國立清華大學
NATIONAL TSING HUA UNIVERSITY

10820ASTR660000
Computational Astrophysics
計算天文物理

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(submit to google classroom)

Problem Set 4

Reading Assignments

1. Read Chapter 2 of the "Scientific Computing: An Introductory Survey" (https://books.google.com.tw/books?id=f6Z8DwAAQBAJ&hl=zh-TW)
2. Read the scipy linear algebra documentation (https://docs.scipy.org/doc/scipy/reference/linalg.html)
3. Given a $M \times N$ matrix A, if $M > N$, the system is called an overdetermined linear system. Read the wikipedia article https://en.wikipedia.org/wiki/Overdetermined_system and https://en.wikipedia.org/wiki/QR_decomposition.
4. Solving the linear least squares of an overdetermined linear system is a common way to do data fitting. Read the wikipedia article https://en.wikipedia.org/wiki/Linear_least_squares.
5. *(Optional)* Read Chapter 3 of the "Scientific Computing: An Introductory Survey" (https://books.google.com.tw/books?id=f6Z8DwAAQBAJ&hl=zh-TW)

Written Assignments

1. Vector Norms. For the vector $\boldsymbol{x} = [-1.6, 1.2]^T$, calculate the first, second, and infinity norms [10pts].
2. Matrix Norms. For the matrix
$$\boldsymbol{A} = \begin{bmatrix} 7 & -3 & 2 \\ 1 & 1 & 5 \\ 2 & -2 & 1 \end{bmatrix}, \tag{1}$$
calculate the first and infinity norms [10pts].
3. (a) Solve the linear system with Gaussian elimination [3pts]
$$\boldsymbol{Ax} = \begin{bmatrix} 1 & 2 & 2 \\ 4 & 6 & 8 \\ 4 & 8 & 10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \\ 10 \end{bmatrix} = \boldsymbol{b} \tag{2}$$
(b) What is the LU factorization of $\boldsymbol{A}$ [4pts]? (c) show that $\boldsymbol{A} = \boldsymbol{LU}$ [3pts]. Please do it step by step and do NOT use a computer.

4. What is the Cholesky factorization of the following matrix [10pts]?

$$\begin{bmatrix} 4 & -1 & -1 \\ -1 & 4 & -1 \\ -1 & -1 & 4 \end{bmatrix} \tag{3}$$

Programming Assignments

1. Consider the linear system:

$$\begin{bmatrix} 1 & 1+\epsilon \\ 1-\epsilon & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1+\epsilon+\epsilon^2 \\ 1 \end{bmatrix}, \tag{4}$$

where ϵ is a small parameter to be specified. The exact solution is trivial

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ \epsilon \end{bmatrix}. \tag{5}$$

Use the Fortran program we developed in the course to solve this system. Experiment with various values for ϵ you try, especially values near $\sqrt{\epsilon_{mach}}$ for your computer, compute an estimate of the condition number of the matrix and the relative error in each component of the solution [20pts].

2. The Cholesky factorization requires only about half as much work and half as much storage as are required for LU factorization of a general matrix by Gaussian elimination. (a) Modify your `linalg.f90` file and implement the below algorithm [10pts]. (b) test your program by solving the matrix in the written assignments problem 4. [10pts]

```
// Algorithm: Cholesky Factorization
for k = 1 to n {
   akk = sqrt(akk)
   for i = k + 1 to n {
      aik = aik / akk
   }
   for j = k + 1 to n {
      for i = k + 1 to n {
         aij = aij - aik*ajk
      }
   }
}
```

3. Consider a linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ has a banded $n \times n$ matrix $\boldsymbol{A} =$

$$\begin{bmatrix} 9 & -4 & 1 & 0 & ... & ... & 0 \\ -4 & 6 & -4 & 1 & ... & ... & 0 \\ 1 & -4 & 6 & -4 & 1 & ... & 0 \\ 0 & 1 & -4 & 6 & -4 & 1 & ... \\ ... & ... & ... & ... & ... & ... & ... \\ ... & ... & 1 & -4 & 6 & -4 & 1 \\ ... & ... & ... & 1 & -4 & 5 & -2 \\ 0 & ... & ... & 0 & 1 & -2 & 1 \end{bmatrix}, \tag{6}$$

Take $b_i = 1$ for each component of the vector $\boldsymbol{b}$. Let $n = 100$, solve the linear system using the LU decompositon in `scipy` and compare the performance with the solver designed for banded matrix (`scipy.linalg.solve_banded`). You could use the function `%timeit` in a jupyter notebook to measure the computing time [20pts].

4. Continue the problem 3, verify that the matrix $\boldsymbol{A}$ has the UL factorization $\boldsymbol{A} = \boldsymbol{R}\boldsymbol{R}^T$, where $\boldsymbol{R}$ is an upper triangular matrix of the form

$$\boldsymbol{R} = \begin{bmatrix} 2 & -2 & 1 & 0 & ... & ... & 0 \\ 0 & 1 & -2 & 1 & ... & ... & ... \\ 0 & 0 & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & 0 \\ ... & ... & ... & 0 & 1 & -2 & 1 \\ ... & ... & ... & ... & 0 & 1 & -2 \\ 0 & ... & ... & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{7}$$

Letting $n = 1000$, solve the linear system using this factorization (two triangular solves). Also solve the system in its original form using a banded system solver as in the previous question. How well do the answers obtained agree with each other? Which approach seems more accurate? What is the condition number of A? [20pts]