Linear Multistep Methods

An extra file for Lecture 3

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1 Introduction and Structural Classification

Linear Multistep Methods (LMMs) achieve high-order accuracy by utilizing approximations from several previous time steps. Consider the foundational initial value problem (IVP):

$$\frac{dy}{dt} = f(t, y), \quad y(t_0) = y_0 \tag{1}$$

Let $h > 0$ denote a constant step size, $t_n = t_0 + nh$, $y_n \approx y(t_n)$, and $f_n = f(t_n, y_n)$. A general linear k-step multistep method is defined as:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{2}$$

where α_j and β_j are real coefficients. We normalize the representation by enforcing $\alpha_k = 1$. The classification of an LMM is strictly dictated by the parameter β_k:

1. **Explicit Methods ($\beta_k = 0$)**: The advanced state y_{n+k} depends exclusively on historical values. The calculation requires no algebraic nonlinear solvers.
2. **Implicit Methods ($\beta_k \neq 0$)**: The advanced derivative $f_{n+k} = f(t_{n+k}, y_{n+k})$ appears on the right-hand side, requiring nonlinear coupled system solves.

The three preeminent families are **Adams-Bashforth** (explicit, integrating historical derivatives), **Adams-Moulton** (implicit, including the target derivative), and **Backward Differentiation Formulas (BDF)** (implicit, differentiating historical states).

2 The Characteristic Polynomials and Consistency

To systematically analyze the local behavior and structural algebraic configuration of a k-step method, we introduce the first and second characteristic polynomials, which fully encapsulate the coefficients of Eq. (2).

Definition 2.1. The **first characteristic polynomial** $\rho(\zeta)$ and the **second characteristic polynomial** $\sigma(\zeta)$ of a linear multistep method are polynomials of a complex variable $\zeta \in \mathbb{C}$, defined respectively as:

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j \tag{3}$$

By matching Taylor series expansions of the discrete difference operator against the continuous field, we map the error coefficients C_q. A linear multistep method is **consistent** with the underlying ODE if it achieves at least first-order accuracy ($p \geq 1$), which requires satisfying the essential relations:

$$\rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1) \tag{4}$$

3 Zero-Stability and the Dahlquist Barriers

For multistep methods, consistency does not automatically guarantee global convergence. We require a stable mapping across the unforced solution paths to prevent round-off perturbations from growing exponentially.

Theorem 3.1 (Dahlquist Root Condition)**.** A linear multistep method is defined as **zero-stable** (or null-stable) if and only if all roots ζ_m of the first characteristic polynomial $\rho(\zeta) = 0$ satisfy:

1. All roots lie within the closed unit disk: $|\zeta_m| \leq 1$.
2. Any root residing on the boundary ($|\zeta_m| = 1$) must be simple (non-repeating).

Dahlquist's Equivalence Theorem establishes that for a consistent LMM, **Zero-Stability** is the necessary and sufficient condition for **Global Convergence**. Maximizing accuracy order p is bound by structural limits:

Theorem 3.2 (Dahlquist's First Order Barrier)**.** The maximum order p of a zero-stable k-step linear multistep method satisfies: $p \leq k + 2$ if k is even, $p \leq k + 1$ if k is odd, and $p \leq k$ if the method is explicit ($\beta_k = 0$).

4 Absolute Stability Analysis and Boundary Locus

To evaluate numerical behavior over long intervals or highly damped trajectories, we apply the general linear multistep scheme (2) to Dahlquist's complex scalar test equation:

$$\frac{dy}{dt} = \lambda y, \quad \mathrm{Re}(\lambda) \leq 0, \quad y(0) = y_0 \tag{5}$$

Substituting $f_{n+j} = \lambda y_{n+j}$ into Eq. (2) and introducing the dimensionless scaled step size parameter $z = \lambda h \in \mathbb{C}$ yields the homogeneous linear recurrence relation $\sum_{j=0}^{k} (\alpha_j - z\beta_j) y_{n+j} = 0$.

Definition 4.1. The algebraic relation dictating the unforced growth of the recurrence step is designated as the **Stability Polynomial** $\pi(\zeta; z)$, defined via the characteristic polynomials as:

$$\pi(\zeta; z) = \rho(\zeta) - z\sigma(\zeta) = 0 \tag{6}$$

The **Region of Absolute Stability** $\mathcal{D}$ contains all values $z \in \mathbb{C}$ for which all roots ζ_m of the stability polynomial (6) reside strictly within or on the closed unit disk ($|\zeta_m| \leq 1$). The boundary of this absolute region, $\partial\mathcal{D}$, corresponds to the locus where at least one root lies exactly on the unit circle, tracking the coordinate $\zeta = e^{i\theta}$ for $\theta \in [0, 2\pi]$. Setting $\pi(e^{i\theta}; z) = 0$ and isolating z yields the classical **Boundary Locus Formula**:

$$z(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})} \tag{7}$$

Unlike one-step methods where the amplification factor is governed by an explicit **Stability Function** $y_{n+1} = R(z)y_n$ mapping a single step, multi-step formulations do not possess a single scalar function $R(z)$ because the state information is distributed across a vector of historical steps $[y_n, \ldots, y_{n+k-1}]^T$. Instead, the stability is fundamentally governed by the root behavior of the polynomial $\pi(\zeta; z)$.

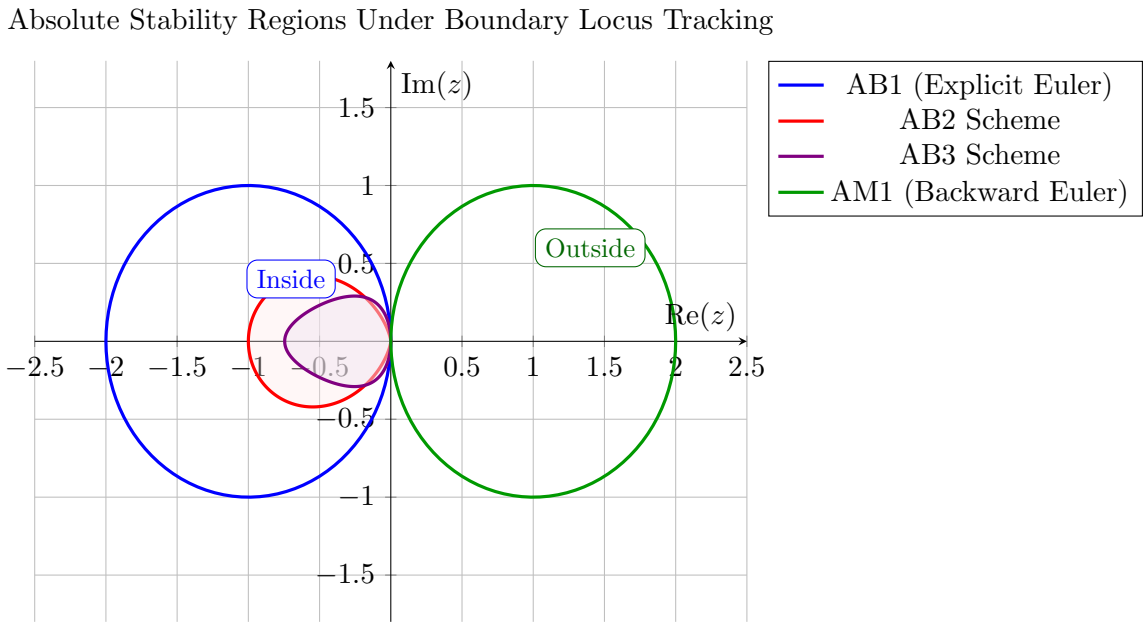


Figure 1: Absolute stability boundaries mapped via Eq. (7). For explicit AB families, the stable domain is inside the boundaries, while for implicit AM1, it covers the exterior left half-plane.

5 Stiff Systems and Dahlquist's Second Barrier

Implicit multi-step methods are essential for solving **stiff differential equations**, which feature heavily coupled processes operating on vastly different time scales. Explicit methods require $h \ll 1$ for stability, making simulations unfeasible. However, A-stability is bounded by severe limitations:

Theorem 5.1 (Dahlquist's Second Stability Barrier)**.** The accuracy configuration of A-stable linear multistep methods is bounded by:

1. No explicit linear multistep method can be A-stable.
2. An implicit linear multistep method can be A-stable if and only if $p \leq 2$.
3. The unique A-stable LMM of order $p = 2$ with the smallest possible error constant is the classical **Trapezoidal Rule** (Adams-Moulton 2).

To circumvent this barrier, higher-order BDF methods ($p \geq 3$) give up full A-stability to achieve **$A(\alpha)$-stability**, leaving only a narrow unstable wedge around the imaginary vertical axis.

BDF Order (p)	1	2	3	4	5	6
Zero-Stable?	Yes	Yes	Yes	Yes	Yes	Yes
A-Stable?	Yes	Yes	No	No	No	No
Max Wedge Angle (α)	90°	90°	86°	73°	51°	17°

Table 1: Stability configuration of BDF methods. Above order $p = 6$, BDF methods lose zero-stability.

6 Conclusion

Linear multistep methods maximize computational efficiency by utilizing historical calculations. Their numerical configuration requires balancing consistency, zero-stability, and absolute stability under the boundaries established by Dahlquist's structural barriers.