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.
- Example: start with the ODE, integration from x_n to x_{n+k},

$$\mathbf{y}(x_{n+k}) - \mathbf{y}(x_n) = \int_{x_n}^{x_{n+k}} \mathbf{f}(x, \mathbf{y}) dx.$$

  With appropriate numerical quadrature rules for the integral $\Rightarrow$ linear multstep methods.

- Examples: $\mathbf{y}_{n+1} \approx \mathbf{y}_n + \frac{h}{2}(f_{n+1} + f_n)$.

$$\mathbf{y}_{n+1} \approx \mathbf{y}_{n-1} + \frac{h}{3}(\mathbf{f}_{n-1} + 4\mathbf{f}_n + \mathbf{f}_{n+1}).$$

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

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

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.
- For implicit methods: $\mathbf{u}_{n+k}$ obtained as solution of nonlinear equation

$$\begin{aligned}
\mathbf{u}_{n+k} &= \beta_k\mathbf{f}(x_{n+k}, \mathbf{u}_{n+k}) + \mathbf{g}_n, \\
\mathbf{g}_n &= h\sum_{s=0}^{k-1}\beta_s\mathbf{f}_{n+s} - \sum_{s=0}^{k-1}\alpha_s\mathbf{u}_{n+s}.
\end{aligned}$$

Linear Multistep Methods

- Successive iteration (fixed-point iteration) for the nonlinear equation:

$$\mathbf{u}_{n+k}^{[v]} = h\beta_k \mathbf{f}(x_{n+k}, \mathbf{u}_{n+k}^{[v-1]}) + \mathbf{g}_n, \ v = 1, 2, \ldots$$

$\mathbf{u}_{n+k}^{[v]} \to \mathbf{u}_{n+k}$, as $v \to \infty$.

Theorem

Assume $\mathbf{f}$ *is Lipschitz continuous for variable* $\mathbf{y}$ *with Lipschitz constant* L, *and* $\lambda \equiv h|\beta_k|L < 1$, *then the above nonlinear equation has a unique solution* $\mathbf{u}_{n+k} = \lim_{v\to\infty} \mathbf{u}_{n+k}^{[v]}$, *and*

$$\|\mathbf{u}_{n+k}^{[v]} - \mathbf{u}_{n+k}\| \leqslant \frac{\lambda^v}{1-\lambda} \|\mathbf{u}_{n+k}^{[1]} - \mathbf{u}_{n+k}^{[0]}\|, \ v = 1, 2, \ldots$$

Truncation Error; Consistency

- Residual Operator:

$$(R\mathbf{y})(x) \equiv \mathbf{y}'(x) - \mathbf{f}(x, \mathbf{y}), \;\; \mathbf{y} \in C^1[a, b]$$

$$(R_h\mathbf{u})_n \equiv \frac{1}{h}\sum_{s=0}^{k} \alpha_s \mathbf{u}_{n+s} - \sum_{s=0}^{k} \beta_s \mathbf{f}(x_{n+s}, \mathbf{u}_{n+s}), \;\; \mathbf{u} = \{\mathbf{u}_n\} \in \Gamma_h[a, b],$$

- Truncation error: $(\mathbf{T}_h)_n = (R_n\mathbf{y})_n, \;\; n = 0, 1, \ldots, N.$
- Consistency: $\|\mathbf{T}_h\|_\infty \to \mathbf{0}$, as $h \to 0$.
- Order p: $\|\mathbf{T}_h\|_\infty = O(h^p)$, as $h \to 0$.
- Principal error function $\boldsymbol{\tau}$: $(\mathbf{T}_h)_n = \boldsymbol{\tau}(x_n)h^p + O(h^{p+1})$, as $h \to 0$.

Truncation Error

- Truncation error:

$$(\mathbf{T}_h)_n = \frac{1}{h}\sum_{s=0}^{k} \alpha_s \mathbf{y}_{n+s} - \sum_{s=0}^{k} \beta_s \mathbf{y}'_{n+s}, \;\; n = 0, 1, \dots, N$$

- With Taylor series expansion:

$$\mathbf{y}(x_{n+s}) = \mathbf{y}(x_n) + sh\mathbf{y}'(x_n) + \frac{1}{2}(sh)^2\mathbf{y}''(x_n) + \cdots$$

$$\mathbf{y}'(x_{n+s}) = \mathbf{y}(x_n) + sh\mathbf{y}''(x_n) + \frac{1}{2}(sh)^2\mathbf{y}'''(x_n) + \cdots$$

- Then we have

$$(\mathbf{T}_h)_n = \frac{1}{h}(\sum_{s=0}^{k} \alpha_s)\mathbf{y}(x_n) + (\sum_{s=0}^{k}(s\alpha_s - \beta_s))\mathbf{y}'(x_n) + O(h)$$

Truncation Error;Consistency;Characteristic Polynomials

- Consistency $(\mathbf{T}_h)_n \to 0$ as $h \to 0$ implies consistency conditions

$$\sum_{s=0}^{k} \alpha_s = 0, \quad \sum_{s=0}^{k} s\alpha_s = \sum_{s=0}^{k} \beta_s.$$

- Introduce characteristic polynomials

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

- Consistency conditions $\Rightarrow$

$$\alpha(1) = 0, \quad \alpha'(1) = \beta(1).$$

- MORE Results using characteristic polynomials (later).

Local Description; Ω-degree

- From local truncation error:

$$\sum_{s=0}^{k} \alpha_s \mathbf{y}(x_{n+s}) - h \sum_{s=0}^{k} \beta_s \mathbf{y}'(x_{n+s}) = h(\mathbf{T}_h)_n.$$

- Define linear operator $L_h : C^1[\mathbf{R}] \to C^1[\mathbf{R}]$,

$$(L_h z)(x) = \sum_{s=0}^{k} \alpha_s z(x+sh) - h \sum_{s=0}^{k} \beta_s z'(x+sh), \; z \in C^1[\mathbf{R}].$$

- Given a set of linearly independent "gauge functions" $\{\omega_r(x)\}_{r=0}^{\infty}$, and define $\Omega_p = \text{Span}\{\omega_0, \omega_1, \ldots, \omega_p\}$
- Ω-degree p of the method:

$$L_h \omega = 0, \; \forall \omega \in \Omega_p, \forall h > 0.$$

Local Description

- Ω_p closed under translation if $\omega(x) \in \Omega_p$ implies $\omega(x+c) \in \Omega_p$
- Ω_p closed under scaling if $\omega(x) \in \Omega_p$ implies $\omega(cx) \in \Omega_p$

Theorem

- *If Ω_p closed under translation, then the method has Ω-degree p iff*

$$(L_h\omega)(0) = 0, \;\; \forall \omega \in \Omega_p, \forall h > 0.$$

- *if Ω_p closed under translation and scaling, then the method has Ω-degree p iff*

$$(L_1\omega)(0) = 0, \;\; \forall \omega \in \Omega_p.$$

Local Description

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

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

- For $\Omega_m = \mathbf{P}_m$, Ω-degree referred as algebraic (or polynomial) degree.
- The method has algebraic degree p if $Lu = 0, \; \forall u \in \mathbf{P}_p$, equivalently,

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

- Examples: Explicit two-step methods: what α's, β's? what polynomial degree p? $\mathbf{u}_{n+2} + \alpha_1 \mathbf{u}_{n+1} + \alpha_0 \mathbf{u}_n = h(\beta_1 \mathbf{f}_{n+1} + \beta_0 \mathbf{f}_n)$.

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 function 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.

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 $\mathbf{y} \in C^{p+2}[a,b]$,

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