Computational Physics; February–May 2024
Assignment 1
Due: Thursday, 21 March 2024

Instructions

- When you are asked to write a code, submit your code by posting it to Github and sending the Github link.
- Otherwise, solve problems manually, or when you are asked for a number as an answer, submit your response in writing.
- Submit assignments by email to the TAs.

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1. Consider the system of linear equations

$$\begin{aligned} x_1 + \frac{1}{2}x_2 &= \frac{5}{21}, \\ \frac{1}{2}x_1 + \frac{1}{3}x_2 &= \frac{11}{84}. \end{aligned} \tag{1}$$

   (a) Assuming a decimal computer with two digits, solve this system using Gaussian elimination.

   (b) For the same computer, solve this system using Conjugate Gradient method.

   (c) Which method gives the better answer?

2. Do the same as above for

$$\begin{aligned} 0.1x_1 + 0.2x_2 &= 0.3, \\ 0.2x_1 + 113x_2 &= 113.2. \end{aligned} \tag{2}$$

3. The Society for Industrial and Applied Mathematics (SIAM) is an international organization for professional researchers in applied mathematics, computational science, and data science from across the world. With funding from the US government, SIAM has been running a project called "The History of Numerical Analysis and Scientific Computing". This is an effort to document and preserve the history of the scientific computing. As part of this project, in 2004, historian Thomas Haigh (University of Wisconsin) conducted this interview with Jack Dongarra (University of Tennessee), the developer of LAPACK and an important personality in the field of computational linear algebra. The text of the interview is available in PDF on SIAM's web site here: `http://history.siam.org/oralhistories/dongarra.htm`. Read this interview. List three things that you took away from it.

4. Do two iterations of the Relaxation Method with $w = 1.1$ for these systems:

$$\begin{aligned} 3x_1 - x_2 + x_3 &= 1 \\ 3x_1 + 6x_2 + 2x_3 &= 0 \\ 3x_1 + 3x_2 + 7x_3 &= 4 \end{aligned} \tag{3}$$

$$\begin{aligned} 10x_1 - x_2 &= 9 \\ -x_1 + 10x_2 - 2x_3 &= 7 \\ -2x_2 + 10x_3 &= 6 \end{aligned} \tag{4}$$

$$\begin{aligned} 10x_1 + 5x_2 &= 6 \\ 5x_1 + 10x_2 - 4x_3 &= 25 \\ -4x_2 + 8x_3 - x_4 &= -11 \\ -x_3 + 5x_4 &= -11 \end{aligned} \tag{5}$$

$$\begin{aligned} 4x_1 + x_2 + x_3 + x_5 &= 6 \\ -x_1 - 3x_2 + x_3 + x_4 &= 6 \\ 2x_1 + x_2 + 5x_3 - x_4 - x_5 &= 6 \\ -x_1 - x_2 - x_3 + 4x_4 &= 6 \\ 2x_2 - x_3 + x_4 + 4x_5 &= 6 \end{aligned} \tag{6}$$

5. Same as above but this time use $w = 1.3$.

6. Spend 15 minutes browsing through the chapters titled 'BLAS Support', 'Linear Algebra', and 'Eigensystems' in the GSL Reference Manual.

7. For the same four systems as in problem number 4 above, do two iterations of the Jacobi method, with 0 as the initial guess.

8. Repeat above with Gauss-Seidel method.

9. Solve the first of the above four systems using the Jacobi method. Stop when the relative change between iterations is smaller than 0.1% under the ℓ_∞ norm.

10. Repeat above with Gauss-Seidel method.

11. Solve the above four systems using `numpy.linalg.solve`.

12. Spend 15 minutes reading the code for `numpy.linalg.solve`.

13. Use GSL to compute the LU decomposition of the above four matrices. In your code, demonstrate that the LU decomposition is correct.

14. Show that the Thomas method is $\mathcal{O}(n)$.

15. Reduce the problem of inverting a complex matrix to that of inverting real matrices.

16. The vector

$$\mathbf{x} = \begin{bmatrix} 7.859713071 \\ 0.422926408 \\ -0.073592239 \\ -0.540643016 \\ 0.010626163 \end{bmatrix}$$

solves the equation

$$\begin{bmatrix} 0.2 & 0.1 & 1 & 1 & 0 \\ 0.1 & 4 & -1 & 1 & -1 \\ 1 & -1 & 60 & 0 & -2 \\ 1 & 1 & 0 & 8 & 4 \\ 0 & -1 & -2 & 4 & 700 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}.$$

Write Python code to solve this equation using Jacobi, Gauss-Seidel, Relaxation, and Conjugate Gradient methods. (Use $w = 1.25$ for the relaxation method.) In each case, stop when the difference between the approximate solution vector and the true solution written above is less than 0.01. (In other words, have a tolerance of 0.01.) Mention how many iterations you need in each method to reach this accuracy.

17. Write a Python code that produces the QR decomposition of

$$\mathbf{A} = \begin{bmatrix} 5 & -2 \\ -2 & 8 \end{bmatrix}$$

using `numpy.linalg.qr`. Use the decomposition to calculate the eigenvalues of the matrix. Compare your result with that produced by `numpy.linalg.eigh`.

18. Write a Python code to apply the Power Method to find the dominant eigenvalue and eigenvector of the matrix

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

Your eigenvalue should be accurate to within a percent.

19. Use `numpy.linalg.svd` and compute the Singular Value Decomposition of the following matrices:

$$\begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix} \tag{8}$$

$$\begin{bmatrix} 2 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{9}$$

$$\begin{bmatrix} 2 & 1 \\ -1 & 1 \\ 1 & 1 \\ 2 & -1 \end{bmatrix} \tag{10}$$

$$\begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & 1 & -1 \end{bmatrix} \tag{11}$$

$$\begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & 1 & -1 \end{bmatrix} \tag{12}$$

$$\begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{13}$$

Report the time taken by each computation. Demonstrate that the decomposition is correct.

20. What is Principle Component Analysis (PCA)? How is it related to Singular Value Decomposition (SVD)? Give an example situation in which you could use PCA.

21. List the names of LAPACK, GSL, and Numpy functions to do the following computations:

    (a) Solving a system of linear equations using Gaussian Elimination with Pivoting
    (b) Solving a system of linear equations using the Jacobi method
    (c) Solving a system of linear equations using the Gauss-Seidel method
    (d) Solving a system of linear equations using the Relaxation method
    (e) Solving a system of linear equations using the Conjugate Gradient method
    (f) Obtaining the LU decomposition of a matrix
    (g) Obtaining the QR decomposition of a matrix
    (h) Obtaining the Singular Value Decomposition of a matrix
    (i) Obtaining the eigenvalues of a real symmetric matrix
    (j) Obtaining the eigenvalues of a complex Hermitian matrix
    (k) Obtaining the eigenvalues of a general real or complex $n \times n$ matrix

22. For a three-digit decimal computer, solve the following system using Gaussian elimination with partial pivoting:

$$
\begin{aligned}
\pi x_1 - e x_2 + \sqrt{2} x_3 - \sqrt{3} x_4 &= \sqrt{11}, \\
\pi^2 x_1 + e x_2 - e^2 x_3 + \frac{3}{7} x_4 &= 0, \\
\sqrt{5} x_1 - \sqrt{6} x_2 + x_3 - \sqrt{2} x_4 &= \pi, \\
\pi^3 x_1 + e^2 x_2 - \sqrt{7} x_3 + \frac{1}{9} x_4 &= \sqrt{2}.
\end{aligned} \tag{14}
$$