Ordinary Differential Equations: Linear Multistep Methods

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Sources

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:

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

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

$$
\alpha_0 \neq 0
$$

$$
|\alpha_k| + |\beta_k| \neq 0
$$

$y_0, \ldots, y_{k-1}$ must be specified
Examples

- forward Euler

\[ y_0 = c \text{ given, } y_n = y_{n-1} + hf_{n-1} \]

- backward Euler

\[ y_0 = c \text{ given, } y_n = y_{n-1} + hf_n \]

- Trapezoidal rule

\[ y_0 = c \text{ given, } y_n = y_{n-1} + \frac{h}{2}(f_n + f_{n-1}) \]
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:

\[ P'(t) = f_{n-1} \]
\[ P(t) = tf_{n-1} + c \]
\[ y_{n-1} = t_{n-1}f_{n-1} + c \rightarrow c = y_{n-1} - t_{n-1}f_{n-1} \]
\[ y_n = P(t_n) \]
\[ = t_nf_{n-1} + y_{n-1} - t_{n-1}f_{n-1} \]
\[ = y_{n-1} + hf_{n-1} \]
Example

Trapezoidal rule:

\[ P'(t) = \frac{(t - t_{n-1})}{(t_n - t_{n-1})} f_n - \frac{(t - t_n)}{(t_n - t_{n-1})} f_{n-1} \]

\[ P(t) = \frac{1}{2h} \left[ (t - t_{n-1})^2 f_n - (t - t_n)^2 f_{n-1} \right] + c \]

\[ c = y_{n-1} + \frac{h}{2} f_{n-1} \]

\[ y_n = \frac{1}{2h} \left[ (t_n - t_{n-1})^2 f_n \right] + y_{n-1} + \frac{h}{2} f_{n-1} \]

\[ = y_{n-1} + \frac{h}{2} (f_n + f_{n-1}) \]
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:

$$P(t) = \frac{(t - t_{n-1})}{(t_n - t_{n-1})} y_n - \frac{(t - t_n)}{(t_n - t_{n-1})} y_{n-1}$$

$$P'(t) = \frac{1}{h} (y_n - y_{n-1})$$

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

$$y_n = y_{n-1} + h f_n$$
Linear multistep methods are recurrences and can be defined in terms of their characteristic polynomials.

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

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

Various properties can be analyzed and expressed in terms of these polynomials.
We have using Taylor series of $y(t)$

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

$$
d_n = N_h[y(t)]
$$

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

**DEFINITION:** 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 $d_n = C_{p+1} h^p y^{(p+1)}(t_n) + O(h^{p+1})$. 

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

\[
C_0 = \sum_{j=0}^{k} \alpha_j \quad C_1 = -\sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j
\]

\[
C_2 = \sum_{j=1}^{k} \frac{j^2}{2} \alpha_j + \sum_{j=1}^{k} j\beta_j \quad C_3 = -\sum_{j=1}^{k} \frac{j^3}{6} \alpha_j - \sum_{j=1}^{k} \frac{j^2}{2} \beta_j
\]

\[
C_4 = \sum_{j=1}^{k} \frac{j^4}{24} \alpha_j + \sum_{j=1}^{k} \frac{j^3}{6} \beta_j
\]
**Consistency**

**LEMMA:** We have

\[ C_0 = \rho(1) \quad \text{and} \quad C_1 = \rho'(1) - \sigma(1) \]

and therefore a method is consistent if and only if

\[ \rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1) \]
Examples

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

forward Euler:

\[
\alpha_0 = 1, \quad \alpha_1 = -1, \quad \beta_0 = 0, \quad \beta_1 = 1 \\
C_0 = 1 - 1 = 0, \quad C_1 = 1 - 0 - 1 = 0 \\
C_2 = -\frac{1}{2} + 1 = \frac{1}{2}
\]

AB(k=2):

\[
\alpha_0 = 1, \quad \alpha_1 = -1, \quad \alpha_2 = 0, \quad \beta_0 = 0, \quad \beta_1 = \frac{3}{2}, \quad \beta_2 = -\frac{1}{2} \\
C_0 = 1 - 1 = 0, \quad C_1 = 1 + 0 + 0 - \frac{3}{2} + \frac{1}{2} = 0 \\
C_2 = -\frac{1}{2} + 0 + \frac{3}{2} - 1 = 0, \quad C_3 = \frac{1}{6} + 0 - \frac{3}{4} + 2 = \frac{5}{12}
\]
Examples

Adams-Moulton: \( k \)-step, order \( k + 1 \), implicit family

AM(k=1) (trapezoidal):

\[
\alpha_0 = 1, \quad \alpha_1 = -1, \quad \beta_0 = \frac{1}{2}, \quad \beta_1 = \frac{1}{2}
\]

\[
C_0 = 1 - 1 = 0, \quad C_1 = 1 - \frac{1}{2} - \frac{1}{2} = 0
\]

\[
C_2 = -\frac{1}{2} + \frac{1}{2} = 0, \quad C_3 = -\frac{1}{6}(-1) - \frac{1}{2}(\frac{1}{2}) = -\frac{1}{12}
\]
Examples

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

AM(k=2):

\[ \alpha_0 = 1, \quad \alpha_1 = -1, \quad \alpha_2 = 0, \quad \beta_0 = 0, \quad \beta_1 = \frac{3}{2}, \quad \beta_2 = -\frac{1}{2} \]

\[ C_0 = 1 - 1 = 0, \quad C_1 = -1 + 2 + 0 - \frac{5}{12} - \frac{8}{12} + \frac{1}{12} = 0 \]

\[ C_2 = -\frac{1}{2} + \frac{8}{12} - \frac{2}{12} = 0, \quad C_3 = -\frac{1}{6}(-1 + 0) - \frac{1}{2}(\frac{8}{12} - \frac{4}{12}) = 0 \]

\[ C_4 = \frac{1}{24}(-1) + \frac{1}{6} \cdot \frac{8}{12} - \frac{8}{6} \cdot \frac{1}{12} = -\frac{1}{24} \]
Examples

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

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(2):

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

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

\[ C_2 = \frac{1}{2}(-\frac{4}{3} + \frac{4}{3}) = 0, \; C_3 = -\frac{1}{6}(-\frac{4}{3} + \frac{8}{3}) = -\frac{2}{9} \]
The first order differential equation has been replaced with a $k$—th order difference equation.

- starting values must be given and be $O(h^p)$ 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:** 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, $\xi_i$, of $\rho(\xi)$ satisfy $|\xi_i| \leq 1$ and roots with unit magnitude are simple.

**THEOREM:** If a linear multistep method is consistent, satisfies the root condition, and has initial values that are $O(h^p)$ 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:** A linear multistep method is strongly stable if all of the roots, \( \xi_i \), of \( \rho(\xi) \) satisfy \( |\xi_i| < 1 \) except the principal root \( \xi = 1 \).

**DEFINITION:** A linear multistep methods is weakly stable if it is 0-stable but not strongly stable.

**EXAMPLE:** Consider Milne’s method

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

The characteristic polynomial \( \rho(\xi) = \xi^2 - 1 \) and \( \xi_i = \pm 1 \). When applied to \( y' = \lambda y \) the recurrence is dominated by 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.)
Stability

- All one-step methods are 0-stable.
- Adams methods have $\rho(\xi) = \xi^k - \xi^{k-1}$ and are strongly stable.
- 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
Absolute Stability Regions

BDF 1,2,3

k=1

k=2

k=3
Stiffness and Stability

• BDF 1 and 2 A-stable, strongly stable, stiff decay
• BDF’s trade absolute stability for stiff decay
• $A(\alpha)$ – stability is stability in a wedge around real axis – still too restrictive
• stiff stability is accurate around origin and absolutely stable for large negative $Re(\lambda)$.
**Predictor Corrector Pairs**

- Implicit methods use explicit methods to predict value at $t_n$ to start nonlinear solution process.
- Functional iteration OK for nonstiff problems
- 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
- Variable stepsize, variable order, method selection are all available in good software
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