Mathematical Tripos Part IB: Lent 2010

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 ρ obeys the root condition.*[2]

Examples revisited For the Adams–Bashforth method (4.8) we have $\rho(w) = (w-1)w$ and the root condition is obeyed. However, for (4.9) we obtain $\rho(w) = (w-1)(w-2)$, the root condition fails and we deduce that there is no convergence.

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 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 (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

$$\begin{aligned}\frac{w(w-1)}{\log w} &= \frac{\xi+\xi^2}{\log(1+\xi)} = \frac{\xi+\xi^2}{\xi - \frac12\xi^2 + \frac13\xi^3 - \cdots} = \frac{1+\xi}{1 - \frac12\xi + \frac13\xi^2 - \cdots}\\ &= (1+\xi)[1 + (\tfrac12\xi - \tfrac13\xi^2) + (\tfrac12\xi - \tfrac13\xi^2)^2 + \mathcal{O}\big(\xi^3\big)] = 1 + \tfrac32\xi + \tfrac{5}{12}\xi^2 + \mathcal{O}\big(\xi^3\big)\\ &= 1 + \tfrac32(w-1) + \tfrac{5}{12}(w-1)^2 + \mathcal{O}\big(|w-1|^3\big) = -\tfrac{1}{12} + \tfrac23 w + \tfrac{5}{12}w^2 + \mathcal{O}\big(|w-1|^3\big)\,.\end{aligned}$$

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

$$\boldsymbol{y}_{n+2} - \boldsymbol{y}_{n+1} = h[-\tfrac{1}{12}\boldsymbol{f}(t_n, \boldsymbol{y}_n) + \tfrac23\boldsymbol{f}(t_{n+1}, \boldsymbol{y}_{n+1}) + \tfrac{5}{12}\boldsymbol{f}(t_{n+2}, \boldsymbol{y}_{n+2})].$$

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,

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

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

[1]Corrections and suggestions to these notes should be emailed 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/PartIB/Handouts.html`.

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

Lemma *The explicit form of the s-step BDF method is*

$$\rho(w)=\sigma_s\sum_{l=1}^{s}\frac{1}{l}w^{s-l}(w-1)^l, \qquad \text{where} \qquad \sigma_s=\left(\sum_{l=1}^{s}\frac{1}{l}\right)^{-1}. \tag{4.10}$$

Proof Set $v=w^{-1}$, therefore the order condition $\rho(w)=\sigma_s w^s\log w+\mathcal{O}\big(|w-1|^{s+1}\big)$ becomes

$$\sum_{l=0}^{s}\rho_l v^{s-l}=-\sigma_s\log v+\mathcal{O}\big(|v-1|^{s+1}\big)\,, \qquad v\to 1.$$

But $\log v=\log(1+(v-1))=\sum_{l=1}^{\infty}(-1)^{l-1}(v-1)^l/l$, consequently

$$\sum_{l=0}^{s}\rho_{s-l}v^l=\sigma_s\sum_{l=1}^{s}\frac{(-1)^l}{l}(v-1)^l.$$

Brief manipulation and a restoration of $w=v^{-1}$ yield

$$\sum_{l=0}^{s}\rho_l w^l=\sigma_s\sum_{l=1}^{s}\frac{(-1)^l}{l}w^{s-l}(1-w)^l$$

and we pick σ_s so that $\rho_s=1$, collecting powers of w^s on the right of the last displayed equation. $\square$

Example Let $s=2$. Substitution in (4.10) 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 $s\le 6$. 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 $w(x)\equiv 1$, $0\le x\le 1$, 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 $\boldsymbol{y}'=\boldsymbol{f}(t,\boldsymbol{y})$?