

1. In numerical solution of boundary value problems in differential equations, we can sometimes use the physics of the problem not only to enforce boundary conditions but also to maintain high-order accuracy near the boundary. For example, we may know the heat flux through a surface or displacement of a beam specified at one end. We can use this information to produce better estimates of the derivatives near the boundary.

Suppose we want to numerically solve the following boundary value problem with Neumann boundary conditions:

$$\frac{d^2y}{dx^2} + y = x^3, \quad 0 \leq x \leq 1$$

with $y'(0) = y'(1) = 0$. We discretize the domain using grid points $x_i = (i - 0.5)h$, $i \in \{1, 2, \dots, N\}$. In this problem, y_i is the numerical estimate of y at x_i . By using a finite difference scheme, we can estimate y_i'' in terms of linear combinations of y_i 's and transform the ODE into a linear system of equations.

- Derive a fourth order Pade approximation for the second derivative at the i^{th} node involving only its neighbors $i \pm 1$, i.e., obtain y_i'' involving $y_{i\pm 1}$, y_i and $y_{i\pm 1}''$. Note that this is applicable only at $i \in \{2, 3, \dots, N - 1\}$
- For the left boundary, derive a third order Pade scheme to approximate y_1'' in the following form:

$$y_1'' + b_2 y_2'' = a_1 y_1 + a_2 y_2 + a_3 y_3 + a_4 y'(0) + O(h^3)$$

- Repeat the above for the left boundary.
- Use the finite difference formulae derived above, to obtain a linear system for y_i'' . Explicitly write down the entries in the matrix and the right hand side.
- Compare the numerical and exact solution by varying $n \in \{10, 20, 50, 100, 200, 500, 1000\}$. Plot the error (computed using the max-norm as a function of n) on a log-log plot. Discuss your result.
- How are the Neumann boundary conditions enforced into the discretized boundary value problem?