Chapter 5
Initial Value Problems for ODEs: One-Step Methods

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One-Step Methods

- Initial Value Problem (IVP) for First-oder ODEs:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}), \ a \leqslant x \leqslant b; \quad \mathbf{y}(a) = \mathbf{y}_0. \tag{1}$$

- One-step methods:
  - grid: $a = x_0 < x_1 < \cdots < x_N = b$,
  - grid size $h_n = x_{n+1} - x_n, \ n = 0, 1, \ldots, N-1$.
  - grid function $\{\mathbf{u}_n\}, \ n = 0, 1, \ldots, N$
  - one-step updating formula: for $n = 0, 1, \ldots, N-1$,

$$\begin{aligned} x_{n+1} &= x_n + h_n \\ \mathbf{u}_{n+1} &= \mathbf{u}_n + h_n \mathbf{\Phi}(x_n, \mathbf{u}_n; h_n) \end{aligned}$$

- Stability, Convergence and Error Estimate.

One-Step Methods

- Note that
$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(x, \mathbf{y})$$
$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{h_n} = \mathbf{\Phi}(x_n, \mathbf{u}_n; h_n)$$
- Residual operators R and R_h on $C^1[a,b]$ and $\Gamma_h[a,b]$ respectively,
$$(R\mathbf{y})(x) = \mathbf{y}'(x) - \mathbf{f}(x, \mathbf{y}), \quad \forall \mathbf{y} \in C^1[a,b];$$
$$(R_h\mathbf{u})_n = \frac{1}{h_n}(\mathbf{u}_{n+1} - \mathbf{u}_n) - \mathbf{\Phi}(x_n, \mathbf{u}_n; h_n), \ n = 0, 1, \ldots, N-1;$$
$$\forall \mathbf{u} = \{\mathbf{u}_n\} \in \Gamma_h[a,b].$$

Stability

Definition

The method is called stable on $[a, b]$ if there exists a constant $K > 0$ not dependent on h such that for an arbitrary grid h on $[a, b]$, and for arbitrary two grid functions $\mathbf{v}, \mathbf{w} \in \Gamma_h[a, b]$, there holds

$$\|\mathbf{v} - \mathbf{w}\|_\infty \leqslant K(\|\mathbf{v}_0 - \mathbf{w}_0\| + \|R_h\mathbf{v} - R_h\mathbf{w}\|_\infty), \quad \mathbf{v}, \mathbf{w} \in \Gamma_h[a, b],$$

for all h with $|h|$ sufficiently small.

- Not sensitive to small perturbations of initial conditions, and round-off errors. For example: if $\mathbf{v}, \mathbf{w}$ are numerical solutions as

$$R_h\mathbf{v} = 0, \quad \mathbf{v}_0 = \mathbf{y}_0$$
$$R_h\mathbf{w} = \boldsymbol{\epsilon}, \quad \mathbf{w}_0 = \mathbf{y}_0 + \boldsymbol{\eta}_0$$

then stability implies $\|\mathbf{v} - \mathbf{w}\|_\infty \leqslant K(\|\boldsymbol{\eta}_0\| + \|\boldsymbol{\epsilon}\|_\infty)$

Stability

Theorem

If $\Phi(x, \mathbf{y}; h)$ *satisfies a Lipschitz condition with respect to the* $\mathbf{y}$*-variables,*

$$\|\Phi(x, \mathbf{y}; h) - \Phi(x, \mathbf{y}^*; h)\| \leqslant M\|\mathbf{y} - \mathbf{y}^*\|, \quad \textit{on } [a, b] \times \mathbf{R}^d \times [0, h_0],$$

then the method is stable. (Proof with following lemma.)

Lemma

Let $\{e_n\}$ *be a sequence of real numbers satisfying*

$$e_{n+1} \leqslant a_n e_n + b_n, \quad n = 0, 1, \ldots, N-1,$$

where $a_n > 0$ *and* b_n *real, then*

$$e_n \leqslant E_n, \ E_n = (\prod_{k=0}^{n-1} a_k)e_0 + \sum_{k=0}^{n-1}(\prod_{l=k+1}^{n-1} a_l)b_k, \ n = 0, 1, \ldots, N.$$

Convergence

Definition

Let $a = x_0 < \cdots < x_N = b$ be a grid on $[a, b]$ with grid length $|h| = \max_{1 \leqslant n \leqslant N}(x_n - x_{n-1})$, let $\mathbf{u} = \{\mathbf{u}_n\}$ be the grid function defined by the method, and $\mathbf{y} = \{\mathbf{y}_n\}$ be the grid function induced by the exact solution. Then the method is said to converge on $[a, b]$ if there holds

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

Theorem

If the method is consistent and stable on $[a, b]$, then it converges. Moreover, if $\mathbf{\Phi}$ has order p, then

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

Proof.

Asymptotics of Global Errors

Theorem

Assume that

- $\boldsymbol{\Phi}(x, \mathbf{y}; h) \in C^2$ *on* $[a, b] \times \mathbf{R}^d \times [0, h_0]$*;*
- $\boldsymbol{\Phi}$ *is a method of order* $p \geqslant 1$ *admitting a principal error function* $\boldsymbol{\tau}(x, \mathbf{y}) \in C$ *on* $[a, b] \times \mathbf{R}^d$*.*
- $\mathbf{e}(x)$ *is the solution of the linear initial value problem*

$$\frac{d\mathbf{e}}{dx} = \mathbf{f}_{\mathbf{y}}(x, \mathbf{y}(x))\mathbf{e} + \boldsymbol{\tau}(x, \mathbf{y}(x)), \; a \leqslant x \leqslant b,$$
$$\mathbf{e}(a) = 0.$$

Then, for $n = 0, 1, \ldots, N$*,*

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

Estimation of Global Errors

Theorem

Assume that

- $\mathbf{\Phi}(x, \mathbf{y}; h) \in C^2$ *on* $[a, b] \times \mathbf{R}^d \times [0, h_0]$;
- $\mathbf{\Phi}$ *is a method of order* $p \geqslant 1$ *admitting a principal error function* $\boldsymbol{\tau}(x, \mathbf{y}) \in C$ *on* $[a, b] \times \mathbf{R}^d$.
- *an estimate* $\mathbf{r}(x, \mathbf{y}; h)$ *is available for the principal error function that satisfies* $\mathbf{r}(x, \mathbf{y}; h) = \boldsymbol{\tau}(x, \mathbf{y}) + O(h), \quad h \to 0,$ *uniformly on* $[a, b] \times \mathbf{R}^d$;
- *along with the* $\{\mathbf{u}_n\}$, *we generate the the grid function* $\mathbf{v} = \{\mathbf{v}_n\}$,

$$\mathbf{v}_{n+1} = \mathbf{v}_n + h[\mathbf{f}_\mathbf{y}(x_n, \mathbf{u}_n)\mathbf{v}_n + \mathbf{r}(x_n, \mathbf{u}_n; h)]$$

Then, for $n = 0, 1, \ldots, N$,

$$\mathbf{u}_n - \mathbf{y}(x_n) = \mathbf{v}_n h^p + O(h^{p+1}) \text{ as } h \to 0.$$

Stiff Problems; A-Stability

- The Jacobian matrix $\mathbf{f_y}$ has eigenvalues with very large negative real parts along with others of normal magnitude.
- Need to use unrealistically small step lengths in standard numerical ODE methods.
- A-stable methods are desired.
- Model problem: linear initial value problem

$$\frac{d\mathbf{y}}{dx} = \mathbf{A}\mathbf{y},\ 0 \leqslant x < \infty;\ \mathbf{y}(a) = \mathbf{y}_0.$$

where $\mathbf{A} \in \mathbf{R}^{d\times d}$ is a constant matrix with eigenvalues in the left half-plane:

$$Re\lambda_i(\mathbf{A}) < 0,\ i = 1, 2, \ldots, d$$

A-Stability

- Model problem: linear initial value problem

$$\frac{d\mathbf{y}}{dx} = \mathbf{A}\mathbf{y},\ 0 \leqslant x < \infty;\ \mathbf{y}(a) = \mathbf{y}_0.$$

with eigenvalues of $\mathbf{A} \in \mathbf{R}^{d\times d}$ in the left half-plane:

$$Re\lambda_i(\mathbf{A}) < 0,\ i = 1, 2, \ldots, d$$

- solution decays exponentially, $\mathbf{y}(x) \to \mathbf{0}$ as $x \to \infty$
- One-step method $\mathbf{\Phi}$

$$\mathbf{y}_{next} = \mathbf{y} + h\mathbf{\Phi}(x, y; h) = \phi(h\mathbf{A})\mathbf{y},$$

where ϕ is the stability function of the method.

A-Stability

- Truncation error:

$$\mathbf{T}(x, \mathbf{y}; h) = \mathbf{\Phi}(x, \mathbf{y}; h) - \frac{1}{h}[\mathbf{y}(x+h) - \mathbf{y}(x)] = \frac{1}{h}[\phi(h\mathbf{A}) - e^{h\mathbf{A}}]\mathbf{y}$$

- Approximate solution $\mathbf{u} = \{\mathbf{u}_n\}$ with uniform grid with grid length h:

$$\mathbf{u}_{n+1} = \phi(h\mathbf{A})\mathbf{u}_n,\ n = 0, 1, \ldots; \mathbf{u}_0 = \mathbf{y}_0;$$

  hence

$$\mathbf{u}_{n+1} = [\phi(h\mathbf{A})]^n \mathbf{u}_0, \quad n = 0, 1, 2, \ldots.$$

- $\lim_{n\to\infty} \mathbf{u}_n = \mathbf{0}$ if and only if

$$\lim_{n\to\infty} [\phi(h\mathbf{A})]^n = \mathbf{0}$$

  if and only if $|\phi(h\lambda_i(\mathbf{A}))| < 1, \quad$ for $i = 1, 2, \ldots, d$.

A-Stability

Definition

A one-step method Φ is called A-stable if the function ϕ associated with Φ is defined in the left half of the complex plane and satisfies

$$|\phi(z)| < 1 \text{ for all } z \text{ with } Rez < 0.$$

- Examples A-stable mthods.
- Methods that are not A-stable, what is the region of absolute stability,

$$D_A = \{z \in \mathbf{C} : |\phi(z)| < 1\}.$$

Padé Approximation

- Approximate an analytic function with a rational function in a neighborhood containing 0.

Definition

The Padé approximation $R[n,m](z)$ to the function $g(z)$ is the rational function

$$R[n,m](z) = \frac{P(z)}{Q(z)}, \;\; P \in \mathbf{P}_m, Q \in \mathbf{P}_n,$$

satisfying

$$g(z)Q(z) - P(z) = Q(z^{n+m+1}) \text{ as } z \to 0.$$

Padé Approximation

- Let $N = n + m$,

$$R(z) = \frac{P(z)}{Q(z)} = \frac{p_0 + p_1 z + \cdots + p_n z^n}{q_0 + q_1 z + \cdots + q_m z^m}.$$

  with $q_0 = 1$ normalized. ($N + 1$ total parameters)

- Determine the coefficients such that

$$R^{(k)}(0) = g^{(k)}(0), \text{ for } k = 0, 1, \ldots, N$$

- Determine the coefficients such that $g(z) - R(z)$ has a zero of multiplicity of $N + 1$ at $z = 0$.

Padé Approximation

- Assume Maclaurin series of $g(z) = \sum_{i=0}^{\infty} a_i z^i$, determine the coefficients such that

$$\left(\sum_{i=0}^{\infty} a_i z^i\right)(1 + q_1 z + \cdots + q_m z^m) - (p_0 + p_1 z + \cdots + p_n z^n)$$

  has no terms of degree $\leqslant N$.

- The coefficient of z^k is

$$(\sum_{i=0}^{k} a_i q_{k-i}) - p_k$$

- Hence $N + 1$ equations for determining the parameters

$$\sum_{i=0}^{k} a_i q_{k-i} = p_k, \ \ k = 0, 1, \ldots, N$$

Padé Approximation

Theorem

The Padé approximation $R[n,m]$ to the exponential function $g(z) = e^z$ is given by

$$P[n,m](z) = \sum_{k=0}^{m} \frac{m!(n+m-k)!}{(m-k)!(n+m)!} \frac{z^k}{k!},$$

$$Q[n,m](z) = \sum_{k=0}^{n} (-1)^k \frac{n!(n+m-k)!}{(n-k)!(n+m)!} \frac{z^k}{k!}.$$

Moreover,

$$e^z - \frac{P[n,m](z)}{Q[n,m](z)} = C_{n,m} z^{n+m+1} + \cdots ,$$

where

$$C_{n,m} = (-1)^n \frac{n!m!}{(n+m)!(n+m-1)!}.$$

Padé Approximation

Theorem

If the function ϕ associated with the one-step method Φ is either the Padé approximation $\phi(z) = R[n,n](z)$ of e^z, or the Padé approximation $\phi(z) = R[n+1,n]$ of e^z, $n = 0, 1, \ldots$, then Φ is A-stable.