1. COMPOSITE OPERATORS

1.1. Ordinary differential equations

An n^{th}-order ordinary differential equation given in explicit form

$$y^{(n)} = f(t, y, y', \dots, y^{(n-1)}) \tag{1}$$

is a statement of equality between the action of two operators. On the left hand side the linear differential operator

$$\mathscr{L} = \frac{\mathrm{d}}{\mathrm{d}t^n}$$

acts upon a sufficiently smooth function, $y \in C^{(n)}(\mathbb{R})$, $\mathscr{L}: C^{(n)}(\mathbb{R}) \to C(\mathbb{R})$. On the right hand side, a nonlinear operator $\mathscr{F}$ acts upon the independent variable t and the first $n-1$ derivatives

$$\mathscr{F}: \mathbb{R} \times C(\mathbb{R}) \times \cdots \times C^{(n-1)}(\mathbb{R}).$$

An associated function $f: \mathbb{R}^{n+1} \to \mathbb{R}$ has values given by

$$f(t) = f(t, y(t), y'(t), \dots, y^{(n-1)}(t)).$$

The numerical solution of (1) seeks to find an approximant of y through:

1. Approximation of the differentiation operator $\mathscr{L}$;
2. Approximation of the nonlinear operator $\mathscr{F}$;
3. Approximation of the equality between the effect of the two operators

$$\mathscr{L}(y) = \mathscr{F}(t, y, \dots, y^{(n-1)}).$$

These approximation problems shall be considered one-by-one, starting with approximation of $\mathscr{L}$ assuming that the action of $\mathscr{F}$ is exactly represented through knowledge of f.

Note that an n^{th}-order differential equation can be restated as a system of n first-order equations

$$\boldsymbol{z}' = \boldsymbol{F}(t, \boldsymbol{z}) \tag{2}$$

by introducing

$$\boldsymbol{z} = [\ z_1\ \ z_2\ \ \dots\ \ z_{n-1}\ \ z_n\ ]^T = [\ y\ \ y'\ \ \dots\ \ y^{(n-2)}\ \ y^{(n-1)}\ ]^T,$$

$$\boldsymbol{F}(t, \boldsymbol{z}) = [\ z_2(t)\ \ z_3(t)\ \ \dots\ \ z_n(t)\ \ f(t, z_1(t), \dots, z_n(t))\ ]^T.$$

Approximation of the differentiation operator for the problem

$$y' = f(t, y) \tag{3}$$

can readily be extended to the individual equations of system (2).

Construction of approximants to (3) is first considered for the initial value problem (IVP)

$$y' = f(t, y), y(0) = y_0. \tag{4}$$

The two procedures are:

1. Approximation of the differentiation operator;
2. Differentiation of an approximation of y.

Often the two approaches leads to the same algorithm. The problem (4) has a unique solution over some rectangle $R = [0, T] \times [y_1, y_2]$ in the ty-plane if f is Lipschitz-continuous, stated as the existence of $K \in \mathbb{R}_+$ such that

$$|f(t, y_2) - f(t, y_1)| \leqslant K |y_2 - y_1|.$$

Note that Lipschitz continuity is a stronger condition than standard continuity in that it states $|f(t,y_2)-f(t,y_1)| = \mathcal{O}(|y_2-y_1|)$. Differentiability implies Lipschitz continuity.

Consider approximation of $\mathrm{d}/\mathrm{d}t$ through forward finite differences

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{h}\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \cdots - \right), \tag{5}$$

and denote by y_i the approximation of $y(t)$, $y_i \cong y(t_i)$ at the equidistant sample points $t_i = ih$. Evaluation of (2) with a k^{th} order truncation of (5) then gives

$$f(t_i, y(t_i)) = \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)(t_i) \cong \frac{1}{h}\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \cdots - (-1)^k \frac{1}{k}\Delta^k\right).$$

Euler forward scheme. For $k=1$, the resulting scheme is

$$\frac{1}{h}\Delta y_i = \frac{y_{i+1}-y_i}{h} = f(t_i, y_i) = f_i \Rightarrow y_{i+1} = y_i + hf_i,$$

where $f_i \cong f(t_i, y(t_i))$, and is known as the Euler forward scheme. New values are obtained from previous values. Such methods are said to be *explicit schemes*. As to be expected from the truncation of (5) to the first term in the series, the scheme is first-order accurate. This can be formally established by evaluation of the error at step i

$$e_i = y(t_i) - y_i.$$

At the next step, $e_{i+1} = y(t_{i+1}) - y_i$, and subtraction of the two errors gives upon Taylor-series expansion

$$e_{i+1} - e_i = y(t_{i+1}) - y(t_i) - (y_{i+1} - y_i) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\xi_i) - y(t_i) - hf_i.$$

Since $f_i = f(t_i, y(t_i))$, the one-step error is given by

$$\tau_i = e_{i+1} - e_i = \frac{h^2}{2}y''(\xi_i).$$

After N steps,

$$e_N - e_0 = \frac{h^2}{2}\sum_{i=1}^{N} y''(\xi_i).$$

Assuming $e_0 = 0$ (exact representation of the initial condition),

$$e_N \leqslant \frac{Nh^2}{2}\|y''\|_\infty.$$

Numerical solution of the initial value problem is carried out over some finite interval $[0,T]$, with $T = Nh$, hence

$$e_N \leqslant h\frac{T}{2}\|y''\|_\infty = \mathcal{O}(h), \tag{6}$$

indeed with first-order convergence.

Alternatively, one could use the backward or centered finite difference approximations of the derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{h}\left(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \cdots\right) = \frac{1}{h}\left(\delta - \frac{1}{24}\delta^3 + \frac{3}{640}\delta^5 - \cdots - \right). \tag{7}$$

Backward Euler scheme. Truncation of the backward operator at first order gives

$$f(t_i, y(t_i)) = \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)_i \cong \frac{1}{h}(\nabla y)_i = \frac{y_i - y_{i-1}}{h} \Rightarrow y_i = y_{i-1} + hf_i = y_{i-1} + hf(t_i, y_i).$$

Note now that the unknown value y_i appears as an argument to f, with $f_i = f(t_i, y_i)$, the approximation of the exact slope $f(t_i, y(t_i))$. Some procedure to solve the equation

$$y_i - y_{i-1} - hf(t_i, y_i) = 0,$$

must be introduced in order to advance the solution from t_{i-1} to t_i. Such methods are said to be *implicit schemes*. The same type of error analysis as in the forward Euler case again leads to the conclusion that the one-step error is $\mathcal{O}(h^2)$, while the overall error over a finite interval $[0,T]$ satisfies (6), and is first-order.

Leapfrog scheme. Truncation of the centered operator at first order gives

$$f(t_i, y(t_i)) = \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)_i \cong \frac{1}{h}(\delta y)_i = \frac{y_{i+1/2} - y_{i-1/2}}{h} \Rightarrow y_{i+1/2} = y_{i-1/2} + hf_i = y_{i-1/2} + hf(t_i, y_i).$$

The higher-order accuracy of the centered finite differences leads to a more accurate numerical solution of the problem (4). The one-step error is third-order accurate,

$$e_{i+1/2} - e_{i-1/2} = y(t_{i+1/2}) - y(t_{i-1/2}) + hf(t_i, y_i) = \frac{h^3}{3} y'''(\xi_i),$$

and the overall error over interval $[0, T = Nh]$ is second-order accurate

$$e_N \leqslant \frac{h^2}{3} T \, \|y'''\|_\infty .$$