solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$. What can you say about the attenuation of the sequence $\{a_i^{(k)}\}_{k=1,2,\ldots}$ for different values of i?

```
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                               Tal-n [ [ so(8)] = CxT = | C1 max | [ so(8)] T x7
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         \chi^{(t+1)} = -D^{\dagger} A_{x}^{(e)} + \chi^{(e)} + \rho^{\dagger} b = D^{\dagger} (b - (b - (L+D+U)\chi^{(e)}) = D^{\dagger} (b - (L+U)\chi^{(e)}) O(7101).
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