Imperial College London
Department of Mathematics
Dr Igor Shevchenko

Numerical Solution of Ordinary Differential Equations

I pledge that the work submitted for this coursework, both the report and the MATLAB code, is my own unassisted work unless stated otherwise.

CID........................ 01724711

Are you a Year 4 student?.. yes

Coursework 3

Fill in your CID and include the problem sheet in the coursework. Before you start working on the coursework, read the coursework guidelines. Any marks received for this coursework are only indicative and may be subject to moderation and scaling. *The mastery component is marked with a star.*

Exercise 1 (Predictor-Corrector Methods) — % of course mark: /6.0

a) Develop a predictor-corrector method based on the explicit and implicit LMMs you developed in Coursework 2.

b) Calculate the local truncation error of the predictor-corrector method.

c) Find the region and interval of absolute stability of the predictor-corrector method.

d) Find the region and interval of absolute stability of the explicit and implicit LMMs developed in Coursework 2 and compare them with those of the predictor-corrector method.

Exercise 2 (Predictor-Corrector and Nonlinear Systems) — % of course mark: /7.0

Solve the initial value problem (1) describing the chemical reaction of Robertson with the predictor-corrector method developed in Exercise 1.

$$\begin{cases} x' = -0.04x + 10^4 yz, \\ y' = 0.04x - 10^4 yz - 3 \cdot 10^7 y^2, \\ z' = 3 \cdot 10^7 y^2, \end{cases} \tag{1}$$

$$x(0) = 1, \; y(0) = z(0) = 0, \; t = [0, 100].$$

Exercise 3 (Implicit LMM and Nonlinear Systems) — % of course mark: /7.0

a) Solve the initial value problem for the Rabinovich–Fabrikant system (2) with the implicit LMM developed in Coursework 2. Use the Fixed point iteration method and Newton method to solve the nonlinear system of equations.

$$\begin{cases} x' = y(z - 1 + x^2) + \gamma x, \\ y' = x(3z + 1 - x^2) + \gamma y, \\ z' = -2z(\alpha + xy), \end{cases} \tag{2}$$

$$x(0) = -1.0, \; y(0) = 0.0, \; z(0) = 0.5, \; \alpha = 1.1, \; \gamma = 0.87, \; t = [0, 50].$$

b) Compare the number of iterations and execution time of the Fixed point iteration method and Newton method.

Exercise 4 (LMM and Absolute Stability) **% of course mark:** **/4.0★**

Find the coefficients α_2, α_0, β_0 of the LMM

$$x_{n+3} + \alpha_2 x_{n+2} + \alpha_0 x_n = h\beta_0 f_n$$

that give a convergent LMM, with the largest interval of absolute stability, when applied to

$$x' = \lambda x, \; Re(\lambda) < 0\,.$$

What is this largest interval?

Coursework mark: **% of course mark**

Coursework Guidelines

Below is a set of guidelines to help you understand what coursework is and how to improve it.

Coursework

- The coursework requires more than just following what has been done in the lectures, some amount of individual work is expected.
- The coursework report should describe in a concise, clear, and coherent way of what you did, how you did it, and what results you have.
- The report should be understandable to the reader with the mathematical background, but unfamiliar with your current work.
- Do not bloat the report by paraphrasing or presenting the results in different forms.
- Use high-quality and carefully constructed figures with captions and annotated axis, put figures where they belong.
- All numerical solutions should be presented as graphs.
- Use tables only if they are more explanatory than figures. The maximum table length is a half page.
- All figures and tables should be embedded in the report. The report should contain all discussions and explanations of the methods and algorithms, and interpretations of your results and further conclusions.
- The report should be typeset in LaTeX or Word Editor and submitted as a single pdf-file.
- The maximum length of the report is ten A4-pages (additional 3 pages is allowed for Year 4 students); the problem sheet is not included in these ten pages.
- Do not include any codes in the report.
- Marks are not based solely on correctness. The results must be described and interpreted. The presentation and discussion is as important as the correctness of the results.

Codes

- You cannot use third party numerical software in the coursework.
- The code you developed should be well-structured and organised, as well as properly commented to allow the reader to understand what the code does and how it works.
- All codes should run out of the box and require no modification to generate the results presented in the report.

Submission

- The coursework submission must be made via Turnitin on your Blackboard page. You must complete and submit the coursework anonymously, **the deadline is 1pm on the date of submission** (unless stated otherwise). The coursework should be submitted via two separate Turnitin drop boxes as a pdf-file of the report and a zip-file containing MATLAB (m-files only) or Python (py-files only) code. The code should be in the directory named `CID_Coursework#`. The report and the zip-file should be named as `CID_Coursework#.pdf` and `CID_Coursework#.zip` , respectively. The executable MATLAB (or Python) scripts for the exercises should be named as follows: exercise1.m, exercise2.m, etc.

Numerical Solution of Ordinary Differential Equations
Coursework 3

CID:01724711

November 2022

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1.1

We use the Predictor

$$x_{n+3} - \frac{3}{2}x_{n+2} + \frac{1}{2}x_{n+1} = \frac{h}{24}(41f_{n+2} - 40f_{n+1} + 11f_n) \tag{1}$$

and the Corrector

$$x_{n+3} - \frac{3}{2}x_{n+2} + \frac{1}{2}x_{n+1} = \frac{h}{24}(24f_{n+3} - 31f_{n+2} + 32f_{n+1} - 13f_n) \tag{2}$$

to develop the predictor-corrector method.

$$\begin{aligned}
&\textbf{Predict} && \hat{x}_{n+1} = \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(41f(t_n, x_n) - 40f(t_{n-1}, x_{n-1}) + 11f(t_{n-2}, x_{n-2}))\\
&\textbf{Evaluate} && f(t_{n+1}, \hat{x}_{n+1})\\
&\textbf{Correct} && x_{n+1} = \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(24f(t_{n+1}, \hat{x}_{n+1}) - 31f(t_n, x_n) + 32f(t_{n-1}, x_{n-1}) - 13f(t_{n-2}, x_{n-2}))\\
&\textbf{Evaluate} && f(t_{n+1}, x_{n+1})
\end{aligned} \tag{3}$$

1.2

To find the LTE we use the continuous forms for the predictor and the corrector and the taylor expansions up to $\mathcal{O}(h^5)$ and use the fact that $f(t_n, x_n) = x'(t_n)$

$$
\begin{aligned}
\hat{x}(t_{n+1}) &= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(x'(t_n) - 40x'(t_{n-1}) + 11x'(t_{n-2})) \\
x(t_{n+1}) &= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(24\hat{x}'(t_{n+1}) - 31x'(t_n) + 32x'(t_{n-1}) - 13x'(t_{n-2})) \\
&= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + h(\frac{3}{2}x'_n - \frac{1}{2}x'_{n-1} + \frac{h}{24}(x^{''}(t_n) - 40x^{''}(t_{n-1}) + 11x^{''}(t_{n-2}))) \\
&+ \frac{h}{24}(-31x'(t_n) + 32x'(t_{n-1}) - 13x'(t_{n-2})) \quad \textbf{(writing } x^{(i)}(t_n) \textbf{ as } x^{(i)}\textbf{)} \\
&= \frac{3}{2}x - \frac{1}{2}(x - hx' + \frac{h^2}{2}x^{''} - \frac{h^3}{6}x''' + \frac{h^4}{24}x^{''''}) \\
&+ h(\frac{3}{2}x' - \frac{1}{2}(x' - hx^{''} + \frac{h^2}{2}x^{'''} - \frac{h^3}{6}x^{''''}) \\
&+ \frac{h}{24}(41x'' - 40(x'' - hx''' + \frac{h^2}{2}x'''') + 11(x'' - 2hx^{'''} + 2h^2x^{''''})) \\
&+ \frac{h}{24}(-31x' + 32(x' - hx^{''} + \frac{h^2}{2}x^{'''} - \frac{h^3}{6}x^{''''}) \\
&- 13(x' - 2hx^{''} + 2h^2x^{'''} - \frac{4}{3}h^3x^{''''})) + \mathcal{O}(h^5) \\
&= x + hx'(\frac{1}{2} + \frac{3}{2} - \frac{1}{2} - \frac{31}{24} + \frac{32}{24} - \frac{13}{24}) \\
&+ h^2x^{''}(-\frac{1}{4} + \frac{1}{2} + \frac{41}{24} - \frac{40}{24} + \frac{11}{24} - \frac{32}{24} + \frac{26}{24}) \\
&+ h^3x^{'''}(\frac{1}{12} - \frac{1}{4} + \frac{40}{24} - \frac{22}{24} + \frac{16}{24} - \frac{26}{24}) \\
&+ h^4x^{''''}(-\frac{1}{48} + \frac{1}{12} - \frac{20}{24} + \frac{22}{24} - \frac{32}{6 \times 24} + \frac{13 \times 4}{24 \times 3}) \\
&= x(t_n) + hx'(t_n) + \frac{h^2}{2}x^{''}(t_n) + \frac{h^3}{6}x^{'''}(t_n) + \frac{31}{48}h^4x^{''''}(t_n) + \mathcal{O}(h^5)
\end{aligned} \tag{4}
$$

$$\Rightarrow x(t+h) - x(t_{n+1}) = -\frac{29}{48}h^4x^{''''}(t_n) + \mathcal{O}(h^5) = \mathcal{O}(h^4)$$

So the LTE is of order 4.

1.3

We first must find the stability polynomial of the predictor-corrector method by applying the method to $x' = \lambda x$.

$$
\begin{aligned}
\hat{x}_{n+1} &= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(41\lambda x_n - 40\lambda x_{n-1} + 11\lambda x_{n-2}) \textbf{ (sub into corrector)} \\
x_{n+1} &= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \lambda h(\frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(41\lambda x_n - 40\lambda x_{n-1} + 11\lambda x_{n-2})) \\
&+ \frac{h}{24}(-31\lambda x_n + 32\lambda x_{n-1} - 13\lambda x_{n-2}) \\
&= \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \hat{h}(\frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{\hat{h}}{24}(41x_n - 40x_{n-1} + 11x_{n-2})) \\
&+ \frac{\hat{h}}{24}(-31x_n + 32x_{n-1} - 13x_{n-2}) \\
&= x_n(\frac{3}{2} + \frac{3}{2}\hat{h} + \frac{41}{24}\hat{h}^2 - \frac{31}{24}\hat{h}) \\
&+ x_{n-1}(-\frac{1}{2} - \frac{\hat{h}}{2} - \frac{40}{24}\hat{h}^2 + \frac{32}{24}\hat{h}) \\
&+ x_{n-2}(\frac{11}{24}\hat{h}^2 - 13\frac{13}{24}\hat{h})
\end{aligned} \tag{5}
$$

$$\Rightarrow p(r) = r^3 - (\frac{3}{2} + \frac{5}{24}\hat{h} + \frac{41}{24}\hat{h}^2)r^2 - (-\frac{1}{2} + \frac{5\hat{h}}{6} - \frac{40}{24}\hat{h}^2)r - (\frac{11}{24}\hat{h}^2 - 13\frac{13}{24}\hat{h})$$

Using Sympy we obtain solutions for $\hat{h}$

$$\begin{aligned}\hat{h}_1 =& 0.5*(-5.0*r**2 - 20.0*r - 98.5849887153212*sqrt(0.404979936207429*r**5 - r**4 \\ &+ 0.924374935692973*r**3 - 0.332750282950921*r**2 + 0.000823129951641115*r \\ &+ 0.0173886202284186) + 13.0)/(41.0*r**2 - 40.0*r + 11.0)\end{aligned} \tag{6}$$

$$\begin{aligned}\hat{h}_2 =& 0.5*(-5.0*r**2 - 20.0*r + 98.5849887153212*sqrt(0.404979936207429*r**5 - r**4 \\ &+ 0.924374935692973*r**3 - 0.332750282950921*r**2 + 0.000823129951641115*r \\ &+ 0.0173886202284186) + 13.0)/(41.0*r**2 - 40.0*r + 11.0)\end{aligned} \tag{7}$$

We apply the boundary locus method by letting $r = e^{is}$, $s \in [0, 2\pi)$ and plotting the $\hat{h}_1, \hat{h}_2$ values for these r.

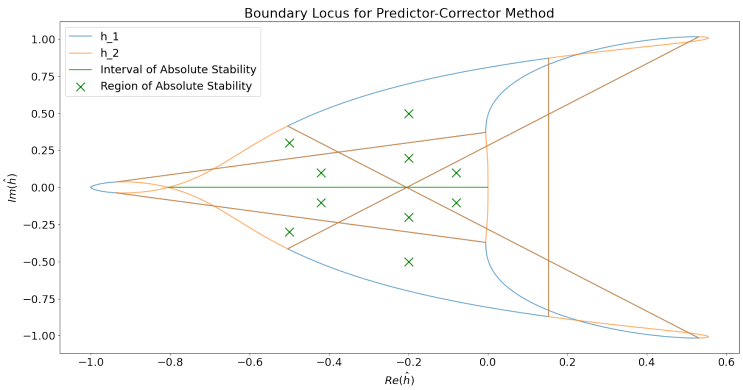


Figure 1: Plot of Boundary Locus for Predictor-Corrector

To find the region and interval of absolute stability we try values of $\hat{h}$ along the real axis in each region shown on the boundary (here we try $\hat{h} \in (-2, -0.9, -0.5, -0.1, 0.1, 1)$) locus plugged into the solutions for r of the stability polynomial and test the three roots for the strict root condition. The Interval and Region of Absolute stability is the part corresponding to the tried $\hat{h}$ that gives r roots satisfying the strict root condition. The Interval of Absolute Stability was obtained to be

$$\hat{h} \in (-0.8048, 0)$$

.

1.4

We repeat the idea in the previous task for both the predictor and corrector separately. For the predictor we obtain

$$p(r) = r^3 - \frac{3}{2}r^2 + \frac{1}{2}r - \frac{\hat{h}}{24}(41r^2 - 40r + 11)$$

$$\hat{h} = 12*r*(2*r**2 - 3*r + 1)/(41*r**2 - 40*r + 11)$$

and for the corrector we obtain

$$p(r) = r^3 - \frac{3}{2}r^2 + \frac{1}{2}r - \frac{\hat{h}}{24}(24r^3 - 31r^2 + 32r - 13)$$

$$\hat{h} = 12 * r * (2 * r * *2 - 3 * r + 1)/(24 * r * *3 - 31 * r * *2 + 32 * r - 13)$$

Again applying the boundary locus method by letting $r = e^{is}, s \in [0, 2\pi)$ and plotting the $\hat{h}$ values for these r. We obtain the Boundary Loci. To find the region and interval of absolute stability we again try values of $\hat{h}$ along the real axis in each region shown on the boundary (here we try $\hat{h} \in (-1, 0, -0.5)$ for the Predictor and $\hat{h} \in (-1, 0, 0.1, 5)$ for the Corrector) locus plugged into the solutions for r of the stability polynomials and test the three roots for the strict root condition. The Interval and Region of Absolute stability is the part corresponding to the tried $\hat{h}$ that gives r roots satisfying the strict root condition. For the Predictor the Interval of Absolute Stability was obtained to be

$$\hat{h} \in (-0.782, 0)$$

For the Corrector the Interval of Absolute Stability was obtained to be

$$\hat{h} \in (-\infty, 0)$$

The interval for the Predictor-Corrector is a subinterval of the interval for the Corrector but the interval for the Predictor is a subinterval of the interval of the Predictor-Corrector. If we take the intersection of the two intervals for the Predictor and Corrector separately we obtain something an interval very similar to the interval of the Predictor-Corrector.

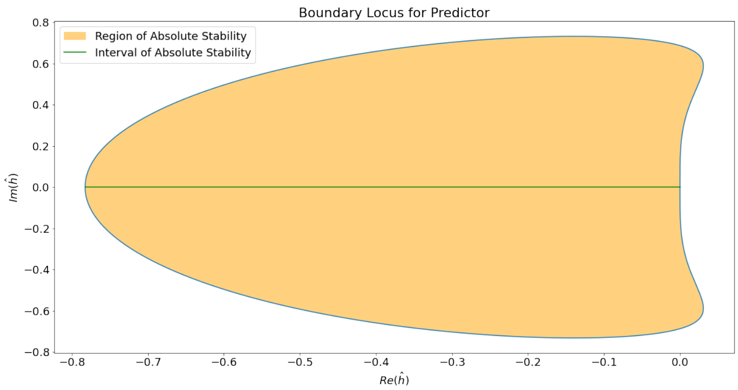


Figure 2: Plot of Boundary Locus for Predictor

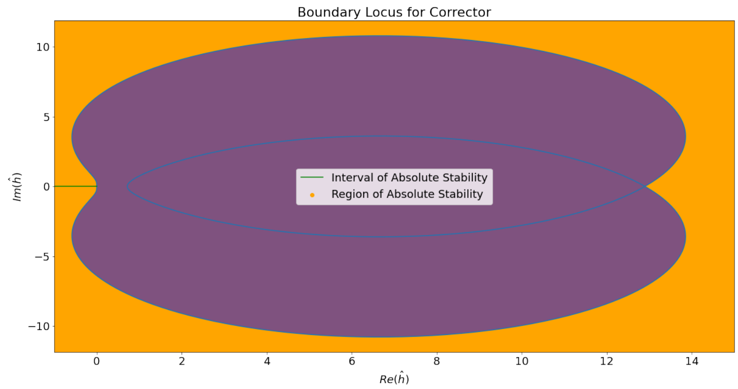


Figure 3: Plot of Boundary Locus for Corrector

2

To apply the Predictor-Corrector method we first need to generate X_1, X_2 since only $X_0 = (1, 0, 0)$ is given and the Predictor-Corrector Method is a three step method. We use the Euler method for this to generate $X_1 = (9.999960e{-}01, 4.000000e{-}06, 0.000000e{+}00)$, $X_2 = (9.999920e-01, 7.951984e-06, 4.800000e-08)$ using a value of $h = 10^{-4}$ and f to be the right hand side of the IVP. Then we are able to apply

$$
\begin{aligned}
\textbf{Predict} \quad & \hat{x}_{n+1} = \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(41f(t_n, x_n) - 40f(t_{n-1}, x_{n-1}) + 11f(t_{n-2}, x_{n-2})) \\
\textbf{Evaluate} \quad & f(t_{n+1}, \hat{x}_{n+1}) \\
\textbf{Correct} \quad & x_{n+1} = \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(24f(t_{n+1}, \hat{x}_{n+1}) - 31f(t_n, x_n) + 32f(t_{n-1}, x_{n-1}) - 13f(t_{n-2}, x_{n-2})) \\
\textbf{Evaluate} \quad & f(t_{n+1}, x_{n+1})
\end{aligned}
\tag{8}
$$

Robertson's autocatalytic chemical reaction IVP is a classic example of a stiff system of ODEs. So we must make sure to take h small enough for the solution to be stable. We plot the solution and observe $y(t)$ to look like constant 0. So in the next plot we increase the scale of y by 10^4 and are able to observe non constant behaviour. We then plot the 3D version of the solution to see how the reaction evolves in space over time.

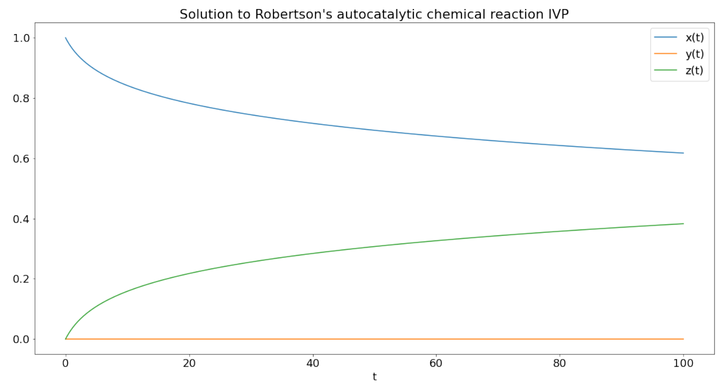


Figure 4: Predictor Corrector Solution for each Component to IVP

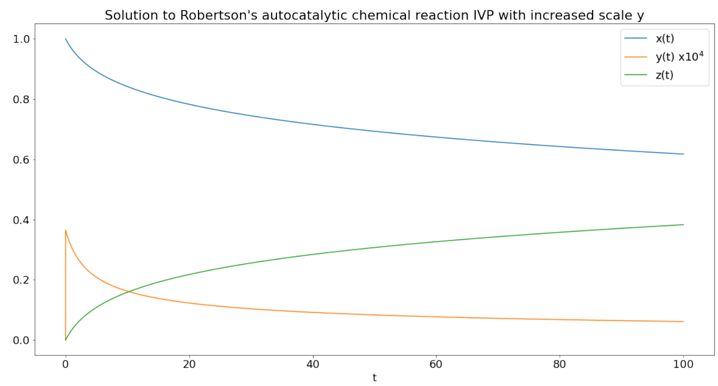
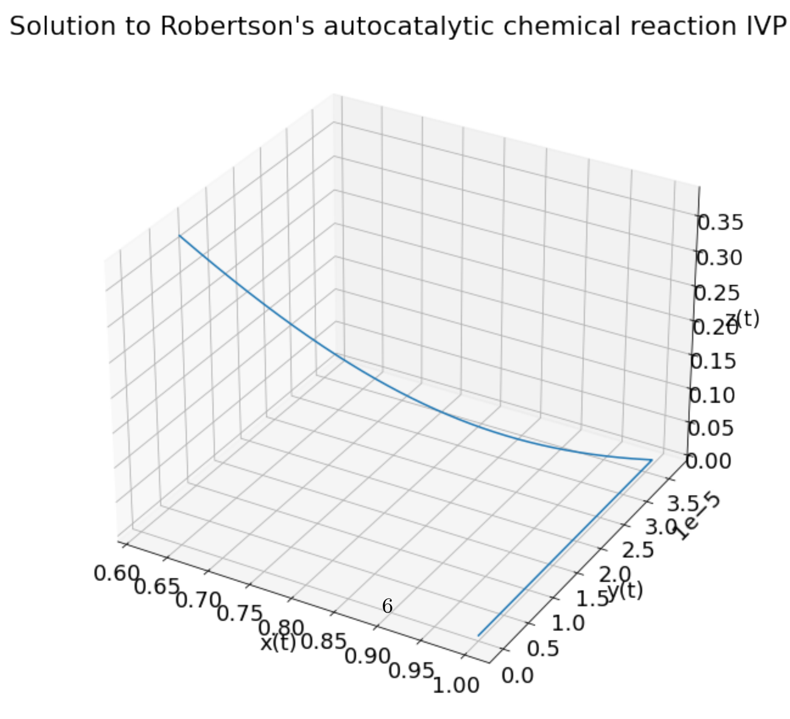


Figure 5: Predictor Corrector Solution for each component with increased y scale to IVP



3

3.1

We will use the following LMM to solve the Rabinovich–Fabrikant system.

$$x_{n+3} - \frac{3}{2}x_{n+2} + \frac{1}{2}x_{n+1} = \frac{h}{24}(24f_{n+3} - 31f_{n+2} + 32f_{n+1} - 13f_n) \tag{9}$$

Rewriting the indices and batching implicit and explicit parts together we obtain

$$x_{n+1} = g_n + hf_{n+1} \tag{10}$$

$$g_n = \frac{3}{2}x_n - \frac{1}{2}x_{n-1} + \frac{h}{24}(-31f_n + 32f_{n-1} - 13f_{n-2}) \tag{11}$$

$$f_n = \begin{pmatrix} y_n(z_n - 1 + x_n^2) +_n \\ x_n(3z_n + 1 - x_n^2) + \gamma y_n \\ -2z_n(\alpha + x_n y_n) \end{pmatrix}, \gamma = 0.87, \alpha = 1.1 \tag{12}$$

Using Newton Method we write

$$F\begin{pmatrix} x_{n+1} \\ y_{n+1} \\ z_{n+1} \end{pmatrix} = \begin{pmatrix} x_{n+1} \\ y_{n+1} \\ z_{n+1} \end{pmatrix} - g_n - hf_{n+1} \tag{13}$$

Partially differentiating w.r.t the $n+1$ terms we obtain

$$F'\begin{pmatrix} x_{n+1} \\ y_{n+1} \\ z_{n+1} \end{pmatrix} = \begin{pmatrix} 1 - 2hy_{n+1}x_{n+1} - h\gamma & -h(z_{n+1} - 1 + x_{n+1}^2) & -hy_{n+1} \\ -h(3z_{n+1} + 1 - 3x_{n+1}^2) & 1 - h\gamma & -3hx_{n+1} \\ 2hy_{n+1}z_{n+1} & 2hx_{n+1}z_{n+1} & 1 + 2h(\alpha + x_{n+1}y_{n+1}) \end{pmatrix} \tag{14}$$

Again we must generate X_1, X_2 using Euler and then we are able to apply the Newton Method. We use $h = 10^{-4}$, maximum iteration of 1000000 and stopping criterion at $\epsilon = 10^{-4}$ We observe a chaotic attractor.

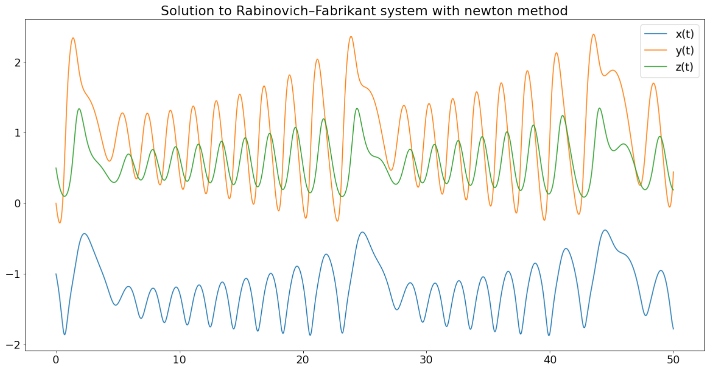


Figure 6: Solution to RF System with Newton Method

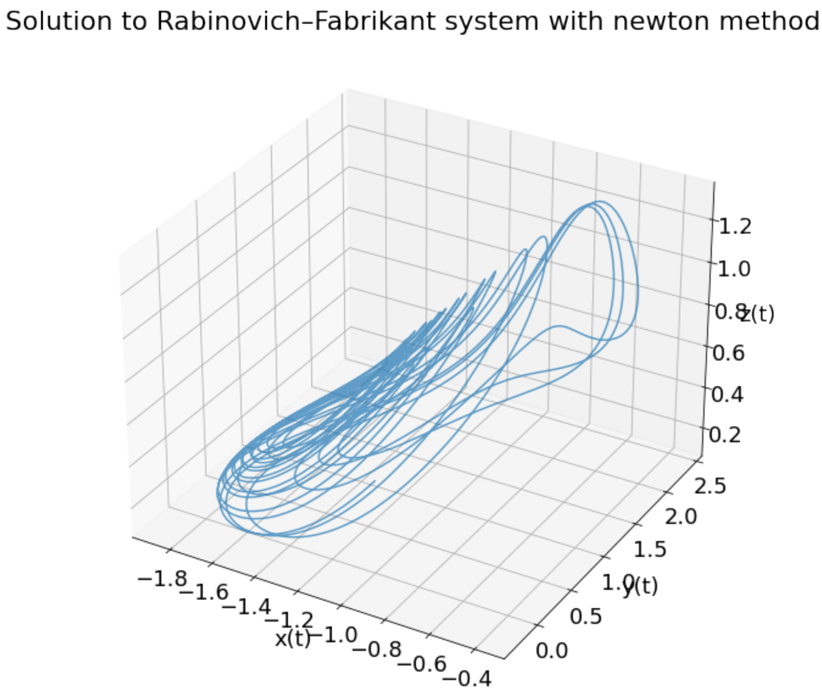


Figure 7: Solution to RF System with Newton Method

Implementing the fixed point method is far simpler than Newton since we do not need to precalculate the jacobian. We again use $h = 10^{-4}$, maximum iteration of 1000000 and stopping criterion at $\epsilon = 10^{-4}$. We observe that the solutions are very similar.

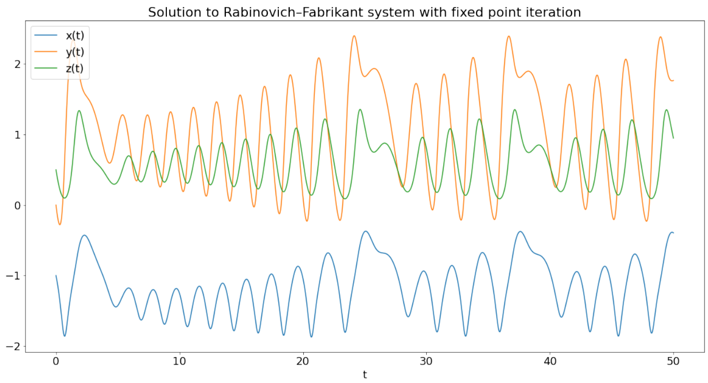


Figure 8: Solution to RF System with fixed point iteration

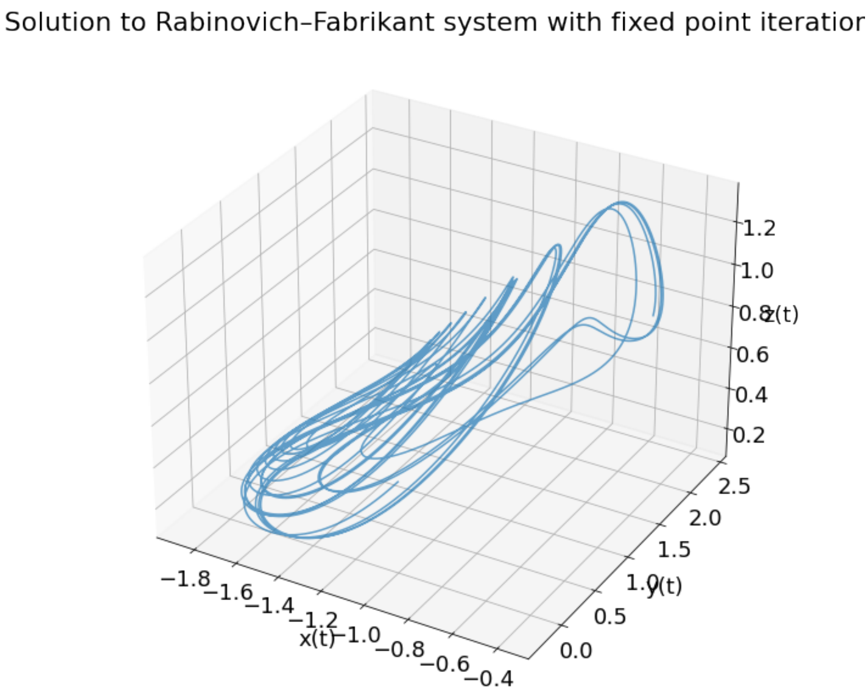


Figure 9: Solution to RF System with fixed point iteration

3.2

We would like to compare the number of iterations and execution time of the Fixed point iteration method and Newton method for this system to see which one is preferable. For Fixed point iteration method we have 731014 iterations and it takes 32.491426944732666 seconds to solve whereas the for the Newton Method we have 724069 iterations and it takes 78.63206505775452 seconds to run. So fixed point iteration has more iterations but takes less time than Newton method. This is most likely due to the expensive operation of inverting the Jacobian. Since Fixed point iteration takes less than half the time of the Newton Method and the difference in iterations is under 10000 we would think to prefer the fixed point iteration for this system.

4

We know by the Dahlquist equivalence theorem that

LMM is convergent $\iff$ it is both consistent and zero-stable

First we set some constraints on the coefficients using consistency.

$$\rho(1) = 0, \rho'(1) = \sigma(1)$$

$$\rho(r) = r^3 + \alpha_2 r^2 + \alpha_0, \sigma(r) = \beta_0$$

$$\Rightarrow \alpha_0 = -1 - \alpha_2, \beta_0 = 3 + 2\alpha_2$$

So we can now express the whole LMM and its characteristic polynomials via just α_2. Requiring zero-stability we need the roots of

$$\rho(r) = r^3 + \alpha_2 r^2 - (1 + \alpha_2)$$

to satisfy the root condition. We solve for r to obtain

$$r_1 = 1, r_2 = -\frac{\alpha_2}{2} - \frac{\sqrt{\alpha_2^2 - 2\alpha_2 - 3}}{2} - \frac{1}{2}, r_3 = -\frac{\alpha_2}{2} + \frac{\sqrt{\alpha_2^2 - 2\alpha_2 - 3}}{2} - \frac{1}{2}$$

Requiring the three roots to satisfy the root condition we obtain

$$\frac{3}{2} < \alpha_2 \leq -1$$

So now we are free to choose any α_2 in that interval and we will be able to find the other coefficients using the relation above and have a convergent LMM by the Dahlquist equivalence theorem. So to find the the largest interval of absolute stability we begin by plotting a few boundary loci for various α_2 in the interval to see if we can spot any pattern. For this we first find the stability polynomial to be

$$p(r) = r^3 + \alpha_2 r^2 - (1 + \alpha_2) - \hat{h}(3 + 2\alpha_2)$$

Solving for $\hat{h}$ and letting $r = e^{is}, s \in [0, 2\pi)$ and plotting the $\hat{h}$ values for these r for various α_2 we see an emerging pattern. The shape for the boundary locus is always the same but it is stretched as α_2 is decreased. For each locus to find the interval of absolute stability we try values of $\hat{h}$ along the real axis in each region shown on the locus plugged into the solutions for r of the stability polynomial and test the three roots for the strict root condition. The Interval and Region of Absolute stability is the part corresponding to the tried $\hat{h}$ that gives r roots satisfying the strict root condition. We find that the interval lies in the smallest region in the centre of the locus for all α_2

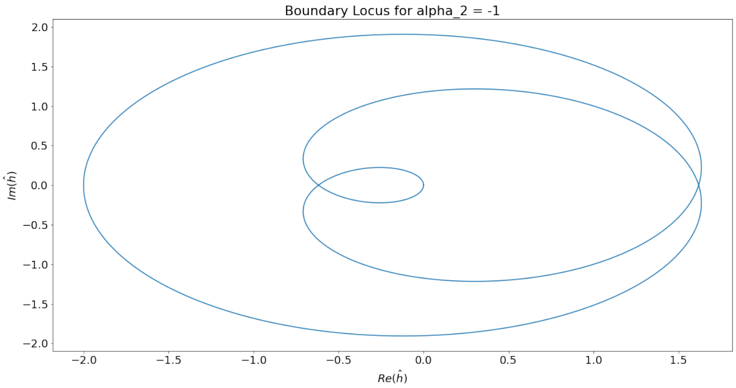


Figure 10: Boundary Locus for $\alpha_2 = -1$

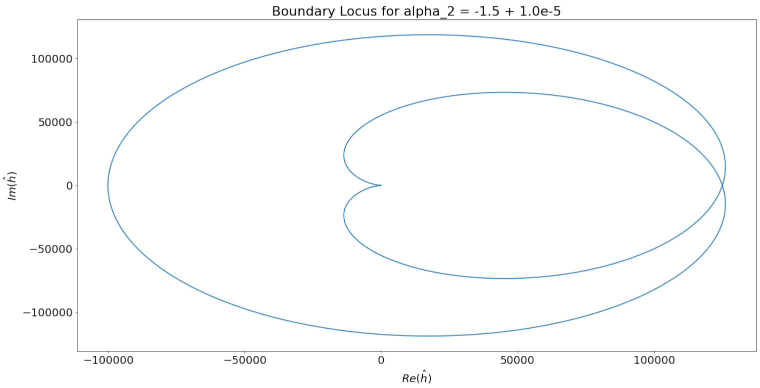


Figure 11: Boundary Locus for $\alpha_2 = -\frac{3}{2} + \epsilon$

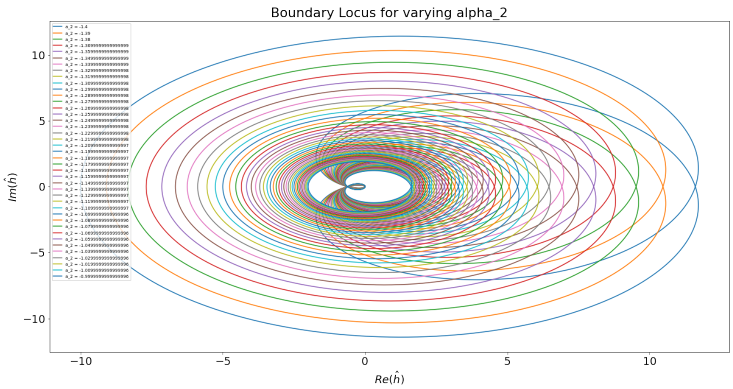


Figure 12: Boundary Locus for all possible α_2

We zoom in on the lower end of the region of absolute stability and observe that as α_2 increases from $-\frac{3}{2}$ to -1 the interval of absolute stability minutely increases in size as it is bounded above at 0 and the lower end decreases minutely. So $\alpha_2 = -1$ gives the greatest interval of absolute stability. By zooming in even more for $\alpha_2 = -1$ we obtain the interval to be

$$\hat{h} \in (-0.618034, 0)$$

and

$$\alpha_2 = -1, \alpha_0 = 0, \beta_0 = 1$$

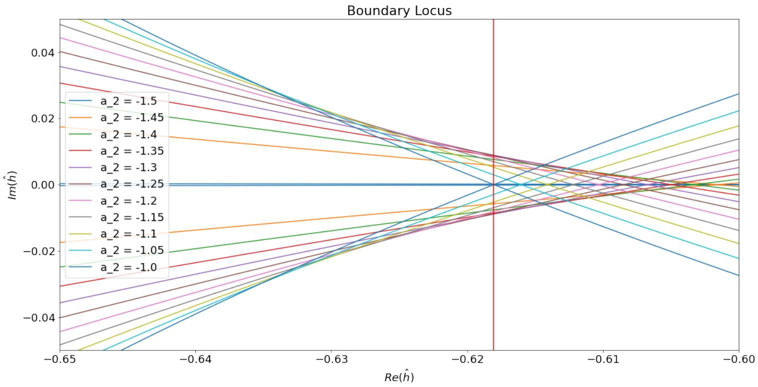


Figure 13: Boundary Locus for all possible α_2 zoomed into the lower end of Absolute stability interval

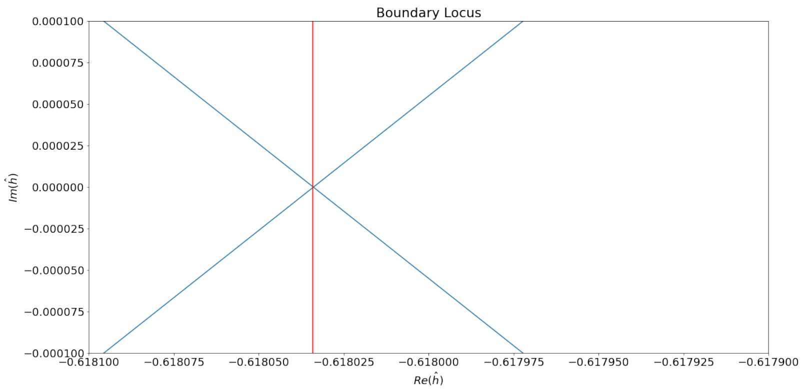


Figure 14: Boundary Locus for $\alpha_2 = -1$ zoomed into the lower end of Absolute stability interval