

Math 6630: Analysis of Numerical Methods, II

Solvers for initial value problems, Part IV

See Ascher and Petzold 1998, Chapters 1-5

Akil Narayan¹

¹Department of Mathematics, and Scientific Computing and Imaging (SCI) Institute
University of Utah



$$\mathbf{u}'(t) = \mathbf{f}(t; \mathbf{u}),$$

$$\mathbf{u}_n \approx \mathbf{u}(t_n)$$

$$\mathbf{u}_{n+1} \approx \mathbf{u}_n + \int_{t_n}^{t_{n+1}} \mathbf{f}(t, \mathbf{u}(t)) dt$$

$$\mathbf{u}(0) = \mathbf{u}_0.$$

We have previously discussed

- Simple schemes: forward/backward Euler, Crank-Nicolson
- Consistency and LTE
- 0-stability and scheme convergence
- absolute/A-stability and consequences
- multi-stage (Runge-Kutta) methods

Finally, we'll discuss multi-step schemes.

To begin we review some basic concepts about (univariate) polynomial interpolation:

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a scalar function, and let x_0, \dots, x_n be any distinct points on \mathbb{R} .

Theorem

There is a unique polynomial $p(x)$ of degree n such that $f(x_j) = p(x_j)$ for all $j = 0, \dots, n$.

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One way to construct this polynomial is via [divided differences](#). Define

$$f[x_j] = f(x_j), f[x_j, \dots, x_{j+l}] = \frac{f[x_{j+1}, \dots, x_{j+l}] - f[x_j, \dots, x_{j+l-1}]}{x_{j+l} - x_j},$$

which are approximations to ℓ th derivatives. Then,

$$p(x) = \sum_{\ell=0}^n f[x_0, \dots, x_j] \prod_{j=0}^{\ell-1} (x - x_j).$$

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If $x_j = x_0 + jk$ for some $k > 0$, then expressions simplify considerably and more explicit formulas can be derived.

Simple theory for linear difference equations parallels linear differential equations:

$$u^{(s)}(t) + \sum_{j=1}^s \alpha_j u^{(s-j)}(t) = 0, \quad u^{(j)}(0) = u_0^j, \quad j = 0, \dots, s-1.$$

Solve for a function $u(t)$, $t > 0$. The order is $s > 0$.

$$u_n + \sum_{j=1}^s \alpha_j u_{n-j} = 0, \quad u_{n-j} = u_{n-j,0}, \quad j = 1, \dots, s.$$

Solve for a sequence u_ℓ , $\ell \geq 0$. The order is $s > 0$.

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$$\text{Ansatz } u(t) = e^{zt} \implies p(z) := \sum_{j=0}^s \alpha_j z^{s-j} = 0, \quad (\alpha_0 = 1)$$

Solutions take the form $u(t) \sim e^{z_j t}$, where z_1, \dots, z_s are the roots of p .

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Solutions $u(t)$ are stable if $\Re z_j \leq 0$. (Asymptotically stable if $\Re z_j < 0$.)

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Solutions u_n are stable if $|z_j| \leq 1$. (Asymptotically stable if $|z_j| < 1$.)

For the IVP,

$$\mathbf{u}'(t) = \mathbf{f}(t; \mathbf{u}),$$

$$\mathbf{u}(0) = \mathbf{u}_0.$$

$$\mathbf{u}_n \approx \mathbf{u}(t_n)$$

a general s -step multi-step scheme with timestep k has the form,

$$\frac{du}{dt} \approx \sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}_{n+1-j}), \quad \alpha_j, \beta_j \in \mathbb{R}$$

$\approx \int_{t_n}^{t_{n+1}} f(t, u(t)) dt$

For the IVP,

$$\begin{aligned} \mathbf{u}'(t) &= \mathbf{f}(t; \mathbf{u}), & \mathbf{u}(0) &= \mathbf{u}_0. \\ \mathbf{u}_n &\approx \mathbf{u}(t_n) \end{aligned}$$

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Comments:

- $s = 1$ corresponds to a general single-step (and single-stage) method

$$\alpha_0 \mathbf{u}_{n+1} + \alpha_1 \mathbf{u}_n = k \beta_0 \mathbf{f}(t_{n+1}, \mathbf{u}_{n+1}) + k \beta_1 \mathbf{f}(t_n, \mathbf{u}_n)$$

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- We can rescale the equation by a constant without changing anything: we fix this freedom by setting $\alpha_0 = 1$.

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- To avoid some minor pathologies, we typically assume that either $\alpha_j \neq 0$ or $\beta_j \neq 0$ for every j .
- $\beta_0 \neq 0$ corresponds to an implicit method. $\beta_0 = 0$ is an explicit method.

To simplify notation, we will assume the ODE is autonomous ($\mathbf{f}(t, \mathbf{u}) = \mathbf{f}(\mathbf{u})$), and will abbreviate $\mathbf{f}(\mathbf{u}_j)$ as \mathbf{f}_j . Then the multi-step method takes the form,

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Generally speaking, the constants are chosen so that:

- The α_j approximate $\frac{d}{dt} \mathbf{u}(t_n)$
- The β_j approximate $\frac{1}{k} \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(r)) dr$

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There are some miscellaneous issues we'll answer later, e.g.,

- If $s \geq 2$, how is \mathbf{u}_1 computed from \mathbf{u}_0 ?
- Must we fix the time-step k ?

A warmup: single-step specializations

D09-S07(a)

Specializing to single-step methods ($s = 1$) yields a transparent family of methods:

$$\mathbf{u}_{n+1} + \alpha_1 \mathbf{u}_n = k (\beta_0 \mathbf{f}_{n+1} + \beta_1 \mathbf{f}_n).$$

(Recall $\alpha_0 = 1$)

A warmup: single-step specializations

D09-S07(b)

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With this restriction, then we have

$$\mathbf{u}_{n+1} - \mathbf{u}_n = k (\beta_0 \mathbf{f}_{n+1} + \beta_1 \mathbf{f}_n),$$

and hence the right hand side should approximate $\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(r)) dr$, requiring $\beta_0 + \beta_1 = 1$ for consistency.

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Then our general family of methods is

$$\mathbf{u}_{n+1} = \mathbf{u}_n + k (\beta \mathbf{f}_{n+1} + (1 - \beta) \mathbf{f}_n),$$

specializing to,

- $\beta = 0$: Forward Euler
- $\beta = 1$: Backward Euler
- $\beta = 1/2$: Crank-Nicolson

Can we derive 2-step methods?

$$s=2$$

$$\alpha_0 u_{n+1} + \alpha_1 u_n + \alpha_2 u_{n-1} = k\beta_0 f_{n+1} + k\beta_1 f_n + k\beta_2 f_{n-1}$$

- set $\alpha_0 = 1$
- explicit scheme: $\beta_0 = 0$

$$u_{n+1} + \alpha_1 u_n + \alpha_2 u_{n-1} = k\beta_1 f_n + k\beta_2 f_{n-1} \quad \alpha_1, \alpha_2, \beta_1, \beta_2 = ?$$

enforce consistency by "minimizing" LTE.

$$\text{LTE} = \frac{1}{k} (u(t_{n+1}) + \alpha_1 u(t_n) + \alpha_2 u(t_{n-1})) - \beta_1 f(t_n, u(t_n)) - \beta_2 f(t_{n-1}, u(t_{n-1}))$$

Taylor expand @ $t = t_{n-1}$

$$\begin{aligned} \text{abbreviations: } u &= u(t_{n-1}) \\ u' &= u'(t_{n-1}) \\ &\vdots \\ u^{(j)} &= u^{(j)}(t_{n-1}) \end{aligned}$$

$$u(t_{n+1}) = u + 2ku' + \frac{(2k)^2}{2} u'' + \frac{(2k)^3}{6} u''' + \dots$$

$$\text{using: } u' = f, \quad u^{(j)} = \frac{d^{j-1}}{dt^{j-1}} f(t, u(t))$$

$$\begin{aligned} f(t_n, u(t_n)) &= f + kf' + \frac{k^2}{2} f'' + \frac{k^3}{6} f''' + \dots \\ &= u' + ku'' + \frac{k^2}{2} u''' + \dots \end{aligned}$$

$$\begin{aligned} \text{LTE} &= \frac{1}{k} \left(u + 2ku' + 2k^2 u'' + \frac{4}{3} k^3 u''' + \dots \right) \\ &\quad + \frac{\alpha_1}{k} \left(u + ku' + \frac{k^2}{2} u'' + \frac{k^3}{6} u''' + \dots \right) \\ &\quad + \frac{\alpha_2}{k} u \end{aligned}$$

$$-\beta_1 [u' + k u'' + \frac{k^2}{2} u''' + \dots]$$

$$-\beta_2 u'$$

$$\frac{1}{k}: 1 + \alpha_1 + \alpha_2 = 0$$

$$1: 2 + \alpha_1 - \beta_1 - \beta_2 = 0$$

$$k: 2 + \frac{\alpha_1}{2} - \beta_1 = 0 \longrightarrow 4 + \alpha_1 - 2\beta_1 = 0$$

$$k^2: \frac{4}{3} + \frac{\alpha_1}{6} - \beta_1/2 = 0 \longrightarrow 8 + \alpha_1 - 3\beta_1 = 0$$

↓

$$4 - \beta_1 = 0$$

$$\beta_1 = 4, \alpha_1 = 4$$

$$\alpha_2 = -5, \beta_2 = 2$$

$$\Rightarrow u_{n+1} + 4u_n - 5u_{n-1} = 4f_n + 2f_{n-1}$$

$$\text{LTE} = O(k^3)$$

(This didn't work...??)

There are two major classes of most popular multi-step methods. The first is the family of *Adams* methods.

For these methods we start with,

$$\mathbf{u}(t_{n+1}) = \mathbf{u}(t_n) + \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(r))dr,$$

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The β_j are chosen as a quadrature rule to approximate the integral:

$$\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(r))dr \approx k \sum_{j=0}^s \beta_j \mathbf{f}_{n+1-j}$$

Note that we are using points *outside* the interval of intergration (if $s > 1$).

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Note that we are using points *outside* the interval of integration (if $s > 1$). Again, the particular type of scheme depends on whether we want an implicit or an explicit method:

- $\beta_0 = 0$ yields explicit methods (one fewer parameter to invest in LTE reduction)
- $\beta_0 \neq 0$ yields implicit methods

The choice of **explicit** path yields the family of **Adams-Bashforth** methods.

$$\mathbf{u}_{n+1} - \mathbf{u}_n = k \sum_{j=1}^s \beta_j \mathbf{f}_{n+1-j}.$$

The β_j coefficients are used to ensure high-order LTE. E.g., two equivalent strategies:

- Expand in Taylor series, match terms by setting β_j
- Interpolate a degree- $(s - 1)$ polynomial on data at t_{n+1-s}, \dots, t_n , integrate the polynomial. The resulting coefficients multiplying the data are the β_j .

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Coefficients for the Adams-Bashforth methods with order=steps:

	β_1	β_2	β_3	β_4	β_5	β_6
$p = s = 1$	1					
$p = s = 2$	$\frac{3}{2}$	-1				
$p = s = 3$	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$			
$p = s = 4$	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$		
$p = s = 5$	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$	
$p = s = 6$	$\frac{4277}{1440}$	$-\frac{7923}{1440}$	$\frac{9982}{1440}$	$-\frac{7298}{1440}$	$\frac{2877}{1440}$	$-\frac{475}{1440}$

The choice of **implicit** path yields the family of **Adams-Moulton** methods.

$$\mathbf{u}_{n+1} - \mathbf{u}_n = k \sum_{j=0}^s \beta_j \mathbf{f}_{n+1-j}.$$

The β_j coefficients are used to ensure high-order LTE.

The same strategies as before are usable.

Note that technically we can take $s = 0$ here, which yields backward Euler. (Though you'd still call this a 1-step method.)

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The same strategies as before are usable.

Note that technically we can take $s = 0$ here, which yields backward Euler. (Though you'd still call this a 1-step method.) Coefficients for the Adams-Moulton methods with order=steps+1:

	β_0	β_1	β_2	β_3	β_4	β_5
$p - 1 = s = 1$	$\frac{1}{2}$	$\frac{1}{2}$				
$p - 1 = s = 2$	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$			
$p - 1 = s = 3$	$\frac{9}{24}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$		
$p - 1 = s = 4$	$\frac{251}{720}$	$\frac{646}{720}$	$-\frac{264}{720}$	$\frac{106}{720}$	$-\frac{19}{720}$	
$p - 1 = s = 5$	$\frac{475}{1440}$	$\frac{1427}{1440}$	$-\frac{798}{1440}$	$\frac{482}{1440}$	$-\frac{173}{1440}$	$\frac{27}{1440}$

The Adams family of methods is not particularly robust for stiff problems.

As an alternative, consider the general form:

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}_{n+1-j}),$$

and now instead let us focus effort on setting $\beta_j = 0$ for $j > 0$, and choosing α_j to approximate $y'(t_n)$ to high order:

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k\beta_0 \mathbf{f}_{n+1}.$$

This is the family of (implicit) [backward differentiation formulas \(BDF\)](#) methods.

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This is the family of (implicit) **backward differentiation formulas (BDF)** methods. Again, the BDF coefficients are

	β_0	α_0	α_1	α_2	α_3	α_4	α_5	α_6
$p = s = 1$	1	1	-1					
$p = s = 2$	$\frac{2}{3}$	1	$-\frac{4}{3}$	$\frac{1}{3}$				
explicitly computable: $p = s = 3$	$\frac{6}{11}$	1	$-\frac{18}{11}$	$\frac{9}{11}$	$-\frac{2}{11}$			
$p = s = 4$	$\frac{12}{25}$	1	$-\frac{48}{25}$	$\frac{36}{25}$	$-\frac{16}{25}$	$\frac{3}{25}$		
$p = s = 5$	$\frac{60}{137}$	1	$-\frac{300}{137}$	$\frac{300}{137}$	$-\frac{200}{137}$	$\frac{75}{137}$	$-\frac{12}{137}$	
$p = s = 6$	$\frac{60}{147}$	1	$-\frac{360}{147}$	$\frac{450}{147}$	$-\frac{400}{147}$	$\frac{225}{147}$	$-\frac{72}{147}$	$\frac{10}{147}$

It's much easier to compute order conditions for multi-step methods (compared to multi-stage ones).

In particular, to compute the LTE for the scheme,

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}_{n+1-j}),$$

we need to compute the residual for the expression

$$\frac{1}{k} \sum_{j=0}^s \alpha_j \mathbf{u}(t_{n+1-j}) - \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}(t_{n+1-j})).$$

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Noting that $\mathbf{u}'(t) = \mathbf{f}(t, \mathbf{u}(t))$, the above expression is equivalent to,

$$\frac{1}{k} \sum_{j=0}^s \alpha_j \mathbf{u}(t_{n+1-j}) - \sum_{j=0}^s \beta_j \mathbf{u}'(t_{n+1-j}),$$

and hence we can compute order conditions simply by computing Taylor expansions of \mathbf{u} and \mathbf{u}' .

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The $\mathcal{O}(1/k)$ terms from the above come from Taylor expansions of the α_j terms, implying that we require,

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For consistency (LTE vanishing as $k \downarrow 0$), we likewise require the $\mathcal{O}(1)$ terms to vanish, i.e.,

$$\sum_{j=0}^s (s-j)\alpha_j - \sum_{j=0}^s \beta_j = 0.$$

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These two expressions are evaluations of certain *characteristic* polynomials:

$$\left. \begin{aligned} \rho(w) &= \sum_{j=0}^s \alpha_j w^{s-j} \\ \sigma(w) &= \sum_{j=0}^s \beta_j w^{s-j} \end{aligned} \right\} \implies \begin{aligned} \rho(1) &= 0 \\ \rho'(1) &= \sigma(1) \end{aligned}$$

$$\text{LTE} = \frac{1}{k} \sum_{j=0}^s \alpha_j \mathbf{u}(t_{n+1-j}) - \sum_{j=0}^s \beta_j \mathbf{u}'(t_{n+1-j}),$$

$$\rho(w) = \sum_{j=0}^s \alpha_j w^{s-j}$$

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We have shown the following:

Theorem

A multi-step method is consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$.

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We have shown the following:

Theorem

A multi-step method is consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$.

Of course, to attain more than first-order accuracy, we require more conditions.

The characteristic polynomials are also integral in determining 0-stability:

Theorem

An s -step linear multi-step method is 0-stable if and only if the roots w_1, \dots, w_s of $\rho(w)$ all satisfy $|w_i| \leq 1$, and any roots satisfying $|w_i| = 1$ are simple. (Terminologically: “ ρ satisfies the root condition”)

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Why is this related to 0-stability? Recall that the essential message of 0-stability is that

Initial data perturbations of size ϵ lead to numerical solutions with errors $C\epsilon$ for small enough ϵ .

(I.e., the k -asymptotic LTE behavior bounds the actual error in the numerical method up to a constant.)

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Note: we only require control of perturbations for vanishingly small ϵ .

It turns out that while phrased as perturbations to initial data, this is conceptually similar to perturbations of \mathbf{f} , and under an ODE well-posedness result, is equivalent to considering perturbations of $\mathbf{f} = \mathbf{0}$.

I.e., it's enough to check controlled perturbations for $\mathbf{u}' = \mathbf{0}$
(This is why it's called 0-stability.)

So if we only need to consider a linear multistep method for $\mathbf{u}' = \mathbf{0}$ to account for 0-stability, this means the scheme reads,

$$\sum_{j=0}^s \alpha_j u_{n+1-j} = 0,$$

say with starting conditions $u_0 = \cdots = u_{s-1} = 0$.

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If we replace the initial data of 0's by perturbations, then the exact solution to the difference equation, assuming unique roots w_1, \dots, w_s of ρ , is,

$$u_n \sim \epsilon_1 w_1^n + \dots + \epsilon_s w_s^n$$

where $\epsilon_1, \dots, \epsilon_s$ are dependent on the initial data perturbations.

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The exact solution to this problem is $u_n = 0$. As $k \downarrow 0$, then $n \uparrow \infty$. I.e., our perturbed solution is bounded relative to 0 iff $|w_j| < 1$ for all j .

$|w_j| = 1$ is allowed for simple roots, but for repeated roots with multiplicity m , then $|u_n| \sim n^{m-1} |w_j| = n^{m-1}$, which is unbounded in n for $m > 1$.

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Hence, 0-stability is equivalent to the roots of ρ lying within the unit circle (and on the boundary for simple roots).

0-stability examples

D09-S17(a)

Example: any one-step ($s = 1$) method is 0-stable, since $\rho(w) = w - 1$.

$$u_{n+1} + \alpha_1 u_n = \beta_0 f_{n+1} + \beta_1 f_n$$

$\Downarrow \alpha_1 = -1$ by consistency

$$\rho(w) = w - 1$$

0-stability examples

D09-S17(b)

Example: any one-step ($s = 1$) method is 0-stable, since $\rho(w) = w - 1$.

Example: All Adams- methods are 0-stable, since $\rho(w) = w^s - w^{s-1}$.

$$u_{n+1} + \alpha_1 u_n = k \sum_{j=0}^s \beta_j f_{n+j}$$

$$\alpha_1 = -1 \text{ (consistency)} \Rightarrow \rho(w) = w^s - w^{s-1} = w^{s-1}(w-1)$$

0-stability examples

D09-S17(c)

Example: any one-step ($s = 1$) method is 0-stable, since $\rho(w) = w - 1$.

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Example: All BDF methods for $s \leq 6$ are 0-stable. Any BDF method with $s > 6$ is unstable.

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Example: All BDF methods for $s \leq 6$ are 0-stable. Any BDF method with $s > 6$ is unstable.

There are reasonable-looking methods that violate 0-stability:

$$\mathbf{u}_{n+1} + 4\mathbf{u}_n - 5\mathbf{u}_{n-1} = k(4\mathbf{f}_n + 2\mathbf{f}_{n-1}),$$

and these methods are actually quite unstable.

$$\rho(w) = w^2 + 4w - 5 = (w+5)(w-1)$$

$$w = 1, -5$$

$$\textcircled{2}$$

Just like our analysis for simple Euler-type schemes, 0-stability and consistency *are* convergence.

Theorem (Dahlquist Equivalence Theorem)

Consider an s -step multistep method where the startup values $\mathbf{u}_0, \dots, \mathbf{u}_{s-1}$ are generated in a consistent way ($\mathbf{u}_j \rightarrow \mathbf{u}(0)$ as $k \downarrow 0$ for $j = 0, \dots, s-1$.)

Such a linear multistep method is convergent if and only if it is consistent and 0-stable.

I.e.,:

A linear multistep method is convergent if and only if $\rho(1) = 0$, $\rho'(1) = \sigma(1)$, and ρ satisfies the root condition.

(When convergent, a linear multistep method has order of convergence equal to the order p of the LTE.)

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(When convergent, a linear multistep method has order of convergence equal to the order p of the LTE.)

Note that 1 is *always* a root of ρ for multistep methods of interest.

Methods for which 1 is the *only* unity-modulus root are *strongly* stable. (Otherwise, they are weakly stable.)

We have a similar notion of absolute stability for multi-step methods: We require that the iteration,

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}_{n+1-j}),$$

produces solutions \mathbf{u}_n that do not grow exponentially in n for the test equation $u' = \lambda u$.

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This results in the difference equation,

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k\lambda \sum_{j=0}^s \beta_j \mathbf{u}_{n+1-j},$$

whose characteristic equation is,

$$\rho(w) = k\lambda\sigma(w) \stackrel{z=\lambda k}{=} z\sigma(w).$$

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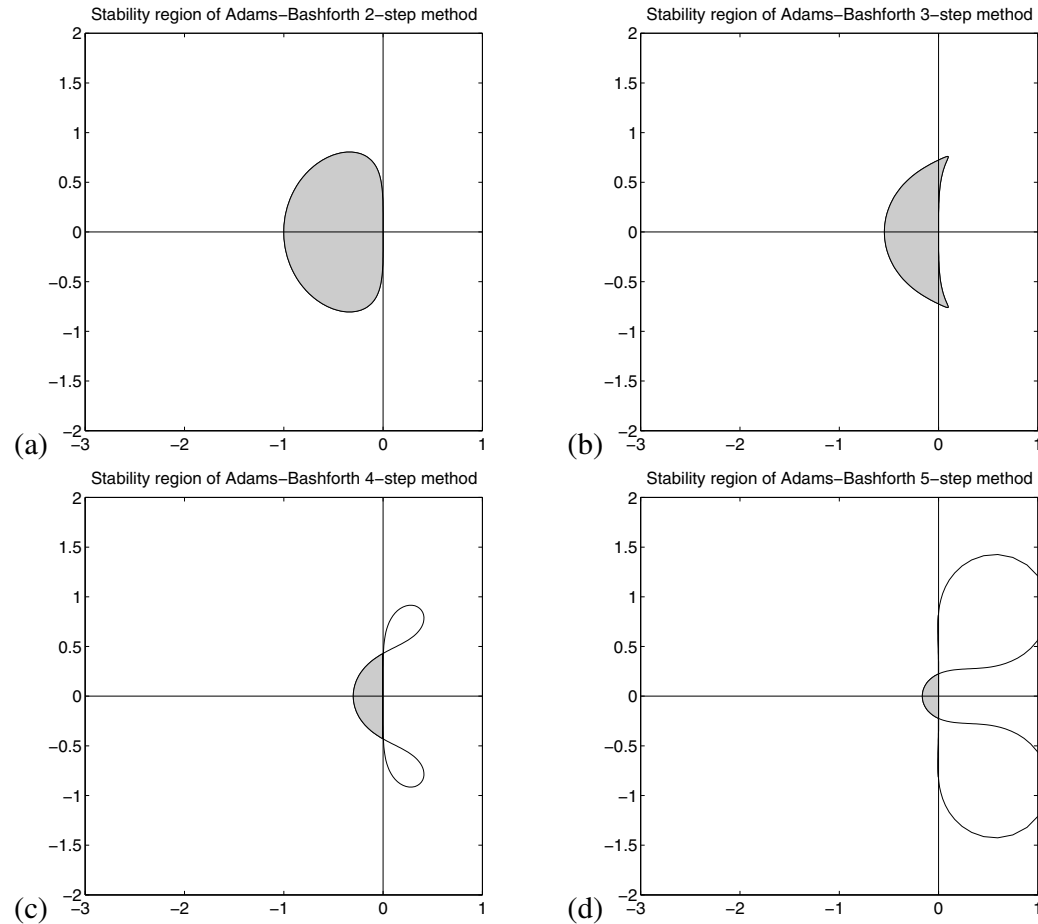
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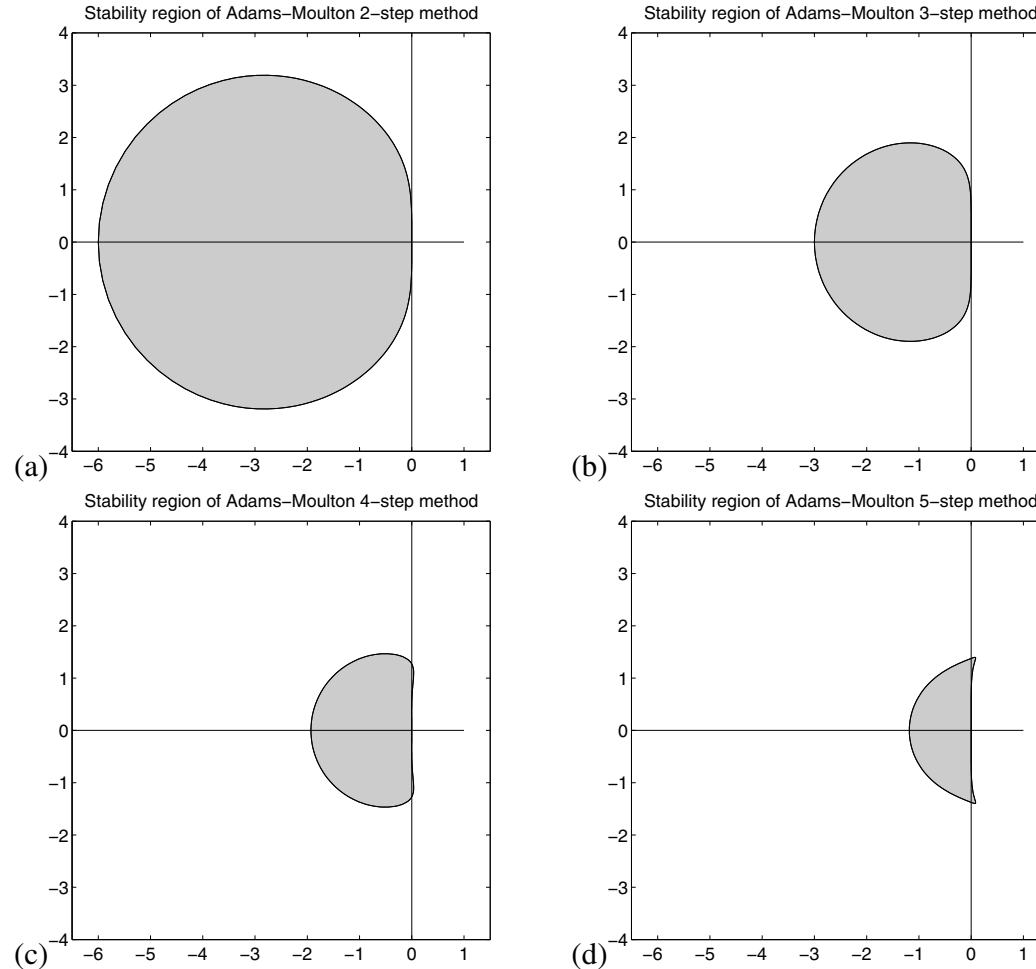
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Thus, we say that the region of (absolute) stability for the scheme is the set of z values such that $\rho(w) - z\sigma(w)$ has roots w_1, \dots, w_s all satisfying $|w_j| < 1$, with $|w_j| = 1$ allowed for simple roots. (I.e., $z \in \text{ROS}$ means $\rho(\cdot) - z\sigma(\cdot)$ satisfies the root condition.)

(Note that $0 \in \text{ROS} \iff 0\text{-stability}$.)



LeVeque 2007, Figure 7.2



There are some somewhat dissapointing results about efficacy of multistep methods:

Theorem (First Dahlquist Barrier)

For an s -step multistep method that is 0-stable:

- An explicit method can have order of accuracy at most $p = s$.*
- If s is odd, the order of accuracy can be at most $p = s + 1$.*
- If s is even, the order of accuracy can be at most $p = s + 2$.*

(Note that consistent s -step methods explicitly have $2s - 1$ degrees of freedom.)

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(Note that consistent s -step methods explicitly have $2s - 1$ degrees of freedom.)

Theorem (Second Dahlquist Barrier)

No A-stable explicit multistep methods exist.

An implicit A-stable multistep method has order of accuracy at most $p = 2$.

Startup

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+1-j} = k \sum_{j=0}^s \beta_j \mathbf{f}(t_{n+1-j}, \mathbf{u}_{n+1-j}),$$

How to start from $n = 0$ if $s > 1$?

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Usually accomplished with Runge-Kutta methods of similar order.

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Predictor-corrector methods

Explicit and implicit methods are frequently used in *predictor-corrector* frameworks, e.g.,:

- An explicit approximation to \mathbf{u}_{n+1} is computed with an Adams-Bashforth method.
- This approximation is used as an emulator for the unknown $\mathbf{u}(t_{n+1})$ on the right-hand side of an Adams-Moulton method.

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Predictor-corrector methods are an example from a more general class of methods called *general linear methods*, which encompass both multi-stage and multi-step methods.

-  Ascher, Uri M. and Linda R. Petzold (1998). *Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations*. SIAM. ISBN: 978-1-61197-139-2.
-  Butcher, J. C. (2006). “General Linear Methods”. In: *Acta Numerica* 15, pp. 157–256. ISSN: 1474-0508, 0962-4929. DOI: 10.1017/S0962492906220014.
-  LeVeque, Randall J. (2007). *Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems*. SIAM. ISBN: 978-0-89871-783-9.