

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 7

7 Multistep methods

7.1 Order of the multistep methods

Definition 7.1 (Multistep methods) It is often useful to use several past solution values in computing a new value. Thus, assuming that $\mathbf{y}_n, \mathbf{y}_{n+1}, \dots, \mathbf{y}_{n+s-1}$ are available, where $s \geq 1$, we say that

$$\sum_{m=0}^s a_m \mathbf{y}_{n+m} = h \sum_{m=0}^s b_m \mathbf{f}_{n+m}, \quad n = 0, 1, \dots, \quad (7.1)$$

where $a_s = 1$, and $\mathbf{f}_{n+m} = \mathbf{f}(t_{n+m}, \mathbf{y}_{n+m})$, is an s -step method. If $b_s = 0$, the method is *explicit*, otherwise it is *implicit*. If $s \geq 2$, we need to obtain extra *starting values* $\mathbf{y}_1, \dots, \mathbf{y}_{s-1}$ by different time-stepping method.

Theorem 7.2 The multistep method (7.1) is of order $p \geq 1$ if and only if

$$\sum_{m=0}^s a_m = 0, \quad \sum_{m=0}^s m^k a_m = k \sum_{m=0}^s m^{k-1} b_m, \quad k = 1..p. \quad (7.2)$$

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

$$\begin{aligned} \sum_{m=0}^s a_m \mathbf{y}(t_{n+m}) - h \sum_{m=0}^s b_m \mathbf{y}'(t_{n+m}) &= \sum_{m=0}^s a_m \sum_{k=0}^{\infty} \frac{(mh)^k}{k!} \mathbf{y}^{(k)}(t_n) - h \sum_{m=0}^s b_m \sum_{k=1}^{\infty} \frac{(mh)^{k-1}}{(k-1)!} \mathbf{y}^{(k)}(t_n) \\ &= \left(\sum_{m=0}^s a_m \right) \mathbf{y}(t_n) + \sum_{k=1}^{\infty} \frac{h^k}{k!} \left(\sum_{m=0}^s m^k a_m - k \sum_{m=0}^s m^{k-1} b_m \right) \mathbf{y}^{(k)}(t_n). \end{aligned}$$

Thus, to obtain the local truncation error of order $\mathcal{O}(h^{p+1})$ regardless of the choice of $\mathbf{y}$, it is necessary and sufficient that the coefficients at h^k vanish for $k \leq p$, i.e., that (7.2) are satisfied. $\square$

Remark 7.3 Since the Taylor expansion of polynomials of degree p contains only $\mathcal{O}(h^k)$ terms with $k \leq p$, the multistep method is of order p if and only if

$$\sum_{m=0}^s a_m Q(t_{n+m}) = h \sum_{m=0}^s b_m Q'(t_{n+m}), \quad \forall Q \in \mathcal{P}_p.$$

In particular, taking $Q(x) = x^k$ for $k = 0..p$ and $t_{n+m} = m, h = 1$, we obtain (7.2).

Given a multistep method (7.1), we define two polynomials of degree s :

$$\rho(w) = \sum_{m=0}^s a_m w^m, \quad \sigma(w) = \sum_{m=0}^s b_m w^m.$$

Theorem 7.4 The multistep method (7.1) is of order $p \geq 1$ if and only if

$$\rho(e^z) - z\sigma(e^z) = \mathcal{O}(z^{p+1}), \quad z \rightarrow 0. \quad (7.3)$$

Proof. Expanding again into Taylor series,

$$\begin{aligned} \rho(e^z) - z\sigma(e^z) &= \sum_{m=0}^s a_m e^{mz} - z \sum_{m=0}^s b_m e^{mz} = \sum_{m=0}^s a_m \sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k - z \sum_{m=0}^s b_m \sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k \\ &= \sum_{k=0}^{\infty} \frac{z^k}{k!} \sum_{m=0}^s m^k a_m - \sum_{k=1}^{\infty} \frac{z^k}{(k-1)!} \sum_{m=0}^s m^{k-1} b_m \\ &= \left(\sum_{m=0}^s a_m \right) + \sum_{k=1}^{\infty} \frac{z^k}{k!} \left(\sum_{m=0}^s m^k a_m - k \sum_{m=0}^s m^{k-1} b_m \right). \end{aligned}$$

The theorem follows from (7.2). $\square$

The reason that (7.3) is equivalent to (7.2) (and that their proofs are almost identical) is due to the (informal) relation between the Taylor series and the exponent e^{hD} , where $D = \frac{d}{dx}$ is the operator of differentiation. Namely

$$f(x+h) = (I + hD + \frac{1}{2}h^2D^2 + \dots) f(x) = e^{hD} f(x).$$

Example 7.5 The 2-step Adams–Bashforth method is

$$y_{n+2} - y_{n+1} = h \left[\frac{3}{2} f_{n+1} - \frac{1}{2} f_n \right]. \quad (7.4)$$

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

$$\begin{aligned} \rho(e^z) - z\sigma(e^z) &= [1 + 2z + \frac{1}{2}(2z)^2 + \frac{1}{6}(2z)^3] - [1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3] - \frac{3}{2}z[1 + z + \frac{1}{2}z^2] + \frac{1}{2}z + \mathcal{O}(z^4) \\ &= \frac{5}{12}z^3 + \mathcal{O}(z^4). \end{aligned}$$

Hence the method is of order 2.

7.2 Convergence

Definition 7.6 (Convergence of a multistep method) Let a multistep method (7.1) be applied to the usual ODE (6.1), and let $\hat{e}(h)$ and $e(h)$ be the numbers

$$\hat{e}(h) := \max \|y(t_i) - y_i\| : i = 0 \dots s-1, \quad e(h) := \max \|y(t_i) - y_i\| : i = 0 \dots N\}.$$

The method is defined to be convergent if, for every ODE, the limits $h \rightarrow 0$ and $\hat{e}(h) \rightarrow 0$ imply $e(h) \rightarrow 0$.

Example 7.7 (Absence of convergence) Consider the 2-step method

$$y_{n+2} + 4y_{n+1} - 5y_n = h(4f_{n+1} + 2f_n). \quad (7.5)$$

Now

$$\rho(w) = w^2 + 4w - 5 \quad \sigma(w) = 4w + 2,$$

and it is easy to verify that the method is of order 3.

Let us apply it, however, to the trivial ODE $y' = 0$, $y(0) = 1$. Hence a single step reads $y_{n+2} + 4y_{n+1} - 5y_n = 0$ and the general solution of this recursion is $y_n = c_1 1^n + c_2 (-5)^n$, where c_1, c_2 are arbitrary constants, which are determined by $y_0 = 1$ and our value of y_1 . If $y_1 \neq 1$, i.e. if there is a small error in our starting values, then $c_2 \neq 0$, thus $|y_n| \rightarrow \infty$ and we cannot recover the exact solution $y(t) \equiv 1$.

As a more convincing example, we may consider ODE $y' = -y$, $y(0) = 1$, with the exact solution $y(t) = e^{-t}$. Even if we take the exact $y_1 = e^{-h}$, the sequence (y_n) from (7.5) will grow like $h^4(-5)^n$, hence no convergence.

So, it is not only the order that matters.

Definition 7.8 (Root condition) We say that a polynomial p obeys the *root condition* if all its zeros reside in $|w| \leq 1$ and all zeros of unit modulus are simple. (If ρ obeys the root condition, the method (7.1) is sometimes said to be *zero-stable*.)

Theorem 7.9 (The Dahlquist equivalence theorem) The multistep method (7.1) is convergent if and only if it is of order $p \geq 1$ and the polynomial ρ obeys the root condition.

For the method (7.4) we have $\rho(w) = w(w-1)$, and the root condition is obeyed. However, for (7.5) we obtain $\rho(w) = (w+5)(w-1)$, the root condition fails and we deduce that there is no convergence.