

# Numerical Solutions to Differential Equations

## Lecture Notes #7 — Linear Multistep Methods

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## Outline

- 1 Introduction and Recap
  - Linear Multistep Methods, Historical Overview
  - Zero-Stability
- 2 Limitations on Achievable Order
  - The First Dahlquist Barrier
  - Example: 2-step, Order 4 — Simpson's Rule
- 3 Stability Theory
  - Model Problem  $\rightsquigarrow$  Stability Polynomial
  - Visualization: The Boundary Locus Method
  - Backward Differentiation Formulas

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  $\{(t_{n-k}, y_{n-k}); k = 0, \dots, s\}$  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:

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

and the same LMM applied to a slightly perturbed system

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

Perturbations are typically due to discretization and round-off.

## Defining Zero-Stability

(Review)

## Definition (Zero-stability)

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

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

whenever

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

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

## Interpreting Zero-Stability

(Formalized)

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

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

## 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**

$$|r_j| \leq 1, \quad j = 1, 2, \dots, k$$

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  $(s + 2)$ .

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## 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

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

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

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

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?**

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**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.

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

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

$$y_{n+1} \sim y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{6}y'''_n + \frac{h^4}{24}y_n^{(4)} + \frac{h^5}{120}y_n^{(5)} + \mathcal{O}(h^6)$$

$$y_{n-1} \sim y_n - hy'_n + \frac{h^2}{2}y''_n - \frac{h^3}{6}y'''_n + \frac{h^4}{24}y_n^{(4)} - \frac{h^5}{120}y_n^{(5)} + \mathcal{O}(h^6)$$

---

$$\text{LHS} \sim 2hy'_n + \frac{h^3}{3}y'''_n + \frac{h^5}{60}y_n^{(5)} + \mathcal{O}(h^7)$$

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$$4f_n \sim 4f_n$$

$$f_{n+1} \sim f_n + hf'_n + \frac{h^2}{2}f''_n + \frac{h^3}{6}f'''_n + \frac{h^4}{24}f_n^{(4)} + \frac{h^5}{120}f_n^{(5)} + \mathcal{O}(h^6)$$

$$\text{RHS} \sim \frac{h}{3} \left[ 6f_n + h^2f''_n + \frac{h^4}{12}f_n^{(4)} + \mathcal{O}(h^6) \right]$$

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

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

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

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### Simpson's Rule — Local Truncation Error

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

## Linear Stability Theory for LMMs

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

$$y'(t) = \lambda y(t), \quad \operatorname{Re}(\lambda) \leq 0$$

and search for the region  $\hat{h} = (h\lambda)$  where the LMM does not grow exponentially.

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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...

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

## Linear Stability Theory for LMMs, II

We have

$$\sum_{j=0}^k [\alpha_j - h\beta_j\lambda] \mathbf{y}_{n+j} = \mathbf{0}$$

A general solution of this difference equation is

$$y_n = r_0 r^n$$

where  $r$  is a root of the characteristic polynomial

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

$\pi(r, \hat{h})$  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  $\hat{h}$ , if for that  $\hat{h}$  all the roots of the stability polynomial  $\pi(r, \hat{h})$  satisfy  $|r_j| < 1$ ,  $j = 1, 2, \dots, s$ , and to be **absolutely unstable** for that  $\hat{h}$  otherwise.

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## 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  $\hat{h}$ -plane, if it is absolutely stable for all  $\hat{h} \in \mathcal{R}_A$ . 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  $\pi(r, \hat{h})$  is  $e^{i\theta}$ .

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

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

Solving for  $\hat{h}$  gives

Method: Boundary Locus

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



## The Region of Absolute Stability for Simpson's Method

Consider Simpson's Rule, and its characteristic polynomials

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

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

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.

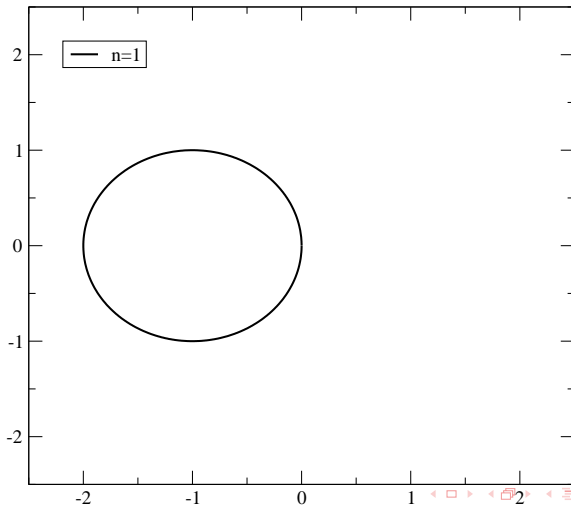
**Simpson's Rule has a zero-area region of absolute stability**  
(Bummer).

## 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.

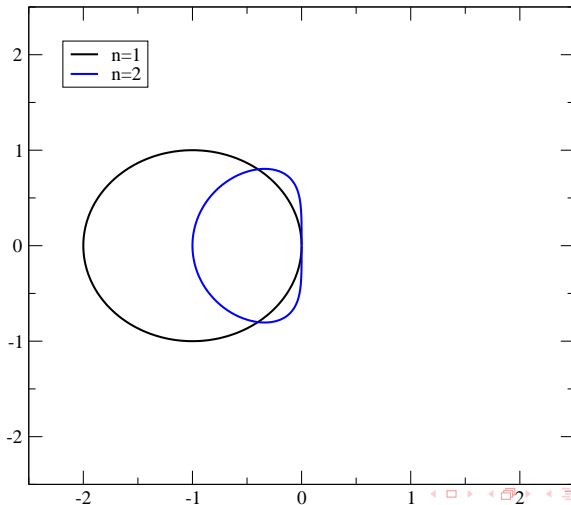
## Stability Regions for Adams-Bashforth Methods

### Adams-Bashforth Methods Stability Regions



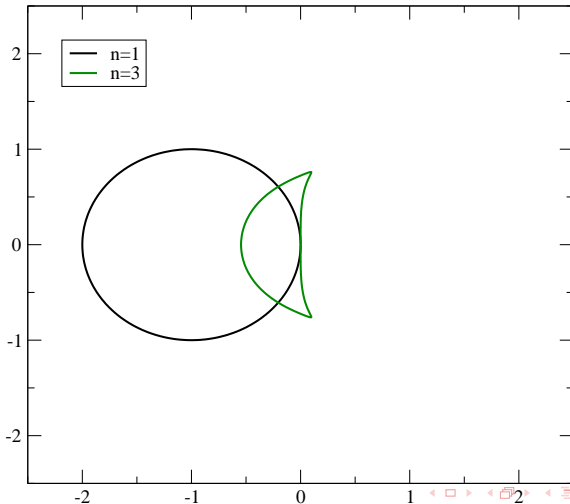
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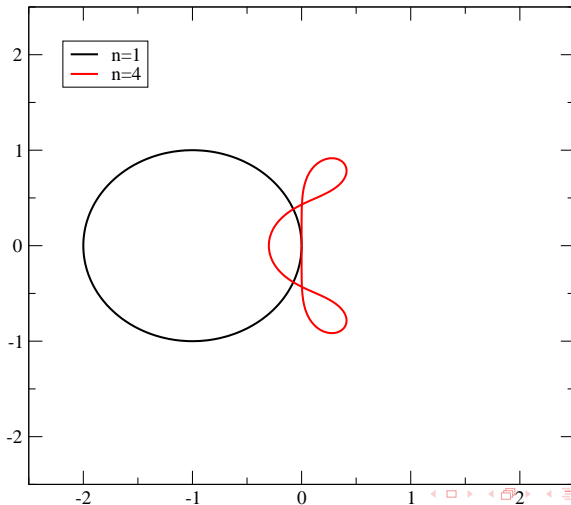
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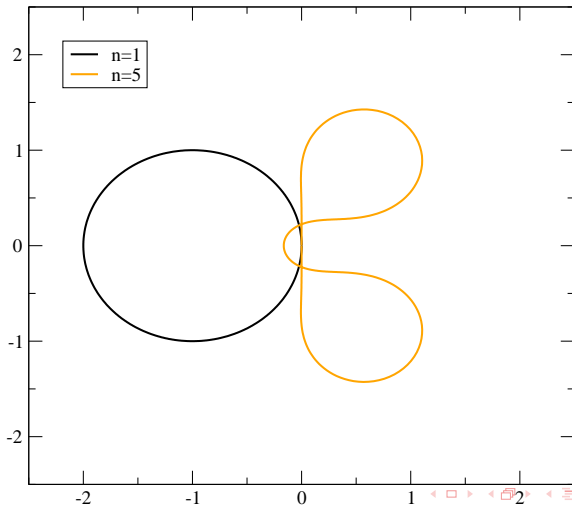
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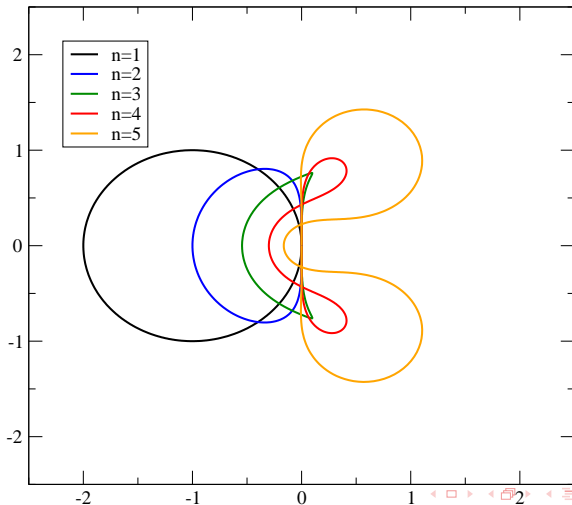
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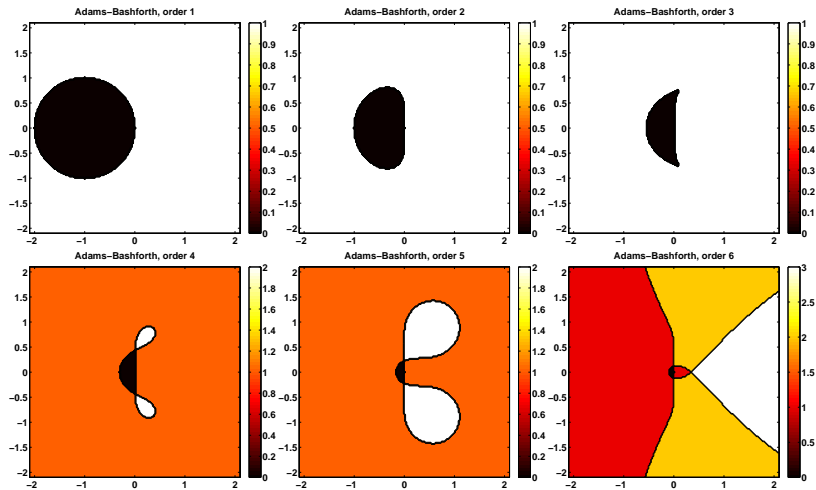
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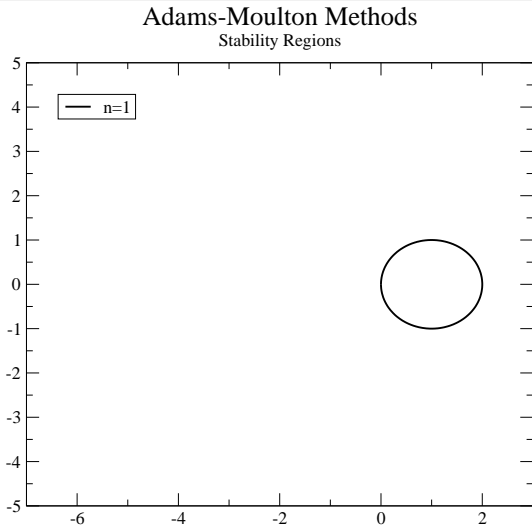


# Stability Regions for Adams-Bashforth Methods

$|r_\nu| > 1$  count

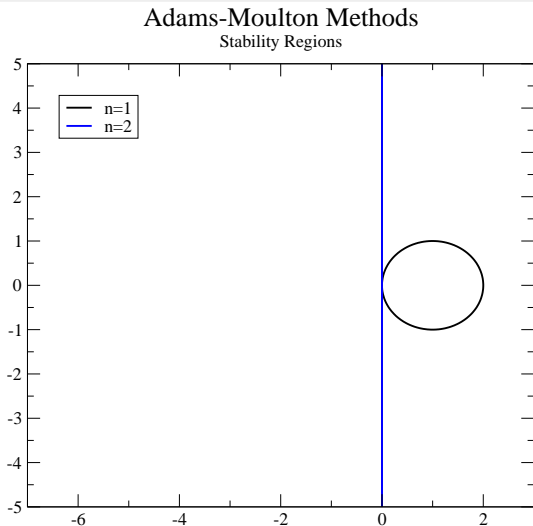


## Stability Regions for Adams-Moulton Methods



**The Exterior of the circle!**

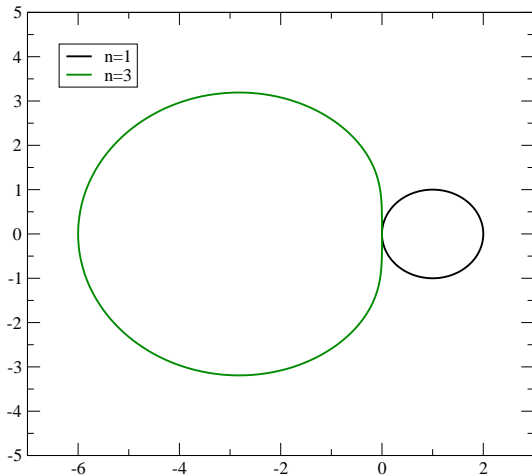
## Stability Regions for Adams-Moulton Methods



**The left half plane!**

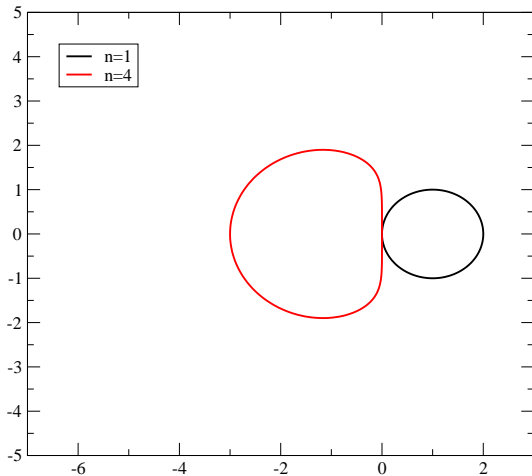
## Stability Regions for Adams-Moulton Methods

### Adams-Moulton Methods Stability Regions



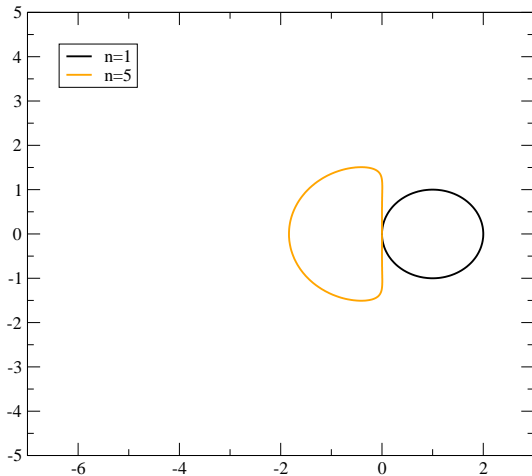
## Stability Regions for Adams-Moulton Methods

Adams-Moulton Methods  
Stability Regions



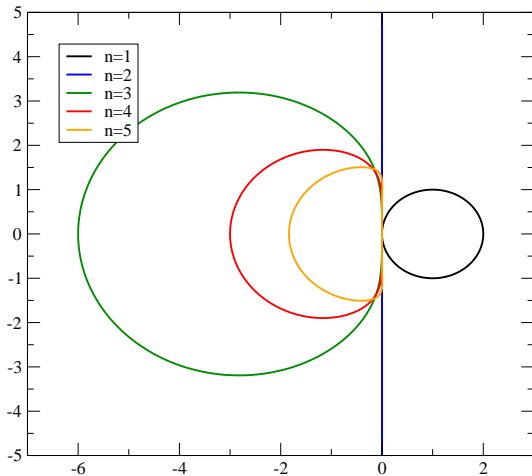
# Stability Regions for Adams-Moulton Methods

## Adams-Moulton Methods Stability Regions



# Stability Regions for Adams-Moulton Methods

## Adams-Moulton Methods Stability Regions



## 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  $\lambda : \operatorname{Re}(\lambda) < 0$ :

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

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

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

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

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

1/IV

The  $k$ th order BDF is derived by constructing the polynomial interpolant through the points

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

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

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

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

$$\nabla y_{n+1} = \left[ y_{n+1} - y_n \right], \quad \nabla^2 y_{n+1} = \frac{1}{2} \left[ \nabla y_{n+1} - \nabla y_n \right], \quad \dots$$

## 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

$$\left. \frac{d}{ds} \binom{-s}{j} \right|_{s=0}$$

Massive application of the product rule gives us

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

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

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:

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

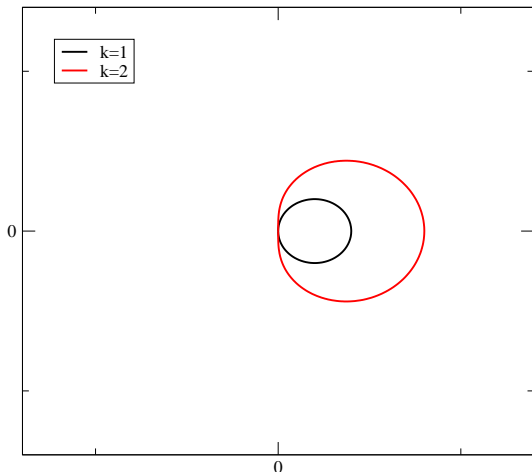
BDFs,  $k = 1, 2, \dots, 6$ 

$k$	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.

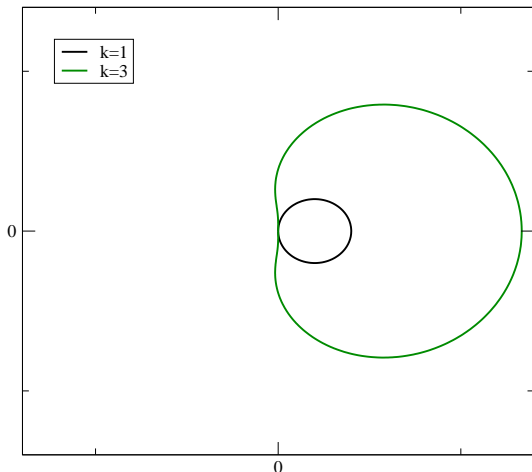
## Stability Regions for BDF Methods

BDF Methods  
Stability Regions



## Stability Regions for BDF Methods

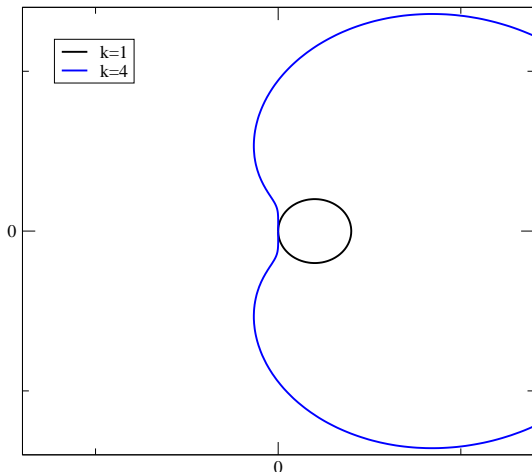
BDF Methods  
Stability Regions





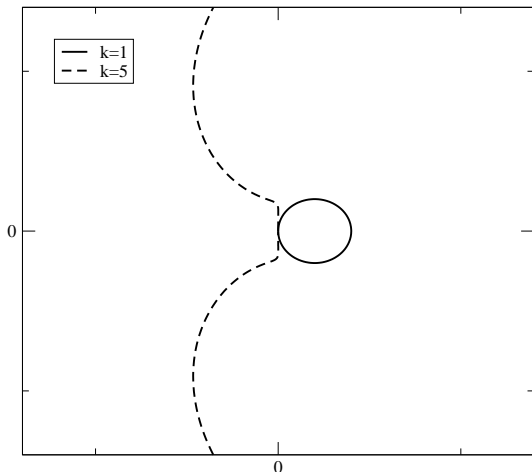
## Stability Regions for BDF Methods

BDF Methods  
Stability Regions



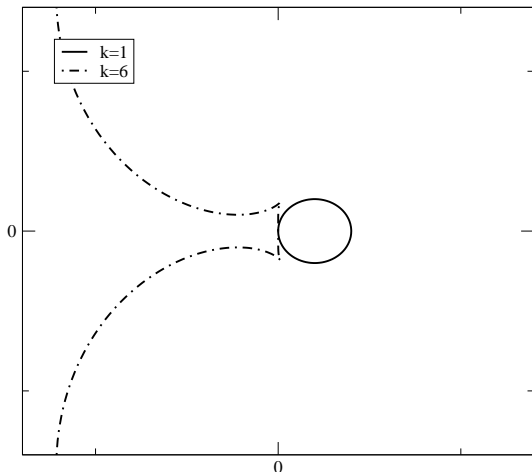
## Stability Regions for BDF Methods

BDF Methods  
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## Stability Regions for BDF Methods

### BDF Methods Stability Regions



## Stability Regions for BDF Methods

BDF Methods  
Stability Regions

