Numerical Solution of Ordinary Differential Equations
Coursework 3

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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 $f(t_n, x_n) = x'(t_n)$

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

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

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.

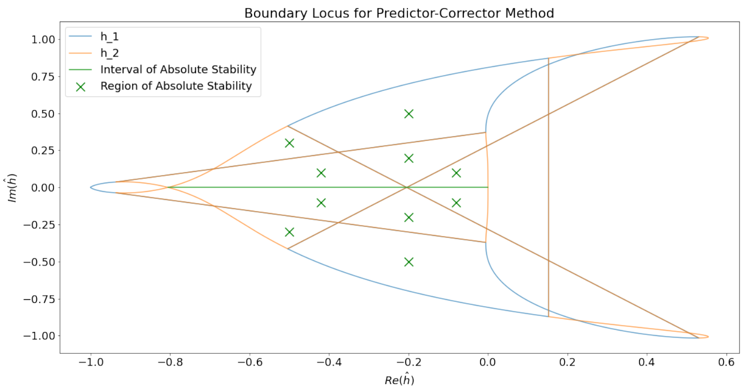


Figure 1: Plot of Boundary Locus for Predictor-Corrector

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.

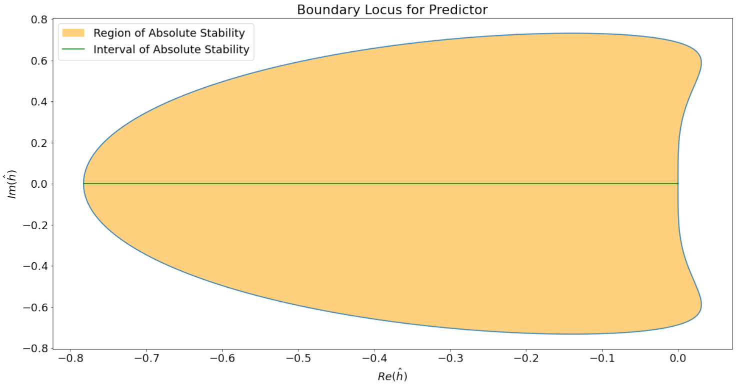


Figure 2: Plot of Boundary Locus for Predictor

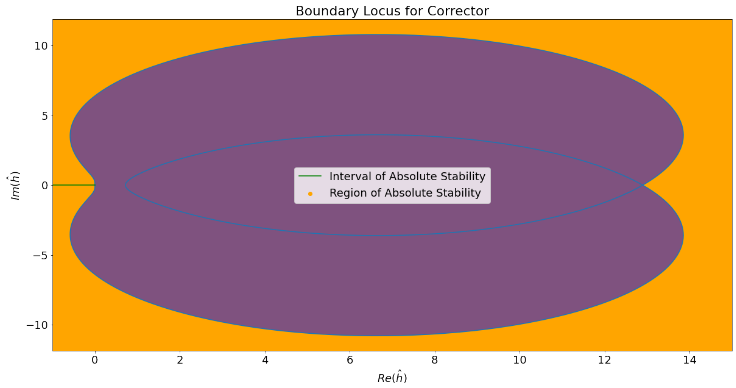


Figure 3: Plot of Boundary Locus for Corrector

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.

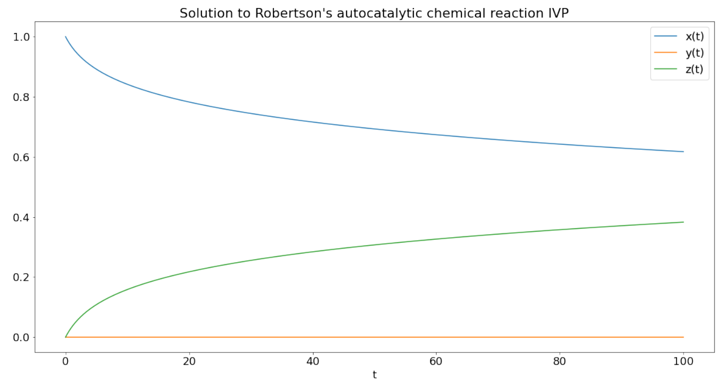


Figure 4: Predictor Corrector Solution for each Component to IVP

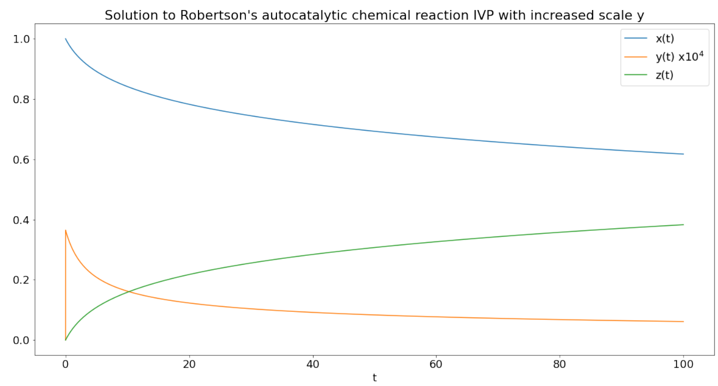
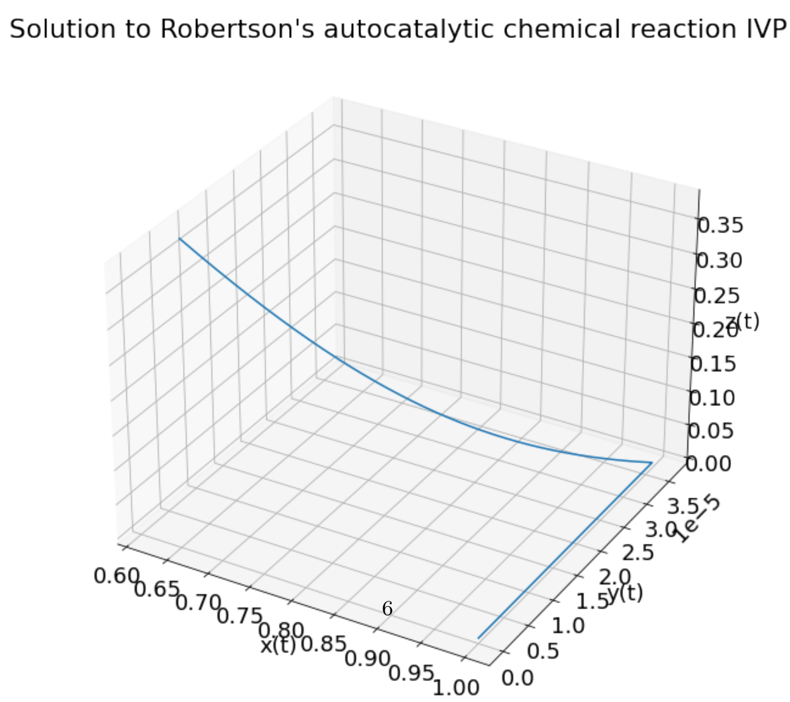


Figure 5: Predictor Corrector Solution for each component with increased y scale to IVP



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.

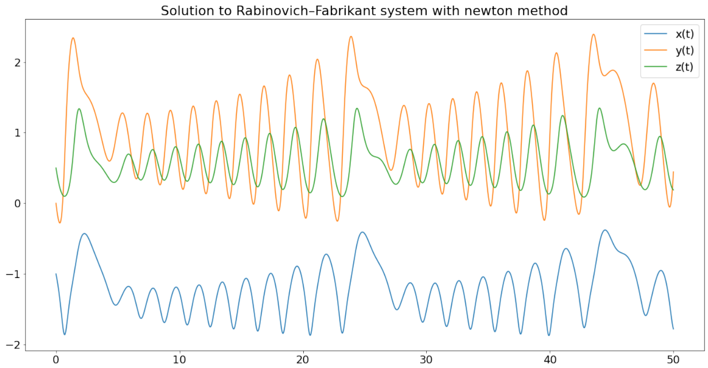


Figure 6: Solution to RF System with Newton Method

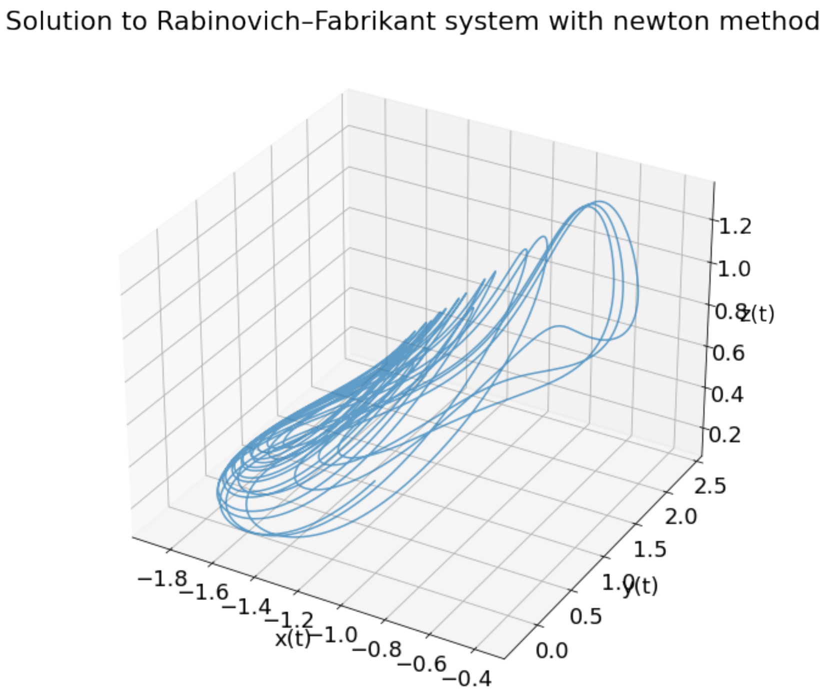


Figure 7: Solution to RF System with Newton Method

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.

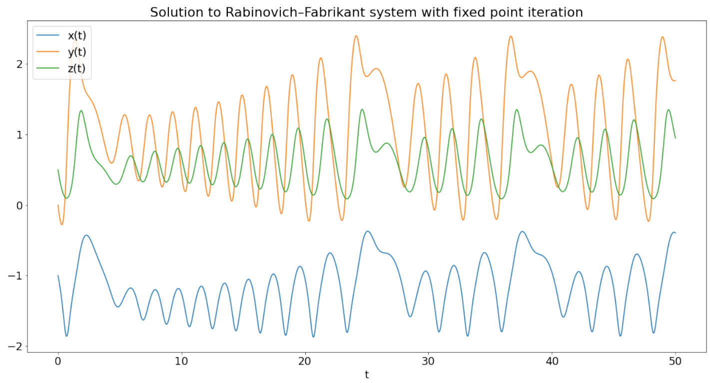


Figure 8: Solution to RF System with fixed point iteration

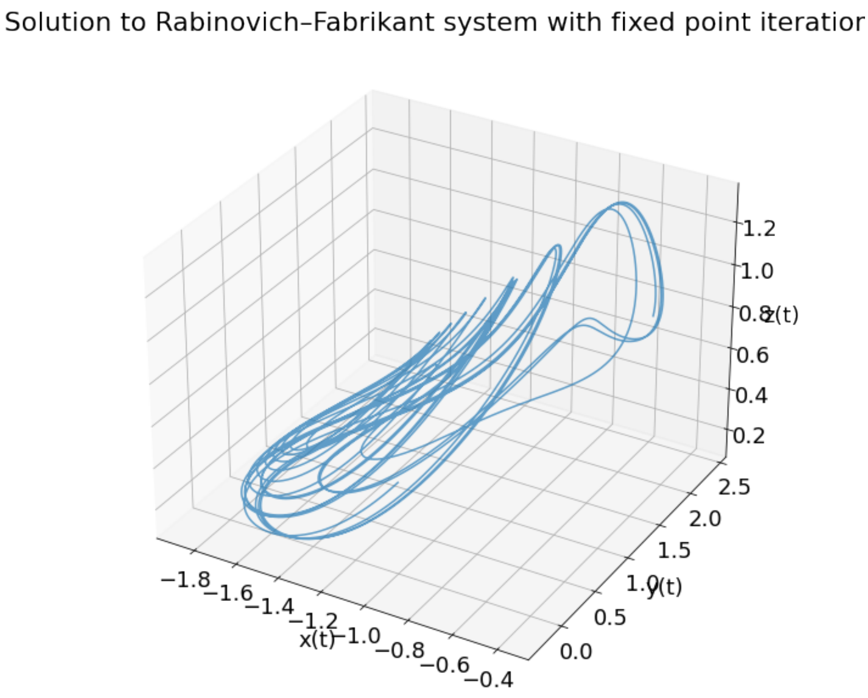


Figure 9: Solution to RF System with fixed point iteration

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

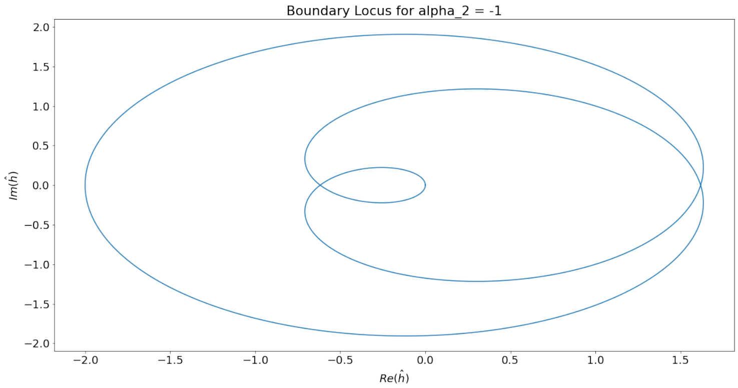


Figure 10: Boundary Locus for $\alpha_2 = -1$

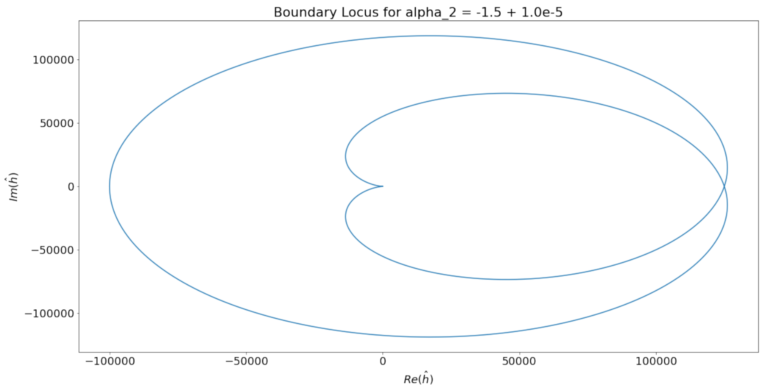


Figure 11: Boundary Locus for $\alpha_2 = -\frac{3}{2} + \epsilon$

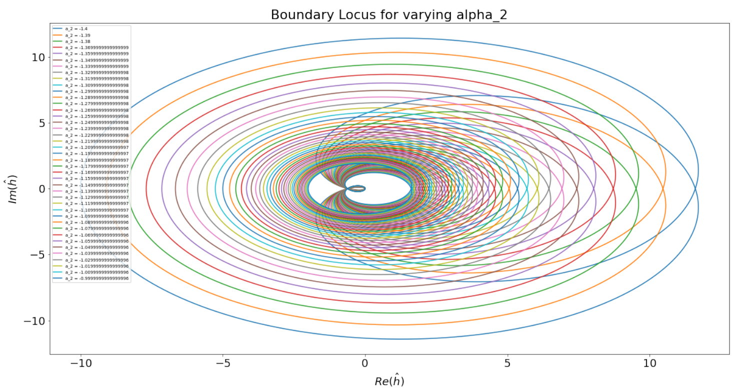


Figure 12: Boundary Locus for all possible α_2

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

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

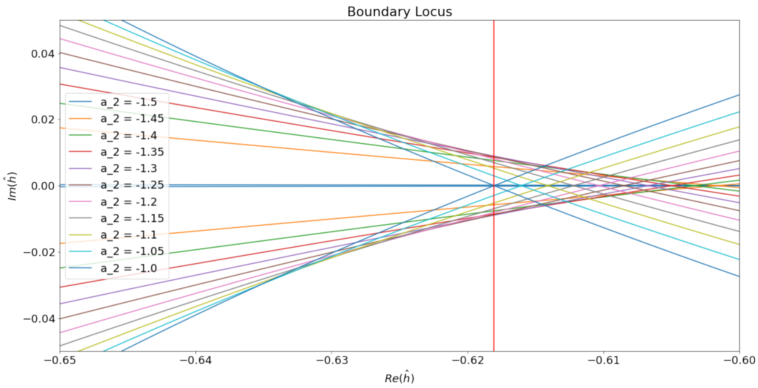


Figure 13: Boundary Locus for all possible α_2 zoomed into the lower end of Absolute stability interval

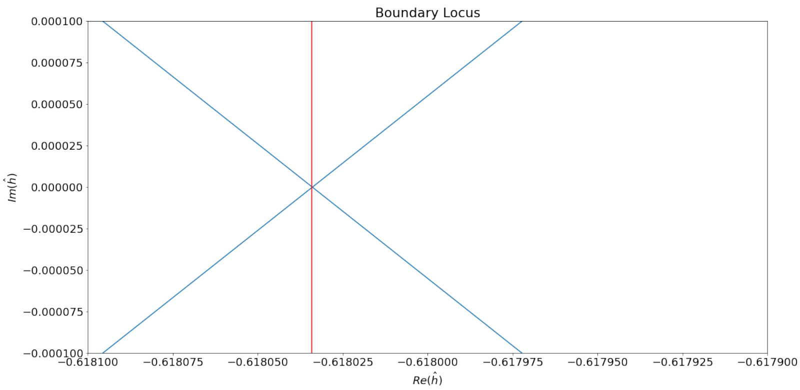


Figure 14: Boundary Locus for $\alpha_2 = -1$ zoomed into the lower end of Absolute stability interval