

Mathematical Tripos Part IB: Lent 2020

Numerical Analysis – Lecture 8¹

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

Theorem (The Dahlquist equivalence theorem) *The multistep method (4.5) is convergent iff it is of order $p \geq 1$ and the polynomial ρ obeys the root condition.*²

Example For the Adams–Bashforth method (see last lecture) we have $\rho(w) = (w - 1)w$ and the root condition is obeyed. Also we saw that the Adams–Bashforth has order 2. By the Dahlquist equivalence theorem it is convergent.

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

$$\mathbf{y}_{n+2} - 2\mathbf{y}_{n+1} + \mathbf{y}_n = 0. \quad (4.10)$$

Here $\rho(w) = w^2 - 2w + 1 = (w - 1)^2$ and $\sigma(w) = 0$. We have $\rho(e^z) - z\sigma(e^z) = (e^z - 1)^2 = (z + O(z^2))^2 = z^2 + O(z^3)$ and so the method has order 1. However ρ does not obey the root condition since the zero $w = 1$ has multiplicity 2. In fact the method (4.10) is obviously not convergent since it does not use the function $\mathbf{f}$ which defines the ODE!

A technique A useful procedure to generate multistep methods which are convergent and of high order is as follows. According to (4.6), order $p \geq 1$ 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*,

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

and (4.6) implies order at least $s + 1$.

Example 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

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

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

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

BDF methods For reasons that will be made clear in the sequel, we wish to consider s -step, s -order methods s.t. $\sigma(w) = \sigma_s w^s$ for some $\sigma_s \in \mathbb{R} \setminus \{0\}$. In other words,

$$\sum_{l=0}^s \rho_l \mathbf{y}_{n+l} = h\sigma_s \mathbf{f}(t_{n+s}, \mathbf{y}_{n+s}), \quad n = 0, 1, \dots$$

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

²If ρ obeys the root condition, the method (4.5) is sometimes said to be *zero-stable*: we will not use this terminology.

Such methods are called *backward differentiation formulae (BDF)*.

Theorem The explicit form of the s -step BDF method is

$$\rho(w) = \sigma_s \sum_{l=1}^s \frac{1}{l} w^{s-l} (w-1)^l, \quad \text{where} \quad \sigma_s = \left(\sum_{l=1}^s \frac{1}{l} \right)^{-1}. \quad (4.11)$$

Proof We are looking for ρ such that the order condition $\rho(w) = \sigma_s w^s \log w + \mathcal{O}(|w-1|^{s+1})$ for $w \rightarrow 1$ holds. Note that

$$\log(w) = -\log\left(\frac{1}{w}\right) = -\log\left(1 - \frac{w-1}{w}\right) = \sum_{l=1}^{\infty} \frac{(w-1)^l}{l \cdot w^l}.$$

With the choice of $\rho(w)$ given in (4.11) we get

$$\rho(w) - \sigma_s w^s \log(w) = -\sigma_s \sum_{l=s+1}^{\infty} \frac{1}{l} (w-1)^l w^{s-l} = \mathcal{O}(|w-1|^{s+1}) \quad (w \rightarrow 1)$$

and so the order condition is satisfied. The value of σ_s in (4.11) is such that $\rho_s = 1$. □

Example Let $s = 2$. Substitution in (4.11) yields $\sigma_2 = \frac{2}{3}$ and simple algebra results in $\rho(w) = w^2 - \frac{4}{3}w + \frac{1}{3}$. Hence the 2-step BDF is

$$\mathbf{y}_{n+2} - \frac{4}{3}\mathbf{y}_{n+1} + \frac{1}{3}\mathbf{y}_n = \frac{2}{3}h\mathbf{f}(t_{n+2}, \mathbf{y}_{n+2}).$$

Remark We cannot take it for granted that BDF methods are convergent. It is possible to prove that they are convergent iff $s \leq 6$. They *must not* be used outside this range!

4.3 Runge–Kutta methods

Recalling quadrature We may approximate

$$\int_0^h f(t)dt \approx h \sum_{l=1}^{\nu} b_l f(c_l h),$$

where the weights b_l are chosen in accordance with an explicit formula from Lecture 5 (with weight function $w \equiv 1$). This *quadrature formula* is exact for all polynomials of degree $\nu - 1$ and, provided that $\prod_{k=1}^{\nu} (x - c_k)$ is orthogonal w.r.t. the weight function $w(x) \equiv 1$, $0 \leq x \leq 1$, the formula is exact for all polynomials of degree $2\nu - 1$.

Suppose that we wish to solve the ‘ODE’ $y' = f(t)$, $y(0) = y_0$. The exact solution is $y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t)dt$ and we can approximate it by quadrature. In general, we obtain the time-stepping scheme

$$y_{n+1} = y_n + h \sum_{l=1}^{\nu} b_l f(t_n + c_l h) \quad n = 0, 1, \dots$$

Here $h = t_{n+1} - t_n$ (the points t_n need not be equispaced). Can we generalize this to genuine ODEs of the form $\mathbf{y}' = \mathbf{f}(t, \mathbf{y})$?