Numerical Solution of Ordinary Differential Equations

A first order differential equation may be expressed as follows:

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

The problem

$$\begin{cases} \text{Solve:} & \frac{dy}{dx} = f(x,y) \\ \text{Subject to:} & y(x_0) = y_0 \end{cases} \tag{1}$$

is called an *initial-value problem.* The first equation gives the slope of the curve y at any point x, and the second equation specifies one particular value of the function $y(x)$.

Existence. Will every initial-value problem have a solution? No, some assumptions must be made about $f(x,y)$, and even then we can only expect the solution to exist in a neighborhood of $x = x_0$. As an example of what could happen, consider

$$\begin{cases} \dfrac{dy}{dx} =1 + y^2 \\ y(0) =0 \end{cases}$$

The solution curve starts at $x = 0$ with slope one; that is, $y'(0) = 1$. Since the slope is positive, $y(x)$ is *increasing* near $x = 0$. Therefore, the expression $1 + y^2$ is also increasing. Hence, y' is increasing. Since y and y' are both increasing and are related by the equation $y' = 1 + x^2$, we can expect that at some finite value of x there will be no solution; that is, $y(x) = +\infty$. As a matter of fact, this occurs at $x = \pi/2$ because the *analytic solution* of the initial-value problem is $y(x) = \tan x$.

Theorem 1. *If $f(x,y)$ is continuous in a rectangle R centered at (x_0, y_0), say*

$$R =\{(x,y) : |x - x_0| \le \alpha, \quad |y - y_0| \le \beta\} \tag{2}$$

then the initial-value problem (1) has a solution $y(x)$ for $|x - x_0| \le min\,(\alpha, \beta/M)$, where M is the maximum of $|f(x,y)|$ in the rectangle R.

Uniqueness. It can happen, even if $F(x,y)$ is continuous, that the initial-value problem does not have a unique solution. A simple example of this phenomenon is given by the problem

$$\begin{cases} \dfrac{dy}{dx} =y^{2/3} \\ y(0) =0 \end{cases}$$

It is obvious that the zero function, $y(x) \equiv 0$, is a solution of this problem. Another solution is the function

$$y(x) = \frac{1}{27}x^3$$

To prove that the initial-value problem (1) has a *unique solution* in a neighborhood of $x = x_0$, it is necessary to assume somewhat more about $f(x,y)$. Here are the usual theorems on this.

Theorem 2. *If $f(x,y)$ and $\frac{\partial f(x,y)}{\partial x}$ are continuous in a rectangle R defined by (2), then the initial-value problem (1) has a unique solution in the interval $|x - x_0| \le min\,(\alpha, \beta/M)$.*

Theorem 3. *If $f(x,y)$ is continuous in the strip*

$$a \le x \le b, \quad -\infty < y < \infty$$

and satisfies there an inequality

$$|f(x,y_1) - f(x,y_2)| \le L|y_1 - y_2| \tag{3}$$

then the initial-value problem (1) has a unique solution in the interval $[a,b]$.

The Inequality (3) is called a *Lipschitz condition* in the second variable. We see immediately that this condition is *stronger* than continuity.

In the numerical solution of differential equations, we rarely expect to obtain the solution directly as a *formula* giving $y(x)$ as a function of x. Instead, we usually construct a table of function values of the form

$$\begin{array}{cccccc} x_0 & x_1 & x_2 & x_3 & \cdots & x_m \\ \hline y_0 & y_1 & y_2 & y_3 & \cdots & y_m \end{array} \tag{4}$$

Here, y_i is the computed approximation value of $y(x_i)$, our notation for the *exact* solution at x_i. From a table such as (4), a spline function or other approximating function can be constructed. However, most numerical methods for solving ordinary differential equations produce such a table first.

♣ **Taylor-Series Method**. For the Taylor-series method, it is necessary to assume that various partial derivatives of $f(x,y)$ exist. To illustrate the method we take a concrete example:

$$\begin{cases} y' = \cos x - \sin y + x^2 \\ y(-1) = 3 \end{cases} \tag{5}$$

At the heart of the procedure is the Taylor series for y, which we write as

$$y(x+h) = x(h) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y'''(x) + \frac{h^4}{4!}y^{(4)}(x) + \cdots \tag{6}$$

The derivative appearing here can be obtained from the differential equation (5). They are

$$\begin{aligned} y'' &= -\sin x - y'\cos y + 2x \\ y''' &= -\cos x - y''\cos y + (y')^2 \sin y + 2 \\ y^{(4)} &= \sin x - y'''\cos y + 3y'y''\sin y + (y')^3 \cos y \end{aligned}$$

At this point, our patience wears thin and we decide to use only terms up to and including h^4 in the Formula (6). The term that we have not included start with a term in h^5, and they constitute collectively the *truncation error* inherent in our procedure. The resulting numerical method is said to be of *order 4*.

Here is an algorithm for this method and the problem (5).

Algorithm for Taylor-Series Method

INPUT : The initial $x_0 = -1$; the initial $y_0 = 3$; the step size h; integer n.

FOR $k = 1, 2, \ldots, n$ DO

$y' := f(x, y) = \cos x - \sin y + x^2$

$y'' := df(x, y) = -\sin x - y' \cos y + 2x$

$y''' := d^2 f(x, y) = -\cos x - y'' \cos y + (y')^2 \sin y + 2$

$y^{(4)} := d^3 f(x, y) = \sin x - y''' \cos y + 3y'y'' \sin y + (y')^3 \cos y$

$y := y + h(y' + \frac{h}{2}(y'' + \frac{h}{3}(y''' + \frac{h}{4} y^{(4)})))$

$x := x + h$

OUTPUT: k, x, y

END

♣ **Euler's Method**. The Taylor-series method with $n = 1$ is called *Euler's method.* It looks like this:

$$y(x + h) = y(x) + hf(x, y)$$

This formula has the obvious advantage of not requiring any differentiation of $f(x, y)$. This advantage is offset by the necessity of taking small values for h to gain acceptable precision. Still, the method serves as a useful example and is of great importance theoretically since existence theorems can be based on it.

Example. Apply the Euler's method to the initial-value problem

$$\begin{cases} y' = 2x + y \\ \quad y(0) = 1, \end{cases} \tag{7}$$

where $h = 0.2$ and $n = 5$

Solution.

$$\begin{aligned}
x_1 &= x_0 + h = 0.2, f(x_0, y_0) = f(0, 1) = 1.000, && (n = 1)\\
y_1 &= y_0 + hf(x_0, y_0) = 1.000 + 0.2(1.000) = 1.200 \\
x_2 &= x_1 + h = 0.4, f(x_1, y_1) = f(0.2, 1.200) = 1.600, && (n = 2)\\
y_2 &= y_1 + hf(x_1, y_1) = 1.200 + 0.2(1.600) = 1.520 \\
x_3 &= x_2 + h = 0.6, f(x_2, y_2) = f(0.4, 1.520) = 2.320, && (n = 3)\\
y_3 &= y_2 + hf(x_2, y_2) = 1.520 + 0.2(2.320) = 1.984 \\
x_4 &= x_3 + h = 0.8, f(x_3, y_3) = f(0.6, 1.984) = 3.184, && (n = 4)\\
y_4 &= y_3 + hf(x_3, y_3) = 1.984 + 0.2(3.184) = 2.621 \\
x_5 &= x_4 + h = 1.0, f(x_4, y_4) = f(0.8, 2.621) = 4.221, && (n = 5)\\
y_5 &= y_4 + hf(x_4, y_4) = 2.621 + 0.2(4.221) = 3.465.
\end{aligned}$$

♣ **Runge-Kutta Methods**. The Taylor-series method has the drawback of requiring some analysis prior to programming it. We shall have to determine formulae for y'', y''', and $y^{(4)}$ by successive differentiation in (1). Then these functions will have to be programmed.

The Runge-Kutta methods avoid this difficulty although they do imitate the Taylor-series method by means of clever combinations of values of $f(x, y)$.

♡ **Second Order Runge-Kutta Method**. Let us begin with the Taylor series for $f(x, y)$:

$$y(x + h) = y(x) + hy'(x) + \frac{h^2}{2!} y''(x) + \frac{h^3}{3!} y''(x) + \frac{h^4}{4!} y^{(4)}(x) + \cdots \tag{8}$$

From the differential equation, we have

$$\begin{aligned} y'(x) &= f \\ y''(x) &= f_x + f_y y' = f_x + f_y f \\ y'''(x) &= f_{xx} + f_{xy} f + [f_x + f_y f] f_y + f[f_{xy} + f_{yy} f] \\ &etc \end{aligned}$$

The first three terms in Equation (8) can be written now in the form

$$\begin{aligned} y(x+h) =& y(x) + hf(x,y) + \frac{1}{2}h^2[f_x(x,y) + f(x,y)f_y(x,y)] + O(h^3) \\ =& y(x) + \frac{1}{2!}hf(x,y) + \frac{1}{2}h[f(x,y) + hf_x(x,y) + hf(x,y)f_y(x,y)] + O(h^3) \end{aligned} \tag{9}$$

In order to eliminate the partial derivatives in Equation (9), we use the Taylor series in two variables for

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

Thus Equation (9) becomes

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

Hence, the formula for advancing the solution is

$$y(x+h) = y(x) + \frac{h}{2}f(x,y) + \frac{h}{2}f(x+h, y+hf(x,y))$$

or equivalently

$$y(x+h) = y(x) + \frac{1}{2}(F_1 + F_2) \tag{10}$$

where

$$\begin{cases} F_1 = hf(x,y) \\ F_2 = hf(x+h, y+F_1) \end{cases}$$

This formula can be used repeatedly to advance the solution one step at a time. It is called a *Second-Order Runge-Kutta Method.* It is also known as *Heun's Method.*

♡ **Fourth Order Runge-Kutta Method**. The higher-order Runge-Kutta formulae are very tedious to derive, and we shall not do so. The formulae are rather elegant, however, and are easily programmed once the have been derived. Here are the formulae for the *classical Fourth-Order Runge-Kutta Method:*

$$y(x+h) = y(x) + \frac{1}{6}(F_1 + 2F_2 + 2F_3 + F_4) \tag{10}$$

where

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

This is called a fourth-order method because it reproduces the terms in Taylor series up to and including the one involving h^4. The error is therefore $O(h^5)$.

Algorithm for Fourth-Order Runge-Kutta Method

INPUT : The function $f(x, y)$; The initial x_0; the initial y_0; the step size h; integer n.

FOR $k = 1, 2, \ldots, n$ DO

$F_1 := hf(x, y)$

$F_2 := hf(x + \frac{1}{2}h, y + \frac{1}{2}F_1)$

$F_3 := hf(x + \frac{1}{2}h, y + \frac{1}{2}F_2)$

$F_4 := hf(x + h, y + F_3)$

$y := y + \frac{1}{6}[F_1 + 2F_2 + 2F_3 + F_4]$

$x := x + h$

OUTPUT: k, x, y

END

Example. Apply the fourth-order Runge-Kutta method to the initial-value problem

$$\begin{cases} y' = 2x + y \\ \quad y(0) = 1, \end{cases} \tag{7}$$

where $h = 0.2$ and $n = 2$

Solution.

$F_1 = hf(x_0, y_0) = 0.2f(0, 1) = 0.2(1) = 0.2,$ $(n = 1)$

$x_0 + \frac{h}{2} = 0 + \frac{1}{2}(0.2) = 0.1$ and $y_0 + \frac{1}{2}F_1 = 1 + \frac{1}{2}(0.2) = 1.1,$

$F_2 = hf(x_0 + \frac{h}{2}, y_0 + \frac{F_1}{2}) = 0.2f(0.1, 1.1) = 0.2(1.3) = 0.26$

$y_0 + \frac{1}{2}F_2 = 1 + \frac{1}{2}(0.26) = 1.13,$

$F_3 = hf(x_0 + \frac{h}{2}, y_0 + \frac{F_2}{2}) = 0.2f(0.1, 1.13) = 0.2(1.33) = 0.266$

$x_0 + h = 0 + 0.2 = 0.2$ and $y_0 + \frac{1}{2}F_3 = 1 + 0.266 = 1.266,$

$F_4 = hf(x_0 + h, y_0 + F_3) = 0.2f(0.2, 1.266) = 0.2(1.666) = 0.3332$

$y_1 = 1 + \frac{1}{6}[F_1 + 2F_2 + 2F_3 + F_4] = 1 + \frac{1}{6}(0.2 + 0.52 + 0.532 + 0.332) = 1.2642$

$F_1 = hf(x_1, y_1) = 0.2f(0.2, 1.2642) = 0.2(1.6642) = 0.33284,$ $(n = 2)$

$x_1 + \frac{h}{2} = 0.2 + \frac{1}{2}(0.2) = 0.3$ and $y_1 + \frac{1}{2}F_1 = 1.2642 + \frac{1}{2}(0.33284) = 1.43062,$

$F_2 = hf(x_1 + \frac{h}{2}, y_1 + \frac{F_1}{2}) = 0.2f(0.3, 1.43062) = 0.2(2.03062) = 0.40612$

$y_1 + \frac{1}{2}F_2 = 1.2642 + \frac{1}{2}(0.40612) = 1.46726,$

$F_3 = hf(x_1 + \frac{h}{2}, y_1 + \frac{F_2}{2}) = 0.2f(0.3, 1.43062) = 0.2(2.06726) = 0.41345$

$x_1 + h = 0.2 + 0.2 = 0.4$ and $y_1 + \frac{1}{2}F_3 = 1.2642 + 0.41345 = 1.67765,$

$F_4 = hf(x_1 + h, y_1 + F_3) = 0.2f(0.4, 1.67765) = 0.2(2.47765) = 0.49553$

$y_2 = 1.2642 + \frac{1}{6}[F_1 + 2F_2 + 2F_3 + F_4] = 1.2642 + \frac{1}{6}(0.33284 + 0.81224 + 0.8269 + 0.49553 = 1.6754$