ODE – Explicit Runge-Kutta methods - example

First-order initial value problem

We want to approximate the solution $\mathbf{Y}(x)$ of a system of first-order ordinary differential equations

$$\mathbf{Y}'(x) = \mathbf{F}(x, \mathbf{Y}(x)) \quad \text{with an initial condition } \mathbf{Y}(x_0) = \mathbf{Y}^{(0)}, \tag{1}$$

where

$$\mathbf{Y}(x) = \begin{bmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_n(x) \end{bmatrix}, \mathbf{Y}'(x) = \begin{bmatrix} y_1'(x) \\ y_2'(x) \\ \vdots \\ y_n'(x) \end{bmatrix}, \mathbf{F}(x, \mathbf{Y}) = \begin{bmatrix} f_1(x, y_1, y_2, \ldots, y_n) \\ f_2(x, y_1, y_2, \ldots, y_n) \\ \vdots \\ f_n(x, y_1, y_2, \ldots, y_n) \end{bmatrix}$$

Explicit Runge-Kutta methods

- numerical one step methods for finding an approximation of the solution, using explicit formulas (there is no need to solve any equations). Moreover, there is no need to compute any derivatives of the function $\mathbf{F}$ – instead, at every step, repeated function evaluations at different points are used only.

Euler's method

The simplest and least accurate method (first-order accuracy) is Euler's method, which extrapolates the derivative at the starting point of each interval to find the next function value:

- choose a step size h
- for $i = 0, 1, 2, \ldots$
  1. compute the derivative $\mathbf{K}$ of the vector function $\mathbf{Y}$ as
     $\mathbf{K} = \mathbf{F}(x_i, \mathbf{Y}^{(i)})$
  2. compute
     $x_{i+1} = x_i + h$
     $\mathbf{Y}^{(i+1)} = \mathbf{Y}^{(i)} + h\,\mathbf{K}$

Midpoint (or Collatz) method

An example of a second-order Runge-Kutta method (with second-order accuracy) is midpoint method, also called Collatz method. First, initial derivative at the starting point of each interval is used to find a trial point halfway across the interval. Second, this midpoint derivative is computed and used to make step across the full length of the interval. The trial midpoint is discarded once its derivative has been calculated and used.

- choose a step size h
- for $i = 0, 1, 2, \ldots$
  1. compute the trial midpoint $[x_p, \mathbf{Y}_p]$ using Euler's method with $\frac{1}{2}h$:

     $\mathbf{K}_1 = \mathbf{F}(x_i,\, \mathbf{Y}^{(i)})$

     $x_p = x_i + \frac{1}{2}h$

     $\mathbf{Y}_p = \mathbf{Y}^{(i)} + \frac{1}{2}h\,\mathbf{K}_1$
  2. compute the derivative $\mathbf{K}_2$ at the trial midpoint $[x_p, \mathbf{Y}_p]$ as

     $\mathbf{K}_2 = \mathbf{F}(x_p,\, \mathbf{Y}_p)$
  3. compute $\mathbf{Y}^{(i+1)}$ using derivative at the trial midpoint:

     $x_{i+1} = x_i + h$

     $\mathbf{Y}^{(i+1)} = \mathbf{Y}^{(i)} + h\,\mathbf{K}_2$

The classical fourth-order Runge-Kutta method (RK4)

This is the most often used, fourth-order, Runge-Kutta formula. It uses three trial points to make a guess of the direction, which is then used to make step across the full length of the interval. These trial points are discarded once their derivatives have been calculated and used.

- choose a step size h
- for $i = 0, 1, 2, \ldots$
  1. compute the first trial midpoint $[x_p, \mathbf{Y}_p]$ using Euler's method
     with step size $\frac{1}{2}h$:

     $\mathbf{K}_1 = \mathbf{F}(x_i,\, \mathbf{Y}^{(i)})$

     $x_p = x_i + \frac{1}{2}h$

     $\mathbf{Y}_p = \mathbf{Y}^{(i)} + \frac{1}{2}h\,\mathbf{K}_1$
  2. compute the second trial midpoint $[x_p, \mathbf{Y}_q]$, using the derivative
     at the first trial midpoint $[x_p, \mathbf{Y}_p]$ and a step size $\frac{1}{2}h$:

     $\mathbf{K}_2 = \mathbf{F}(x_p,\, \mathbf{Y}_p)$

     $\mathbf{Y}_q = \mathbf{Y}^{(i)} + \frac{1}{2}h\,\mathbf{K}_2$
  3. compute trial endpoint $[x_{i+1}, \mathbf{Y}_e]$, using the derivative
     at the second trial midpoint $[x_p, \mathbf{Y}_q]$ and a step size h:

     $\mathbf{K}_3 = \mathbf{F}(x_p,\, \mathbf{Y}_q)$

     $\mathbf{Y}_e = \mathbf{Y}^{(i)} + h\,\mathbf{K}_3$
  4. compute $\mathbf{Y}^{(i+1)}$ using weighted average of derivatives
     at the initial point and at all three trial points:

     $x_{i+1} = x_i + h$

     $\mathbf{K}_4 = \mathbf{F}(x_{i+1},\, \mathbf{Y}_e)$

     $\mathbf{Y}^{(i+1)} = \mathbf{Y}^{(i)} + \frac{1}{6}h\,(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4)$

Example 1 - from the previous tutorial, with RK4 added

Consider Cauchy problem $\quad y' = \dfrac{y}{x^2}\,, \quad y(1) = 2\ .$

Compute an approximate value of $y(1.4)$ using RK4 with step sizes $h = 0.2$ and $h = 0.4$ and compare its performance with previous results summarized in the first four columns of Table 1: exact solution, Euler's method with step size $h = 0.1$ and midpoint method with step size $h = 0.2$.

Solution

Computation for $h = 0.2,\ x_0 = 1,\ y_0 = 2$:

- $\mathbf{i = 0}$

  1. $k_1 = \dfrac{y_0}{(x_0)^2} = \dfrac{2}{1^2} = 2$

     $x_p = x_0 + \frac{1}{2}h = 1 + 0.1 = 1.1$

     $y_p = y_0 + \frac{1}{2}h\,k_1 = 2 + 0.1 \cdot 2 = 2.2$
  2. $k_2 = \dfrac{y_p}{(x_p)^2} = \dfrac{2.2}{1.1^2} = 1.8182$

     $y_q = y_0 + \frac{1}{2}h\,k_2 = 2 + 0.1 \cdot 1.8182 = 2.1818$
  3. $k_3 = \dfrac{y_q}{(x_p)^2} = \dfrac{2.1818}{1.1^2} = 1.8032$

     $y_e = y_0 + h\,k_3 = 2 + 0.2 \cdot 1.8032 = 2.3606$
  4. $k_4 = \dfrac{y_e}{(x_1)^2} = \dfrac{2.3606}{1.2^2} = 1.6393$

     $x_1 = x_0 + h = 1 + 0.2 = 1.2$

     $y_1 = y_0 + \frac{1}{6}h\,(k_1 + 2k_2 + 2k_3 + k_4) =$

     $= 2 + \frac{1}{30} \cdot (2 + 2 \cdot 1.8182 + 2 \cdot 1.8032 + 1.6393) = 2.3627$

     $y(1.2)$ is approximately equal to $y_1 = 2.3627$.
     This is the second value at the fifth column.

- $\mathbf{i = 1}$

  1. $k_1 = \dfrac{y_1}{(x_1)^2} = \dfrac{2.3627}{1.2^2} = 1.6408$

     $x_p = x_1 + \frac{1}{2}h = 1.2 + 0.1 = 1.3$

     $y_p = y_1 + \frac{1}{2}h\,k_1 = 2.3627 + 0.1 \cdot 1.6408 = 2.5268$
  2. $k_2 = \dfrac{y_p}{(x_p)^2} = \dfrac{2.5268}{1.3^2} = 1.4952$

     $y_q = y_1 + \frac{1}{2}h\,k_2 = 2.3627 + 0.1 \cdot 1.4952 = 2.5122$

3. $k_3 = \dfrac{y_q}{x_p^2} = \dfrac{2.5122}{1.3^2} = 1.4865$

   $y_e = y_1 + h\, k_3 = 2.3627 + 0.2 \cdot 1.4865 = 2.6600$

4. $k_4 = \dfrac{y_e}{(x_2)^2} = \dfrac{2.6600}{1.4^2} = 1.3572$

   $x_2 = x_1 + h = 1.2 + 0.2 = 1.4$

   $y_2 = y_1 + \frac{1}{6}h\,(k_1 + 2k_2 + 2k_3 + k_4) =$

   $= 2.3627 + \frac{1}{30} \cdot (1.6408 + 2 \cdot 1.4952 + 2 \cdot 1.4865 + 1.3572) = 2.6614$

   $y(1.4)$ is approximately equal to $y_2 = 2.6614$. The last two values at fifth column are computed by the same process for $i = 2$ and $i = 3$.

Using above process with $h = 0.4$ we obtain values presented at the last column of Table 1.

Our results show that midpoint method gives more precise solution than Euler's method, even in the case when double step size is used (which represents comparable work, because within every step the derivative is computed twice). RK4 method gives the best results, even in the case when quadruple step size is used (which represents comparable work, because within every step the derivative is computed four times).

x_i	exact $y(x_i)$	$h = 0.1$ Euler's y_i	$h = 0.2$ midpoint y_i	$h = 0.2$ RK4 y_i	$h = 0.4$ RK4 y_i
1	2.0000	2.0000	2.0000	2.0000	2.0000
1.1	2.1903	2.2000			
1.2	2.3627	2.3818	2.3636	2.3627	
1.2	2.5191	2.5472			
1.4	2.6614	2.6979	2.6628	2.6614	2.6617
1.5	2.7912	2.8356			
1.6	2.9100	2.9616	2.9115	2.9100	
1.7	3.0190	3.0773			
1.8	3.1192	3.1838	3.1209	3.1193	3.1196

Table 1: **Example 1**. The first column represents values of x, where the approximate solution is computed. At the second column there is exact solution, the third column presents approximate solution obtained by Euler's method with step size $h = 0.1$, at the fourth column there is midpoint method with the step size $h = 0.2$ and the last two columns present approximate solution obtained by RK4 method with step sizes $h = 0.2$ and $h = 0.4$, respectively.

Appendix – Optional

The idea behind the RK methods - illustration on 2-nd order explicit methods

Let us consider the equation $y' = f(x,y)$.
The 2-nd order RK methods have a general form of

$$\begin{aligned} x_{i+1} &= x_i + h \\ y_{i+1} &= y_i + h\,(a_1 k_1 + a_2 k_2)\,, \end{aligned}$$

where

$$\begin{aligned} k_1 &= f(x_i, y_i) \\ k_2 &= f(x_i + p_1 h, y_i + q_{11} k_1\, h)\,. \end{aligned}$$

For the midpoint method, $a_1 = 0,\ a_2 = 1,\ p_1 = q_{11} = \frac{1}{2}$.

The **midpoint** method is of the 2-nd order, because it has the *Local Truncation Error (LTE)* of order $\mathcal{O}(h^3)$ (local and global truncation errors and order of method will be discussed in more detail later).

The question is: Is there any other **explicit RK method of the 2-nd order**, i.e. with LTE of order $\mathcal{O}(h^3)$?

Let $y(x)$ be the exact solution given by the initial condition $y(x_i) = y_i$.
The first three terms of the Taylor expansion are

$$y(x_i + h) = y(x_i) + y'(x_i)\,h + \frac{1}{2}\,y''(x_i)\,h^2 + \mathcal{O}(h^3).$$

Using $y'' = \dfrac{\mathrm{d}y'}{\mathrm{d}x} = \dfrac{\mathrm{d}f(x,y(x))}{\mathrm{d}x} = \dfrac{\partial f}{\partial x} + \dfrac{\partial f}{\partial y}\dfrac{\mathrm{d}y}{\mathrm{d}x}$ (chain rule) and $\dfrac{\mathrm{d}y}{\mathrm{d}x} = f$ leads to

$$y(x_i + h) = y_i + f(x_i,y_i)\,h + \frac{1}{2}\left(\frac{\partial f}{\partial x}(x_i,y_i) + \frac{\partial f}{\partial y}(x_i,y_i)\,f(x_i,y_i)\right)\,h^2 + \mathcal{O}(h^3). \quad (2)$$

The term k_2 can be written using Taylor expansion in 2 variables as
$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1\, h) = f(x_i,y_i) + \dfrac{\partial f}{\partial x}(x_i,y_i)\,p_1 h + \dfrac{\partial f}{\partial y}(x_i,y_i)\,q_{11} k_1\, h + \mathcal{O}(h^2)$,
which together with $k_1 = f(x_i,y_i)$ can be substituted to the RK formula as

$$\begin{aligned} y_{i+1} &= y_i + h\,(a_1 k_1 + a_2 k_2) \\ &= y_i + h\,(a_1 f(x_i,y_i) + a_2[f(x_i,y_i) + \frac{\partial f}{\partial x}(x_i,y_i)\,p_1 h + \frac{\partial f}{\partial y}(x_i,y_i)\,q_{11} f(x_i,y_i)\,h + \mathcal{O}(h^2)]) \\ &= y_i + h\,(a_1 + a_2) f(x_i,y_i) + h^2\left(a_2\,p_1 \frac{\partial f}{\partial x}(x_i,y_i) + a_2\,q_{11} f(x_i,y_i)\frac{\partial f}{\partial y}(x_i,y_i)\right) + \mathcal{O}(h^3). \end{aligned}$$

Comparing this with the expansion (2), we get $a_1 + a_2 = 1,\ a_2\,p_1 = \frac{1}{2},\ a_2\,q_{11} = \frac{1}{2}$.

Heun's method: $a_1 = \frac{1}{2},\ a_2 = \frac{1}{2},\ p_1 = q_{11} = 1$

Ralston's method: $a_1 = \frac{1}{3},\ a_2 = \frac{2}{3},\ p_1 = q_{11} = \frac{3}{4}$