intellectual flexibility

1) Newton's method

$$F(x) = 0$$

$$x^{(i+1)} = x^{(i)} - (F'(x^{(i)}))^{-1} F(x^{(i)})$$

2) implicit Euler method

ODE $\quad x'(t) = f(x(t)), \quad x(0) = x_0$

$$x_{k+1} = x_k + \tau f(x_{k+1})$$

$$F(x_{k+1}) = x_k + \tau f(x_{k+1}) - x_{k+1} \overset{!}{=} 0$$

$$F(x) = x_k + \tau f(x) - x$$

3) linear implicit Euler

$$F(x) = x_k + \tau f(x) - x$$

$$F'(x) = \tau f'(x) - 1$$

1 step of Newton with $x^{(0)} = x_k$

scalar problem (not a system)

$$x^{(1)} = x^{(0)} - (F'(x^{(0)}))^{-1} F(x^{(0)})$$

$$= x^{(0)} - \frac{x^{(0)} + \tau f(x^{(0)}) - x^{(0)}}{\tau f'(x^{(0)}) - 1}$$

$$= x_k - \frac{\tau f(x_k)}{\tau f'(x_k) - 1}$$

$$=: x_{k+1}$$

initial value problem

$$x'(t) = f(x(t)), \quad 0 < t \le T$$

$$x(0) = x_0$$

$$x : [0, T] \to \mathbb{R}^d$$

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix}$$

$$f : \mathbb{R}^d \to \mathbb{R}^d$$

Existence & uniqueness:
Picard - Lindelöf

assumption: f Lipschitz, i.e.,

$$\| f(x) - f(y) \| < L \, \| x - y \|$$
$$\forall x, y \in \mathbb{R}^d$$

$\Rightarrow$ existence & uniqueness $\forall \, T > 0$

examples

1. Dahlquist's test equation

$$f(x) = \lambda x \qquad d = 1, \lambda \in \mathbb{R}$$

$$x(t) = x_0 e^{\lambda t}$$

flow operator (solution operator)

$$x_0 \longrightarrow \phi^t x_0 = x(t)$$

$$t \text{ fixed}: \quad \mathbb{R}^d \ni x_0 \longrightarrow \phi^t x_0 \in \mathbb{R}^d$$

semigroup property:

$$\boxed{\phi^{t+\tau} x_0 = \phi^\tau(\phi^t x_0) = \phi^\tau \phi^t x_0}$$

1. example: $\phi^t x_0 = x_0 e^{\lambda t}$

2. Population of bacteria

$$x' = q x - k x^2, \quad x(0) = x_0, \; d = 1$$

$q > 0$ birth rate, $k > 0$ competition rate

$$\phi^t x_0 = \frac{x_0 q e^{qt}}{q + (e^{qt} - 1) k x_0} \quad t \geqslant 0$$

Discretization:

grid: $t_k = k\tau$, $k = 0, \dots, n$

uniform time step: $\tau = T/n$

$\phi^t x_0$: exact sol. after time t

$\psi^\tau x$: approx. sol. after $\tau > 0$

intended: $\psi^\tau x \approx \phi^\tau x$

single step method:

$$x_{k+1} = \psi^\tau x_k, \quad x_k \approx x(t_k)$$

semigroup property implies:

$$\begin{aligned} x(t_{k+1}) &= x(t_k + \tau) \\ &= \phi^{t_k+\tau} x_0 = \phi^\tau \phi^{t_k} x_0 \\ &= \phi^\tau x(t_k) \end{aligned}$$

consistency with order p

Def.: $\| \Psi^\tau x - \phi^\tau x \| \leq C \tau^{p+1}$

Taylor expansion of Ψ^τ, ϕ^τ at $\tau = 0$

Let $d = 1$, for simplicity:

$$\phi^\tau x = y(\tau) = y(0) + y'(0)\tau + \frac{1}{2} y''(\xi)\tau^2$$

$$0 < \xi < \tau$$

$$(\phi^\tau)' x = \phi^{\tau\prime} x = y'(\tau) = f(y(\tau))$$

$$\Leftrightarrow y'(0) = f(y(0)) = f(x)$$

$$y(0) = \phi^0 x = x$$

$$y''(0) = \frac{d}{d\tau} f(y(\tau)) \Big|_{\tau=0}$$

$$= f'(y(\tau))\, y'(\tau) \Big|_{\tau=0}$$

$$= f'(x) f(x)$$

and so on

$$\psi^{\tau} x = \psi^{0} x + (\psi^{0} x)' \tau + \frac{1}{2} (\psi^{\xi} x)'' \tau^{2}$$

$$\psi^{0} x = x$$

higher order derivatives depend on ψ^{τ}

systematic construction of consistent discretizations with arbitrary order

fundamental theorem of calculus:

$$x'(t) = f(x(t))$$

$$x(t_{k+1}) = x(t_k) + \int_{t_k}^{t_{k+1}} f(x(s))\, ds$$

$$= x(t_k) + \int_{t_k}^{t_{k+1}} f(\phi^s x(t_k))\, ds$$

construction of Ψ^τ by quadrature rule

$$\int_{t_k}^{t_{k+1}} f(x(s))\, ds \approx f(x(t_k))\, \tau$$

$$\Leftrightarrow \quad x_{k+1} = x_k + \tau f(x_k)$$

$$= \Psi^\tau x_k$$

$$\Psi^\tau x = x + \tau f(x)$$

1. explicit Euler method:

$$\Psi^{\tau} x = x + \tau f(x)$$

consistency

Taylor expansion of ϕ^{τ}:

$$\phi^{\tau} x = x + \tau f(x) + O(\tau^2)$$

$$\| \Psi^{\tau} x - \phi^{\tau} x \| =$$

$$\| x + \tau f(x) - (x + \tau f(x) + O(\tau^2)) \|$$

$$= O(\tau^2)$$

$\Rightarrow$ consistency with order $p = 1$

2. linear implicit Euler

$$x_{k+1} = x_k - \frac{\tau f(x_k)}{\tau f'(x_k) - 1} =: \Psi^\tau x_k$$

$$\Psi^{\tau\,\prime} x = -\frac{f(x)}{\tau f'(x) - 1} + \frac{\tau f(x)}{(\tau f'(x) - 1)^2} f'(x)$$

$$\Psi^{\tau\,\prime} x \Big|_{\tau=0} = f(x), \quad \Psi^0 x = x$$

$$\Psi^\tau x = x + \tau f(x) + O(\tau^2)$$

$$\Phi^\tau x = x + \tau f(x) + O(\tau^2)$$

$\Rightarrow$ consistency

3. Runge - Kutta methods

a) $$\int_{t_k}^{t_{k+1}} f(\phi^{r} x(t_k))\, dr$$

$$\approx \tau \sum_{i=1}^{s} f(\phi^{\tau_i} x(t_k))\, b_i$$

b) approximate $\phi^{\tau_i} x(t_k)$

in the same way

$$\psi^{\tau} x = x + \tau \sum_{i=1}^{s} b_i k_i$$

$$k_i = f\left(x + \tau \sum_{j=1}^{s} a_{ij} k_j\right)$$

$$i = 1, \dots, s$$

s - stage Runge - Kutta method

Butcher scheme

$$\begin{array}{c|c} & A \\ \hline & b \end{array} \qquad A = (a_{ij})_{i,j=1}^{s}, \quad b = (b_i)_{i=1}^{s}$$

examples:

- explicit Euler

$$\Psi^\tau x = x + \tau f(x) = x + \tau \cdot 1 \cdot k_1$$

$$k_1 = f(x + \tau \cdot 0 \cdot k_1)$$

$$\begin{array}{c|c} & 0 \\ \hline & 1 \end{array}$$

- implicit Euler

$$\Psi^\tau x = x + \tau f(\Psi^\tau x) = x + \tau \cdot 1 \cdot k_1$$

$$k_1 = f(x + \tau \cdot 1 \cdot k_1)$$

$$\begin{array}{c|c} & 1 \\ \hline & 1 \end{array}$$

- implicit midpoint rule

$$\Phi^\tau = x + \frac{\tau}{2}\left(f(x) + f(\Phi^\tau x)\right)$$

$$= x + \tau \left(\frac{1}{2} k_1 + \frac{1}{2} k_2 \right)$$

$$k_1 = f(x) = f(x + \tau(0 \cdot k_1 + 0 k_2))$$

$$k_2 = f(\Phi^\tau x) = f\left(x + \tau\left(\frac{1}{2} k_1 + \frac{1}{2} k_2\right)\right)$$

$$\begin{array}{|cc} 0 & 0 \\ 1/2 & 1/2 \\ \hline 1/2 & 1/2 \end{array}$$

- Runge-Kutta-4

$$\begin{array}{|cccc} 0 & - & & 0 \\ 1/2 & 0 & & \vert \\ 0 & 1/2 & 0 & \vert \\ 0 & 0 & 1 & 0 \\ \hline 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

arbitrary order: Butcher trees

Butcher (1933 - ...)

Stability w.r.t. perturbations

Lipschitz continuity of f:

$$\| f(x) - f(y) \| \leq L \, \| x - y \| \quad \forall\, x, y \in \mathbb{R}^d$$

implies Lipschitz continuity of flow operator ϕ^t

$$\| \phi^t x - \phi^t y \| \leq e^{tL} \| x - y \| \quad \forall\, x, y \in \mathbb{R}^d,\ t \geq 0$$

Proof: Gronwall lemma

Definition Ψ^τ is called stable, if

$$\| \Psi^\tau x - \Psi^\tau y \| \leq e^{\tau \gamma L} \| x - y \| \quad \forall\, x, y \in \mathbb{R}^d,\ \tau \geq 0$$

with some $\gamma = \gamma(A, b) \geq 1$

example:

- explicit Euler method

$$\Psi^{\tau} x = x + \tau f(x)$$

$$\| \Psi^{\tau} x - \Psi^{\tau} y \|$$

$$= \| x + \tau f(x) - (y + \tau f(y)) \|$$

$$\leq \| x - y \| + \tau \| f(x) - f(y) \|$$

$$\leq (1 + \tau L) \| x - y \|$$

$$\leq (1 + \tau L + \frac{1}{2!} \tau^2 L^2 \ldots) \| x - y \|$$

$$\leq e^{\tau L} \| x - y \|$$

<=> stable with $\gamma = 1$

Theorem:

- all explicit RK methods are stable
- $A \geq 0, b \geq 0 \Rightarrow \gamma = 1$

Convergence with order p

$$\max_{k=0,\dots,n} \| x_k - x(t_k) \| \leq C \tau^p$$

Theorem (Paradigm)

consistency with order p

$+$

stability

of the discrete flow Ψ^τ imply

convergence with order p

Proof:

consistency:

$$\phi^{\tau} x_k - \psi^{\tau} x_k = \varepsilon_k = O(\tau^{p+1})$$

stability:

$$\| x(t_k) - x_k \| \leq e^{t_k \gamma L} \sum_{i=0}^{k-1} \| \varepsilon_i \|$$

proof by induction

convergence:

$$\max_{k=1,\dots,n} \| x(t_k) - x_k \| \leq e^{T \gamma L} \sum_{i=0}^{n-1} \| \varepsilon_i \| \leq e^{T \gamma L} \underbrace{n \tau}_{=T} O(\tau^{p})$$