Overview

- ODE review
- First-order ODE initial value problem
- Differential operator approximation from polynomial interpolants
  - forward Euler scheme
  - backward Euler scheme
  - Leapfrog scheme
- Schemes based upon numerical quadrature
  - Adams-Bashforth schemes
  - Adams-Moulton schemes
- Forward Euler analysis
- General analysis techniques: convergence = consistency + stability

- An n^{th}-order ordinary differential equation given in explicit form

$$y^{(n)} = \frac{\mathrm{d}^n y}{\mathrm{d}t^n} = f\left(t, y, y', \ldots, y^{(n-1)}\right).$$

- The problem is to determine the function $y\colon \mathbb{R} \to \mathbb{R}$, $y \in C^{(n)}(\mathbb{R})$
- y is not given directly but as an equality between two operators acting on y

$$\mathcal{L}y = f(t, y, y', \ldots, y^{(n-1)}), \mathcal{L} = \frac{\mathrm{d}^n}{\mathrm{d}t^n}, f\colon \mathbb{R}^{n+1} \to \mathbb{R}.$$

- An n^{th} order ODE is equivalent to a system of n first-order ODEs

$$\boldsymbol{z}' = \boldsymbol{F}(t, \boldsymbol{z})$$

where

$$\boldsymbol{z} = \begin{bmatrix} z_1 & z_2 & \ldots & z_{n-1} & z_n \end{bmatrix}^T = \begin{bmatrix} y & y' & \ldots & y^{(n-2)} & y^{(n-1)} \end{bmatrix}^T,$$

$$\boldsymbol{F}(t, \boldsymbol{z}) = \begin{bmatrix} z_2(t) & z_3(t) & \ldots & z_n(t) & f(t, z_1(t), \ldots, z_n(t)) \end{bmatrix}^T.$$

This leads to the central role of numerical solution of first-order ODEs.

- The initial value problem (IVP) for $y: \mathbb{R} \to \mathbb{R}$ is

$$y' = f(t, y), y(0) = y_0.$$

- IVP has a *unique* solution for $(t, y) \in [0, T] \times [y_1, y_2]$ if f Lipschitz-continuous

$$\exists K \in \mathbb{R}_+ \text{such that} \, |f(t, y_2) - f(t, y_1)| \leqslant K \, |y_2 - y_1|.$$

  $|f(t, y_2) - f(t, y_1)| = \mathcal{O}(|y_2 - y_1|)$ $|f_2 - f_1|$ goes to zero as $|y_2 - y_1|$.

- Lipschitz is more restrictive than continuity ($\forall \varepsilon > 0, \exists \delta_\varepsilon$ such that $|t_2 - t_1| < \delta_\varepsilon \Rightarrow |y(t_2) - y(t_1)| < \varepsilon$ (no relation between how $|t_2 - t_1|$,$|y_2 - y_1|$ go to zero

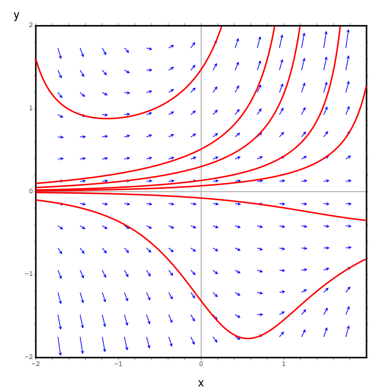

Figure 1. To solve an ODE IVP is to find a specific integral curve.

- Approaches to numerical solution of $\mathcal{L}y = f(t, y)$, $\mathcal{L} = \mathrm{d}/\mathrm{d}t$
  - Approximation of the differentiation operator $\mathcal{L}$, $\mathcal{L} \cong \mathcal{D}$
  - Approximation of the nonlinear operator f, $f \cong g$
  - Approximation of the equality between effect of two operators $\mathcal{D}y = g(t, y)$
- Methods from approximating $\mathcal{L} = \mathrm{d}/\mathrm{d}t$, $f_i = f(t_i, y_i)$
  - *Forward Euler* (an *explicit* method, next y value given directly)

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t_i) \cong \frac{y(t_{i+1}) - y(t_i)}{t_{i+1} - t_i} = \frac{y_{i+1} - y_i}{h} \Rightarrow y_{i+1} = y_i + h f_i, i = 0, 1, 2, \ldots$$

  - *Backward Euler* (an *implicit* method, must solve an equation to find y_i)

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t_i) \cong \frac{y(t_i) - y(t_{i-1})}{t_i - t_{i-1}} = \frac{y_i - y_{i-1}}{h} \Rightarrow y_i = y_{i-1} + h f(t_i, y_i), i = 1, 2, \ldots$$

  - *Leapfrog* (centered finite difference)

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t_i) \cong \frac{y_{i+1/2} - y_{i-1/2}}{t_{i+1/2} - t_{i-1/2}} = f_i \Rightarrow y_{i+1/2} = y_{i-1/2} + h f_i,$$

- Integrate $y' = f(t, y)$ over time step $[t_i, t_{i+1}]$, $y_{i+1} - y_i = \int_{t_i}^{t_{i+1}} f(t, y(t))\,\mathrm{d}t$
- Approximate f on data set $\mathcal{D} = \{(t_i, y_i), (t_{i-1}, y_{i-1}), \ldots, (t_{i+1-s}, y_{i+1-s})\}$

$$f(t, y(t)) \cong \sum_{k=1}^{s} \ell_k(t)\, f_k,\; f_k = f(t_{i+1-k}, y(t_{i+1-k})) \cong f(t_{i+1-k}, y_{i+1-k}).$$

- The resulting schemes are known as *Adams-Bashforth explicit methods*

$$y_{i+1} = y_i + \sum_{k=1}^{s} \left(\int_{t_i}^{t_{i+1}} \ell_k(t)\,\mathrm{d}t \right) f_k = y_i + h \sum_{k=1}^{s} b_k\, f_{i+1-k},$$

s	b_1	b_2	b_3	b_4
1	1			
2	$\frac{3}{2}$	$-\frac{1}{2}$		
3	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$	

Table 1. Adams-Bashforth scheme coefficients.

- Integrate $y' = f(t, y)$ over time step $[t_i, t_{i+1}]$, $y_{i+1} - y_i = \int_{t_i}^{t_{i+1}} f(t, y(t))\,\mathrm{d}t$
- Approximate f on data set $\mathcal{D} = \{(t_{i+1}, y_{i+1}), (t_i, y_i), \ldots, (t_{i+2-s}, y_{i+2-s})\}$

$$f(t, y(t)) \cong \sum_{k=0}^{s-1} \ell_k(t)\, f_k,\; f_k = f(t_{i+1-k}, y(t_{i+1-k})) \cong f(t_{i+1-k}, y_{i+1-k}).$$

- The resulting schemes are known as *Adams-Moulton implicit methods*

$$y_{i+1} = y_i + \sum_{k=1}^{s} \left(\int_{t_i}^{t_{i+1}} \ell_k(t)\,\mathrm{d}t \right) f_k = y_i + h \sum_{k=1}^{s} b_k\, f_{i+1-k},$$

s	b_0	b_1	b_2	b_3
1	1			
2	$\frac{1}{2}$	$\frac{1}{2}$		
3	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$	

Table 2. Adams-Moulton scheme coefficients.

- Introduce error at step i, $e_i = y(t_i) - y_i$. ($y(t_i)$ denotes the exact value)

$$e_{i+1} - e_i = y(t_{i+1}) - y(t_i) - (y_{i+1} - y_i) \Rightarrow$$

$$e_{i+1} - e_i = h y'(t_i) + \frac{h^2}{2} y''(\xi_i) - y(t_i) - h f(t_i, y(t_i)) = \frac{h^2}{2} y''(\xi_i).$$

- At each step forward Euler introduces an error (*the one-step error*)

$$\tau_i = e_{i+1} - e_i = \frac{h^2}{2} y''(\xi_i).$$

- After N steps

$$e_N - e_0 = \frac{h^2}{2} \sum_{i=1}^{N} y''(\xi_i).$$

- Exact start $e_0 = 0$. Obtain for $T = Nh$, that *FE is first-order of accuracy*.

$$e_N \leqslant \frac{Nh^2}{2} \|y''\|_\infty = h \frac{T}{2} \|y''\|_\infty = \mathcal{O}(h)$$

- Introduce error at step i, $e_i = y(t_i) - y_i$. ($y(t_i)$ denotes the exact value)

$$e_{i+1} - e_i = y(t_{i+1}) - y(t_i) - (y_{i+1} - y_i) \Rightarrow$$

$$e_{i+1} - e_i = y(t_{i+1}) - y(t_{i+1}) + h y'(t_{i+1}) - \frac{h^2}{2} y''(\xi_i) - h f(t_{i+1}, y(t_{i+1})).$$

- At each step backward Euler introduces an error (*the one-step error*)

$$\tau_i = e_{i+1} - e_i = -\frac{h^2}{2} y''(\xi_i).$$

- After N steps

$$e_N - e_0 = \frac{h^2}{2} \sum_{i=1}^{N} y''(\xi_i).$$

- Exact start $e_0 = 0$. Obtain for $T = Nh$, that *BE is first-order of accuracy*.

$$e_N \leqslant \frac{Nh^2}{2} \|y''\|_\infty = h \frac{T}{2} \|y''\|_\infty = \mathcal{O}(h)$$

- Introduce error at step i, $e_i = y(t_i) - y_i$. ($y(t_i)$ denotes the exact value)

$$e_{i+1} - e_i = y(t_{i+1}) - y(t_i) - (y_{i+1} - y_i) \Rightarrow$$

$$\tau_i = e_{i+1} - e_i = y(t_{i+1}) - y(t_i) - h\,f(t_{i+1/2}, y(t_{i+1/2})) \Rightarrow$$

$$\tau_i = y(t_{i+1/2}) + \frac{h}{2}\,y'(t_{i+1/2}) + \frac{h^2}{4}y''(t_{i+1/2}) + \frac{h^3}{8}y'''(\xi_i) - \dots$$

$$\dots y(t_{i+1/2}) + \frac{h}{2}\,y'(t_{i+1/2}) - \frac{h^2}{4}y''(t_{i+1/2}) + \frac{h^3}{8}y'''(\eta_i) - h\,f(t_{i+1/2}, y(t_{i+1/2}))$$

- At each step leapfrog introduces an error (*the one-step error*)

$$\tau_i = e_{i+1} - e_i = \frac{h^3}{4}\left[\frac{y'''(\xi_i) + y'''(\eta_i)}{2}\right] = \frac{h^3}{8}y'''(\zeta_i).$$

- After N steps with $T = Nh$, that *LF is second-order of accuracy*.

$$e_N \leqslant \frac{Nh^3}{8}\|y'''\|_\infty = h^2\,\frac{T}{8}\|y''\|_\infty = \mathcal{O}(h^2)$$

- Consider a small initial error in forward Euler $\tilde{y}_0 = y_0 + \epsilon$ (e.g., floating point)

$$y' = \lambda y \Rightarrow y_{i+1} = y_i + h\lambda y_i = (1 + h\lambda) y_i = (1 + z) y_i$$

- After N steps FE with a perturbed initial condition gives

$$\tilde{y}_N = (1 + z)^N (y_0 + \epsilon) = y_N + (1 + z)^N \epsilon = y_N + e_N$$

- For $|1 + z| > 1$ the error e_N increases without bound. The forward Euler scheme is said to be *unstable*.
- How to approach this? First, precisely define a convergent sequence of approximations $\{y_n\}_{n \in \mathbb{N}}$ for the solution $y(t_n)$ of the IVP $y' = f(t, y)$, $y(0) = y_0$, over the time interval $[0, T]$, $t_n = nh$, $h = T/N$. A numerical method (scheme) is said to be convergent if

$$\lim_{\substack{h \to 0 \\ Nh = T}} y_N = y(T).$$

- Analytical calculations of the above limit are however difficult.

- Consider the model problem $y' = \lambda y$, $y(0) = y_0$, $\lambda \leqslant 0$ with solution

$$y(t) = e^{\lambda t} y_0 \Rightarrow y(t_n) = e^{n\lambda h} y_0.$$

- Now, consider a perturbation of the initial conditions

$$\tilde{y}(T) = e^{\lambda T}(y_0 + \delta) \Rightarrow \varepsilon = \tilde{y}(T) - y(T) = e^{\lambda T}\delta.$$

- Error ε is maintained small if $\lambda \leqslant 0$. How does a numerical scheme behave?
- Forward Euler: $y_N = (1+z)^N y_0$. Exponential decay of analytical solution only if

$$-\frac{2}{\lambda} > h > 0.$$

- The above is known as a *stability condition*.
- In the limit of $h \to 0$, the error $e_N \leqslant h\frac{T}{2}\|y''\|_\infty$ also goes to zero. This is known as *consistency*.
- In general a numerical scheme is convergent iff it is stable *and* consistent.