Lecture 18

Numerical Approximations for IVP

MA 322: Scientific Computing

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1 Runge-Kutta Methods

Eulers method is only first-order accurate; nevertheless, it is simple and cheap to implement because, to obtain y_{n+1} from y_n, we only require a single evaluation of the function f, at (x_n, y_n). RungeKutta methods aim to achieve higher accuracy by sacrificing the efficiency of Eulers method through re-evaluating $f(\cdot,\cdot)$ at points intermediate between $(x_n, y(x_n))$ and $(x_{n+1}, y(x_{n+1}))$. Consider, for example, the following family of methods:

$$y_{n+1} = y_n + h(ak_1 + bk_2), \tag{1}$$

where

$$k_1 \;=\; f(x_n, y_n), \;\; k_2 = f(x_n + \alpha h, y_n + \beta h k_1), \tag{2}$$

and where the parameters a, b, α and β are to be determined.

Note that Eulers method is a member of this family of methods, corresponding to $a = 1$ and $b = 0$. In fact, improved Euler method is also a part of this family. However, we are now seeking methods that are at least second-order accurate. Recall the general one step method

$$y_{n+1} = y_n + h\Phi(x_n, y_n; h). \tag{3}$$

So that the equation (1) can be written as

$$y_{n+1} = y_n + h(ak_1 + bk_2) = y_n + h\Phi(x_n, y_n; h), \tag{4}$$

with

$$\Phi(x_n, y_n; h) = af(x_n, y_n) + bf(x_n + \alpha h, y_n + \beta h f(x_n, y_n)). \tag{5}$$

By the previous lecture, a method from this family will be consistent if, and only if

$$\lim_{h\to 0} \Phi(x_n, y_n; h) = f(x_n, y_n), \tag{6}$$

which yields $a + b = 1$. Further conditions on the parameters are found by attempting to maximize the order of accuracy of the method. Last lecture, we have derived following error bound

Theorem 1.1 Consider the general one step method (3). We assume that Φ is continuous in a region $R \subset \mathbb{R}^2$ containing the initial point (x_0, y_0) and there exists a positive constant L_Φ such that

$$|\Phi(x, y; h) - \Phi(x, z; h)| \le L_\Phi |y - z| \;\; \forall\, (x, y),\; (x, z) \in R. \tag{7}$$

Then we have following error bound

$$|e_k| \le \exp^{L_\Phi(x_k - x_0)} |e_0| + \Big[\frac{\exp^{L_\Phi(x_k-x_0)} - 1}{L_\Phi}\Big] T, n = 0,\ 1,\ 2, \ldots,\ n, \tag{8}$$

where $T = \max_{0\le k\le n-1} |T_k|$, $\;T_k = \frac{y(x_{k+1}) - y(x_k)}{h} - \Phi(x_k, y(x_k); h)$.

Using above result, we have discussed the convergence of improved Euler method. Note that the convergence of (3) depends on $T = \max_{0\le k\le n-1} |T_k|$. To determine a bound for T, we need the higher derivatives of $y(x)$, which are obtained by differentiating the function f:

$$\begin{aligned}
y'(x_n) &= f, \\
y''(x_n) &= f_x + f_y y' = f_x + f_y f, \\
y'''(x_n) &= f_{xx} + f_{xy} f + (f_{xy} + f_{yy} f) f + f_y (f_x + f_y f),
\end{aligned}$$

and so on; in these expressions the subscripts x and y denote partial derivatives, and all functions appearing on the right-hand sides are to be evaluated at $(x_n, y(x_n))$. We also need to expand $\Phi(x_n, y(x_n); h)$ in powers of h, giving (with the same notational conventions as before)

$$\begin{aligned}\Phi(x_n, y(x_n); h) &= af + b(f + \alpha h f_x + \beta h f f_y + \frac{1}{2}(\alpha h)^2 f_{xx} \\ &\qquad + \alpha\beta h^2 f f_{xy} + \frac{1}{2}(\beta h)^2 f^2 f_{yy} + \mathrm{O}(h^3)).\end{aligned}$$

Then, we obtain

$$\begin{aligned}T_n &= \frac{y(x_{n+1}) - y(x_n)}{h} - \Phi(x_n, y(x_n); h) \\ &= f + \frac{1}{2}h(f_x + f f_y) \\ &\quad + \frac{1}{6}h^2(f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y(f_x + f_y f)) \\ &\quad - \{af + b(f + \alpha h f_x + \beta h f f_y + \frac{1}{2}(\alpha h)^2 f_{xx} \\ &\qquad + \alpha\beta h^2 f f_{xy} + \frac{1}{2}(\beta h)^2 f^2 f_{yy} + \mathrm{O}(h^3))\}\end{aligned}$$

As $1 - a - b = 0$, the term $(1 - a - b)f$ is equal to 0. The coefficient of the term in h is

$$\frac{1}{2}(f_x + f f_y) - b\alpha f_x - b\beta f f_y$$

which vanishes for all functions f provided that

$$b\alpha = b\beta = \frac{1}{2}.$$

The method is therefore second-order accurate if

$$\beta = \alpha, \quad a = 1 - \frac{1}{2\alpha}, \quad b = \frac{1}{2\alpha}, \quad \alpha \neq 0,$$

showing that there is a one-parameter family of second-order methods of this form, parametrised by $\alpha \neq 0$. Evidently there is no choice of the free parameter α which will make this method third-order accurate for all functions f.

A similar but more complicated analysis is used to construct Runge Kutta methods of higher order. One of the most frequently used methods of the RungeKutta family is often known as the classical fourth-order method:

$$y_{n+1} = y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4),$$

where

$$\begin{aligned}k_1 &= f(x_n, y_n), \\ k_2 &= f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1), \\ k_3 &= f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2), \\ k_4 &= f(x_n + h, y_n + hk_3).\end{aligned}$$

Here k_2 and k_3 represent approximations to the derivative y' at points on the solution curve, intermediate between $(x_n, y(x_n))$ and $(x_{n+1}, y(x_{n+1}))$, and $\Phi(x_n, y_n; h)$ is a weighted average of the k_i, $i = 1, 2, 3, 4$. For the numerical example, see Table 6.24 of the book by Atkinson (An introduction to Numerical Analysis).