Numerical Solutions to Differential Equations

Lecture Notes #7 — Linear Multistep Methods

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Outline

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 $\{(t_{n-k}, y_{n-k});\ k = 0, \ldots, s\}$ 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 Hirschenfelder — Backward difference methods.

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

Modern Theory

1956 Dahlquist

1962 Henrici

Introducing Zero-Stability (Review)

Consider the LMM applied to a noise-free problem:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}$$
$$y_\mu = \eta_\mu(h), \quad \mu = 0, 1, \ldots, k-1$$

and the same LMM applied to a slightly perturbed system

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} + \delta_{n+k}$$
$$y_\mu = \eta_\mu(h) + \delta_\mu, \quad \mu = 0, 1, \ldots, k-1$$

Perturbations are typically due to discretization and round-off.

Defining Zero-Stability (Review)

Definition (Zero-stability)

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

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

whenever

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

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

Interpreting Zero-Stability (Formalized)

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

$$\sum_{j=0}^{k} \alpha_j z_{n+j} = \widehat{\delta}_{n+k}$$
$$z_\mu = \widehat{\delta}_\mu, \quad \mu = 0, 1, \ldots, k-1$$

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.

A Simple Criterion for Zero-Stability (Review)

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**

$$|r_j| \le 1, \quad j = 1, 2, \ldots, k$$

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

Theorem (Convergence)

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

The First Dahlquist Barrier, I/III — Statement

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...)

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

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

The First Dahlquist Barrier, II/III — Newton-Cotes Errors

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*

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

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

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

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

The First Dahlquist Barrier, III/III — Comments

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

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

$$\begin{array}{rcl}
y_{n+1} & \sim & y_n + hy_n' + \frac{h^2}{2}y_n'' + \frac{h^3}{6}y_n''' + \frac{h^4}{24}y_n^{(4)} + \frac{h^5}{120}y_n^{(5)} + \mathcal{O}(h^6) \\
y_{n-1} & \sim & y_n - hy_n' + \frac{h^2}{2}y_n'' - \frac{h^3}{6}y_n''' + \frac{h^4}{24}y_n^{(4)} - \frac{h^5}{120}y_n^{(5)} + \mathcal{O}(h^6) \\
\hline
\text{LHS} & \sim & 2hy_n' + \frac{h^3}{3}y_n''' + \frac{h^5}{60}y_n^{(5)} + \mathcal{O}(h^7)
\end{array}$$

$$\begin{array}{rcl}
f_{n-1} & \sim & f_n - hf_n' + \frac{h^2}{2}f_n'' - \frac{h^3}{6}f_n''' + \frac{h^4}{24}f_n^{(4)} - \frac{h^5}{120}f_n^{(5)} + \mathcal{O}(h^6) \\
4f_n & \sim & 4f_n \\
f_{n+1} & \sim & f_n + hf_n' + \frac{h^2}{2}f_n'' + \frac{h^3}{6}f_n''' + \frac{h^4}{24}f_n^{(4)} + \frac{h^5}{120}f_n^{(5)} + \mathcal{O}(h^6) \\
\hline
\text{RHS} & \sim & \frac{h}{3}\left[6f_n + h^2 f_n'' + \frac{h^4}{12}f_n^{(4)} + \mathcal{O}(h^6)\right]
\end{array}$$

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

$$\begin{aligned} \text{LHS} &\sim 2hy_n' + \frac{h^3}{3}y_n''' + \frac{h^5}{60}y_n^{(5)} + \mathcal{O}(h^7) \\ \text{RHS} &\sim \frac{h}{3}\left[6f_n + h^2 f_n'' + \frac{h^4}{12}f_n^{(4)} + \mathcal{O}(h^6)\right] \end{aligned}$$

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

$$\begin{aligned} \text{LHS} &\sim 2hf_n + \frac{h^3}{3}f_n'' + \frac{h^5}{60}f_n^{(4)} + \mathcal{O}(h^7) \\ \text{RHS} &\sim 2hf_n + \frac{h^3}{3}f_n'' + \frac{h^5}{24}f_n^{(4)} + \mathcal{O}(h^7) \end{aligned}$$

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

Simpson's Rule — Local Truncation Error

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

Linear Stability Theory for LMMs

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

$$y'(t) = \lambda y(t), \quad Re(\lambda) \le 0$$

and search for the region $\widehat{h} = (h\lambda)$ 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...

$$\sum_{j=0}^{k}\left[\alpha_j - h\beta_j\lambda\right] y_{n+j} = 0$$

Linear Stability Theory for LMMs, II

We have

$$\sum_{j=0}^{k}\left[\alpha_j - h\beta_j\lambda\right] y_{n+j} = 0$$

A general solution of this difference equation is

$$y_n = r_0 r^n$$

where r is a root of the characteristic polynomial

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

$\pi(r,\widehat{h})$ 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 $\widehat{h}$, if for that $\widehat{h}$ all the roots of the stability polynomial $\pi(r,\widehat{h})$ satisfy $|r_j| < 1$, $j = 1, 2, \ldots, s$, and to be **absolutely unstable** for that $\widehat{h}$ 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 $\widehat{h}$-plane, if it is absolutely stable for all $\widehat{h} \in \mathcal{R}_A$. 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 $\pi(r, \widehat{h})$ is $e^{i\theta}$.

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

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

Solving for $\widehat{h}$ gives

Method: Boundary Locus

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

The Region of Absolute Stability for Simpson's Method

Consider Simpson's Rule, and its characteristic polynomials

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

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

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

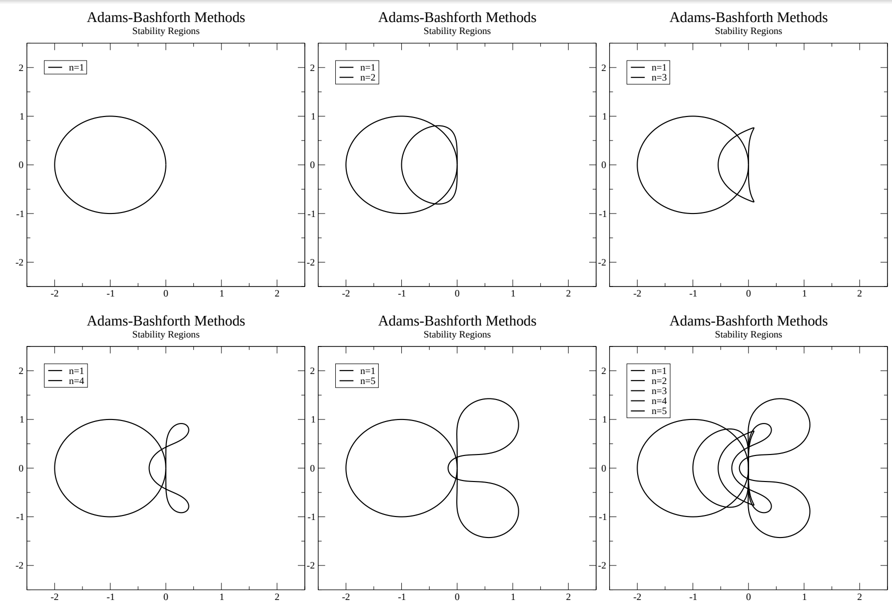
$$\widehat{h}(\theta) = 3\frac{e^{2i\theta} - 1}{e^{2i\theta} + 4e^{i\theta} + 1} = 3\frac{e^{i\theta} - e^{-i\theta}}{e^{i\theta} + 4 + e^{-i\theta}} = \frac{6i\sin\theta}{4 + 2\cos\theta} = \frac{3i\sin\theta}{2 + \cos\theta}$$

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).

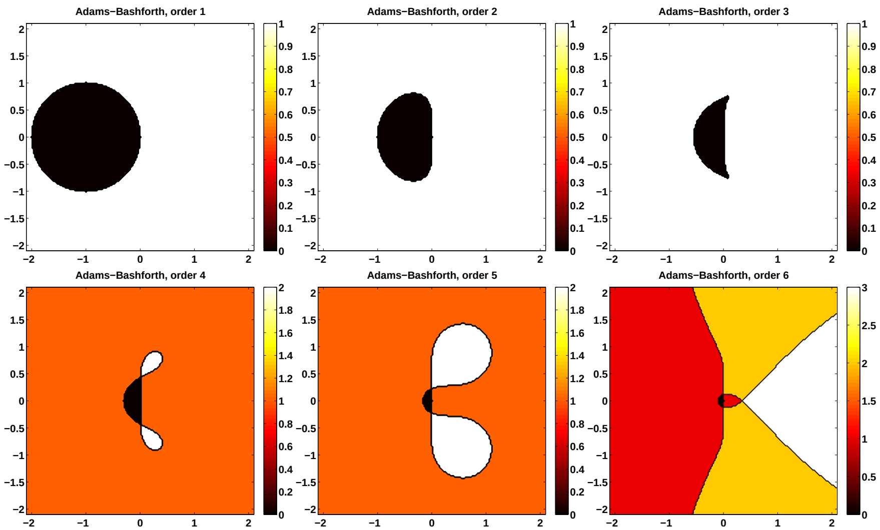
Optimal Methods are not so Optimal after all...

- 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.

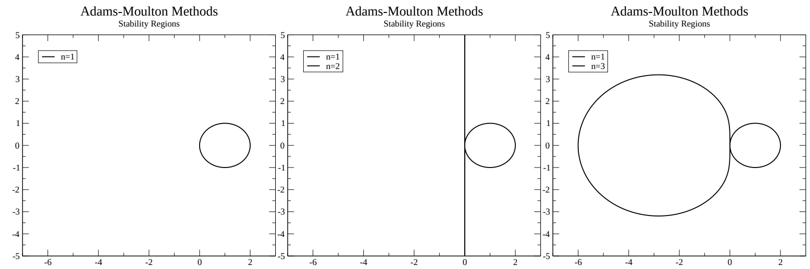
Stability Regions for Adams-Bashforth Methods



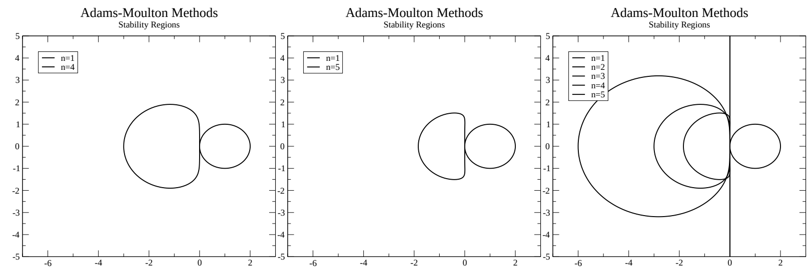
Stability Regions for Adams-Bashforth Methods $|r_\nu| > 1$ count



Stability Regions for Adams-Moulton Methods



The exterior of the circle! The left half plane!



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 $\lambda : Re(\lambda) < 0$:

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

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

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

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

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.**

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).

Deriving BDF I/IV

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

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

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

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

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

Deriving BDF II/IV

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

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

Deriving BDF III/IV

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

$$\frac{d}{ds}\binom{-s}{j}\bigg|_{s=0}$$

Massive application of the product rule gives us

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

That is

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

Deriving BDF IV/IV

We now have

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

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

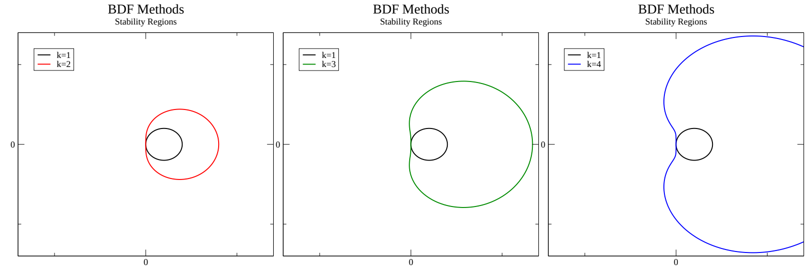
$$\left[\sum_{j=1}^{k} \frac{1}{j} \right]^{-1} \sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = h \left[\sum_{j=1}^{k} \frac{1}{j} \right]^{-1} f_{n+1}$$

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

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