Numerical Analysis Hilary Term 2023
Lecture 15–16: Multistep methods

Linear multi-step methods

Runge-Kutta methods deliver an approximate solution to

$$\mathbf{y}' = \mathbf{f}(x, \mathbf{y}), \qquad \mathbf{y}(x_0) = \mathbf{y}_0, \tag{1}$$

but tacitly assume that it is possible to evaluate the right-hand side $\mathbf{f}(x, \mathbf{y})$ anywhere (and use a lot of such function evaluations). Instead, linear multi-step methods require values of $\mathbf{f}$ at grid points only.

Definition 1. *Let $X > x_0$ be a final time, $N, k \in \mathbb{N}$, $N \geq k$, $h := (X - x_0)/N$, and $x_n := x_0 + hn$. A* linear k-step method *is an iterative method that computes the approximation $\mathbf{y}_{n+k}$ to $\mathbf{y}(x_{n+k})$ by solving*

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}(x_{n+j}, \mathbf{y}_{n+j}), \tag{2}$$

where $\{\alpha_j\}_{j=0}^{k}$ and $\{\beta_j\}_{j=0}^{k}$ are real coefficients. To avoid degenerate cases, we assume that $\alpha_k \neq 0$ and that $\alpha_0^2 + \beta_0^2 \neq 0$.

Note that if $\beta_k = 0$, the method is explicit.

It is also possible to construct multi-step methods on nonequidistant grids, and good timestepping software does so for you.

In the same way Runge-Kutta methods are summarized with Butcher tables, linear multi-step methods can be summarized with two polynomials.

Definition 2. *For the k-step method defined by (2),*

$$\rho(z) = \sum_{j=0}^{k} \alpha_j z^j \quad \text{and} \quad \sigma(z) = \sum_{j=0}^{k} \beta_j z^j \tag{3}$$

are called the first *and* second characteristic polynomials*.*

Example 3. *A simple linear 3-step method can be constructed using Simpson's quadrature rule. Indeed,*

$$\begin{aligned}\mathbf{y}(x_{n+1}) &= \mathbf{y}(x_{n-1}) + \textstyle\int_{x_{n-1}}^{x_{n+1}} \mathbf{f}(x, \mathbf{y}(x))\,\mathrm{d}x \\ &\approx \mathbf{y}(x_{n-1}) + \tfrac{2h}{6}\left(\mathbf{f}(x_{n-1}, \mathbf{y}(x_{n-1})) + 4\mathbf{f}(x_n, \mathbf{y}(x_n)) + \mathbf{f}(x_{n+1}, \mathbf{y}(x_{n+1}))\right).\end{aligned}$$

This motivates the following linear 2-step method

$$\mathbf{y}_{n+2} - \mathbf{y}_n = h\left(\frac{2}{6}\mathbf{f}(x_n, \mathbf{y}_n) + \frac{8}{6}\mathbf{f}(x_{n+1}, \mathbf{y}_{n+1}) + \frac{2}{6}\mathbf{f}(x_{n+2}, \mathbf{y}_{n+2})\right) \tag{4}$$

Its first and second characteristic polynomials are

$$\rho(z) = z^2 - 1 \quad \text{and} \quad \sigma(z) = \frac{2}{6}(z^2 + 4z + 1). \tag{5}$$

There is a formal calculus that can be used to construct families of multi-step methods.

Definition 4. *For a fixed small $h > 0$, we define:*

- *the shift operator* $E : \mathbf{y}(x) \mapsto \mathbf{y}(x+h)$,
- *its inverse* $E^{-1} : \mathbf{y}(x) \mapsto \mathbf{y}(x-h)$,
- *the difference operator* $\Delta : \mathbf{y}(x) \mapsto \mathbf{y}(x) - \mathbf{y}(x-h)$,
- *the identity operator* $\mathbf{I} : \mathbf{y}(x) \mapsto \mathbf{y}(x)$,
- *and the differential operator* $D : \mathbf{y}(x) \mapsto \mathbf{y}'(x)$.

Lemma 5. *Suppose that $\mathbf{y}(x)$ is analytic (hence infinitely differentiable) at x. Then formally, $hD = -\log(\mathbf{I} - \Delta)$.*

Proof. First, using Taylor expansion, we can show that

$$\begin{aligned} E\mathbf{y}(x) &= \mathbf{y}(x) + h\mathbf{y}'(x) + \tfrac{h^2}{2}\mathbf{y}''(x) + \dots \\ &= \mathbf{y}(x) + hD\mathbf{y}(x) + \tfrac{h^2}{2}D^2\mathbf{y}(x) + \dots = \exp(hD)\mathbf{y}(x)\,, \end{aligned}$$

and thus, $E = \exp(hD)$. This implies that $hD = \log(E)$.

Then, using the definition, we see that $E^{-1} = \mathbf{I} - \Delta$, and thus $E = (\mathbf{I} - \Delta)^{-1}$.

Therefore, $hD = \log(E) = \log((\mathbf{I} - \Delta)^{-1}) = -\log(\mathbf{I} - \Delta)$. □

Example 6. *We can construct a multi-step method using the previous lemma. Indeed, by Taylor expansion of the logarithm* $\log(1-x) = -\sum_{i=1}^{\infty} x^i/i$,

$$hD = -\log(\mathbf{I} - \Delta) = \left(\Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots\right)\,, \tag{6}$$

and thus

$$h\mathbf{f}(x_n, \mathbf{y}(x_n)) = \left(\Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots\right)\mathbf{y}(x_n)\,. \tag{7}$$

To construct a family of multi-step methods, we truncate the infinite series at different orders and replace $\mathbf{y}(x_n)$ with $\mathbf{y}_n$. These methods are called backward differentiation formulas, *and their simplest instances are*

$$\begin{aligned} \mathbf{y}_n - \mathbf{y}_{n-1} &= h\mathbf{f}(x_n, \mathbf{y}_n)\,, \quad \textit{(implicit Euler)} \\ \tfrac{3}{2}\mathbf{y}_n - 2\mathbf{y}_{n-1} + \tfrac{1}{2}\mathbf{y}_{n-2} &= h\mathbf{f}(x_n, \mathbf{y}_n)\,, \\ \tfrac{11}{6}\mathbf{y}_n - 3\mathbf{y}_{n-1} + \tfrac{3}{2}\mathbf{y}_{n-2} - \tfrac{1}{3}\mathbf{y}_{n-3} &= h\mathbf{f}(x_n, \mathbf{y}_n)\,. \end{aligned}$$

Example 7. *Explicit Euler's method arises from truncating the series*

$$hD = \left(\Delta - \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \dots\right)E\,, \tag{8}$$

which can be derived similarly.

Example 8. *Another two important families are the* Adams-Moulton methods *and the* Adams-Bashforth methods*, which originate from the formal equalities*

$$E\Delta = h\left(\mathbf{I} - \tfrac{1}{2}\Delta - \tfrac{1}{12}\Delta^2 - \tfrac{1}{24}\Delta^3 - \tfrac{19}{720}\Delta^4 + \dots\right) D\,,$$
$$E\Delta = h\left(\mathbf{I} + \tfrac{1}{2}\Delta + \tfrac{5}{12}\Delta^2 + \tfrac{3}{8}\Delta^3 + \tfrac{251}{720}\Delta^4 + \dots\right) D\,,$$

respectively.

For example, writing $\mathbf{f}_{n+i} = \mathbf{f}_{n+i}(x_{n+i}, \mathbf{y}_{n+i})$ *for simplicity, the three-step Adams–Moulton method is (an implicit method)*

$$\mathbf{y}_{n+3} = \mathbf{y}_{n+2} + \frac{1}{24} h\left(9\mathbf{f}_{n+3} + 19\mathbf{f}_{n+2} - 5\mathbf{f}_{n+1} - 9\mathbf{f}_n\right),$$

and the four-step Adams-Bashforth method is (explicit)

$$\mathbf{y}_{n+4} = \mathbf{y}_{n+3} + \frac{1}{24} h\left(55\mathbf{f}_{n+3} - 59\mathbf{f}_{n+2} + 37\mathbf{f}_{n+1} - 9\mathbf{f}_n\right)$$

To compute $\mathbf{y}_k$ with a linear k-step method, we need the values $\mathbf{y}_0, \dots, \mathbf{y}_{k-1}$. These (except $\mathbf{y}_0$) must be approximated with either a one-step method or another multi-step method that uses fewer steps. At any rate, they will contain numerical errors. Clearly, a meaningful multistep method should be robust with respect to small perturbations of these initial values.

Definition 9. *A linear k-step method is said to be* zero-stable *if there is a constant $K > 0$ such that for every $N \in \mathbb{N}$ sufficiently large and for any two different sets of initial data $\mathbf{y}_0, \dots, \mathbf{y}_{k-1}$ and $\tilde{\mathbf{y}}_0, \dots, \tilde{\mathbf{y}}_{k-1}$, the two sequences $\{\mathbf{y}_n\}_{n=0}^N$ and $\{\tilde{\mathbf{y}}_n\}_{n=0}^N$ that stem from the linear k-step method with $h = (X - x_0)/N$ satisfy*

$$\max_{0 \le n \le N} \|\mathbf{y}_n - \tilde{\mathbf{y}}_n\| \le K \max_{j \le k-1} \|\mathbf{y}_j - \tilde{\mathbf{y}}_j\|\,. \tag{9}$$

Zero-stability of a k-step method can be verified algebraically with the following property, which is known as the *root condition*.

Definition 10. *A linear k-step method satisfies the* root condition *if all zeros of its first characteristic polynomial $\rho(z)$ lie inside the closed unit disc, and every zero that lies on the unit circle is simple.*

Theorem 11. *A linear multi-step method is zero-stable for any ODE $\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y})$ with Lipschitz right-hand side, if and only if the linear multi-step method satisfies the root condition.*

This theorem implies that zero-stability of a multi-step method can be determined by merely considering its behavior when applied to the trivial differential equation $y' = 0$; it is for this reason that it is called *zero*-stability.

Consistency and convergence

Definition 12. *The* consistency error *of a linear k-step method with $\sigma(1) \neq 0$ is*

$$\boldsymbol{\tau}(h) = \frac{\sum_{j=0}^{k} \alpha_j \mathbf{y}(x_j) - h \sum_{j=0}^{k} \beta_j \mathbf{y}'(x_j)}{h \sum_{j=0}^{k} \beta_j}, \tag{10}$$

where $\mathbf{y}$ is a smooth function.

Definition 13. *A linear multi-step method has* (consistency) order p *if $\boldsymbol{\tau}(h) = O(h^p)$.*

By adequate Taylor expansion, we can obtain the following theorem.

Theorem 14. *A linear multi-step method has consistency order p if and only if $\sigma(1) \neq 0$ and*

$$\sum_{j=0}^{k} \alpha_j = 0 \quad \textit{and} \quad \sum_{j=0}^{k} \alpha_j j^q = q \sum_{j=0}^{k} \beta_j j^{q-1} \quad \textit{for} \quad q = 1, \ldots, p\,. \tag{11}$$

Definition 15. *A multi-step method is said to be* consistent *if these conditions are satisfied at least for $p = 1$.*

Theorem 16. *A linear multi-step method is consistent iff*

$$\rho(1) = 0 \quad \textit{and} \quad \rho'(1) = \sigma(1) \neq 0. \tag{12}$$

In general, these conditions can be reformulated more elegantly.

Theorem 17. *Equation (11) is equivalent to $\rho(e^h) - h\sigma(e^h) = O(h^{p+1})$.*

To define the concept of convergence for linear k-step methods, we need to specify some criteria about the choice of the starting conditions.

Definition 18. *A set of starting conditions $\mathbf{y}_i = \boldsymbol{\eta}_i(h)$, $i = 0, \ldots, k-1$ is consistent with the initial value $\mathbf{y}_0$ if $\boldsymbol{\eta}_s(h) \to \mathbf{y}_0$ as $h \to 0$ for every $s = 0, \ldots, k-1$.*

Definition 19. *A linear k-step method is* convergent *if, for every initial value problem $\mathbf{y} = \mathbf{f}(x, \mathbf{y})$, $\mathbf{y}(x_0) = \mathbf{y}_0$ (that satisfies the assumptions of Picard's theorem) and for any choice of consistent starting conditions*

$$\mathbf{y}_0 = \boldsymbol{\eta}_0(h), \ldots, \mathbf{y}_{k-1} = \boldsymbol{\eta}_{k-1}(h)\,, \tag{13}$$

we have that

$$\lim_{h \to 0} \mathbf{y}_N = \mathbf{y}(X) \quad (\textit{with } N = (X - x_0)/h) \tag{14}$$

Theorem 20 (Dahlquist's Equivalence Theorem). *For consistent linear k-step method with consistent starting values, zero-stability is necessary and sufficient for convergence.*

Moreover, if $\boldsymbol{\tau}(h) = O(h^p)$ and $\|\mathbf{y}(x_s) - \boldsymbol{\eta}_s(h)\| = O(h^p)$ for $s = 0, \ldots, k-1$, then $\max_{0 \leq n \leq N} \|\mathbf{y}(x_n) - \mathbf{y}_n\| = O(h^p)$.

For Runge–Kutta methods, we showed that one can construct s-stage methods of order $2s$. Unfortunately, it is not possible to construct linear k-step methods of order $2k$ without violating the zero-stability requirement.

Theorem 21 (The first Dahlquist-barrier). *The order p of a zero-stable linear k-step method satisfies*

- $p \leq k+2$ *if k is even,*
- $p \leq k+1$ *if k is odd,*
- $p \leq k$ *if $\beta_k/\alpha_k \leq 0$ (in particular if the method is explicit).*

Stability of linear multi-step methods Similar to one-step methods, stability is investigated by applying a linear multi-step method to the Dahlquist test equation $y' = zy$, $z \in \mathbb{C}$, $y(0) = 1$, and $h = 1$. Recall that the solution to this ODE is $y(x) = \exp(zx)$, that $|y(x)| \to 0$ as $t \to \infty$ whenever $\text{Re}(z) < 0$, and that we call its numerical approximation $\{y_n\}_{n\in\mathbb{N}}$ (absolutely) stable if $y_n \to 0$ as $n \to \infty$ when $\text{Re}(z) < 0$.

Our goal is to investigate when the sequence $\{y_n\}_{n\in\mathbb{N}}$ computed with a linear k-step method is stable. First of all, note that the n-th iterate y_n satisfies

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = \sum_{j=0}^{k} \beta_j z y_{n+j}\,, \quad \text{or equivalently,} \quad \sum_{j=0}^{k} (\alpha_j - z\beta_j) y_{n+j} = 0\,. \tag{15}$$

With the following lemma from the theory of difference equations, we know that y_n is of the form

$$y_n = p_1(n) r_1^n + \ldots + p_\ell(n) r_\ell^n\,, \tag{16}$$

where the r_js are the roots of the polynomial $\pi(x) = \sum_{j=0}^{k} (\alpha_j - z\beta_j) x^j$, and the $p_j(n)$s are polynomials of degree $m_j - 1$, where m_j is the multiplicity of r_j.

Lemma 22. *Let $\{\gamma_i\}_{i=0}^{k}$ be real coefficients and let $\{x_i\}_{i=0}^{k-1}$ be initial values. Let $\{x_n\}_{n\in\mathbb{N}}$ be the sequence defined by the kth order linear difference equation*

$$\sum_{i=0}^{k} \gamma_i x_{n+i} = 0 \quad . \tag{17}$$

Then, x_n is of the form

$$x_n = p_1(n) r_1^n + \ldots + p_\ell(n) r_\ell^n\,, \tag{18}$$

where $r_1, \ldots, r_\ell$ are the roots of the polynomial $\pi(x) = \sum_{i=0}^{k} \gamma_i x^i$ and $p_1, \ldots, p_\ell$ are polynomials of degree $m_1 - 1, \ldots, m_\ell - 1$, where m_i is the multiplicity of r_i.

With (16), we can fully analyze the asymptotic behavior of $\{y_n\}_{n\in\mathbb{N}}$. Indeed:

- if $\pi(x)$ has a zero r_j outside the unit disc, than y_n grows as $|r_j|^n$,
- if an r_j is on the unit circle and has multiplicity $m_j > 1$, then $y_n \sim n^{m_j - 1}$,

- otherwise, $y_n \to 0$ geometrically as $n \to \infty$.

This computation shows that the polynomial π plays a crucial role in this stability analysis. Therefore, similarly to one-step methods, we introduce the following definitions.

Definition 23. *The* stability polynomial *of a linear k-step method is*

$$\pi(x) = \pi(x; z) := \sum_{j=0}^{k} (\alpha_j - z\beta_j) x^j = \rho(x) - z\sigma(x) . \tag{19}$$

Definition 24. *The* stability domain *of a linear multistep method is*

$$S := \{z \in \mathbb{C} : \textit{if } \pi(x; z) = 0, \textit{ then } |x| \le 1; \textit{ multiple zeros satisfy } |x| < 1\} . \tag{20}$$

Note that $0 \in S$ if the method is zero-stable (as $\pi(x; 0) = \rho(x)$).

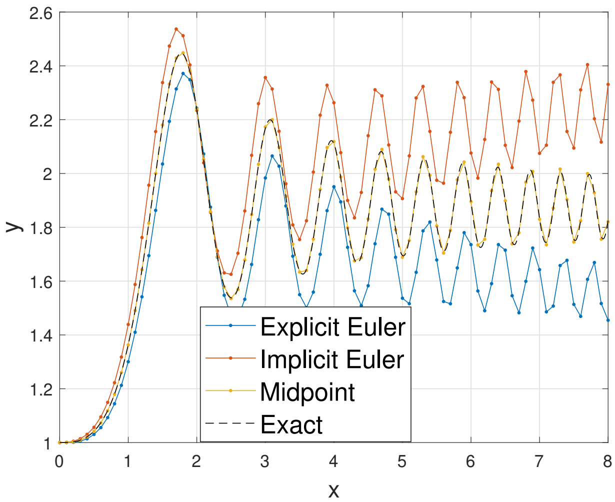
Dahlquist's second barrier theorem places sharp limits on the stability domains of linear multi-step methods.

Theorem 25 (Dahlquist's second barrier). *An A-stable linear multi-step method must be implicit and of order $p \le 2$. The trapezium rule is the second-order A-stable linear multi-step method with the smallest error constant.*

It is possible to break the Dahlquist barrier by hybridising between multi-stage and multi-step methods. Such methods are called *general linear methods*[1].

Example 26. *We conclude with an example illustrating some of the results. Consider the scalar IVP $y' = \sin(x^2)y$, $y(0) = 1$. We use explicit Euler, implicit Euler, implicit midpoint, explicit 4-stage Runge-Kutta, and 4th order Adam-Bashforth method to solve it.*

Here are the solutions.



We now look at the error $y(x_n) - y_n$, shown in Figure 1. There we also examine the multistep method

$$\mathbf{y}_{n+2} = -4\mathbf{y}_{n+1} + 5\mathbf{y}_n + h(4\mathbf{f}(x_{n+1}, \mathbf{y}_{n+1}) - 2\mathbf{f}(x_n, \mathbf{y}_n)) \tag{21}$$

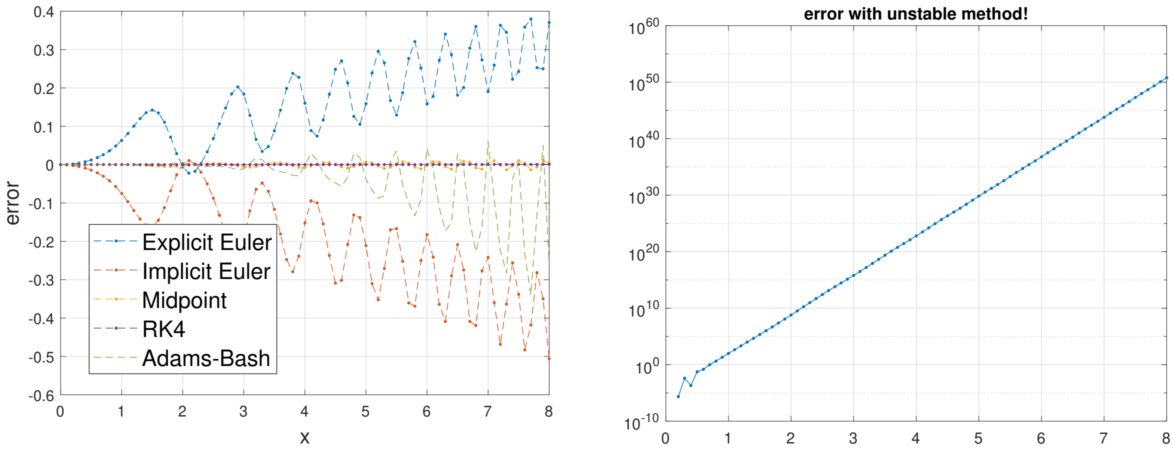
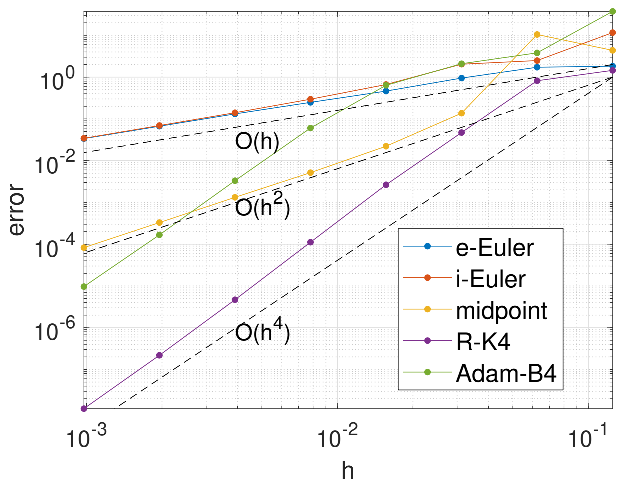


Figure 1: Errors with stable methods (left) and an unstable method (21)

which has consistency order 3, but is not zero-stable; we thus expect it to not converge. In fact the solution blows up and the error diverges to ∞*—it hardly gets any worse than that!*

Finally, we can vary the step size h *and examine the convergence as* $h \to 0$*. Higher-order methods should have better accuracy especially for small* h*. We confirm this in the figure (note the loglog scale).*



(MATLAB code is lec16_demo.m)

This concludes this course—for further courses related to numerical analysis, check out e.g.

- Numerical Solution of Differential Equations (Part B)
- Approximation of Functions (Part C)
- Numerical Linear Algebra (Part C)
- Finite Element Method for PDEs (Part C)
- Continuous Optimisation (Part C)

[1]See *General linear methods*, J. C. Butcher, Acta Numerica (2006).