Chapter 6
Initial Value Problems for ODEs: Multistep Methods

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Numerical Methods for ODEs

- IVP for ODE:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}),\ a \leqslant x \leqslant b;\ \mathbf{y}(a) = \mathbf{y}_0.$$

- Approximation $\{\mathbf{u}_n \approx \mathbf{y}(x_n)\}$ at discrete points $\{x_n\}$: grid function $\{\mathbf{u}_n\}$ on a grid

$$a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b$$

- One-step method: Chap 5.
- Multistep method: in a k-step method, $\mathbf{u}_{n+k}$ is determined with information from previous k points, $\mathbf{u}_{n+k-1}, \mathbf{u}_{n+k-2}, \ldots, \mathbf{u}_n$. k is called the step number (index) of the method.

Linear Multistep Methods

- Assume uniform grid legnth h.
- General k-step method: for $n = 0, 1, 2, \ldots, N-k$,

$$\begin{aligned}&\mathbf{u}_{n+k} + \alpha_{k-1}\mathbf{u}_{n+k-1} + \cdots + \alpha_0\mathbf{u}_n \\ &= h[\beta_k\mathbf{f}_{n+k} + \beta_{k-1}\mathbf{f}_{n+k-1} + \cdots + \beta_0\mathbf{f}_n],\end{aligned}$$

  with $\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_{k-1}$ provided.
  If $\beta_k = 0$: explicit methods. If $\beta_k \neq 0$: implicit methods.
- Truncation error: $(\mathbf{T}_h)_n = (R_n\mathbf{y})_n,\ n = 0, 1, \ldots, N.$

$$\begin{aligned}(R_h\mathbf{y})_n &\equiv \frac{1}{h}\sum_{s=0}^{k}\alpha_s\mathbf{y}_{n+s} - \sum_{s=0}^{k}\beta_s\mathbf{f}(x_{n+s}, \mathbf{y}_{n+s}) \\ &= \frac{1}{h}\sum_{s=0}^{k}\alpha_s\mathbf{y}_{n+s} - \sum_{s=0}^{k}\beta_s\mathbf{y}'(x_{n+s})\end{aligned}$$

Truncation Error; Consistency; Order of Method

- Using Taylor expansion of $\mathbf{y}(x_{n+s})$ and $\mathbf{y}'(x_{n+s})$ at x_n:

$$(\mathbf{T}_h)_n = \frac{1}{h}[C_0\mathbf{y}(x_n) + C_1 h\mathbf{y}'(x_n) + C_2 h^2\mathbf{y}''(x_n) + \cdots]$$

with

$$C_0 = \sum_{s=0}^{k} \alpha_s$$

$$C_1 = \sum_{s=1}^{k} s\alpha_s - \sum_{s=0}^{k} \beta_s$$

$$C_2 = \sum_{s=1}^{k} \frac{s^2}{2!}\alpha_s - \sum_{s=1}^{k} s\beta_s$$

$$C_q = \sum_{s=1}^{k} \frac{s^q}{q!}\alpha_s - \sum_{s=1}^{k} \frac{s^{q-1}}{(q-1)!}\beta_s, \quad q \geqslant 2$$

Truncation Error; Consistency; Order of Method

- The method is of order p if and only if:

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

Then,

$$(\mathbf{T}_h)_n = C_{p+1} h^p \mathbf{y}^{(p+1)}(x_n) + O(h^{p+1}).$$

Truncation Error; Consistency; Order of Method

- Linear functional $L : C^1[\mathbf{R}] \to \mathbf{R}$:

$$Lu = \sum_{s=0}^{k} [\alpha_s u(s) - \beta_s u'(s)], \ u \in C^1[\mathbf{R}].$$

- The method has algebraic (or polynomial) degree p if $Lu = 0, \ \forall u \in \mathbf{P}_p$, equivalently,

$$Lt^r = 0, \ r = 0, 1, \ldots, p.$$

- Using Peano Kernel representation of linear functional L to represent the truncation error.

Peano Kernel of Linear Functionals

- Denote local solution $\mathbf{v}(t) \equiv \mathbf{y}(x_n + th),\ 0 \leqslant t \leqslant k$, then

$$L\mathbf{v} = \sum_{s=0}^{k} [\alpha_s \mathbf{v}(s) - \beta_s \mathbf{v}'(s)] = h(\mathbf{T}_h)_n.$$

- For the linear functional L, Define p-th Peano kernel

$$\lambda_p(\sigma) = L_{(t)}(t-\sigma)_+^p = \sum_{s=0}^{k} [\alpha_s (s-\sigma)_+^p - \beta_s p (s-\sigma)_+^{p-1}],\ p \geqslant 1,$$

- Peano representation of the functional L,

$$L\mathbf{v} = \frac{1}{p!} \int_0^k \lambda_p(\sigma) \mathbf{v}^{(p+1)}(\sigma) d\sigma.$$

- L is definite of order p if λ_p is of the same sign for $\sigma \in [0,\ k]$.

Peano Kernel of Linear Functionals

- L is definite of order p, then

$$L\mathbf{v} = l_{p+1}\mathbf{v}^{(p+1)}(\bar{\sigma}),\ 0 < \bar{\sigma} < k;\ l_{p+1} = L\frac{t^{p+1}}{(p+1)!}$$

Theorem

A multistep method of polynomial degree p has order p whenever the exact solution $\mathbf{y}(x)$ is in the smoothness class $C^{p+1}[a,b]$. If the associated functional L is definite, then

$$(\mathbf{T}_h)_n = l_{p+1}\mathbf{y}^{(p+1)}(\bar{x}_n)h^p,\ x_n < \bar{x}_n < x_{n+k}.$$

Moreover, for the principal error function $\boldsymbol{\tau}$ of the method, whenever definite or not, we have if $\mathbf{y} \in C^{p+2}[a,b]$,

$$\boldsymbol{\tau}(x) = l_{p+1}\mathbf{y}^{(p+1)}(x).$$

Adams-type Multistep Method

- We konw

$$\mathbf{y}(x_{n+k}) = \mathbf{y}(x_{n+k-1}) + \int_{x_{n+k-1}}^{x_{n+k}} \mathbf{y}'(x)dx.$$

- Use polynomial interpolation of $\mathbf{y}'$ with the following nodes
  - $x_n, x_{n+1}, \ldots, x_{n+k-1}$: Adams-Bashford Method; Explicit
  - $x_{n+1}, x_{n+2}, \ldots, x_{n+k}$: Adams-Moutton Method; Implicit

Adams-Bashford Method; kth-order

- Using polynomial interpolation of degree $\leqslant k-1$:

$$\mathbf{y}' = \mathbf{p}_{k-1}(\mathbf{y}'; x_n, \ldots, x_{n+k-1}) + \mathbf{r}_n$$

- Then

$$\mathbf{y}(x_{n+k}) = \mathbf{y}(x_{n+k-1}) + h \sum_{s=0}^{k-1} \beta_{k,s} \mathbf{y}'(x_{n+s}) + h\mathbf{r}_n,$$

with

$$\beta_{k,s} = \int_0^1 \prod_{r=0, r\neq s}^{k-1} \frac{t+k-1-r}{s-r} dt, \;\; s = 0, 1, \ldots, k-1.$$

$$\mathbf{r}_n = \gamma_k h^k \mathbf{y}^{(k+1)}(\bar{x}_n), x_n < \bar{x}_n < x_{n+k-1}; \gamma_k = \int_0^1 \begin{pmatrix} t+k-1 \\ k \end{pmatrix} dt$$

Adams-Bashford Method; kth-order

- Truncation error and principal error function:

$$(\mathbf{T}_h)_n = \mathbf{r}_n = \gamma_k \mathbf{y}^{(k+1)}(\bar{x}_n)h^k + O(h^{k+1})$$

$$\boldsymbol{\tau}(x) = \gamma_k \mathbf{y}^{(k+1)}(x)$$

- The k-step method:

$$\mathbf{u}_{n+k} = \mathbf{u}_{n+k-1} + h\sum_{s=0}^{k-1} \beta_{k,s}\mathbf{f}(x_{n+s}, \mathbf{u}_{n+s}),$$

Remark

Formulas can also be derived if using Newton's form of the interpolation polynomial.

Adams-Moulton Method; kth-order

- Using polynomial interpolation of degree $\leqslant k-1$:

$$\mathbf{y}' = \mathbf{p}_{k-1}(\mathbf{y}'; x_{n+1}, \ldots, x_{n+k}) + \mathbf{r}_n^*$$

- Then

$$\mathbf{y}(x_{n+k}) = \mathbf{y}(x_{n+k-1}) + h\sum_{s=1}^{k} \beta_{k,s}^* \mathbf{y}'(x_{n+s}) + h\mathbf{r}_n^*,$$

with

$$\beta_{k,s}^* = \int_0^1 \prod_{r=1, r\neq s}^{k} \frac{t+k-1-r}{s-r} dt, \;\; s = 1, \ldots, k.$$

$$\mathbf{r}_n^* = \gamma_k^* h^k \mathbf{y}^{(k+1)}(\bar{x}_n^*), x_n < \bar{x}_n^* < x_{n+k-1}; \gamma_k^* = \int_{-1}^{0} \begin{pmatrix} t+k-1 \\ k \end{pmatrix} dt$$

Adams-Moulton Method; kth-order

- Truncation error and principal error function:

$$(\mathbf{T}_h^*)_n = \mathbf{r}_n^* = \gamma_k^* \mathbf{y}^{(k+1)}(\bar{x}_n^*) h^k + O(h^{k+1})$$

$$\boldsymbol{\tau}^*(x) = \gamma_k^* \mathbf{y}^{(k+1)}(x)$$

- The $k-1$-step method:

$$\mathbf{u}_{n+k} = \mathbf{u}_{n+k-1} + h \sum_{s=1}^{k} \beta_{k,s}^* \mathbf{f}(x_{n+s}, \mathbf{u}_{n+s}),$$

Remark

Formulas can also be derived if using Newton's form of the interpolation polynomial.

Examples of Adams-type Method

- First-order Adams Method
  - Adams-Bashford: Forward Euler's method
  - Admas-Moulton: Backward Euler's method.
- Fourth-order Adams Method
  - Adams-Bashford:

$$\mathbf{y}_{n+4} \approx \mathbf{y}_{n+3} + \frac{h}{24}[55\mathbf{f}_{n+3} - 59\mathbf{f}_{n+2} + 37\mathbf{f}_{n+1} - 9\mathbf{f}_n].$$

  - Admas-Moulton:

$$\mathbf{y}_{n+4} \approx \mathbf{y}_{n+3} + \frac{h}{24}[9\mathbf{f}_{n+4} + 19\mathbf{f}_{n+3} - 5\mathbf{f}_{n+2} + \mathbf{f}_{n+1}]$$

Predictor-Corrector Method

- Pairs of an explicit and implicit multstep method, of the same order.
- Explicit formula to predict next approximation (Predictor); Implicit formula to correct it (Corrector).
- Explicit k-step method of order k: with coefficients α_s, β_s.
- Implicit $k-1$-step method of order k: with coefficients α_s^*, β_s^*.
- PECE method ("P" for predict, "E" for evaluate, "C" for correct)

$$\mathring{\mathbf{u}}_{n+k} = -\sum_{s=0}^{k-1} \alpha_s \mathbf{u}_{n+s} + h \sum_{s=0}^{k-1} \beta_s \mathbf{f}_{n+s}$$

$$\mathbf{u}_{n+k} = -\sum_{s=1}^{k-1} \alpha_s^* \mathbf{u}_{n+s} + h\{\beta_k^* \mathbf{f}(x_{n+k}, \mathring{\mathbf{u}}_{n+k}) + \sum_{s=1}^{k-1} \beta_s^* \mathbf{f}_{n+s}\}$$

Predictor-Corrector Method

- Truncation error:

$$(\mathbf{T}_h^{PECE})_n = \frac{1}{h}\sum_{s=1}^{k}\alpha_s^*\mathbf{y}(x_{n+s}) - \{\beta_k^*\mathbf{f}(x_{n+k},\mathring{\mathbf{y}}_{n+k}) + \sum_{s=1}^{k-1}\beta_s^*\mathbf{y}'(x_{n+s})\}$$

$$\mathring{\mathbf{y}}_{n+k} = -\sum_{s=0}^{k-1}\alpha_s\mathbf{y}(x_{n+s}) + h\sum_{s=0}^{k-1}\beta_s\mathbf{y}'(x_{n+s}).$$

- We have

$$\begin{aligned}(\mathbf{T}_h^{PECE})_n &= \frac{1}{h}\sum_{s=1}^{k}\alpha_s^*\mathbf{y}(x_{n+s}) - \sum_{s=1}^{k}\beta_s^*\mathbf{y}'(x_{n+s}) \\ &\quad + \beta_k^*[\mathbf{y}'(x_{n+k}) - \mathbf{f}(x_{n+k},\mathring{\mathbf{y}}_{n+k})] \\ &= l_{k+1}^*h^k\mathbf{y}^{(k+1)}(\bar{x}_n^*) + \beta_k^*[\mathbf{f}(x_{n+k},\mathbf{y}(x_{n+k})) - \mathbf{f}(x_{n+k},\mathring{\mathbf{y}}_{n+k})]\end{aligned}$$

Predictor-Corrector Method

- Using Lipschitz continuity of $\mathbf{f}$.
- And using truncation error for the predictor

$$\mathbf{y}(x_{n+k}) - \mathring{\mathbf{y}}_{n+k} = l_{k+1} h^{k+1} \mathbf{y}^{(k+1)}(\bar{x}_n) = h \times \text{ the truncation error}$$

- Then we have

$$\|(\mathbf{T}_h^{PECE})\|_\infty \leqslant (l_{k+1}^* + hL|l_{k+1}\beta_k^*|)\|\mathbf{y}^{(k+1)}\|_\infty h^k \leqslant Ch^k$$

- Example: k-th order Adams-Bashford as Predictor; k-th order Adams-Moulton as Corrector.

Homogeneous Equation

- Homogeneous difference equation (LHS of the k-step method):

$$v_{n+k} + \alpha_{k-1} v_{n+k-1} + \cdots + \alpha_0 v_n = 0, \ n = 0, 1, \ldots.$$

- Characteristic Polynomial

$$\alpha(t) = \sum_{s=0}^{k} \alpha_s t^s, \quad (\alpha_k = 1).$$

- Characteristic Equation: $\alpha(t) = 0$.
- Distinct roots: $\{t_s\}$ of multiplicity m_s, for $s = 1, \ldots, k'$.
- v_n, for $n = 0, 1, \ldots$, given by

$$v_n = \sum_{s=1}^{k'} \left(\sum_{r=0}^{m_s - 1} c_{rs} n^r \right) t_s^n$$

Root Condition

- Homogeneous difference equation (LHS of the k-step method):

$$v_{n+k} + \alpha_{k-1} v_{n+k-1} + \cdots + \alpha_0 v_n = 0, \;\; n = 0, 1, \ldots.$$

Theorem

We have $|v_n| \leqslant M$, all $n \geqslant 0$, for every solution $\{v_n\}$ of the homogeneous equation, with M depending on the starting values $v_0, v_1, \ldots, v_{k-1}$ (but not n) if and only if

$$\text{(root condition)} \qquad \alpha(t_s) = 0 \text{ implies } \begin{cases} \text{either } |t_s| < 1 \\ \text{or } |t_s| = 1, \;\; m_s = 1. \end{cases}$$

Inhomogeneous Difference Equation

- Inhomogeneous Difference Equation (k-step method)

$$v_{n+k} + \alpha_{k-1} v_{n+k-1} + \cdots + \alpha_0 v_n = \phi_{n+k}, \ n = 0, 1, \ldots .$$

Theorem

There exists a constant $M > 0$, independent of n, such that

$$|v_n| \leqslant M\{\max_{0 \leqslant s \leqslant k-1} |v_s| + \sum_{m=k}^{n} |\phi_m|\}, \ n = 0, 1, \ldots .$$

for every solution $\{v_n\}$ of the above equation, and for every $\{\phi_{n+k}\}$, if and only if the characteristic polynomial $\alpha(t)$ satisfies the root condition.

Stability

Definition

The k-step method is called stable on $[a,b]$ if there exits a constant $K>0$ not depending on h such that for an arbitrary (uniform) grid h on $[a,b]$, and for arbitrary two grid function $\mathbf{v},\mathbf{w}\in\Gamma_h[a,b]$, there holds

$$\|\mathbf{v}-\mathbf{w}\|_\infty \leqslant K\left(\max_{0\leqslant s\leqslant k-1}\|\mathbf{v}_s-\mathbf{w}_s\| + \|R_h\mathbf{v}-R_h\mathbf{w}\|_\infty\right),$$

for all h sufficiently small.

- Denote $\mathcal{F}=\{\mathbf{f} : \mathbf{f}$ is Lipschitz continuous on $[a,b]$ with $L=L_f\}$

Theorem

The multistep method is stable for every $\mathbf{f}\in\mathcal{F}$ if and only if its characteristic polynomial satisfies the root condition.

Convergence

Definition

Consider a uniform grid on $[a, b]$ with grid length h. Let $\mathbf{u} = \{\mathbf{u}_n\}$ be the grid function obtained by the multistep method on $[a, b]$, with starting approximation $\mathbf{u}_s$ for $s = 0, \ldots, k-1$. Let $\mathbf{y} = \{\mathbf{y}_n\}$ be the grid function induced by the exact solution. The multistep method is said to converge on $[a, b]$ if there holds

$$\|\mathbf{u} - \mathbf{y}\|_\infty \to 0 \text{ as } h \to 0$$

whenever $\mathbf{u}_s \to \mathbf{y}_0$ as $h \to 0, \; s = 0, 1, \ldots, k-1$

Theorem

The multistep method converges for all $\mathbf{f} \in \mathcal{F}$ if and only if it is consistent and stable. If it has order p and $\mathbf{u}_s - \mathbf{y}_s = O(h^p)$, $s = 0, 1, \ldots, k-1$, then

$$\|\mathbf{u} - \mathbf{y}\|_\infty = O(h^p) \textit{ as } h \to 0$$

Asymptotic of Global Error

Theorem

Assume that

(1) $\mathbf{f}(x, \mathbf{y}) \in C^2$ *on* $[a, b] \times \mathbf{R}^d$

(2) the multistep method is table and has order p

(3) the exact solution $\mathbf{y}$ *is of class* $C^{p+2}[a, b]$

(4) the starting approximation satisfy $\mathbf{u}_s - \mathbf{y}_s = O(h^{p+1})$, *as* $h \to 0$

(5) $\mathbf{e}(x)$ *is the solution of the linear initial value problem*

$\frac{d\mathbf{e}}{dx} = \mathbf{f}_y(x, \mathbf{y}(x))\mathbf{e} - \mathbf{y}^{(p+1)}(x), \; \mathbf{e}(a) = 0$

Then for $n = 0, \ldots, N$,

$$\mathbf{u}_n - \mathbf{y}_n = C_{k,p} h^p \mathbf{e}(x_n) + O(h^{p+1}), \; \text{as } h \to 0$$

where $C_{k,p}$ *is the error constant,*

$$C_{k,p} = \frac{l_{p+1}}{\sum_{s=0}^{k} \beta_s}, \; l_{p+1} = L\frac{t^{p+1}}{(p+1)!}$$

Order and Stability

Problems:

- Construct a multistep method of maximum algebraic degree, with $\alpha(t)$ satisfying the root condition
- Determine the maximum algebraic degree among all k-step methods whose $\alpha(t)$ satisfy the root condition.

Analytic Characterization of Order

- Characteristic polynomials for k-step method:

$$\alpha(t) = \sum_{s=0}^{k} \alpha_s t^s. \ \beta(t) = \sum_{s=0}^{k} \beta_s t^s$$

- Define define

$$\delta(\xi) = \frac{\alpha(\xi)}{\ln \xi} - \beta(\xi), \ \xi \in \mathbf{C}$$

Theorem

The multistep method has (exact) polynomial of degree p if and only if $\delta(\xi)$ has a zero of (exact) multiplicity p at $\xi = 1$.

Example !

Stable Methods fo Maximum Order

Theorem

- *If k is odd, the every stable k-step method has order $p \leqslant k+1$*
- *if k is even, then every stable k-step method has order $p \leqslant k+2$, the order being $k+2$ if and only if $\alpha(t)$ has all its zeros on the circumference of the unit circle.*

Stiff Problems: A-Stability

- Model problem:

$$\frac{dy}{dx} = \lambda y, \quad 0 \leqslant x < \infty, \quad Re\lambda < 0$$

- Exact solution: $y(x) \to 0$ as $x \to \infty$.
- Expect numerical solution $u_n \to 0$ as $n \to \infty$.

Definition

A multistep method is called A-stable if, when applied to the model problem, it produces a grid function $\{u_n\}_{n=0}^{\infty}$ satisfying

$$u_n \to 0 \text{ as } n \to \infty$$

regardless of the choice of starting values. (assuming uniform grid)

Stiff Problems: A-Stability

- The multistep method for the model problem gives:

$$\sum_{s=0}^{k} \alpha_s u_{n+s} = h\lambda \sum_{s=0}^{k} \beta_s u_{n+s}$$

with characteristic polynomial:

$$\alpha(t) = \sum_{s=0}^{k} \alpha_s t^s, \ \beta(t) = \sum_{s=0}^{k} \beta_s t^s$$

Stiff Problems: A-Stability

- Re-writting the method as

$$\sum_{s=0}^{k} \alpha_s u_{n+s} - h\lambda \sum_{s=0}^{k} \beta_s u_{n+s} = 0$$

$$\sum_{s=0}^{k} (\alpha_s - h\lambda\beta_s) u_{n+s} = 0$$

- new characteristic polynomial

$$\tilde{\alpha}(t) = \sum_{s=0}^{k} (\alpha_s - h\lambda\beta_s) t^s = \alpha(t) - \tilde{h}\beta(t), \;\; \tilde{h} = h\lambda \in \mathbf{C}.$$

- Solution $u_n \to 0$ as $n \to \infty$ if absolute values of zeros of $\tilde{\alpha}$ strictly less than 1

Stiff Problems: A-Stability

- The multistep method is A-stable if and only if

$$\{\tilde{\alpha}(\xi) = 0,\ Re\lambda < 0\} \text{ implies } |\xi| < 1.$$

Equivalently,

$$\{\tilde{\alpha}(\xi) = 0,\ |\xi| \geqslant 1\} \text{ implies } Re\lambda \geqslant 0.$$

- $\tilde{\alpha}(\xi) = 0$ implies

$$\tilde{h} = h\lambda = \frac{\alpha(\xi)}{\beta(\xi)}$$

- Then A-stability is characterized by the condition

$$Re\frac{\alpha(\xi)}{\beta(\xi)} \geqslant 0 \text{ if } |\xi| \geqslant 1.$$

Stiff Problems: A-Stability

Theorem

If the multistep method is A-stable, then it has order $p = 2$ *and error constant* $C_{k,p} \leqslant -\frac{1}{12}$. *The trapezoidal rule is the only A-stable method for which* $p = 2$ *and* $C_{k,p} = -\frac{1}{12}$.

- A-stable multistep method is second order accurate !
- Note the difference compared to implicit Runge-Kutta method.

A(α)-Stability

- Region of A-stability

$$\mathcal{D}_A = \{\tilde{h} \in \mathbf{C} : \tilde{\alpha}(\xi) = 0 \text{ implies } |\xi| < 1\}$$

Note: A-stability requires the left half plane $Re\tilde{h} < 0$ to be contained in $\mathcal{D}_A$. Many applications only require part of the left plane to be contained in $\mathcal{D}_A$.

- Wedge-like region

$$W_\alpha = \{\tilde{h} \in \mathbf{C} : |arg(-\tilde{h})| < \alpha,\ \tilde{h} \neq 0\},\ 0 < \alpha < \frac{\pi}{2}.$$

Definition

The multistep method is said to be A(α)-stable, $0 < \alpha < \frac{\pi}{2}$, if $W_a \subset \mathcal{D}_A$.

- Multistep method with order $p > 2$ and are A(α)-stable for suitable α.