Numerical Analysis – Lecture 10[1]

Definition 3.10 *(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

$$\sum_{l=0}^{s} \rho_l \boldsymbol{y}_{n+l} = h \sum_{l=0}^{s} \sigma_l \boldsymbol{f}(t_{n+l}, \boldsymbol{y}_{n+l}), \qquad n = 0, 1, \ldots, \tag{3.4}$$

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.
Let $\rho(w) = \sum_{l=0}^{s} \rho_l w^l$, $\sigma(w) = \sum_{l=0}^{s} \sigma_l w^l$.

Theorem 3.11 *The multistep method (3.4) is of order $p \geq 1$ iff*

$$\rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) = \mathcal{O}\big(z^{p+1}\big), \qquad z \to 0. \tag{3.5}$$

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

$$\sum_{l=0}^{s} \rho_l = 0, \qquad \sum_{l=0}^{s} l^k \rho_l = k \sum_{l=0}^{s} l^{k-1} \sigma_l, \qquad k = 1, 2, \ldots, p. \tag{3.6}$$

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 (3.6). □

Example 3.12 The 2-step *Adams–Bashforth method* is

$$\boldsymbol{y}_{n+2} - \boldsymbol{y}_{n+1} = h[\tfrac{3}{2} \boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - \tfrac{1}{2} \boldsymbol{f}(t_n, \boldsymbol{y}_n)]. \tag{3.7}$$

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

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

[1] Please email all corrections and suggestions to these notes 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/PartII/Handouts.html`.

Hence the method is of order 2.

Example 3.13 *(Absence of convergence)* Consider the 2-step method

$$\boldsymbol{y}_{n+2} - 3\boldsymbol{y}_{n+1} + 2\boldsymbol{y}_n = \tfrac{1}{12}h[13\boldsymbol{f}(t_{n+2}, \boldsymbol{y}_{n+2}) - 20\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) - 5\boldsymbol{f}(t_n, \boldsymbol{y}_n)]. \tag{3.8}$$

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 (3.8) does not converge!* As a more general point, it is important to realise that many 'plausible' multistep methods may not be convergent and we need a theoretical tool to allow us to check for this feature.

Definition 3.14 We say that a polynomial obeys the *root condition* if all its zeros reside in $|w| \le 1$ and all zeros of unit modulus are simple.

Theorem 3.15 (The Dahlquist equivalence theorem) *The multistep method (3.4) is convergent iff it is of order $p \ge 1$ and the polynomial ρ obeys the root condition.*[2]

Examples 3.12 & 3.13 revisited For the Adams–Bashforth method (3.7) we have $\rho(w) = (w-1)w$ and the root condition is obeyed. However, for (3.8) we obtain $\rho(w) = (w-1)(w-2)$, the root condition fails and we deduce that there is no convergence.

Technique 3.16 A useful procedure to generate multistep methods which are convergent and of high order is as follows. According to (3.5), order $p \ge 1$ implies $\rho(1) = 0$. Choose an arbitrary s-degree polynomial ρ that obeys the root condition and such that $\rho(1) = 0$. To maximize order, we let σ be the s-degree (alternatively, $(s-1)$-degree for explicit methods) polynomial arising from the truncation of the Taylor expansion of

$$\frac{\rho(w)}{\log w}$$

about the point $w = 1$. Thus, for example, for an *implicit method*,

$$\sigma(w) = \frac{\rho(w)}{\log w} + \mathcal{O}\big(|w-1|^{s+1}\big) \qquad \Rightarrow \qquad \rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) = \mathcal{O}\big(z^{s+2}\big)$$

and (3.5) implies order at least $s+1$.

Example 3.17 The choice $\rho(w) = w^{s-1}(w-1)$ corresponds to *Adams methods:* Adams–Bashforth methods if $\sigma_s = 0$, whence the order is s, otherwise order-$(s+1)$ (but implicit) Adams–Moulton methods. For example, letting $s = 2$ and $\xi = w - 1$, we obtain the 3rd-order Adams–Moulton method by expanding

$$\begin{aligned}
\frac{w(w-1)}{\log w} &= \frac{\xi + \xi^2}{\log(1+\xi)} = \frac{\xi + \xi^2}{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \cdots} = \frac{1+\xi}{1 - \frac{1}{2}\xi + \frac{1}{3}\xi^2 - \cdots} \\
&= (1+\xi)[1 + (\tfrac{1}{2}\xi - \tfrac{1}{3}\xi^2) + (\tfrac{1}{2}\xi - \tfrac{1}{3}\xi^2)^2 + \mathcal{O}\big(\xi^3\big)] = 1 + \tfrac{3}{2}\xi + \tfrac{5}{12}\xi^2 + \mathcal{O}\big(\xi^3\big) \\
&= 1 + \tfrac{3}{2}(w-1) + \tfrac{5}{12}(w-1)^2 + \mathcal{O}\big(|w-1|^3\big) = -\tfrac{1}{12} + \tfrac{2}{3}w + \tfrac{5}{12}w^2 + \mathcal{O}\big(|w-1|^3\big).
\end{aligned}$$

Therefore the 2-step, 3rd-order Adams–Moulton method is

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

[2] If ρ obeys the root condition, the method (3.4) is sometimes said to be *zero-stable:* we will not use this terminology.