
Numerical Analysis Hilary Term 2024
Lecture 16: Multistep methods

Linear multi-step methods

Runge-Kutta methods deliver an approximate solution to

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

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 are more parsimonious, requiring values of \mathbf{f} at grid points only. That is, these methods re-use quantities that have already been computed, and thus available without extra computation.

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

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

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.

Non-examinable: 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),

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

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,

$$\begin{aligned} \mathbf{y}(x_{n+1}) &= \mathbf{y}(x_{n-1}) + \int_{x_{n-1}}^{x_{n+1}} \mathbf{f}(x, \mathbf{y}(x)) \, dx \\ &\approx \mathbf{y}(x_{n-1}) + \frac{2h}{6} (\mathbf{f}(x_{n-1}, \mathbf{y}(x_{n-1})) + 4\mathbf{f}(x_n, \mathbf{y}(x_n)) + \mathbf{f}(x_{n+1}, \mathbf{y}(x_{n+1}))) . \end{aligned}$$

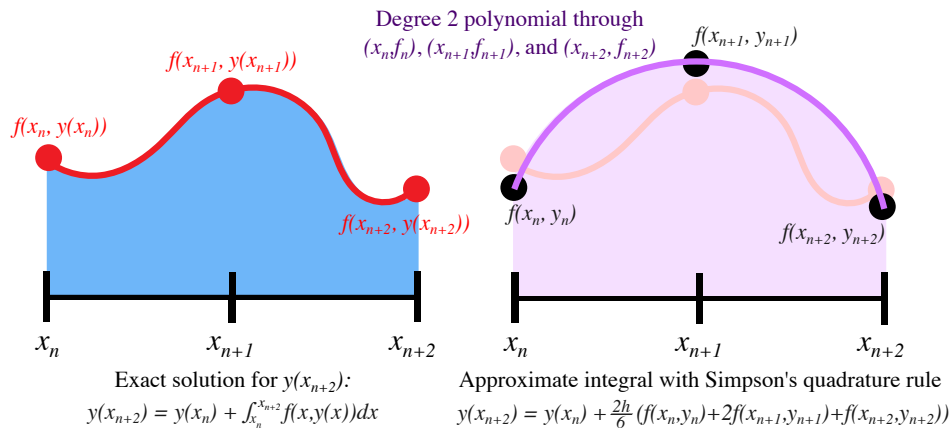
This motivates the following linear 2-step method

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

Its first and second characteristic polynomials are

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

Here's an illustration.



Example 4. Two important families of multistep methods are Adams-Moulton methods and the Adams-Bashforth methods. The three-step Adams-Moulton method is (an implicit method)

$$\mathbf{y}_{n+3} = \mathbf{y}_{n+2} + \frac{1}{24}h (9\mathbf{f}_{n+3} + 19\mathbf{f}_{n+2} - 5\mathbf{f}_{n+1} - 9\mathbf{f}_n), \quad (6)$$

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

$$\mathbf{y}_{n+4} = \mathbf{y}_{n+3} + \frac{1}{24}h (55\mathbf{f}_{n+3} - 59\mathbf{f}_{n+2} + 37\mathbf{f}_{n+1} - 9\mathbf{f}_n) \quad (7)$$

(If you're curious how they can be derived, see the non-examinable material at the end).

The methods listed above are all good ('convergent') methods, in that they compute solutions that converge to the exact ones as the step size $h \rightarrow 0$. Now let us look at

$$\mathbf{y}_{n+2} = -4\mathbf{y}_{n+1} + 5\mathbf{y}_n + h(4\mathbf{f}(x_{n+1}, \mathbf{y}_{n+1}) - 2\mathbf{f}(x_n, \mathbf{y}_n)) \quad (8)$$

and

$$\mathbf{y}_{n+3} = -2\mathbf{y}_{n+2} + \mathbf{y}_{n+1} + 2\mathbf{y}_n + h(2\mathbf{f}(x_{n+3}, \mathbf{y}_{n+3}) + \mathbf{f}(x_{n+2}, \mathbf{y}_{n+2}) + 3\mathbf{f}(x_n, \mathbf{y}_n)). \quad (9)$$

These methods are consistent—method (8) has consistency order 3, and (9) has 2 (see below for the precise definition). However, these methods are catastrophically bad—as $h \rightarrow 0$, the error does not decrease, it grows unboundedly! Our next goal is to understand why the methods in Examples 3 and 4 converge, while methods like (8), (9) do not.

Consistency+Zero-Stability \Rightarrow Convergence To gain insight, let us examine what happens to \mathbf{y}_n as $h \rightarrow 0$ in (9). For tiny h and $n = O(1)$, the recursion effectively yields $\mathbf{y}_{n+3} + 2\mathbf{y}_{n+2} - \mathbf{y}_{n+1} - 2\mathbf{y}_n = 0$. How does \mathbf{y}_n behave? This is a difference equation, and one way to solve it is as follows: (as in "Note" in lecture 12) we rewrite (assuming for simplicity \mathbf{y}_n are scalars)

$$\begin{bmatrix} \mathbf{y}_{n+3} \\ \mathbf{y}_{n+2} \\ \mathbf{y}_{n+1} \end{bmatrix} = \begin{bmatrix} -2 & 1 & 2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y}_{n+2} \\ \mathbf{y}_{n+1} \\ \mathbf{y}_n \end{bmatrix} =: A \begin{bmatrix} \mathbf{y}_{n+2} \\ \mathbf{y}_{n+1} \\ \mathbf{y}_n \end{bmatrix}.$$

Since this holds for all n , it follows immediately that (noting that the eigenvalues of A are $-2, 1, -1$)

$$\begin{bmatrix} \mathbf{y}_{n+2} \\ \mathbf{y}_{n+1} \\ \mathbf{y}_n \end{bmatrix} = A^n \begin{bmatrix} \mathbf{y}_2 \\ \mathbf{y}_1 \\ \mathbf{y}_0 \end{bmatrix} = X \begin{bmatrix} (-2)^n & & \\ & 1^n & \\ & & (-1)^n \end{bmatrix} X^{-1} \begin{bmatrix} \mathbf{y}_2 \\ \mathbf{y}_1 \\ \mathbf{y}_0 \end{bmatrix} \quad (10)$$

for an invertible matrix X of A 's eigenvectors. Now since $(-2)^n$ blows up to $\pm\infty$, so does \mathbf{y}_n ; regardless of f ! Finally, notice that the matrix $A = \begin{bmatrix} -2 & 1 & 2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$ has the same

structure as the companion matrix from lecture 8!¹ Thus the eigenvalues of A are equal to the roots of the first characteristic polynomial $\rho(z) = z^3 + 2y^2 - y - 2 = 0$.

More generally, given any multistep method, any root of $\rho(z)$ outside the unit disk will lead to similar blowups. What about roots on the unit circle? The answer is that they are fine if they are simple roots; however multiple roots on the unit circle leads to divergence². This motivates the following definition:

Definition 5. *A linear k -step method satisfies the root condition if all roots of its first characteristic polynomial $\rho(z)$ lie inside the closed unit disc, and every root that lies on the unit circle is simple.*

The root condition is thus a necessary condition for a multistep method to be convergent. The remarkable result by Dahlquist is that this property is also sufficient, as long as the method is consistent, which is a straightforward condition. That is, "Consistency + root condition \Rightarrow Convergence". Finally, the root condition can be shown to be identical to the so-called *zero-stability* (which we define and explain in the non-examinable appendix³). Thus Dahlquist's theorem is colloquially often known as

"Consistency + (Zero-)Stability \Rightarrow Convergence".

This result has sometimes been called the Fundamental Theorem of Numerical Analysis. It explains why the method (9) does not converge (the roots of $\rho(z)$ are -5 and 1 , violating the root condition), whereas the other ones are convergent (by checking consistency, and that the root condition is satisfied).

To state Dahlquist's theorem precisely, let us define consistency properly for multistep methods.

¹This is why we're solving the difference equation this way. You may well have seen other ways to solve it.

²This is because companion matrices cannot have eigenvalues of geometric multiplicity 2 or more, because $A - \lambda I$ has rank deficiency at most one. Put another way, if there is a multiple eigenvalue, A must have a Jordan block of the form $J_\lambda = \begin{bmatrix} \lambda & 1 \\ & \lambda \end{bmatrix}$. If $|\lambda| = 1$, then $\|J_\lambda^n\|_2 \rightarrow \infty$ as $n \rightarrow \infty$.

³Note that the word 'stability' in zero-stability is used in a rather different way than the stability we've been discussing, as in A -stability and L -stability, which relate to the question 'how small is small enough for h '. If confused, think of zero-stability as an exceptional use of the word.

Definition 6. The consistency error of a linear k -step method with $\sigma(1) \neq 0$ is

$$\tau(h) = \frac{\sum_{j=0}^k \alpha_j \mathbf{y}(x_j) - h \sum_{j=0}^k \beta_j \mathbf{y}'(x_j)}{h \sum_{j=0}^k \beta_j}, \quad (11)$$

where \mathbf{y} is a smooth function. A linear multi-step method has (consistency) order p if $\tau(h) = O(h^p)$.

As in Runge-Kutta methods, The consistency error here is defined to model the local error of the method; for example it reduces to that for one-step methods when $k = 1$ and $\alpha_k = 1$.

By a simple Taylor expansion of \mathbf{y} , we can obtain the following theorem.

Theorem 7. A linear multi-step method has consistency order p if and only if $\sigma(1) \neq 0$ and

$$\sum_{j=0}^k \alpha_j = 0 \quad \text{and} \quad \sum_{j=0}^k \alpha_j j^q = q \sum_{j=0}^k \beta_j j^{q-1} \quad \text{for } q = 1, \dots, p. \quad (12)$$

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

From the above theorem we see that a linear multi-step method is consistent iff

$$\rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1) \neq 0. \quad (13)$$

In general, these conditions can be reformulated more elegantly (nonexaminable): Equation (12) is equivalent to $\rho(e^h) - h\sigma(e^h) = O(h^{p+1})$.

To discuss convergence precisely for linear k -step methods, we need to specify some criteria about the choice of the starting conditions. Below, we say that a set of starting conditions $\mathbf{y}_i = \boldsymbol{\eta}_i(h)$, $i = 0, \dots, k-1$ is consistent with the initial value \mathbf{y}_0 if $\boldsymbol{\eta}_s(h) \rightarrow \mathbf{y}_0$ as $h \rightarrow 0$ for every $s = 0, \dots, k-1$.

We are now ready to state Dahlquist's Equivalence Theorem.

Theorem 8 (Dahlquist's Equivalence Theorem). For a consistent linear k -step method with consistent starting values, the root condition (=zero-stability) is necessary and sufficient for convergence, that is, $\lim_{h \rightarrow 0} \mathbf{y}_N = \mathbf{y}(X)$ (with $N = (X - x_0)/h$).

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

The proof is long and non-examinable, but you should understand the statement.

Stability of linear multi-step methods Now that we understand convergence of multi-step methods, we turn to stability⁴. 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 $|y(x)| \rightarrow 0$ as $t \rightarrow \infty$ whenever $\text{Re}(z) < 0$, and that we call its numerical approximation $\{y_n\}_{n \in \mathbb{N}}$ (asymptotically) stable if $y_n \rightarrow 0$ as $n \rightarrow \infty$ when $\text{Re}(z) < 0$.

⁴Not to be confused with zero-stability, which was crucial for convergence; here we mean the analogues of A-stability, L-stability, that is, related to the question of 'how small does h need to be?'

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

$$\sum_{j=0}^k \alpha_j y_{n+j} = \sum_{j=0}^k \beta_j z y_{n+j}, \quad \text{or equivalently,} \quad \sum_{j=0}^k (\alpha_j - z\beta_j) y_{n+j} = 0. \quad (14)$$

By an argument similar to that surrounding (10), we obtain

$$y_n = p_1(n)r_1^n + \dots + p_\ell(n)r_\ell^n, \quad (15)$$

where the r_j s 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 .

With (15), 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, then 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, $y_n \rightarrow 0$ geometrically as $n \rightarrow \infty$.

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

$$\pi(x) = \pi(x; z) := \sum_{j=0}^k (\alpha_j - z\beta_j)x^j = \rho(x) - z\sigma(x). \quad (16)$$

The stability domain of a linear multistep method is

$$S := \{z \in \mathbb{C} : \text{if } \pi(x; z) = 0, \text{ then } |x| \leq 1; \text{ multiple zeros satisfy } |x| < 1\}. \quad (17)$$

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.

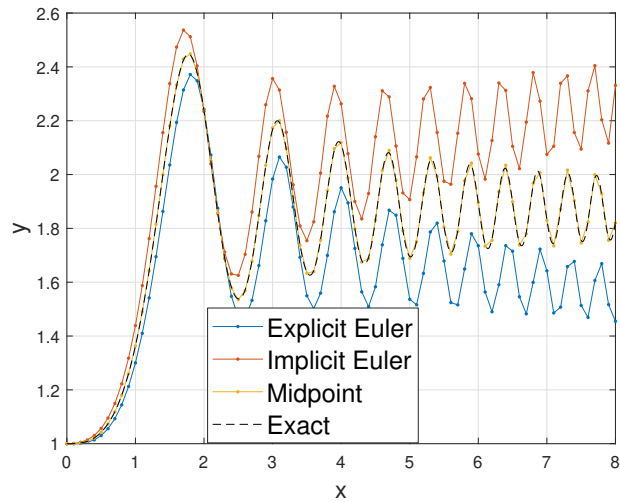
Theorem 10 (Dahlquist's second barrier). *An A -stable linear multi-step method must be implicit and of order $p \leq 2$. The trapezium rule is the second-order A -stable linear multi-step method with the smallest error constant.*

The proof is long and omitted, and non-examinable. It is possible to break the Dahlquist barrier by hybridising between multi-stage (Runge-Kutta) and multi-step methods. Such methods are called *general linear methods*⁵.

Example 11. *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.

⁵See *General linear methods*, J. C. Butcher, Acta Numerica (2006).



We now look at the error $y(x_n) - y_n$, shown in Figure 1. There we also examine the unstable multistep method (8), which 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!

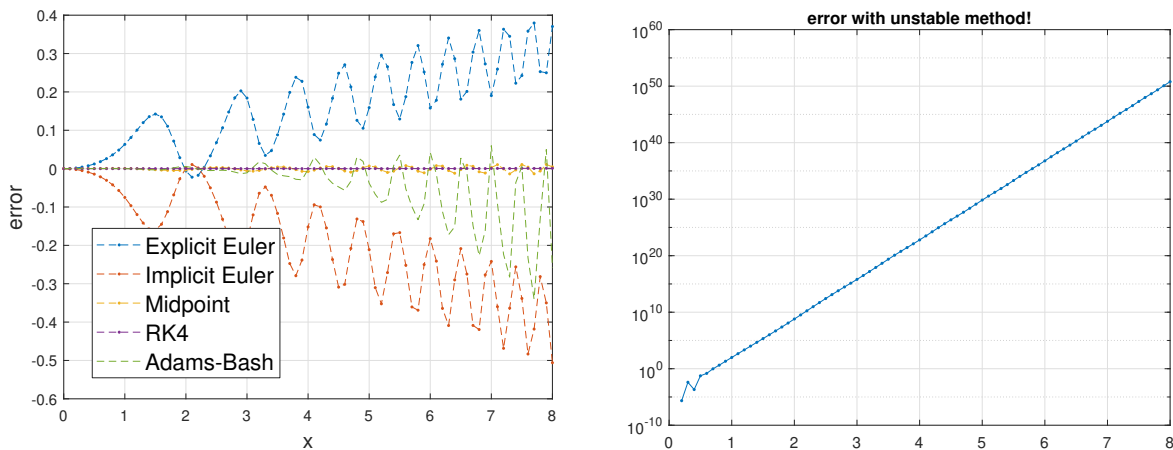
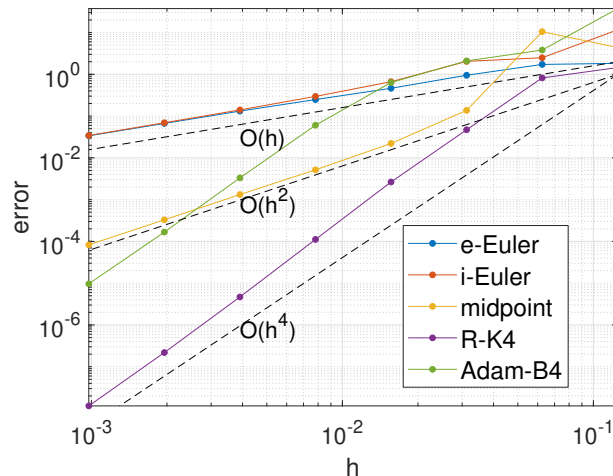


Figure 1: Errors with stable methods (left) and an unstable method (8)

Finally, we can vary the step size h and examine the convergence as $h \rightarrow 0$. 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*)

Summary of lectures 12–15 Here is a summary and key takeaways from the last part of the course on numerical solution of IVPs:

- Euler’s method; explicit and implicit methods. Implicit methods are more expensive, but sometimes achieve higher order, and more importantly, more stable (can be A-stable, L-stable).
- Consistency error (local error as $h \rightarrow 0$), order of accuracy (global error) and convergence (does computed \mathbf{y} tend to the exact solution as $h \rightarrow 0$?).
- Runge-Kutta methods, which achieve higher order of accuracy by evaluating $f(x, y)$ at ‘intermediate points’. Convergence (relatively straightforward from the theorem in Lecture 12) and stability (A-stable, L-stable).
- Multistep methods, which achieve higher order of accuracy by using previously computed solutions. Convergence (requires zero-stability) and stability (A-stable).

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

- Numerical Solution of Partial Differential Equations (Part B)
- Approximation of Functions (Part C, offered –2023)
- Numerical Linear Algebra (Part C)
- Finite Element Method for PDEs (Part C)
- Continuous Optimisation (Part C)

The remainder is nonexaminable.

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

Definition 12. 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 13. 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

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

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

Example 14. We can construct a multi-step method using the previous lemma. Indeed, by Taylor expansion of the logarithm $\log(1 - x) = -\sum_{i=1}^{\infty} x^i/i$,

$$hD = -\log(\mathbf{I} - \Delta) = \left(\Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots \right), \quad (18)$$

and thus

$$h\mathbf{f}(x_n, \mathbf{y}(x_n)) = \left(\Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots \right) \mathbf{y}(x_n). \quad (19)$$

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

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

Example 15. Explicit Euler's method arises from truncating the series

$$hD = \left(\Delta - \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \dots \right) E, \quad (20)$$

which can be derived similarly.

Using the formal equalities

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

we can derive the Adams-Moulton methods (6) and Adams-Bashforth methods (7).

More on zero-stability 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 (e.g. Runge-Kutta) 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 16. 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

$$\max_{0 \leq n \leq N} \|\mathbf{y}_n - \tilde{\mathbf{y}}_n\| \leq K \max_{j \leq k-1} \|\mathbf{y}_j - \tilde{\mathbf{y}}_j\|. \quad (21)$$

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

Definition 17. 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 18. 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*.

The first Dahlquist barrier theorem 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 (this result is non-examinable).

Theorem 19 (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).