Numerical integration of ODEs

- → implicit methods : predictor / corrector approach
- → multi-step methods
- → symplectic integration methods

Implicit methods

$$\begin{cases} \dot{\vec q} = \vec f(\vec q, t) \\ \vec q(0) = \vec q_0 \end{cases}$$

$$\vec q_{n+1} = \vec{\mathcal{Y}}_n(\overset{d}{\vec q_{n+1}}, \vec q_n, \dots)$$

ex. backward Euler

$$\vec q_{n+1} = \vec q_n + h\,\underline{\vec f(\vec q_{n+1}, t_n + h)}$$

$$\underline{\vec q^{\,(0)}_{n+1}} \to \vec q^{\,(1)}_{n+1} = \vec q_n + h\,\vec f(q^{(0)}_{n+1}, t_n + h) + o(\underline{\underline{h^2}})$$

$$\to \vec q^{\,(2)}_{n+1} =$$

"predictor"

good guess : Forward Euler

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

$$= \vec q_{n+1} + o(h^2)$$

"corrector"

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

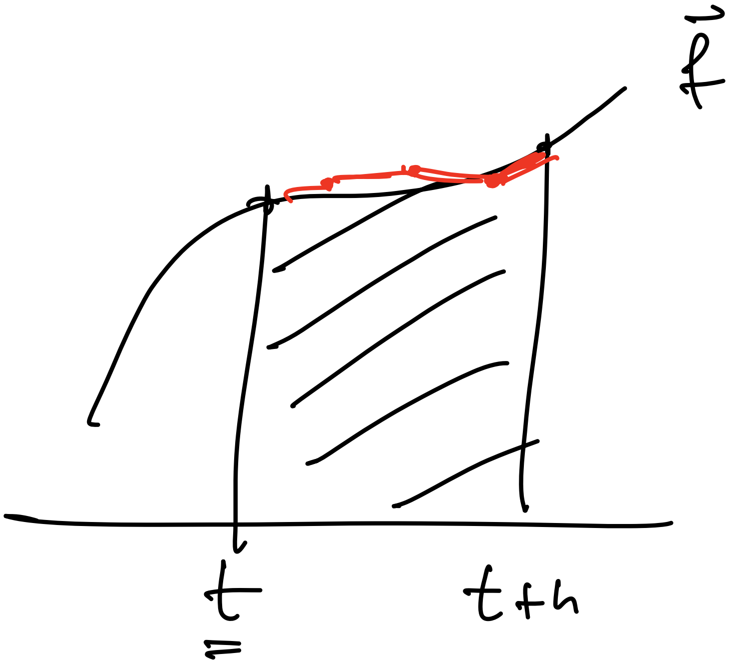
$$= \vec q_n + \boxed{h\,\vec f(\vec q_{n+1}, t_n + h)} + o(h^2)$$

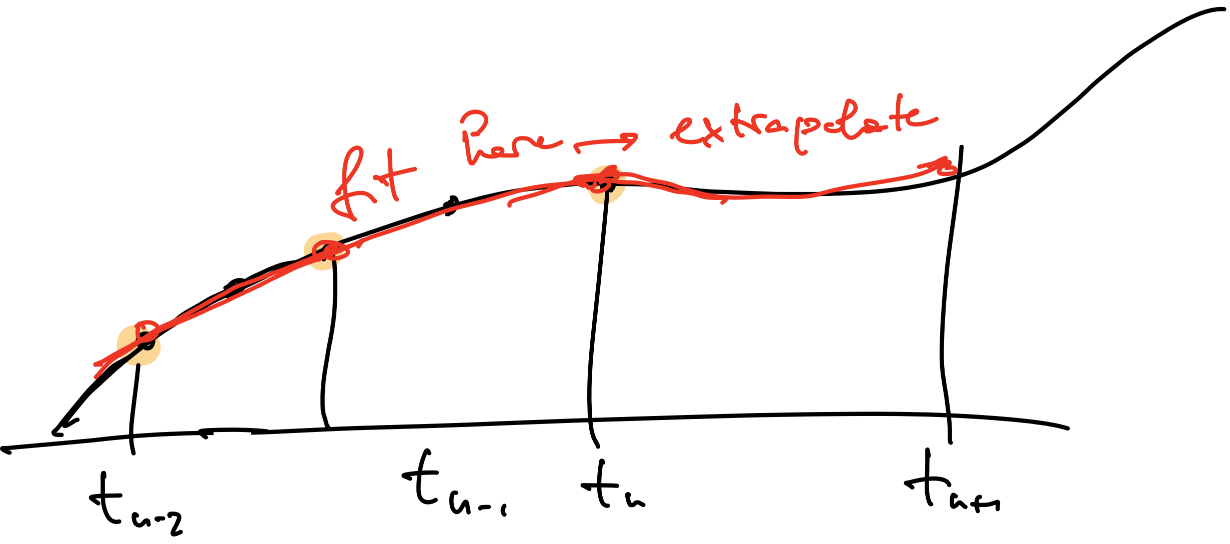
the same up to $\mathcal{O}(h^3)$

Order-p implicit method:

$\left\{\begin{array}{l} \text{one "predictor" step with order-p explicit method } \vec{q}^{\,(0)}_{n+1}; \\ \text{one "corrector" step} \rightarrow \vec{q}^{\,(1)}_{n+1} \end{array}\right.$

Multi-step methods (alternatives to RK)





s- step methods

$$\vec{y}_{n+1} = \underset{=}{\vec{y}_n}\left((\vec{y}_{n+1}), \vec{y}_n, \dots, \vec{y}_{\underline{n-s+1}}; \vec{f}, h\right)$$

<u>advantage</u>: s- step method can be of order $\underline{p=s}$

example (Adams- Bashforth)

$\underline{s=2}$

$$\vec{y}_{n+1} = \vec{y}_n + h\left[\frac{3}{2}\vec{f}(\vec{y}_n, t_n) - \frac{1}{2}\vec{f}(\vec{y}_{n-1}, t_{n-1})\right]$$

⊙ Explicit multi-step methods are not <u>A-stable</u>

⊙ Implicit multi-step methods are at most of order $\underline{p=2}$.

⊙ There are no multi-step which are <u>symplectic</u>

Symplectic integration methods

Goal : numerical integration method which conserve at least quantities exactly conserved by the problem

Hamilton's equations $\underline{\vec z} = (\vec p, \vec q) \in \mathbb{R}^{2N}$

$\vec p$: momenta

$\vec q$: positions

$$\mathcal{H}(\vec p, \vec q) \ : \quad \begin{cases} \dot{\vec p} = -\vec\nabla_{\vec q}\,\mathcal{H} \\ \dot{\vec q} = \vec\nabla_{\vec p}\,\mathcal{H} \end{cases}$$

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

conservation

$$(\vec p(0), \vec q(0)) \Rightarrow (\vec p(t), \vec q(t))$$ Hamiltonian flow

$$\dot{\underline{\vec z}} = \boxed{J}\, \vec\nabla_{\vec z}\,\mathcal{H}$$

$$(\dot{\vec p}, \dot{\vec q}) \quad \underset{-}{} \quad \Rightarrow \left(\vec\nabla_{\vec p}\mathcal{H},\ \overset{\perp}{\underline{\vec\nabla_{\vec q}\mathcal{H}}}\right)$$

$$J = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

$$\vec{z}(t+h) = \vec{z}(t) + h\, J \vec{\nabla}_{\vec{z}} \mathcal{H}[\vec{z}(t)] + \ldots$$

$$= \underbrace{\left(\mathbb{1} + \underbrace{\boxed{h}\, \underbrace{J \vec{\nabla}_{\vec{z}} \mathcal{H}[\;\cdot\;]}_{}}_{}\right)}_{} \vec{z}(t) + \ldots$$

$\vec{\varphi} : J \vec{\nabla} \mathcal{H}[\underline{\underline{\vec{z}}}] \to$ vector

map: $\vec{\varphi} : \vec{z} \in \mathbb{R}^{2N} \to \vec{\varphi}[\vec{z}] = \underline{\underline{\vec{z}'}}$

Jacobian of $\vec{\varphi}$

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

$\uparrow$

$$= \ldots \begin{pmatrix} -\mathcal{H}_{qp} & -\mathcal{H}_{qq} \\ \mathcal{H}_{pp} & \mathcal{H}_{pq} \end{pmatrix}$$

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

$\ldots$

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

Hamiltonian map

$$\vec{z}(0) \to \vec{z}(t)$$

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

formal solution

$$\vec{z}(t) = \underbrace{\exp\{t J \vec{\nabla}_z \mathcal{H}[.]\}}_{} [\vec{z}(0)]$$

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

$$= \mathbb{1} + t J \nabla_z \mathcal{H}[\vec{z}(0)]$$

$$+ \frac{t^2}{2} J \nabla_z \mathcal{H}[J \nabla_z \mathcal{H}[\vec{z}(0)]]$$

$$+ \cdots$$

Hamiltonian map

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

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

Jacobian matrix for $\vec{\vartheta}$

$$\underline{\underline{S}} = \frac{\partial \vec{\vartheta}}{\partial \vec{z}} = e^{t \underline{\underline{L}}}$$

$\underline{\underline{S}}$: $\boxed{S^T \underline{\underline{J}} S = \underline{\underline{J}}}$ <u>symplectic</u> matrix

$\uparrow$

orthogonal matrix $O^T \underline{\mathbb{1}} O = \underline{\mathbb{1}}$

<u>symplectic integrator</u> : numerical integration method with a symplectic Jacobian matrix

$$\vec{q} \to \vec{z}$$

$\vec{z}_n \to \vec{z}_{n+1}$ map

$$\vec{z}_{n+1} = \vec{\varrho}[\vec{z}_n]$$

Jacobian $\frac{d\vec{z}}{dZ} \rightarrow$ symplectic

IDEA : Hamilton flow is symplectic AND it conserves $\mathcal{H}$

=> any symplectic map conserves something

→ "hope" : something $\simeq \mathcal{H}$

How to build a symplectic method?

RK methods

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1m} \\ c_2 & \vert & & & \vert \\ \vdots & \vert & & & \vert \\ c_m & a_{m1} & & & a_{mm} \\ \hline & b_1 & b_2 & \cdots & b_m \end{array}$$

M matrix: $b_k a_{kl} + b_l a_{lk} - b_k b_l$

if $M = 0$ => method is symplectic

e.g. implicit midpoint $\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}$

$\underline{M=0}$

Building symplectic integrators

$$\mathcal{H}(\vec{z}) = T(\vec{p}) + U(\vec{q})$$

$$\downarrow$$

$$\dot{\vec{z}} = \left(-\nabla_q U(\vec{q}),\ \nabla_{\vec{p}} T(\vec{p})\right)$$

$$= \vec{Q}[\vec{z}] + \vec{R}[\vec{z}]$$

$$\vec{Q}[\vec{z}] = \left(0,\ \nabla_{\vec{p}} T(\cdot)\right)[\vec{p}, \vec{q}]$$

$$\vec{R}[\vec{z}] = \left(-\underline{\underline{\nabla_{\vec{q}}}} U(\cdot),\ 0\right)[\vec{p}, \underset{\uparrow}{\vec{q}}]$$

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

$$= \exp\left\{t\left(\vec{Q}[\cdot] + \vec{R}[\cdot]\right)\right\}[\vec{z}(0)]$$

$\vec{Q}$, $\vec{R}$ maps do not commute

$$\neq \exp(t\vec{Q})\left[\exp(t\vec{R})\,[\vec{z}(0)]\right]$$

$$\boxed{e^{h(\vec{Q}+\vec{R})} = e^{h\vec{Q}}\, e^{h\vec{R}} + \underline{O(h^2)}}$$

h small

$$e^{h(\vec{Q}+\vec{R})} = e^{h/2\,\vec{Q}}\, e^{h\vec{R}}\, e^{h/2\,\vec{Q}} + O(h^3)$$

$$\simeq (\mathbb{1}+h\vec{Q})(\mathbb{1}+h\vec{R}) + O(h^2)$$

defines a method of order 1

$$(\mathbb{1}+h\vec{Q})(\mathbb{1}+h\vec{R})\,(\vec{p}(t), \vec{q}(t)) + O(h^2)$$

$$= (\mathbb{1}+h\vec{Q})\Big[\underbrace{(\vec{p}(t), \vec{q}(t)) + h\,(-\nabla_q U(\vec{q}(t)), 0)}_{(\underbrace{\vec{p}(t) - h\nabla_{\vec{q}} U}_{\vec{p}(t+h) + O(h^2)},\ \vec{q}(t))}\Big] \quad O(h^2)$$

$$= (\vec{p}(t+h), \vec{q}(t)) + h\,(0, \nabla_{\vec{p}} T(\vec{p}(t+h))) + O(h^2)$$

$$= \left(\vec{p}(t+h),\ \vec{q}(t+h)\right) + o(h^2)$$

$$\left\{\begin{aligned} \vec{p}(t+h) &= \vec{p}(t) - h\,\nabla_{\vec{q}}\, U(\vec{q}(t)) \\ \vec{q}(t+h) &= \vec{q}(t) + h\,\nabla_{\vec{p}}\, T(\vec{p}(t+h)) \end{aligned}\right]$$

Verlet's method

$$\left\{\begin{aligned} \vec{p}_{n+1} &= \vec{p}_n - h\,\nabla_q\, U(\vec{q}_n) \\ \vec{q}_{n+1} &= \vec{q}_n + h\,\nabla_p\, T(\vec{p}_{n+1}) \end{aligned}\right.$$