

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 8

8 Multistep methods (contd)

8.1 Construction

Technique 8.1 A useful procedure to generate multistep methods which are convergent and of high order is as follows. According to (7.2), 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 polynomial of degree s for implicit methods (alternatively, of degree $(s-1)$ for explicit methods) 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*,

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

and (7.3) implies order at least $s+1$ (for explicit methods order s).

Example 8.2 The choice $\rho(w) = w^{s-1}(w-1)$ corresponds to *Adams methods*:

- 1) *Adams–Bashforth methods* if $b_s = 0$, hence explicit, with the order s (e.g. (7.4) for $s = 2$),
- 2) *Adams–Moulton methods* if $b_s \neq 0$, hence implicit, but with the order $(s+1)$.

For example, letting $s = 2$ and $\xi = w - 1$, we obtain the 3rd-order Adams–Moulton method by expanding

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

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

$$\mathbf{y}_{n+2} - \mathbf{y}_{n+1} = h \left[\frac{5}{12} \mathbf{f}_{n+2} + \frac{2}{3} \mathbf{f}_{n+1} - \frac{1}{12} \mathbf{f}_n \right].$$

(If we cut expansion at $1 + \frac{3}{2}\xi = 1 + \frac{3}{2}(w-1) = \frac{3}{2}w - \frac{1}{2}$, we get explicit 2-step 2nd-order method (7.4).)

Method 8.3 (BDF) As another exercise in applying Technique 8.1 (and for future applications) let us construct s -step s -order methods such that $\sigma(w) = b_s w^s$ for some non-zero b_s , say $b_s = 1$. In other words,

$$\sum_{m=0}^s a_m \mathbf{y}_{n+m} = h \mathbf{f}_{n+s}, \quad n = 0, 1, \dots \quad (8.1)$$

Such methods are called *backward differentiation formulae (BDF)*, and their coefficients (a_m) can be obtained from the following expression.

Lemma 8.4 The polynomial $\rho(w) = \sum_{m=0}^s a_m w^m$ of the s -step s -order BDF method (8.1) has the form

$$\rho(w) = \sum_{k=1}^s \frac{1}{k} w^{s-k} (w-1)^k. \quad (8.2)$$

Proof. We need to fulfill the s -order condition $\rho(e^z) - z\sigma(e^z) = \mathcal{O}(z^{s+1})$ which, with $w = e^z$ and $\sigma(w) = w^s$, becomes

$$\rho(w) = w^s \log w + \mathcal{O}(|w-1|^{s+1}).$$

But we have $\log w = -\log\left(\frac{1}{w}\right) = -\log\left(1 - \frac{w-1}{w}\right)$, and $\log(1-x) = -\sum_{k=1}^{\infty} \frac{1}{k} x^k$, therefore

$$w^s \log w = w^s \sum_{k=1}^s \frac{1}{k} \left(\frac{w-1}{w}\right)^k + \mathcal{O}(|w-1|^{s+1}),$$

and the first term is a polynomial of degree s , hence the result. $\square$

Example 8.5 For $s = 2$, we obtain $\frac{3}{2}\mathbf{y}_{n+2} - 2\mathbf{y}_{n+1} + \frac{1}{2}\mathbf{y}_n = h\mathbf{f}_{n+2}$, or with the standard normalization $a_s = 1$

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

Warning. We cannot take it for granted that BDF methods are convergent (i.e. that $\rho(w)$ in (8.2) satisfies the root condition). In fact, this is the case if and only if $s \leq 6$, so they can be used within this range only.

Method 8.6 Let us look at construction of both Adams methods and BDF formulae from a different (although equivalent) point of view, namely using the polynomial criterion for the p -order methods:

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

1) For Adams methods, the left-hand side is $Q(s) - Q(s-1) = \int_{s-1}^s Q'(t) dt$, therefore letting $q = Q'$ we are looking for the quadrature formula (of numerical integration)

$$\int_{s-1}^s q(t) dt = \sum_{m=0}^s b_m q(m),$$

which should be valid for all polynomials q of degree s (if $b_s \neq 0$) or of degree $s-1$ (if $b_s = 0$). By the Lagrange interpolating formula, we can write q as $q(t) = \sum_{m=0}^s \ell_m(t)q(m)$, where ℓ_m are the fundamental Lagrange polynomials satisfying $\ell_m(k) = \delta_{mk}$, and it follows that

$$b_m = \int_{s-1}^s \ell_m(t) dt, \quad \ell_m(t) = \frac{\omega(t)}{(t-m)\omega'(m)}, \quad \omega(t) = \prod_{m=0}^s (t-m).$$

2) For BDF, we are looking for the formulae of numerical (backward) differentiation instead,

$$\sum_{m=0}^s a_m Q(m) = Q'(s),$$

which should be valid for all polynomials of degree s . Again, from the Lagrange interpolating formula $Q(t) = \sum_{m=0}^s \ell_m(t)Q(m)$, it follows that $a_m = \ell'_m(s)$, and using explicit form of ℓ_m given above we derive

$$a_s = \sum_{m=1}^s \frac{1}{m}, \quad a_m = \frac{(-1)^{s-m}}{s-m} \binom{s}{m}.$$

8.2 Higher order and convergence (non-examinable)

Lemma 8.7 *There is no s -step methods of order $2s+1$. The implicit and explicit methods of order $2s$ and $2s-1$, respectively, do exist and are unique.*

Example 8.8 For $s = 1$ and $s = 2$ the highest order (implicit) methods have the form

$$1) \quad \text{one-step order 2: } \mathbf{y}_{n+1} - \mathbf{y}_n = h \left(\frac{1}{2}\mathbf{f}_{n+1} + \frac{1}{2}\mathbf{f}_n \right) \quad [\text{trapezoidal rule}],$$

$$2) \quad \text{two-step order 4: } \mathbf{y}_{n+2} - \mathbf{y}_n = h \left(\frac{1}{3}\mathbf{f}_{n+2} + \frac{4}{3}\mathbf{f}_{n+1} + \frac{1}{3}\mathbf{f}_n \right) \quad [\text{Simpson rule}].$$

Obviously, the root condition for both methods is fulfilled. However, for $s \geq 3$, the s -step methods of order $2s$ do not satisfy the root condition, and that makes them not very useful for numerical implementation. In fact, we should not go very far in our search for the higher order multistep methods because of the following restriction.

Theorem 8.9 (The first Dalquist barrier) *If an s -step method converges, then it has the order*

$$p \leq \begin{cases} s & \text{for explicit methods,} \\ s+1 & \text{if } s \text{ is odd,} \\ s+2 & \text{if } s \text{ is even.} \end{cases}$$

So, in Example 8.2, the Adams-Bashforth methods are optimal in the sense that they attain the bound $p = s$ for explicit methods, and the Adams-Moulton methods for odd s are also optimal, with $p = s+1$.

An optimal implicit method with even number of steps s with order $p = s+2$ is given for example by $\rho(w) = w^s - 1$. This method corresponds to the quadrature (where $q = Q'$, with $Q \in \mathcal{P}_{s+2}$)

$$\int_0^s q(t) dt = \sum_{m=0}^s b_m q(m) \quad \forall q \in \mathcal{P}_{s+1}.$$