1 Ordinary differential equations

Many physical problems can be reformulated in terms of a system of *ordinary differential equations* (ODEs),

$$\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y}), \tag{1}$$

with an initial condition

$$\mathbf{y}(x_0) = \mathbf{y}_0, \tag{2}$$

where $\mathbf{y}$ and $\mathbf{f}(x, \mathbf{y})$ are generally understood as column-vectors.

1.1 Runge-Kutta methods

Runge-Kutta methods are one-step methods where the solution $\mathbf{y}$ is advanced by one step $h = x_1 - x_0$ as

$$\mathbf{y}_1 = \mathbf{y}_0 + h\mathbf{k}, \tag{3}$$

where $\mathbf{k}$ is a cleverly chosen (vector) constant. The Runge-Kutta methods are distinguished by their *order*: a method has order p if its error is $O(h^{p+1})$ for small h, or, in other words, if the solution of an ODEs is a polynomial of the order p the ODEs is integrated exactly by the method.

The first order Runge-Kutta method is simply the Euler's method

$$\mathbf{k} = \mathbf{f}(x_0, \mathbf{y}_0). \tag{4}$$

Second order Runge-Kutta method advances the solution by an auxiliary evaluation of the derivative, e.g. the *half-step method*,

$$\begin{aligned} \mathbf{k}_0 &= \mathbf{f}(x_0, \mathbf{y}_0)\ , \\ \mathbf{y}_{1/2} &= \mathbf{y}_0 + \frac{h}{2}\mathbf{k}_0\ , \\ \mathbf{k}_{1/2} &= \mathbf{f}(x_{1/2}, \mathbf{y}_{1/2})\ , \\ \mathbf{k} &= \mathbf{k}_{1/2}\ , \end{aligned} \tag{5}$$

or the *two-point method*,

$$\begin{aligned} \mathbf{k}_0 &= \mathbf{f}(x_0, \mathbf{y}_0), \\ \mathbf{k}_1 &= \mathbf{f}(x_1, \mathbf{y}_0 + h\mathbf{k}_0), \\ \mathbf{k} &= \frac{1}{2}(\mathbf{k}_0 + \mathbf{k}_1)\ . \end{aligned} \tag{6}$$

These two methods can be combined into a third order method,

$$\mathbf{k} = \frac{1}{6}\mathbf{k}_0 + \frac{4}{6}\mathbf{k}_{1/2} + \frac{1}{6}\mathbf{k}_1\ . \tag{7}$$

Higher order Runge-Kutta methods have been devised, with the most commonly used being the famous Runge-Kutta-Fehlberg fourth-fifth order method implemented in the renowned **rkf45** (now superseded by netlib.org/ode/rksuite).

1.2 Multi-step and predictor-corrector methods

Multi-step methods try to use the information about the function gathered at the previous steps. They are generally not *self-starting* as there are no previous points at the start of the integration. The first step should be done with a one-step method.

Predictor-corrector methods use extra iterations to improve the solution.

1.2.1 A two-step method

For example, having the two points, $\mathbf{y}_0$ and $\mathbf{y}_1$, the sought function $\mathbf{y}$ can be approximated in the vicinity of the point x_1 as

$$\bar{\mathbf{y}}(x) = \mathbf{y}_1 + \mathbf{y}_1' \cdot (x - x_1) + \mathbf{c} \cdot (x - x_1)^2, \tag{8}$$

where the coefficient $\mathbf{c}$ can be found from the condition $\mathbf{y}(x_0) = \mathbf{y}_0$,

$$\mathbf{c} = \frac{\mathbf{y}_0 - \mathbf{y}_1 - \mathbf{y}_1' \cdot (x_0 - x_1)}{(x_0 - x_1)^2}. \tag{9}$$

Now $\mathbf{y}_2$ can be calculated as $\bar{\mathbf{y}}(x_2)$ from (8).

1.2.2 A predictor-corrector method

Having the two-step approximation $\bar{\mathbf{y}}(x)$ one can estimate $\bar{\mathbf{f}}_2 = \mathbf{f}(x_2, \bar{\mathbf{y}}(x_2))$. Using this new information one can improve the approximation (8) by one order, namely

$$\bar{\bar{\mathbf{y}}}(x) = \bar{\mathbf{y}}(x) + \mathbf{d} \cdot (x - x_1)^2(x - x_0). \tag{10}$$

The coefficient $\mathbf{d}$ can be found from the condition $\bar{\bar{\mathbf{y}}}'(x_2) = \bar{\mathbf{f}}_2$,

$$\mathbf{d} = \frac{\bar{\mathbf{f}}_2 - \mathbf{y}_1' - 2\mathbf{c} \cdot (x_2 - x_1)}{2(x_2 - x_1)(x_2 - x_0) + (x_2 - x_1)^2}. \tag{11}$$

Equation (10) gives a better estimate, $\mathbf{y}_2 = \bar{\bar{\mathbf{y}}}(x_2)$, of the function at the point x_2.

In this context the formula (8) is referred to as *predictor*, and (10) as *corrector*. The difference between the two gives an estimate of the error.

1.3 Step-size control

The *tolerance* τ is the maximal accepted error on the given integration step consistent with the required absolute (δ) and relative (ϵ) accuracies to be achieved in the integration of an ODEs. Under assumption of random distribution of errors on the integration steps from a to b the tolerance, according to the central limit theorem, scales as a square root of the step-size h,

$$\tau = (\epsilon||y|| + \delta)\sqrt{\frac{h}{b-a}}. \qquad (12)$$

The error of the integration method on a given step can be estimated e.g. by comparing the solutions for a full-step and two half-steps (the *Runge principle*),

$$\mathrm{err} = \frac{||y_{\mathrm{full-step}} - y_{\mathrm{two-half-steps}}||}{2^p - 1}, \qquad (13)$$

where p is the order of the algorithm used.

The step is accepted if the error is smaller than tolerance. The next step can be estimated according to the (empirical) prescription

$$h_{\mathrm{next}} = h_{\mathrm{previous}} \times \left(\frac{\mathrm{tol}}{\mathrm{err}}\right)^{\mathrm{Power}} \times \mathrm{Safety}, \qquad (14)$$

where power ≈ 0.25, Safety ≈ 0.95. It is better to pick such formula, that the full-step and two half-step calculations share the evaluations of the function $\mathbf{f}(x, \mathrm{y})$ which would increase the efficiency of the algorithm.