Set 19: Ordinary Differential Equations: Linear Multistep Methods

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Foundations of Computational Math 2

Spring 2013

Sources

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Linear One-step Methods

general form $\alpha_0 y_n + \alpha_1 y_{n-1} = h(\beta_0 f_n + \beta_1 f_{n-1})$

forward Euler $y_n = y_{n-1} + h f_{n-1}$

$$y_n - y_{n-1} = h f_{n-1}$$

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = 0, \;\; \beta_1 = 1$$

backward Euler $y_n = y_{n-1} + h f_n$

$$y_n - y_{n-1} = h f_n$$

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = 1, \;\; \beta_1 = 0$$

Trapezoidal rule $y_n = y_{n-1} + \frac{h}{2}(f_n + f_{n-1})$

$$y_n - y_{n-1} = h(\frac{1}{2} f_n + \frac{1}{2} f_{n-1})$$

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = 1/2, \;\; \beta_1 = 1/2$$

General Form of Linear Multistep Methods

Assume $h_n = h$ and let $f_n = f(t_n, y_n)$ where y_n is a point on the numerical solution.

$k-$ step Linear multistep methods are of the form:

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = h \sum_{j=0}^{k} \beta_j f_{n-j}$$

$$\mathcal{N}_h[y_n] = \frac{\sum_{j=0}^{k} \alpha_j y_{n-j}}{h} - \sum_{j=0}^{k} \beta_j f_{n-j}$$

$$\alpha_0 \neq 0$$

y_{n-k} and/or f_{n-k} involved $\Rightarrow |\alpha_k| + |\beta_k| \neq 0$

Initial conditions must be specified $\quad y_0, \ldots, y_{k-1}$

Questions

How does the form of linear multistep methods affect the following?

- Derivation of methods
- Consistency of methods
- 0 and absolute stability of methods
- Convergence of methods

Derivations

Various derivations of these methods are possible depending on the family.

- algebraic constraints
- difference operator calculus
- interpolation and integration
- interpolation and differentiation

Adams Methods

$$y(t_n) = y(t_{n-1}) + \int_{t_{n-1}}^{t_n} f(t, y(t))dt$$

Adams-Bashforth – explicit methods, $k-$step, order k

- let $P'(t)$ interpolate $f_{n-1}, \ldots, f_{n-k}$
- Define the integration constant so that $P(t_{n-1}) = y_{n-1}$
- The method is given by $y_n = P(t_n)$

Adams-Moulton – implicit methods, $k-$step, order $k+1$

- let $P'(t)$ interpolate $f_n, f_{n-1}, \ldots, f_{n-k}$
- Define the integration constant so that $P(t_{n-1}) = y_{n-1}$
- The method is given by $y_n = P(t_n)$

Example

Forward Euler:

$$P'(t) = f_{n-1}$$

$$P(t) = tf_{n-1} + c$$

$$y_{n-1} = P(t_{n-1}) \rightarrow y_{n-1} = t_{n-1}f_{n-1} + c \rightarrow c = y_{n-1} - t_{n-1}f_{n-1}$$

$$\begin{aligned} y_n &= P(t_n) \\ &= t_n f_{n-1} + y_{n-1} - t_{n-1}f_{n-1} \\ &= y_{n-1} + hf_{n-1} \end{aligned}$$

Example

Trapezoidal rule:

$$
\begin{aligned}
P'(t) &= \frac{(t - t_{n-1})}{(t_n - t_{n-1})} f_n - \frac{(t - t_n)}{(t_n - t_{n-1})} f_{n-1} \\
P(t) &= \frac{1}{2h} \left[(t - t_{n-1})^2 f_n - (t - t_n)^2 f_{n-1} \right] + c \\
y_{n-1} &= P(t_{n-1}) \rightarrow c = y_{n-1} + \frac{h}{2} f_{n-1} \\
y_n &= \frac{1}{2h} \left[(t_n - t_{n-1})^2 f_n \right] + y_{n-1} + \frac{h}{2} f_{n-1} \\
&= y_{n-1} + \frac{h}{2} (f_n + f_{n-1})
\end{aligned}
$$

Adams Bashforth Coefficients

For all k $\beta_0 = 0$,$\alpha_0 = 1$ and $\alpha_1 = -1$, step and order are k.

k		1	2	3	4	5	6
1	β_j	1					
2	$2\beta_j$	3	-1				
3	$12\beta_j$	23	-16	5			
4	$24\beta_j$	55	-59	37	-9		
5	$720\beta_j$	1901	-2774	2616	-1274	251	
6	$1440\beta_j$	4277	-7923	9982	-7298	2877	-475

Adams Moulton Coefficients

For all k $\alpha_0 = 1$ and $\alpha_1 = -1$, order is $k+1$ (except for Backward Euler).

k		0	1	2	3	4	5
1	β_j	1					
2	$2\beta_j$	1	1				
3	$12\beta_j$	5	8	-1			
4	$24\beta_j$	9	19	-5	1		
5	$720\beta_j$	251	646	-264	106	-19	
6	$1440\beta_j$	475	1427	-798	482	-173	27

Note. Two one-step methods in table.

Backward Differentiation Methods

BDF – implicit methods, $k-$step, order k

- let $P(t)$ interpolate $y_n, y_{n-1}, \ldots, y_{n-k}$
- The method is given by $P'(t_n) = f_n$

Backward Euler:

$$
\begin{aligned}
P(t) &= \frac{(t - t_{n-1})}{(t_n - t_{n-1})} y_n - \frac{(t - t_n)}{(t_n - t_{n-1})} y_{n-1} \\
P'(t) &= \frac{1}{h}(y_n - y_{n-1}) \\
f_n &= \frac{1}{h}(y_n - y_{n-1}) \\
y_n &= y_{n-1} + h f_n
\end{aligned}
$$

BDF Coefficients

For all k, $\alpha_0 = 1$ and order is k.

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

Characteristic Polynomials

Linear multistep methods are recurrences and can be defined in terms of their characteristic polynomials. (see the text for analytical methods for solving linear recurrences)

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = h \sum_{j=0}^{k} \beta_j f_{n-j}$$

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^{k-j}, \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^{k-j}$$

$$\rho'(\xi) = \sum_{j=0}^{k-1} (k-j)\alpha_j \xi^{k-j-1}$$

Characteristic Polynomials

forward Euler $\quad y_n - y_{n-1} = hf_{n-1}$

$$\rho(\xi) = \xi - 1, \quad \sigma(\xi) = 1$$

backward Euler $\quad y_n - y_{n-1} = hf_n$

$$\rho(\xi) = \xi - 1, \quad \sigma(\xi) = \xi$$

Trapezoidal rule $\quad y_n - y_{n-1} = h(\frac{1}{2}f_n + \frac{1}{2}f_{n-1})$

$$\rho(\xi) = \xi - 1, \quad \sigma(\xi) = \frac{1}{2}\xi + \frac{1}{2}$$

Consistency

We have using Taylor series of $y(t)$

$$\mathcal{N}_h[y_n] = \frac{\sum_{j=0}^{k} \alpha_j y_{n-j}}{h} - \sum_{j=0}^{k} \beta_j f_{n-j}$$

$$d_n = \mathcal{N}_h[y(t)]$$

$$hd_n = C_0 y(t) + C_1 h y'(t) + \cdots + C_q h^q y^{(q)}(t) + \cdots$$

Definition 19.1. The linear multistep method is consistent of order p if and only if

$$C_0 = C_1 = \cdots = C_p = 0 \text{ and } C_{p+1} \neq 0.$$

We have $d_n = C_{p+1} h^p y^{(p+1)}(t_n) + \mathcal{O}(h^{p+1})$.

Consistency

Closed forms are known for the C_i. The first few are:

$$C_0 = \sum_{j=0}^{k} \alpha_j \qquad C_1 = -\sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j$$

$$C_2 = \sum_{j=1}^{k} \frac{j^2}{2}\alpha_j + \sum_{j=1}^{k} j\beta_j \qquad C_3 = -\sum_{j=1}^{k} \frac{j^3}{6}\alpha_j - \sum_{j=1}^{k} \frac{j^2}{2}\beta_j$$

$$C_4 = \sum_{j=1}^{k} \frac{j^4}{24}\alpha_j + \sum_{j=1}^{k} \frac{j^3}{6}\beta_j$$

Consistency

Theorem 19.1. *A method is consistent if and only if*

$$\rho(1) = 0 \quad \textit{and} \quad \rho'(1) = \sigma(1)$$

Proof. We have $C_0 = \rho(1)$ and

$$C_0 = 0 \to C_1 = \rho'(1) - \sigma(1).$$

The result follows from $C_0 = C_1 = 0$.

$\square$

Examples

Adams-Bashforth: $k-$step, order k, explicit family

AB(k=1),forward Euler:

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = 0, \;\; \beta_1 = 1$$

$$C_0 = 1 - 1 = 0, \;\; C_1 = 1 - 0 - 1 = 0$$

$$C_2 = -\frac{1}{2} + 1 = \frac{1}{2}$$

AB(k=2):

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \alpha_2 = 0, \;\; \beta_0 = 0, \;\; \beta_1 = \frac{3}{2}, \;\; \beta_2 = -\frac{1}{2}$$

$$C_0 = 1 - 1 = 0, \;\; C_1 = 1 + 0 + 0 - \frac{3}{2} + \frac{1}{2} = 0$$

$$C_2 = -\frac{1}{2} + 0 + \frac{3}{2} - 1 = 0, \;\; C_3 = \frac{1}{6} + 0 - \frac{3}{4} + 2 = \frac{5}{12}$$

Examples

Adams-Moulton: $k-$step, order $k+1$, implicit family

AM(k=1) (trapezoidal):

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = \frac{1}{2}, \;\; \beta_1 = \frac{1}{2}$$

$$C_0 = 1 - 1 = 0, \;\; C_1 = 1 - \frac{1}{2} - \frac{1}{2} = 0$$

$$C_2 = -\frac{1}{2} + \frac{1}{2} = 0, \;\; C_3 = -\frac{1}{6}(-1) - \frac{1}{2}(\frac{1}{2}) = -\frac{1}{12}$$

Examples

Adams-Moulton: $k-$step, order $k+1$, implicit family

AM(k=2):

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \alpha_2 = 0, \;\; \beta_0 = \frac{5}{12}, \;\; \beta_1 = \frac{8}{12}, \;\; \beta_2 = -\frac{1}{12}$$

$$C_0 = 1 - 1 = 0, \;\; C_1 = 1 + 0 - \frac{5}{12} - \frac{8}{12} + \frac{1}{12} = 0$$

$$C_2 = -\frac{1}{2} + \frac{8}{12} - \frac{2}{12} = 0, \;\; C_3 = -\frac{1}{6}(-1+0) - \frac{1}{2}(\frac{8}{12} - \frac{4}{12}) = 0$$

$$C_4 = \frac{1}{24}(-1) + \frac{1}{6}\frac{8}{12} - \frac{8}{6}\frac{1}{12} = -\frac{1}{24}$$

Examples

Backward Differentiation Method: $k-$step, order k, implicit family

BDF(k=1), backward Euler:

$$\alpha_0 = 1, \;\; \alpha_1 = -1, \;\; \beta_0 = 1, \;\; \beta_1 = 0$$

$$C_0 = 1 - 1 = 0, \;\; C_1 = 1 - 1 = 0, \;\; C_2 = \frac{1}{2}(-1) = -\frac{1}{2}$$

BDF(k=2):

$$\alpha_0 = 1, \;\; \alpha_1 = -\frac{4}{3}, \;\; \alpha_2 = \frac{1}{3}, \;\; \beta_0 = \frac{2}{3}, \;\; \beta_1 = 0, \;\; \beta_2 = 0$$

$$C_0 = 1 - \frac{4}{3} + \frac{1}{3} = 0, \;\; C_1 = \frac{4}{3} - \frac{2}{3} - \frac{2}{3} = 0,$$

$$C_2 = \frac{1}{2}(-\frac{4}{3} + \frac{4}{3}) = 0, \;\; C_3 = -\frac{1}{6}(-\frac{4}{3} + \frac{8}{3}) = -\frac{2}{9}$$

0-Stability of Linear Multistep Methods

- The first order differential equation has been replaced with a $k-$th order difference equation.
- starting values must be given and be $\mathcal{O}(h^p)$ accurate.
- spurious roots of the difference equation can not help.
- spurious roots of the difference equation must be prevented from damaging the solution

0-Stability of Linear Multistep Methods

- The 0-stability definition used earlier based on the Lipschitz continuity of $\mathcal{N}_h^{-1}$ can be difficult to work with.
- 0-stability for linear multistep methods can be stated in terms of their performance on the test problem $y' = 0$.
- A method is 0-stable if the numerical solution to $y' = 0$ remains bounded when the extra initial conditions are perturbed.
- characterization comes from standard difference equation results
- useful linear multistep methods require an additional property – strong stability

0-Stability, Consistency, Convergence

Definition 19.2. The linear multistep method with characteristic polynomials $\rho(\xi)$ and $\sigma(\xi)$ is

- consistent if and only if

$$\rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1)$$

- satisfies the root condition if all roots, ξ_i, of $\rho(\xi)$ satisfy $|\xi_i| \leq 1$ and roots with unit magnitude are simple.

Theorem 19.2. *If a linear multistep method is consistent, satisfies the root condition, and has initial values that are $\mathcal{O}(h^p)$ accurate, then the method is convergent to order p.*

Example of Unstable Consistent Method (Petzold)

The method

$$y_n = -4y_{n-1} + 5y_{n-2} + 4hf_{n-1} + 2hf_{n-2}$$

is the most accurate two-step explicit method in terms of local truncation error. It does not satisfy the root condition however since

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

Consider solving $y' = 0$, with $y_0 = 0$ and $y_1 = \epsilon$ to see disastrous effect of instability.

Strong Stability

Definition 19.3. A linear multistep method is strongly stable if all of the roots, ξ_i, of $\rho(\xi)$ satisfy $|\xi_i| < 1$ except the principal root $\xi = 1$.

Definition 19.4. A linear multistep methods is weakly stable if it is 0-stable but not strongly stable.

Theorem 19.3. *(Dahlquist) A strongly stable k-step method can have at most order $k + 1$*

Example

Example 19.1. Consider Milne's method

$$y_n = y_{n-2} + \frac{h}{3}(f_n + 4f_{n-1} + f_{n-2})$$

$$\rho(\xi) = \xi^2 - 1, \text{roots are} \quad \xi_i = \pm 1 \rightarrow \text{weakly stable}$$

$$\sigma(\xi) = \frac{1}{3}\xi^2 + \frac{4}{3}\xi + \frac{1}{3}$$

$$\rho(1) = 0, \quad \rho'(1) = 2 = \sigma(1) \rightarrow \text{consitent}$$

When applied to $y' = \lambda y$ the recurrence is dominated by a term related to the spurious root at -1 for any $\lambda < 0$ and is unstable.

To be stable and accurate it should be dominated by the principal root.

$0-$**Stability**

- All one-step methods are 0-stable.
- weakly stable methods should be avoided due to absolute stability difficulties
- Adams methods have $\rho(\xi) = \xi^k - \xi^{k-1}$ and are strongly stable.
- Adams Moulton have maximum order.
- BDF methods are strongly stable for $k = 1, \ldots, 6$ and unstable thereafter.

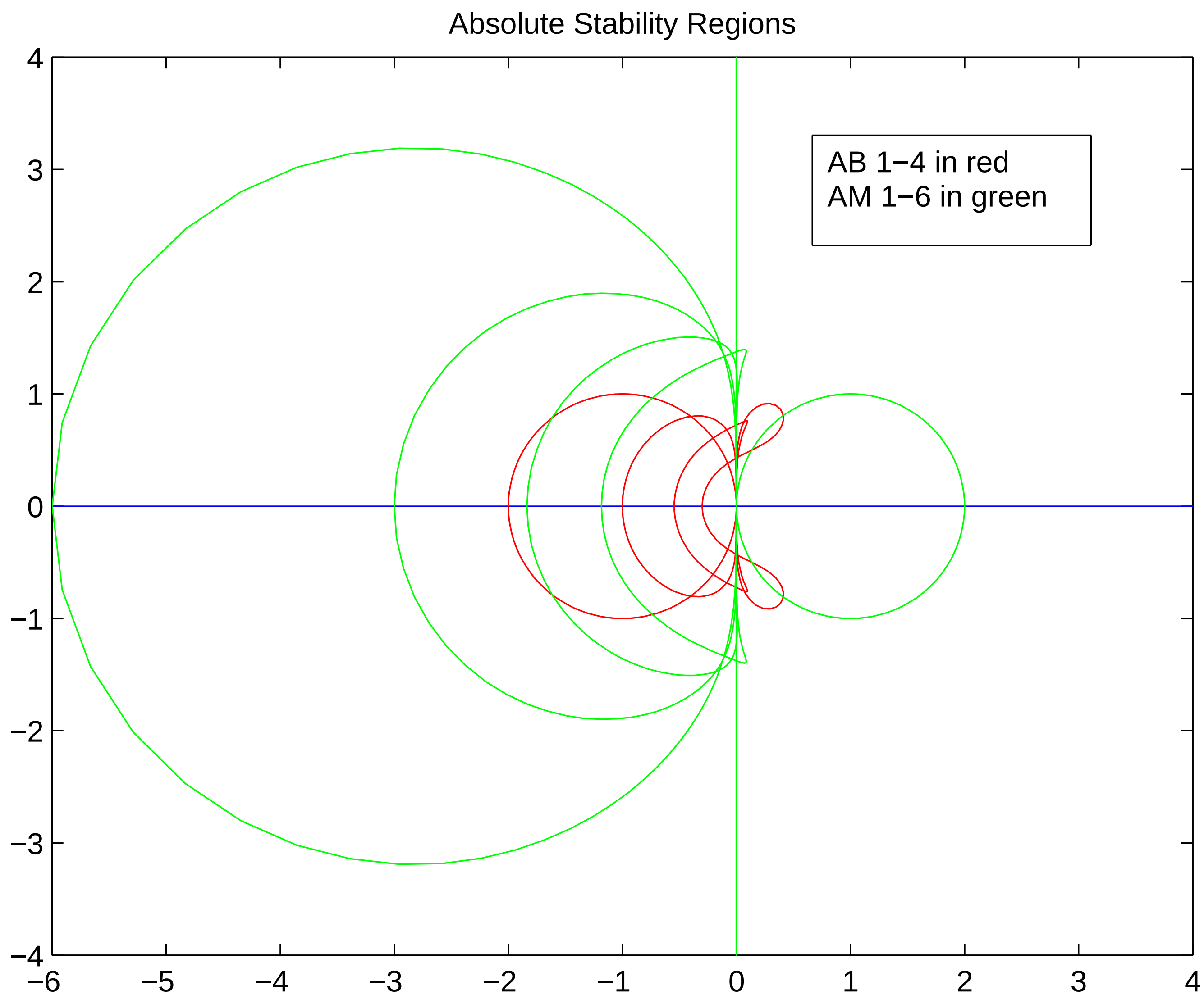
Absolute Stability Region

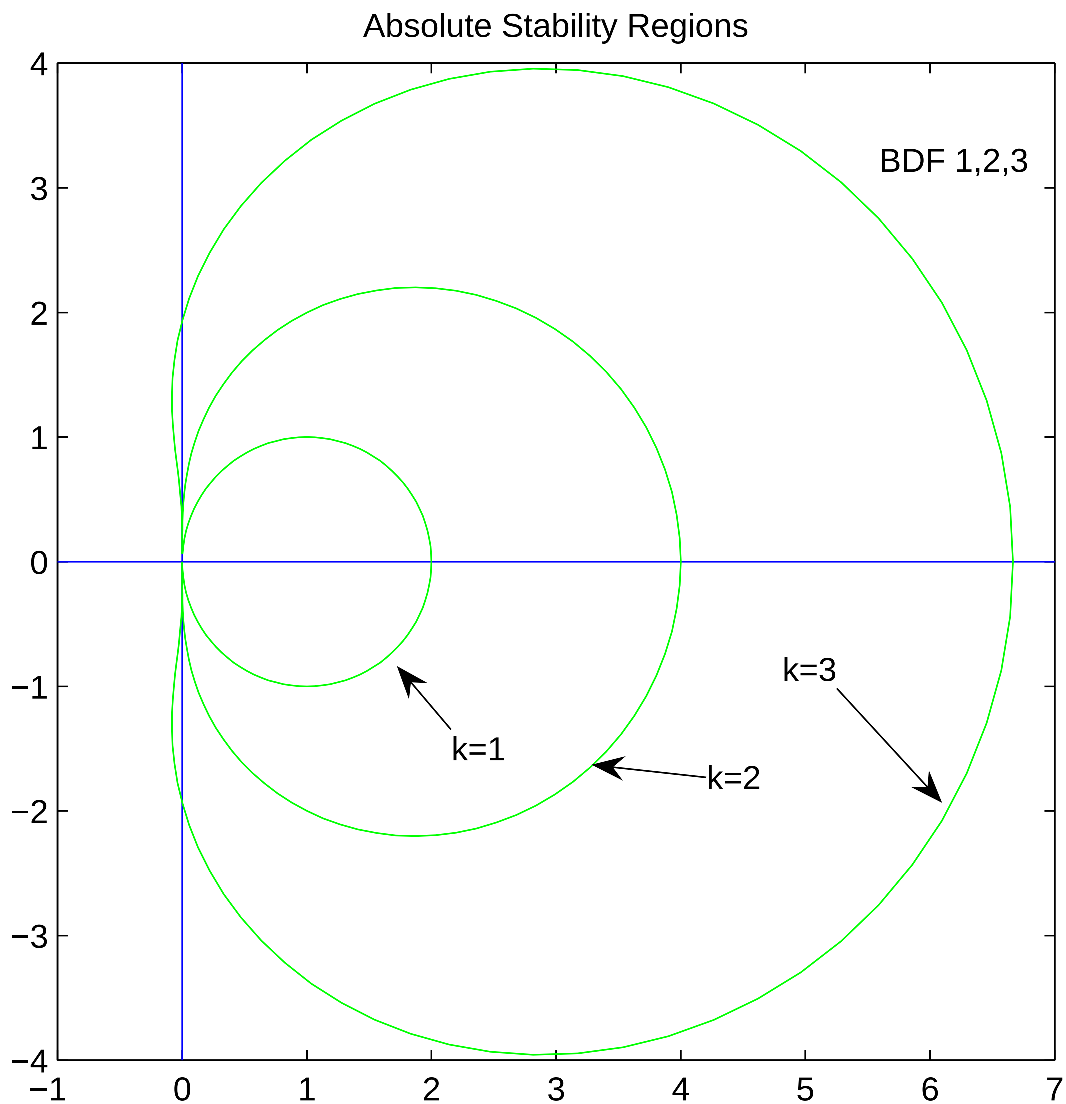
- test problem: $y' = \lambda y$
- applying method yields $\sum_{j=0}^{k} \alpha_j y_{n-j} = h\lambda \sum_{j=0}^{k} \beta_j y_{n-j}$
- characteristic polynomial for homogeneous difference equation

$$\rho(\xi) - h\lambda\sigma(\xi) = 0$$

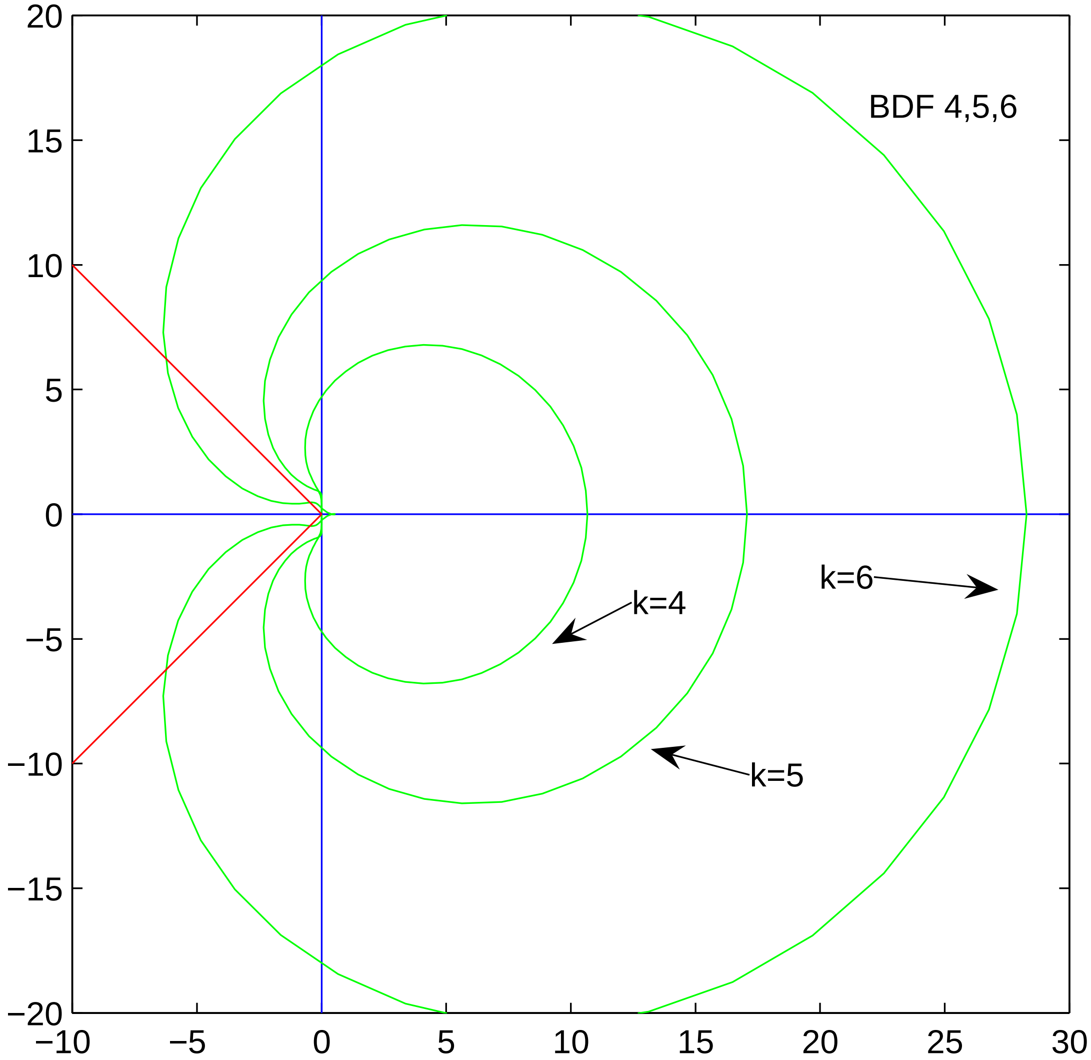
- $|y_n|$ does not grow for if roots satisfy $|\xi_i| \leq 1$
- roots are a function of $h\lambda$
- Boundary of absolute stability region for $h\lambda = z \in \mathbb{C}$

$$z = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}$$


Absolute Stability Regions
AB 1−4 in red
AM 1−6 in green
4
3
2
1
0
−1
−2
−3
−4
−6
−5
−4
−3
−2
−1
0
1
2
3
4



Absolute Stability Regions
BDF 1,2,3
k=1
k=2
k=3
4
3
2
1
0
−1
−2
−3
−4
−1
0
1
2
3
4
5
6
7


BDF 4,5,6
k=4
k=5
k=6
20
15
10
5
0
−5
−10
−15
−20
−10
−5
0
5
10
15
20
25
30

Predictor Corrector Pairs

- Implicit methods use explicit methods to predict value at t_n to start nonlinear solution process.
- Functional iteration for nonstiff problems

$$y_n^{(i)} = h\beta_0 f(t_n, y_n^{(i-1)}) + \text{other terms}$$

- Newton or other superlinear method needed for stiff problems
- error can be estimated from predictor/corrector difference
- fixed number of corrector iterations may be used – $P(EC)^m E$ methods – functional iteration corrector truncated
- variable stepsize, variable order, method selection are all available in good software

Error Estimation

Recall local error, ℓ_n, discretization (local truncation) error, d_n are related, i.e., $\ell_n \approx h_n d_n$. Given the normalization $\alpha_0 = 1$ for a linear multistep method and the resulting d_n we have

$$\text{predictor: } h\hat{d}_n = \hat{C}_{p+1} h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2})$$

$$\text{corrector: } hd_n = C_{p+1} h^p y^{(p+1)}(t_n) + O(H^{p+1})$$

$$y_n - y_n^0 = (C_{p+1} - \hat{C}_{p+1}) h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2})$$

$$\ell_n^{est} = hd_n^{est} = \frac{C_{p+1}}{(C_{p+1} - \hat{C}_{p+1})}(y_n - y_n^0)$$

Given tolerance, ϵ, basic idea is to control step and order so that

$$|\ell_n^{est}| < \epsilon$$

Comments

- AB cheaper than AM and BDF
- same order or same steps AM better error and stability than AB
- As steps increase AM and AB improve error and reduce stability region.
- BDFs are superstable and have stiff decay
- As steps increase BDF improve error and increase instability region.

Things Not Treated

- variable step methods,representations, and adjustments
  - representations: Nordsieck, modified divided differences
  - high order starting
  - asymptotics when only the last stepsize changes
  - heuristics
- Boundary value problems and methods
  - finite difference methods and nonlinear equations
  - shooting methods
- Differential Algebraic theory and methods.
  - index of a DAE
  - consistent initial conditions
  - symplectic and geometric integrators