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.

First Name .... Marwan

Family Name......... Riach

CID 01349928

Coursework 4

Before you start working on this coursework, please read coursework wines. Fill in this page and include it as a cover sheet to your report, otherwise the coursework will not be marked. 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.* **Make sure both the report and the code are located in the directory CW4_FirstName_FamilyName_CID.**

Exercise 1 (Convergence) **% of course mark: /3.0**

Study and explain the behaviour of the AB(5) method

$$\mathbf{x}_{n+5} = \mathbf{x}_{n+4} + \frac{h}{720}\left(1901\mathbf{f}_{n+4} - 2774\mathbf{f}_{n+3} + 2616\mathbf{f}_{n+2} - 1274\mathbf{f}_{n+1} + 251\mathbf{f}_n\right)$$

for the initial value problem

$$\mathbf{x}' = \begin{pmatrix} -2 & 1 \\ s-2 & 1-s \end{pmatrix}\mathbf{x}, \quad \mathbf{x}(t_0) = [1,1]^{\mathrm{T}}, \quad t = (0, 10000h],$$

where h is the time step, and $s = 10^{17}$.

Exercise 2 (Explicit Runge–Kutta methods) **% of course mark: /3.0**

Derive the order conditions for 4-stage explicit Runge–Kutta (ERK) methods of order 4. Develop your own ERK method of order 4. Find its region and interval of absolute stability.

Exercise 3 (Implicit Runge–Kutta methods) **% of course mark: /4.0**

Derive the order conditions for 2-stage implicit Runge–Kutta (IRK) methods of order 4. Develop your own 4-stage IRK method of order 4. Find its region and interval of absolute stability.

Exercise 4 (Runge-Kutta methods for systems of ODEs) **% of course mark: /5.0**

Solve the initial value problem describing the chemical reaction of Robertson

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

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

with both ERK and IRK methods developed in Exercise 2 and 3, respectively. Use the Newton method together with the IRK method.

Exercise 5 (Runge-Kutta methods for systems of ODEs) % of course mark: /5.0★

Solve the initial value problem for the Rabinovich–Fabrikant system on a sphere of radius $r = 3$ with the IRK you have developed in Exercise 3

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

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

Use the Newton method together with the IRK method.
Recommended text: E. Hairer, C. Lubich, G. Wanner "Geometric Numerical Integration Structure-Preserving Algorithms for Ordinary Differential Equations". Berlin, Heidelberg; Springer Berlin Heidelberg. [**Chapter IV. Conservationof First Integrals and Methods on Manifolds**]

Coursework mark: % of course mark

In order to produce the plots and figures in this document, run the *exercise.m* files in the CW4 repository in MATLAB.

1 Exercise One (Convergence)

Prior to solving the initial value problem, we will establish that the AB(5) method itself is both zero-stable and consistent. This will ensure that the method is convergent. We will also compute the interval of absolute stability so that we know which h values to use for the numerical solution to the IVP. The interval of absolute stability will be obtained numerically since to obtain it analytically would require us to obtain the root of a quintic polynomial which is not able to be generalised (as shown using Galois theory which is beyond the scope of this course).

The IVP is as follows:

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x}$$

$$A = \begin{pmatrix} -2 & 1 \\ s-2 & 1-s \end{pmatrix},\ \mathbf{x_0} = \begin{pmatrix} 1 \\ 1 \end{pmatrix},\ t = (0, 10000h],\ s = 10^{17}$$

The first and second characteristic polynomials of AB(5) are:

$$\rho(r) = r^5 - r^4$$
$$\sigma(r) = \frac{1}{720}(1901r^4 - 2774r^3 + 2616r^2 - 1274r + 251)$$

For consistency, we require the following:

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

Verifying this:

$$\rho(1) = 1^5 - 1^4 = 0$$
$$\rho'(1) = 5 * 1^4 - 4 * 1^3 = 1$$
$$\sigma(1) = \frac{1}{720}(1901 * 1^4 - 2774 * 1^3 + 2616 * 1^2 - 1274 * 1 + 251) = \frac{720}{720} = 1 = \rho'(1)$$

Thus, the method is consistent. For zero-stability, we require the roots of the first characteristic polynomial to all be less than or equal to one with all roots of size one being simple. One can easily see that $\rho(r) = r^5 - r^4$ has roots 1 and 0 with order 1 and 4 respectively. Ergo, the method is zero-stable and consistent and hence convergent.

To compute the interval of absolute stability, we start by applying $x' = \lambda x$ to the AB(5) method which gives:

$$x_{n+5} = x_{n+4} + \frac{\hat{h}}{720}(1901x_{n+4} - 2774x_{n+3} + 2616x_{n+2} - 1274x_{n+1} + 251x_n)$$

This gives us the following stability polynomial:

$$p(r) = r^5 - (1 + \frac{1901\hat{h}}{720})r^4 + \frac{2774\hat{h}}{720}r^3 - \frac{2616\hat{h}}{720}r^2 + \frac{1274\hat{h}}{720}r - \frac{251\hat{h}}{720}$$

Setting it equal to zero and substitution of $r = e^{is}$ for $s \in [0, 2\pi]$ yields the following:

$$p(r) = r^5 - (1 + \frac{1901\hat{h}}{720})r^4 + \frac{2774\hat{h}}{720}r^3 - \frac{2616\hat{h}}{720}r^2 + \frac{1274\hat{h}}{720}r - \frac{251\hat{h}}{720} = 0$$
$$\Rightarrow \hat{h} = \frac{r^4 - r^5}{-\frac{1901}{720}r^4 + \frac{2774}{720}r^3 - \frac{2616}{720}r^2 + \frac{1274}{720}r - \frac{251}{720}}$$
$$\Rightarrow \hat{h} = \frac{e^{4is} - e^{5is}}{-\frac{1901}{720}e^{4is} + \frac{2774}{720}e^{3is} - \frac{2616}{720}e^{2is} + \frac{1274}{720}e^{is} - \frac{251}{720}}$$

The locus of the points for which the stability polynomial has the root $|r| = 1$ is given below:

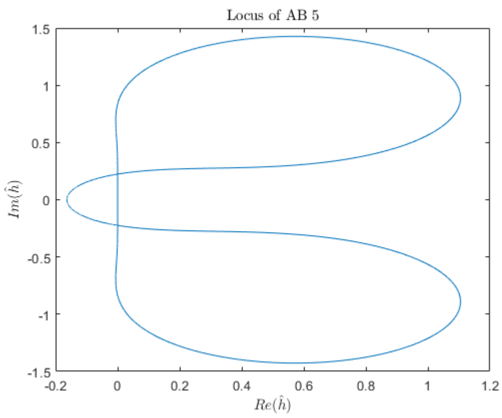


Figure 1: The locus of points for which the stability polynomial has the root $|r| = 1$

The interval of absolute stability ends where the hump appears just after -0.2 in Figure 1. Numerically according to MATLAB, the value at which the interval ends is -0.163339382937743 which is approximately $-\frac{49}{300}$. Thus, the interval of absolute stability for AB(5) is approximately $\hat{h} \in (-\frac{49}{300}, 0)$.

The eigenvalues of our matrix A are λ = -1, -s and this gives eigenvectors $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 2-s \end{pmatrix}$ respectively.

The interval of absolute stability for AB(5) is approximately $\hat{h} \in (-\frac{49}{300}, 0)$. Since the system of ODEs is of order 2, we have to find to the smallest interval of absolute stability; this will be given by the eigenvalue of -s.

When $\lambda = -s$, $\hat{h} \in (-\frac{49}{300}, 0) \Rightarrow h \in (0, \frac{49}{300s})$, and so to investigate how the global error behaves, we will investigate with time steps just inside and just outside the given interval for h.

The analytical solution to the IVP is:

$$\mathbf{x} = c_1 e^{-t}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + c_2 e^{-st}\begin{pmatrix} 1 \\ 2-s \end{pmatrix} = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix}$$

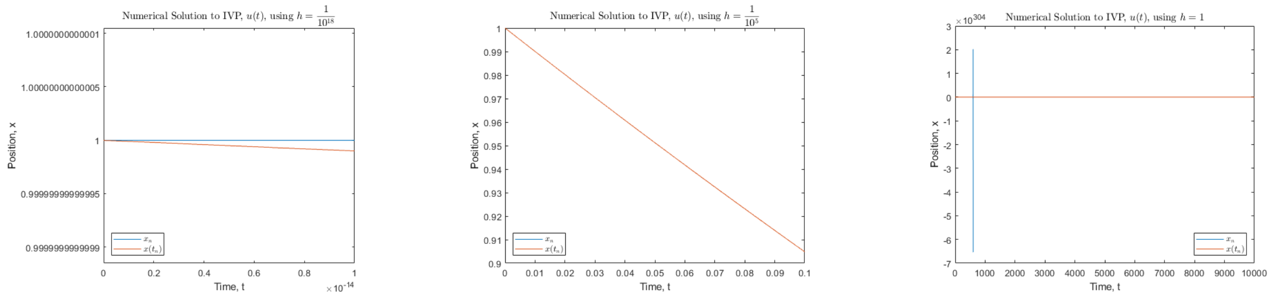
Considering the boundary conditions of the IVP, it follows that:

$$c_1 + c_2 = 1,$$
$$c_1 + (2-s)c_2 = 1,$$
$$\Rightarrow c_1 = 1, \ c_2 = 0$$

Giving us:

$$\mathbf{x} = e^{-t}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

In the *exercise1.m* file, the AB5 method has been coded and the output for three numerical solutions is given below. In order to carry out the AB5 method, the Euler method, AB2, AB3, and AB4 methods were used.



(a) $h = \frac{1}{10^{18}}$ (b) $h = \frac{1}{10^5}$ (c) $h = 1$

Figure 2: Numerical and analytical solution for $u(t)$

The interval of convergence for this IVP with AB5 is $h \in (0, \frac{49}{3 \cdot 10^{19}})$ and of the above three figures, the first is the only to lie in this interval. The reason for the apparent divergence in the solution is that a value of $h = 10^{-18}$ is extremely granular and MATLAB sees $1 + 10^{-18}$ as being equal to 1.

Despite $h = 10^{-5}$ lying outside the interval of absolute stability, there is no divergence to the solution in the time frame, $t \in [0, 0.1]$, making this the most accurate of the three solutions when using MATLAB. Were the time frame extended, divergence would become apparent.

The final figure uses the large time step $h = 1$ and divergence can clearly be seen by the blue line spiking downwards.

2 Exercise Two and Three (Implicit and Explicit RK Methods)

We will begin first with finding an implicit method of our own of order 4 and verifying this by finding the LTE of the 4-stage implicit method. This can then be used in the subsequent section to find the order conditions of explicit RK methods of order 4, since explicit RK methods are simply a special case of implicit RK methods.

In order for a RK method to be implicit, the Butcher table need only not be lower triangular. Therefore, if one element above the lower triangle is non-zero, we have ourselves an implicit RK method. The following Butcher table represents a possible 4-stage implicit RK method since $a_{44} \neq 0$. This will be the form of our derived implicit method of order 4:

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
c_2 & a_{21} & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & a_{44} \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}
$$

with

$$c_i = \sum_{j=1}^{4} a_{ij}, \; i = 1, 2, 3, 4$$

$$
\begin{aligned}
k_1 &= f(t_n, x_n) \\
k_2 &= f(t_n + c_2 h, x_n + a_{21} h k_1) \\
k_3 &= f(t_n + c_3 h, x_n + a_{31} h k_1 + a_{32} h k_2) \\
k_4 &= f(t_n + c_4 h, x_n + a_{41} h k_1 + a_{42} h k_2 + a_{43} h k_3 + a_{44} h k_4)
\end{aligned}
$$

with the method being as follows:

$$x_{n+1} = x_n + h(b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4) \tag{1}$$

We will Taylor expand (1) up to its 4th degree of h so that we can ensure the LTE is $O(h^5)$.

The double Taylor expansion of a function, f, is as follows:

$$f(t+ah,x+bh) = f(t,x) + ahf_t + bhf_x + \frac{h^2}{2}(a^2 f_{tt} + 2abf_{tx} + b^2 f_{xx})$$
$$+\frac{h^3}{6}(a^3 f_{ttt} + 3a^2 bf_{ttx} + 3ab^2 f_{txx} + b^3 f_{xxx}) + O(h^4)$$

Applying this to (1) for each individual k_i (except k_1 which is trivial) gives:

$$\begin{aligned}
k_2 = f(t_n + c_2 h, x_n + a_{21}hk_1) &= f(t,x) + c_2 hf_t + a_{21}k_1 hf_x + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2 a_{21}k_1 f_{tx} + (a_{21}k_1)^2 f_{xx}) \\
&+\frac{h^3}{6}(c_2^3 f_{ttt} + 3c_2^2 a_{21}k_1 f_{ttx} + 3c_2(a_{21}k_1)^2 f_{txx} + (a_{21}k_1)^3 f_{xxx}) + O(h^4) \\
&= f(t,x) + c_2 hf_t + a_{21}fhf_x + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2 a_{21}ff_{tx} + (a_{21}f)^2 f_{xx}) \\
&+\frac{h^3}{6}(c_2^3 f_{ttt} + 3c_2^2 a_{21}ff_{ttx} + 3c_2(a_{21}f)^2 f_{txx} + (a_{21}f)^3 f_{xxx}) + O(h^4)
\end{aligned}$$
$$= f + c_2 h(f_t + ff_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx}) + \frac{h^3}{6}(c_2^3 f_{ttt} + 3c_2^3 ff_{ttx} + 3c_2^3 f^2 f_{txx} + c_2^3 f^3 f_{xxx}) + O(h^4)$$

$$k_3 = f(t_n + c_3 h, x_n + a_{31}hk_1 + a_{32}hk_2) = f(t,x) + c_3 hf_t + (a_{31}k_1 + a_{32}k_2)hf_x + \frac{h^2}{2}(c_3^2 f_{tt} + 2c_3(a_{31}k_1 + a_{32}k_2)f_{tx}$$
$$+(a_{31}k_1 + a_{32}k_2)^2 f_{xx}) + \frac{h^3}{6}(c_3^3 f_{ttt} + 3c_3^2(a_{31}k_1 + a_{32}k_2)f_{ttx} + 3c_3(a_{31}k_1 + a_{32}k_2)^2 f_{txx} + (a_{31}k_1 + a_{32}k_2)^3 f_{xxx})$$
$$+O(h^4)$$

Substitution of $k_2 \approx f + c_2 h(f_t + ff_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx})$ where only terms up to h^4 when compounded are considered into k_3 gives:

$$k_3 = f + c_3 hf_t + (a_{31}f + a_{32}(f + c_2 hf_t + a_{21}fhf_x + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2 a_{21}ff_{tx} + (a_{21}f)^2 f_{xx})))hf_x$$
$$+\frac{h^2}{2}(c_3^2 f_{tt} + 2c_3(a_{31}f + a_{32}(f + c_2 hf_t + a_{21}fhf_x))f_{tx} + (a_{31}f + a_{32}(f + c_2 hf_t + a_{21}fhf_x))^2 f_{xx}) +$$
$$\frac{h^3}{6}(c_3^3 f_{ttt} + 3c_3^2(a_{31}f + a_{32}f)f_{ttx} + 3c_3(a_{31}f + a_{32}f)^2 f_{txx} + (a_{31}f + a_{32}f)^3 f_{xxx}) + O(h^4)$$

Using $c_2 = a_{21}$ and $c_3 = a_{31} + a_{32}$ gives:

$$k_3 = f + c_3 hf_t + (c_3 f + a_{32}(c_2 hf_t + c_2 fhf_x + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + (c_2 f)^2 f_{xx})))hf_x$$
$$+\frac{h^2}{2}(c_3^2 f_{tt} + 2c_3(c_3 f + c_2 a_{32}h(f_t + ff_x))f_{tx} + (c_3 f + c_2 a_{32}h(f_t + ff_x))^2 f_{xx}) +$$
$$\frac{h^3}{6}(c_3^3 f_{ttt} + 3c_3^3 ff_{ttx} + 3c_3^3 f^2 f_{txx} + c_3^3 f^3 f_{xxx}) + O(h^4)$$
$$= f + hc_3(f_t + ff_x) + \frac{h^2}{2}(2a_{32}c_2 f_x(f_t + ff_x) + c_3^2(f_{tt} + 2ff_{tx} + f^2 f_{xx})) + \frac{h^3}{6}((6c_2 c_3 a_{32}f_t + (6c_2 c_3 a_{32} + 3a_{32}c_2^2)ff_x)ff_{xx}$$
$$+(6c_3 c_2 a_{32}f_t + (6c_3 c_2 a_{32} + 6a_{32}c_2^2)ff_x)f_{tx} + 3a_{32}c_2^2 f_x f_{tt} + c_3^3(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx})) + O(h^4)$$

For k_4, we will substitute in k_1, k_2, k_3 up to their second order where appropriate and we will plug in k_4 up to h^2 where suitable and do this recursively until we have obtained all terms up to and including h^3. We will also make use of the fact that $c_4 = a_{41} + a_{42} + a_{43} + a_{44}$, $k_2 \approx f + c_2 h(f_t + ff_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx})$, and $k_3 \approx f + hc_3(f_t + ff_x) + h^2(a_{32}c_2 f_x(f_t + ff_x) + \frac{c_3^2}{2}(f_{tt} + 2ff_{tx} + f^2 f_{xx}))$:

$$
\begin{aligned}
k_4 = f(t_n + c_4h, x_n + a_{41}hk_1 + a_{42}hk_2 + a_{43}hk_3 + a_{44}hk_4) = f(t,x) + c_4hf_t + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)hf_x \\
+\frac{h^2}{2}(c_4^2 f_{tt} + 2c_4(a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)f_{tx} + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)^2 f_{xx}) \\
+\frac{h^3}{6}(c_4^3 f_{ttt} + 3c_4^2(a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)f_{ttx} + 3c_4(a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)^2 f_{txx} \\
+(a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)^3 f_{xxx}) + O(h^4) \\
= f + c_4hf_t + (a_{41}f + a_{42}(f + c_2h(f_t + ff_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx})) + a_{43}(f + hc_3(f_t + ff_x) + \\
h^2(a_{32}c_2f_x(f_t + ff_x) + \frac{c_3^2}{2}(f_{tt} + 2ff_{tx} + f^2 f_{xx}))) + a_{44}(f + c_4hf_t + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)hf_x \\
+\frac{h^2}{2}(c_4^2 f_{tt} + 2c_4(a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)f_{tx} + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 + a_{44}k_4)^2 f_{xx})))hf_x \\
+\frac{h^2}{2}(c_4^2 f_{tt} + 2c_4(a_{41}f + a_{42}(f + c_2h(f_t + ff_x)) + a_{43}(f + hc_3(f_t + ff_x)) + a_{44}(f + c_4hf_t + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 \\
+a_{44}k_4)hf_x))f_{tx} + (a_{41}f + a_{42}(f + c_2h(f_t + ff_x)) + a_{43}(f + hc_3(f_t + ff_x)) + a_{44}(f + c_4hf_t + (a_{41}k_1 + a_{42}k_2 + a_{43}k_3 \\
+a_{44}k_4)hf_x))^2 f_{xx}) + \frac{h^3}{6}(c_4^3 f_{ttt} + 3c_4^3 ff_{ttx} + 3c_4^3 f^2 f_{txx} + c_4^3 f^3 f_{xxx}) + O(h^4)
\end{aligned}
$$

$$
\begin{aligned}
= f + c_4hf_t + (a_{41}f + a_{42}(f + c_2h(f_t + ff_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx})) + a_{43}(f + hc_3(f_t + ff_x) + \\
h^2(a_{32}c_2f_x(f_t + ff_x) + \frac{c_3^2}{2}(f_{tt} + 2ff_{tx} + f^2 f_{xx}))) + a_{44}(f + c_4hf_t + (a_{41}f + a_{42}(f + c_2h(f_t + ff_x)) \\
+a_{43}(f + hc_3(f_t + ff_x)) + a_{44}(f + c_4hf_t + c_4fhf_x))hf_x + \frac{h^2}{2}(c_4^2 f_{tt} + 2c_4^2 ff_{tx} + c_4^2 f^2 f_{xx})))hf_x \\
+\frac{h^2}{2}(c_4^2 f_{tt} + 2c_4(a_{41}f + a_{42}(f + c_2h(f_t + ff_x)) + a_{43}(f + hc_3(f_t + ff_x)) + a_{44}(f + c_4hf_t + fc_4hf_x))f_{tx} \\
+(c_4^2 f^2 + 2hfc_4(f_t + ff_x)(c_2a_{42} + c_3a_{43} + c_4a_{44}))f_{xx}) + \frac{h^3}{6}(c_4^3 f_{ttt} + 3c_4^3 ff_{ttx} + 3c_4^3 f^2 f_{txx} + c_4^3 f^3 f_{xxx}) + O(h^4)
\end{aligned}
$$

Collecting the terms by the coefficients of h^p we obtain the following:

$$
\begin{aligned}
k_4 = f + h(c_4(f_t + ff_x)) + \frac{h^2}{2}(2f_x(f_t + ff_x)(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + \frac{c_4^2}{2}(f_{tt} + 2f_{tx}f + f^2 f_{xx})) \\
+\frac{h^3}{6}(c_4^3(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx}) + 6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)(f_t + ff_x)(f_{tx} + ff_{xx}) + \\
3(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2)f_x(f_{tt} + 2ff_{tx} + f^2 f_{xx}) + 6(a_{43}a_{32}c_2 + a_{44}(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_x^2(f_t + ff_x)) + O(h^4)
\end{aligned}
$$

$$
\begin{aligned}
k_4 = f + h(c_4(f_t + ff_x)) + \frac{h^2}{2}(2f_x(f_t + ff_x)(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + \frac{c_4^2}{2}(f_{tt} + 2f_{tx}f + f^2 f_{xx})) \\
+\frac{h^3}{6}(c_4^3(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx}) \\
+(6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)f_t + (6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + 3(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))ff_x)ff_{xx} + \\
(6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)f_t + (6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + 6(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))ff_x)f_{tx} \\
+3(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2)f_xf_{tt} + \\
6(a_{43}a_{32}c_2 + a_{44}(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_x^2(f_t + ff_x)) + O(h^4)
\end{aligned}
$$

From lecture 15, we know that the Taylor expansion of the exact solution is given by:

$$
x(t_{n+1}) = x(t_n) + hf + \frac{h^2}{2}(f_t + ff_x) + \frac{h^3}{6}(f_{tt} + 2f_{tx}f + f_{xx}f^2 + f_x(f_t + f_xf)) + O(h^4)
$$

In order to verify that our method will be of order 4, we will need to expand the above Taylor expansion to a further degree of accuracy, so that the residue is $O(h^5)$. This will involve differentiating the h^3 term, using the chain rule and partial derivatives rule. The coefficient of $\frac{h^4}{24}$ is as follows:

$$f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx} + f_{xx}(3ff_t + 3f^2 f_x) + f_{tx}(3f_t + 5ff_x) + f_{tt}f_x + f_x^2(f_t + ff_x)$$

This then makes the Taylor expansion of the exact solution:

$$x(t_{n+1}) = x(t_n) + hf + \frac{h^2}{2}(f_t + ff_x) + \frac{h^3}{6}(f_{tt} + 2f_{tx}f + f_{xx}f^2 + f_x(f_t + f_x f))$$
$$+\frac{h^4}{24}(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx} + 3ff_{xx}(f_t + ff_x) + f_{tx}(3f_t + 5ff_x) + f_{tt}f_x + f_x^2(f_t + ff_x)) + O(h^5)$$

The local truncation error is given by:

$$x(t_{n+1}) - x_{n+1}$$

Plugging in the k values into $x_{n+1} = x_n + h(b_1k_1 + b_2k_2 + b_3k_3 + b_4k_4)$ yields:

$$x_n + hb_1f + b_2(fh + c_2h^2(f_t + ff_x) + \frac{h^3}{2}(c_2^2 f_{tt} + 2c_2^2 ff_{tx} + c_2^2 f^2 f_{xx}) + \frac{h^4}{6}(c_2^3 f_{ttt} + 3c_2^3 ff_{ttx} + 3c_2^3 f^2 f_{txx} + c_2^3 f^3 f_{xxx}))$$
$$+b_3(fh + h^2 c_3(f_t + ff_x) + \frac{h^3}{2}(2a_{32}c_2 f_x(f_t + ff_x) + c_3^2(f_{tt} + 2ff_{tx} + f^2 f_{xx}))+$$
$$\frac{h^4}{6}((6c_2c_3a_{32}f_t + (6c_2c_3a_{32} + 3a_{32}c_2^2)ff_x)ff_{xx} + (6c_3c_2a_{32}f_t + (6c_3c_2a_{32} + 6a_{32}c_2^2)ff_x)f_{tx} + 3a_{32}c_2^2 f_x f_{tt}$$
$$+c_3^3(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx})))$$
$$+b_4(fh + h^2(c_4(f_t + ff_x)) + \frac{h^3}{2}(2f_x(f_t + ff_x)(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + \frac{c_4^2}{2}(f_{tt} + 2f_{tx}f + f^2 f_{xx}))$$
$$+\frac{h^4}{6}(c_4^3(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx})$$
$$+(6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)f_t + (6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + 3(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))ff_x)ff_{xx}+$$
$$(6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)f_t + (6c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + 6(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))ff_x)f_{tx}$$
$$+3(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2)f_x f_{tt}+$$
$$6(a_{43}a_{32}c_2 + a_{44}(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_x^2(f_t + ff_x))) + O(h^5)$$

Tidying up the above expression by grouping together the terms by the degree of h gives:

$$= x_n + h(b_1 + b_2 + b_3 + b_4)f + h^2(b_2c_2 + b_3c_3 + b_4c_4)(f_t + ff_x)$$
$$+\frac{h^3}{2}((b_2c_2^2 + b_3c_3^2 + b_4c_4^2)(f_{tt} + 2f_{tx}f + f^2 f_{xx}) + (2a_{32}b_3c_2 + 2b_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_x(f_t + ff_x))$$
$$+\frac{h^4}{6}((b_2c_2^3 + b_3c_3^3 + b_4c_4^3)(f_{ttt} + 3ff_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx})$$
$$+((6b_3c_2c_3a_{32} + 6b_4c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_t + (6b_3c_2c_3a_{32} + 3b_3a_{32}c_2^2 + 6b_4c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4)$$
$$+3b_4(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2)ff_x)ff_{xx}) + ((6b_3c_3c_2a_{32} + 6b_4c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_t$$
$$+(6b_3c_3c_2a_{32} + 6b_3a_{32}c_2^2 + 6b_4c_4(a_{42}c_2 + a_{43}c_3 + a_{44}c_4) + 6b_4(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))ff_x)f_{tx}$$
$$+(3a_{32}b_3c_2^2 + 3b_4(a_{42}c_2^2 + a_{43}c_3^2 + a_{44}c_4^2))f_x f_{tt} + 6b_4(a_{43}a_{32}c_2 + a_{44}(a_{42}c_2 + a_{43}c_3 + a_{44}c_4))f_x^2(f_t + ff_x)))$$

Comparing the coefficients of the IRK with the Taylor expansion and equating them produces the following order conditions:

$$
\begin{aligned}
b_1+b_2+b_3+b_4 &= 1,\\
b_2c_2+b_3c_3+b_4c_4 &= \frac{1}{2},\\
b_2c_2^2+b_3c_3^2+b_4c_4^2 &= \frac{1}{3},\\
a_{32}b_3c_2+b_4(a_{42}c_2+a_{43}c_3+a_{44}c_4) &= \frac{1}{6},\\
b_2c_2^3+b_3c_3^3+b_4c_4^3 &= \frac{1}{4},\\
b_3c_2c_3a_{32}+b_4c_4(a_{42}c_2+a_{43}c_3+a_{44}c_4) &= \frac{1}{8},\\
a_{32}b_3c_2^2+b_4(a_{42}c_2^2+a_{43}c_3^2+a_{44}c_4^2) &= \frac{1}{12},\\
b_4(a_{43}a_{32}c_2+a_{44}(a_{42}c_2+a_{43}c_3+a_{44}c_4)) &= \frac{1}{24}
\end{aligned}
$$

The following Butcher tableau gives a 4-stage IRK method that satisfies the above conditions. The coefficients were derived by fixing $a_{44}=1$ and then choosing the b and c values so that the first and second order conditions were met. The other values were then chosen to satisfy the remaining order conditions, working backwards:

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{3} & 0 & 0 & 0\\
\frac{2}{3} & -\frac{1}{3} & 1 & 0 & 0\\
1 & 1 & 0 & -1 & 1\\
\hline
 & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8}
\end{array}
$$

The order conditions for 4-stage explicit RK methods can be easily derived from the aforementioned conditions by setting $a_{44}=0$ as setting this to zero gives the standard form of an explicit 4-stage RK method:

$$
\begin{aligned}
1st: b_1+b_2+b_3+b_4 &= 1,\\
2nd: b_2c_2+b_3c_3+b_4c_4 &= \frac{1}{2},\\
3rd: b_2c_2^2+b_3c_3^2+b_4c_4^2 &= \frac{1}{3},\\
a_{32}b_3c_2+b_4(a_{42}c_2+a_{43}c_3) &= \frac{1}{6},\\
4th: b_2c_2^3+b_3c_3^3+b_4c_4^3 &= \frac{1}{4},\\
b_3c_2c_3a_{32}+b_4c_4(a_{42}c_2+a_{43}c_3) &= \frac{1}{8},\\
a_{32}b_3c_2^2+b_4(a_{42}c_2^2+a_{43}c_3^2) &= \frac{1}{12},\\
b_4a_{43}a_{32}c_2 &= \frac{1}{24}
\end{aligned}
$$

The following Butcher tableau gives a 4-stage ERK method that satisfies the above conditions. The coefficients were derived by fixing b_4, a_{43}, a_{32}, c_2 and ensuring that none of them were zero and that they satisfied the final condition and then working backwards:

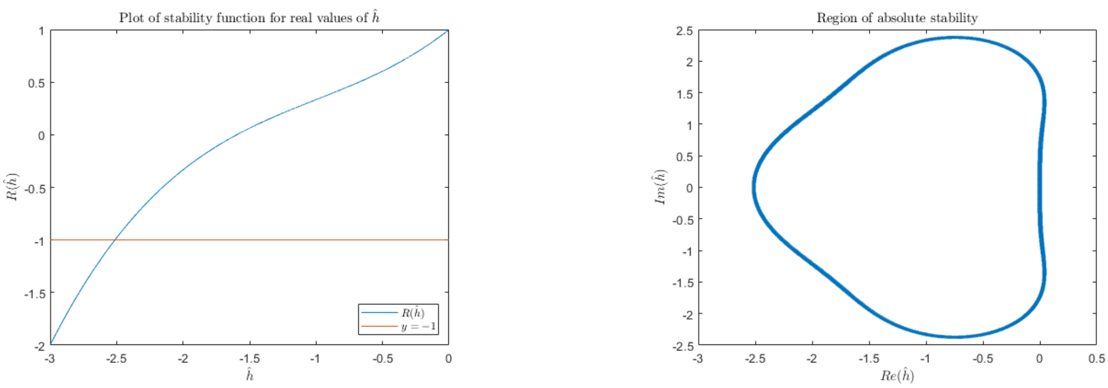
$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{3} & \frac{1}{6} & 0 & 0\\
1 & 0 & -2 & 3 & 0\\
\hline
 & \frac{1}{6} & -\frac{1}{3} & 1 & \frac{1}{6}
\end{array}
$$

Starting first with our 4-stage implicit RK method, the region and interval of absolute stability can be obtained by applying the method to the equation $x' = \lambda x$.

$$\begin{aligned}
k_1 &= f(t_n, x_n),\\
k_2 &= f(t_n + \frac{h}{3}, x_n + \frac{h}{3}k_1),\\
k_3 &= f(t_n + \frac{2h}{3}, x_n - \frac{h}{3}k_1 + hk_2),\\
k_4 &= f(t_n + h, x_n + hk_1 - hk_3 + hk_4),\\
x_{n+1} &= x_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4)
\end{aligned}$$

$$\begin{aligned}
k_1 &= \lambda x_n,\\
k_2 &= \lambda(x_n + \frac{h}{3}\lambda x_n),\\
k_3 &= \lambda(x_n - \frac{h}{3}\lambda x_n + h(\lambda(x_n + \frac{h}{3}\lambda x_n))),\\
k_4 &= \lambda(x_n + h\lambda x_n - h\lambda(x_n - \frac{h}{3}\lambda x_n + h(\lambda(x_n + \frac{h}{3}\lambda x_n))) + hk_4),\\
k_4 &= \frac{\lambda(x_n + h\lambda x_n - h\lambda(x_n - \frac{h}{3}\lambda x_n + h(\lambda(x_n + \frac{h}{3}\lambda x_n))))}{1-\hat{h}}, \hat{h} := h\lambda\\
x_{n+1} &= x_n + \frac{hx_n}{8}(\lambda + 3(\lambda + \lambda^2\frac{h}{3}) + 3(\lambda - \frac{h}{3}\lambda^2 + h\lambda^2 + \frac{h^2}{3}\lambda^3) + \frac{(\lambda + h\lambda^2 - h(\lambda^2 - \frac{h}{3}\lambda^3 + h(\lambda^3 + \frac{h}{3}\lambda^4))}{1-\hat{h}})\\
x_{n+1} &= x_n + \frac{x_n}{8}(7\hat{h} + 3\hat{h}^2 + \hat{h}^3 + \frac{(\hat{h} - \frac{2}{3}\hat{h}^3 - \frac{1}{3}\hat{h}^4)}{1-\hat{h}})\\
x_{n+1} &= x_n(1 + \frac{1}{8}(7\hat{h} + 3\hat{h}^2 + \hat{h}^3 + \frac{(\hat{h} - \frac{2}{3}\hat{h}^3 - \frac{1}{3}\hat{h}^4)}{1-\hat{h}})) = R(\hat{h})x_n
\end{aligned}$$

The interval of absolute stability is the set of real $\hat{h}$ such that $|R(\hat{h})| < 1$ and the region is the area in the complex plane for which $|R(\hat{h})| < 1$. The plots below show the interval and region. The first plot shows how we found the point at which the interval of absolute stability ends, since it is the point of intersection. $\hat{h} \in (-2.52985, 0)$ is the interval of absolute stability for our implicit RK method.



(a) Finding the stability interval

(b) Region of absolute stability

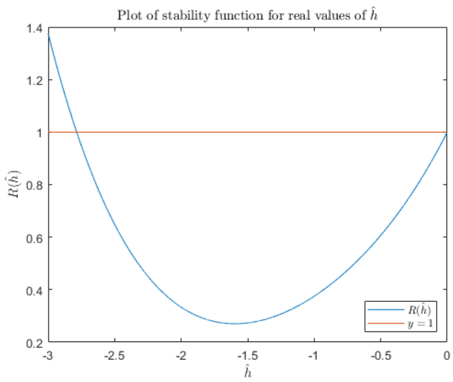
Figure 3: Method to find interval of absolute stability and locus plot of region of absolute stability

Now we consider our 4-stage explicit RK method. The region and interval of absolute stability can be obtained by applying the method to the equation $x' = \lambda x$.

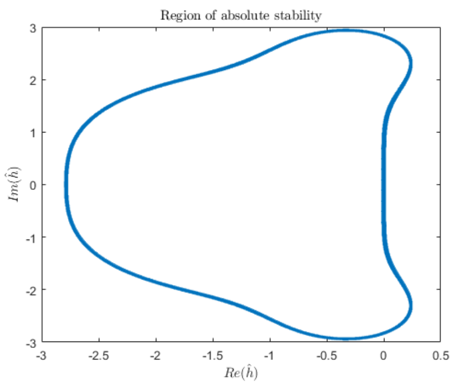
$$\begin{aligned} k_1 &= f(t_n, x_n), \\ k_2 &= f(t_n + \frac{h}{2}, x_n + \frac{h}{2}k_1), \\ k_3 &= f(t_n + \frac{h}{2}, x_n + \frac{h}{3}k_1 + \frac{h}{6}k_2), \\ k_4 &= f(t_n + h, x_n - 2hk_2 + 3hk_3), \\ x_{n+1} &= x_n + \frac{h}{6}(k_1 - 2k_2 + 6k_3 + k_4) \end{aligned}$$

$$k_1 = \lambda x_n,$$
$$k_2 = \lambda(x_n + \frac{h}{2}\lambda x_n),$$
$$k_3 = \lambda(x_n + \frac{h}{3}\lambda x_n + \frac{h}{6}(\lambda(x_n + \frac{h}{2}\lambda x_n))) = \lambda(x_n + \frac{h}{2}\lambda x_n + \frac{h^2}{12}\lambda^2 x_n),$$
$$k_4 = \lambda(x_n - 2h\lambda(x_n + \frac{h}{2}\lambda x_n) + 3h\lambda(x_n + \frac{h}{2}\lambda x_n + \frac{h^2}{12}\lambda^2 x_n)),$$
$$x_{n+1} = x_n + \frac{hx_n}{6}(\lambda - 2(\lambda + \lambda^2\frac{h}{2}) + 6(\lambda + \frac{h}{2}\lambda^2 + \frac{h^2}{12}\lambda^3) + \lambda - 2h\lambda^2(1 + \frac{h}{2}\lambda) + 3h\lambda^2(1 + \frac{h}{2}\lambda + \frac{h^2}{12}\lambda^2))$$
$$x_{n+1} = x_n + \frac{x_n}{6}(6\hat{h} + 3\hat{h}^2 + \hat{h}^3 + \frac{1}{4}\hat{h}^4)$$
$$x_{n+1} = x_n(1 + \hat{h} + \frac{1}{2}\hat{h}^2 + \frac{1}{6}\hat{h}^3 + \frac{1}{24}\hat{h}^4) = R(\hat{h})x_n$$

The interval of absolute stability is the set of real $\hat{h}$ such that $|R(\hat{h})| < 1$ and the region is the area in the complex plane for which $|R(\hat{h})| < 1$. The plots below show the interval and region. The first plot shows how we found the point at which the interval of absolute stability ends, since it is the point of intersection. $\hat{h} \in (-2.79268, 0)$ is the interval of absolute stability for our explicit RK method.



(a) Finding the stability interval



(b) Region of absolute stability

Figure 4: Method to find interval of absolute stability and locus plot of region of absolute stability

In Butcher Tableau form, the standard 2-stage implicit RK method is as follows:

$$\begin{array}{c|cc} c_1 & a_{11} & a_{12} \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array}$$

To derive the order 4 conditions, we will Taylor expand k_1 and k_2 up to $O(h^4)$ and then ensure that the coefficients are equivalent to the Taylor expansion of the exact solution contained herein.

$$k_1 = f(t_n + c_1 h, x_n + a_{11}hk_1 + a_{12}hk_2) = f + h(c_1 f_t + (a_{11}k_1 + a_{12}k_2)f_x) + \frac{h^2}{2}(c_1^2 f_{tt} + 2c_1(a_{11}k_1 + a_{12}k_2)f_{tx}$$
$$+(a_{11}k_1 + a_{12}k_2)^2 f_{xx}) + \frac{h^3}{6}(c_1^3 f_{ttt} + 3c_1^2(a_{11}k_1 + a_{12}k_2)f_{ttx} + 3c_1(a_{11}k_1 + a_{12}k_2)^2 f_{txx} + (a_{11}k_1 + a_{12}k_2)^3 f_{xxx})$$
$$+O(h^4)$$

$$k_2 = f(t_n + c_2 h, x_n + a_{21}hk_1 + a_{22}hk_2) = f + h(c_2 f_t + (a_{21}k_1 + a_{22}k_2)f_x) + \frac{h^2}{2}(c_2^2 f_{tt} + 2c_2(a_{21}k_1 + a_{22}k_2)f_{tx}$$
$$+(a_{21}k_1 + a_{22}k_2)^2 f_{xx}) + \frac{h^3}{6}(c_2^3 f_{ttt} + 3c_2^2(a_{21}k_1 + a_{22}k_2)f_{ttx} + 3c_2(a_{21}k_1 + a_{22}k_2)^2 f_{txx} + (a_{21}k_1 + a_{22}k_2)^3 f_{xxx})$$
$$+O(h^4)$$

Now we will substitute k_1 and k_2 up to order h^p such that all terms up to and including h^3 are covered. We will begin with k_1:

$$k_1 = f + h(c_1 f_t + c_1 f f_x) + h^2((a_{11}c_1 + a_{12}c_2)(f_t + f_x f)f_x)$$
$$+h^3((a_{11}(c_1 a_{11} + c_2 a_{12}) + a_{12}(c_1 a_{21} + c_2 a_{22}))(f_t + f f_x)f_x^2 + \frac{1}{2}(c_1^2 a_{11} + c_2^2 a_{12})(f_{tt} + 2f f_{tx} + f^2 f_{xx})f_x)$$
$$+$$
$$\frac{h^2}{2}(c_1^2 f_{tt} + 2c_1^2 f f_{tx} + c_1^2 f^2 f_{xx}) + \frac{h^3}{2}(2c_1(a_{11}c_1 + a_{12}c_2)(f_t + f f_x)f_{tx} + 2c_1 f(a_{11}c_1 + a_{12}c_2)(f_t + f f_x)f_{xx})$$
$$+$$
$$\frac{h^3}{6}(c_1^3(f_{ttt} + 3f f_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx}))$$
$$+$$
$$O(h^4)$$

Grouping together the terms by their degree of h gives:

$$k_1 = f + hc_1(f_t + f f_x) + \frac{h^2}{2}(2(a_{11}c_1 + a_{12}c_2)(f_t + f_x f)f_x + c_1^2(f_{tt} + 2f f_{tx} + f^2 f_{xx}))+$$
$$\frac{h^3}{6}(c_1^3(f_{ttt} + 3f f_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx}) + 6c_1(a_{11}c_1 + a_{12}c_2)(f_t + f f_x)f_{tx} + 6c_1(a_{11}c_1 + a_{12}c_2)(f_t + f f_x)f f_{xx}+$$
$$6(a_{11}(c_1 a_{11} + c_2 a_{12}) + a_{12}(c_1 a_{21} + c_2 a_{22}))(f_t + f f_x)f_x^2 + 3(c_1^2 a_{11} + c_2^2 a_{12})(f_{tt} + 2f f_{tx} + f^2 f_{xx})f_x)$$

By symmetry, k_2 can be written as follows:

$$k_2 = f + hc_2(f_t + f f_x) + \frac{h^2}{2}(2(a_{21}c_1 + a_{22}c_2)(f_t + f_x f)f_x + c_2^2(f_{tt} + 2f f_{tx} + f^2 f_{xx}))+$$
$$\frac{h^3}{6}(c_2^3(f_{ttt} + 3f f_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx}) + 6c_2(a_{21}c_1 + a_{22}c_2)(f_t + f f_x)f_{tx} + 6c_2(a_{21}c_1 + a_{22}c_2)(f_t + f f_x)f f_{xx}+$$
$$6(a_{21}(c_1 a_{11} + c_2 a_{12}) + a_{22}(c_1 a_{21} + c_2 a_{22}))(f_t + f f_x)f_x^2 + 3(c_1^2 a_{21} + c_2^2 a_{22})(f_{tt} + 2f f_{tx} + f^2 f_{xx})f_x)$$

Comparing $x_{n+1} = x_n + h(b_1k_1 + b_2k_2)$ with the Taylor expansion of the exact solution gives the following order conditions:

$$
\begin{gathered}
1st : b_1 + b_2 = 1, \\
2nd : b_1c_1 + b_2c_2 = \frac{1}{2}, \\
3rd : b_1c_1^2 + b_2c_2^2 = \frac{1}{3}, \\
b_1(a_{11}c_1 + a_{12}c_2) + b_2(a_{21}c_1 + a_{22}c_2) = \frac{1}{6}, \\
4th : b_1c_1^3 + b_2c_2^3 = \frac{1}{4}, \\
b_1c_1(a_{11}c_1 + a_{12}c_2) + b_2c_2(a_{21}c_1 + a_{22}c_2) = \frac{1}{8}, \\
b_1(c_1^2a_{11} + c_2^2a_{12}) + b_2(c_1^2a_{21} + c_2^2a_{22}) = \frac{1}{12}, \\
b_1(a_{11}(c_1a_{11} + c_2a_{12}) + a_{12}(c_1a_{21} + c_2a_{22})) + b_2(a_{21}(c_1a_{11} + c_2a_{12}) + a_{22}(c_1a_{21} + c_2a_{22})) = \frac{1}{24}
\end{gathered}
$$

If the above order conditions are satisfied, then a 2-stage implicit RK method will be of order 4. Running the $exercise2and3.m$ file will produce the figures in this section.

3 Exercise Four (RK methods for systems of ODEs)

The IVP is as follows:

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

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

The Explicit LMM used is as follows:

$$
\begin{gathered}
k_1 = f(t_n, x_n), \\
k_2 = f(t_n + \frac{h}{2}, x_n + \frac{h}{2}k_1), \\
k_3 = f(t_n + \frac{h}{2}, x_n + \frac{h}{3}k_1 + \frac{h}{6}k_2), \\
k_4 = f(t_n + h, x_n - 2hk_2 + 3hk_3), \\
x_{n+1} = x_n + \frac{h}{6}(k_1 - 2k_2 + 6k_3 + k_4)
\end{gathered}
$$

$$
\mathbf{x_n} = \begin{pmatrix} x_n \\ y_n \\ z_n \end{pmatrix}, \quad \mathbf{f_n} = \begin{pmatrix} -0.04x_n + 10^4y_nz_n \\ 0.04x_n - 10^4y_nz_n - 3 \cdot 10^7y_n^2 \\ 3 \cdot 10^7y_n^2 \end{pmatrix}, \quad \mathbf{x_0} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
$$

The solution to the IVP using the ERK method is given below. A 3D plot was avoided since the y component is miniscule relative to the others.

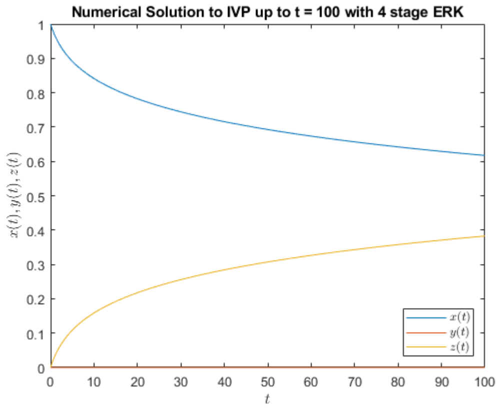


Figure 5: ERK solution to the IVP using $h = 10^{-4}$

The Implicit LMM used is as follows:

$$\begin{aligned}
k_1 &= f(t_n, x_n),\\
k_2 &= f(t_n + \frac{h}{3}, x_n + \frac{h}{3}k_1),\\
k_3 &= f(t_n + \frac{2h}{3}, x_n - \frac{h}{3}k_1 + hk_2),\\
k_4 &= f(t_n + h, x_n + hk_1 - hk_3 + hk_4),\\
x_{n+1} &= x_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4)
\end{aligned}$$

As the method is implicit, we will require the Newton method to obtain the value of k_4 which in this instance has three elements since our IVP has three dimensions. We will denote the ith element of k_4 as $k_4(i)$. Up to k_4, all k values are explicit and so in the context of finding k_4 they, along with x_n, are constants. We will denote all terms in f except for k_4 as a constant, a, with components a_1, a_2 and a_3 ($a = x_n + hk_1 - hk_3$). Furthermore, since at no point is f dependent on t, we will consider f as only taking in one argument.

The $\mathbf{F}$ in our Newton method is given as:

$$\mathbf{F}(k_4) = k_4 - f(a + hk_4) = \begin{pmatrix} k_4(1) \\ k_4(2) \\ k_4(3) \end{pmatrix} - f\begin{pmatrix} a_1 + hk_4(1) \\ a_2 + hk_4(2) \\ a_3 + hk_4(3) \end{pmatrix}$$
$$= \begin{pmatrix} k_4(1) + 0.04(a_1 + hk_4(1)) - 10^4(a_2 + hk_4(2))(a_3 + hk_4(3)) \\ k_4(2) - 0.04(a_1 + hk_4(1)) + 10^4(a_2 + hk_4(2))(a_3 + hk_4(3)) + 3 \cdot 10^7(a_2 + hk_4(2))^2 \\ k_4(3) - 3 \cdot 10^7(a_2 + hk_4(2))^2 \end{pmatrix}$$

The Jacobian matrix, $\mathbf{F}'(k_4)$, is computed by taking the partial derivatives of $\mathbf{F}$ with respect to $k_4(1), k_4(2)$ and $k_4(3)$. The matrix is as follows:

$$\mathbf{F}'(k_4) = \begin{pmatrix} 1 + 0.04h & -10^4h(a_3 + hk_4(3)) & -10^4h(a_2 + hk_4(2)) \\ -0.04h & 1 + 10^4h(a_3 + hk_4(3)) + 6 \cdot 10^7h(a_2 + hk_4(2)) & 10^4h(a_2 + hk_4(2)) \\ 0 & -6 \cdot 10^7h(a_2 + hk_4(2)) & 1 \end{pmatrix}$$

This thus makes the Newton method:

$$k_4^{i+1} = k_4^i - \mathbf{F}'(k_4^i)^{-1}\mathbf{F}(k_4^i), \; i = 0, 1, 2, ..., M.$$

To execute the implicit method with the Newton method we require an initial guess, k_4^0. Consider the following:

$$k_4 = f(t_n + h, x_n + hk_1 - hk_3 + hk_4) \approx f(t_n + h, x_n + hk_1 - hk_3 + hf(t_n, x_n)) = f(t_n + h, x_n + 2hk_1 - hk_3)$$

We will therefore estimate our value of k_4 for k_4^0 as $f(t_n + h, x_n + 2hk_1 - hk_3)$ which we know the value of.

To speed up the implementation of the algorithm we will add a stopping criterion with a tolerance of $\epsilon = 10^{-5}$ to stop us always having to iterate through M times for each time step.

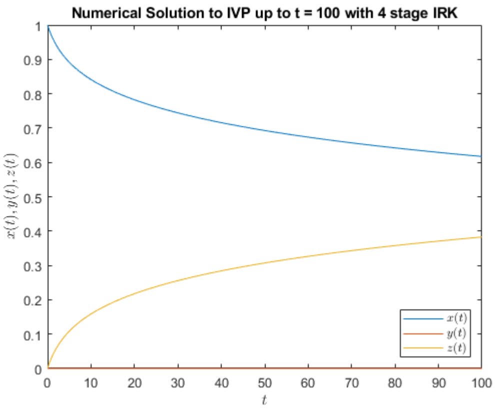


Figure 6: IRK solution to the IVP using $h = 10^{-4}$ and $M = 5$

Both solutions given by the two methods are identical, corroborating the strength of each of them. Running the $exercise4.m$ file will produce the figures in this section.

4 Exercise Five (RK methods for systems of ODEs - Mastery)

The IVP is as follows:

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

$$x(0) = -1,\ y(0) = 0,\ z(0) = 0.5,\ t \in [0, 50]$$

$$\alpha = 1.1,\ \gamma = 0.87$$

The Implicit LMM used is as follows:

$$\begin{aligned} k_1 &= f(t_n, x_n), \\ k_2 &= f(t_n + \frac{h}{3}, x_n + \frac{h}{3}k_1), \\ k_3 &= f(t_n + \frac{2h}{3}, x_n - \frac{h}{3}k_1 + hk_2), \\ k_4 &= f(t_n + h, x_n + hk_1 - hk_3 + hk_4), \\ x_{n+1} &= x_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4) \end{aligned}$$

$$\mathbf{x_n} = \begin{pmatrix} x_n \\ y_n \\ z_n \end{pmatrix}, \quad \mathbf{f_n} = \begin{pmatrix} y_n(z_n - 1 + x_n^2) + \gamma x_n \\ x_n(3z_n + 1 - x_n^2) + \gamma y_n \\ -2z_n(\alpha + x_n y_n) \end{pmatrix}, \quad \mathbf{x_0} = \begin{pmatrix} -1 \\ 0 \\ 0.5 \end{pmatrix}$$

As this method is implicit, we will require the Newton method to obtain the value k_4. This IRK method is the same as in question 4 so we will proceed in the same way, accounting for the different f in this question.

The $\mathbf{F}$ in our Newton method is given as:

$$\mathbf{F}(k_4) = k_4 - f(a + hk_4) = \begin{pmatrix} k_4(1) \\ k_4(2) \\ k_4(3) \end{pmatrix} - f\begin{pmatrix} a_1 + hk_4(1) \\ a_2 + hk_4(2) \\ a_3 + hk_4(3) \end{pmatrix}$$
$$= \begin{pmatrix} k_4(1) - (a_2 + hk_4(2))(a_3 + hk_4(3) - 1 + (a_1 + hk_4(1))^2) - \gamma(a_1 + hk_4(1)) \\ k_4(2) - (a_1 + hk_4(1))(3a_3 + 3hk_4(3) + 1 - (a_1 + hk_4(1))^2) - \gamma(a_2 + hk_4(2)) \\ k_4(3) + 2(a_3 + hk_4(3))(\alpha + (a_1 + hk_4(1))(a_2 + hk_4(2))) \end{pmatrix}$$

The Jacobian matrix, $\mathbf{F}'(k_4)$, is computed by taking the partial derivatives of $\mathbf{F}$ with respect to $k_4(1), k_4(2)$ and $k_4(3)$. The matrix is as follows. As the matrix entries are long, this has been split up into the first two columns and the last column:

$$\begin{pmatrix} 1 - 2h(a_2 + hk_4(2))(a_1 + hk_4(1)) - \gamma h & -h(a_3 + hk_4(3) - 1 + (a_1 + hk_4(1))^2) \\ h(2(a_1 + hk_4(1))^2 - (3a_3 + 3hk_4(3) + 1 - (a_1 + hk_4(1)^2)) & 1 - \gamma h \\ 2(a_3 + hk_4(3))(ha_2 + k_4(2)) & 2(a_3 + hk_4(3))(ha_1 + k_4(1)) \end{pmatrix}$$

$$\begin{pmatrix} -h(a_2 + hk_4(2)) \\ -3h(a_1 + hk_4(1)) \\ 1 + 2h(\alpha + (a_1 + hk_4(1))(a_2 + hk_4(2))) \end{pmatrix}$$

This thus makes the Newton method:

$$k_4^{i+1} = k_4^i - \mathbf{F}'(k_4^i)^{-1}\mathbf{F}(k_4^i), \ i = 0, 1, 2, ..., M.$$

The initial value, k_4^0, is derived using the same method as in exercise 4.

Now that we have our implicit method tailored to this IVP, we can attempt to solve this IVP on a sphere of radius 3 which we will determine. To do this, we will consider algorithm 4.2 from Chapter IV of "Geometric Numerical Integration Structure Preserving Algorithms for Ordinary Differential Equations". This necessitates that our initial value lies on the manifold (which in this case is a sphere of radius 3).

The general equation of a sphere or radius 3 is as follows:

$$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = 3^2$$

Given our initial values, if we choose x_0, y_0 and z_0 as below, then our initial condition will lie on the manifold and ergo algorithm 4.2 will be applicable:

$$(x + 1)^2 + (y - 3)^2 + (z - 0.5)^2 = 3^2$$

The algorithm is executed by marching forwards one step using our IRK method and then projecting that result on the above sphere. The projection we consider will project the line connecting the result to the centre of the sphere. This involves finding the length of the vector, scaling the vector so that the length is equal to the radius of the sphere, and then finally changing back to the original coordinate system in order to obtain the projection. This is then repeated for however many steps are in the entire algorithm. Solutions for a method with and without projection onto a sphere are given overleaf.

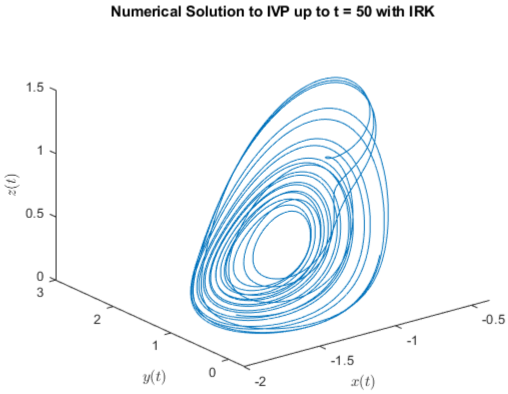


Figure 7: IRK solution to the IVP using $h = 10^{-4}$ and $M = 5$ with no projection

The Rabinovich–Fabrikant equations with the given parameters and initial conditions exhibit chaotic behaviour, as can be seen in Figure 7. Figure 8 shows the sphere onto which the solution is projected which is represented by the red line.

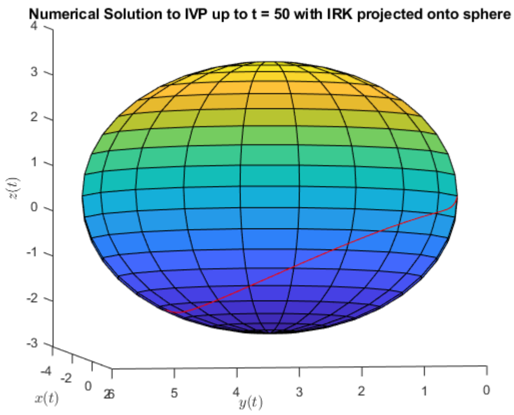


Figure 8: IRK solution to the IVP using $h = 10^{-4}$ and $M = 5$ with each step being projected onto a sphere. The red line in Figure 8 represents the solution projected onto the sphere