LECTURE 21: ORDINARY DIFFERENTIAL EQUATIONS - SINGLE STEP METHODS

1. Ordinary differential equations

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

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

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

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

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

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

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

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

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

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

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

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)

$$y' = f(t, y), y(0) = y_0.$$
 (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

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

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

Consider approximation of d/dt through forward finite differences

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

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

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

2. Differentiation operator approximation from polynomial interpolants

2.1. 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,

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

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

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

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

$$e_N \leqslant h \frac{T}{2} \| y^{\prime \prime} \|_{\infty} = \mathcal{O}(h), \tag{6}$$

indeed with first-order convergence.

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

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

2.2. Backward Euler scheme

Truncation of the backward operator at first order gives

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

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.

2.3. 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,

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

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

$$e_N \leqslant \frac{h^2}{3} T \, \| y^{\prime \prime \prime} \|_{\infty}$$