Mathematical Tripos Part IB: Lent 2010

Numerical Analysis – Lecture 7[1]

Order: The *order* of a general numerical method $\boldsymbol{y}_{n+1} = \boldsymbol{\varphi}_h(t_n, \boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_n)$ for the solution of (4.1) is the largest integer $p \geq 0$ such that

$$\boldsymbol{y}(t_{n+1}) - \boldsymbol{\varphi}_h(t_n, \boldsymbol{y}(t_0), \boldsymbol{y}(t_1), \ldots, \boldsymbol{y}(t_n)) = \mathcal{O}\big(h^{p+1}\big)$$

for all $h > 0$, $n \geq 0$ and all sufficiently smooth functions $\boldsymbol{f}$ in (4.1). Note that, unless $p \geq 1$, the 'method' is an unsuitable approximation to (4.1): in particular, $p \geq 1$ is necessary for convergence.

The order of Euler's method: We now have $\boldsymbol{\varphi}_h(t, \boldsymbol{y}) = \boldsymbol{y} + h\boldsymbol{f}(t, \boldsymbol{y})$. Substituting the exact solution of (4.1), we obtain from the Taylor theorem

$$\boldsymbol{y}(t_{n+1}) - [\boldsymbol{y}(t_n) + h\boldsymbol{f}(t_n, \boldsymbol{y}(t_n))] = [\boldsymbol{y}(t_n) + h\boldsymbol{y}'(t_n) + \tfrac{1}{2}h^2\boldsymbol{y}''(t_n) + \cdots] - [\boldsymbol{y}(t_n) + h\boldsymbol{y}'(t_n)] = \mathcal{O}\big(h^2\big)$$

and we deduce that Euler's method is of order 1.

Theta methods: We consider methods of the form

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h[\theta\boldsymbol{f}(t_n, \boldsymbol{y}_n) + (1-\theta)\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1})], \qquad n = 0, 1, \ldots, \tag{4.4}$$

where $\theta \in [0, 1]$ is a parameter:

- If $\theta = 1$, we recover Euler's method.
- if $\theta \in [0, 1)$ then the *theta method* (4.4) is *implicit:* Each time step requires the solution of N (in general, nonlinear) algebraic equations for the unknown vector $\boldsymbol{y}_{n+1}$.
- The choices $\theta = 0$ and $\theta = \frac{1}{2}$ are known as

  Backward Euler: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1})$,

  Trapezoidal rule: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \frac{1}{2}h[\boldsymbol{f}(t_n, \boldsymbol{y}_n) + \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1})]$.

Solution of nonlinear algebraic equations can be done by iteration. For example, for backward Euler, letting $\boldsymbol{y}_{n+1}^{[0]} = \boldsymbol{y}_n$, we may use

Direct iteration $\quad \boldsymbol{y}_{n+1}^{[j+1]} = \boldsymbol{y}_n + h\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}^{[j]})$;

Newton–Raphson: $\quad \boldsymbol{y}_{n+1}^{[j+1]} = \boldsymbol{y}_{n+1}^{[j]} - \left[I - h\frac{\partial \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}^{[j]})}{\partial \boldsymbol{y}}\right]^{-1} [\boldsymbol{y}_{n+1}^{[j]} - \boldsymbol{y}_n - h\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}^{[j]})]$;

Modified Newton–Raphson: $\quad \boldsymbol{y}_{n+1}^{[j+1]} = \boldsymbol{y}_{n+1}^{[j]} - \left[I - h\frac{\partial \boldsymbol{f}(t_n, \boldsymbol{y}_n)}{\partial \boldsymbol{y}}\right]^{-1} [\boldsymbol{y}_{n+1}^{[j]} - \boldsymbol{y}_n - h\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}^{[j]})]$

The order of the theta method: It follows from (4.4) and Taylor's theorem that

$$\begin{aligned}
&\boldsymbol{y}(t_{n+1}) - \boldsymbol{y}(t_n) - h[\theta\boldsymbol{y}'(t_n) + (1-\theta)\boldsymbol{y}'(t_{n+1})] \\
&= [\boldsymbol{y}(t_n) + h\boldsymbol{y}'(t_n) + \tfrac{1}{2}h^2\boldsymbol{y}''(t_n) + \tfrac{1}{6}h^3\boldsymbol{y}'''(t_n)] - \boldsymbol{y}(t_n) - \theta h\boldsymbol{y}'(t_n) \\
&\quad - (1-\theta)h[\boldsymbol{y}'(t_n) + h\boldsymbol{y}''(t_n) + \tfrac{1}{2}h^2\boldsymbol{y}'''(t_n)] + \mathcal{O}\big(h^4\big) \\
&= (\theta - \tfrac{1}{2})h^2\boldsymbol{y}''(t_n) + (\tfrac{1}{2}\theta - \tfrac{1}{3})h^3\boldsymbol{y}'''(t_n) + \mathcal{O}\big(h^4\big).
\end{aligned}$$

Therefore the theta method is of order 1, except that the trapezoidal rule is of order 2.

4.2 Multistep methods

It is often useful to use past solution values in computing a new value. Thus, assuming that $\boldsymbol{y}_n, \boldsymbol{y}_{n+1}, \ldots, \boldsymbol{y}_{n+s-1}$ are available, where $s \geq 1$, we say that

$$\sum_{l=0}^{s} \rho_l \boldsymbol{y}_{n+l} = h \sum_{l=0}^{s} \sigma_l \boldsymbol{f}(t_{n+l}, \boldsymbol{y}_{n+l}), \qquad n = 0, 1, \ldots, \tag{4.5}$$

[1]Corrections and suggestions to these notes should be emailed to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartIB/Handouts.html`.

where $\rho_s = 1$, is an s-step method. If $\sigma_s = 0$, the method is *explicit,* otherwise it is *implicit.*
If $s \ge 2$, we need to obtain extra *starting values* $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{s-1}$ by different time-stepping method.
Let $\rho(w) = \sum_{l=0}^{s} \rho_l w^l$, $\sigma(w) = \sum_{l=0}^{s} \sigma_l w^l$.

Theorem *The multistep method (4.5) is of order $p \ge 1$ iff*

$$\rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) = \mathcal{O}\big(z^{p+1}\big)\,, \qquad z \to 0. \tag{4.6}$$

Proof. Substituting the exact solution and expanding into Taylor series about t_n,

$$\begin{aligned}\sum_{l=0}^{s} \rho_l \boldsymbol{y}(t_{n+l}) - h \sum_{l=0}^{s} \sigma_l \boldsymbol{y}'(t_{n+l}) &= \sum_{l=0}^{s} \rho_l \sum_{k=0}^{\infty} \frac{1}{k!} \boldsymbol{y}^{(k)}(t_n) l^k h^k - h \sum_{l=0}^{s} \sigma_l \sum_{k=0}^{\infty} \frac{1}{k!} \boldsymbol{y}^{(k+1)}(t_n) l^k h^k \\ &= \left(\sum_{l=0}^{s} \rho_l\right) \boldsymbol{y}(t_n) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{l=0}^{s} l^k \rho_l - k \sum_{l=0}^{s} l^{k-1} \sigma_l\right) h^k \boldsymbol{y}^{(k)}(t_n).\end{aligned}$$

Thus, to obtain $\mathcal{O}\big(h^{p+1}\big)$ regardless of the choice of $\boldsymbol{y}$, it is necessary and sufficient that

$$\sum_{l=0}^{s} \rho_l = 0, \qquad \sum_{l=0}^{s} l^k \rho_l = k \sum_{l=0}^{s} l^{k-1} \sigma_l, \qquad k = 1, 2, \ldots, p. \tag{4.7}$$

On the other hand, expanding again into Taylor series,

$$\begin{aligned}\rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) &= \sum_{l=0}^{s} \rho_l \mathrm{e}^{lz} - z \sum_{l=0}^{s} \sigma_l \mathrm{e}^{lz} = \sum_{l=0}^{s} \rho_l \left(\sum_{k=0}^{\infty} \frac{1}{k!} l^k z^k\right) - z \sum_{l=0}^{s} \sigma_l \left(\sum_{k=0}^{\infty} \frac{1}{k!} l^k z^k\right) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{l=0}^{s} l^k \rho_l\right) z^k - \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \left(\sum_{l=0}^{s} l^{k-1} \sigma_l\right) z^k \\ &= \left(\sum_{l=0}^{s} \rho_l\right) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{l=0}^{s} l^k \rho_l - k \sum_{l=0}^{s} l^{k-1} \sigma_l\right) z^k.\end{aligned}$$

The theorem follows from (4.7). □

Example The 2-step *Adams–Bashforth method* is

$$\boldsymbol{y}_{n+2} - \boldsymbol{y}_{n+1} = h[\tfrac{3}{2} \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - \tfrac{1}{2} \boldsymbol{f}(t_n, \boldsymbol{y}_n)]. \tag{4.8}$$

Therefore $\rho(w) = w^2 - w$, $\sigma(w) = \frac{3}{2} w - \frac{1}{2}$ and

$$\rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) = [1 + 2z + 2z^2 + \tfrac{4}{3} z^3] - [1 + z + \tfrac{1}{2} z^2 + \tfrac{1}{6} z^3] - \tfrac{3}{2} z[1 + z + \tfrac{1}{2} z^2] + \tfrac{1}{2} z + \mathcal{O}\big(z^4\big) = \tfrac{5}{12} z^3 + \mathcal{O}\big(z^4\big)\,.$$

Hence the method is of order 2.

Example *(Absence of convergence)* Consider the 2-step method

$$\boldsymbol{y}_{n+2} - 3\boldsymbol{y}_{n+1} + 2\boldsymbol{y}_n = \tfrac{1}{12} h[13 \boldsymbol{f}(t_{n+2}, \boldsymbol{y}_{n+2}) - 20 \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - 5 \boldsymbol{f}(t_n, \boldsymbol{y}_n)]. \tag{4.9}$$

Now $\rho(w) = w^2 - 3w + 2$, $\sigma(w) = \frac{1}{12}(13w^2 - 20w - 5)$ and it is easy to verify that the method is of order 2. Let us apply it, however, to the trivial ODE $y' = 0$, $y(0) = 1$. Hence a single step reads $y_{n+2} - 3y_{n+1} + 2y_n = 0$ and the general solution of this recursion is $y_n = c_1 + c_2 2^n$, $n = 0, 1, \ldots$, where c_1, c_2 are arbitrary constants, which are determined by $y_0 = 1$ and our value of y_1. In general, $c_2 \neq 0$. Suppose that $h \to 0$ and $nh \to t > 0$. Then $n \to \infty$, thus $|y_n| \to \infty$ and *we cannot recover the exact solution* $y(t) \equiv 1$. (This remains true even if we force $c_2 = 0$ by our choice of y_1, because of the presence of roundoff errors.)
We deduce that *the method (4.9) does not converge!* As a more general point, it is important to realise that many 'plausible' multistep methods may fail to be convergent and we need a theoretical tool to allow us to check for this feature.