Simulation Methods Problem Set 2

Leonardo Bocchi

March 26, 2023

Exercise 1
In order to integrate $y' = f(x, y)$ we want to use a Runge-Kutta method of the form

$$y_{n+1} = y_n + h(c_1 k_1 + c_2 k_2)$$

with

$$k_1 = f(x_n + a_h, y_n + hak_1), \quad k_2 = f(x_n + b_h, y_n + hbk_1)$$

1. Using what we have seen in the theoretical part, determine which relations have to satisfy the coefficients a, b, c_1, c_2 in order to have global order of convergence equal to 3.
2. Find the regions of stability corresponding to these methods.
3. (optional) Determine which methods are stable.

1.
For the Runge-Kutta method to have global order of convergence equal to 3, it needs to satisfy the following

$$|y(x_n + h) - y_{n+1}| \leq Kh^4$$

Meaning that the error is of the order $\mathcal{O}(h^4)$. We can start by doing a Taylor expansion of $y(x_n + h)$ which assumes the following form

$$y(x_n + h) = y_n + hf + \frac{h^2}{2}(f_x + f_y f) + \frac{h^3}{6}(f_{xx} + 2f_{xy} + f_{yy} f^2) + \frac{h^3}{6}(f_y f_x + f_y^2 f) + \mathcal{O}(h^4)$$

We now want to apply the same expansion to point y_{n+1} defined by the given Runge-Kutta method. To do so, we have to expand the terms k_1 and k_2 which are the application of f to the point (x_n, y_n) with an increment of ah and bh respectively. Since this is an implicit Runge-Kutta method, when taking derivatives the k_1 gives more derivatives of f itself, but of one order greater than the instance before.
By expanding k_1 and k_2 we obtain the following expressions

$$k_1 = fah(f_x + f_y f) + a^2 h^2 (f_y f_x + f_y^2 f) + \frac{a^2 h^2}{2}(f_{xx} + 2f(xy)f + f_{yy} f^2) + \mathcal{O}(h^3)$$
$$k_2 = f + bh(f_x + f_y f) + abh^2 (f_y f_x + f_y^2 f) + \frac{b^2 h^2}{2}(f_{xx} + 2f_{xy} f + f_{yy} f^2) + \mathcal{O}(h^3)$$

Substituting these into the expression of y_{n+1} of the Runge-Kutta method we obtain the following

$$y_{n+1} = y_n + h(c_1 + c_2)f + h^2(c_1 a + c_2 b)(f_x + f_y f) +$$
$$+ \frac{h^3}{2}(c_1 a^2 + c_2 b^2)(f_{xx} + 2f_{xy} f + f_{yy} f^2) + h^3(c_1 a^2 + c_2 ab)(f_y f_x + f_y^2 f) + \mathcal{O}(h^4)$$

By comparing it with the Taylor expansion of $y(x_n + h)$ we can subtract term by term such that each term of order $\mathcal{O}(h^3)$ or higher is canceled out, and the error $|y(x_n + h) - y_{n+1}|$ is of the order $\mathcal{O}(h^4)$
By doing so, we obtain the following restrictions for the parameters a, b, c_1, c_2

$$c_1 + c_2 = 1$$
$$c_1 a + c_2 b = \frac{1}{2}$$
$$c_1 a^2 + c_2 b^2 = \frac{1}{3}$$
$$c_1 a^2 + c_2 ab = \frac{1}{6}$$

Which results in the following values for the parameters

$$c_1 = \frac{3}{4},\ c_2 = \frac{1}{4},\ a = \frac{1}{3},\ b = 1$$

2.

To find the region of stability of this Runge-Kutta method, we can consider the Cauchy problem

$$y' = f(x, y)$$
$$y(0) = y_0$$

Which has a solution of the form

$$y(x) = y_0 e^{\lambda x}$$

With $\lambda \in \mathbb{C}$. In this case, we have that we can write k_1 and k_2 as

$$k_1 = \lambda(y_n + ahK_1) = \lambda(y_n + \frac{1}{3}hk_1)$$
$$k_2 = \lambda(y_n + bhk_1) = \lambda(y_n + hk_1)$$

From which we can obtain k_1 and k_2

$$k_1 = \frac{3\lambda}{3 - \lambda h} y_n$$
$$k_2 = \frac{\lambda(3 + 2\lambda h)}{3 - \lambda h} y_n$$

So now we can write y_{n+1} by substituting the values of k_1 and k_2

$$y_{n+1} = y_n + h\left(\frac{3}{4}\frac{3\lambda}{3 - \lambda h} y_n + \frac{1}{4}\frac{\lambda(3 + 2\lambda h)}{3 - \lambda h} y_n\right) = \left(\frac{4(3 - \lambda h) + 9\lambda h + \lambda h(3 + 2\lambda h)}{4(3 - \lambda h)}\right) y_n =$$

$$= \frac{12 + 5\lambda h + 3\lambda h + 2\lambda^2 h^2}{4(3 - \lambda h)} y_n = \frac{12 + 8\lambda h + 2\lambda^2 h^2}{4(3 - \lambda h)} y_n = \frac{6 + 4\lambda h + \lambda^2 h^2}{2(3 - \lambda h)} y_n$$

This makes it easy to see that the method will be stable, meaning the numerical solution remains bounded for $n \to \infty$ if the absolute value of the coefficient in front of y_n is less than 1

$$\left|\frac{6 + 4\lambda h + \lambda^2 h^2}{2(3 - \lambda h)}\right| < 1$$

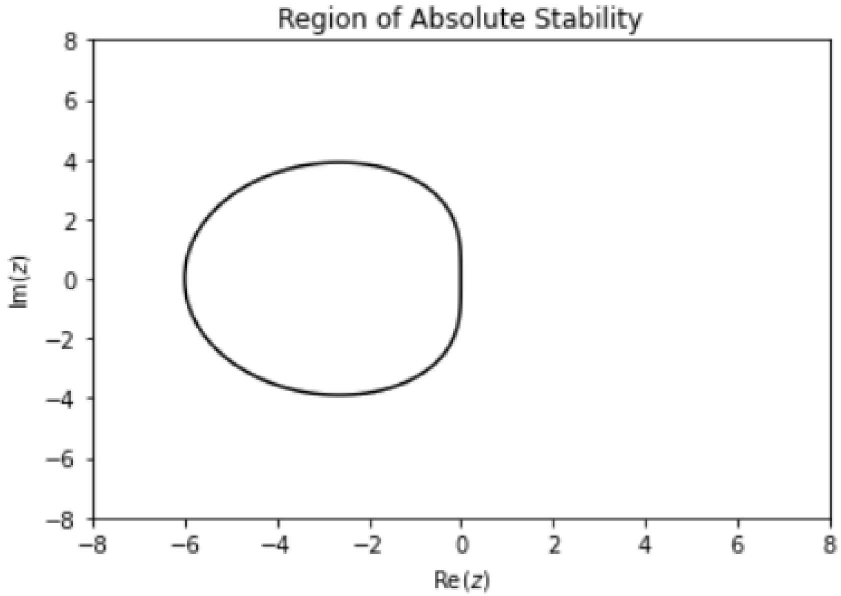
The region of stability is thus defined as the values of $\lambda \in \mathbb{C}$ that satisfy the above-obtained inequality.

3.

To determine which methods are stable, we need to analyze the regions of stability of each method. We can visualize the region of stability defined in point 2 using, for example, the following python program,

```python
import numpy as np
import matplotlib.pyplot as plt

# Define the stability function
R = lambda z: abs((6 + 4*z + z**2)/(2*(3 - z)))

# Define the real and imaginary ranges for z
ZR = np.linspace(-8, 8, 100)
ZI = np.linspace(-8, 8, 100)
ZH = np.empty((len(ZI), len(ZR)), dtype=complex)
for i, zi in enumerate(ZI):
    for j, zr in enumerate(ZR):
        ZH[i, j] = zr + 1j*zi

# Evaluate the stability function on a grid of z values
STAB = np.empty((len(ZI), len(ZR)))
for i, zi in enumerate(ZI):
    for j, zr in enumerate(ZR):
        STAB[i, j] = R(ZH[i, j])

# Create a contour plot of the stability function
plt.contourf(ZR, ZI, STAB, levels=[0, 1], colors=['white', 'gray'])
plt.contour(ZR, ZI, STAB, levels=[0, 1], colors='k')

# Add title and labels
plt.title('Region of Absolute Stability')
plt.xlabel(r'$\mathrm{Re}(z)$')
plt.ylabel(r'$\mathrm{Im}(z)$')

# Show the plot
plt.show()
```

Which outputs the visualization of the stability region



Region of Absolute Stability
8
6
4
2
0
−2
−4
−6
−8
Im(z)
−8
−6
−4
−2
0
2
4
6
8
Re(z)