Numerical Methods I

Assignment III

Due: April 3, 2019

Consider the $N \times N$ circulant matrix $\mathbf{C}$ with elements given by

$$\mathbf{C}_{ij} = \epsilon\ \delta(i,j) + \delta(i, j+1 \bmod N) + \delta(i, j-1 \bmod N). \tag{1}$$

Here δ is the Kronecker delta function and $i, j = 0, 1, 2 \ldots N-1$. For example, the matrix for $N = 4$ is

$$\mathbf{C} = \begin{pmatrix} \epsilon & 1 & 0 & 1 \\ 1 & \epsilon & 1 & 0 \\ 0 & 1 & \epsilon & 1 \\ 1 & 0 & 1 & \epsilon \end{pmatrix}. \tag{2}$$

1. For general $N > 2$, determine the eigenvalues λ_i and the corresponding (complex) eigenvectors $|\lambda_i\rangle$ of $\mathbf{C}$. Use these to construct a diagonalizing matrix $\mathbf{M}$ such that

   $$\mathbf{D} = \mathbf{M}^{-1}\mathbf{C}\mathbf{M}, \tag{3}$$

   with $\mathbf{D}_{ij} = \lambda_i\ \delta(i,j)$. For what values of ϵ is this procedure singular?

   (5 Marks)

2. Write a program to perform the matrix multiplication in Eq. (3). Plot the error between the numerically computed diagonal elements of $\mathbf{D}$ and the exact answer for $N = 2^n$ (with $n = 2, 3 \ldots 10$).

   (10 Marks)

3. Consider the matrix

   $$\mathbf{B} = \alpha\mathbf{C} + \beta\mathbf{D}. \tag{4}$$

   For an α and β of your choice, write a program to perform a direct triangular decomposition of $\mathbf{B}$ using the Gaussian elimination algorithm. Use this to compute the determinant $\det(\mathbf{B})$ for $N = 2^n$ (with $n = 2, 3 \ldots 10$).

   (15 Marks)

4. Write a program to perform the LU decomposition $\mathbf{B} = \mathbf{L}\mathbf{U}$ where $\mathbf{L}$ is a lower triangular and $\mathbf{U}$ is an upper triangular matrix. Defining

   $$\mathbf{L}|\mathbf{y}\rangle = |\mathbf{1}\rangle, \quad \mathbf{U}|\mathbf{x}\rangle = |\mathbf{y}\rangle, \tag{5}$$

   use forward and back substitution respectively in the above equations to solve the linear system

   $$\mathbf{B}|\mathbf{x}\rangle = |\mathbf{1}\rangle. \tag{6}$$

   Here $|\mathbf{1}\rangle$ is a column vector with all elements equal to 1. Choose $N = 2^n$ (with $n = 2, 3 \ldots 10$).

   (20 Marks)