Numerical Methods for the Solution of Differential Equations (AM 213B)
Homework 1 Solution

Question 1. Let $f(x)$ be a continuously differentiable function defined over the interval $[0, 1]$.

a) **(10 points)** Derive the four-point finite-difference backward differentiation formula (BDF3) approximation of the first derivative of f.

$$f'(x_j) \simeq \frac{11f(x_j) - 18f(x_{j-1}) + 9f(x_{j-2}) - 2f(x_{j-3})}{6\Delta x} \tag{1}$$

b) **(10 points)** Prove that (1) converges with order 3 in Δx to the analytical derivative $f'(x_j)$.

c) **(10 points)** Show numerically that (1) converges with order 3 by applying it to the periodic function

$$f(x) = \log\left(2 + \sin(2\pi x)\right) \qquad x \in [0, 1]. \tag{2}$$

To this end, plot the derivative of the function (2) and the finite difference approximation (1) you obtain on the evenly-spaced grid

$$x_j = \frac{j}{n} \qquad j = 0, \ldots, n \tag{3}$$

for $n = 20$ and $n = 60$ (two different Figures). In another Figure, plot the maximum pointwise error between the analytical and numerical derivatives evaluated on the grid (3), i.e.,

$$e(n) = \max_{j=0,\ldots,n} \left| f'(x_j) - \frac{1}{\Delta x}\left(\frac{11}{6}f(x_j) - 3f(x_{j-1}) + \frac{3}{2}f(x_{j-2}) - \frac{1}{3}f(x_{j-3})\right)\right|, \tag{4}$$

as a function of n, for n up to 10^4 (see the log-log plot in Figure 9 of the course note 1).

Answers:

a) To derive the three-point finite-difference backward differentiation formula (BDF3) we consider the third-order Lagrange polynomial interpolating $f(x)$ at the evenly-spaced set of grid points $\{x_{j-3}, x_{j-2}, x_{j-1}, x_j\}$

$$\Pi_3 f(x) = f(x_j)l_j(x) + f(x_{j-1})l_{j-1}(x) + f(x_{j-2})l_{j-2}(x) + f(x_{j-3})l_{j-3}(x). \tag{5}$$

The characteristic polynomials corresponding to the grid points are defined as

$$l_j(x) = \frac{(x-x_{j-1})}{(x_j-x_{j-1})}\frac{(x-x_{j-2})}{(x_j-x_{j-2})}\frac{(x-x_{j-3})}{(x_j-x_{j-3})} = \frac{(x-x_{j-1})}{\Delta x}\frac{(x-x_{j-2})}{2\Delta x}\frac{(x-x_{j-3})}{3\Delta x}, \tag{6}$$

$$l_{j-1}(x) = \frac{(x-x_j)}{(x_{j-1}-x_j)}\frac{(x-x_{j-2})}{(x_{j-1}-x_{j-2})}\frac{(x-x_{j-3})}{(x_{j-1}-x_{j-3})} = \frac{(x-x_j)}{-\Delta x}\frac{(x-x_{j-2})}{\Delta x}\frac{(x-x_{j-3})}{2\Delta x}, \tag{7}$$

$$l_{j-2}(x) = \frac{(x-x_j)}{(x_{j-2}-x_j)}\frac{(x-x_{j-1})}{(x_{j-2}-x_{j-1})}\frac{(x-x_{j-3})}{(x_{j-2}-x_{j-3})} = \frac{(x-x_j)}{-2\Delta x}\frac{(x-x_{j-1})}{-\Delta x}\frac{(x-x_{j-3})}{\Delta x}, \tag{8}$$

$$l_{j-3}(x) = \frac{(x-x_j)}{(x_{j-3}-x_j)}\frac{(x-x_{j-1})}{(x_{j-3}-x_{j-1})}\frac{(x-x_{j-2})}{(x_{j-3}-x_{j-2})} = \frac{(x-x_j)}{-3\Delta x}\frac{(x-x_{j-1})}{-2\Delta x}\frac{(x-x_{j-2})}{-\Delta x}. \tag{9}$$

The first derivative of each polynomial evaluated at x_j is

$$l'_j(x_j) = \frac{1}{6\Delta x^3}\left(6\Delta x^2 + 3\Delta x^2 + 2\Delta x^2\right) = \frac{11}{6\Delta x}, \tag{10}$$

$$l'_{j-1}(x_j) = -\frac{1}{2\Delta x^3}\left(6\Delta x^2\right) = -\frac{3}{\Delta x}, \tag{11}$$

$$l'_{j-2}(x_j) = \frac{1}{2\Delta x^3}\left(3\Delta x^2\right) = \frac{3}{2\Delta x}, \tag{12}$$

$$l'_{j-3}(x_j) = -\frac{1}{6\Delta x^3}\left(2\Delta x^2\right) = -\frac{1}{3\Delta x}. \tag{13}$$

Hence,

$$f'(x_j) \simeq \frac{d\Pi_3 f(x_j)}{dx} = \frac{1}{\Delta x}\left(\frac{11}{6}f(x_j) - 3f(x_{j-1}) + \frac{3}{2}f(x_{j-2}) - \frac{1}{3}f(x_{j-3})\right) \tag{14}$$

which proves (1).

b) To prove that (14) converges to $f'(x_j)$ with order 3 we use Taylor series.To this end, we write $f(x_{j-k})$ as $f(x_j - k\Delta x)$ for $k = 1, 2, 3$ and expand around $\Delta x = 0$ to obtain

$$f(x_j - k\Delta x) = f(x_j) - f'(x_j)k\Delta x + \frac{1}{2}f''(x_j)k^2(\Delta x)^2 - \frac{1}{6}f'''(x_j)k^3(\Delta x)^3 + \frac{1}{24}f''''(x_j)k^4(\Delta x)^4 + \cdots, \tag{15}$$

Substituting (15) into (14) yields

$$\begin{aligned}
&-3f(x_{j-1}) + \frac{3}{2}f(x_{j-2}) - \frac{1}{3}f(x_{j-3}) = \\
&-3f(x_j) + 3f'(x_j)\Delta x - \frac{3}{2}f''(x_j)(\Delta x)^2 + \frac{3}{6}f'''(x_j)(\Delta x)^3 - \frac{3}{24}f''''(x_j)(\Delta x)^4 \\
&+\frac{3}{2}f(x_j) - \frac{6}{2}f'(x_j)\Delta x + \frac{12}{4}f''(x_j)(\Delta x)^2 - \frac{24}{12}f'''(x_j)(\Delta x)^3 + \frac{48}{48}f''''(x_j)(\Delta x)^4 \\
&-\frac{1}{3}f(x_j) + \frac{3}{3}f'(x_j)\Delta x - \frac{9}{6}f''(x_j)(\Delta x)^2 + \frac{27}{18}f'''(x_j)(\Delta x)^3 - \frac{81}{72}f''''(x_j)(\Delta x)^4 + \cdots,
\end{aligned} \tag{16}$$

i.e.

$$-3f(x_{j-1})+\frac{3}{2}f(x_{j-2})-\frac{1}{3}f(x_{j-3}) = -\frac{11}{6}f(x_j)+f'(x_j)\Delta x-\frac{1}{4}f''''(x_j)(\Delta x)^4+o\left((\Delta x)^4\right). \quad (17)$$

The last equation implies that

$$\left|f'(x_j)-\frac{1}{\Delta x}\left(\frac{11}{6}f(x_j)-3f(x_{j-1})+\frac{3}{2}f(x_{j-2})-\frac{1}{3}f(x_{j-3})\right)\right| = \frac{(\Delta x)^3}{4}\left|f''''(x_j)\right|+o\left((\Delta x)^4\right), \quad (18)$$

i.e., the backward differentiation formula (14) (or (1)) coverges with order 3 in Δx.

c) The first derivative of the function (2) is easily obtained as

$$f'(x) = \frac{2\pi\cos(2\pi x)}{2+\sin(2\pi x)} \qquad x \in [0,1]. \quad (19)$$

In Figure 1 we demonstrate numerically that the backward differentiation formula (1) converges with order 3 in Δx. In fact, the slope of the pointwise error (4) versus n in a log-log plot is -3.

These plots are obtained by running the Matlab code `plot_BDF_error.m`. To compute the derivative at $\{x_0, x_1, x_2\}$ we added three ghost nodes to the left of $x_0 = 0$ and used the periodicity of the function f.

Question 2. Consider the two-dimensional linear system of ODEs

$$\begin{cases} \dfrac{d\boldsymbol{y}}{dt} = \boldsymbol{A}\boldsymbol{y} \\ \boldsymbol{y}(0) = \boldsymbol{y}_0 \end{cases} \quad (20)$$

where

$$\boldsymbol{y}_0 = \begin{bmatrix} -3 \\ 1 \end{bmatrix}, \qquad \text{and} \qquad \boldsymbol{A} = \begin{bmatrix} -1 & 3 \\ -3 & -1 \end{bmatrix}. \quad (21)$$

a) **(15 points)** Compute the analytical solution of (20)-(21) and plot $y_1(t)$ versus t, $y_2(t)$ versus t, and $y_2(t)$ versus $y_1(t)$ for $t \in [0, 10]$.

b) **(20 points)** Write a computer code to compute the numerical solution of the initial value problem (20) using the three-stage Runge-Kutta method (RK3) defined by the Butcher array

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/3 & 1/3 & 0 & 0 \\ 2/3 & 0 & 2/3 & 0 \\ \hline & 1/4 & 0 & 3/4 \end{array}$$

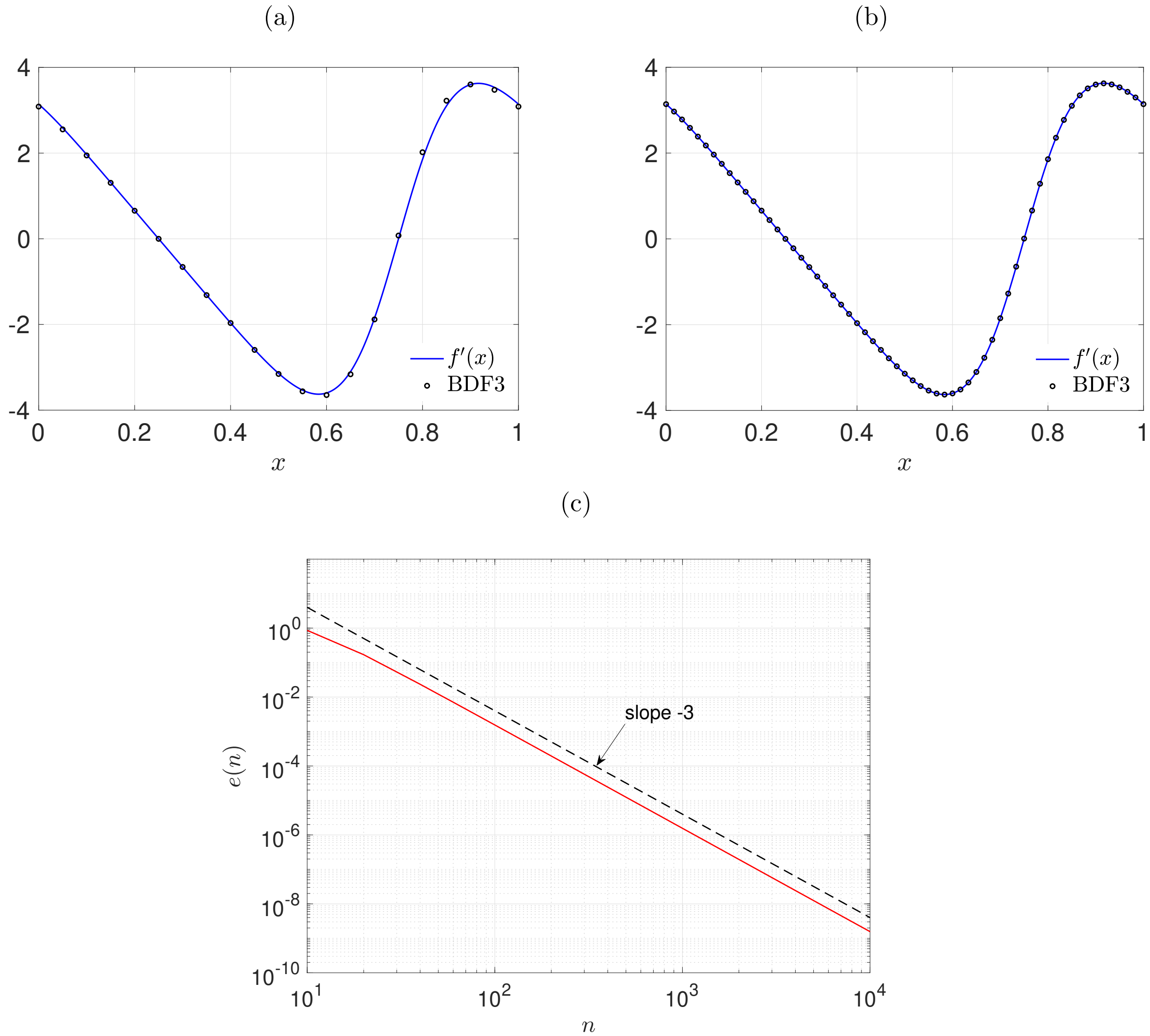

Figure 1: Numerical approximation of the derivative (19) obtained using the BDF formula (1) for $n = 20$ (a) and $n = 60$ (b). We also demonstrate that the pointwise error (4) decays as n^{-3}, i.e. that the BDF formula (1) is of order 3 in Δx.

and the three-step Adams-Moulton method[1] (AM3)

$$\boldsymbol{u}_{k+3} = \boldsymbol{u}_{k+2} + \frac{\Delta t}{24}\left[9\boldsymbol{f}\left(\boldsymbol{u}_{k+3}, t_{k+3}\right) + 19\boldsymbol{f}\left(\boldsymbol{u}_{k+2}, t_{k+2}\right) - 5\boldsymbol{f}\left(\boldsymbol{u}_{k+1}, t_{k+1}\right) + \boldsymbol{f}\left(\boldsymbol{u}_{k}, t_{k}\right)\right]. \tag{22}$$

[1]Note that since the system is linear, i.e., $\boldsymbol{f}(\boldsymbol{y}) = \boldsymbol{A}\boldsymbol{y}$, the implementation of the implicit Adams-Moulton method does not require a nonlinear solver, but only one linear solve at each time step. To start-up the AM3 method, i.e., to compute $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$, use the RK3 method.

To this end,

c) **(5 points)** Provide the explicit formulations of RK3 and AM3 tailored for the linear dynamical system (20)-(21), i.e., for $\boldsymbol{f}(\boldsymbol{y}) = \boldsymbol{A}\boldsymbol{y}$.

d) **(20 points)** Study convergence of the numerical solution you obtain with RK3 and AM3 as a function of Δt. To this end, run simulations for different values of Δt, i.e., $\Delta t = \{0.1, 0.05, 0.005, 0.0005\}$, fixed final time $T = 10$, and plot the error

$$e_2(t_k) = \|\boldsymbol{u}_k - \boldsymbol{y}(t_k)\|_2 \qquad k = 0, 1, \dots \tag{23}$$

in logarithmic scale versus time for each case. In (23), $\boldsymbol{y}(t_k)$ denotes the analytical solution of (20)-(21) evaluated at time t_k while $\boldsymbol{u}_k$ is the numerical solution you obtain with AM3 or RK3.

e) **(10 points)** Plot the error (23) at final time in logarithmic scale versus Δt for both AM3 or RK3. What is the order of convergence you observe numerically for AM3 and RK3?

Answers:

(a) The analytical solution of the ODE system (20)-(21) is

$$\boldsymbol{y}(t) = -3\exp(-t)\begin{bmatrix}\cos(3t)\\ -\sin(3t)\end{bmatrix} + \exp(-t)\begin{bmatrix}\sin(3t)\\ \cos(3t)\end{bmatrix}. \tag{24}$$

In fact, the matrix $\boldsymbol{A}$ can be decomposed as

$$\boldsymbol{A} = \underbrace{\begin{bmatrix}1 & 1\\ i & -i\end{bmatrix}}_{\boldsymbol{P}}\underbrace{\begin{bmatrix}-1+3i & 0\\ 0 & -1-3i\end{bmatrix}}_{\boldsymbol{\Lambda}}\underbrace{\frac{1}{2}\begin{bmatrix}1 & -i\\ 1 & i\end{bmatrix}}_{\boldsymbol{P}^{-1}}, \tag{25}$$

where $\boldsymbol{\Lambda}$ is the diagonal matrix of eigenvalues, and $\boldsymbol{P}$ is the matrix of eigenvectors. We know that the analytical solution can be expressed as

$$\boldsymbol{y}(t) = \boldsymbol{P}\boldsymbol{e}^{\boldsymbol{\Lambda}t}\boldsymbol{P}^{-1}\boldsymbol{y}_0, \tag{26}$$

which after simple algebraic manipulations can be written as in (24). The solution (24) is plotted in Figure 2

b) The given three-stage Runge-Kutta method can be written as

$$\boldsymbol{u}_{k+1} = \boldsymbol{u}_k + \Delta t\left(\frac{1}{4}\boldsymbol{K}_1 + \frac{3}{4}\boldsymbol{K}_3\right), \tag{27}$$

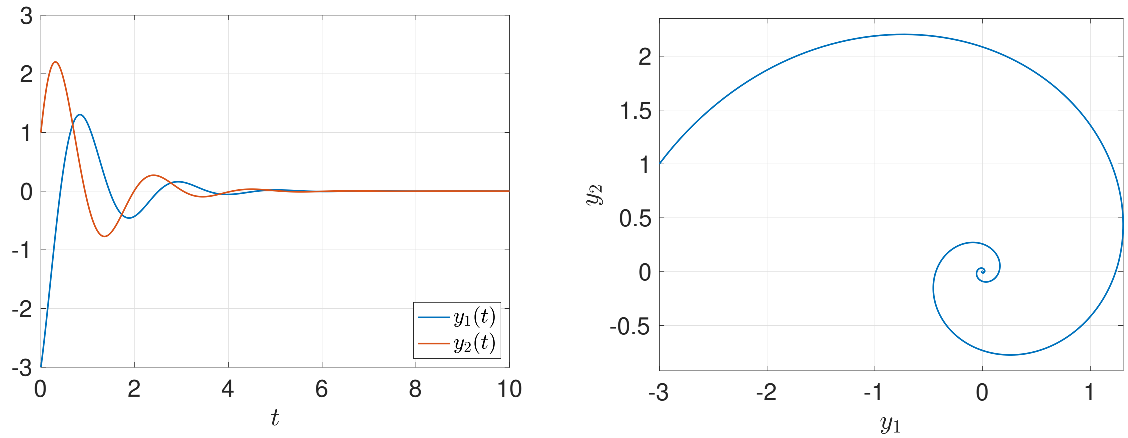

Figure 2: Plot of the analytical solution (24) of the linear system (20)-(21). Note that the origin is a stable spiral.

where

$$\boldsymbol{K}_1 = \boldsymbol{f}(\boldsymbol{u}_k, t_k), \tag{28}$$

$$\boldsymbol{K}_2 = \boldsymbol{f}\left(\boldsymbol{u}_k + \frac{\Delta t}{3}\boldsymbol{K}_1, t_k + \frac{\Delta t}{3}\right), \tag{29}$$

$$\boldsymbol{K}_3 = \boldsymbol{f}\left(\boldsymbol{u}_k + \frac{2\Delta t}{3}\boldsymbol{K}_2, t_k + \frac{2}{3}\Delta t\right). \tag{30}$$

To compute $\boldsymbol{u}_{k+1}$ we first evaluate $\boldsymbol{K}_1$, $\boldsymbol{K}_2$, and $\boldsymbol{K}_3$, and then compute their weighted sum (27). This is implemented in the Matlab file `RK3_Method.m`.

c) The ODE system (20)-(21) is linear, i.e.,

$$\boldsymbol{f}(\boldsymbol{u}_k, t_k) = \boldsymbol{A}\boldsymbol{u}_k. \tag{31}$$

This allows us to write $\boldsymbol{K}_1$, $\boldsymbol{K}_2$ and $\boldsymbol{K}_3$ as

$$\boldsymbol{K}_1 = \boldsymbol{A}\boldsymbol{u}_k, \tag{32}$$

$$\boldsymbol{K}_2 = \boldsymbol{A}\boldsymbol{u}_k + \frac{\Delta t}{3}\boldsymbol{A}^2\boldsymbol{u}_k, \tag{33}$$

$$\boldsymbol{K}_3 = \boldsymbol{A}\boldsymbol{u}_k + \frac{2\Delta t}{3}\boldsymbol{A}^2\boldsymbol{u}_k + \frac{4\Delta t^2}{9}\boldsymbol{A}^3\boldsymbol{u}_k, \tag{34}$$

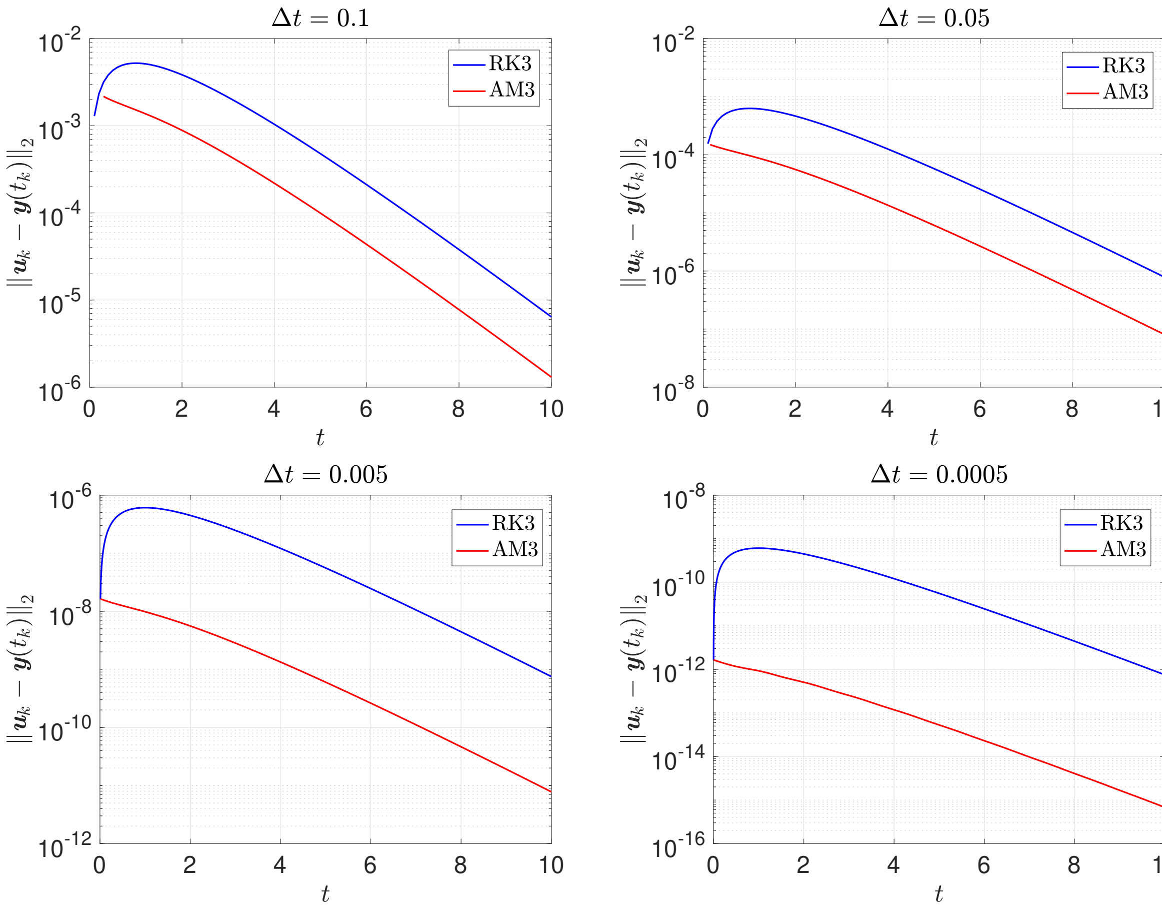

Figure 3: Time dependent errors obtained by solving the linear ODE system (20) with RK3 and AM3 using different Δt.

leading to the explicit scheme

$$\boldsymbol{u}_{k+1} = \boldsymbol{u}_k + \Delta t \boldsymbol{A}\boldsymbol{u}_k + \frac{\Delta t^2}{2}\boldsymbol{A}^2\boldsymbol{u}_k + \frac{\Delta t^3}{3}\boldsymbol{A}^3\boldsymbol{u}_k. \tag{35}$$

In contrast to RK3, the three-step Adams-Moulton (AM3) method, written for linear systems, and given by

$$\boldsymbol{u}_{k+3} = \boldsymbol{u}_{k+2} + \frac{\Delta t}{24}\boldsymbol{A}\left[9\boldsymbol{u}_{k+3} + 19\boldsymbol{u}_{k+2} - 5\boldsymbol{u}_{k+1} + \boldsymbol{u}_k\right] \tag{36}$$

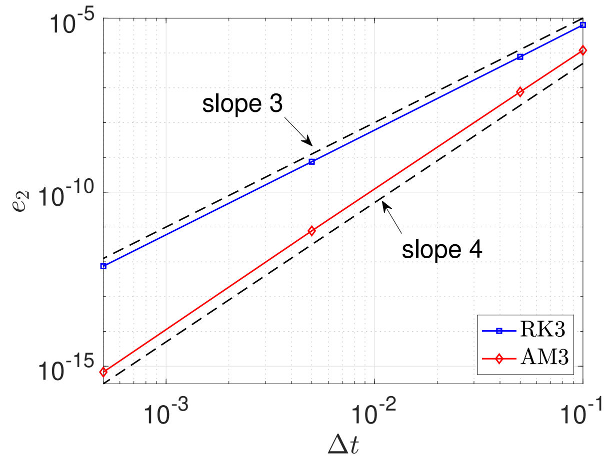

Figure 4: Errors at $t = 10$ obtained by solving the linear ODE system (20) with RK3 and AM3 versus Δt. It is seen that RK3 converges with order 3 while AM3 converges with order 4.

is an implicit numerical scheme. By simple mathematical manipulations we can write (36) as[2]

$$\left(\boldsymbol{I} - \frac{9\Delta t}{24}\boldsymbol{A}\right)\boldsymbol{u}_{k+3} = \boldsymbol{u}_{k+2} + \frac{\Delta t}{24}\boldsymbol{A}\left[19\boldsymbol{u}_{k+2} - 5\boldsymbol{u}_{k+1} + \boldsymbol{u}_k\right]. \tag{38}$$

Hence, at every iteration we need to solve a linear equation. A stable way to compute this matrix inversion in MATLAB is to use the backslash \ operator. For more general nonlinear vector fields, e.g., the ODE system in question 3, we have to use a nonlinear solver.

Note that the AM3 method (36) requires $\boldsymbol{u}_0$ and $\boldsymbol{u}_1$ to compute $\boldsymbol{u}_2$. Since the IVP only gives us the initial condition $\boldsymbol{u}_0$, in the MATLAB script `AM3_Method_Linear.m` we compute $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ by running two steps of the third-order Runge-Kutta method. However, one can choose to start-up AM2 with a method of lower-order (e.g., Euler forward), at the price of carrying on in the integration a larger perturbation due to the truncation error in the first two step.

d) By running the MATLAB script `RK3_AM3_Comparison.m`, we obtain the error plots in Figure 3 for the requested values of Δt.

e) Finally, in Figure 4 we plot the errors (23) at final time $t = 10$ versus Δt. It is seen that RK3 is a third-order method, while AM4 is a fourth-order method. In fact, the slope if the error plot versus Δt in a log-log scale for RK3 and AM3 is 3 and 4, respectively.

[2]Since the system we are solving is two-dimensional, we could invert the matrix $\boldsymbol{I} - 9\Delta t\boldsymbol{A}/24$ appearing at the left hand side of (37) in a pre-processing step and write the scheme (37) as

$$\boldsymbol{u}_{k+3} = \left(\boldsymbol{I} - \frac{9\Delta t}{24}\boldsymbol{A}\right)^{-1}\left(\boldsymbol{u}_{k+2} + \frac{\Delta t}{24}\boldsymbol{A}\left[19\boldsymbol{u}_{k+2} - 5\boldsymbol{u}_{k+1} + \boldsymbol{u}_k\right]\right). \tag{37}$$

This is not possible in high-dimensions since the computation of the inverse matrix may be not be accurate.