# Mathematical Tripos Part IB: Lent 2019

# Numerical Analysis – Lecture 8[1]

**Definition** 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 (The Dahlquist equivalence theorem)*** *The multistep method (4.5) is convergent iff it is of order $p \ge 1$ and the polynomial $\rho$ 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

$$\boldsymbol{y}_{n+2} - 2\boldsymbol{y}_{n+1} + \boldsymbol{y}_n = 0. \tag{4.10}$$

Here $\rho(w) = w^2 - 2w + 1 = (w-1)^2$ and $\sigma(w) = 0$. We have $\rho(\mathrm{e}^z) - z\sigma(\mathrm{e}^z) = (\mathrm{e}^z - 1)^2 = (z + O(z^2))^2 = z^2 + O(z^3)$ and so the method has order 1. However $\rho$ 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 $\boldsymbol{f}$ 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 $p \ge 1$ implies $\rho(1) = 0$. Choose an arbitrary $s$-degree polynomial $\rho$ that obeys the root condition and such that $\rho(1) = 0$. To maximize order, we let $\sigma$ 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 (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

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

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

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

**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,

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

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

[2] If $\rho$ 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*

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

**Proof** We are looking for $\rho$ such that the order condition $\rho(w) = \sigma_s w^s \log w + \mathcal{O}\big(|w-1|^{s+1}\big)$ for $w \to 1$ 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

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

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

**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

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

**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

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

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 $y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t)\mathrm{d}t$ and we can approximate it by quadrature. In general, we obtain the time-stepping scheme

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

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 $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$?