B.Sc.(Hons.) Physics
32221501
Teacher: Mamta

S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 4
Numerov Method

Due Date and Time :
19.08.2022, 11:59PM
Max. Marks : 20

The objective of this assignment is to

- understand the Numerov method for solving IVP.
- realise the order of local and global truncation errors in Numerov Method.

1. (8 marks) **Theory**
   (a) Derive the Numerov method algorithm for solving IVP

$$u''(x) + f(x)u(x) = 0 \quad \text{with} \quad u(a) = u_0, \quad u(a+h) = u_1 \tag{1}$$

   $x \in [a, b]$ and with $h = (b-a)/N$ i.e. you with N intervals or $N+1$ grid points in the interval $[a, b]$.
   (b) Discuss the local and global truncation errors.
   (c) How will you use Numerov method to solve the IVP when the initial conditions given are $u(a) = u_0, \quad u'(a) = du_0$ without affecting the order of local truncation error.
   (d) Now derive the algorithm for

$$u''(x) + f(x)u(x) = r(x) \quad \text{with} \quad u(a) = u_0, \quad u(a+h) = u_1 \tag{2}$$

   (e) Show the steps of numerical computation to solve the following IVP using Numerov method with $N = 4$:

$$u''(x) - (1+x^2)u(x) = 0 \quad \text{with} \quad u(0) = 1, \quad u'(0) = 0. \tag{3}$$

2. (10 marks) **Programming**
   (a) Write a Python code that
      i. solves the IVP (1) with $N+1$ number of grid points.
      ii. plots the final numerical solution $u(x)$ and $u'(x)$ in the range $[a, b]$ along with the solutions obtained by inbuilt function *scipy.integrate.solve_ivp*.
   (b) Validate your code by solving the IVP given in equations (3)
   (c) Print a table with the column heads x_i, u_{num_i}, u_{inbuilt_i}, $E_i = |u_{\text{inbuilt}_i} - y_{\text{num}_i}|$ for $N = 2$ and $N = 4$.
   (d) Now extend your program to solve the IVP for $N = 2^k$ with $k = 1, 2, \ldots, 6$. Plot the solution for each N as points of different style along with the inbuilt solution.

3. (2 marks) **Discussion**
   Interpret and discuss your results.