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

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ODEs

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

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

for $x \in [a, b]$ with an initial condition $y(a) = y_0$.

- IVP for a system of first-order ODEs:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}) \tag{2}$$

for $x \in [a, b]$ with an initial condition $\mathbf{y}(a) = \mathbf{y}_0$, where

$$\mathbf{y} = [y^1, \ldots, y^d]^T, \mathbf{f} = [f^1, \ldots, f^d]^T, \mathbf{y}_0 = [y_0^1, \ldots, y_0^d]^T$$

Numerical Methods for ODEs; One-Step Method

- Approximation $\{\mathbf{u}_n \approx \mathbf{y}(x_n) = \mathbf{y}_n\}$ 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: $\mathbf{u}_{n+1}$ is determined solely from information at x_n, $\mathbf{u}_n$, and step size h with $x_{n+1} = x_n + h$.
  - For a generic point $(x, \mathbf{y})$, a single step of the one-step method:

$$\mathbf{y}_{next} = \mathbf{y} + h\mathbf{\Phi}(x, \mathbf{y}; h), h > 0,$$

    where $\mathbf{\Phi}$ is the approximate difference quotient
  - Local Truncation Error
  - Consistency
  - Order of the method

Euler's Method

- Approximate $\frac{d\mathbf{y}}{dx}$ by forward- or backward-finite difference:

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

- At grid point x_n,
  - Forward-difference: Forward Euler:

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{h} = \mathbf{f}(x_n, \mathbf{u}_n), \quad \Rightarrow \mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_n, \mathbf{u}_n).$$

  - Backward-difference: Backward Euler:

$$\frac{\mathbf{u}_n - \mathbf{u}_{n-1}}{h} = \mathbf{f}(x_n, \mathbf{u}_n), \quad \Rightarrow \mathbf{u}_n = \mathbf{u}_{n-1} + h\mathbf{f}(x_n, \mathbf{u}_n).$$

Forward Euler; Truncation Error; Consistency; Order

- Forward Euler:

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{h} = \mathbf{f}(x_n, \mathbf{u}_n), \quad \Rightarrow \mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_n, \mathbf{u}_n).$$

- Truncation Error:

$$\begin{aligned} \mathbf{T}(x_n, \mathbf{y}_n; h) &= \mathbf{f}(x_n, \mathbf{y}_n) - \frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{h} = \mathbf{y}'(x_n) - \frac{\mathbf{y}(x_n + h) - \mathbf{y}(x_n)}{h} \\ &= \mathbf{y}'(x_n) - \frac{1}{h}[\mathbf{y}(x_n) + h\mathbf{y}'(x_n) + \frac{1}{2}\mathbf{y}''(\xi)h^2 - \mathbf{y}(x_n)] \\ &= -\frac{1}{2}h\mathbf{y}''(\xi) \end{aligned}$$

  where $x_n < \xi < x_n + h$; Assume $\mathbf{y} \in C^2[a, b]$ ($\mathbf{f}$ is C^1), so $\|\mathbf{y}''\| \leqslant C$

- Order: $|\mathbf{T}| \leqslant Ch$, i.e., First-Order
- Consistency: $\lim_{h\to 0} |\mathbf{T}| = 0$

Backward Euler; Truncation Error; Consistency; Order

- Backward Euler:

$$\frac{\mathbf{u}_n - \mathbf{u}_{n-1}}{h} = \mathbf{f}(x_n, \mathbf{u}_n), \quad \Rightarrow \mathbf{u}_n = \mathbf{u}_{n-1} + h\mathbf{f}(x_n, \mathbf{u}_n).$$

- Truncation Error:

$$\begin{aligned}
\mathbf{T}(x_n, \mathbf{y}_n; h) &= \mathbf{f}(x_n, \mathbf{y}_n) - \frac{\mathbf{y}_n - \mathbf{y}_{n-1}}{h} = \mathbf{y}'(x_n) - \frac{\mathbf{y}(x_n) - \mathbf{y}(x_n - h)}{h} \\
&= \mathbf{y}'(x_n) - \frac{1}{h}[\mathbf{y}(x_n) - (\mathbf{y}(x_n) - h\mathbf{y}'(x_n) + \frac{1}{2}\mathbf{y}''(\xi)h^2)] \\
&= \frac{1}{2}h\mathbf{y}''(\xi)
\end{aligned}$$

  where $x_n - h < \xi < x_n$; Assume $\mathbf{y} \in C^2[a,b]$ ($\mathbf{f}$ is C^1), so $\|\mathbf{y}''\| \leqslant C$

- Order: $|\mathbf{T}| \leqslant Ch$, i.e., First-Order
- Consistency: $\lim_{h\to 0} |\mathbf{T}| = 0$

Principal Error Function

For both forward- or backward- Euler method:

$$\mathbf{T}(x_n, \mathbf{y}_n; h) = -\frac{1}{2}h\mathbf{y}''(\xi) = \frac{1}{2}h(\mathbf{f}_x + \mathbf{f}_\mathbf{y}\mathbf{f})(\xi, \mathbf{y}(\xi)) \quad = \frac{1}{2}h(\mathbf{f}_x + \mathbf{f}_\mathbf{y}\mathbf{f})(x_n, \mathbf{y}_n) +$$

so the principal error function is

$$\tau(x_n, \mathbf{y}_n) = -\frac{1}{2}(\mathbf{f}_x + \mathbf{f}_\mathbf{y}\mathbf{f})(x_n, \mathbf{y}_n)$$

Clearly, order of Euler method is 1.

Explicit Method V.S. Implicit Method

- Forward Euler is an explicit method:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_n, \mathbf{u}_n).$$

- Backward Euler is an implicit method:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_{n+1}, \mathbf{u}_{n+1}).$$

If $\mathbf{f}$ is nonlinear in $\mathbf{u}_{n+1}$, compute $\mathbf{u}_{n+1}$ by finding zeros of equation

$$\mathbf{u} - \mathbf{u}_n - h\mathbf{f}(x_n, \mathbf{u}) = 0$$

An Example

- Consider

$$\frac{dy}{dx} = \lambda y, \; x \in (0,1],$$
$$y(0) = y_0.$$

- Forward Euler:

$$u_0 = y_0, \quad u_{n+1} = u_n + h\lambda u_n = (1 + h\lambda) u_n$$

- Backward Euler:

$$u_0 = y_0, \quad u_{n+1} = u_n + h\lambda u_{n+1} \Rightarrow u_{n+1} = u_n/(1 - h\lambda)$$

- Check error: $\max_n |u_n - y(x_n)|$, with $y(x) = y_0 e^{\lambda x}$

Taylor Series Expansion Method

- Taylor Expansion:

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

- Euler's method through linear Taylor expansion:

$$\mathbf{y}(x_{n+1}) \approx \mathbf{y}(x_n) + h\mathbf{y}'(x_n)$$

  suggests the forward Euler's method:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_n, \mathbf{u}_n).$$

- pth-order method through pth-order Taylor series expansion:

$$\mathbf{y}(x_{n+1}) \approx \mathbf{y}(x_n) + h\mathbf{y}'(x_n) + \frac{1}{2}h^2\mathbf{y}''(x_n) + \cdots + \frac{1}{p!}h^p\mathbf{y}^{(p)}(x_n)$$

Taylor Series Expansion Method

- What are $\mathbf{y}'(x_n), \ldots, \mathbf{y}^{(p)}(x_n)$?
- Total derivatives of $\mathbf{f}(x, \mathbf{y})$:

  $\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y}) = \mathbf{f}^{[0]}(x, \mathbf{y})$,

  $\mathbf{y}''(x) = \frac{d\mathbf{f}(x,\mathbf{y})}{dx} = \frac{d\mathbf{f}^{[0]}(x,\mathbf{y})}{dx} = \mathbf{f}_x(x, \mathbf{y}) + \mathbf{f}_{\mathbf{y}}(x, \mathbf{y})\mathbf{f}(x, \mathbf{y}) = \mathbf{f}^{[1]}(x, \mathbf{y})$,

  $\vdots$

  $\mathbf{y}^{(k)} = \mathbf{f}^{[k-1]}(x, \mathbf{y}) = \frac{d\mathbf{f}^{[k-2]}(x,\mathbf{y})}{dx} = \mathbf{f}_x^{[k-2]}(x, \mathbf{y}) + \mathbf{f}_{\mathbf{y}}^{[k-2]}(x, \mathbf{y})\mathbf{f}(x, \mathbf{y})$
- pth-order method:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\{\mathbf{f}^{[0]}(x_n, \mathbf{u}_n) + \frac{1}{2}\mathbf{f}^{[1]}(x_n, \mathbf{u}_n) + \cdots + \frac{1}{p!}h^{p-1}\mathbf{f}^{[p-1]}(x_n, \mathbf{u}_n)\}$$

  i.e., $\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{\Phi}(x_n, \mathbf{u}_n; h)$ with

$$\mathbf{\Phi}(x_n, \mathbf{u}_n; h) = \mathbf{f}^{[0]}(x_n, \mathbf{u}_n) + \frac{1}{2}\mathbf{f}^{[1]}(x_n, \mathbf{u}_n) + \cdots + \frac{1}{p!}h^{p-1}\mathbf{f}^{[p-1]}(x_n, \mathbf{u}_n)$$

Taylor Series Expansion Method

- Truncation error:

$$\begin{aligned}\mathbf{T}(x_n, \mathbf{y}_n; h) &= \mathbf{\Phi}(x_n, \mathbf{y}_n; h) - \frac{1}{h}[\mathbf{y}(x_n + h) - \mathbf{y}(x_n)] \\ &= \mathbf{\Phi}(x_n, \mathbf{y}_n; h) - \sum_{k=0}^{p-1} \mathbf{y}^{(k+1)}(x_n)\frac{h^k}{(k+1)!} - \mathbf{y}^{(p+1)}(\xi)\frac{h^p}{(p+1 \\ &= -\mathbf{y}^{(p+1)}(\xi)\frac{h^p}{(p+1)!}, \ x_n < \xi < x_n + h.\end{aligned}$$

- Order of Method: assume $\|\mathbf{y}^{(p+1)}\| \leqslant C_p$ $(\|\mathbf{f}^{[p]}\| \leqslant C_p)$

$$\|\mathbf{T}(x_n, \mathbf{y}_n; h)\| \leqslant \frac{C_p}{(p+1)!}h^p$$

- Principal error function $\tau(x_n, \mathbf{y}_n) = -\frac{1}{(p+1)!}\mathbf{f}^{[p]}(x_n, \mathbf{y}_n)$

An Example

Consider

$$y'(x) = x^2 \sin(y(x)), \quad y(0) = y_0$$

We can compute

$$\begin{aligned} y''(x) &= 2x \sin(y(x)) + x^2 \cos(y(x)) y'(x) \\ &= 2x \sin(y(x)) + x^4 \cos(y(x)) \sin(y(x)) \end{aligned}$$

Then a second-order method is:

$$u_{n+1} = u_n + h x_n^2 \sin(u_n) + \frac{1}{2} h^2 [2x_n \sin(u_n) + x_n^4 \cos(u_n) \sin(u_n)]$$

Improved Euler Method

- Exact solution:

$$\mathbf{y}(x_{n+1)} = \mathbf{y}(x_n) + \int_{x_n}^{x_{n+1}} \mathbf{f}(x, \mathbf{y}(x))dx$$

- Numerical Integration: e.g.,
  - rectangle rule:

$$\mathbf{y}(x_{n+1)} \approx \mathbf{y}(x_n) + h\mathbf{f}(x_n, \mathbf{y}(x_n)) \Rightarrow \text{ Forward Euler}$$

  - rectangle rule:

$$\mathbf{y}(x_{n+1)} \approx \mathbf{y}(x_n) + h\mathbf{f}(x_{n+1}, \mathbf{y}(x_{n+1})) \Rightarrow \text{ Backward Euler}$$

  - θ-method: for $\theta \in [0, 1]$,

$$\mathbf{y}(x_{n+1)} \approx \mathbf{y}(x_n) + h\{(1-\theta)\mathbf{f}(x_n, \mathbf{y}(x_n)) + \theta\mathbf{f}(x_{n+1}, \mathbf{y}(x_{n+1}))\}$$

Improved Euler Method

- Intuitively, approximating

$$\int_{x_n}^{x_{n+1}} \mathbf{f}(x, \mathbf{y}(x))dx \approx h\mathbf{\Phi}(x_n, \mathbf{y}_n; h)$$

  with high-order accuracy results in high-order methods:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{\Phi}(x_n, \mathbf{u}_n; h)$$

- Maintain explicitness of Euler's method, and improve the order of method.

Improved Euler Method

- Two-stage method example 1:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{f}(x_n + \frac{1}{2}h, \mathbf{u}_n + \frac{1}{2}h\mathbf{f}(x_n, \mathbf{u}_n)),$$

  equivalently,
  $\mathbf{k}_1 = \mathbf{f}(x_n, \mathbf{u}_n)$; $\quad \mathbf{k}_2(x_n, \mathbf{u}_n; h) = \mathbf{f}(x_n + \frac{1}{2}h, \mathbf{u}_n + \frac{1}{2}h\mathbf{k}_1)$;
  $\mathbf{u}_{n+1} = \mathbf{u}_n + h\mathbf{k}_2$.

- Two-stage method example 2:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{1}{2}h[\mathbf{f}(x_n, y_n) + \mathbf{f}(x_n + h, \mathbf{u}_n + h\mathbf{f}(x_n, \mathbf{u}_n))]$$

  equivalently,
  $\mathbf{k}_1(x_n, \mathbf{u}_n) = \mathbf{f}(x_n, y_n)$; $\quad \mathbf{k}_2(x_n, \mathbf{u}_n; h) = \mathbf{f}(x_n + h, \mathbf{u}_n + h\mathbf{k}_1)$;
  $\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{1}{2}h(\mathbf{k}_1 + \mathbf{k}_2)$.

Both have order 2, and maintain explicitness.

Two-Stage Methods

The method:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\boldsymbol{\Phi}(x_n, \mathbf{u}_n; h)$$

with

$$\boldsymbol{\Phi}(x_n, \mathbf{u}_n; h) = \alpha_1 \mathbf{k}_1 + \alpha_2 \mathbf{k}_2$$

and

$$\begin{aligned}\mathbf{k}_1(x_n, \mathbf{u}_n) &= \mathbf{f}(x_n, \mathbf{u}_n)\\ \mathbf{k}_2(x_n, \mathbf{u}_n) &= \mathbf{f}(x_n + \mu h, \mathbf{u}_n + \mu h \mathbf{k}_1).\end{aligned}$$

for appropriate parameters α_1, α_2, μ.

- example 1: $\alpha_1 = 0, \alpha_2 = 1, \mu = 1/2$.
- example 2: $\alpha_1 = \alpha_2 = 1/2, \mu = 1$.

Goal: choose α_1, α_2, μ to maximize order of the method.

Two-Stage Methods

Truncation error:

$$\begin{aligned}\mathbf{T}(x_n, \mathbf{y}_n; h) &= \mathbf{\Phi}(x_n, \mathbf{y}_n; h) - \frac{1}{h}[\mathbf{y}(x_n + h) - \mathbf{y}(x_n)] \\ &= \alpha_1 \mathbf{k}_1(x_n, \mathbf{y}(x_n)) + \alpha_2 \mathbf{k}_2(x_n, \mathbf{y}(x_n); h) - \frac{1}{h}[\mathbf{y}(x_n + h) - \mathbf{y}(x_n)\end{aligned}$$

With Taylor expansion to maximize order of **T**.