13. Numerical solution of Ordinary Differential Equations: Background

Consider the initial value problem (IVP) for a first order ordinary differential equation:

$$dy/dx = f(x, y), \qquad y(x_0) = y_0.$$

The following theorem gives sufficient conditions for existence and uniqueness of a solution.

Theorem 10. *Let $f(x, y)$ satisfy the following conditions:*

(A) $f(x, y)$ is defined and continuous in the strip $x_0 \le x \le b$, $-\infty < y < \infty$, where x_0 and b are finite.

(B) There exists a constant L such that for any $x \in [x_0, b]$ and any two numbers y and y^*, $|f(x, y) - f(x, y^*)| \le L|y - y^*|$.

Then given any number y_0, there exists exactly one function $y(x)$ satisfying: (i) $y(x)$ is continuous and differentiable on $[x_0, b]$, (ii) $y'(x) = f(x, y(x))$, $x \in [x_0, b]$, and (iii) $y(x_0) = y_0$, i.e., the IVP has a unique solution.

It is also possible to view y as a vector with N components, so that the IVP represents a first order system of odes. One way to treat higher order odes is to reduce them to a first order system by introducing additional variables:

Example: $d^2y/dx^2 = f(x, y, dy/dx)$. Set $z = dy/dx$. Then $dz/dx = f(x, y, z)$ and we obtain the first order system:

$$\frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} z \\ f(x, y, z \end{pmatrix} = \begin{pmatrix} f_1(x, y, z) \\ f_2(x, y, z) \end{pmatrix}.$$

13.1. Euler's method.

Our numerical schemes will seek approximations to the solution $y(x)$ at a sequence of points x_i, i.e., we will approximate $y(x_i)$ by a number y_i. We begin by discussing the simplest method, i.e., Euler's method. Set $y_0 = y(x_0)$ and define

$$y_{n+1} = y_n + h_n f(x_n, y_n), \qquad n = 0, 1, \ldots,$$

where $h_n = x_{n+1} - x_n$.

One motivation of this method is that we have approximated the derivative $(dy/dx)(x_n)$ by the forward difference approximation $(y(x_{n+1}) - y(x_n))/(x_{n+1} - x_n)$ and so:

$$y(x_{n+1}) \approx y(x_n) + h_n f(x_n, y(x_n)).$$

We then define our approximations y_n as the value that restores equality, i.e., $y_{n+1} = y_n + h_n f(x_n, y_n)$.

Another motivation for the method is to expand the solution in a Taylor series expansion and neglect higher order terms, i.e.,

$$\begin{aligned} y(x_n + h_n) &= y(x_n) + h_n y'(x_n) + O(h_n^2) \\ &= y(x_n) + h_n f(x_n, y(x_n)) + O(h_n^2) \approx y(x_n) + h_n f(x_n, y(x_n)). \end{aligned}$$

Example: $y' = y \quad y(0) = 1$. Then Euler's method, using a constant step size $h_n = h$, is: $y_{n+1} = y_n + hy_n = (1 + h)y_n$. Hence $y_0 = 1$, $y_1 = 1 + h$, $y_2 = (1 + h)y_1 = (1 + h)^2$, and $y_n = (1 + h)^n$.

We next consider the convergence of Euler's method. Expanding the solution $y(x)$ in a Taylor series, we have

$$y(x_{n+1}) = y(x_n) + h_n f(x_n, y(x_n)) + (h_n^2/2)y''(\xi_n), \qquad x_n \le \xi_n \le x_{n+1}.$$

Neglecting any roundoff errors, the approximation given by Euler's method satisfies:

$$y_{n+1} = y_n + h_n f(x_n, y_n).$$

Let $e_n = y(x_n) - y_n$. Note $e_0 = 0$. Subtracting equations, we get

$$e_{n+1} = e_n + h_n[f(x_n, y(x_n)) - f(x_n, y_n)] + (h_n^2/2)y''(\xi_n),$$

Hence

$$\begin{aligned}|e_{n+1}| &\le |e_n| + h_n|f(x_n, y(x_n)) - f(x_n, y_n)| + (h_n^2/2)|y''(\xi_n)| \\ &\le |e_n| + h_n L e_n + h_n^2 M_2/2 \le (1 + h_n L)|e_n| + h_n^2 M_2/2,\end{aligned}$$

where we assume that $\max |y''(x)| \le M_2$. Consider the case when $h_n = h$ for all n. Then

$$|e_1| \le h^2 M_2/2, \qquad |e_2| \le (1 + hL)|e_1| + h^2 M_2/2 \le [1 + (1 + hL)]h^2 M_2/2,$$
$$|e_3| \le (1 + hL)|e_2| + h^2 M_2/2 \le [1 + (1 + hL) + (1 + hL)^2]h^2 M_2/2.$$

Using the fact that $\sum_{i=0}^{n-1} r^i = (1 - r^n)/(1 - r)$, we get

$$|e_n| \le [1 + (1 + hL) + (1 + hL)^2 + \cdots (1 + hL)^{n-1}]h^2 M_2/2 \le [(1 + hL)^n - 1]hM_2/(2L).$$

Observing that $e^x = 1 + x + e^\xi x^2/2 \ge 1 + x$ for all x, we see that $1 + hL \le e^{hL}$ and hence $(1 + hL)^n \le e^{nhL} = e^{(x_n - x_0)L}$. Thus, we get the error estimate:

$$|e_n| \le \frac{hM_2}{2L}[e^{(x_n - x_0)L} - 1],$$

so the error bound is $O(h)$. This bound is quite pessimistic and not a realistic way to determine a value of h to guarantee a given accuracy. It also requires a bound on y''.

We now consider what this result says about convergence of Euler's method, and first what we mean by convergence in this context.

Let x be a point in the interval $[x_0, b]$ and let $y(x)$ denote the true solution of the IVP at the point x. For each value of the step size h, we will have an approximation to $y(x)$ that we denote by y_n^h, where n will be determined by the equation $x - x_0 = nh$. Thus, as h is decreased, the value of n for which y_n denotes the approximation to $y(x)$ will also change. So for convergence, we want:

$$\lim_{\substack{h \to 0 \\ n \to \infty \\ nh = x}} y_n^h = y(x).$$

Example: For $x_0 = 0$, $x = 1/2$, and the sequence $h = 1/4, 1/8, 1/16, 1/32$, we look for the convergence of $y_2^{1/4}$, $y_4^{1/8}$, $y_8^{1/16}$, $y_{16}^{1/32}$.

Suppose in the error estimate for Euler's method, we keep $x_n = x$ fixed, i.e., we choose n so that $nh = x - x_0$ and let $h \to 0$. Then

$$|y(x) - y_n^h| \le \frac{hM_2}{2L}[e^{(x-x_0)L} - 1] \implies \lim_{\substack{h\to 0\\ n\to\infty\\ nh=x}} |y(x) - y_n^h| = 0,$$

so we have converence of the method as $h \to 0$.

13.2. **Taylor series methods.** Consider the Taylor series of $y(x)$, the solution of the IVP, about $x = x_n$:

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2}y^{(2)}(x_n) + \cdots + \frac{h^k}{k!}y^{(k)}(x_n) + \frac{h^{k+1}}{(k+1)!}y^{(k+1)}(\xi).$$

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

$$y''(x) = f'(x, y(x)) = \frac{d}{dx}f(x, y(x)) = f_x(x, y(x)) + f_y(x, y(x))\frac{dy}{dx}.$$

In general,

$$y^{(k)}(x) = f^{(k-1)}(x, y(x)) = \frac{d}{dx}f^{(k-2)}(x, y(x)) = f_x^{(k-2)}(x, y(x)) + f_y^{(k-2)}(x, y(x))\frac{dy}{dx}.$$

Hence, if $y(x_n)$ were known, we could compute an approximation to $y(x_n + h)$ by using the truncated Taylor series:

$$y(x_n + h) \approx y(x_n) + hf(x_n, y(x_n)) + \frac{h^2}{2}f'(x_n, y(x_n)) + \cdots + \frac{h^k}{k!}f^{(k-1)}(x_n, y(x_n)),$$

i.e., if we denote by y_n the approximation to $y(x_n)$, we can define the Taylor algorithm of order k as the sequence of computations

$$y_{n+1} = y_n + hT_k(x_n, y_n), \qquad n = 0, 1, \ldots,$$

where

$$T_k(x, y) = f(x, y) + \frac{h}{2}f'(x, y) + \cdots + \frac{h^{k-1}}{k!}f^{(k-1)}(x, y).$$

Note: Euler's method is the Taylor algorithm of order 1.

Example: We wish to solve the IVP $y' = 1/x^3 - y/x - y^2$, $y(1) = 2$ by the Taylor algorithm of order 2. Now

$$f(x, y) = \frac{1}{x^3} - \frac{y}{x} - y^2$$

and

$$\begin{aligned} f'(x, y) = f_x(x, y) + f_y(x, y)f(x, y) &= -\frac{3}{x^4} + \frac{y}{x^2} - \left[\frac{1}{x} + 2y\right] f \\ &= -\frac{3}{x^4} + \frac{y}{x^2} - \left[\frac{1}{x} + 2y\right]\left[\frac{1}{x^2} - \frac{y}{x} - y^2\right]. \end{aligned}$$

Then

$$y_{n+1} = y_n + hf(x_n.y_n) + \frac{h^2}{2}f'(x_n, y_n),$$

where $f'(x, y)$ defined above.

Note we can also compute $f'(x,y)$ directly, remembering that y is a function of x, i.e.,

$$f'(x,y) = \frac{d}{dx}\left[\frac{1}{x^3} - \frac{y}{x} - y^2\right] = -\frac{3}{x^4} - \frac{xy'-y}{x^2} - 2yy' = -\frac{3}{x^4} + \frac{y}{x^2} - \left[\frac{1}{x} + 2y\right] y'$$
$$= -\frac{3}{x^4} + \frac{y}{x^2} - \left[\frac{1}{x} + 2y\right]\left[\frac{1}{x^2} - \frac{y}{x} - y^2\right].$$

Definition: The local truncation error for the Taylor series method of order k is defined by:

$$y(x_{n+1}) - y(x_n) - hT_k(x_n, y(x_n)) = \frac{h^{k+1}}{(k+1)!} y^{(k+1)}(\xi_n).$$

The local truncation of Euler's method is $h^2 y^{(2)}(\xi_n)/2$.

The Taylor algorithm of order k is an example of a one-step method, i.e, the value of y_{n+1} only depends on one past value (y_n). One-step methods have the form

$$y_{n+1} = y_n + h\Phi(x_n, y_n), \qquad n = 0, 1, \ldots,$$

Analogously to the Taylor series methods, we define the Local Truncation Error of such methods to be

$$LTE = y(x_{n+1}) - y(x_n) - h\Phi(x_n, y(x_n)).$$

Then we have the following result giving a bound on the global error.

Theorem 11. *If $|\Phi(x,u) - \Phi(x,v)| \le \mathcal{L}|u-v|$ for $a \le x \le b$, $0 < h < h_0$ and all u, v and if the local trucation error is $O(h^{p+1})$, then for any $x_n = x_0 + nh \in [x_0, b]$,*

$$|y(x_n) - y_n| \le C\frac{h^p}{\mathcal{L}}(e^{\mathcal{L}(x_n - x_0)} - 1).$$

The proof of this result is essentially identical to the proof of the error bound for Euler's method.

Although Taylor series methods become increasingly more accurate as k increases, their major disadvantage is that they require calulation of high derivatives of the function f.