Problem 1

Finite difference approximation (3 points). Let $f : \mathbb{R} \to \mathbb{R}$ be a smooth function, and let $x_1 < x_2 < x_3 < x_4$ be four increasing values.

a) Derive a finite difference (FD) approximation for $f''(x_2)$ that is as accurate as possible, based on the four values of $f_1 = f(x_1), \ldots, f_4 = f(x_4)$. Calculate an expression for the dominant term in the error.

b) Write a program to test the FD approximation on the function

$$f(x) = e^{-x} \tan x. \tag{1}$$

Consider step sizes of $H = 10^{-k/100}$ for $k = 100, 101, \ldots, 300$. For each H, set $x_1 = 0$ and $x_4 = H$. Choose x_2 and x_3 as uniformly randomly distributed random numbers over the range from 0 to H.[a] Make a log–log plot showing the absolute error magnitude E of the FD approximation versus H. Use linear regression to fit the data to

$$E = CH^p \tag{2}$$

and determine C and p to three significant figures.[b]

c) **Optional.**[c] Examine and discuss whether your value of the fitted parameter C is consistent with the dominant error term from part (a).

[a] If $x_2 > x_3$, then swap the two values to ensure the ordering is preserved. If $x_2 = x_3$, then choose new random numbers.

[b] Since sample points for the FD approximation are randomly chosen, there will be small variations in the values of C and p that you compute.

[c] Optional questions are not graded.

a) Using the method of undetermined coefficients as explained in class and in textbook, we seek to find coefficients a, b, c, d such that

$$f''(x_2) = af(x_1) + bf(x_2) + cf(x_3) + df(x_4) + E \tag{3}$$

where E is the error term. Using Taylor expansions about x_2, we have

$$f(x_1) = f(x_2) + f'(x_2)(x_1 - x_2) + \frac{f''(x_2)}{2}(x_1 - x_2)^2 + \frac{f^{(3)}(x_2)}{6}(x_1 - x_2)^3 + \frac{f^{(4)}(\xi_1)}{24}(x_1 - x_2)^4, \tag{4}$$

$$f(x_3) = f(x_2) + f'(x_2)(x_3 - x_2) + \frac{f''(x_2)}{2}(x_3 - x_2)^2 + \frac{f^{(3)}(x_2)}{6}(x_3 - x_2)^3 + \frac{f^{(4)}(\xi_3)}{24}(x_3 - x_2)^4, \tag{5}$$

$$f(x_4) = f(x_2) + f'(x_2)(x_4 - x_2) + \frac{f''(x_2)}{2}(x_4 - x_2)^2 + \frac{f^{(3)}(x_2)}{6}(x_4 - x_2)^3 + \frac{f^{(4)}(\xi_4)}{24}(x_4 - x_2)^4, \tag{6}$$

where ξ_i is some point between x_i and x_2. Substituting these into the original equation and collecting terms gives

$$\begin{aligned}
f''(x_2) = {} & (a + b + c + d)f(x_2) && (7)\\
& + (a(x_1 - x_2) + c(x_3 - x_2) + d(x_4 - x_2))f'(x_2) && (8)\\
& + \left(\frac{a(x_1 - x_2)^2}{2} + \frac{c(x_3 - x_2)^2}{2} + \frac{d(x_4 - x_2)^2}{2} \right) f''(x_2) && (9)\\
& + \left(\frac{a(x_1 - x_2)^3}{6} + \frac{c(x_3 - x_2)^3}{6} + \frac{d(x_4 - x_2)^3}{6} \right) f^{(3)}(x_2) && (10)\\
& + \left(\frac{a(x_1 - x_2)^4}{24} f^{(4)}(\xi_1) + \frac{c(x_3 - x_2)^4}{24} f^{(4)}(\xi_3) + \frac{d(x_4 - x_2)^4}{24} f^{(4)}(\xi_4) \right). && (11)
\end{aligned}$$

To ensure that the approximation is exact for polynomials of degree up to 3, we require that the coefficients of $f(x_2)$, $f'(x_2)$, $f''(x_2)$, and $f^{(3)}(x_2)$ match on both sides, leading to the system of equations:

$$a + b + c + d = 0, \tag{12}$$

$$a(x_1 - x_2) + c(x_3 - x_2) + d(x_4 - x_2) = 0, \tag{13}$$

$$\frac{a(x_1 - x_2)^2}{2} + \frac{c(x_3 - x_2)^2}{2} + \frac{d(x_4 - x_2)^2}{2} = 1, \tag{14}$$

$$\frac{a(x_1 - x_2)^3}{6} + \frac{c(x_3 - x_2)^3}{6} + \frac{d(x_4 - x_2)^3}{6} = 0. \tag{15}$$

Problem 2

Mixed boundary value problem (5 points). For a smooth function $u(x)$ and source term $f(x)$, consider the two point boundary value problem (BVP)

$$u'' + u = f(x) \tag{16}$$

on the domain $x \in [0, \pi]$, using the mixed boundary conditions

$$u'(0) - u(0) = 0, \qquad u'(\pi) + u(\pi) = 0. \tag{17}$$

a) Use a mesh width of $h = \pi/n$ where $n \in \mathbb{N}$ and introduce grid points at $x_j = jh$ for $j = 0, 1, \ldots, n$. Construct a second-order accurate finite-difference method for this BVP. Write your method as a linear system of the form $AU = F$.

b) Construct the exact solution $u(x)$ to the BVP when $f(x) = -e^x$.

c) Verify that your method is second-order accurate by solving the BVP with $f(x) = -e^x$ using $n = 20, 40, 80, 160$. For each n, construct the error measure

$$E_n = \sqrt{h \sum_{j=0}^{n} q_j (U_j - u(x_j))^2} \tag{18}$$

where U_j is the numerical solution at x_j. Here, $q_j = \frac{1}{2}$ when $j \in \{0, n\}$ and $q_j = 1$ otherwise. Present your results in a table, and comment on whether the trend in the errors is expected for a second-order method.

Problem 3

Nonlinear BVP (4 points). Consider the nonlinear BVP

$$u''(x) - 80 \cos u(x) = 0 \tag{19}$$

with the boundary conditions $u(0) = 0$ and $u(1) = 10$. Define the mesh width $h = \frac{1}{n}$ for $n \in \mathbb{N}$, and introduce gridpoints $x_j = jh$ for $j = 0, 1, \ldots, n$.

Let U_i be the approximation of $u(x_i)$. From the boundary conditions, $U_0 = 0$ and $U_n = 10$. Let $U = (U_1, U_2, \ldots, U_{n-1})$ be the vector of unknown function values, and write $F(U) = 0$ as the nonlinear system of algebraic equations from the finite-difference approximation, where $F : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$. The components are

$$F_1(U) = \frac{U_2 - 2U_1}{h^2} - 80 \cos U_1, \tag{20}$$

$$F_i(U) = \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} - 80 \cos U_i \qquad \text{for } i = 2, \ldots, n-2, \tag{21}$$

$$F_{n-1}(U) = \frac{10 - 2U_{n-1} + U_{n-2}}{h^2} - 80 \cos U_{n-1}. \tag{22}$$

a) Calculate the Jacobian $J_F \in \mathbb{R}^{(n-1)\times(n-1)}$ for the function F and describe its structure.

b) Use Newton's method to solve the BVP for $n = 100$, using the Jacobian matrix from part (a). Write U^k to indicate the kth Newton step, and start with the initial guess $U^0 = 0$. Terminate Newton's method when the relative step size $\|\Delta U^k\|_2 / \|U^k\|_2$ is less than 10^{-10}. Plot the solution U over the interval $[0, 1]$, and report the value of U_{50} to three significant figures.

Problem 4

FD in a triangular domain (8 points). Let T be a domain in the shape of an equilateral triangle with vertices at $(0,0)$, $(1,0)$, and $(\frac{1}{2}, s)$ where $s = \frac{\sqrt{3}}{2}$. For $n \in \mathbb{N}$, define $h = \frac{1}{n}$, and introduce grid points

$$\mathbf{x}_{i,j} = (h(i + \tfrac{1}{2}j), hsj)) \tag{23}$$

for $0 \le i \le n$, $0 \le j \le n - i$. An example grid for $n = 7$ is shown in Fig. **??**. The grid points on the boundary ∂T correspond to $i = 0$, $j = 0$, or $i + j = n$. All other points are defined as a interior points.

1. Let $u : T \to \mathbb{R}$ be a smooth function, and write $u_{i,j} = u(\mathbf{x}_{i,j})$. For an interior point $\mathbf{x}_{i,j}$, consider the finite difference approximation
$$\nabla_3^2 u_{i,j} = \alpha u_{i,j} + \beta u_{i+1,j} + \gamma u_{i,j-1} + \delta u_{i-1,j+1}. \tag{24}$$
Derive the values of α, β, γ, and δ so that
$$\nabla_3^2 u_{i,j} = \nabla^2 u(\mathbf{x}_{i,j}) + hW + O(h^2) \tag{25}$$
and determine the form of W in terms of partial derivatives of u. By considering the function $u(x, y) = x^3$ show that $\nabla_3^2 u_{i,j}$ is a first-order accurate approximation for $\nabla^2 u(\mathbf{x}_{i,j})$, but it is not second-order accurate.

2. Using your result from part (a), or otherwise, determine the constants $c_0, c_1, \ldots, c_6$ such that the finite difference approximation
$$\begin{aligned}\nabla_6^2 u_{i,j} = {} & c_0 u_{i,j} + c_1 u_{i+1,j} + c_2 u_{i,j-1} + c_3 u_{i-1,j+1} \\ & + c_4 u_{i-1,j} + c_5 u_{i,j+1} + c_6 u_{i+1,j-1}\end{aligned} \tag{26}$$
satisfies $\nabla_6^2 u_{i,j} = \nabla^2 u(\mathbf{x}_{i,j}) + O(h^2)$.

3. Write a program to solve the equation
$$\nabla^2 u = f \tag{27}$$
on the domain T using the boundary conditions that $u(\mathbf{x}) = 0$ for $\mathbf{x} \in \partial T$. Using the method of manufactured solutions, determine the value of $f(x, y)$ such that the solution will be
$$u^{\text{ex}}(x, y) = \left((2y - \sqrt{3})^2 - 3(2x - 1)^2\right) \sin y. \tag{28}$$
Consider values of $n = 10, 20, 40, 80, 160$, and compute the error measure
$$E_n = \sqrt{\frac{s}{2n^2} \sum_{j=1}^{n-1} \sum_{i=1}^{n-j-1} (u_{i,j} - u^{\text{ex}}(\mathbf{x}_{i,j}))^2}. \tag{29}$$
Make a log–log plot of E_n versus n, and use linear regression to fit the data to $E_n = Cn^{-p}$, reporting your values of C and p to three significant figures.

4. Repeat part (c) for the finite difference approximation given in Eq. (26).

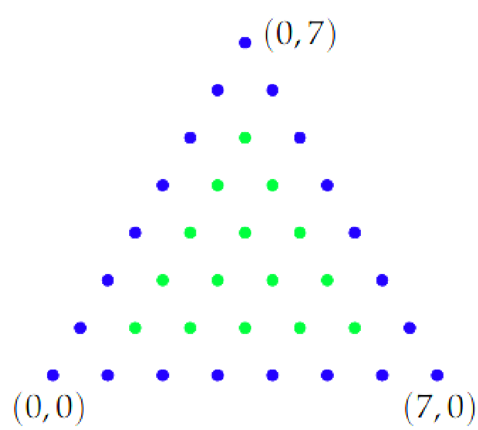

Figure 1: Example of the triangular domain T and numerical grid for the case of $n = 7$. The corner points are labeled with their grid indices (i, j). Blue circles denote the boundary points, and green circles denote the interior points.