Ahmedabad University

School of Arts and Sciences

MAT396/MAT596 - Numerical Methods

End-semester examination

(Monsoon 2024 Semester)

Marks: 40 **Time: 2.5 hours**

Enrolment Number: .....

Date: 3rd December 2024 (8:00 AM to 10:30 AM)

No. of pages: 02

Instructions:

- Every question, except question 3 and parts of question 1, involves coding, i.e. you are required to code a solution in the jupyter notebook. Write all your code in a single jupyter notebook named 'firstname_lastname'.
- Your PCs will not have access to internet during the duration of the exam. At 10:25 AM internet access will be given and you can upload the jupyter notebook to the google form **https://forms.gle/WKA4SE9oxJZnugue6**
- Write answers for non-coding questions in the answer sheet provided. You can use the same answer sheet for rough work.

1. Determine the real roots of $f(x) = 0.5x^2 - 2.5x - 4.5$. **[6]**
   (a) Use the quadratic formula to calculate the roots analytically.
   (b) Write a function that uses the bisection method to determine the highest root. Compute the root accurate up to 6 decimal places and print each iteration of the root along with the error.
   (c) For a choice of initial guesses, arrive at the analytical expression for the number of iterations required to compute the root up to the given accuracy.

2. The ideal gas law for a gas at low temperature and pressure is $PV = nRT$, where P is pressure (in atm), V is volume (in Litres), T is temperature (in Kelvin), n is the number of moles of the gas, and R = 0.0820578 L atm $K^{-1}mol^{-1}$ is the molar gas constant. The van der Waals equation **[5]**

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT \ ,$$

covers the non-ideal case where these assumptions do not hold. Use the ideal gas law to compute an initial guess, followed by Newton's Method applied to the van der Waals equation to find the volume of one mole of oxygen at 320 K and a pressure of 15 atm. For oxygen, a = 1.36 L^2 atm $mole^{-2}$ and b= 0.003183 L/mole. State your initial guess and solution with three significant digits.

3. Use Taylor series expansion to deduce the following approximation: **[4]**

$$f'(x_n) = \frac{f(x_{n-2}) - 8f(x_{n-1}) + 8f(x_{n+1}) - f(x_{n+2})}{12h} + \mathcal{O}(h^4) \ .$$

4. Implement Jacobi method for solving the system of equations **[5]**

$$\begin{pmatrix} 20 & 1 & -2 \\ 3 & 20 & -1 \\ 2 & -3 & 20 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 17 \\ -18 \\ 25 \end{pmatrix}$$

with $\mathbf{x}^{(0)}$. Continue iterating until error $< 10^{-5}$.

5. For the matrix M given below, find the dominant eigenvalue and the corresponding eigen-vector correct to 5 decimal places using Power method: **[5]**

$$M = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & -1 \end{pmatrix} \ .$$

6. Consider the following IVP for a simple harmonic oscillator: **[15]**

$$\frac{d^2x}{dt^2} = -2x/3, \ x(0) = 0.5, \ x'(0) = 0, \ 0 \leq x \leq 25 \ .$$

where x is the position of the oscillator and dx/dt is the velocity. For a step size $h = 0.025$

(a) Use Euler's method to obtain a numerical solution.

(b) Use Modified Euler's method to obtain a numerical solution.

(c) Use the second order Runge-Kutta method to obtain a numerical solution.

(d) Plot the position of the oscillator as a function of time for all methods together on the same graph. Do the same for the velocity of the oscillator.

Hint: The second order ODE can be written in the following vector form of two first order ODEs:

$$\frac{d\vec{X}}{dt} = \vec{F}(\vec{X}, t)$$

with initial conditions: $\vec{X}_0 = \begin{bmatrix} 0.5 \\ 0 \end{bmatrix}$.