Numerical integration of ODEs

→ RK methods

Stability of a Cauchy problem

$$\begin{cases} \dot{\vec{q}} = \vec{f}(\vec{q}, t) \\ \vec{q}(0) = \vec{q}_0 \end{cases} \quad \xrightarrow{\text{perturbed}} \quad \begin{cases} \dot{\vec{z}} = \vec{f}(\vec{z}, t) + \vec{\delta}(t) \\ \vec{z}(0) = \vec{q}_0 + \vec{\delta}_0 \end{cases}$$

$$\|\vec{\delta}(t)\| \leq \underline{\epsilon} \quad \forall t \in [0, t_0] \quad \Longrightarrow \quad \exists C^{>0} : \|\vec{z}(t) - \vec{q}(t)\| \leq C\epsilon \quad \forall t \in [0, t_0]$$

stable Cauchy problem

For a stable Cauchy problem ⟹ zero-stability of a numerical scheme

s-step scheme

$$\sum_{j=0}^{s} \alpha_j \vec{q}_{n+j} = \vec{\Phi}_{\vec{f}}(\vec{q}_n, \dots, \vec{q}_{n+s}; h, t_n)$$

perturbed scheme

$$\sum_{j=0}^{s} \alpha_j \vec{z}_{n+j} = \vec{\Phi}_{\vec{f}}(\vec{z}_n, \dots, \vec{z}_{n+s}; h, t_n) + \vec{\delta}_n$$

$$\vec{z}(0) = \vec{q}_0 + \vec{\delta}_0$$

zero-stable numerical scheme over the interval $[0, t_0]$

$$n \in [0, t_0/h] \qquad \exists S > 0$$

if

$$\|\vec{\delta}_n\| \leq \epsilon \quad \forall n \quad \Longrightarrow \quad \|\vec{z}_n - \vec{q}_n\| \leq S\epsilon$$

consistency of order p $\Longleftrightarrow$ convergence of order p

?

the error made at every step is $\sim o(h^{p+1})$

$\| \vec{q}_n - \underbrace{\vec{q}(t_n)}_{\text{exact}} \| \sim o(h^p)$

(ex. Euler $\vec{q}_{n+1} = \vec{q}_n + h \vec{f}(\vec{q}_n, t_n) + o(h^2)$

$p=1$)

Fundamental theorem of numerical analysis

$\boxed{\begin{array}{l}\text{consistency of order } p \\ \text{zero-stability}\end{array}} \Longleftrightarrow \boxed{\begin{array}{l}\text{convergence} \\ \text{of order } p\end{array}}$

Proof of zero-stability

s-step scheme

$$\sum_{j=0}^{s} \alpha_j \vec{q}_{n+j} = \vec{\Phi}_{\vec{f}} (\vec{q}_n, \dots, \vec{q}_{n+s} ; h, t_n)$$

characteristic polynomial

$$p(x) = \sum_j \alpha_j x^j$$

ex. RK

$$\vec{q}_{n+1} - \vec{q}_n = \sum_i b_i \vec{k}_i (\vec{q}_n, \vec{q}_{n+1}, \vec{f}, h, t_n)$$

$\alpha_0 = -1 \qquad \alpha_1 = 1$

$p(x) = x - 1$

Root condition

$$\boxed{\text{an } s\text{-step numerical scheme is s-stable}} \iff \boxed{\begin{array}{l} p(x) \text{ has roots } p(x_r)=0 \\ |x_r| \le 1, \text{ and roots with } |x_r| = 1 \text{ are simple ones} \end{array}}$$

$|x_r| = 1$ $\quad p(x) = \underbrace{(x - x_r)} \cdots$

RK schemes $\quad p(x) = x - 1 \quad x_r = 1$ ✓

↓

p-th order consistent RK scheme $\implies$ p-th order convergent

Why implicit methods?

s-step scheme

$$\sum_{j=0}^{s} \alpha_j \vec{q}_{n+j} = \vec{\Phi}_{\vec{f}}(\vec{q}_n, \dots, \vec{q}_{n+s}; h, t_n)$$

$\boxed{\text{Stiffness of ODEs}}$

↳ sensitivity to the size of the time step

convergence of order p $\quad \|\vec{q}_n - \vec{q}(t_n)\| \underset{h \to 0}{=} \left(\frac{h}{h_0}\right)^p$

how big is h_0?
The answer is method-dependent

<u>Example</u> :

$$\begin{cases} \dot{y} = -ay = f(y) \\ y(0) = y_0 \end{cases} \qquad (a>0)$$

$$y(t) = y_0 e^{-at}$$

<u>Forward Euler</u>

$$y_{n+1} = y_n - h a y_n = y_n(1-ha)$$

$$= y_{n-1}(1-ha)^2 = \dots$$

$$= \underset{(1)}{y_0}\, (1-ha)^{n+1}$$

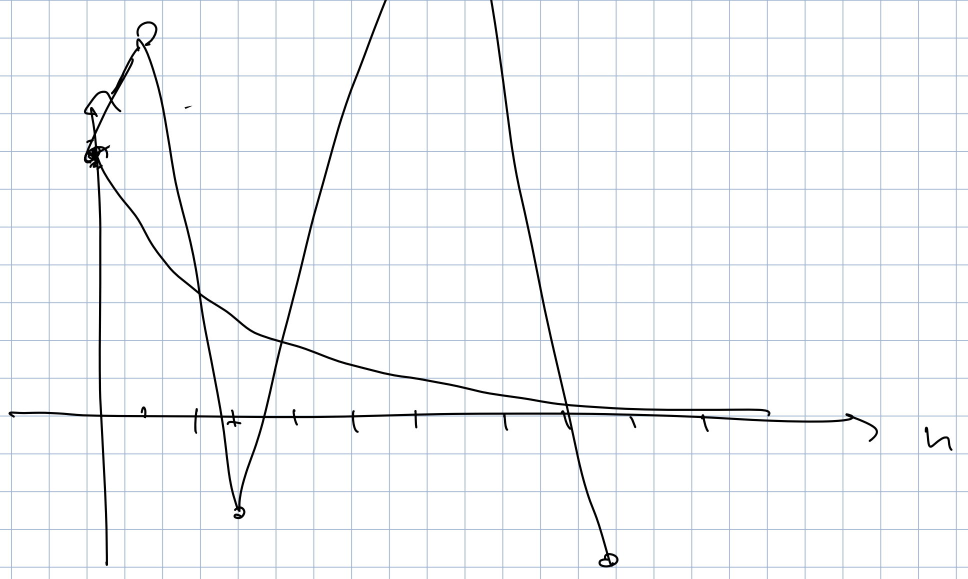
exp. decreasing with n if $|1-ha| < 1$

$$|1-ha|^n = e^{-n|\log|1-ha||}$$

$$|1-ha| < 1 \qquad ha < 2 \qquad \boxed{h < \frac{2}{a}}$$

<u>otherwise</u> :

$$|1-ha| > 1$$



Backward Euler :

$$y_{n+1} = y_n - ha\, y_{n+1}$$

$$y_{n+1} = \frac{y_n}{1+ha} = \dots = \frac{y_0}{(1+ha)^{n+1}}$$

$1+ha > 1$ exponentially decreasing regardless of h

Absolute stability (A - stability)

how does a scheme solve the following Cauchy problem?

$$\begin{cases} \dot{y} = +\lambda y \\ y(0) = y_0 \end{cases} \qquad \lambda \in \mathbb{C}$$

$$(\lambda = -a \in \mathbb{R})$$

Linear stability domain of a method = portion of the complex plane

$$\mathcal{D} = \{ h\lambda \in \mathbb{C} \mid y_n \xrightarrow[n \to \infty]{} 0 \}$$

example

Forward Euler:

$$\mathcal{D}_{FE} = \{ h\lambda \in \mathbb{C} \mid |1 + h\lambda| < 1 \}$$

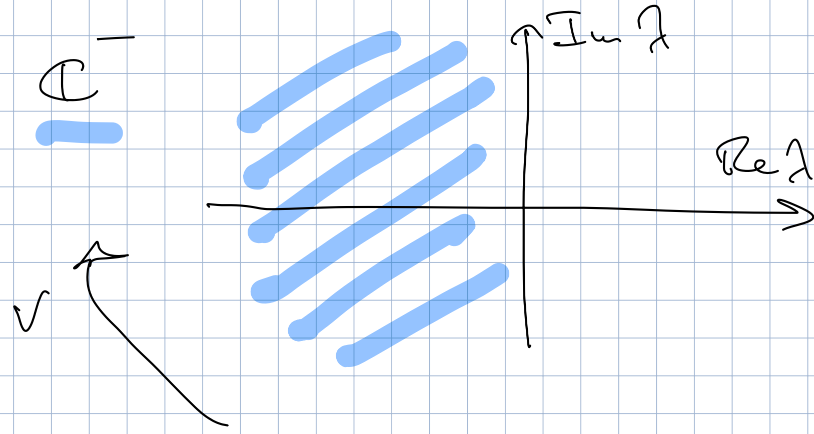
Backward Euler

$$\mathcal{D}_{BE} = \{ h\lambda \in \mathbb{C} \mid |1 - h\lambda| > 1 \}$$

$\uparrow$

prove that: $\operatorname{Re}\lambda < 0 \quad \forall h$

$$\mathcal{D}_{BE} \equiv \underline{\mathbb{C}^-}$$



A-stability of a method $=$ $\mathbb{C}^- \subseteq \mathcal{D}$

1) No explicit RK method is A-stable
2) Gauss-Legendre RK methods are A-stable

ex. $p=1$ implicit Euler

$p=2$ implicit mid point $\leftarrow$

...

Implicit methods: predictor-corrector method

simply: self-consistent solution defining an implicit method can be achieved (within the precision of the method) in one step

In general

f

$$\vec{y}_{n+1} = \vec{\mathcal{Y}}_n(\vec{y}_{n+1}, \vec{y}_n ; \vec{f}, h) + \underline{o(h^{p+1})}$$

the self-consistent solution may be costly.

But: finite error at each step

ex. implicit Euler

$$\vec{y}_{n+1} = \vec{y}_n + h \vec{f}(\vec{y}_{n+1}, t_{n+1})$$

explicit Euler: first guess

$$\vec{y}_{n+1}^{(0)} = \vec{y}_n + h \vec{f}(\vec{y}_n, t_n) + o(h^2)$$

"predictor"

$$\vec{y}_{n+1}^{(1)} = \vec{y}_n + \vec{f}(\vec{y}_{n+1}^{(0)}, t_{n+1}) + o(h^2) \quad \text{"corrector"}$$

$$|\vec{y}_{n+1}^{(1)} - \vec{y}_{n+1}^{(0)}| = o(h^2)$$

$$= \vec{y}_n + \vec{f}(\vec{y}_{n+1}^{(1)} + o(h^2), t_{n+1}) + o(h^2)$$

Other methods: multi-step methods $(s \geq 2)$

ex.: linear multi-step methods are not A-stable.

No linear multi-step method is symplectic (?)

Symplectic integration schemes

Solution of Hamilton's equations

particles described by $\vec{q}\,,\ \vec{p} \in \mathbb{R}^N$

positions, momenta

$$\vec{z} = (\vec{p}, \vec{q}) \in \mathbb{R}^{2N} \quad (N \text{ particles})$$

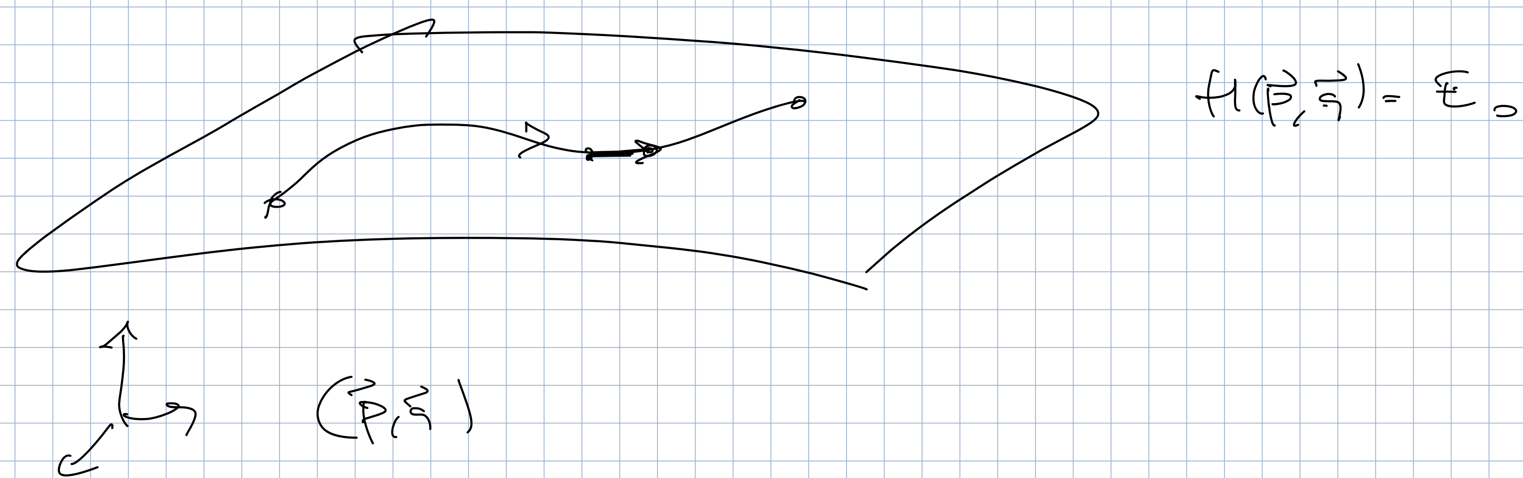
$$H = H(\vec{p}, \vec{q}, t) \quad \text{Hamiltonian}$$

$$\begin{cases} \dot{\vec{p}} = -\vec{\nabla}_{\vec{q}} H \\ \dot{\vec{q}} = \nabla_{\vec{p}} H \end{cases}$$

specific interest: closed systems (no time dependence)

solution

$$\frac{d}{dt} H(\vec{p}(t), \vec{q}(t)) = 0$$



numerical solution to Ham.'s equations will not conserve H exactly!

num. scheme: map $\vec{z}_n \to \vec{z}_{n+1}$

Property of Hamilton flow $(\vec{p}(t), \vec{q}(t)) = \vec{z}(t)$

$$\begin{cases} \dot{\vec{p}} = -\vec{\nabla}_q H \\ \dot{\vec{q}} = \vec{\nabla}_p H \end{cases}$$

$$\dot{\vec{z}} = \Big(\underbrace{-\vec{\nabla}_{\vec{q}} H}_{\dot{\vec{p}}}, \underbrace{\vec{\nabla}_{\vec{p}} H}_{\dot{\vec{q}}}\Big)$$

$$(\vec{\nabla}_{\vec{p}}, \vec{\nabla}_{\vec{q}}) H = \vec{\nabla} H$$

$$\dot{\vec{z}}(t) = J \, \vec{\nabla} H [\vec{z}(t)] \qquad J = \left(\begin{array}{c|c} 0 & -1\!\!1 \\ \hline 1\!\!1 & 0 \end{array}\right)$$

$1\!\!1_{N \times N}$

infinitesimal evolution $t \to t+h$

$$\frac{\vec{z}(t+h) - \vec{z}(t)}{h} = J \, \vec{\nabla} H [\vec{z}(t)] + o(h)$$

$$\vec{z}(t+h) = (1\!\!1 + h J \vec{\nabla} H [\cdot]) \; \vec{z}(t) + o(h^2)$$

map in phase space

$$\vec{\varphi} : \quad \vec{z} \in \mathbb{R}^{2N} \to \vec{z}' = J \vec{\nabla} H [\vec{z}] \in \mathbb{R}^{2N}$$

(matrix)

Jacobian of a map

$$L = \text{"}\frac{\partial \vec{\varphi}}{\partial \vec{z}}\text{"} = J \left\{ \frac{\partial^2 H}{\partial z_i \partial z_j} \right\}$$

$z_i = p_i, q_i$

$$\dots = h \left(\begin{array}{c|c} -H_{qp} & -H_{qq} \\ \hline H_{pp} & H_{pq} \end{array}\right) \to 4 \; N \times N \text{ blocks}$$

$$H_{qp} = \left\{ \frac{\partial^2 H}{\partial q_i \partial p_j} \right\} \qquad H_{qq} = \left\{ \frac{\partial^2 H}{\partial q_i \partial q_j} \right\}$$

$$= H_{pq} \qquad H_{pp} = \left\{ \frac{\partial^2 H}{\partial p_i \partial p_j} \right\}$$

property : $\underline{L^T J + J L = 0}$

(you can prove)

$\downarrow$

Hamilton flow : map $\vec{z}(0) \longrightarrow \vec{z}(t)$

$$\dot{\vec{z}}(t) = J \vec{\nabla} H [\vec{z}(t)]$$

formal solution :

$$\vec{z}(t) \overset{u}{=} \exp\left(t J \vec{\nabla} H\right) [\vec{z}(0)]$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \underbrace{J \vec{\nabla} H [J \vec{\nabla} H [\ldots J \vec{\nabla} H [\vec{z}(0)]] \ldots]}_{n \text{ times}}$$

Hamilton map

$$\vec{\vartheta} : \vec{z} \in \mathbb{R}^{2N} \to \vec{\vartheta}[\vec{z}] = \exp(t J \vec{\nabla} H) [\vec{z}]$$

$$\vec{\vartheta} = e^{t \vec{\varphi}}$$

Jacobian matrix

$$S = \frac{\partial \vec{\vartheta}}{\partial \vec{z}} = e^{tL}$$

$$L^T J + J L = 0$$

$$\boxed{S^T J S = J} \quad \text{symplectic matrices} \qquad J = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

(orthogonal matrices $S^T S = \mathbb{1}$) $\qquad \mathbb{1}_{2N\times 2N} = \begin{pmatrix} \mathbb{1}_{N\times N} & 0 \\ 0 & \mathbb{1}_{N\times N} \end{pmatrix}$

Symplectic integration scheme : map with a symplectic Jacobian

$$\vec{z}_{n+1} = \vec{\rho}\,(\vec{z}_n) \qquad \frac{d\vec{\rho}}{d\vec{z}} \text{ is a symplectic matrix}$$

$$\vec{\rho}\,[\vec{z}] = e^{hJ\vec{\nabla}K}\,[\vec{z}]$$

associated with a function $K = K(\vec{p}, \vec{q})$ which is conserved

$$K \simeq H$$

Are RK methods symplectic ?

M-matrix

$$M_{kl} = b_k a_{kl} + b_l a_{lk} - b_k b_l$$

$$\begin{array}{c|ccc|}
c_1 & a_{11} & a_{12} & \\
c_2 & & | & - \\
\vdots & & & \\
c_m & & | & \\
\hline
 & b_1 & - \; - & b_m
\end{array}$$

if $M = \emptyset$ $\Rightarrow$ symplectic

↳ zero matrix

ex. implicit mid-point rule

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array} \qquad b_1 = 1 \qquad a_{11} = \frac{1}{2}$$

Famous symplectic integrators: Verlet's scheme

Störmer-Verlet's schemes

$$H(\vec{z}) = \underbrace{T(\vec{p})}_{\text{kinetic}} + \underbrace{V(\vec{q})}_{\text{potential}}$$

$$e^{tJ\vec{\nabla}H} = e^{t(-\vec{\nabla}_q V,\ \vec{\nabla}_p T)}$$

$$= e^{t(\vec{Q}+\vec{R})}$$

$$\vec{R} = (-\vec{\nabla}_{\vec{q}} V,\ 0) \qquad \vec{Q} = (0,\ \vec{\nabla}_p T)$$

$$e^{t(\vec{Q}+\vec{R})} \neq e^{t\vec{Q}}\, e^{t\vec{R}} \qquad e^{A+B} \stackrel{?}{=} e^{A} e^{B}$$

for A, B matrices

$$\simeq e^{t\vec{Q}}_{T}\ e^{t\vec{R}}_{T} + O(t^2)$$

Verlet scheme $t \to t+h$

$$\vec{z}_{n+1} \simeq \mathbb{1} + h\vec{Q}\,\left[(\mathbb{1} + h\vec{R})\,[\vec{z}_n]\right]$$

$$\begin{cases} \vec{p}_{n+1} = \vec{p}_n - h\,\vec{\nabla}_q V(\vec{q}_n) \\ \vec{q}_{n+1} = \vec{q}_n + h\,\vec{\nabla}_p T(\vec{p}_{n+1}) \end{cases}$$

$\vec{p}_n$

Euler