MULTI-STEP METHODS FOR ODEs

We already gave one example of a <u>multistep</u> method for solving

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

Adams-Basforth (AB2): second order

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

explicit two-step

<u>NOTE</u>: One could also write

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

but LeVeque uses the first form.

A general Linear Multistep Method (LMM) with r steps: ②

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

Here we assume τ is constant and fixed (not adaptive)

The coefficients α and β determine the method. Two important classes of methods include
Adams-Bashforth, Adams-Moulton, Backwards Differentiation Formulae (BDF)

Adams methods

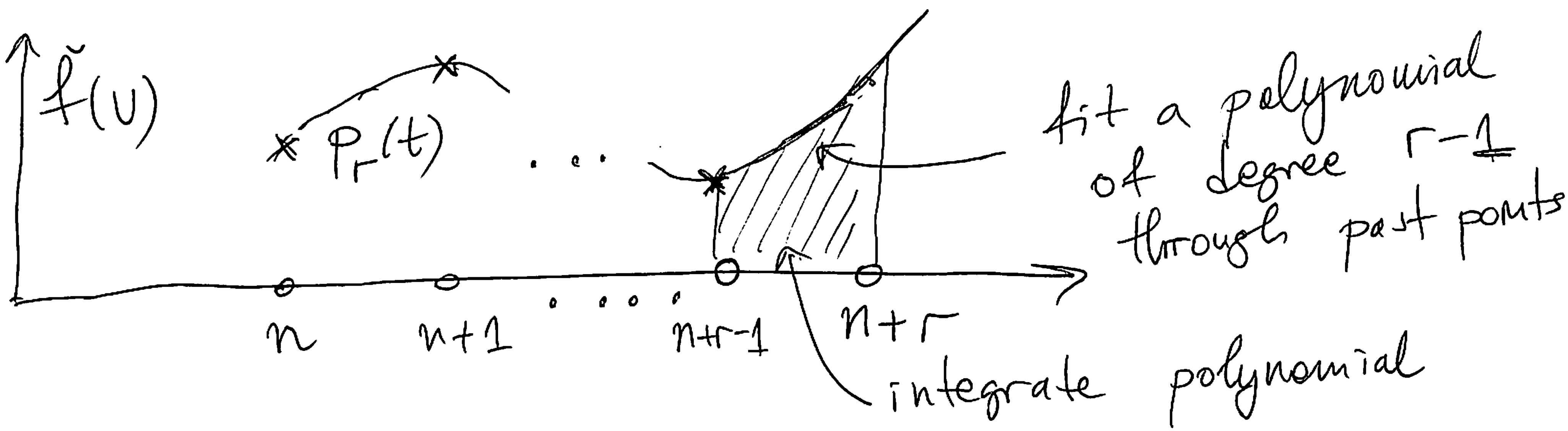
(3)

$$U^{n+r} = U^{n+r-1} + \tau \sum_{j=0}^{r} \beta_j f(U^{n+j}, t_{n+j})$$

So here $\alpha_r = 1$, $\alpha_{r-1} = -1$, all others zero

If $\underline{\beta_r = 0}$ $\rightarrow$ explicit AB

$\beta_r \neq 0$ $\rightarrow$ implicit AM (Adams-Moulton)



$$u^{n+r} = U^{n+r-1} + \int_{t_{n+r-1}}^{t_{n+r}} f(u(t))\,dt$$ ④

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

where $P_r(t)$ is the intepolating polynomial for <u>past</u> points.

<u>AB 3</u>:

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

Third-order accurate

Computing the local truncation error and the order of accuracy of the LTE is done as for one-step methods: Plug exact solution in iteration and do Taylor series. 5

<u>Implicit AM</u> methods:

AM2 - two step but <u>third</u> order:

$$U^{n+2} = U^{n+1} + \frac{k}{12}\left[-f(U^{n}) + 8f(U^{n+1}) + \underbrace{5f(U^{n+2})}_{\text{implicit}}\right]$$

<u>(AB-AM)2</u> Explicit third-order:
Compute $U^{n+2,*}$ using AB2
then do AM2 replacing U^{n+2} with $U^{n+2,*}$
(and <u>iterate</u>?)

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Multistep methods are not self-starting.
To get the r initial values, use a one step method with LTE of order $O(\tau^p)$ for p-th order

this is enough because we don't need LTE $= O(\tau^{p-1})$ as we are doing only a fixed (small) number of steps.

So use Euler to generate U^0, U^1 for AB2

Or use Richardson extrapolation for higher order

Or use RK3 / RK4 etc.

Best to use RK of the same order as multistep to avoid initial error build-up

Backward Differentiation Formulas

Implicit BDF schemes

are good for stiff equations.

Here $\beta_0 = \beta_1 = \ldots = \beta_{r-1} = 0$ and α's are obtained by fitting a polynomial through U's (not $f(U)$'s like Adams) including U^{n+r} and then differentiating the polynomial at t_{n+r}: $\boxed{f(U^{n+2}) = p'(t_{n+2})}$

always implicit

BDF 2 scheme:

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

Rewrite BDF2 as

$$\boxed{U^{n+2} = \frac{4}{3}U^{n+1} - \frac{1}{3}U^{n} + \frac{2}{3} f(U^{n+2})}$$

Consider an implicit-explicit scheme for

$$u'(t) = \underbrace{f(u,t)}_{\text{not stiff}} + \underbrace{g(u,t)}_{\text{stiff}}$$

We need to approximate explicitly

$$f(U^{n+2}) \simeq \underbrace{2f(U^{n+1}, t_{n+1}) - f(U^{n}, t_n)}_{\text{Linear extrapolation as in AB2}}$$

Putting this into BDF2 we get a "semi-implicit" BDF2 (SBDF2) popular when the imaginary eigenvalues are not the stiff ones:

SBDF2

$$U^{n+1} = \frac{4}{3}U^n - \frac{1}{3}U^{n-1} + \underbrace{\frac{2}{3}\tau g(U^{n+1}, t^{n+1})}_{\text{implicit}}$$

$$+ \frac{2}{3}\tau\left[\underbrace{f(U^n, t^n) - f(U^{n-1}, t^{n-1})}_{\text{explicit}}\right]$$

Recall also the trapezoidal BDF2 (TR-BDF)

Trap to midpoint: $U^{n+1/2,*} = U^n + \frac{\tau}{4}\left(f(U^n) + f(U^{n+1/2,*})\right)$

BDF2 using midpoint: $U^{n+1} = \frac{1}{3}\left(4U^{n+1/2,*} - U^n + \tau f(U^{n+1})\right)$

This is an L-stable one-step scheme of 2nd order

(Zero) Stability of Multistep Schemes

Are multistep methods convergent if the $LTE = O(\tau^p)$, $p \geq 2$?

Apply scheme to

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

For one-step methods, we get $u^k = 0$ for all k.

But for multistep methods, the previous values of u will not be exact but have some perturbation, and this <u>may</u> grow

An r-step method is <u>convergent</u> if solving $u' = f(u,t)$ with Lipshitz f continuous in u with <u>initial values</u> that satisfy:

$$\lim_{\tau \to 0} U^{\nu}(k) = u(0), \quad \nu = 0, \dots, r-1,$$

for every $T > 0$ at which ODE has a unique solution

$$\lim_{\tau \to 0} U^{T/\tau} = u(T)$$

So the initial values are only required to be accurate as $\tau \to 0$.

Example non-convergent LMM

$$U^{n+2} - 3U^{n+1} + 2U^{n} = -\tau f(U^n)$$

Apply this to $f = 0$:

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

$$\Rightarrow \quad U^n = 2U^0 - u^1 + 2^n (U^1 - U^0)$$

grows with n

So if $U^1 \neq U^0$ we will get a U^n that blows up even for the trivial ODE!

Let's see when $U^n \to 0$ for large n

Linear recurrence (difference) relations

Consider

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

with given $u^0, u^1, \dots, u^{r-1}$

For every simple root of

$$\rho(\xi) = \sum_{j=0}^{r} \alpha_r \xi^j$$ — characteristic polynomial of LMM

$$\rho(\xi_i) = 0$$

a linearly independent solution is

$$u^n = \xi_i^n$$

For a doubly repeated root

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

two linearly independent solutions are

$$U^n = \xi_j^n \text{ and } V^n = n\xi_j^n$$

and similarly for higher order roots.

General solution

$$u^n = \underbrace{\sum_{j=1}^{n_1} c_j \xi_j^n}_{\text{distinct roots}} + \underbrace{\sum_{k=1}^{n_2} \tilde{c}_k n \xi_k^n}_{\text{repeated roots}} + \dots$$

We want the coefficients not to grow with time, so we want

$$\boxed{|\xi_j| \leq 1 \text{ for simple roots}}$$

If we have a repeated root:

$|\xi_k| < 1$ then $\xi_k^n \to 0$ so OK

But if $|\xi_k| = 1$, then we could get a term like

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

$$\Rightarrow U^{T/\tau} = \dots + O(N\tau) = \dots + O(1)$$

so NOT convergent

Def: An LMM is <u>zero-stable</u> if all simple roots have modulus less than or equal to 1, and all repeated roots have modulus < 1.

E.g. Adams methods have

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

so 1 is a simple root and zero a repeated root.

$\Rightarrow$ $\boxed{\text{All Adams methods are zero-stable}}$

Define also another characteristic polynomial

$$\sigma(\zeta) = \sum_{j=0}^{r} \beta_j \zeta^j$$

Talyor series shows that

An LMM is consistent if

$$\sum_{j=0}^{r} \alpha_j = 0 \qquad \sum_{j=0}^{r} j\alpha_j = \sum_{j=0}^{r} \beta_j$$

$$\boxed{\rho(1) = 0 \qquad \sigma(1) = \rho'(1)}$$

$\Rightarrow$ 1 is always a root for all consistent LMMs

DAHLQUIST equivalence theorem

An LMM that is consistent and zero-stable is convergent

$$\boxed{\text{consistency} + \text{zero-stability} \iff \text{convergence}}$$

A single step (one-step) method has only one root $\xi_1 = 1$ so it is convergent.

Note that zero stability is about the limit $\tau \to 0$, <u>not</u> about finite time step size.

So we need to also examine absolute stability.

Absolute stability of LMMs

Apply an LMM to $u' = \lambda u$

$$\sum_{j=0}^{r} \alpha_j U^{n+j} = k \sum_{j=0}^{r} \beta_j \lambda U^{n+j}$$

$$\Rightarrow \sum_{j=0}^{r} \underbrace{(\alpha_j - z\beta_j)}_{\text{New coefficients}} U^{n+j} = 0 \quad \ldots (*)$$

Recall $\boxed{z = \lambda \tau}$

Define $\boxed{\pi(\xi; z) = \rho(\xi) - z\sigma(\xi)}$

Solution does not blow up if roots of $\pi(\xi; z)$ satisfy root condition

The region of absolute stability of an LMM is :

$$\boxed{S = \left\{ z \in \mathbb{C} \;\middle|\; \begin{array}{l} \text{Simple roots of } \pi(\zeta; z) \\ \text{are } \leq 1 \text{ in magnitude,} \\ \text{repeated ones } < 1 \end{array} \right\}}$$

We can plot S by taking the <u>boundary of S</u> :

$$\pi(e^{i\theta}; z) = 0 \qquad 0 < \theta \leq 2\pi$$

$$\Rightarrow \quad z = \rho(e^{i\theta}) / \sigma(e^{i\theta}) = z(\theta)$$

Consider <u>BDF</u> methods

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

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As $|z| \to \infty$

$$\pi(\xi; z) \to -z\,\sigma(\xi)$$

so roots of π match roots of σ

But σ has $\emptyset$ as its only root. $\Rightarrow$

$$\boxed{\text{All BDF methods are stable as } |z| \to \infty}$$

so they <u>could</u> be L-stable if they are A-stable

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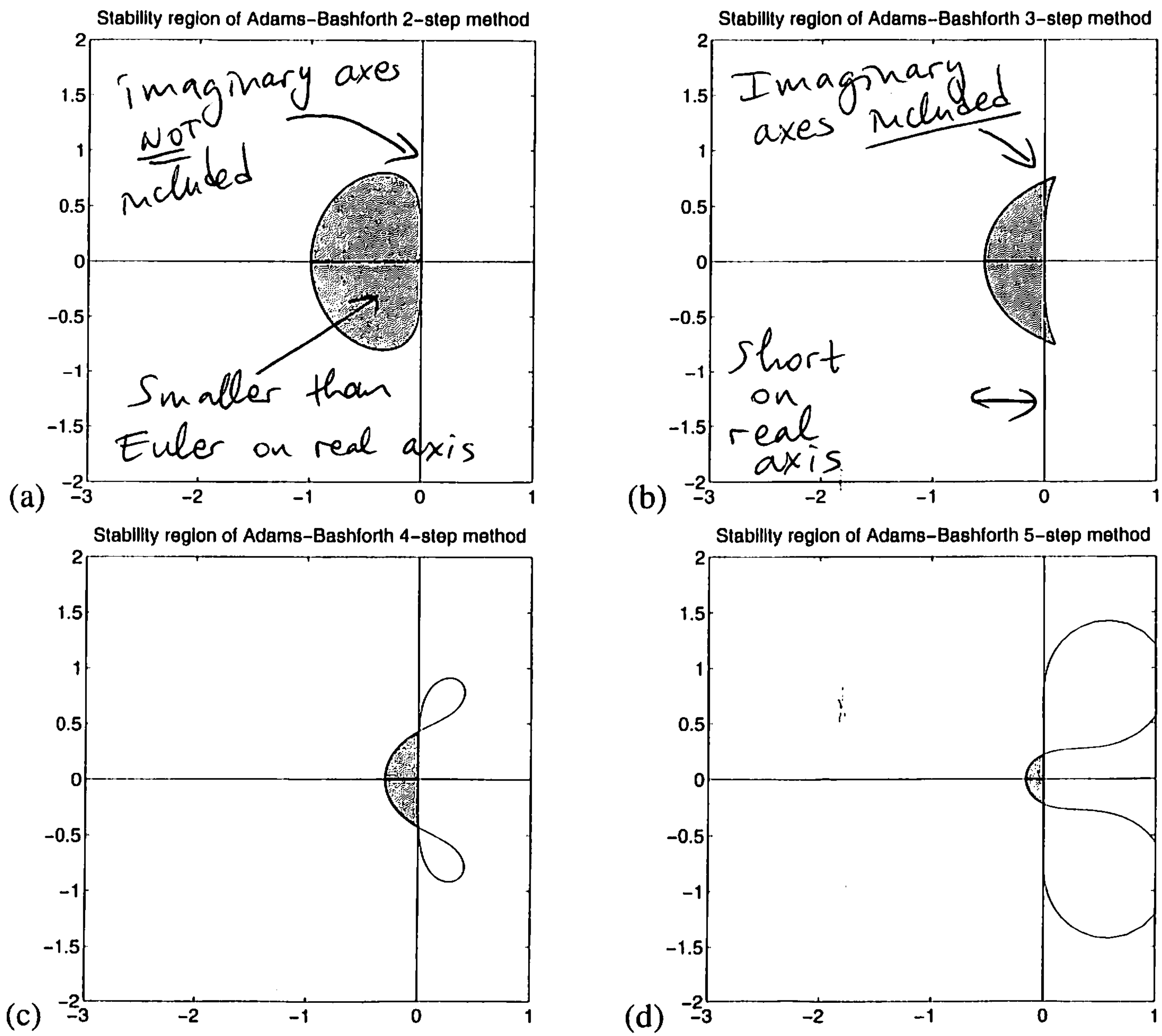
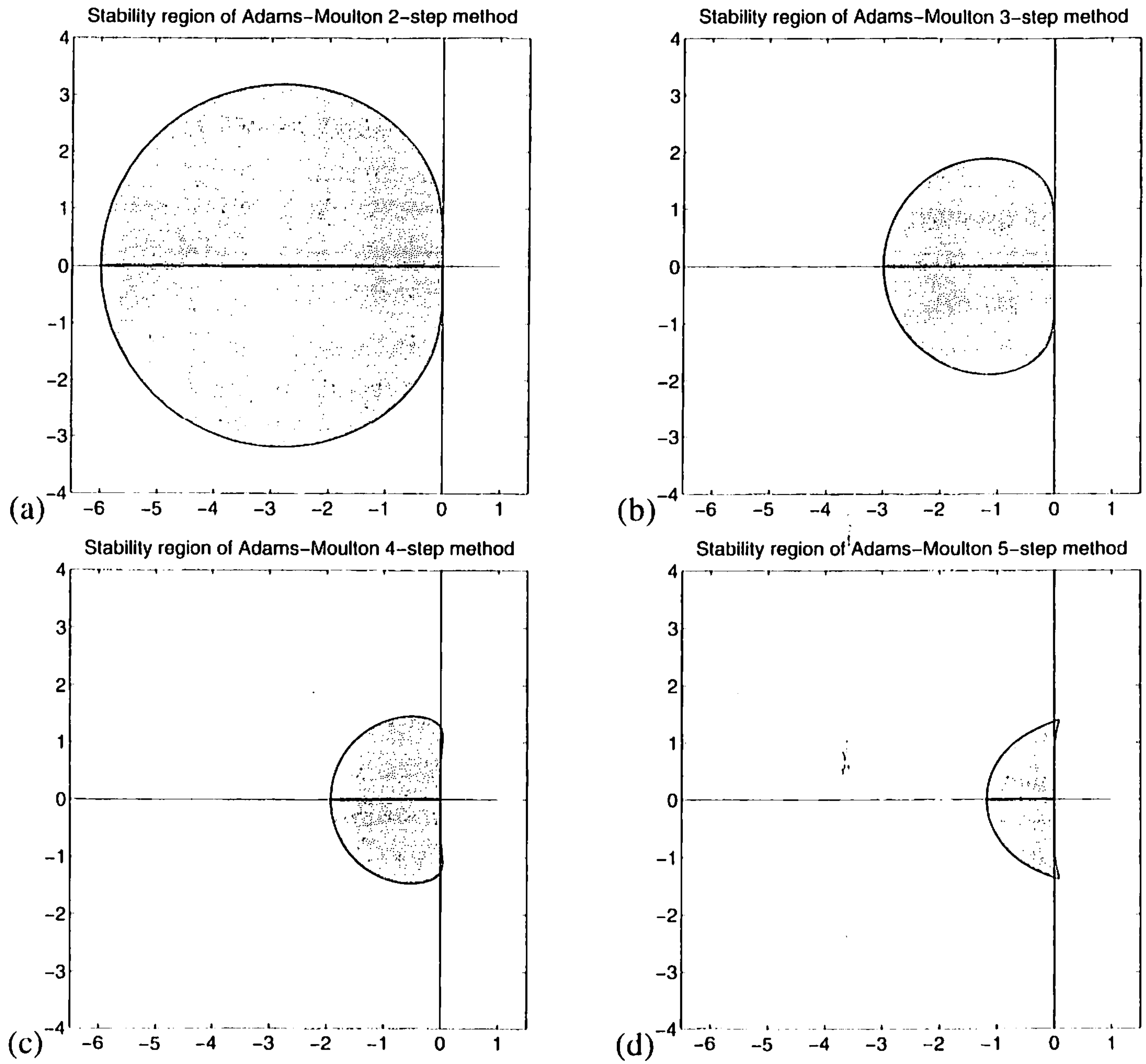

Stability region of Adams-Bashforth 2-step method
Imaginary axes NOT included
Smaller than Euler on real axis
(a)
Stability region of Adams-Bashforth 3-step method
Imaginary axes included
Short on real axis
(b)
Stability region of Adams-Bashforth 4-step method
(c)
Stability region of Adams-Bashforth 5-step method
(d)

None are A-stable!



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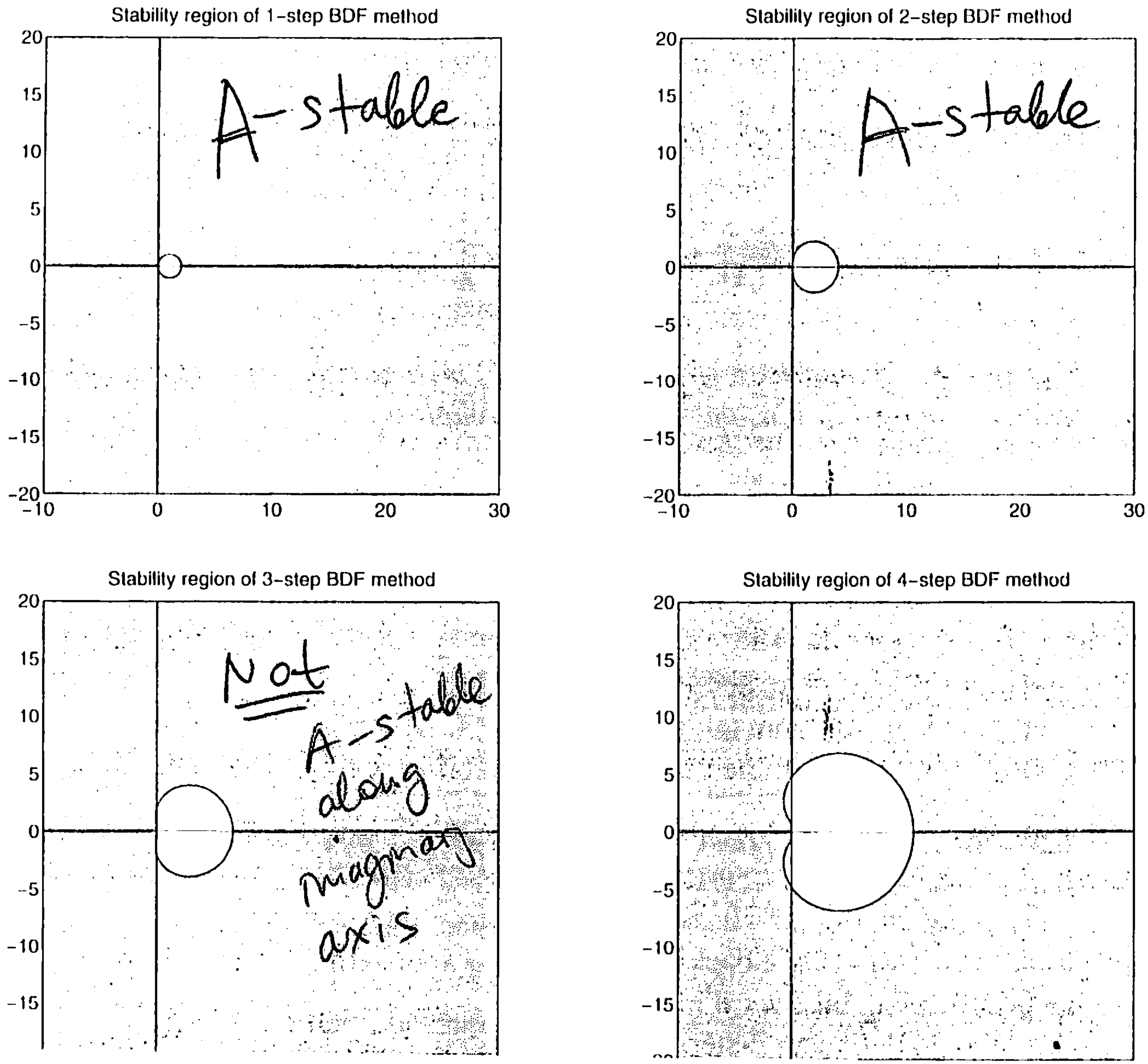
Stability region of 1-step BDF method
A-stable
Stability region of 2-step BDF method
A-stable
Stability region of 3-step BDF method
Not A-stable along imaginary axis
Stability region of 4-step BDF method
20
15
10
5
0
-5
-10
-15
-20
-10
0
10
20
30

Dahlquist order barriers

1. A zero-stable LMM with r steps can at most have order of accuracy

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

and implicit

2. An explicit LMM cannot be A-stable (same as for RK)

3. An implicit A-stable LMM cannot be more than 2nd order (e.g. BDF2)