Abstract

This document corresponds to the solution of the second list of exercises in the Simulation Methods course.

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

$$k_1 = f(x_n + ah, y_n + hak_1), \quad k_2 = f(x_n + bh, y_n + hbk_1).$$

(a) 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.

(b) Find the regions of stability corresponding to these methods.

(c) (optional) Determine which methods are stable.

Proof. Let us start by solving *(a)*. In order to have a global order of convergence equal to 3, we need the following:

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

We need to compute the Taylor expansion of y_{n+1} as a function of h and compare it with the Taylor expansion of the real solution evaluated in $x_n + h$, i.e., the Taylor expansion of $y(x_n + h)$. Let us start with the Taylor expansion of y_{n+1}. To proceed, we will compute separately the Taylor expansions of k_1 and k_2.

$$\begin{aligned} k_1 = \Bigg[& f(x_n, y_n) + h \left(f_x(x_n + ah, y_n + ahk_1)a + f_y(x_n + ah, y_n + ahk_1) \left(ak_1 + ha\frac{dk_1}{dh} \right) \right) + \\ & \frac{h^2}{2} \Bigg(a^2 f_{xx}(x_n + ah, y_n + ahk_1) + 2a^2 \left(k_1 + h\frac{dk_1}{dh} \right) f_{xy}(x_n + ah, y_n + ahk_1) + \\ & f_{yy}(x_n + ah, y_n + ahk_1) \left(ak_1 + ha\frac{dk_1}{dh} \right)^2 + \\ & f_y(x_n + ah, y_n + ahk_1) \left(2a\frac{dk_1}{dh} + ha\frac{d^2k_1}{dh^2} \right) \Bigg) + \mathcal{O}(h^3) \Bigg] \Bigg|_{h=0} . \end{aligned}$$

where f_x and f_y are the partial derivative of f with respect the variables x and y respectively. Now, we are going to evaluate at $h = 0$ and we will skip the point in which f is evaluated since will be always the same, (x_n, y_n). The last expresion becomes:

$$k_1 = f + ha(f_x + f_y f) + \frac{h^2}{2} \left(a^2 f_{xx} + 2a^2 k_1 f_{xy} + a^2 k_1^2 f_{yy} + 2a \left(\frac{dk_1}{dh} \right) f_y \right) + \mathcal{O}(h^3).$$

Notice that still needs to be added the derivative of k_1 evaluated at $h = 0$. Finally, we obtain the following expression:

$$k_1 = f + ah(f_x + f_y f) + a^2 h^2 (f_y f_x + f_y^2 f) + \frac{a^2 h^2}{2} \left(f_{xx} + 2f_{xy} f + f_{yy} f^2 \right) + \mathcal{O}(h^3).$$

Similarly, we can compute the Taylor expansion of k_2. Notice that

$$k_2 = f + hb(f_x + f_y f) + \frac{h^2}{2}\left(b^2 f_{xx} + 2b^2 k_1 f_{xy} + b^2 k_1^2 f_{yy} + 2b\left(\frac{dk_1}{dh}\right) f_y\right) + \mathcal{O}(h^3).$$

Again, adding the Taylor expression of k_1 and its derivative, we obtain the following.

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

Finally, notice that the Taylor expansions of y_{n+1} as a function of h have the following form:

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

We have to compare this with the Taylor expansion of $y(x_n + h)$, i.e.,

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

Therefore, comparing these terms, we obtain that

$$||y(x_n + h) - y_{n+1}|| \leqslant Kh^4 \iff \begin{cases} c_1 + c_2 = 1 \\ c_1 a + c_2 b = \frac{1}{2} \\ c_1 a^2 + c_2 ab = \frac{1}{6} \\ \frac{1}{2}(c_1 a^2 + c_2 b^2) = \frac{1}{6} \end{cases}$$

The solution of the system of equations is $a = \frac{1}{3}, b = 1, c_1 = \frac{3}{4}$ and $c_2 = \frac{1}{4}$.

Let us continue with exercise *(b)*. We need to compare our method with the solution of the Cauchy problem

$$\begin{cases} \dot{y} = \lambda y \\ y(0) = y_0 \end{cases}$$

Notice that, setting $f(x, y) = \lambda y$, we can obtain an expression for k_1 and k_2.

$$k_1 = \lambda(y_n + hak_1) \iff k_1 = \frac{\lambda y_n}{1 - \lambda ha},$$

$$k_2 = \lambda(y_n + hbk_1) \iff k_2 = \lambda y_n\left(1 + \frac{\lambda hb}{1 - \lambda ha}\right).$$

All together,

$$y_{n+1} = y_n + c_1 h\left(\frac{\lambda y_n}{1 - \lambda ha}\right) + c_2 h\lambda y_n\left(1 + \frac{\lambda hb}{1 - \lambda ha}\right).$$

Let us define a complex variable $z := \lambda h$. The above equation can be written as follows:

$$y_{n+1} = y_n\left[1 + \left(\frac{c_1 z}{1 - za}\right) + c_2 z\left(1 + \frac{zb}{1 - za}\right)\right].$$

In this way, defining $R(z) := 1 + \left(\frac{c_1 z}{1-za}\right) + c_2 z\left(1 + \frac{zb}{1-za}\right)$, the stability region is given by the set $S = \{z \in \mathbb{C}; |R(z)| \leqslant 1\}$. To get an idea of what this region is (using the previous coefficients), we have implemented a small python code (attached in the delivery) that shows the region, see Figure 1.

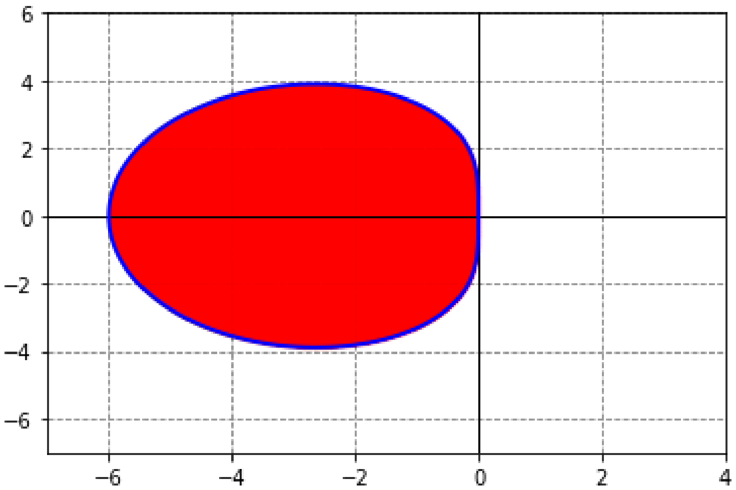

Figure 1: Stability region of the previous method.

Let us finish this exercise by solving *(c)*. Recall that a method is said to be stable if for $z \in \mathbb{C}$, $\{\mathrm{Re}(z) < 0\} \subseteq S$. Notice that, if we choose $z = -7$, using the previous method, $\mathrm{Re}(z) < 0$ but $R(-7) \approx 1.35$, i.e., $|R(-7)| > 1$, thus $z \notin S$. We can conclude that the previous method is not stable. $\square$

Exercise 2 *(optional) Consider the Runge method of order 3:*

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

Compute the error when one uses this method to integrate the Cauchy problem $x''+x = 0, x(0) = 1, x'(0) = 1$ from $t = 0$ until $t = 1$ and step h small, using the following procedure:

(a) Define the complex variable $z = x + ix'$ and write the Cauchy problem and the method of Runge using this variable.

(b) Compute n iterates of this method with stepsize $h = 1/n$.

(c) If we define $r_k = |z_k|$ and $\theta_k = Arg(z_k)$, prove that

$$r_n = a_0 + a_1 h^m + \mathcal{O}(h^m), \quad Arg(z_n) = b_0 + b_1 h^s + \mathcal{O}(h^s)$$

giving the values of the constants a_0, a_1, b_0, b_1, m and s.

(d) If $z(t) = x(t) + ix'(t)$ is the solution of the Cauchy problem and $r(t) = |z(t)|$, $\theta(t) = Arg(z(t))$, compute $r(1) - r_n$ and $\theta(1) - \theta_n$ as functions of $h = 1/n$.

Proof. Let us start by solving *(a)*. Making the proposed change of variables $z = x + ix'$, we can see that $x = z - ix'$ and $x' = z' - ix''$. Since $x'' = -x$, $x' = z' + ix$ and substituting this into the first equation, we obtain that $x = z - ix' = z - i(z' + ix) = z - iz' + x$. Therefore, $z - iz' = 0$. Regarding the initial condition, notice that $z(0) = x(0) + ix'(0) = 1$. Our Cauchy problem is

$$\begin{cases} z' = -iz := f(t, z) \\ z(0) = 1 \end{cases}$$

Now, let us apply the same change of variable to the Runge-Kutta method. Notice that the proposed Runga-Kutta has the following associated scheme:

$$z_{n+1} = z_n + \frac{h}{6}(k_1 + 4k_2 + k_4),$$

where

$$\begin{aligned} k_1 &= f(t_n, z_n), & k_2 &= f(t_n + \frac{h}{2}, z_n + \frac{h}{2}k_1) \\ k_3 &= f(t_n + h, z_n + hk_2), & k_4 &= f(t_n + h, z_n + hk_3) \end{aligned}$$

where $t_0 = 0$ and $z_0 = 1$. Notice that

$$\begin{aligned} k_1 &= -iz_n \\ k_2 &= f\left(\frac{h}{2}, \left(1 - \frac{hi}{2}\right) z_n\right) = \left(-i - \frac{h}{2}\right) z_n \\ k_3 &= f\left(h, \left(1 - hi - \frac{h^2}{2}\right) z_n\right) = \left(-i - h + \frac{ih^2}{2}\right) z_n \\ k_4 &= f\left(h, \left(1 - hi - h^2 + \frac{ih^3}{2}\right) z_n\right) = \left(-i - h + ih^2 + \frac{h^3}{2}\right) z_n \end{aligned}$$

Finally, the method becomes

$$z_{n+1} = z_n + \left(\frac{h}{6}(-6i - 3h + ih^2 + h^3/2)\right) z_n = \left(1 - hi - \frac{h^2}{2} + \frac{ih^3}{6} + \frac{h^4}{12}\right) z_n.$$

This finish the proof of *(a)*. Let us continue with *(b)*. We want to compute n iterates of this method with stepsize $h = 1/n$. Notice that the previous equation becomes:

$$z_{n+1} = \left(1 - \frac{i}{n} - \frac{1}{2n^2} + \frac{i}{6n^3} + \frac{1}{12n^4}\right) z_n.$$

Therefore, n iterates of this method with stepsize $h = 1/n$ lead to the following iterative scheme

$$z_n = \left(1 - \frac{i}{n} - \frac{1}{2n^2} + \frac{i}{6n^3} + \frac{1}{12n^4}\right)^n z_0 = \left(1 - \frac{i}{n} - \frac{1}{2n^2} + \frac{i}{6n^3} + \frac{1}{12n^4}\right)^n$$

since $z_0 = 1$.

I skip *(c)* and *(d)* since the whole exercise was optional.

□