

Problem 1

Finite difference approximation (3 points). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ 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 $f_1 = f(x_1), \dots, f_4 = f(x_4)$. Calculate an expression for the dominant term in the error.
- (b) Write a program to test the FD approximation on the function

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

Consider step sizes of $H = 10^{-k/100}$ for $k = 100, 101, \dots, 300$. 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

$$E = CH^p \quad (2)$$

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).

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

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

^cOptional questions are not graded.

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

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

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

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

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

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

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

$$f''(x_2) = (a + b + c + d)f(x_2) \quad (7)$$

$$+ (a(x_1 - x_2) + c(x_3 - x_2) + d(x_4 - x_2))f'(x_2) \quad (8)$$

$$+ \left(\frac{a(x_1 - x_2)^2}{2} + \frac{c(x_3 - x_2)^2}{2} + \frac{d(x_4 - x_2)^2}{2} \right) f''(x_2) \quad (9)$$

$$+ \left(\frac{a(x_1 - x_2)^3}{6} + \frac{c(x_3 - x_2)^3}{6} + \frac{d(x_4 - x_2)^3}{6} \right) f^{(3)}(x_2) \quad (10)$$

$$+ \left(\frac{a(x_1 - x_2)^4}{24} f^{(4)}(\xi_1) + \frac{c(x_3 - x_2)^4}{24} f^{(4)}(\xi_3) + \frac{d(x_4 - x_2)^4}{24} f^{(4)}(\xi_4) \right). \quad (11)$$

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:

$$a + b + c + d = 0, \quad (12)$$

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

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

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

Solving this system yields the coefficients:

$$\begin{aligned} a &= \frac{2x_2 - x_3 - x_4}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)}, \\ b &= \frac{2x_2 - x_1 - x_4}{(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)}, \\ c &= \frac{2x_2 - x_1 - x_4}{(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)}, \\ d &= \frac{2x_2 - x_1 - x_3}{(x_4 - x_1)(x_4 - x_2)(x_4 - x_3)}. \end{aligned}$$

The dominant term in the error is given by

$$E = \left(\frac{a(x_1 - x_2)^4}{24} f^{(4)}(\xi_1) + \frac{c(x_3 - x_2)^4}{24} f^{(4)}(\xi_3) + \frac{d(x_4 - x_2)^4}{24} f^{(4)}(\xi_4) \right). \quad (16)$$

So we have a third-order accurate finite difference approximation for $f''(x_2)$.

- (b) See the attached code file `714Hw1.py` for the implementation of the finite difference approximation and the testing on the function $f(x) = e^{-x} \tan x$. The log-log plot of the absolute error magnitude E versus H is shown below, along with the results of the linear regression fit to $E = CH^p$ showing the values of C and p to three significant figures.

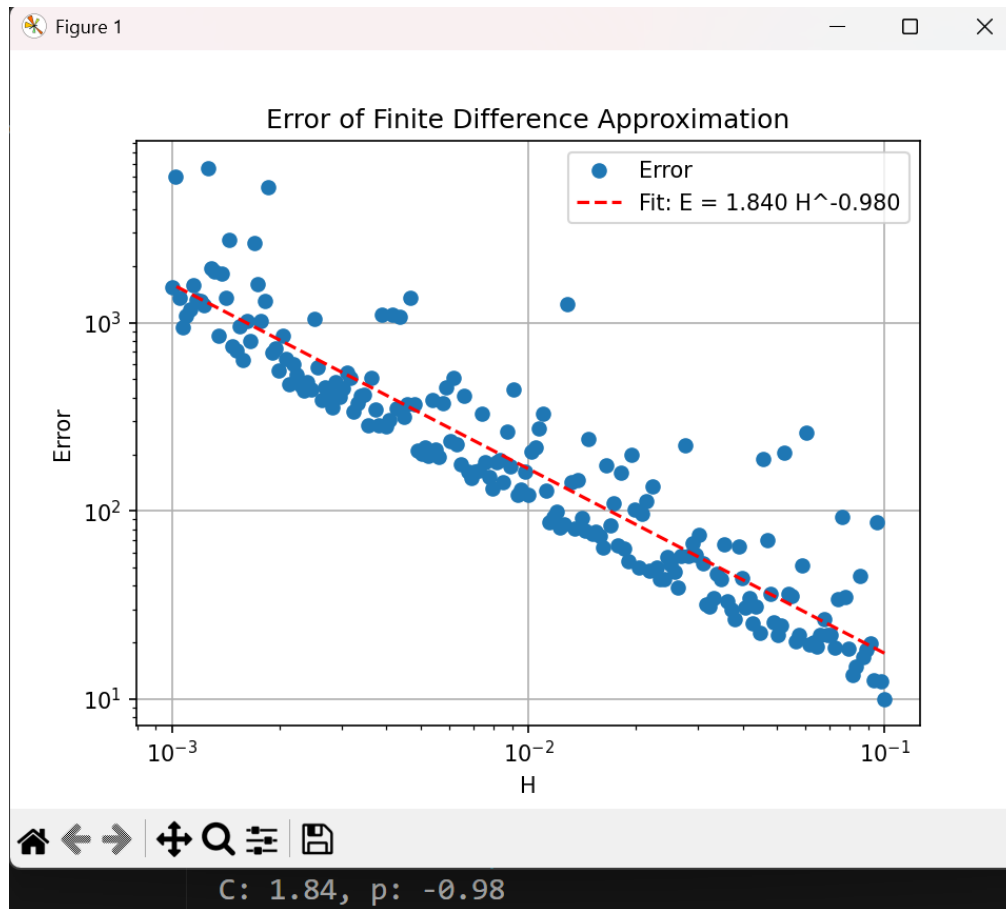


Figure 1: Log-log plot of absolute error magnitude E versus step size H . The dashed line represents the linear regression fit to $E = CH^p$.

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)

$$u'' + u = f(x) \quad (17)$$

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

$$u'(0) - u(0) = 0, \quad u'(\pi) + u(\pi) = 0. \quad (18)$$

- (a) Use a mesh width of $h = \pi/n$ where $n \in \mathbb{N}$ and introduce grid points at $x_j = jh$ for $j = 0, 1, \dots, n$. 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

$$E_n = \sqrt{h \sum_{j=0}^n q_j (U_j - u(x_j))^2} \quad (19)$$

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.

- (a) Consider the following:

As given in the problem statement, we have the differential equation

$$u''(x) + u(x) = f(x), \quad x \in [0, \pi]$$

with boundary conditions

$$\begin{aligned} u'(0) - u(0) &= 0, \\ u'(\pi) + u(\pi) &= 0. \end{aligned}$$

We discretize the domain using a uniform grid with mesh width $h = \pi/n$ and grid points $x_j = jh$ for $j = 0, 1, \dots, n$. Let U_j be the approximation of $u(x_j)$. We will use a second-order central difference approximation for the second derivative at interior points. So for each interior point $j = 1, 2, \dots, n-1$, we have

$$u''(x_j) \approx \frac{U_{j-1} - 2U_j + U_{j+1}}{h^2}.$$

Substituting this into the differential equation gives

$$\frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} + U_j = f(x_j), \quad j = 1, 2, \dots, n-1.$$

so the matrix (for the interior points) will be a tridiagonal matrix of the form

$$A = \frac{1}{h^2} \begin{pmatrix} -2 + h^2 & 1 & 0 & \cdots & 0 \\ 1 & -2 + h^2 & 1 & \cdots & 0 \\ 0 & 1 & -2 + h^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -2 + h^2 \end{pmatrix}.$$

Next, we need to incorporate the boundary conditions. For the first boundary condition at $x = 0$, we can use a the second order accurate forward difference approximation for $u'(0)$:

$$u'(0) \approx \frac{-3U_0 + 4U_1 - U_2}{2h}.$$

Substituting this into the boundary condition gives

$$\begin{aligned} \frac{-3U_0 + 4U_1 - U_2}{2h} - U_0 &= 0 \\ \frac{U_0(-3 - 2h) + 4U_1 - U_2}{2h} &= 0. \end{aligned}$$

We can then incorporate this into the first row of the matrix A and the first entry of the vector F . The first row of A becomes

$$A_{0,:} = \frac{1}{2h} \begin{pmatrix} -3-2h & 4 & -1 & 0 & \cdots & 0 \end{pmatrix}, F_0 = 0.$$

For the second boundary condition at $x = \pi$, we can use a second-order accurate backward difference approximation for $u'(\pi)$:

$$u'(\pi) \approx \frac{3U_n - 4U_{n-1} + U_{n-2}}{2h}.$$

Substituting this into the boundary condition gives

$$\begin{aligned} \frac{3U_n - 4U_{n-1} + U_{n-2}}{2h} + U_n &= 0 \\ \frac{U_n(3+2h) - 4U_{n-1} + U_{n-2}}{2h} &= 0. \end{aligned}$$

We can then incorporate this into the last row of the matrix A and the last entry of the vector F . The last row of A becomes

$$A_{n,:} = \frac{1}{2h} \begin{pmatrix} 0 & \cdots & 0 & 1 & -4 & 3+2h \end{pmatrix}, F_n = 0.$$

Thus, we have that the linear system $AU = F$ is given by

$$AU = \begin{pmatrix} \frac{-3-2h}{2h} & \frac{4}{2h} & \frac{-1}{2h} & 0 & \cdots & 0 \\ \frac{1}{h^2} & \frac{-2+h^2}{h^2} & \frac{1}{h^2} & 0 & \cdots & 0 \\ 0 & \frac{1}{h^2} & \frac{-2+h^2}{h^2} & \frac{1}{h^2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{h^2} & \frac{-2+h^2}{h^2} \\ 0 & \cdots & 0 & \frac{1}{2h} & \frac{-4}{2h} & \frac{3+2h}{2h} \end{pmatrix} \begin{pmatrix} U_0 \\ U_1 \\ U_2 \\ \vdots \\ U_{n-1} \\ U_n \end{pmatrix} = \begin{pmatrix} 0 \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{n-1}) \\ 0 \end{pmatrix} = F.$$

Since we used second-order accurate finite difference approximations for both the interior points and the boundary conditions, the overall method is second-order accurate.

- (b) To construct the exact solution to the BVP when $f(x) = -e^x$, we first solve the corresponding homogeneous equation

$$u''(x) + u(x) = 0.$$

The characteristic equation is $r^2 + 1 = 0$, which has solutions $r = i$ and $r = -i$. Thus, the general solution to the homogeneous equation is

$$u_h(x) = C_1 \cos x + C_2 \sin x,$$

where C_1 and C_2 are constants to be determined by the boundary conditions.

Next, we find a particular solution to the non-homogeneous equation. We can use the method of undetermined coefficients and try a particular solution of the form

$$u_p(x) = Ae^x,$$

where A is a constant to be determined. Substituting this into the differential equation gives

$$Ae^x + Ae^x = -e^x,$$

which simplifies to

$$2Ae^x = -e^x.$$

Dividing both sides by e^x (which is never zero), we find

$$2A = -1 \implies A = -\frac{1}{2}.$$

Thus, a particular solution is

$$u_p(x) = -\frac{1}{2}e^x.$$

The general solution to the non-homogeneous equation is then

$$u(x) = u_h(x) + u_p(x) = C_1 \cos x + C_2 \sin x - \frac{1}{2}e^x.$$

Now, we apply the boundary conditions to determine C_1 and C_2 . The first boundary condition is

$$u'(0) - u(0) = 0.$$

We first compute $u'(x)$:

$$u'(x) = -C_1 \sin x + C_2 \cos x - \frac{1}{2}e^x.$$

Evaluating at $x = 0$ gives

$$\begin{aligned} u(0) &= C_1 - \frac{1}{2}, \\ u'(0) &= C_2 - \frac{1}{2}. \end{aligned}$$

Applying the first boundary condition:

$$\begin{aligned} u'(0) - u(0) = 0 &\implies (C_2 - \frac{1}{2}) - (C_1 - \frac{1}{2}) = 0 \\ &\implies C_2 - C_1 = 0 \\ &\implies C_1 = C_2. \end{aligned}$$

For the second boundary condition at $x = \pi$:

$$\begin{aligned} u(\pi) &= C_1 \cos \pi + C_2 \sin \pi - \frac{1}{2}e^\pi = -C_1 - \frac{1}{2}e^\pi, \\ u'(\pi) &= -C_1 \sin \pi + C_2 \cos \pi - \frac{1}{2}e^\pi = C_2(-1) - \frac{1}{2}e^\pi = -C_2 - \frac{1}{2}e^\pi. \end{aligned}$$

The boundary condition is $u'(\pi) + u(\pi) = 0$, so:

$$\begin{aligned} (-C_2 - \frac{1}{2}e^\pi) + (-C_1 - \frac{1}{2}e^\pi) &= 0 \\ -(C_1 + C_2) - e^\pi &= 0 \\ C_1 + C_2 &= -e^\pi. \end{aligned}$$

But from above, $C_1 = C_2$, so $2C_1 = -e^\pi$, hence $C_1 = C_2 = -\frac{1}{2}e^\pi$.

Therefore, the exact solution is

$$u(x) = -\frac{1}{2}e^\pi \cos x - \frac{1}{2}e^\pi \sin x - \frac{1}{2}e^x.$$

- (c) See the attached code file `714Hw1.py` for the implementation of the finite difference method and the error calculation. The results for $n = 20, 40, 80, 160$ are presented in the following table:

Problem 3

Nonlinear BVP (4 points). Consider the nonlinear BVP

$$u''(x) - 80 \cos u(x) = 0 \tag{20}$$

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 $j = 0, 1, \dots, n$.

Let U_i be the approximation of $u(x_i)$. From the boundary conditions, $U_0 = 0$ and $U_n = 10$. Let $U = (U_1, U_2, \dots, U_{n-1})$ 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 $F : \mathbb{R}^{n-1} \rightarrow \mathbb{R}^{n-1}$. The components are

$$F_1(U) = \frac{U_2 - 2U_1}{h^2} - 80 \cos U_1, \tag{21}$$

$$F_i(U) = \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} - 80 \cos U_i \quad \text{for } i = 2, \dots, n-2, \tag{22}$$

$$F_{n-1}(U) = \frac{10 - 2U_{n-1} + U_{n-2}}{h^2} - 80 \cos U_{n-1}. \tag{23}$$

- Calculate the Jacobian $J_F \in \mathbb{R}^{(n-1) \times (n-1)}$ for the function F and describe its structure.
- Use Newton's method to solve the BVP for $n = 100$, using the Jacobian matrix from part (a). Write U^k to indicate the k th 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.

(a) We calculate the Jacobian matrix J_F of the function F . The Jacobian matrix is defined as

$$(J_F)_{ij} = \frac{\partial F_i}{\partial U_j}.$$

We compute the partial derivatives for each component of F :

- For $i = 1$:

$$\begin{aligned}\frac{\partial F_1}{\partial U_1} &= -\frac{2}{h^2} + 80 \sin U_1, \\ \frac{\partial F_1}{\partial U_2} &= \frac{1}{h^2}, \\ \frac{\partial F_1}{\partial U_j} &= 0 \quad \text{for } j > 2.\end{aligned}$$

- For $2 \leq i \leq n-2$:

$$\begin{aligned}\frac{\partial F_i}{\partial U_{i-1}} &= \frac{1}{h^2}, \\ \frac{\partial F_i}{\partial U_i} &= -\frac{2}{h^2} + 80 \sin U_i, \\ \frac{\partial F_i}{\partial U_{i+1}} &= \frac{1}{h^2}, \\ \frac{\partial F_i}{\partial U_j} &= 0 \quad \text{for } j < i-1 \text{ or } j > i+1.\end{aligned}$$

- For $i = n-1$:

$$\begin{aligned}\frac{\partial F_{n-1}}{\partial U_{n-2}} &= \frac{1}{h^2}, \\ \frac{\partial F_{n-1}}{\partial U_{n-1}} &= -\frac{2}{h^2} + 80 \sin U_{n-1}, \\ \frac{\partial F_{n-1}}{\partial U_j} &= 0 \quad \text{for } j < n-2.\end{aligned}$$

Thus, the Jacobian matrix J_F has the following tridiagonal structure:

$$J_F = \begin{pmatrix} -\frac{2}{h^2} + 80 \sin U_1 & \frac{1}{h^2} & 0 & \cdots & 0 \\ \frac{1}{h^2} & -\frac{2}{h^2} + 80 \sin U_2 & \frac{1}{h^2} & \cdots & 0 \\ 0 & \frac{1}{h^2} & -\frac{2}{h^2} + 80 \sin U_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -\frac{2}{h^2} + 80 \sin U_{n-1} \end{pmatrix}.$$

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

$$\mathbf{x}_{i,j} = (h(i + \frac{1}{2}j), hs j) \quad (24)$$

for $0 \leq i \leq n$, $0 \leq j \leq n - i$. 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 interior points.

1. Let $u : T \rightarrow \mathbb{R}$ 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

$$\nabla_3^2 u_{i,j} = \alpha u_{i,j} + \beta u_{i+1,j} + \gamma u_{i,j-1} + \delta u_{i-1,j+1}. \quad (25)$$

Derive the values of α , β , γ , and δ so that

$$\nabla_3^2 u_{i,j} = \nabla^2 u(\mathbf{x}_{i,j}) + hW + O(h^2) \quad (26)$$

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, \dots, c_6 such that the finite difference approximation

$$\begin{aligned} \nabla_6^2 u_{i,j} = & c_0 u_{i,j} + c_1 u_{i+1,j} + c_2 u_{i,j-1} + c_3 u_{i-1,j+1} \\ & + c_4 u_{i-1,j} + c_5 u_{i,j+1} + c_6 u_{i+1,j-1} \end{aligned} \quad (27)$$

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

$$\nabla^2 u = f \quad (28)$$

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

$$u^{\text{ex}}(x, y) = \left((2y - \sqrt{3})^2 - 3(2x - 1)^2 \right) \sin y. \quad (29)$$

Consider values of $n = 10, 20, 40, 80, 160$, and compute the error measure

$$E_n = \sqrt{\frac{s}{2n^2} \sum_{j=1}^{n-1} \sum_{i=1}^{n-j-1} (u_{i,j} - u^{\text{ex}}(\mathbf{x}_{i,j}))^2}. \quad (30)$$

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. (27).

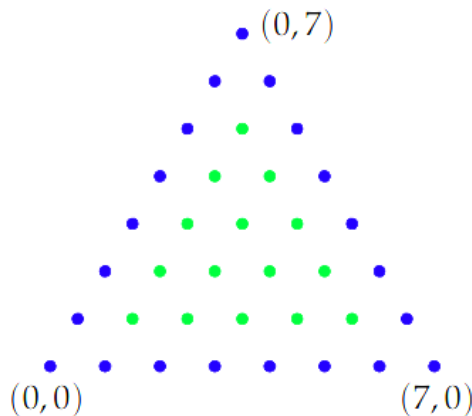


Figure 1: Example of the triangular domain T and numerical grid for the case of $n = 7$. The corner points are labeled with their grid indices (i, j) . Blue circles denote the boundary points, and green circles denote the interior points.