LINEAR MULTISTEP METHODS (LMMs)

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We already gave one example of a (linear) multistep method for solving the (system of) ODE(s):

$$u'(t) = f(u(t), t)$$

namely the Adams-Bashforth (AB2) second-order method:

$$u^{n+2} = u^{n+1} + \frac{\tau}{2}\left(3f^{n+1} - f^{n}\right)$$

time step size

This is an explicit two step scheme.

More commonly written as

$$u^{n+1} = u^{n} + \frac{\tau}{2}\left(3f^{n} - f^{n-1}\right)$$

future present past

It requires storing f^{n-1} (but not u^{n-1}).

A general r-step Linear Multistep Method (LMM) takes the form:

$$\sum_{j=0}^{r} \alpha_j u^{(n+j)} = \tau \sum_{j=0}^{r} \beta_j f^{(n+j)}$$

For LMMs we will assume τ is fixed and not adaptive, as adaptivity is hard with multistep methods.

Three classes of LMMs:

A) Adams methods

$\alpha_r = 1$, $\alpha_{r-1} = -1$, $\alpha_{j \le r-2} = 0$

① Adams-Bashforth

$\beta_r = 0 \longrightarrow$ explicit

② Adams(-Bashforth)-Moulton

$\beta_r \neq 0 \longrightarrow$ implicit

B) Backwards Differentiation Formulas

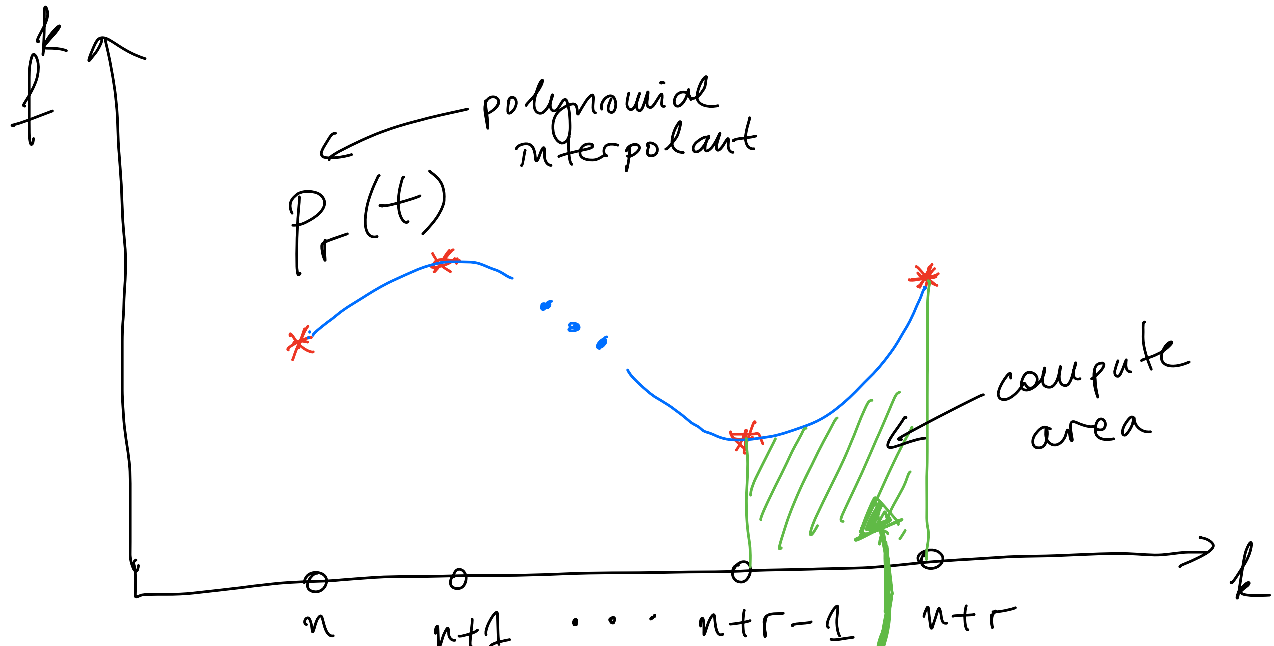
$\beta_j = 0$, $j = 0 \ldots r-1$ $\rightarrow$ implicit

Stores past values of u not f

Adams Methods

$$u^{n+r} = u^{n+r-1} + \tau \sum_{j=0}^{r} \beta_j f^{n+j}$$

Basic idea: Fit a polynomial of degree $r-1$ through past values of f^k: interpolate (+extrapolate) the r.h.s of ODE



$$u^{n+r} = u^{n+r-1} + \int_{t=t^{n+r-1}}^{t^{n+r}} f(u(t),t)\,dt$$

$$u^{n+r} \simeq u^{n+r-1} + \int_{t=t^{n+r-1}}^{t=t^{n+r}} P_r(t)\, dt$$

Simple algebra to compute interpolant. If method is explicit the last time step is <u>extrapolated</u>

AB3 scheme (third order)

$$u^{n+3} = u^{n+2} + \frac{\tau}{12}\left[5f^{n} - 16f^{n+1} + 23f^{n+2}\right]$$

Computing the LTE to confirm the order of accuracy is just as for RK schemes:

Plug exact solution into the scheme and do Taylor series

$$u^{n+1} = u^{n} + \frac{\tau}{2}\left(3f^{n} - f^{n-1}\right) \quad \text{AB2}$$

$$u((n+1)\tau) = u(n\tau) + \frac{\tau}{2}\Big[3f(u(n\tau), n\tau) - f(u((n-1)\tau, (n-1)\tau)\Big] + LTE * \tau$$

expand around (u^{n}, t^{n})

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$$\begin{cases} u'(t) = f(u(t),t) & \cdots\cdots (*) \\ u''(t) = \dfrac{\partial f}{\partial u}(u(t),t)\,u'(t) + \dfrac{\partial f}{\partial t}(u(t),t) \end{cases}$$

$$\cancel{u(n\tau)} + u'(n\tau)\tau + \frac{1}{2}u''(n\tau)\tau^2 + O(\tau^3)$$

$$= \cancel{u(n\tau)} + \frac{\tau}{2}\Big\{3f(u(n\tau),n\tau) -$$

$$\Big[f(u(n\tau),n\tau) + \frac{\partial f}{\partial u}(u(n\tau),n\tau)\big(\underbrace{u((n+1)\tau) - u(n\tau)}_{u'(n\tau)\tau}\big)$$

$$+ \frac{\partial f}{\partial t}(u(n\tau),n\tau)\tau + O(\tau^2)\Big] + LTE$$

Use $(*)$

$$\cancel{f(u(n\tau),n\tau)\tau} + \frac{\tau^2}{2}\Big[\cancel{\frac{\partial f}{\partial u}(u(t),t)u'(t)} + \cancel{\frac{\partial f}{\partial t}(u(t),t)}\Big]$$

$$= \cancel{f(u(n\tau),n\tau)\tau} + \cancel{\frac{\tau^2}{2}\frac{\partial f}{\partial u}(\dots)} + \cancel{\frac{\tau^2}{2}\frac{\partial f}{\partial t}(\dots)} +$$

$$+ O(\tau^3) + LTE$$

$$\Rightarrow \quad LTE = O(\tau^3) \Rightarrow \text{third order}$$

These sort of calculations are best done using symbolic algebra (Maple, Mathematica) Or, better, use error estimates for polynomial interpolation!

AM2 (Adams-Moulton two step):

$$u^{n+2} = u^{n+1} + \frac{\tau}{12}\left[-f^{n} + 8f^{n+1} + 5f^{n+2}\right]$$

implicit

One can get another $\underline{\text{explicit}}$ 2^{nd} order scheme by combining AB2 with AM2 in a predictor-corrector fashion:

AB2-AM2 $\underbrace{\text{two-stage}}_{\text{linear multi-stage}}$ $\underbrace{\text{two-step}}_{\text{multi-step}}$ scheme:

$$\begin{cases} u^{n+2,*} = u^{n+1} + \frac{\tau}{2}\left(3f^{n+1} - f^{n}\right) & \text{AB2 predictor} \\ u^{n+2} = u^{n+1} + \frac{\tau}{12}\left(-f^{n} + 8f^{n+1} + 5f(u^{n+2,*}, t^{n+2})\right) & \text{AM2 corrector} \end{cases}$$

One could iterate this multiple times but there is rarely a benefit of that - use AM2 with Newton's method solver instead.

LMMs are not self-starting

To do r initial steps, use a one-step method of order p−1, if order of LMM is p.

Order p−1 is OK since we do a finite (small) number of initial steps so error does not accumulate.

- For AB2/AM2 use one step of Euler
- For AB3/AM2 use RK2 (midpoint or trapezoidal)

To avoid any large errors in the initial steps, usually an RK of order $\underline{P}$ is used in practice.

Backwards Differentiation Formulas (BDF)

$$\underbrace{\frac{1}{\tau}\sum_{j=0}^{r} \alpha_j u^{n+j}}_{} = f^{n+r} \approx u'((n+r)\tau)$$

finite-difference approximation of derivative $u'((n+r)\tau)$ using past values of u.

Interpolate $r+1$ values of u with a polynomial of degree r to get a scheme of order r:

$$f^{n+r} = p_r'((n+r)\tau)$$

BDF schemes are good for stiff systems of equations.

BDF 1 $\equiv$ Backwards Euler

$$\frac{u^{n+1} - u^n}{\tau} = f(u^{n+1}, (n+1)\tau)$$

BDF2 scheme (2nd order implicit)

$$\frac{3u^{n+2} - 4u^{n+1} + u^{n}}{2\tau} = f^{n+2}$$

$$\Rightarrow u^{n+2} = \frac{1}{3}\left(4u^{n+1} - u^{n} + 2\tau f^{n+2}\right)$$

Trapezoidal BDF2: TR-BDF2

$$\begin{cases} u^{n+1/2,*} = u^{n} + \frac{\tau}{4}\left(f^{n} + f^{n+1/2,*}\right) \quad \leftarrow \text{implicit} \\ \text{Trapezoidal to midpoint (predictor)} \\ u^{n+1} = \frac{1}{3}\left(4u^{n+1/2,*} - u^{n} + \tau f^{n+1}\right) \quad \text{implicit} \end{cases}$$

BDF2 from u^{n}, $u^{n+1/2,*}$ with time-step size $\tau/2$ (corrector)

(One of the simplest) L-stable schemes of 2nd order.

It is used when solving PDEs

Zero Stability of LMMs

When do LMMs converge?

Let's apply the scheme to a linear equation

$$\begin{cases} u'(t) = 0 \\ u(0) = 0 \end{cases}$$

A one-step method would give $u^k = 0 \quad \forall k$, so stable.

BUT, in an LMM, not necessarily

Previous r values will have some roundoff errors / perturbations.

We don't want those to grow.

Also, previous values have some error since method is not exact.

We should only require initial values to be $= u^0 \simeq u(0)$ as $\tau \to 0$.

Take an ODE $u' = f(u,t)$ where f is Lipshitz continuous in u and ODE has a unique solution up to time T.

$$
\begin{cases}
\text{An } r\text{-step LMM converges if} \\
\forall u^{\nu} \text{ s.t. } \lim\limits_{\tau \to 0} u^{\nu} = u(0), \quad \nu = 0, \dots, r-1 \\
\lim\limits_{\tau \to 0} u^{T/\tau} = u(T)
\end{cases}
$$

Here is a <u>non-convergent</u> LMM:

$$u^{n+2} - 3u^{n+1} + 2u^{n} = -\tau f^{n}$$

Apply to $f = 0$:

$$u^{n+2} - 3u^{n+1} + 2u^{n} = 0 \leftarrow \text{reccurence relation}$$

$$\Rightarrow \quad u^{n} = 2u^{0} - u^{1} + \underbrace{2^{n}}_{\text{grows exponentially}} (\underbrace{u^{1} - u^{0}}_{\text{non-zero}})$$

which will <u>blow</u> up for $n \gg 1$!

We need to understand when linear reccurence relations blow up. Consider

$$(**) \ldots \sum_{j=0}^{r} \alpha_j u^{n+j} = 0 \quad (\text{since } f \equiv 0)$$

For every simple root ξ_i of

$$\begin{cases} \rho(\xi) = \sum_{j=0}^{r} \alpha_j \xi^j & \text{— characteristic polynomial of LMM} \\ \rho(\xi_i) = 0 \end{cases}$$

a linearly independent solution of $(**)$ is $u^n = \xi_i^n$.

For a double (repeated) root,

$$\rho(\xi_j) = 0 \quad \& \quad \rho'(\xi_j = 0)$$

two linearly independent solutions of $(**)$ are

$$u^n = \xi_j^n \quad \& \quad u^n = n\,\xi_j^n$$

etc. for roots of multiplicity >2.

General solution of (**):

$$u^n = \sum_{j=1}^{n_1} c_j^{(1)} \xi_j^n + \sum_{k=1}^{n_2} c_k^{(2)} n \xi_k^n + \sum_{\ell=1}^{n_3} c_\ell^{(3)} n^2 \xi_\ell^n + \dots$$

We want the coefficients <u>not</u> to grow with time. This requires that

$$|\xi_j| \le 1 \quad \text{for simple roots}$$

$$|\xi_j| < 1 \quad \text{for repeated roots}$$

To see why take a double root. If $|\xi_k| = 1$, then we get a term

$$u^n = \dots + n\, O(\tau) \Rightarrow$$

$$u^{T/\tau} = \dots + O(N\tau) = \dots + O(T)$$

<u>not</u> convergent

Adams methods:

$$\rho(\xi) = \xi^r - \xi^{r-1} = (\xi - 1)\,\xi^{r-1}$$

$$\Rightarrow \begin{cases} \xi_1 = 1 & \text{is a simple root} \\ \xi_2 = 0 & \text{is a root of multiplicity } r-1 \end{cases}$$

$\Rightarrow$ All Adams methods are zero-stable

Note that $\xi_1 = 1$ is always a root for any consistent LMM.

$$\sum_{j=0}^{r} \alpha_j u^{(n+j)} = \tau \sum_{j=0}^{r} \beta_j f^{(n+j)}$$

$$\sum_j \alpha_j \left(u^n + f^n (j\tau) + O(\tau^2)\right) = \tau \sum_j \beta_j \left(f^n + O(\tau)\right) \Rightarrow$$

$$\begin{cases} O(\tau^0): & \sum_j \alpha_j = 0 \\ O(\tau^1): & \sum_j j\alpha_j = \sum_j \beta_j \end{cases}$$

$$\sigma(\xi) = \sum_j \beta_j \xi^j$$

$$\begin{cases} O(\tau^0) : & \rho(1) = 0 \Rightarrow 1 \text{ is a root} \\ O(\tau^1) : & \rho'(1) = \sigma(1) \end{cases}$$

Dahlquist equivalence theorem

consistency + zero stability $\Longleftrightarrow$ convergence

Note: A one step method has only one root $\xi_1 = 1$ so it is convergent, as we proved earlier.

Absolute stability of LMMs

Zero stability is about the limit $\tau \to 0$, and we want a finite τ. So we need to look at absolute stability:

$$u' = \lambda u$$

$$\sum_{j=0}^{r} \alpha_j u^{n+j} = \tau \sum_{j=0}^{r} \beta_j \lambda u^{n+j}$$

reccurence relation $\rightarrow$ $$\sum_{j=0}^{r} (\alpha_j - z\beta_j) u^{n+j} = 0$$

where recall $z = \lambda \tau$

Define polynomial

$$\pi(\xi; z) = \rho(\xi) - z\sigma(\xi)$$

LMM is absolutely stable if roots of π satisfy root conditions ($|\text{simple roots}| \leq 1$, $|\text{multiple roots}| < 1$)

Stability region S for an LMM

$$S = \left\{ z \in \mathbb{C} \;\middle|\; \begin{array}{l} |\text{simple roots of } \pi(\xi;z)| \le 1 \\ |\text{multiple roots}| < 1 \end{array} \right\}$$

We can plot the boundary of S by rendering the parametric curve:

$$\pi(e^{i\theta}; z) = 0, \quad 0 < \theta \le 2\pi$$

$$\Rightarrow \quad z(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}, \quad 0 < \theta \le 2\pi$$

is the boundary of S.

Take BDF methods, for example:

$$\sigma(\xi) = \beta_r \xi^r$$

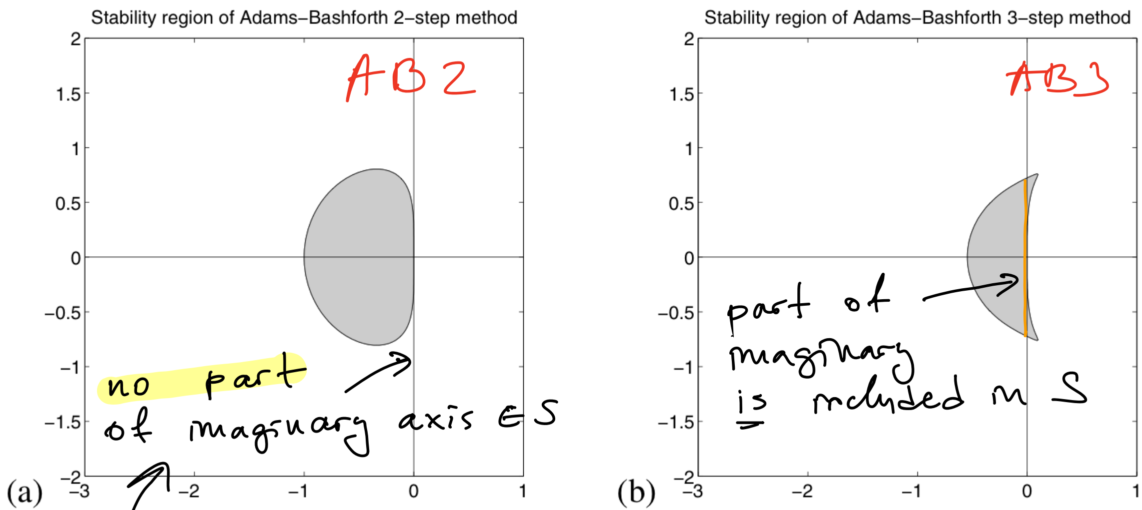
As $|z| \to \infty \Rightarrow \pi(\xi; z) \to -z\sigma(\xi)$

so roots of π match roots of σ as $|z| \to \infty$. But the only root of $\sigma(\xi)$ is $\xi_r = 0 \Rightarrow$

All BDF methods are stable as $|z| \to \infty$

Corrolary: An A-stable LMM is L-stable

This is why BDF is great for very stiff equations.



Not good for hyperbolic PDEs

good for hyperbolic PDEs

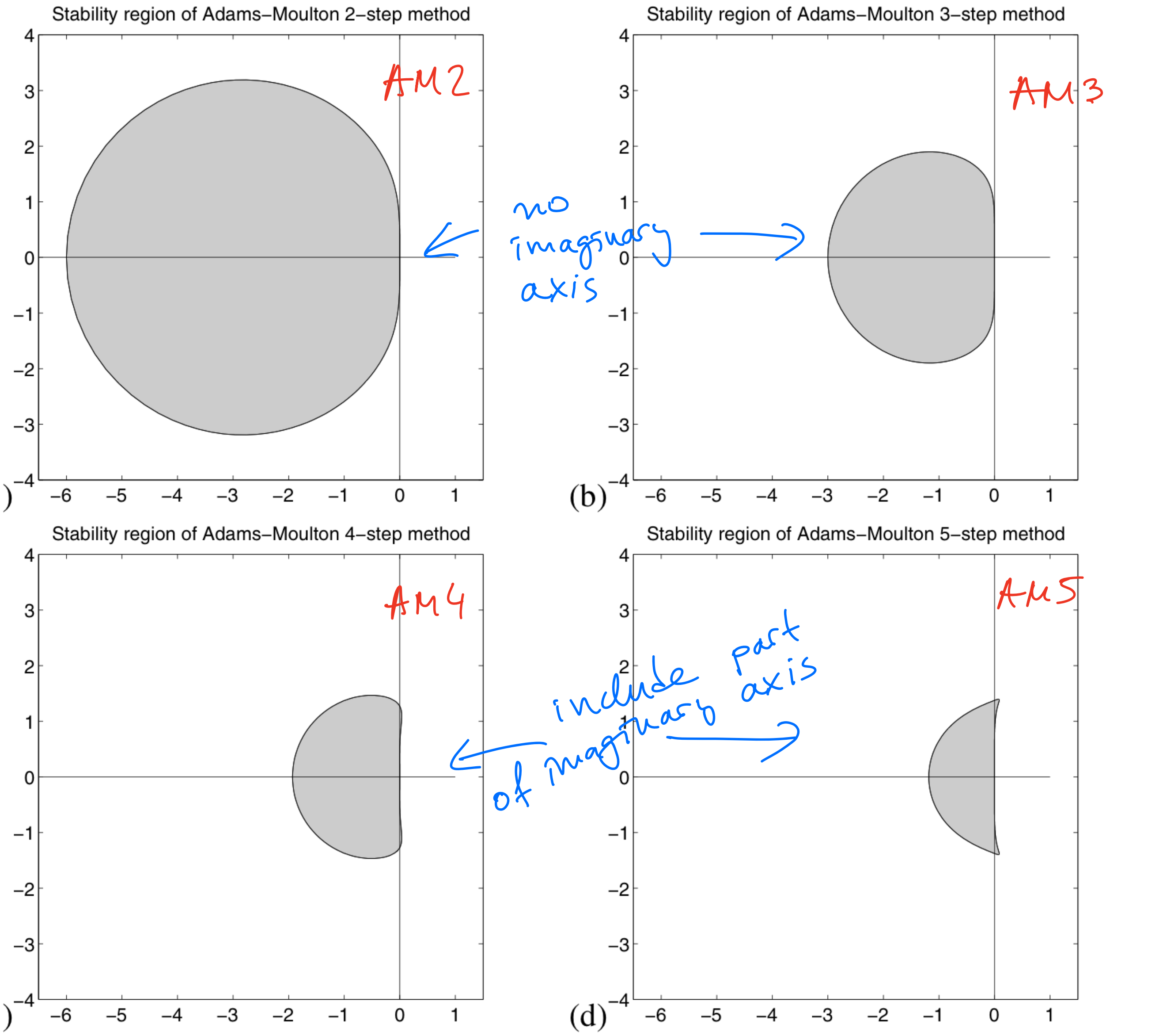
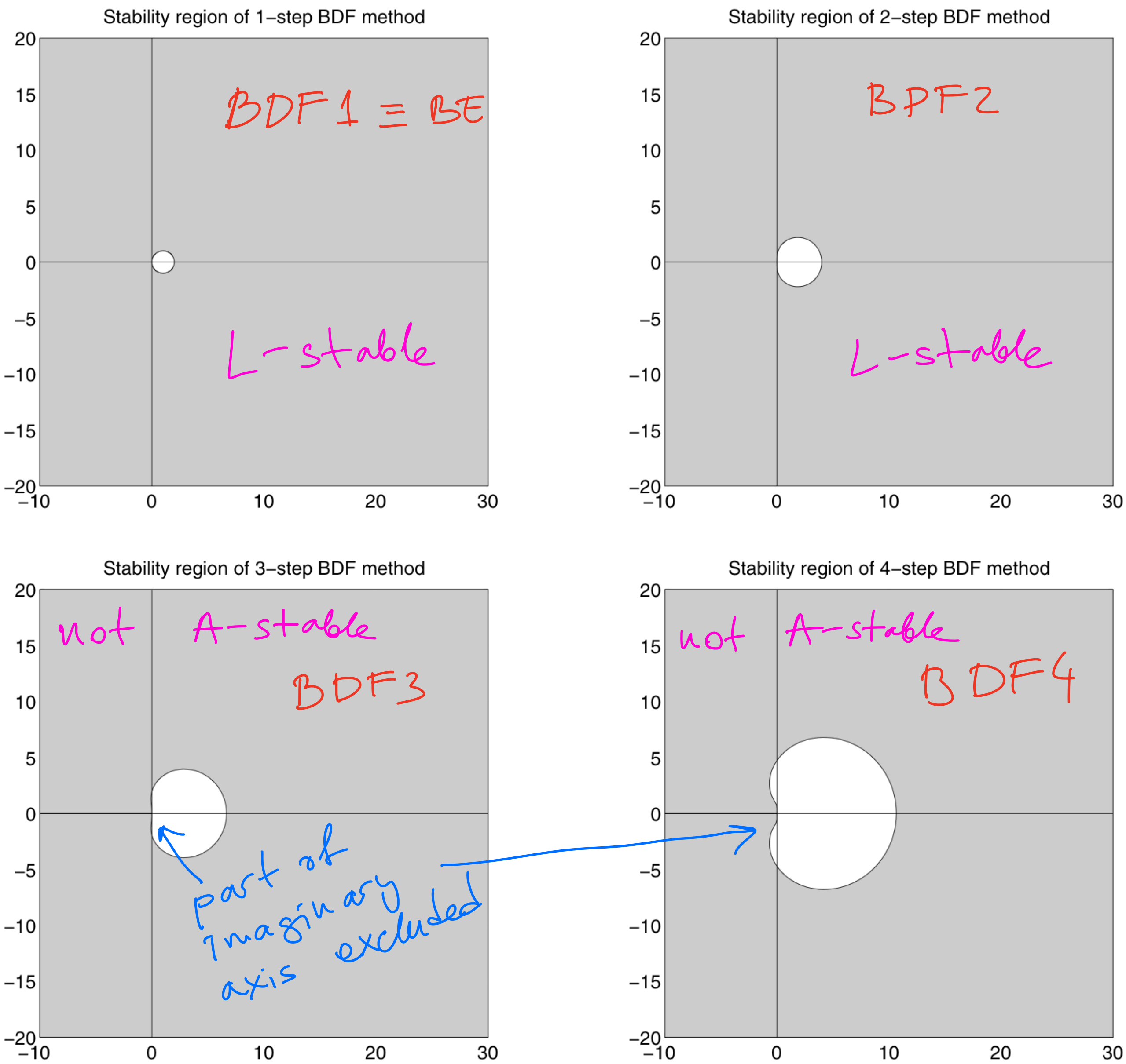


Figure 7.3. *Stability regions for some Adams–Moulton methods.*

General rule: For non-A-stable classes of methods (e.g., explicit), the stability region shrinks as the order of accuracy increases.

Explicit methods are never A-stable



Lesson: Going higher order brings issues with absolute stability. To be good for ODEs with purely imaginary eigenvalues, explicit schemes must be <u>at least 3rd order</u>

These can be turned into theorems called the Dahlquist order barriers

① A zero-stable r-step LMM can at most have order of accuracy:

If implicit $\begin{cases} r+1 & \text{if } r \text{ is } \underline{\text{odd}} \\ r+2 & \text{if } r \text{ is even} \end{cases}$

If explicit : r

② An explicit LMM <u>cannot</u> be A-stable (same as for RK)

③ An implicit A-stable LMM cannot be more than 2nd order accurate (so best is BDF2!)