Numerical Analysis [WI4014TU]
Assignment 2

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Consider the following boundary-value problem:

$$-\frac{d^2u_i}{dx^2} = f_i, \quad x \in (0,3); \tag{1}$$

$$u_i(0) = 1, \quad u_i(3) = 1, \quad i = 1, 2;$$

with the source functions

$$f_1(x) = 3x + 2, \quad f_2(x) = x^2 + 3x + 2, \quad x \in [0,3] \tag{2}$$

1. Find the exact solutions $u_1^{ex}(x)$ and $u_2^{ex}(x)$ of the problem (1) corresponding to $f_1(x)$ and $f_2(x)$ given in (2).

Solution: For $i = 1$:

$$-\frac{d^2u_1}{dx^2} = f_1 = 3x - 2$$

$$\implies u_1 = -\frac{x^3}{2} + x^2 - C_1x - C_2$$

Using the given boundary conditions;

$$u(0) = 1 \implies C_2 = -1$$

$$u(3) = 1 \implies 1 = \frac{-27}{2} + 9 - 3C_1 + 1$$

$$\implies C_1 = -\frac{3}{2}$$

$$\therefore u_1^{ex} = -\frac{x^3}{2} + x^2 + \frac{3}{2}x + 1$$

Similarly, for $i = 2$:

$$-\frac{d^2u_2}{dx^2} = f_2 = x^2 + 3x - 2$$

$$\implies u_2 = -\frac{x^4}{12} - \frac{x^3}{2} + x^2 - C_1x - C_2$$

Using the given boundary conditions;

$$u(0) = 1 \implies C_2 = -1$$

$$u(3) = 1 \implies 1 = -\frac{27}{4} - \frac{27}{2} + 9 - 3C_1 + 1$$

$$\implies C_1 = -\frac{15}{4}$$

$$\therefore \implies u_2^{ex} = -\frac{x^4}{12} - \frac{x^3}{2} + x^2 + \frac{15}{4}x + 1$$

2. Discretisze the problem (1) using the Finite-Difference Method (FDM) on a uniform grid obtained by dividing the $[0, 3]$ interval into $n = 5$ sub-intervals of equal length.

   (a) What is the step size h? How many internal and boundary points do you get? How many unknowns does your numerical problem have?

   (b) Write down the $\mathcal{O}(h^2)$ finite-difference (FD) approximation of the (negative) second derivative operator, including the explicit remainder term

   (c) Write down all discrete FD equations for your problem, explicitly computing numerical constants

   (d) Write out the system matrix A and the right-hand-side vectors $\mathbf{f_1}$ and $\mathbf{f_2}$, for the source functions (2)

   (e) Compute the theoretical eigenvalues of A and present then as a column of a LaTeX table in your report.

   (f) Compute the first 4 (smallest) eigenvalues of the negative second derivative operator and present them as the second column in your table

Solution:

(a) The step size of the FDM is determined using the formula:

$$h = \frac{b-a}{N}$$

where h is the step size, b and a are the grid boundary values, and N is the number of steps. For $N = 5$, the step size $h = 0.6$. number of internal points $= 4$, and number of boundary points $= 2$. We will get total 4 unknowns for the 4 internal nodes.

(b) The $\mathcal{O}(h^2)$ FD approximation is given by the following formula:

$$\mathcal{O}(h^2) = \left| -u_i'' - \left(\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2}\right) \right| \tag{3}$$

From the Taylor series expansion, we derive:

$$-u_i'' = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} + \frac{u_i^{(4)}}{12}h^2 + \cdots$$

Now, for f_1:

$$u_1^{(4)} = \frac{d^4}{dx^4}(-\frac{x^3}{2} + x^2 + \frac{3}{2}x + 1)$$

$$\implies u_1^{(4)} = 0$$

This is because the 4^{th} derivative of a cubic function is 0. Using the Taylor series expansion (ignoring the higher order terms) and the obtained result in 3, we get

$$\mathcal{O}(h^2) = \left| \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} - (\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2}) \right|$$

$$\implies \mathcal{O}(h^2) = |0| = 0$$

Similarly, for f_2:

$$u_2^{(4)} = \frac{d^4}{dx^4}(-\frac{x^4}{12} - \frac{x^3}{2} + x^2 + \frac{15}{4}x + 1)$$

$$\implies u_2^{(4)} = -2$$

Using the Taylor series expansion (ignoring the higher order terms) and the obtained result in (3), we get

$$\mathcal{O}(h^2) = \left| \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} - \frac{2 \times 0.6^2}{12} - (\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2}) \right|$$

$$\implies \mathcal{O}(h^2) = \left| -\frac{2 \times 0.6^2}{12} \right| = 0.06$$

(c) Using subscripts 1 and 2 for source functions $\mathbf{f_1}$ and $\mathbf{f_2}$, the discrete FD equations are as follows:
For $\mathbf{f_1}$:

$$u_{10} = 1 \qquad \text{left BC}$$

$$\frac{-1}{h^2}(u_{10} - 2u_{11} + u_{12}) = f_{11}$$

$$\frac{-1}{h^2}(u_{11} - 2u_{12} + u_{13}) = f_{12}$$

$$\frac{-1}{h^2}(u_{14} - 2u_{13} + u_{14}) = f_{13}$$

$$\frac{-1}{h^2}(u_{13} - 2u_{14} + u_{15}) = f_{14}$$

$$u_{15} = 3 \qquad \text{right BC}$$

Inserting the numerical constants, the final system of equations look like as follows:

$$-2u_{11} + u_{12} = \frac{-116}{125} = -0.928$$
$$u_{11} - 2u_{12} + u_{13} = \frac{-72}{125} = -0.576$$
$$u_{14} - 2u_{13} + u_{14} = \frac{-153}{125} = -1.224$$
$$u_{13} - 2u_{14} = \frac{-359}{125} = -2.872$$

Following the same procedure for $\mathbf{f_2}$, we get the final system of equations as:

$$-2u_{21} + u_{22} = \frac{-661}{625} = -1.0576$$
$$u_{21} - 2u_{22} + u_{23} = \frac{-684}{625} = -1.0944$$
$$u_{24} - 2u_{23} + u_{24} = \frac{-1494}{625} = -2.3904$$
$$u_{23} - 2u_{24} = \frac{-3091}{625} = -4.9456$$

(d) In general terms, the matrix form of the FD discretized 1D Poisson equation looks like

$$A\mathbf{u} = \mathbf{f}$$

$$\implies -\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} f_1 + \frac{u_0}{h^2} \\ f_2 \\ f_3 \\ f_4 + \frac{u_5}{h^2} \end{bmatrix}$$

$$\text{where } -\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \quad \text{is the system matrix } A$$

Substituting the values, we get:

For $\mathbf{f_1}$:

$$-\frac{1}{0.36}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 2.57778 \\ 1.6 \\ 3.4 \\ 7.97778 \end{bmatrix}$$

Similarly, for $\mathbf{f_2}$:

$$-\frac{1}{0.36}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 2.937778 \\ 3.04 \\ 6.64 \\ 13.737778 \end{bmatrix}$$

(e) The theoretical eigenvalues for the FD system matrix A are given by the formula:

$$\lambda_i = \frac{4}{h^2}\sin^2(\frac{\pi}{2}\cdot\frac{i}{N}); \qquad i = 1, 2, \cdots, (N-1)$$

Since, these eigenvalues are independent of the source function, these will be same for $\mathbf{f_1}$ as well as $\mathbf{f_2}$. The theoretical eigenvalues are given in Table 1.

(f) The eigenvalues of the negative second derivative operator are given using the formula:

$$\tilde{\lambda}_i = \left(\frac{\pi i}{D}\right)^2; \qquad i = 1, 2, \cdots$$

Using this formula, we can compute the first 4 (smallest) eigenvalues of the original continuous problem. These are given in Table 1.

Table 1: Eigenvalues.

Theoretical e-values	First 4 e-values	np.linalg.eig
1.061016698	1.096622711	1.0610167
3.838794476	4.3864908845	3.83879448
7.272316635	9.869604401	7.27231664
10.05009441	17.54596338	10.0500944187837

3. Construct a uniform grid and display the source functions and the exact solutions.

Solution: To construct a uniform grid, based on the problem statement, the variables `x[]` and `bc[]` are defined which store the boundary nodes and $u(x)$ at those nodes respectively. We need another variable for the number of sub-intervals, `n`, which is taken as input from the user.

```
xgrid, h = np.linspace(x[0], x[1], N+1, retstep=True)
```

The command `np.linspace()` returns the discretized 1D domain, stored in `xgrid` and the step size is stored in `h`.
The Python plot for f_1 and f_2, and u_1^{ex} and u_2^{ex} for $n = 5$ is given in Figure 1, and Figure 2 respectively.

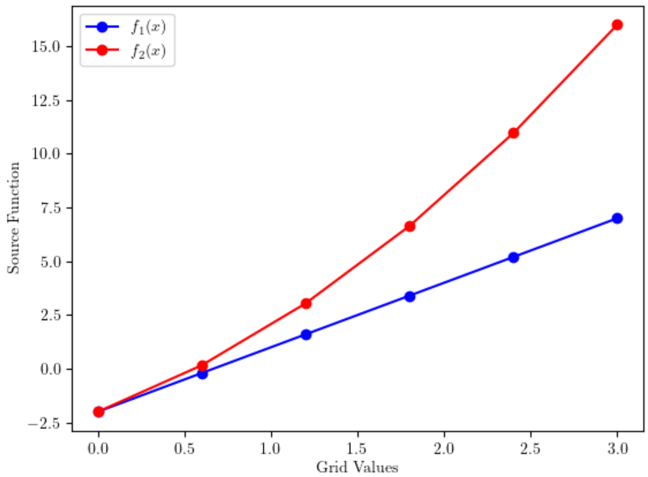

Figure 1: Source function $\mathbf{f_1}$ and $\mathbf{f_2}$.

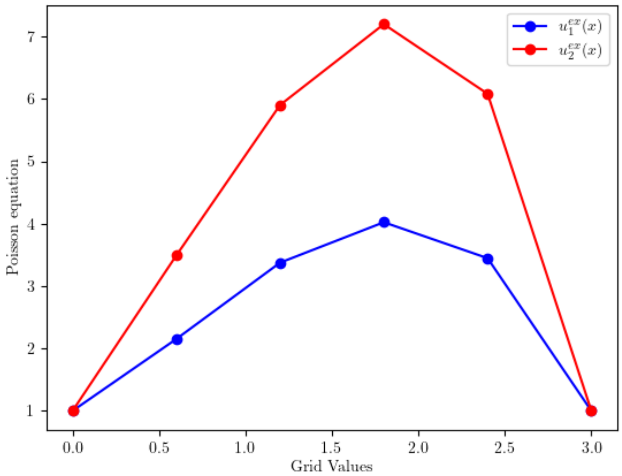

Figure 2: Exact solution for $n = 5$ sub-intervals, and $h = 0.6$ grid spacing.

4. Assemble the Finite-Difference (negative) Laplacian matrix.

Solution:
Structure of the FD negative Laplacian matrix is given in Figure 3. The eigenvalues computed using `np.linalg.eig()` are given in the third column of Table 1.

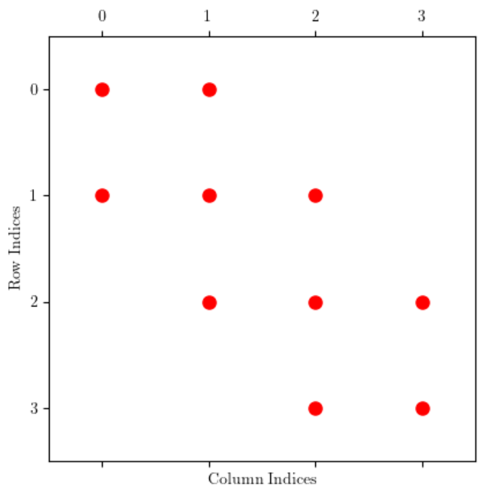

Figure 3: Structure of the system matrix A for $n = 5$.

5. Solve the linear algebraic problem.

Solution: The plot for numerical solutions u_1 and u_2 and exact solutions u_1^{ex} and u_2^{ex} with source functions f_1 and f_2 at $n = 5$ is given in Figure 4. Solid lines represent the exact solution, and dashed lines represent the numerical solution. Blue corresponds to source function f_1 and red corresponds to the source function f_2.

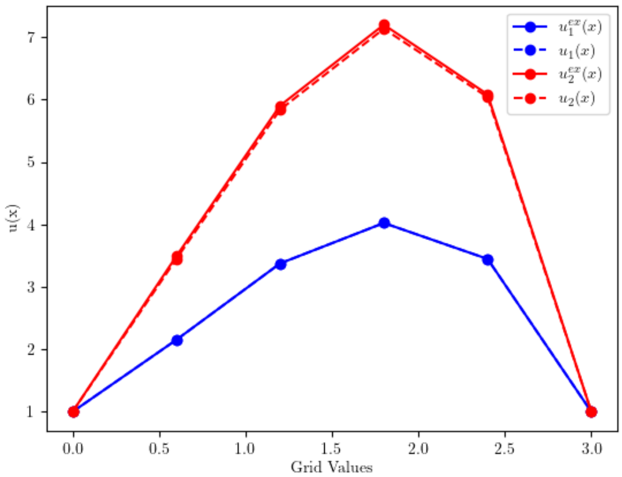

Figure 4: Numerical solution vs the Exact solution with source function $\mathbf{f_1}$ and $\mathbf{f_2}$ for $n = 5$.

6. Analyze your results.

Solution: The global error between numerical and exact solution for $n = 5$ is calculated using the RMSE (Root Mean Squared Error) method, the formula for which is given by:

$$\epsilon = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n-1}|u_i - \tilde{u}_i|^2}$$

The global errors computed for source functions f_1 and f_2 are:

$$\epsilon_1 = 3.33066907 \times 10^{-16}$$

$$\epsilon_2 = 5.50694107 \times 10^{-2}$$

These are close to the $\mathcal{O}(h^2)$ that we manually calculated in question 2(b).

The logarithm of the global error as a function of n is given in Figure 5. The fluctuation in the error calculation of $u_1(x)$ is due to the round-off errors caused in the python function `numpy.sum()`. For $u_2(x)$, we can see that as we increase the number of sub-intervals, the error reduces exponentially.

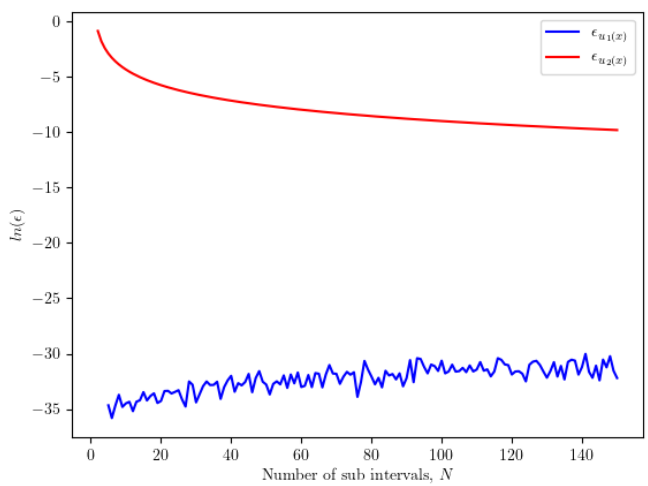

Figure 5: Rate of Convergence of the Finite-Difference Method