Derivation of Runge-Kutta method

The first-order ODE is defined as:

$$y' = S(x, y), y(x_0) = y_0$$

Let's say we wish to compute y_{i+1} in the following fashion:

$$K_0 = hS(x_i, y_i), (1)$$

$$K_1 = hS(x_i + \alpha h, y_i + \beta K_0), (2)$$

$$y_{i+1} = y_i + aK_0 + bK_1, (3)$$

where a, b, α, β are constants to be determined.

The slope is defined as $S(x, y)$, which is a function of both x and y.
We use the following notation:
x_i: the starting value of x, at the beginning step.
h: the step size.
$x_{i+1} = x_i + h$: the value of x at the end of the step.
$y_i = y(x_i)$: the starting value of y at the beginning of the step.
$y_{i+1} = y(x_{i+1})$: the value of y at the end of the step.
$S(x_i, y_i)$: the slope evaluated at (x_i, y_i).

Using Taylor's series, we could express the right hand of Eq. (3) as:

$$y_{i+1} = y(x_i + h) \approx y(x_i) + h\left.\frac{dy}{dx}\right|_{x_i} + \frac{h^2}{2}\left.\frac{d^2y}{dx^2}\right|_{x_i}, (4)$$

Remember,

$$\frac{d^2y}{dx^2} = \frac{dS(x, y)}{dx} = \frac{\partial S(x, y)}{\partial x} + \frac{\partial S(x, y)}{\partial y}\frac{dy}{dx}, (5)$$

Then, Eq. (4) can be written as:

$$\begin{aligned} y_{i+1} = y(x_i + h) &\approx y(x_i) + h\left.\frac{dy}{dx}\right|_{x_i} + \frac{h^2}{2}\left.\frac{d^2y}{dx^2}\right|_{x_i} \\ &= y(x_i) + h\left.\frac{dy}{dx}\right|_{x_i} + \frac{h^2}{2}\left.\frac{\partial S(x, y)}{\partial x}\right|_{(x_i, y_i)} + \frac{h^2}{2}\frac{dy}{dx}\left.\frac{\partial S(x, y)}{\partial y}\right|_{(x_i, y_i)}, (6) \end{aligned}$$

Because we define:

$$\left.\frac{dy}{dx}\right|_{x_i} = S(x_i, y_i)$$

Eq. (6) can be written as:

$$y_{i+1} = y_i + hS(x_i, y_i) + \frac{h^2}{2}\left.\frac{\partial S}{\partial x}\right|_{(x_i, y_i)} + \frac{h^2}{2}S(x_i, y_i)\left.\frac{\partial S}{\partial y}\right|_{(x_i, y_i)}, (7)$$

To continue, we can expand K_1 term in Eq. (2) as:

$$K_1 = hS(x_i + \alpha h, y_i + \beta K_0) = h\left[S(x_i, y_i) + \alpha h\left.\frac{\partial S}{\partial x}\right|_{(x_i, y_i)} + \beta K_0\left.\frac{\partial S}{\partial y}\right|_{(x_i, y_i)}\right], (8)$$

Plug Eq. (1) into Eq. (8), we get:

$$K_1 = hS(x_i + \alpha h, y_i + \beta K_0) = h\left[S(x_i, y_i) + \alpha h \frac{\partial S}{\partial x}\bigg|_{(x_i, y_i)} + \beta S(x_i, y_i) \frac{\partial S}{\partial y}\bigg|_{(x_i, y_i)}\right], (9)$$

Then, the right hand of Eq. (3) becomes:

$$y_{i+1} = y_i + aK_0 + bK_1 = y_i + ahS(x_i, y_i) + bh\left[S(x_i, y_i) + \alpha h \frac{\partial S}{\partial x}\bigg|_{(x_i, y_i)} + \beta S(x_i, y_i) \frac{\partial S}{\partial y}\bigg|_{(x_i, y_i)}\right], (10)$$

Further simplify gives:

$$y_{i+1} = y_i + ahS(x_i, y_i) + bhS(x_i, y_i) + b\alpha h^2 \frac{\partial S}{\partial x}\bigg|_{(x_i, y_i)} + b\beta h^2 S(x_i, y_i) \frac{\partial S}{\partial y}\bigg|_{(x_i, y_i)}, (11)$$

From Eq. (7), we also have:

$$y_{i+1} = y_i + hS(x_i, y_i) + \frac{h^2}{2} \frac{\partial S}{\partial x}\bigg|_{(x_i, y_i)} + \frac{h^2}{2} S(x_i, y_i) \frac{\partial S}{\partial y}\bigg|_{(x_i, y_i)}, (12)$$

Compare Eq. (11), and Eq. (12), we get:

$$\begin{cases} a + b = 1 \\ b\alpha = \dfrac{1}{2} \\ b\beta = \dfrac{1}{2} \end{cases}, (13)$$

There are infinite solutions of Eq. (13). Let's give some special cases:

Special case 1: $a = 0, b = 1, \alpha = \beta = \frac{1}{2}$

Then the solution of the ODE is defined as:

$$\begin{cases} K_0 = hS(x_i, y_i) \\ K_1 = hS(x_i + \dfrac{1}{2}h, y_i + \dfrac{1}{2}K_0) \\ y_{i+1} = y_i + K_1 \end{cases}$$

This is basically the Midpoint method.

Special case 2: $a = b = \frac{1}{2}, \alpha = \beta = 1$

Then the solution of the ODE is defined as:

$$\begin{cases} K_0 = hS(x_i, y_i) \\ K_1 = hS(x_i + h, y_i + K_0) \\ y_{i+1} = y_i + \dfrac{1}{2}(K_0 + K_1) \end{cases}$$

This is basically the Heun's method.

Both the Midpoint and Heun's methods are special cases of the 2nd order Runge-Kutta (RK2) method. Similar to the derivation of RK2 method, we could derive the 4th order Runge-Kutta (RK4) methods. To derive RK4 methods, we need to save higher order terms for the Taylor series.

We first write the general form of RK4 method as:

$$K_0 = hS(x_i, y_i)$$

$$K_1 = hS(x_i + \alpha_1 h, y_i + \beta_1 K_0)$$

$$K_2 = hS(x_i + \alpha_2 h, y_i + \beta_2 K_1)$$

$$K_3 = hS(x_i + \alpha_3 h, y_i + \beta_3 K_2)$$

$$y_{i+1} = y_i + aK_0 + bK_1 + cK_2 + dK_3$$

Using Taylor expansion on y_{i+1}, and on K_1, K_2, K_3, and compare terms, we get equations linking the constants of $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, a, b, c, d$, and there are infinite solutions of these constants. Within these solutions, the most popular one is:

$$\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = \frac{1}{2}$$

$$\alpha_3 = \beta_3 = 1$$

$$a = d = \frac{1}{6}$$

$$b = c = \frac{1}{3}$$

Then, the RK4 method is given by:

$$K_0 = hS(x_i, y_i)$$

$$K_1 = hS(x_i + \frac{1}{2}h, y_i + \frac{1}{2}K_0)$$

$$K_2 = hS(x_i + \frac{1}{2}h, y_i + \frac{1}{2}K_1)$$

$$K_3 = hS(x_i + h, y_i + K_2)$$

$$y_{i+1} = y_i + \frac{1}{6}(K_0 + 2K_1 + 2K_2 + K_3)$$