Numerical Differentiation

Numerical Differentiation

Suppose a given function f has continuous first derivative and f'' exists. From Taylor's theorem

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(\xi)h^2, \quad , h > 0,$$

where ξ is between x and $x+h$, one has

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\xi) = \frac{f(x+h) - f(x)}{h} + O(h).$$

Hence it is reasonable to use the approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

the forward finite difference scheme.

difference, and the error involved is

The forward difference is an $O(h)$ scheme.

$$|e| = \frac{h}{2}|f''(\xi)| \leq \max_{t\in(x,x+h)} |f''(t)|.$$

error is called the truncation error and is unavoidable because the Taylor series is truncated

Similarly one can derive the backward finite difference approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

which has the same order of truncation error as the forward finite difference scheme.

In theory, the truncation error $e \to 0$ as $h \to 0$. However, the roundoff error will kick in when h is small.

This is because when h is small

$$x \approx x + h \quad \Longrightarrow \quad f(x) \approx f(x+h)$$

since f is continuous.

The forward difference is an $O(h)$ scheme. An $O(h^2)$ scheme can also be derived from the Taylor's theorem

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(\xi_1)h^3 \\ f(x-h) &= f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(\xi_2)h^3, \end{aligned}$$

where ξ_1 is between x and $x+h$ and ξ_2 is between x and $x-h$. Hence

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{1}{6}[f'''(\xi_1) + f'''(\xi_2)]h^3$$

and

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{12}[f'''(\xi_1) + f'''(\xi_2)]h^2$$

Let

$$M = \max_{z\in[x-h,x+h]} f'''(z) \quad \text{and} \quad m = \min_{z\in[x-h,x+h]} f'''(z).$$

If f''' is continuous on $[x-h, x+h]$, then by the intermediate value theorem, there exists $\xi \in [x-h, x+h]$ such that $f(\xi) = \frac{1}{2}[f'''(\xi_1) + f'''(\xi_2)]$. Hence

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}f'''(\xi)h^2 = \frac{f(x+h) - f(x-h)}{2h} + O(h^2).$$

This is called center difference approximation and the truncation error is

$$|e| = \frac{h^2}{6}f'''(\xi)$$

Similarly, we can derive an $O(h^2)$ scheme from Taylor's theorem for $f''(x)$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}f^{(4)}(\xi)h^2,$$

where ξ is between $x-h$ and $x+h$.

Polynomial Interpolation Method

A general approach for numerical differentiation is to use polynomial interpolation.

For a given function f (or a set of function values)

we find a polynomial p such that $p \approx f$ and expect $p' \approx f'$.

Suppose that $n+1$ points, $x_0, x_1, \ldots, x_n$, and values of f, $f(x_0), f(x_1), \ldots, f(x_n)$, have been given or evaluated, we apply the Lagrange polynomial interpolation scheme to derive

$$p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x), \qquad \text{where} \qquad \ell_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}.$$

Since $f(x)$ can be written as

$$f(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w(x),$$

where

$$w(x) = \prod_{j=0}^{n} (x - x_j),$$

we have, by taking derivative,

$$f'(x) = \sum_{i=0} n f(x_i)\ell_i'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) + \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x).$$

Note that

$$w'(x) = \sum_{j=0}^{n} \prod_{i=0, i\neq j}^{n} (x - x_i).$$

Hence a reasonable approximation for the first derivative of f is

$$f'(x) \approx \sum_{i=0}^{n} f(x_i)\ell_i'(x).$$

When $x = x_k$ for some $0 \le k \le n$,

$$w(x_k) = 0 \quad \text{and} \quad w'(x_k) = \prod_{i=0, i\neq k}^{n} (x_k - x_i).$$

Hence

$$f'(x_k) = \sum_{i=0}^{n} f(x_i)\ell_i'(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0, i\neq k}^{n} (x_k - x_i).$$

Richardson Extrapolation Method

Again from the Taylor's theorem

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) + \frac{h^6}{6!}f^{(6)}(x) + \cdots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x) + \frac{h^6}{6!}f^{(6)}(x) + \cdots$$

we have

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!}f'''(x) + \frac{2h^5}{5!}f^{(5)}(x) + \cdots,$$

and, consequently,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2}{3!}f'''(x) + \frac{h^4}{5!}f^{(5)}(x) + \cdots\right].$$

Denote

$$L \equiv f'(x) \quad \text{and} \quad \phi(h) = \frac{f(x+h) - f(x-h)}{2h}.$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2}{3!} f'''(x) + \frac{h^4}{5!} f^{(5)}(x) + \cdots\right].$$

Then equation can be expressed as

$$L = \phi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots .$$

This yields the $O(h^2)$ central difference scheme.

Consider

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2}{3!} f'''(x) + \frac{h^4}{5!} f^{(5)}(x) + \cdots\right].$$

Now replace h with $\frac{h}{2}$ in the Taylor's expansion, one has instead

$$f'(x) = \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h} - \left[\frac{1}{3!}\left(\frac{h}{2}\right)^2 f'''(x) + \frac{1}{5!}\left(\frac{h}{2}\right)^4 f^{(5)}(x) + \cdots\right]$$

This gives

$$L = \phi(\frac{h}{2}) + \frac{1}{4}a_2h^2 + \frac{1}{16}a_4h^4 + \frac{1}{64}a_6h^6 + \cdots ,$$

or, equivalently,

$$4L = 4\phi(\frac{h}{2}) + a_2h^2 + \frac{1}{4}a_4h^4 + \frac{1}{16}a_6h^6 + \cdots .$$

$$3L = 4\phi(\frac{h}{2}) - \phi(h) - \frac{3}{4}a_4h^4 - \frac{15}{16}a_6h^6 + \cdots .$$

This yields an $O(h^4)$ approximation scheme

$$f'(x) = L = \frac{4}{3}\phi(\frac{h}{2}) - \frac{1}{3}\phi(h) - \frac{1}{4}a_4h^4 - \frac{5}{16}a_6h^6 + \cdots .$$

Richardson Extrapolation Method

We may repeat this idea by letting

$$\psi(h) = \frac{4}{3}\phi(\frac{h}{2}) - \frac{1}{3}\phi(h).$$

Then

$$L = \psi(h) + b_4h^4 + b^6h^6 + \cdots$$

and also

$$16L = 16\psi(\frac{h}{2}) + b_4h^4 + \frac{1}{4}b_6h^6 + \cdots .$$

Subtract () from () to give

$$15L = 16\psi(\frac{h}{2}) - \psi(h) - \frac{3}{4}b_6h^6 + \cdots .$$

It leads to an $O(h^6)$ approximation

$$f'(x) = L = \frac{16}{15}\psi(\frac{h}{2}) - \frac{1}{15}\psi(h) - \frac{1}{20}b_6h^6 + \cdots .$$

Numerical Solutions of Ordinary Differential Equations

initial-value problems (IVP) $$\begin{cases} y' = f(x, y), & x \in \mathbb{R} \\ y(x_0) = y_0, \end{cases}$$

where y is a function of x, f is a function of y and x, x_0 is called the initial point, and y_0 the initial value. The numerical values of $y(x)$ on an interval containing x_0 are to be determined.

Existence and Uniqueness of Solutions

IVP $$\begin{cases} y' = f(x, y), & x \in \mathbb{R} \\ y(x_0) = y_0, \end{cases}$$

Theorem *If $f(x, y)$ is continuous in a region Ω, where*

$$\Omega = \{(x, y) |\ |x - x_0| \le \alpha,\ |y - y_0| \le \beta\}$$

then the IVP has a solution $y(x)$ for $|x - x_0| \le \min\{\alpha, \frac{\beta}{M}\}$, where $M = \max_{(x,y)\in\Omega} |f(x, y)|$.

Theorem 8.2 *If f and $\frac{\partial f}{\partial x}$ are continuous in Ω, then the IVP has a unique solution in the interval $|x - x_0| \le \min\{\alpha, \frac{\beta}{M}\}$.*

Theorem 8.3 *If f is continuous in $a \le x \le b$, $-\infty < y < \infty$ and*

$$|f(x, y_1) - f(x, y_2)| \le L|y_1 - y_2|$$

for some positive constant L, (that is, f is Lipschitz continuous in y), then IVP) has a unique solution in the interval $[a, b]$.

Euler's Method

On of the simplest methods for solving the IVP $\begin{cases} y' = f(x, y), & x \in \mathbb{R} \\ y(x_0) = y_0, \end{cases}$

Note that the slope of the tangent line at x_0 is

$$y'(x_0) = y'_0 = \frac{y_1 - y_0}{h},$$

hence

$$y_1 = y_0 + hy'_0 = y_0 + hf(x_0, y_0)).$$

Repeat this idea at (x_1, y_1) and we get

$$y_2 = y_1 + hy'_1 = y_1 + hf(x_1, y_1),$$

and so on. If x_i are equally spaced, and h is the increment then we have the formulation of Euler's mehtod

$$\begin{aligned} x_{k+1} &= x_k + h = x_0 + (k+1)h \\ y_{k+1} &= y_k + hf(x_k, y_k) \end{aligned}$$

Euler's method is a first-order ($O(h)$) method.

The Improved Euler's method

$$\begin{aligned} x_{k+1} &= x_k + h = x_0 + (k+1)h \\ y^*_{k+1} &= y_k + hf(x_k, y_k) \\ y_{k+1} &= y_k + \frac{h}{2}\left[f(x_k, y_k) + f(x_{k+1}, y^*_{k+1})\right] \end{aligned}$$

Example 1: Euler Method

Use Euler's method with $h = 0.1$ to find approximate values for the solution of the initial value problem

$$y' + 2y = x^3 e^{-2x}, \quad y(0) = 1$$

at $x = 0.1, 0.2, 0.3$.

Solution

We rewrite Equation as

$$y' = -2y + x^3 e^{-2x}, \quad y(0) = 1,$$

which is of the form Equation , with

$$f(x, y) = -2y + x^3 e^{-2x},\ x_0 = 0, \text{ and } y_0 = 1.$$

Euler's method yields

$$\begin{aligned} y_1 &= y_0 + hf(x_0, y_0) \\ &= 1 + (0.1)f(0, 1) = 1 + (0.1)(-2) = 0.8, \end{aligned}$$

$$\begin{aligned} y_2 &= y_1 + hf(x_1, y_1) \\ &= 0.8 + (0.1)f(0.1, 0.8) = 0.8 + (0.1)\left(-2(0.8) + (0.1)^3 e^{-0.2}\right) = 0.640081873, \end{aligned}$$

$$\begin{aligned} y_3 &= y_2 + hf(x_2, y_2) \\ &= 0.640081873 + (0.1)\left(-2(0.640081873) + (0.2)^3 e^{-0.4}\right) = 0.512601754. \end{aligned}$$

Example 2: Euler Method

Use Euler's method with step sizes $h = 0.1$, $h = 0.05$, and $h = 0.025$ to find approximate values of the solution of the initial value problem

$$y' + 2y = x^3 e^{-2x}, \quad y(0) = 1$$

at $x = 0, 0.1, 0.2, 0.3, \ldots, 1.0$. Compare these approximate values with the values of the exact solution

$$y = \frac{e^{-2x}}{4}(x^4 + 4),$$

x	$h = 0.1$	$h = 0.05$	$h = 0.025$	Exact
0.0	1.000000000	1.000000000	1.000000000	1.000000000
0.1	0.800000000	0.810005655	0.814518349	0.818751221
0.2	0.640081873	0.656266437	0.663635953	0.670588174
0.3	0.512601754	0.532290981	0.541339495	0.549922980
0.4	0.411563195	0.432887056	0.442774766	0.452204669
0.5	0.332126261	0.353785015	0.363915597	0.373627557
0.6	0.270299502	0.291404256	0.301359885	0.310952904
0.7	0.222745397	0.242707257	0.252202935	0.261398947
0.8	0.186654593	0.205105754	0.213956311	0.222570721
0.9	0.159660776	0.176396883	0.184492463	0.192412038
1.0	0.139778910	0.154715925	0.162003293	0.169169104

$$y_{exact}(1) - y_{approx}(1) \approx \begin{cases} 0.0293 \text{with} h = 0.1, \\ 0.0144 \text{ with } h = 0.05, \\ 0.0071 \text{ with } h = 0.025. \end{cases}$$

Based on this scanty evidence, you might guess that the error in approximating the exact solution at a **fixed value of** x by Euler's method is roughly halved when the step size is halved. You can find more evidence to support this conjecture by examining Table 3.1.2 , which lists the approximate values of $y_{exact} - y_{approx}$ at $x = 0.1, 0.2, \ldots, 1.0$.

Table 3.1.2 : Errors in approximate solutions of $y' + 2y = x^3 e^{-2x}$, $y(0) = 1$, obtained by Euler's method.

x	$h = 0.1$	$h = 0.05$	$h = 0.0.25$
0.1	0.0187	0.0087	0.0042
0.2	0.0305	0.0143	0.0069
0.3	0.0373	0.0176	0.0085
0.4	0.0406	0.0193	0.0094
0.5	0.0415	0.0198	0.0097
0.6	0.0406	0.0195	0.0095
0.7	0.0386	0.0186	0.0091
0.8	0.0359	0.0174	0.0086
0.9	0.0327	0.0160	0.0079
1.0	0.0293	0.0144	0.0071

Truncation Error in Euler's Method

we will now show that under reasonable assumptions on f there's a constant K such that

the error in approximating the solution of the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0,$$

at a given point $b > x_0$ by Euler's method with step size $h = (b - x_0)/n$ satisfies the inequality

$$|y(b) - y_n| \le Kh,$$

where K is a constant independent of n.

There are two sources of error (not counting roundoff) in Euler's method:

1. The error committed in approximating the integral curve by the tangent line

$$y = y(x_i) + f(x_i, y(x_i))(x - x_i).$$

2. The error committed in replacing $y(x_i)$ by y_i

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

We call the error in this approximation the **local truncation error at the** ith step, and denote it by T_i; thus,

$$T_i = y(x_{i+1}) - y(x_i) - hf(x_i, y(x_i)).$$

we will now use **Taylor's theorem** to estimate T_i, assuming for simplicity that f, f_x, and f_y are continuous and bounded for all (x, y). Then y'' exists and is bounded on $[x_0, b]$. To see this, we differentiate

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

to obtain

$$\begin{aligned} y''(x) &= f_x(x, y(x)) + f_y(x, y(x))y'(x) \\ &= f_x(x, y(x)) + f_y(x, y(x))f(x, y(x)). \end{aligned}$$

Since we assumed that f, f_x and f_y are bounded, there's a constant M such that

$$|f_x(x, y(x)) + f_y(x, y(x))y'(x)| \le M \quad x_0 < x < b$$

which implies that

$$|y''(x)| \le M, \quad x_0 < x < b$$

Since $x_{i+1} = x_i + h$, Taylor's theorem implies that

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(\tilde{x}_i),$$

where $\tilde{x}_i$ is some number between x_i and x_{i+1}.

. Since $y'(x_i) = f(x_i, y(x_i))$ this can be written as $$y(x_{i+1}) = y(x_i) + hf(x_i, y(x_i)) + \frac{h^2}{2}y''(\tilde{x}_i),$$

or, equivalently,

$$y(x_{i+1}) - y(x_i) - hf(x_i, y(x_i)) = \frac{h^2}{2}y''(\tilde{x}_i).$$

Comparing this with Equation $T_i = y(x_{i+1}) - y(x_i) - hf(x_i, y(x_i)).$

$$T_i = \frac{h^2}{2}y''(\tilde{x}_i).$$

Recalling Equation $|y''(x)| \le M, \quad x_0 < x < b$

$$|T_i| \le \frac{Mh^2}{2}, \quad 1 \le i \le n.$$

local truncation error of Euler's method is **of order** h^2, which we write as $O(h^2)$.

Since the local truncation error for Euler's method is $O(h^2)$, it is reasonable to expect that halving h reduces the local truncation error by a factor of This is true, but halving the step size also requires twice as many steps to approximate the solution at a given point. To analyze the overall effect of truncation error in Euler's method, it is useful to derive an equation relating the errors

$$e_{i+1} = y(x_{i+1}) - y_{i+1} \quad \text{and} \quad e_i = y(x_i) - y_i.$$

To this end, recall that

$$y(x_{i+1}) = y(x_i) + hf(x_i, y(x_i)) + T_i$$

and

$$y_{i+1} = y_i + hf(x_i, y_i).$$

Subtracting Equation

$$e_{i+1} = e_i + h\left[f(x_i, y(x_i)) - f(x_i, y_i)\right] + T_i.$$

The last term on the right is the local truncation error at the ith step. The other terms reflect the way errors made at **previous steps** affect e_{i+1}. Since $|T_i| \le Mh^2/2$, we see

$$|e_{i+1}| \le |e_i| + h|f(x_i, y(x_i)) - f(x_i, y_i)| + \frac{Mh^2}{2}. \quad (3$$

Since we assumed that f_y is continuous and bounded, the mean value theorem implies that

$$f(x_i, y(x_i)) - f(x_i, y_i) = f_y(x_i, y_i^*)(y(x_i) - y_i) = f_y(x_i, y_i^*)e_i,$$

where y_i^* is between y_i and $y(x_i)$. Therefore

$$|f(x_i, y(x_i)) - f(x_i, y_i)| \le R|e_i|$$

for some constant R. From this and Equation ,

$$|e_{i+1}| \le (1 + Rh)|e_i| + \frac{Mh^2}{2}, \quad 0 \le i \le n-1.$$

For convenience, let $C = 1 + Rh$. Since $e_0 = y(x_0) - y_0 = 0$, applying Equation 5 repeatedly yields

$$\begin{aligned}
|e_1| &\le \frac{Mh^2}{2} \\
|e_2| &\le C|e_1| + \frac{Mh^2}{2} \le (1 + C)\frac{Mh^2}{2} \\
|e_3| &\le C|e_2| + \frac{Mh^2}{2} \le (1 + C + C^2)\frac{Mh^2}{2} \\
&\vdots
\end{aligned}$$

$$|e_n| \le C|e_{n-1}| + \frac{Mh^2}{2} \le (1 + C + \cdots + C^{n-1})\frac{Mh^2}{2}.$$

Recalling the formula for the sum of a geometric series, we see that

$$1 + C + \cdots + C^{n-1} = \frac{1 - C^n}{1 - C} = \frac{(1 + Rh)^n - 1}{Rh}$$

(since $C = 1 + Rh$). From this and Equation

$$|y(b) - y_n| = |e_n| \le \frac{(1 + Rh)^n - 1}{R} \frac{Mh}{2}.$$

Since Taylor's theorem implies that

$$1 + Rh < e^{rh}$$

(verify),

$$(1 + Rh)^n < e^{nRh} = e^{R(b - x_0)} \quad (\text{since } nh = b - x_0).$$

This and Equation 3.1.17 imply that

$$|y(b) - y_n| \le Kh,$$

with

$$K = M\frac{e^{R(b-x_0)} - 1}{2R}.$$

Because of Equation 3.1.18 we say that the **global truncation error of Euler's method is of order** h, which we write as $O(h)$.

Runge-Kutta Methods

One of the most important methods for solving the IVP

Recall the Taylor's Theorem

$$\begin{aligned} y(x+h) &= y(x) + hy'(x) + \frac{h^2}{2}y'' + \frac{h^3}{2}y''' + \dots \\ &= y(x) + hy'(x) + \frac{h^2}{2}y'' + O(h^3) \end{aligned}$$

By differentiating $y(x)$, we have

$$
\begin{aligned}
y' &= f(x,y) \equiv f \\
y'' &= \frac{d}{dx}f = f_x + f_y y' = f_x + f_y f \\
y''' &= f_{xx} + f\frac{d}{dx}f_y + f_y\frac{d}{dx}f \\
&= f_{xx} + f(\frac{f_y}{dy}\frac{dy}{dx} + f_{yx}) + f_y(f_x + f_y f) \\
&= f_{xx} + f(f_{yx} + f_{yy}f) + f_y(f_x + f_y f)
\end{aligned}
$$

plug in, we get

plug in, we get

$$
\begin{aligned}
y(x+h) &= y + hy' + \frac{h^2}{2}y'' + O(h^3) \\
&= y + hf + \frac{h^2}{2}(f_x + f_y f) + O(h^3) \\
&= y + \frac{h}{2}f + \frac{h}{2}f + \frac{h^2}{2}(f_x + f_y f) + O(h^3) \\
&= y + \frac{h}{2}f + \frac{h}{2}(f + hf_x + hf_y f) + O(h^3)
\end{aligned}
$$

Apply Taylor's Theorem on f

$$f(x+h, y+hf) = f(x,y) + hf_x + hff_y + O(h^2)$$

$$\Rightarrow \quad f + hf_x + hff_y \approx f(x+h, y+hf)$$

$$\Rightarrow \quad y(x+h) = y + \frac{1}{2}hf + \frac{h}{2}f(x+h, y+hf) + O(h^3)$$

Let $\quad F_1 = hf(x,y) \qquad F_2 = hf(x+h, y+F_1)$

Then $\quad y(x+h) = y + \frac{1}{2}(F_1 + F_2)$

This is called the second-order Runge-Kutta method.

Algorithm for second-order Runge-Kutta mehtod :

for $k = 0, 1, 2, \ldots$ **do**

$x_{k+1} = x_k + h = x_0 + (k+1)h$

$F_1 = hf(x_k, y_k)$

$F_2 = hf(x_{k+1}, y_k + F_1)$

$y_{k+1} = y_k + \frac{1}{2}(F_1 + F_2)$

end for

General form of second-order Runge-Kutta method :

$$y(x+h) = y + \omega_1 hf + \omega_2 hf(x+\alpha h, y+\beta hf) + O(h^3)$$

where $\omega_1, \omega_2, \alpha, \beta$ are constants to be defined, and

$$\begin{cases} \omega_1 + \omega_2 = 1 \\ \omega_2 \alpha = \frac{1}{2} \\ \omega_2 \beta = \frac{1}{2} \end{cases} .$$

By letting $\omega_1 = 0, \omega_2 = 1, \alpha = \beta = \frac{1}{2}$ leads to the modified Euler's mehtod.

Fourth-Order Runge-kutta method

$$y(x+h) = y + \frac{1}{6}(F_1 + 2F_2 + 2F_3 + F_4) + O(h^5)$$

where

$$\begin{cases} F_1 = hf(x, y) \\ F_2 = hf(x + \frac{1}{2}h, y + \frac{1}{2}F_1) \\ F_3 = hf(x + \frac{1}{2}h, y + \frac{1}{2}F_2) \\ F_4 = hf(x + h, y + F_3) \end{cases}$$

Algorithm for fourth-order Runge-Kutta mehtod :

for $k = 0, 1, 2, \ldots$ **do**

$x_{k+\frac{1}{2}} = x_k + \frac{1}{2}h$

$x_{k+1} = x_k + h = x_0 + (k+1)h$

$F_1 = hf(x_k, y_k)$

$F_2 = hf(x_{k+\frac{1}{2}}, y_k + \frac{1}{2}F_1)$

$F_3 = hf(x_{k+\frac{1}{2}}, y_k + \frac{1}{2}F_2)$

$F_4 = hf(x_{k+1}, y_k + F_3)$

$y_{k+1} = y_k + \frac{1}{6}(F_1 + 2F_2 + 2F_3 + F_4) + O(h^5)$

end for

Local truncation error in the Runge-Kutta mehtod is the error that arises in each step simply because of the truncated Taylor series. This error is inevitable. The fourth Runge-Kutta method involves a local truncation error of $O(h^5)$.

The Number of function evaluations in the second order method is two and the fourth order is four.

Fourth-Order Runge-kutta method

Example

$$\frac{\mathrm{d}x}{\mathrm{d}t} = F(x,t) = tx^2 + 2x$$

Setting $x_0 = -5$, $t_0 = 0$, $h = 0.4$, the following are the values of k_1, k_2, k_3, and k_4 required to calculate x_1:

$$\begin{aligned} k_1 &= F(x_0, t_0) = F(-5, 0) \\ &= 0 + 2(-5) = -10 \end{aligned}$$

$$\begin{aligned} k_2 &= F\left(x_0 + \frac{h}{2}k_1, t_0 + \frac{h}{2}\right) = F(-5 + 0.2(-10), 0 + 0.2) \\ &= 0.2(-5 + 0.2(-10))^2 + 2 \times (-5 + 0.2(-10)) = -4.2 \end{aligned}$$

$$\begin{aligned} k_3 &= F\left(x_0 + \frac{h}{2}k_2, t_0 + \frac{h}{2}\right) = F(-5 + 0.2(-4.2), 0 + 0.2) \\ &= 0.2(-5 + 0.2(-4.2))^2 + 2 \times (-5 + 0.2(-4.2)) = -4.8589 \end{aligned}$$

$$\begin{aligned} k_4 &= F(x_0 + hk_3, t_0 + h) = F(-5 + 0.4(-4.8589), 0 + 0.4) \\ &= 0.4(-5 + 0.4(-4.8589))^2 + 2 \times (-5 + 0.4(-4.8589)) = 5.3981 \end{aligned}$$

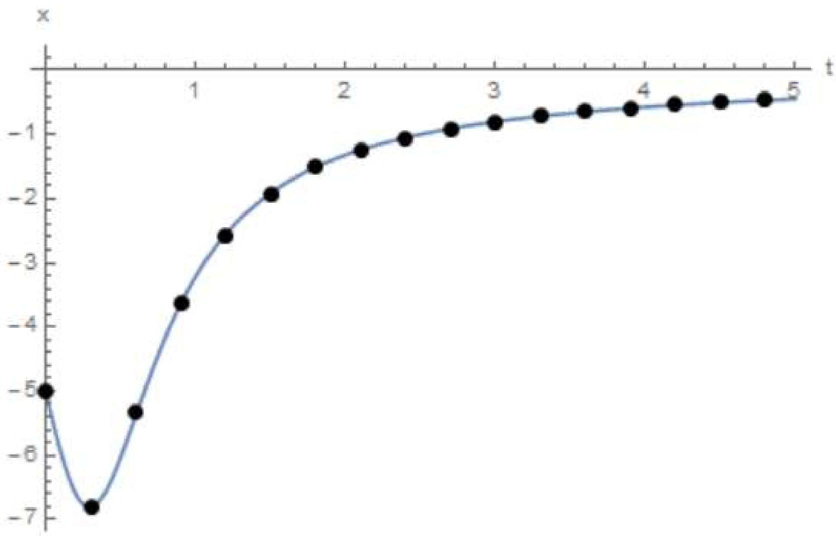
Therefore:

$$x_1 = x_0 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) = -5 + \frac{0.4}{6}(-10 - 2\times4.2 - 2\times4.8589 + 5.3981) = -6.51465$$

4	t	x_i	K1	K2	K3	K4	x_{i+1}
5	0	-5	-10	-4.2	-4.85888	5.398062	-6.51465
6	0.4	-6.51465	3.946955	8.21662	4.495225	8.363611	-3.99903
7	0.8	-3.99903	4.795731	3.161124	4.601764	1.273386	-2.55937
8	1.2	-2.55937	2.741709	1.639871	2.507986	0.762341	-1.77272
9	1.6	-1.77272	1.482614	0.970087	1.328735	0.598829	-1.32745
10	2	-1.32745	0.869336	0.620481	0.779014	0.444957	-1.05323
11	2.4	-1.05323	0.555837	0.423321	0.501973	0.329747	-0.87082
12	2.8	-0.87082	0.381666	0.304644	0.347978	0.24963	-0.74171
13	3.2	-0.74171	0.277018	0.228853	0.254859	0.193961	-0.64582
14	3.6	-0.64582	0.209861	0.177907	0.194609	0.154436	-0.57186
15	4	-0.57186	0.164388	0.142156	0.153477	0.12562	-0.51311
16	4.4	-0.51311	0.132228	0.116153	0.124165	0.104065	-0.46532
17	4.8	-0.46532	0.108664	0.096668	0.102541	0.087562	-0.42567
18	5.2	-0.42567					

Out[155]= $-\frac{20\, e^{2t}}{9 - 5\, e^{2t} + 10\, e^{2t}\, t}$

Out[158]=



Systems and Higher-Order Ordinary Differential Equations

Consider a system of first-order ODE's.

$$\begin{cases} y_1' &= f_1(x, y_1, y_2, \ldots, y_n) \\ y_2' &= f_2(x, y_1, y_2, \ldots, y_n) \\ &\vdots \\ y_n' &= f_n(x, y_1, y_2, \ldots, y_n) \end{cases}$$

with initial conditions

$$\begin{cases} y_1(x_0) &= y_1^0 \\ y_2(x_0) &= y_2^0 \\ &\vdots \\ y_n(x_0) &= y_n^0 \end{cases}$$

Define

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \qquad F = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}, \qquad Y_0 = \begin{bmatrix} y_1^0 \\ y_2^0 \\ \vdots \\ y_n^0 \end{bmatrix}$$

and transform the system into vector form

$$\begin{cases} Y' & = F(x, Y) \\ Y(x_0) & = Y_0 \end{cases}$$

The Runge-Kutta methods can be easily extended to vector form.

Example

$$\begin{cases} y_1' & = y_1 + 4y_2 - e^x \\ y_2' & = y_1 + y_2 + 2e^x \end{cases} \qquad \textit{with initial conditions} \qquad \begin{cases} y_1(0) & = 4 \\ y_2(0) & = \frac{5}{4} \end{cases}$$

Sol: Transform to

$$\begin{aligned} Y' &= \begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} y_1 + 4y_2 - e^x \\ y_1 + y_2 + 2e^x \end{bmatrix} = F(x, Y) \\ Y_0 &= \begin{bmatrix} 4 \\ \frac{5}{4} \end{bmatrix}, \qquad x_0 = 0 \end{aligned}$$

■

Example :

$$\begin{cases} (\sin x)y''' + \cos(xy) + \sin(x^2 + y'') + (y')^3 = \log x \\ y(2) = 7 \\ y'(2) = 3 \\ y''(2) = -4 \end{cases}$$

Sol: Let $u_1 = y, u_2 = y'$, and $u_3 = y''$

$$\begin{aligned} & (\sin x)y''' + \cos(xy) + \sin(x^2 + y'') + (y')^3 = \log x \\ \Rightarrow \quad & (\sin x)u_3' + \cos(xu_1) + \sin(x^2 + u_3) + (u_2)^3 = \log x \\ \Rightarrow \quad & u_3' = \left[\log x - \cos(xu_1) - \sin(x^2 + u_3) - (u_2)^3\right] / \sin x \end{aligned}$$

system:

$$\begin{cases} u_1' &= u_2 \\ u_2' &= u_3 \\ u_3' &= [\log x - \cos(xu_1) - \sin(x^2 + u_3) - u_2^3] / \sin x \end{cases} \qquad \begin{cases} u_1(2) &= 7 \\ u_2(2) &= 3 \\ u_3(2) &= -4 \end{cases}$$

let

$$U = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}, \qquad F = \begin{bmatrix} u_2 \\ u_3 \\ [\log x - \cos(xu_1) - \sin(x^2 + u_3) - u_2^3] / \sin x \end{bmatrix},$$

and

$$U_0 = \begin{bmatrix} 7 \\ 3 \\ -4 \end{bmatrix}, \qquad x_0 = 2.$$

The higher-order ODE becomes

$$\begin{cases} U' &= F(x, U) \\ U(x_0) &= U_0 \end{cases}$$

and can be solved by Runge-Kutta methods.

EXAMPLE

Consider the following BVP

$$7\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - 2\frac{\mathrm{d}y}{\mathrm{d}x} - y + x = 0$$

With the boundary conditions $y(0) = 5$ and $y(20) = 8$. Assuming $h = 2$, use the finite difference method to find a numerical solution to the given BVP. Compare with the exact solution.

SOLUTION

The exact solution can be directly obtained in Mathematica using the DSolve function.

$$y = x + 7.00018e^{-0.261204x} - 0.000178305e^{0.546918x} - 2.$$

The numerical solution is obtained by first discretizing the domain into $n = 10$ intervals with $h = \frac{20}{10} = 2$ and $x_0 = 0, x_1 = 2, x_2 = 4, x_3 = 6, x_4 = 8, x_5 = 10, x_6 = 12, x_7 = 14,$ $x_8 = 16, x_9 = 18, x_{10} = 20$. The values of y at these points are denoted by $y_0, y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8, y_9, y_{10}$. The boundary conditions are given as Dirichlet type with $y_0 = 5$ and $y_{10} = 8$. The remaining 9 unknowns can be obtained by utilizing the basic formulas of the centred finite difference scheme to replace the derivatives in the differential equation. These can be utilized to write 9 equations of the form:

$$7\left(\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}\right) - 2\left(\frac{y_{i+1} - y_{i-1}}{2h}\right) - y_i + x_i = 0$$

This results in the following nine equations (after the substitution $y_0 = 5$ and $y_{10} = 8$):

$$7\left(\frac{y_2 - 2y_1 + 5}{4}\right) - \frac{y_2 - 5}{2} - y_1 + x_1 = 0$$
$$7\left(\frac{y_3 - 2y_2 + y_1}{4}\right) - \frac{y_3 - y_1}{2} - y_2 + x_2 = 0$$
$$7\left(\frac{y_4 - 2y_3 + y_2}{4}\right) - \frac{y_4 - y_2}{2} - y_3 + x_3 = 0$$
$$7\left(\frac{y_5 - 2y_4 + y_3}{4}\right) - \frac{y_5 - y_3}{2} - y_4 + x_4 = 0$$
$$7\left(\frac{y_6 - 2y_5 + y_4}{4}\right) - \frac{y_6 - y_4}{2} - y_5 + x_5 = 0$$
$$7\left(\frac{y_7 - 2y_6 + y_5}{4}\right) - \frac{y_7 - y_5}{2} - y_6 + x_6 = 0$$
$$7\left(\frac{y_8 - 2y_7 + y_6}{4}\right) - \frac{y_8 - y_6}{2} - y_7 + x_7 = 0$$
$$7\left(\frac{y_9 - 2y_8 + y_7}{4}\right) - \frac{y_9 - y_7}{2} - y_8 + x_8 = 0$$
$$7\left(\frac{8 - 2y_9 + y_8}{4}\right) - \frac{8 - y_8}{2} - y_9 + x_9 = 0$$

Rearranging yields the following linear system of equations:

$$\begin{pmatrix} -4.5 & 1.25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.25 & -4.5 & 1.25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.25 & -4.5 & 1.25 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.25 & -4.5 & 1.25 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.25 & -4.5 & 1.25 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.25 & -4.5 & 1.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.25 & -4.5 & 1.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2.25 & -4.5 & 1.25 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.25 & -4.5 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \end{pmatrix} = \begin{pmatrix} -13.25 \\ -4 \\ -6 \\ -8 \\ -10 \\ -12 \\ -14 \\ -16 \\ -28 \end{pmatrix}$$

Solving the above system yields:

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \end{pmatrix} = \begin{pmatrix} 4.19959 \\ 4.51853 \\ 5.50744 \\ 6.89345 \\ 8.50301 \\ 10.2026 \\ 11.824 \\ 13.0018 \\ 12.7231 \end{pmatrix}$$

Combined with $y_0 = 5$ and $y_{10} = 8$, a list plot can be drawn to show the obtained numerical solution. The following figure shows the exact solution (blue curve) with the numerical solution (black dots). The numerical solution provides a very good approximation to the the exact solution!