Runge-Kutta Method

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October 24, 2025

1 Euler method

To begin, let's introduce the simplest method for numerically solving an ordinary differential equation (ODE). This is also known as the (1st order) Runge-Kutta method. The equation to be solved is assumed to be:

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

Here, f(x,y) is a given function. To simplify the notation, we set $y_i = y(x_i)$ and $x_{i+1} = x_i + h$. The initial condition (at i = 0) is given as (x_0, y_0) . If the x-mesh step h is chosen such that $|h| \ll 1$, y_{i+1} can be expanded by a Taylor series in h.

$$y_{i+1} = y(x_i + h)$$

$$= y(x_i) + \frac{dy}{dx} \Big|_{x=x_i} + O[h^2]$$

$$= y_i + f(x_i, y_i)h + O[h^2]$$
(2)

Thus, we obtain the following expression:

$$f(x_i, y_i) = \frac{y_{i+1} - y_i}{h}$$
 (3)

This is correct to the first order in h. The solution is given by the following recurrence relation:

$$\begin{cases} x_{i+1} &= x_i + h \\ y(x_{i+1}) &= y(x_i) + f[x_i, y(x_i)] \end{cases}$$
 (4)

2 2nd order Runge-Kutta method (Heun method)

In a similar manner, y_{i+1} is expanded with respect to h. Writing it out to the second order, we have:

$$y_{i+1} = y(x_i + h)$$

$$= y(x_i) + y'(x_i)h + \frac{1}{2}y''(x_i)h^2 + O[h^3]$$
(5)

$$\Delta y = y_{i+1} - y_i$$

$$= y_1 - y_0$$

$$= y'(x_0)h + \frac{1}{2}y''(x_0)h^2$$
(6)

While the value $y'(x_0)$ was used before, this time let's try selecting another value, $y'(x_1)$, in addition.

$$\Delta y = h[\alpha y'(x_0) + \beta y'(x_1)] \tag{7}$$

where α and β are undetermined constants. Here, $\beta y'(x_1)$ can also be expanded:

$$\beta y'(x_1) = \beta y'(x_0 + h)$$

$$= \beta [y'(x_0) + hy''(x_0) + O(h^2)]$$
(8)

Hence,

$$\Delta y = (\alpha + \beta)y'(x_0)h + \beta y''(x_0)h^2 \tag{9}$$

By comparing Eq. (6) and Eq. (9), the parameters are determined as $\alpha = \beta = \frac{1}{2}$. Finally, the second-order recurrence relation is as follows:

$$\begin{cases} k_{1n} &= hf(x_n, y_n) \\ k_{2n} &= hf(x_n + h, y_n + k_{1n}) \\ y_{n+1} &= y_n + \frac{1}{2}(k_{1n} + k_{2n}) \end{cases}$$
(10)

This is called the 'Heun method' and provides a more accurate solution than the Euler method.

3 4th order Runge-Kutta method (RK4)

Following the same procedure, and considering terms up to the fourth order in h, the following recurrence relations are obtained:

$$\begin{cases}
k_{1n} &= hf(x_n, y_n) \\
k_{2n} &= hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}) \\
k_{3n} &= hf(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}) \\
k_{4n} &= hf(x_n + h, y_n + k_{3n}) \\
y_{n+1} &= y_n + \frac{1}{6}(k_{1n} + 2k_{2n} + 2k_{3n} + k_{4n})
\end{cases}$$
(11)

RK4 is often considered the most reasonable method for solving ODEs numerically. This is because using even higher-order (e.g., 5th order or more) Runge-Kutta calculations may require more computation time than RK4 to achieve the same precision, sometimes making the extra computational cost unjustifiable.