Numerical Solution of Ordinary Differential Equations Coursework 2

CID:01724711

November 2022

1

The general form for a 3 step explicit LMM is

$$\sum_{m=0}^{3} \alpha_m x_{n+m} = h \sum_{m=0}^{3} \beta_m f_{n+m} \quad \text{where} \quad \alpha_m, \beta_m = const \in \mathbb{R}, \alpha_3 = 1, \beta_3 = 0$$

We know by the Dahlquist equivalence theorem that

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

and also by Theorem 8.2 in lectures

The global error of a convergent LMM equals to its order of consistency

Combining these two we have that to find a 3 step LMM with global error of order 3 we need to find α_m, β_m in the above general form such that order of consistency of the LMM is 3 and such that the LMM is zero-stable.
To find the coefficients such that the LMM is consistent of order 3 we find the LDO up to h^4 terms by finding each terms Taylor expansion and set the lower terms to equal 0.

$$\begin{aligned}
\mathcal{L}_h z(t) &= z(t+3h) + \alpha_2 z(t+2h) + \alpha_1 z(t+h) + \alpha_0 z(t) - h[\beta_2 z'(t+2h) + \beta_1 z'(t+h) + \beta_0 z'(t)] \\
&= (1 + \alpha_0 + \alpha_1 + \alpha_2) z(t) \\
&+ (3 + \alpha_1 + 2\alpha_2 - \beta_2 - \beta_1 - \beta_0) h z'(t) \\
&+ (\frac{9}{2} + \frac{\alpha_1}{2} + 2\alpha_2 - 2\beta_2 - \beta_1) h^2 z''(t) \\
&+ (\frac{9}{2} + \frac{\alpha_1}{6} + \frac{4\alpha_2}{3} - 2\beta_2 - \frac{\beta_1}{2}) h^3 z'''(t) \\
&+ (\frac{27}{8} + \frac{\alpha_1}{24} + \frac{2\alpha_2}{3} - \frac{4\beta_2}{3} - \frac{\beta_1}{6}) h^4 z''''(t) \\
&+ \mathcal{O}(h^5)
\end{aligned} \tag{1}$$

We require the first 4 terms to be 0 and the 5th term to be non 0.

$$\begin{aligned} 1+\alpha_0+\alpha_1+\alpha_2 &= 0 \\ 3+\alpha_1+2\alpha_2-\beta_2-\beta_1-\beta_0 &= 0 \\ \frac{9}{2}+\frac{\alpha_1}{2}+2\alpha_2-2\beta_2-\beta_1 &= 0 \\ \frac{9}{2}+\frac{\alpha_1}{6}+\frac{4\alpha_2}{3}-2\beta_2-\frac{\beta_1}{2} &= 0 \\ \frac{27}{8}+\frac{\alpha_1}{24}+\frac{2\alpha_2}{3}-\frac{4\beta_2}{3}-\frac{\beta_1}{6} &\neq 0 \end{aligned} \tag{2}$$

This is only enough to guarantee consistency of the right order. We also require the LMM to be zero-stable. An LMM is said to be zero-stable if its first characteristic polynomial, $p(r)$, satisfies the root condition. A polynomial of degree n is said to satisfy the root condition if all its roots $|r_i| \leq 1, i = 1, ..n$ and any roots that satisfy $|r_k| = 1$ are simple. Hence we require the roots of

$$p(r) = r^3 + \alpha_2 r^2 + \alpha_1 r + \alpha_0 = 0$$

to satisfy the root condition. So we need to find the coefficients $\alpha_2, \alpha_1, \alpha_0$ such that the characteristic polynomial satisfies the root condition. Luckily there is a well known method for this.
Let the cubic equation $ar^3 + br^2 + cr + d = 0$ have the three roots r_1, r_2, r_3. We can now write $ar^3 + br^2 + cr + d = a(r - r_1)(r - r_2)(r - r_3)$.

By multiplying out the right hand side, we have
$ar^3 + br^2 + cr + d = ar_3 - a(r_1 + r_2 + r_3)r_2 + a(r_1r_2 + r_1r_1 + r_2r_3)r - ar_1r_2r_3$

This must hold for all values of r, so corresponding coefficients must be equal. This gives

$$\begin{aligned} -\frac{b}{a} &= r_1 + r_2 + r_3 \\ \frac{c}{a} &= r_1r_2 + r_2r_3 + r_1r_3 \\ -\frac{d}{a} &= r_1r_2r_3 \end{aligned} \tag{3}$$

We observe that the first equation in (2) gives us that one of the roots of the characteristic polynomial is 1. We can arbitrarily choose the other roots so that the root condition is satisfied and find the α coefficients by (3).
Let us choose $r_1 = 0, r_2 = \frac{1}{2}, r_3 = 1$. This gives

$$\alpha_2 = -\frac{3}{2}, \alpha_1 = \frac{1}{2}, \alpha_0 = 0 \tag{4}$$

By subbing in (4) into (2) we obtain

$$\beta_2 = \frac{41}{24}, \beta_1 = -\frac{40}{24}, \beta_0 = \frac{11}{24} \tag{5}$$

Lastly we check $\frac{27}{8} + \frac{\alpha_1}{24} + \frac{2\alpha_2}{3} - \frac{4\beta_2}{3} - \frac{\beta_1}{6} = \frac{19}{48} \neq 0$ so that the order of consistency is indeed 3 and not higher. So by construction we have an explicit 3-step convergent method with the global error of order 3.

$$x_{n+3} - \frac{3}{2}x_{n+2} + \frac{1}{2}x_{n+1} = \frac{h}{24}(41f_{n+2} - 40f_{n+1} + 11f_n) \tag{6}$$

2

The implicit LMM will be developed the same way with the exception that now $\beta_3 \neq 0$

$$\begin{aligned}
\mathcal{L}_h z(t) &= z(t+3h) + \alpha_2 z(t+2h) + \alpha_1 z(t+h) + \alpha_0 z(t) \\
&- h[\beta_3 z'(t+3h)\beta_2 z'(t+2h) + \beta_1 z'(t+h) + \beta_0 z'(t)] \\
&= (1 + \alpha_0 + \alpha_1 + \alpha_2)z(t) \\
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\end{aligned} \tag{8}$$

Again let us choose $r_1 = 0, r_2 = \frac{1}{2}, r_3 = 1$. This gives

$$\alpha_2 = -\frac{3}{2}, \alpha_1 = \frac{1}{2}, \alpha_0 = 0 \tag{9}$$

By subbing in (9) into (8) we obtain a whole family of possible β coefficients since we have 3 equation in 4 variables. We are free to choose one of the variables. We decide to choose $\beta_3 = 1$ for simplicity. With this choice from (8) we obtain

$$\beta_3 = 1, \beta_2 = -\frac{31}{24}, \beta_1 = \frac{32}{24}, \beta_0 = -\frac{13}{24} \tag{10}$$

We are aware that since we chose the roots that give $\alpha_0 = 0$ we cannot have $\beta_0 = 0$ otherwise this will not be a 3 step method. Indeed we see that $\beta_0 \neq 0$ so we do have a 3 step method. Lastly we check $\frac{27}{8} + \frac{\alpha_1}{24} + \frac{2\alpha_2}{3} - \frac{27\beta_3}{8} - \frac{4\beta_2}{3} - \frac{\beta_1}{6} = -\frac{143}{48} \neq 0$ so that the order of consistency is indeed 3 and not higher. So by construction we have an implicit 3-step convergent method with the global error of order 3.

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

3

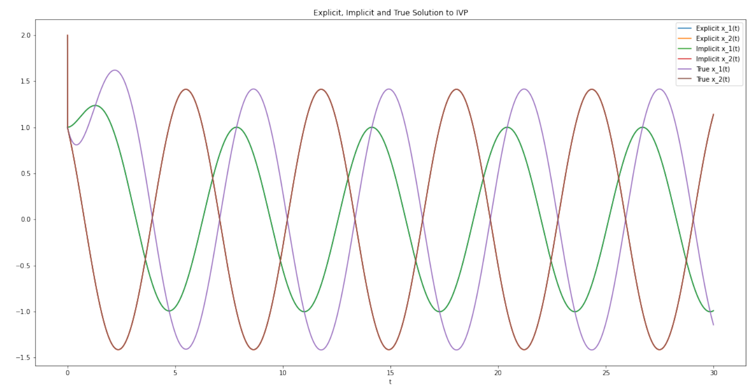

Figure 1: Plot of each component of Explicit, Implicit and True Solution to IVP

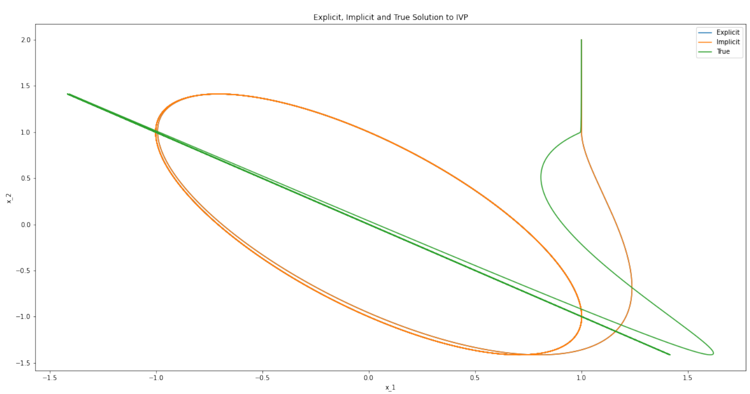

Figure 2: Plot of system of Explicit, Implicit and True Solution to IVP

Now we apply the methods developed in exercises 1 and 2 to the given IVP in exercise 3. Looking at my code it will become apparent that the method used in the implicit LMM was fixed point iteration with $\epsilon = 10^{-4}$ and $M = 1000000$. We observe that the two methods have essentially the exact same solution. We note that the time to solve using the explicit method was 19.2 seconds compared to 38.3 seconds for the implicit method. The latter takes nearly twice as long to solve due to the fixed point iteration necessary to work around the implicitness so currently we may choose to prefer the explicit method. When comparing to the true solution we observe that for both methods the second component is essentially the same as the true solution second component but the same cannot be said for the first component. The behaviour for the first component is caught by the methods as we can see the similarity to that of the first component sinusoidal behaviour of the true solution. The period of the method solutions appear to match up with that of the true solution (however I think that it only appears to have constant period over the small interval we observe and in reality is not constant due to convergence of solutions to the true one) but true solution is slightly delayed and also the amplitude of the true solution is greater than that of the LMM method solution. Both of these differences play an adverse effect on the system behaviour as seen in Figure 2. In the LMM solution the oscillation of the first component begins before it should do and the symmetry between the two components is not captured. As evident from the true solution the two components are reflections in the x axis which results in the line oscillatory behaviour in Figure 2. The slight offsetting in oscillation results in both our methods displaying an elliptical oscillation behaviour. Further, the difference in amplitude of the first component also shows in the system. The major axis of the ellipse is less than the length of the line of the true solution. An interesting experiment would be to observe the system solution using my methods for $t \in [0, \infty)$. I would predict the ellipse would slowly stretch out until it becomes a line oscillation seeing as we have proved for both methods that they converge to the true solution. I will discuss more in 4 about how I obtained the true solution.

4

The true solution was obtained by diagonalizing

$$A = \begin{pmatrix} -1 & 1 \\ 1 & -1000 \end{pmatrix} = PDP^{-1}$$

Then obtaining a decoupled system of equations by using $X = PY$ which are linear with an added term of the same sin and cosine terms as in the original IVP for each component. We can then solve this easily since is two sets of decoupled linear odes with some straightforward separated sin or cosine term. After solving the decoupled system we again apply $X = PY$ to obtain the original solutions.

$$x_1(t) = 1.00099899399489 * sin(t) - 1.00200299798629 * cos(t)$$

$-0.000998997500005635*exp(-1000.001001*t)+2.0030019954863*exp(-0.998999000002073*t)$

$$x_2(t) = -0.997996502514384 * sin(t) + 0.999995492504405 * cos(t)$$

$+0.997999502502125*exp(-1000.001001*t)+0.00200500499346977*exp(-0.998999000002073*t)$

We can now find the maximum global error in the interval $t \in [0, 30]$ and also the global error at $t = 30$. We obtain for the explicit method that the global maximum error in the interval is 1.0458759859598825 , and the global error at $t = 30$ is 0.15398797618005658
We obtain for the implicit method that the global maximum error in the interval is 1.0459695440368237 , and the global error at $t = 30$ is 0.15397479013258686. In these calculation we have used the Euclidean norm in the error. So

$$e_n = ||x(t_n) - x_n||_2$$

Now theoretically.
For $n = 0, 1, 2, ..., N - 1$ we find that
$|e_0| = x(t_0) - x_0 = 0$,
$|e_1| \leq |R_1|$, ...
For explicit

$$\mathcal{L}_h z(t) = \frac{19}{48} h^4 z''''(t) + \mathcal{O}(h^5)$$

For implicit

$$\mathcal{L}_h z(t) = -\frac{143}{48} h^4 z''''(t) + \mathcal{O}(h^5)$$

Using these two and the recurrence between e_{n+1} and e_n we obtain theoretical global error at $t = 30$ to be 0.1552 for implicit and 0.1548 for explicit. We observe that both of these are higher than the practical global errors we observe as we should expect.

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 2

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 (Explicit LMM) **% of course mark: /5.0**

Develop an explicit 3-step convergent method of your own design with the global error of order 3. Note that the methods from the Adams–Bashforth and Adams–Moulton families cannot be used in the development.

Exercise 2 (Implicit LMM) **% of course mark: /5.0**

Develop an implicit 3-step convergent method of your own design with the global error of order 3. Note that the methods from the Adams–Bashforth and Adams–Moulton families cannot be used in the development.

Exercise 3 (Explicit and Implicit LMMs) **% of course mark: /5.0**

Solve the initial value problem

$$\begin{pmatrix} x_1'(t) \\ x_2'(t) \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 1 & -1000 \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} + \begin{pmatrix} 2\sin(t) \\ 1000(\cos(t) - \sin(t)) \end{pmatrix}, \quad \begin{pmatrix} x_1(t_0) \\ x_2(t_0) \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad t = [0, 30] \tag{1}$$

with the explicit and implicit LMM you developed.

Exercise 4 (Global error and LMMs) **% of course mark: /4.0★**

Theoretically estimate the global error of your LMMs and compare it with the global error computed numerically for system (1).

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.

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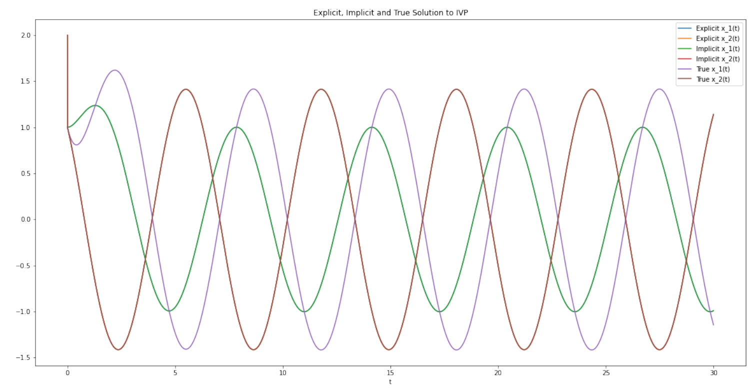


Figure 1: Plot of each component of Explicit, Implicit and True Solution to IVP

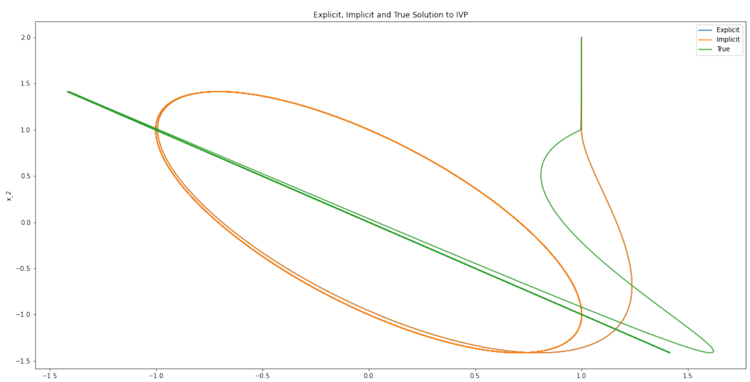


Figure 2: Plot of system of Explicit, Implicit and True Solution to IVP

Now we apply the methods developed in exercises 1 and 2 to the given IVP in exercise 3. Looking at my code it will become apparent that the method used in the implicit LMM was fixed point iteration with $\epsilon = 10^{-4}$ and $M = 1000000$. We observe that the two methods have essentially the exact same solution. We note that the time to solve using the explicit method was 19.2 seconds compared to 38.3 seconds for the implicit method. The latter takes nearly twice as long to solve due to the fixed point iteration necessary to work around the implicitness so currently we may choose to prefer the explicit method. When comparing to the true solution we observe that for both methods the second component is essentially the same as the true solution second component but the same cannot be said for the first component. The behaviour for the first component is caught by the methods as we can see the similarity to that of the first component sinusoidal behaviour of the true solution. The period of the method solutions appear to match up with that of the true solution (however I think that it only appears to have constant period over the small interval we observe and in reality is not constant due to convergence of solutions to the true one) but true solution is slightly delayed and also the amplitude of the true solution is greater than that of the LMM method solution. Both of these differences play an adverse effect on the system behaviour as seen in Figure 2. In the LMM solution the oscillation of the first component begins before it should do and the symmetry between the two components is not captured. As evident from the true solution the two components are reflections in the x axis which results in the line oscillatory behaviour in Figure 2. The slight offsetting in oscillation results in both our methods displaying an elliptical oscillation behaviour. Further, the difference in amplitude of the first component also shows in the system. The major axis of the ellipse is less than the length of the line of the true solution. An interesting experiment would be to observe the system solution using my methods for $t \in [0, \infty)$. I would predict the ellipse would slowly stretch out until it becomes a line oscillation seeing as we have proved for both methods that they converge to the true solution. I will discuss more in 4 about how I obtained the true solution.

4

The true solution was obtained by diagonalizing

$$A = \begin{pmatrix} -1 & 1 \\ 1 & -1000 \end{pmatrix} = PDP^{-1}$$

Then obtaining a decoupled system of equations by using $X = PY$ which are linear with an added term of the same sin and cosine terms as in the original IVP for each component. We can then solve this easily since is two sets of decoupled linear odes with some straightforward separated sin or cosine term. After solving the decoupled system we again apply $X = PY$ to obtain the original solutions.

$$x_1(t) = 1.00099899399489 * sin(t) - 1.00200299798629 * cos(t)$$

$-0.000998997500005635*exp(-1000.001001*t)+2.0030019954863*exp(-0.998999000002073*t)$

$$x_2(t) = -0.997996502514384 * sin(t) + 0.999995492504405 * cos(t)$$

$+0.997999502502125*exp(-1000.001001*t)+0.00200500499346977*exp(-0.998999000002073*t)$

We can now find the maximum global error in the interval $t \in [0, 30]$ and also the global error at $t = 30$. We obtain for the explicit method that the global maximum error in the interval is 1.0458759859598825 , and the global error at $t = 30$ is 0.15398797618005658
We obtain for the implicit method that the global maximum error in the interval is 1.0459695440368237 , and the global error at $t = 30$ is 0.15397479013258686. In these calculation we have used the Euclidean norm in the error. So

$$e_n = ||x(t_n) - x_n||_2$$

Now theoretically.
For $n = 0, 1, 2, ..., N - 1$ we find that
$|e_0| = x(t_0) - x_0 = 0$,
$|e_1| \leq |R_1|$, ...
For explicit

$$\mathcal{L}_h z(t) = \frac{19}{48} h^4 z''''(t) + \mathcal{O}(h^5)$$

For implicit

$$\mathcal{L}_h z(t) = -\frac{143}{48} h^4 z''''(t) + \mathcal{O}(h^5)$$

Using these two and the recurrence between e_{n+1} and e_n we obtain theoretical global error at $t = 30$ to be 0.1552 for implicit and 0.1548 for explicit. We observe that both of these are higher than the practical global errors we observe as we should expect.

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

1

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.

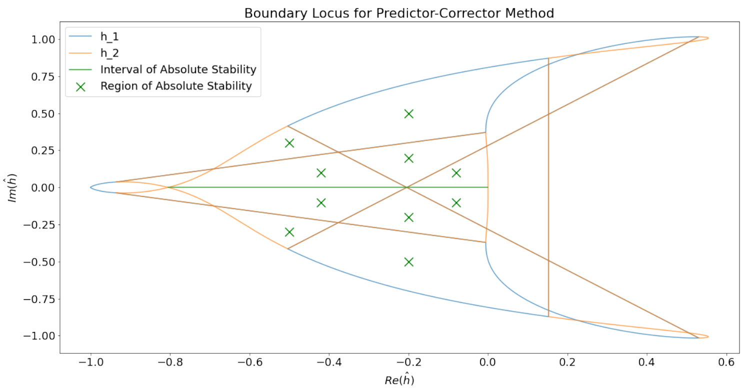


Figure 1: Plot of Boundary Locus for Predictor-Corrector

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.

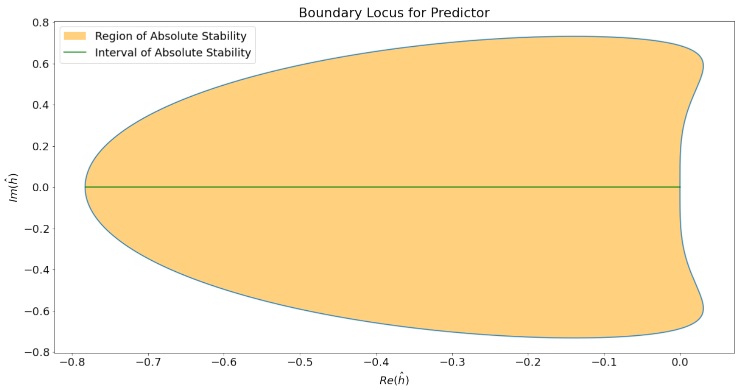


Figure 2: Plot of Boundary Locus for Predictor

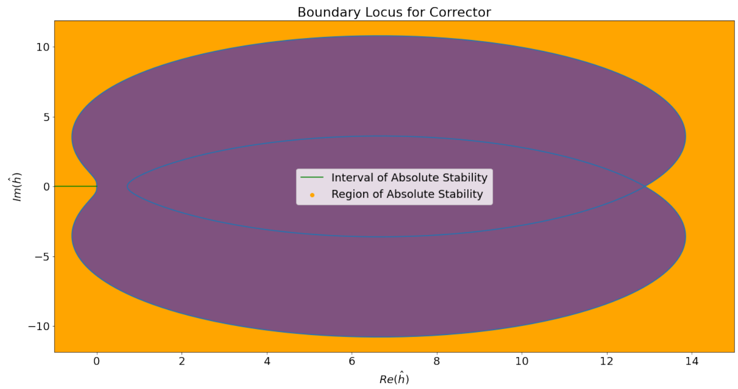


Figure 3: Plot of Boundary Locus for Corrector

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.

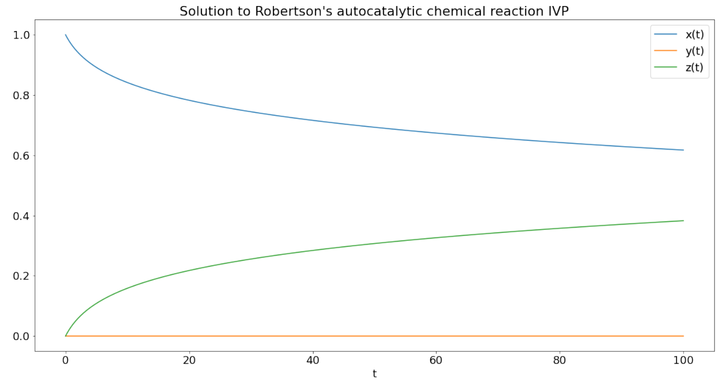


Figure 4: Predictor Corrector Solution for each Component to IVP

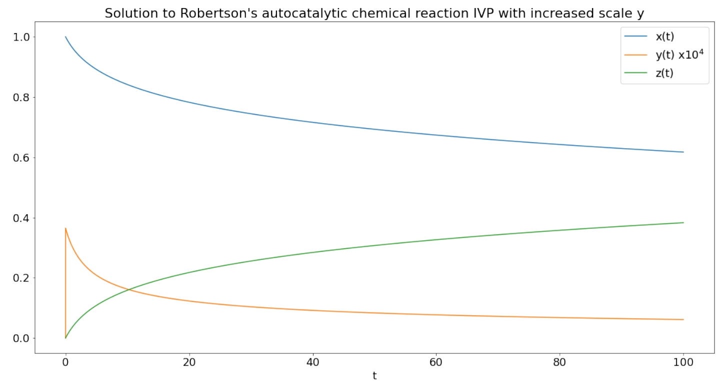
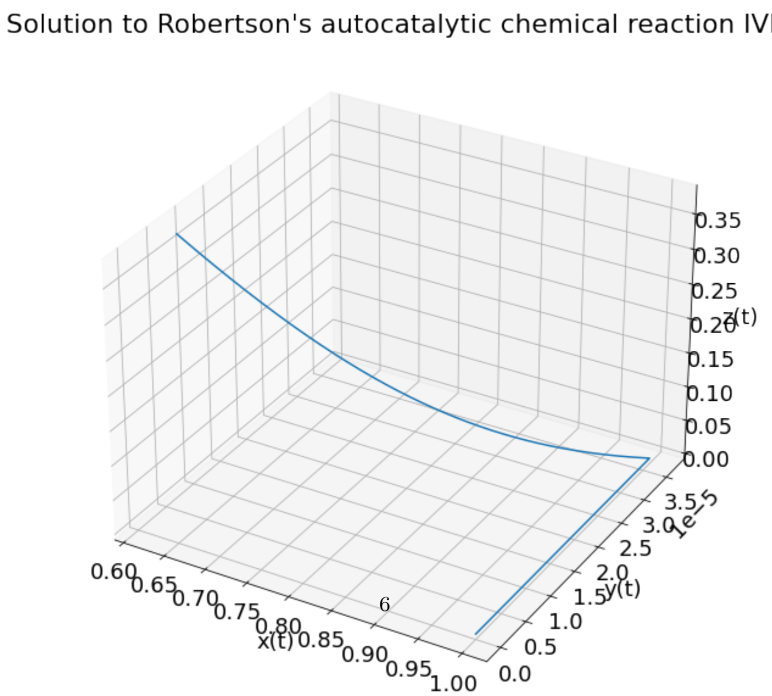


Figure 5: Predictor Corrector Solution for each component with increased y scale to IVP



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.

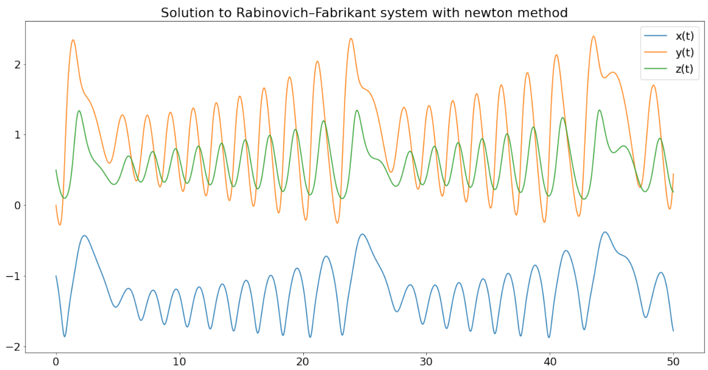


Figure 6: Solution to RF System with Newton Method

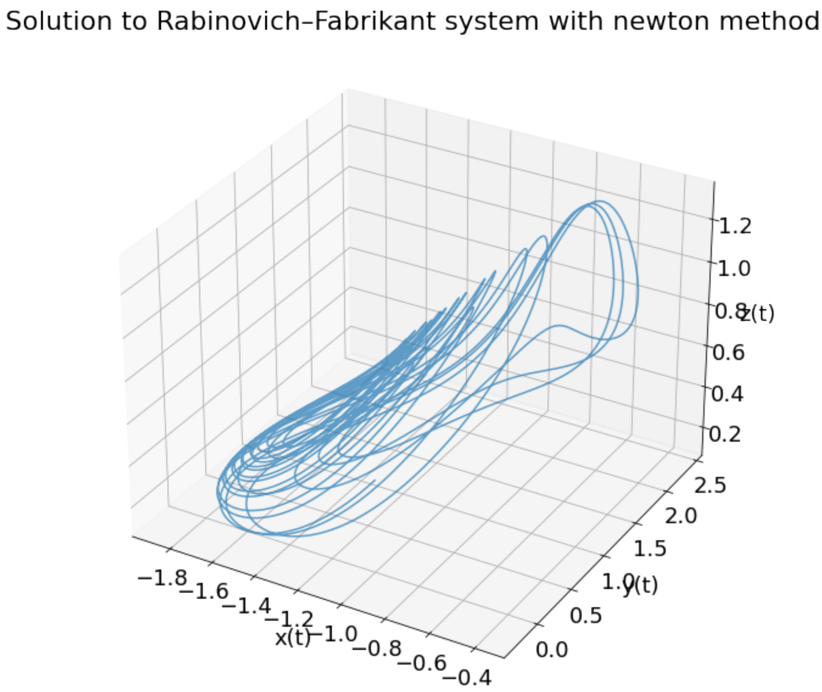


Figure 7: Solution to RF System with Newton Method

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.

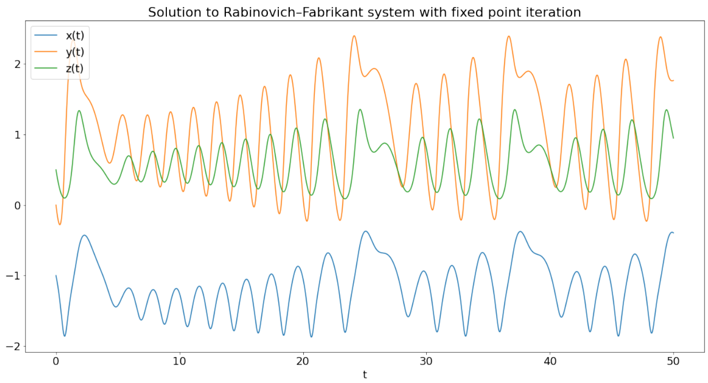


Figure 8: Solution to RF System with fixed point iteration

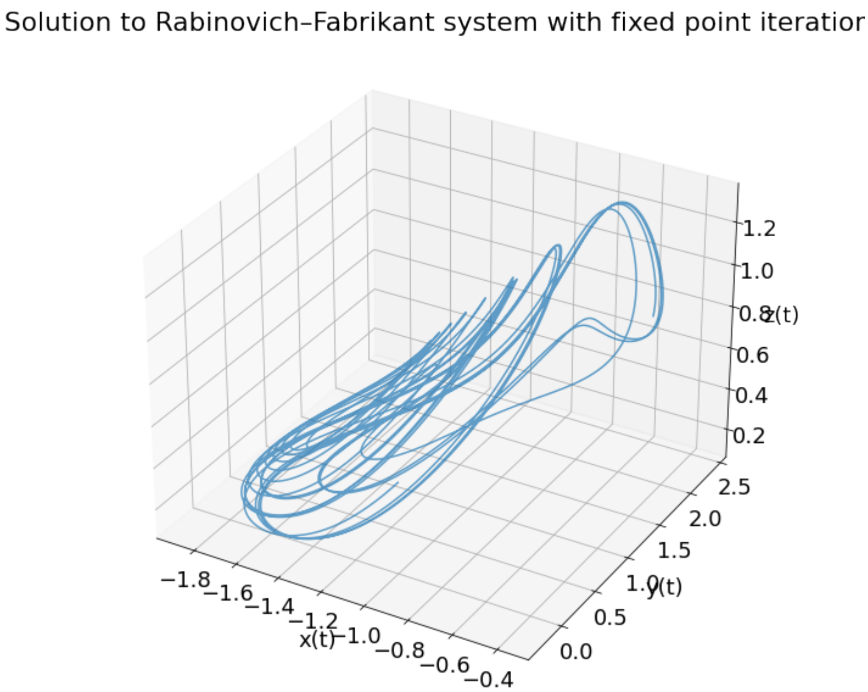


Figure 9: Solution to RF System with fixed point iteration

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

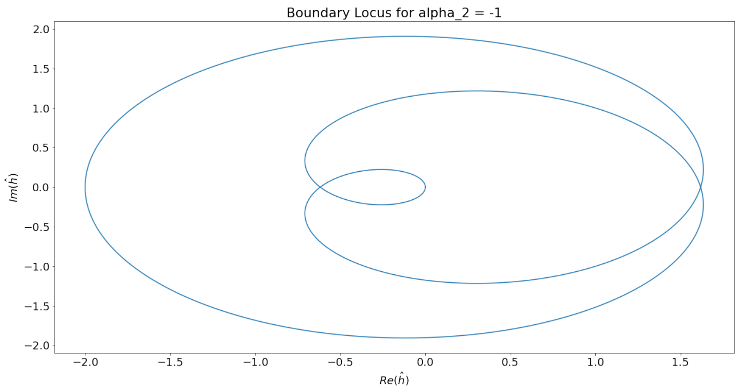


Figure 10: Boundary Locus for $\alpha_2 = -1$

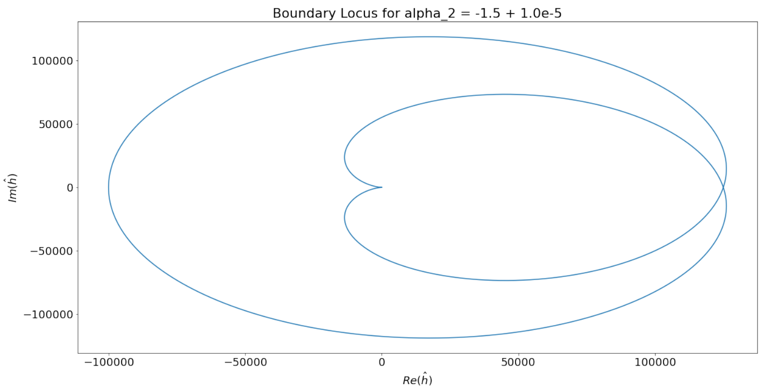


Figure 11: Boundary Locus for $\alpha_2 = -\frac{3}{2} + \epsilon$

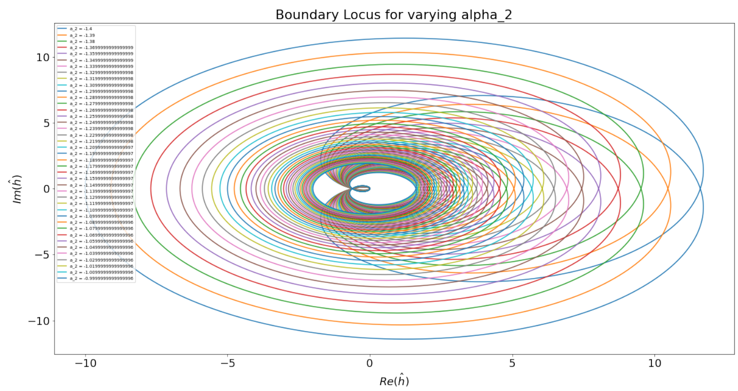


Figure 12: Boundary Locus for all possible α_2

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

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

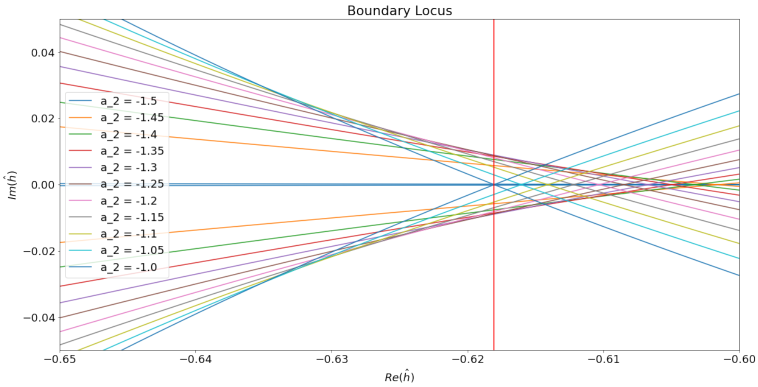


Figure 13: Boundary Locus for all possible α_2 zoomed into the lower end of Absolute stability interval

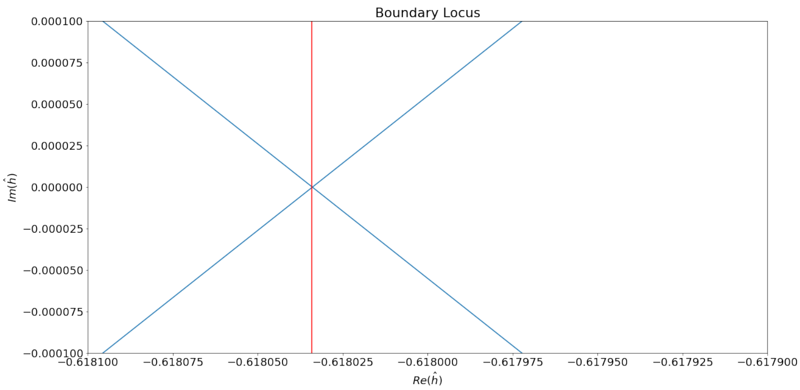


Figure 14: Boundary Locus for $\alpha_2 = -1$ zoomed into the lower end of Absolute stability interval