Math 6630: Numerical Solutions of Partial Differential Equations
Solvers for initial value problems, Part IV

See Ascher and Petzold 1998, Chapters 1-5

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Initial value problems

$$\boldsymbol{u}'(t) = \boldsymbol{f}(t; \boldsymbol{u}), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0.$$

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

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

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.

*
multi-stage

Preliminaries: polynomial interpolation

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

Let $f : \mathbb{R} \to \mathbb{R}$ be a scalar function, and let $x_0, \ldots, x_n$ 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* $j = 0, \ldots, n$.

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

One way to construct this polynomial is via divided differences. Define

$$f[x_j] = f(x_j), \quad f[x_j, \ldots, x_{j+\ell}] = \frac{f[x_{j+1}, \ldots, x_{j+\ell}] - f[x_j, \ldots, x_{j+\ell-1}]}{x_{j+\ell} - x_j},$$

which are approximations to ℓth derivatives. Then,

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

$$\prod_{j=0}^{-1} a_j = 1$$

This is the Newton form of the interpolating polynomial.

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This is the Newton form of the interpolating polynomial.

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

Preliminaries: difference equations

Simple theory for linear difference equations parallels linear differential equations:

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

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

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

Solve for a sequence u_ℓ, $\ell \geqslant 0$. 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 $z_1, \ldots, z_s$ are the roots of p.

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

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

Multi-step methods, I

$f(z) = \frac{az+b}{cz+d}$, $ad - bc \neq 0$

For the IVP,

$$\boldsymbol{u}'(t) = \boldsymbol{f}(t;\boldsymbol{u}), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0.$$

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

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

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

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Comments:

- $s = 1$ corresponds to a general single-step (and single-stage) method
- $s > 1$: we need time history, e.g., $\boldsymbol{u}_{n-2}, \boldsymbol{u}_{n-3}, \ldots$
- We assume $\alpha_0 \neq 0$.
- We can rescale the equation by a constant without changing anything: we fix this freedom by setting $\alpha_0 = 1$.
- 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.

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$= \beta_0 f_{n+1} + \beta_1 f_n + \beta_2 f_{n-1} + \cdots$

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Multi-step methods, II

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

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Generally speaking, the constants are chosen so that:

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

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

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

A warmup: single-step specializations

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

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

(Recall $\alpha_0 = 1$)

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With this restriction, then we have

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

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

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Then our general family of methods is

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

specializing to,

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

The Adams Family

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,

$$\boldsymbol{u}(t_{n+1}) = \boldsymbol{u}(t_n) + \int_{t_n}^{t_{n+1}} \boldsymbol{f}(\boldsymbol{u}(r))\mathrm{d}r,$$

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suggesting that we should take $\alpha_0 = 1$, $\alpha_1 = -1$.

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

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

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 intergration (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

Adams-Bashforth Methods

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

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

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 $t_{n+1-s}, \ldots, t_n$, 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				
$p = s = 3$	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$			
$p = s = 4$	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$		
$p = s = 5$	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$	
$p = s = 6$	$\frac{4277}{1440}$	$-\frac{7923}{1440}$	$\frac{9982}{1440}$	$-\frac{7298}{1440}$	$\frac{2877}{1440}$	$-\frac{475}{1440}$

Adams-Moulton Methods

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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 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.) Coefficients for the Adams-Moulton methods with order=steps+1:

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

Backward Differentiation formulas

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

As an alternative, consider the general form:

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

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:

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

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

	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	$-\frac{4}{3}$	$\frac{1}{3}$				
$p = s = 3$	$\frac{6}{11}$	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	$-\frac{360}{147}$	$\frac{450}{147}$	$-\frac{400}{147}$	$\frac{225}{147}$	$-\frac{72}{147}$	$\frac{10}{147}$

Consistency and order of approximation

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,

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

we need to compute the residual for the expression

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

Consistency and order of approximation

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,

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

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

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

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

Consistency of multi-step methods, I

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

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

$$\sum_{j=0}^{s} \alpha_j = 0.$$

($s=1 \Rightarrow \alpha_0 = 1$, $1 + \alpha_1 = 0$)

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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:

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

Consistency of multi-step methods, II

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

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

$$\sigma(w) = \sum_{j=0}^{s} \beta w^{s-j}$$

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

0-stability: $k \downarrow 0 \Longrightarrow \sum_{j=0}^{s} \alpha_j u_{n+1-j} = 0$

Let's derive a multistep method.

$s=2$, explicit

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

$$u_{n+1} \approx u_{n-1} + 2k u'_{n-1} + \frac{4k^2}{2} u''_{n-1} + \frac{8k^3}{6} u'''_{n-1} + \dots$$

$$u_n \approx u_{n-1} + k u'_{n-1} + \frac{k^2}{2} u''_{n-1} + \frac{k^3}{6} u'''_{n-1} + \dots$$

$$f_n = u'_n \approx u'_{n-1} + k u''_{n-1} + \frac{k^2}{2} u'''_{n-1} + \dots$$

u_{n-1}: $1 + \alpha_1 + \alpha_2 = 0$ $\quad (\rho(1) = 0)$

u'_{n-1}: $2k + \alpha_1 k = \beta_1 k + \beta_2 k$ $\quad (\rho'(1) = \sigma(1))$

u''_{n-1}: $2k^2 + \alpha_1 k^2/2 = \beta_1 k \rightarrow 2 + \alpha_1/2 = \beta_1$

u'''_{n-1}: $\frac{4}{3}k^3 + \alpha_1 k^3/6 = \frac{k^3}{2}\beta_1 \rightarrow 4/3 + \alpha_1/6 = \beta_1/2$

$\Rightarrow -\frac{2}{3} + \frac{1}{6}\alpha_1 = 0$

$\alpha_1 = 4$

$\alpha_2 = -5$

$\beta_1 = 4$

$\beta_2 = 2$

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

2-step explicit method, LTE: k^3. $(p=3)$

0-Stability of multi-step methods

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 $w_1, \ldots, w_s$ of $\rho(w)$ all satisfy $|w_i| \leqslant 1$, and any roots satisfying $|w_i| = 1$ are simple.

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

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

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

and these methods are actually quite unstable.

$w = -5$ ☹

$(w+5)(w-1)$

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

Absolute stability

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

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

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This results in the difference equation,

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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 $w_1, \ldots, w_s$ all satisfying $|w_j| \leqslant 1$.

Forward Euler: $\alpha_0 u_{n+1} + \alpha_1 u_n = \beta_1 f_n$

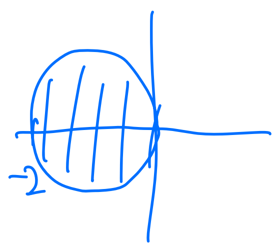
$\alpha_0 = \frac{1}{k} \quad \alpha_1 = -\frac{1}{k}, \quad \beta_1 = 1$

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

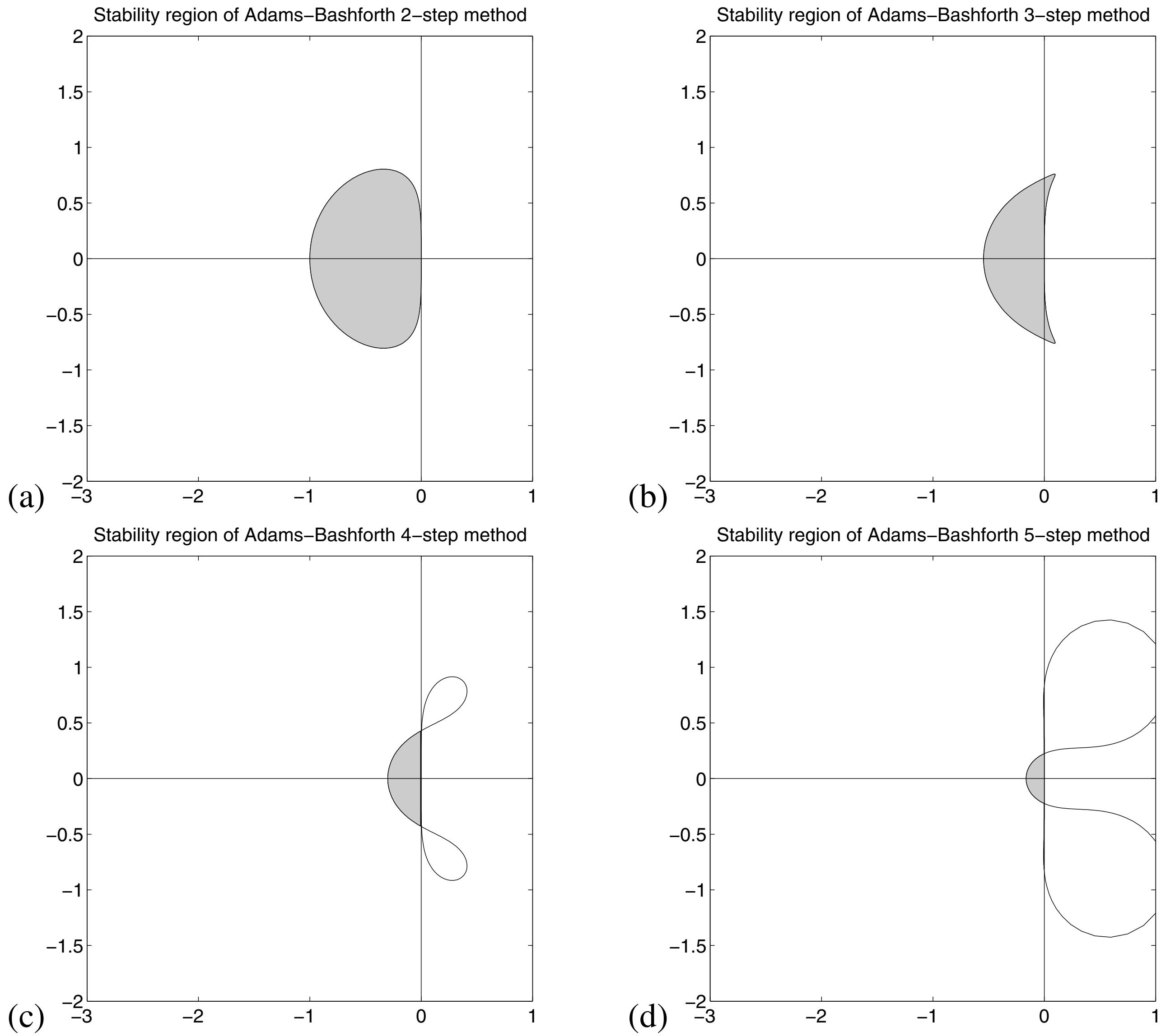
roots of $\rho(w) - z\sigma(w)$

$w - 1 - z \Rightarrow w = z + 1$

when is $|z+1| \le 1$?

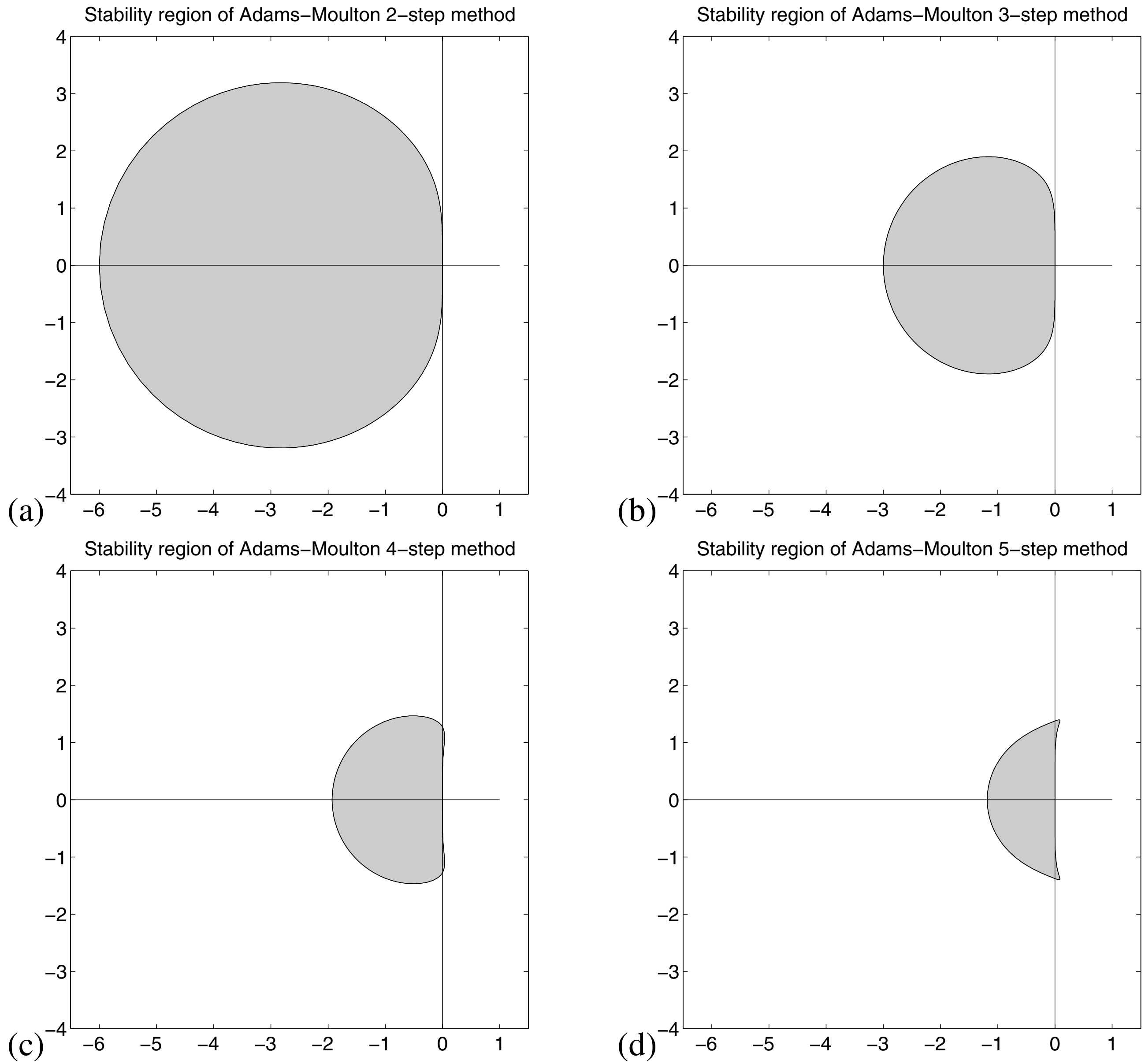


Absolute stability: Adams-Bashforth



LeVeque 2007, Figure 7.2

Absolute stability: Adams-Moulton



LeVeque 2007, Figure 7.3

Odds and ends for multi-step methods

Startup

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

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

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 $\boldsymbol{u}_{n+1}$ is computed with an Adams-Bashforth method.
- This approximation is used as an emulator for the unknown $\boldsymbol{u}(t_{n+1})$ 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.

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