Mathematical Tripos Part IB: Lent 2020

Numerical Analysis – Lecture 7[1]

4.2 Multistep methods

It is often useful to use past solution values in computing a new value to the ODE (4.1). Assuming that $\boldsymbol{y}_n, \boldsymbol{y}_{n+1}, \ldots, \boldsymbol{y}_{n+s-1}$ are available, where $s \geq 1$, we say that

$$\sum_{l=0}^{s} \rho_l \boldsymbol{y}_{n+l} = h \sum_{l=0}^{s} \sigma_l \boldsymbol{f}(t_{n+l}, \boldsymbol{y}_{n+l}), \qquad n = 0, 1, \ldots, \tag{4.4}$$

where $\rho_s = 1$, is an *s-step method*. If $\sigma_s = 0$, the method is *explicit,* otherwise it is *implicit.* If $s \geq 2$, we need to obtain extra *starting values* $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{s-1}$ by different time-stepping method.

Examples: The following are some common multistep methods:

$$\begin{aligned}
\text{Euler:} \quad & \boldsymbol{y}_{n+1} - \boldsymbol{y}_n = h\boldsymbol{f}(t_n, \boldsymbol{y}_n), \\
\text{Implicit Euler:} \quad & \boldsymbol{y}_{n+1} - \boldsymbol{y}_n = h\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}), \\
\text{Trapezoidal rule:} \quad & \boldsymbol{y}_{n+1} - \boldsymbol{y}_n = \tfrac{1}{2}h[\boldsymbol{f}(t_n, \boldsymbol{y}_n) + \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1})] \\
\text{Theta rule:} \quad & \boldsymbol{y}_{n+1} - \boldsymbol{y}_n = h[\theta\boldsymbol{f}(t_n, \boldsymbol{y}_n) + (1-\theta)\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1})] \\
\text{2-step Adams-Bashforth:} \quad & \boldsymbol{y}_{n+2} - \boldsymbol{y}_{n+1} = h[\tfrac{3}{2}\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - \tfrac{1}{2}\boldsymbol{f}(t_n, \boldsymbol{y}_n)] \\
\text{2-step Adams-Moulton:} \quad & \boldsymbol{y}_{n+2} - \boldsymbol{y}_{n+1} = h[\tfrac{5}{12}\boldsymbol{f}(t_{n+2}, \boldsymbol{y}_{n+2}) + \tfrac{2}{3}\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - \tfrac{1}{12}f(t_n, \boldsymbol{y}_n)].
\end{aligned}$$

For example Adams-Bashforth is a 2-step method ($s = 2$) with $\rho_2 = 1, \rho_1 = -1, \rho_0 = 0$ and $\sigma_2 = 0, \sigma_1 = \frac{3}{2}$ and $\sigma_0 = -\frac{1}{2}$. The implicit Euler method, trapezoidal rule, theta rule for $0 \leq \theta < 1$, and Adams-Moulton are *implicit* methods. The reason these are called implicit is that $\boldsymbol{y}_{\boldsymbol{n+s}}$ appears in the right-hand side of (4.4) and so one has to solve a (generally nonlinear) algebraic equation to compute the new value $\boldsymbol{y}_{n+s}$ from the recursion rule.

Our goal is to develop some general tools to study the convergence of multistep methods. We first introduce the definition or *order.*

Order: The *order* of the multistep method (4.4) is the largest integer $p \geq 0$ such that

$$\sum_{l=0}^{s} \rho_l \boldsymbol{y}(t_{n+l}) - h \sum_{l=0}^{s} \sigma_l \boldsymbol{y}'(t_{n+l}) = \mathcal{O}\big(h^{p+1}\big) \tag{4.5}$$

for all sufficiently smooth functions $\boldsymbol{y}$. The order is a local measure of accuracy for the method: it measures the error incurred by applying the rule (4.4), assuming that the correct value of $\boldsymbol{y}$ at the previous points is known. Let us evaluate the order of some of the methods given above:

The order of Euler's method: For Euler's method, the left-hand side of (4.5) is

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

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

The order of the theta method: From Taylor's theorem we have:

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

[1] Corrections and suggestions to these notes should be emailed to `h.fawzi@damtp.cam.ac.uk`.

Therefore the theta method is of order 1, except that the trapezoidal rule ($\theta = 1/2$) is of order 2.

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 (4.4) is of order $p \geq 1$ 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 For the 2-step *Adams–Bashforth method* we have $\rho(w) = w^2 - w$, $\sigma(w) = \frac{3}{2}w - \frac{1}{2}$ and so

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

Hence the method is of order 2.