

Numerical Solutions to Differential Equations

Lecture Notes #7 — Linear Multistep Methods

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Quick Review, Higher Order Methods for $y'(t) = f(t, y)$

Taylor When the Taylor series for $f(t, y)$ is available, we can use the expansion to build higher accurate methods.

RK If the Taylor series is not available (or too expensive), but $f(t, y)$ easily can be computed, then RK-methods are a good option. RK-methods compute / sample / measure $f(t, y)$ in a neighborhood of the solution curve and use those a combination of the values to determine the final step from (t_n, y_n) to (t_{n+1}, y_{n+1}) .

LMM If the Taylor series is not available, and $f(t, y)$ is expensive to compute (could be a lab experiment?), then LMMs are a good idea. Only one new evaluation of $f(t, y)$ needed per iteration. LMMs use more of the history $\{(t_{n-k}, y_{n-k}); k = 0, \dots, s\}$ to build up the step.

Chronology

Methods

1883 Adams and Bashforth introduce the idea of improving the Euler method by letting the solution depend on a longer “history” of computed values. (Now known as Adams-Bashforth schemes)

1925 Nyström proposes another class of LMM methods, $\rho(\zeta) = \zeta^k - \zeta^{k-2}$, explicit.

1926 Moulton developed the implicit version of Adams and Bashforth's idea. (Now known as Adams-Moulton schemes)

1952 Curtiss and Hirschfelder — Backward difference methods.

1953 Milne's methods, $\rho(\zeta) = \zeta^k - \zeta^{k-2}$, implicit.

Modern Theory

1956 Dahlquist

1962 Henrici

Consider the LMM applied to a noise-free problem:

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

$$y_\mu = \eta_\mu(h), \quad \mu = 0, 1, \dots, k-1$$

and the same LMM applied to a slightly perturbed system

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

$$y_\mu = \eta_\mu(h) + \delta_\mu, \quad \mu = 0, 1, \dots, k-1$$

Perturbations are typically due to discretization and round-off.

Definition (Zero-stability)

Let $\{\delta_n, n = 0, 1, \dots, N\}$ and $\{\delta_n^*, n = 0, 1, \dots, N\}$ be any two perturbations of the LMM, and let $\{y_n, n = 0, 1, \dots, N\}$ and $\{y_n^*, n = 0, 1, \dots, N\}$ be the resulting solutions. If there exists constants S and h_0 such that, for all $h \in (0, h_0]$,

$$\|y_n - y_n^*\| \leq S\epsilon, \quad 0 \leq n \leq N$$

whenever

$$\|\delta_n - \delta_n^*\| \leq \epsilon, \quad 0 \leq n \leq N$$

the method is said to be **zero stable**.

Applying the LMM to $z_n = y_n - y_n^*$, $\widehat{\delta}_n = \delta_n - \delta_n^*$ gives:

$$\sum_{j=0}^k \alpha_j z_{n+j} = \widehat{\delta}_{n+k}$$

$$z_\mu = \widehat{\delta}_\mu, \quad \mu = 0, 1, \dots, k-1$$

Interpretation

That is, zero-stability guarantees that a zero-forced system (with zero starting-values) produces errors bounded by the round-off noise.

In infinite precision, the solution stays at zero.

If the roots of the characteristic polynomial

$$\sum_{j=0}^k \alpha_j y_{n+j} = 0, \quad \Leftrightarrow \quad \rho(\zeta) = 0$$

satisfies the **root criterion**

$$|r_j| \leq 1, \quad j = 1, 2, \dots, k$$

then the method is **zero-stable**.

Theorem (Convergence)

*The method is **convergent** if and only if it is consistent and zero-stable.*

Theorem (Germund Dahlquist, 1956)

No zero-stable s -step method can have order exceeding $(s + 1)$ when s is odd, and $(s + 2)$ when s is even.

Definition

A zero-stable s -step method is said to be **optimal** if it is of order $(s + 2)$.

Observation

Simpson's rule is optimal (to be shown...)

$$y_{n+2} - y_n = \frac{h}{3} [f_{n+2} + 4f_{n+1} + f_n]$$

Note: Zero-stability does not give us the whole picture; see **absolute stability**... (coming right up!)

The first Dahlquist barrier reminds us of something from Math 541:

Theorem (Errors for Newton-Cotes Integration Formulas)

Suppose that $\sum_{i=0}^n a_i f(x_i)$ denotes the $(n + 1)$ point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b - a)/n$. Then there exists $\xi \in (a, b)$ for which

$$\int_a^b f(x) dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n) dt,$$

if n is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x) dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n) dt,$$

if n is odd and $f \in C^{n+1}[a, b]$.

- For the Newton-Cotes' formulas: when n is an even integer, the degree of precision (higher order polynomial for which the formula is exact) is $(n + 1)$. When n is odd, the degree of precision is only n .
- For zero-stable s -step LMMs: when s is even, the order is at most $(s + 2)$; when s is odd, the order is at most $(s + 1)$.

Coincidence? — Unlikely!

The LMMs get the next y_{k+1} by integrating over the solution history; and the Newton-Cotes' formulas give the (numerical) integral over an interval.

Simpson's Rule, $y_{n+1} - y_{n-1} = \frac{h}{3}[f_{n+1} + 4f_n + f_{n-1}]$

For **notational convenience**, the points have been re-numbered (index lowered by one), and we expand around the center point (t_n, y_n) :

$$y_{n+1} \sim y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{6}y'''_n + \frac{h^4}{24}y^{(4)}_n + \frac{h^5}{120}y^{(5)}_n + \mathcal{O}(h^6)$$

$$y_{n-1} \sim y_n - hy'_n + \frac{h^2}{2}y''_n - \frac{h^3}{6}y'''_n + \frac{h^4}{24}y^{(4)}_n - \frac{h^5}{120}y^{(5)}_n + \mathcal{O}(h^6)$$

$$\text{LHS} \sim 2hy'_n + \frac{h^3}{3}y'''_n + \frac{h^5}{60}y^{(5)}_n + \mathcal{O}(h^7)$$

$$f_{n-1} \sim f_n - hf'_n + \frac{h^2}{2}f''_n - \frac{h^3}{6}f'''_n + \frac{h^4}{24}f^{(4)}_n - \frac{h^5}{120}f^{(5)}_n + \mathcal{O}(h^6)$$

$$4f_n \sim 4f_n$$

$$f_{n+1} \sim f_n + hf'_n + \frac{h^2}{2}f''_n + \frac{h^3}{6}f'''_n + \frac{h^4}{24}f^{(4)}_n + \frac{h^5}{120}f^{(5)}_n + \mathcal{O}(h^6)$$

$$\text{RHS} \sim \frac{h}{3} \left[6f_n + h^2f''_n + \frac{h^4}{12}f^{(4)}_n + \mathcal{O}(h^6) \right]$$

Simpson's Rule, $\mathbf{y}_{n+1} - \mathbf{y}_{n-1} = \frac{h}{3}[\mathbf{f}_{n+1} + 4\mathbf{f}_n + \mathbf{f}_{n-1}]$, II

$$\text{LHS} \sim 2hy'_n + \frac{h^3}{3}y_n''' + \frac{h^5}{60}y_n^{(5)} + \mathcal{O}(h^7)$$

$$\text{RHS} \sim \frac{h}{3} \left[6f_n + h^2f_n'' + \frac{h^4}{12}f_n^{(4)} + \mathcal{O}(h^6) \right]$$

Use the equation $y'(t) = f(t, y) \Leftrightarrow y^{(k+1)}(t) = f^{(k)}(t, y)$:

$$\text{LHS} \sim 2hf_n + \frac{h^3}{3}f_n'' + \frac{h^5}{60}f_n^{(4)} + \mathcal{O}(h^7)$$

$$\text{RHS} \sim 2hf_n + \frac{h^3}{3}f_n'' + \frac{h^5}{24}f_n^{(4)} + \mathcal{O}(h^7)$$

$$\frac{\text{LHS} - \text{RHS}}{h} = h^4 \left[\frac{1}{60} - \frac{1}{24} \right] f_n^{(4)} + \mathcal{O}(h^6)$$

Simpson's Rule — Local Truncation Error

$$\text{LTE}_{\text{Simpson}}(h) = \mathcal{O}(h^4)$$

Linear Stability Theory for LMMs

As we did for RK-methods we apply our LMMs to the problem

$$y'(t) = \lambda y(t), \quad \text{Re}(\lambda) \leq 0$$

and search for the region $\hat{h} = (h\lambda)$ where the LMM does not grow exponentially.

We get...

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

Thus...

$$\sum_{j=0}^k [\alpha_j - h\beta_j \lambda] \mathbf{y}_{n+j} = \mathbf{0}$$

Linear Stability Theory for LMMs, II

We have

$$\sum_{j=0}^k [\alpha_j - h\beta_j \lambda] \mathbf{y}_{n+j} = \mathbf{0}$$

A general solution of this difference equation is

$$y_n = r_0 r^n$$

where r is a root of the characteristic polynomial

$$0 = \sum_{j=0}^k [\alpha_j - h\beta_j \lambda] r^j = \rho(r) - \hat{h}\sigma(r) = \pi(r, \hat{h})$$

$\pi(r, \hat{h})$ is called the **stability polynomial**.

Linear Stability Theory: Absolute Stability

Definition (Absolute Stability)

A linear multistep method is said to be **absolutely stable** for a given \hat{h} , if for that \hat{h} all the roots of the stability polynomial $\pi(r, \hat{h})$ satisfy $|r_j| < 1$, $j = 1, 2, \dots, s$, and to be **absolutely unstable** for that \hat{h} otherwise.

Definition (Region of Absolute Stability)

The LMM is said to have the **region of absolute stability** \mathcal{R}_A , where \mathcal{R}_A is a region in the complex \hat{h} -plane, if it is absolutely stable for all $\hat{h} \in \mathcal{R}_A$. The intersection of \mathcal{R}_A with the real axis is called the **interval of absolute stability**.

The Boundary Locus Method

The boundary of \mathcal{R}_A , denoted $\partial\mathcal{R}_A$ is given by the points where one of the roots of $\pi(r, \hat{h})$ is $e^{i\theta}$.

$\partial\mathcal{R}_A$ is \hat{h} such that

$$\pi(e^{i\theta}, \hat{h}) = \rho(e^{i\theta}) - \hat{h}\sigma(e^{i\theta}) = 0, \quad \theta \in [0, 2\pi)$$

Solving for \hat{h} gives

Method: Boundary Locus

$$\hat{h}(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}, \quad \theta \in [0, 2\pi)$$

The Region of Absolute Stability for Simpson's Method

Consider Simpson's Rule, and its characteristic polynomials

$$y_{n+2} - y_n = \frac{h}{3} [f_{n+2} + 4f_{n+1} + f_n]$$

$$\rho(\zeta) = \zeta^2 - 1, \quad \sigma(\zeta) = \frac{1}{3} [\zeta^2 + 4\zeta + 1]$$

The $\partial\mathcal{R}_A$ is given by

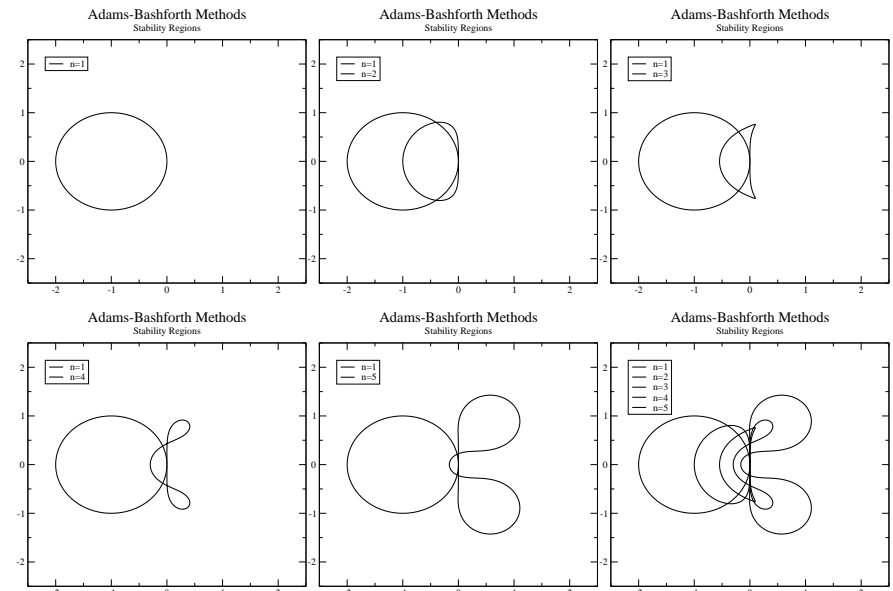
$$\hat{h}(\theta) = 3 \frac{e^{2i\theta} - 1}{e^{2i\theta} + 4e^{i\theta} + 1} = 3 \frac{e^{i\theta} - e^{-i\theta}}{e^{i\theta} + 4 + e^{-i\theta}} = \frac{6i \sin \theta}{4 + 2 \cos \theta} = \frac{3i \sin \theta}{2 + \cos \theta}$$

Hence $\partial\mathcal{R}_A$ is the segment $[-i\sqrt{3}, i\sqrt{3}]$ of the imaginary axis.
Simpson's Rule has a zero-area region of absolute stability (Bummer).

Optimal Methods are not so Optimal after all...

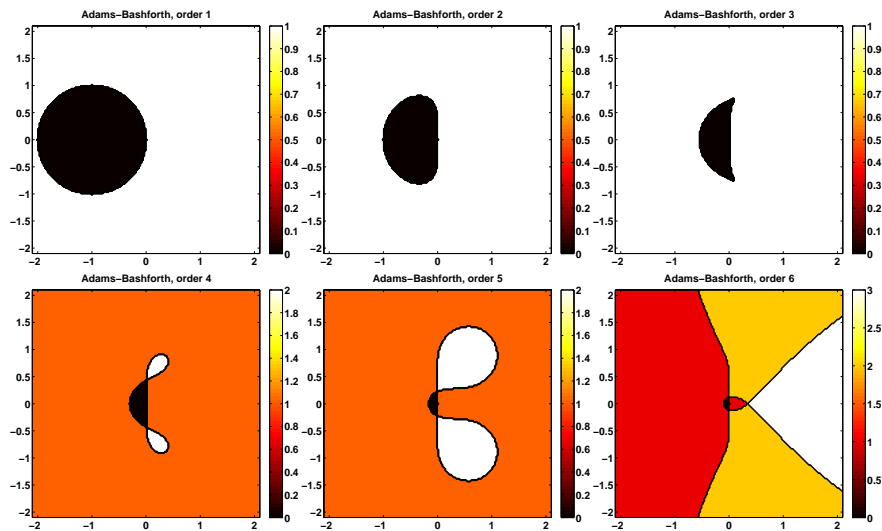
- All optimal methods have regions of absolute stability which are either empty, or essentially useless — they do not contain the negative real axis in the neighborhood of the origin.
- By squeezing out the maximum possible order, subject to zero-stability, the region of absolute stability get squeezed flat.
- “Optimal” methods are essentially useless.

Stability Regions for Adams-Bashforth Methods



Stability Regions for Adams-Bashforth Methods

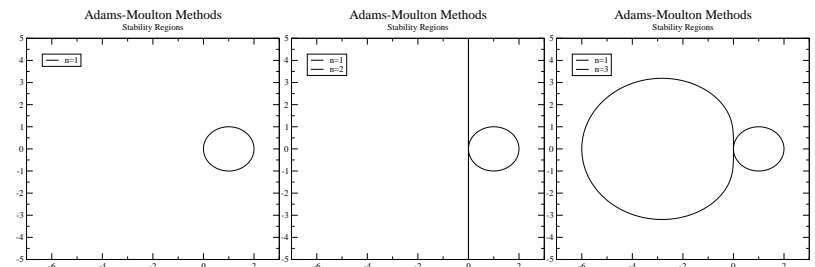
$|r_\nu| > 1$ count



Linear Multistep Methods

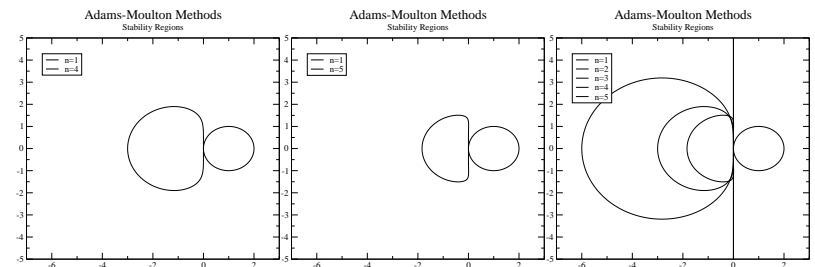
— (21/30)

Stability Regions for Adams-Moulton Methods



The exterior of the circle!

The left half plane!



Linear Multistep Methods

— (22/30)

Absolute Stability Matters!

So far we have seen (only) two methods which produce bounded solutions to the ODE

$$y'(t) = \lambda y(t)$$

for all $\lambda : \text{Re}(\lambda) < 0$:

Implicit Euler (Adams-Moulton, $n = 1$)

$$y_{n+1} = y_n + hf_{n+1}$$

Trapezoidal Rule (Adams-Moulton, $n = 2$)

$$y_{n+1} = y_n + \frac{h}{2} [f_{n+1} + f_n]$$

The size of the stability region located in the left half plane tends to shrink as we require higher order accuracy — **requiring a smaller stepsize h** .

Linear Multistep Methods

— (23/30)

Backward Differentiation Formulas

Can we find high order methods with large stability regions!?

Yes!

The class of Backward Differentiation Formulas (BDF) defined by

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

have large regions of absolute stability.

Note that the right-hand side is simple, but the left-hand side is more complicated (the opposite of Adams-methods).

Linear Multistep Methods

— (24/30)

The k th order BDF is derived by constructing the polynomial interpolant through the points

$$(t_{n+1}, y_{n+1}), (t_n, y_n), \dots, (t_{n-k+1}, y_{n-k+1}),$$

i.e. (after re-numbering the points: $0, 1, \dots, k$)

$$P_k(t) = \sum_{m=0}^k y_{n+m} L_{k,m}(t), \quad \text{where } L_{k,m}(t) = \prod_{\ell=0, \ell \neq m}^k \frac{t - t_\ell}{t_m - t_\ell}$$

and then computing the derivative of this polynomial at the point corresponding to t_{n+1} and setting it equal to f_{n+1} .

Newton's Backward Difference Formula (Math 541) comes in handy. We can write the interpolating polynomial

$$P_k(t_{n+1} + sh) = y_{n+1} + \sum_{j=1}^k (-1)^j \binom{-s}{j} \nabla^j y_{n+1}$$

where Newton's divided differences are

$$\nabla y_{n+1} = [y_{n+1} - y_n], \quad \nabla^2 y_{n+1} = \frac{1}{2} [\nabla y_{n+1} - \nabla y_n], \quad \dots$$

The binomial coefficient is given by

$$\binom{-s}{j} = \frac{-s(-s-1)\cdots(-s-j+1)}{j!} = (-1)^j \frac{s(s+1)\cdots(s+j-1)}{j!}$$

In order to compute $P'_k(t_{n+1})$ we need to compute

$$\left. \frac{d}{ds} \binom{-s}{j} \right|_{s=0}$$

Massive application of the product rule gives us

$$\left. \frac{d}{ds} \binom{-s}{j} \right|_{s=0} = (-1)^j \frac{(j-1)!}{j!} = \frac{(-1)^j}{j}$$

That is

$$hP'_k(t_{n+1}) = \sum_{j=1}^k \frac{(-1)^{2j}}{j} \nabla^j y_{n+1} = \sum_{j=1}^k \frac{1}{j} \nabla^j y_{n+1}$$

We now have

$$\sum_{j=1}^k \frac{1}{j} \nabla^j y_{n+1} = hf_{n+1}$$

Making sure that the coefficient for y_{n+1} is 1:

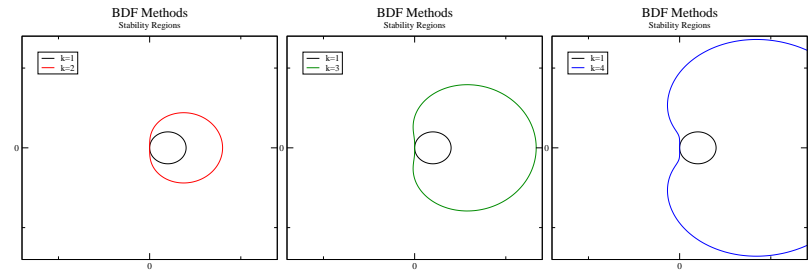
$$\left[\sum_{j=1}^k \frac{1}{j} \right]^{-1} \sum_{j=1}^k \frac{1}{j} \nabla^j y_{n+1} = h \left[\sum_{j=1}^k \frac{1}{j} \right]^{-1} f_{n+1}$$

BDFs, $k = 1, 2, \dots, 6$

k	BDF	LTE
1	$y_{n+1} - y_n = hf_{n+1}$	$-\frac{1}{2}h$
2	$y_{n+1} - \frac{4}{3}y_n + \frac{1}{3}y_{n-1} = \frac{2}{3}hf_{n+1}$	$-\frac{2}{9}h^2$
3	$y_{n+1} - \frac{18}{11}y_n + \frac{9}{11}y_{n-1} - \frac{2}{11}y_{n-2} = \frac{6}{11}hf_{n+1}$	$-\frac{3}{22}h^3$
4	$y_{n+1} - \frac{48}{25}y_n + \frac{36}{25}y_{n-1} - \frac{16}{25}y_{n-2} + \frac{3}{25}y_{n-3} = \frac{12}{25}hf_{n+1}$	$-\frac{12}{125}h^4$
5	$y_{n+1} - \frac{300}{137}y_n + \frac{300}{137}y_{n-1} - \frac{200}{137}y_{n-2} + \frac{75}{137}y_{n-3} - \frac{12}{137}y_{n-4} = \frac{60}{137}hf_{n+1}$	$-\frac{10}{137}h^5$
6	$y_{n+1} - \frac{360}{147}y_n + \frac{450}{147}y_{n-1} - \frac{400}{147}y_{n-2} + \frac{225}{147}y_{n-3} - \frac{72}{147}y_{n-4} + \frac{10}{147}y_{n-5} = \frac{60}{147}hf_{n+1}$	$-\frac{20}{343}h^6$

These are all **zero-stable**. BDFs for $k \geq 7$ are not zero-stable.

Stability Regions for BDF Methods



The exterior(s) / Parts of Left Half Plane

