3. Symplectic integration

The main motivation are Hamiltonian systems.
Let $p, q \in \mathbb{R}^d$ solution of

$$\begin{cases} p' = -\dfrac{\partial H}{\partial q}(p,q) & , \quad p(0) = p_0 \\ q' = \dfrac{\partial H}{\partial p}(p,q) & , \quad q(0) = q_0 \end{cases}$$

Introduce $y \in \mathbb{R}^{2d}$, $y = \begin{pmatrix} p \\ q \end{pmatrix}$. Then:

$$\begin{cases} y' = J^{-1} \nabla H(y) \\ y(0) = y_0 \end{cases} , \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

I $d \times d$ identity

Besides $H(y(t)) = \text{constant}$, the system $y' = J^{-1} \nabla H(y)$ has the property that its flow φ_t is "symplectic". What does this mean?

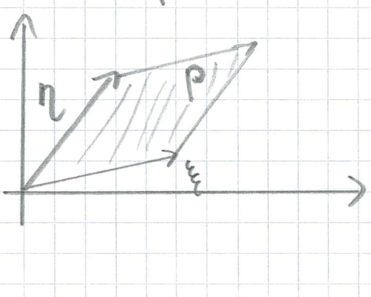
Symplectic transformation:

Linear case: Consider $\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix}$, $\eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix} \in \mathbb{R}^{2d}$

$$\xi^p, \xi^q, \eta^p, \eta^q \in \mathbb{R}^d$$

Define $d=1$: $\omega(\xi, \eta) = \det \begin{pmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{pmatrix} = \xi^p \eta^q - \eta^p \xi^q$

(oriented) area of P:



$d>1$: $\omega(\xi,\eta) = \sum_{i=1}^{d} \det\begin{pmatrix} \xi_i^p & \eta_i^p \\ \xi_i^q & \eta_i^q \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^p \eta_i^q - \eta_i^p \xi_i^q)$

sum of the areas of the projections of some hyper-parallelogram identified by (ξ,η).

Lemma 1: $\omega(\xi,\eta) = \xi^T J \eta$, $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.

with $I \in \mathbb{R}^{d \times d}$.

Proof:

$$\xi^T J \eta = \xi \circ \begin{pmatrix} \eta_1^q \\ \vdots \\ \eta_d^q \\ -\eta_1^p \\ \vdots \\ -\eta_d^p \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^p \eta_i^q - \eta_i^p \xi_i^q) = \omega(\xi,\eta).$$

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Defn.: (symplectic)

A linear map $A: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if

$$A^T J A = J.$$

(Recall: $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$)

Lemma 2: A is symplectic $\iff \omega(A\xi, A\eta) = \omega(\xi,\eta)$ $\forall \xi,\eta \in \mathbb{R}^{2d}$.

Proof: Let A be symplectic:

$\Rightarrow$: $\omega(A\xi, A\eta) \overset{\text{Lemma 1}}{=} \xi^T A^T J A \eta = \xi^T J \eta = \omega(\xi,\eta)$.

$\Leftarrow$: Let $\omega(A\xi, A\eta) = \omega(\xi,\eta)$ $\forall\, \xi,\eta \in \mathbb{R}^{2d}$.

Take $\xi = e_i$, $\eta = e_j$ for some $i,j \in \{1,\dots,2d\}$

$$\overset{\text{Lemma 1}}{\Rightarrow} \quad \underbrace{e_i^T A^T J A e_j}_{(A^TJA)_{ij}} = \underbrace{e_i^T J e_j}_{(J)_{ij}}$$

$$\Rightarrow \quad A^TJA = J \quad \Rightarrow \quad A \text{ is symplectic.}$$

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Rem: In $d=1$: symplecticity $\Leftrightarrow$ volume preserving.

Nonlinear case:

Defn.: (symplectic)

Let $U \subset \mathbb{R}^{2d}$ be an open set.
A differentiable map $g: U \to \mathbb{R}^{2d}$ is called symplectic if $\forall\, y \in U$ it holds

$$g'(y)^T J g'(y) = J \quad . \qquad (g': \text{Jacobian})$$

Likewise, by Lemma 2, g is called symplectic if

$$\omega(g'(y)\xi, g'(y)\eta) = \omega(\xi,\eta) \quad \forall\, \xi,\eta \in \mathbb{R}^{2d},\ y \in U.$$

Lemma: Let $U \subset \mathbb{R}^{2d}$ open, bounded and $\mathrm{Vol}(U) = \int_U dy$.

Then, if $g: U \to \mathbb{R}^{2d}$ is symplectic, then

$$\mathrm{Vol}(g(U)) = \mathrm{Vol}(U).$$

Proof:

$$\int_{g(U)} dy \overset{\substack{\text{change of variable}\\ \downarrow}}{=} \int_U |\det g'(y)|\, dy$$

Now, $g'(y)^T J g'(y) = J$, $\det(J) = 1$
$\uparrow$ g symplectic

$$\Rightarrow (\det(g'(y)))^2 = \det(J) = 1 \Rightarrow |\det(g'(y))| = 1$$

$$\Rightarrow \mathrm{Vol}(g(U)) = \mathrm{Vol}(U).$$

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Rem: Volume preservation $\overset{\text{(counter-example see exercises)}}{\not\Rightarrow}$ symplecticity
$\Leftarrow$

Goal: Flow of Hamiltonian ODE is symplectic.

Preparation: Variational equation

Consider $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$ and $\varphi_t(y_0) = y(t)$ (flow)

Define $\psi(t) = \frac{\partial}{\partial y_0} \varphi_t(y_0)$

$$\Rightarrow \frac{d}{dt}\psi(t) = \frac{d}{dt}\frac{\partial}{\partial y_0}\varphi_t(y_0) = \frac{\partial}{\partial y_0}\frac{d}{dt}\varphi_t(y_0)$$

$$\overset{\frac{d}{dt}\varphi_t = f\circ\varphi_t \text{ (see previous lectures)}}{=} \frac{\partial}{\partial y_0} f(\varphi_t(y_0))$$

$$\overset{\text{chain rule}}{=} f'(\varphi_t(y_0))\frac{\partial}{\partial y_0}\varphi_t(y_0)$$

$$= f'(\varphi_t(y_0))\,\psi(t)$$

$\Rightarrow \psi(t)$ satisfies $\begin{cases} \psi'(t) = f'(\varphi_t(y_0))\,\psi(t) \\ \psi(0) = I \end{cases}$ variational equation associated to $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$.

Rem: If f is Lipschitz continuous and $\frac{\partial f}{\partial y}$ exists and is continuous, then the above formal computation can be justified.

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Theorem: (Poincaré, 1899)

Let $H: U \to \mathbb{R}$ be twice $\overset{\text{cont.}}{\text{differentiable}}$.
Then $\forall t$ the flow φ_t of

$$\begin{cases} y' = J^{-1} \nabla H(y) \\ y(0) = y_0 \end{cases}$$

(Hamiltonian ODE)

is symplectic.

Proof: Consider $\Psi(t) = \frac{\partial}{\partial y_0} \varphi_t(y_0)$:

$$\begin{cases} \Psi'(t) = J^{-1} \overset{\leftarrow \text{ Hessian matrix}}{\nabla^2 H(\varphi_t(y_0))}\, \Psi(t) \\ \Psi(0) = I \end{cases}$$

(variational equation) associated to the Hamiltonian ODE

We need to show that

$$\frac{\partial}{\partial y_0} \varphi_t(y_0)^T \, J \, \frac{\partial}{\partial y_0} \varphi_t(y_0) = J$$

or in other terms

$$\Psi(t)^T J \, \Psi(t) = J .$$

Observe that for $t=0$: $\Psi(0)^T J \, \Psi(0) = J$.
Hence, we have to show that $\frac{d}{dt}\left(\Psi(t)^T J \, \Psi(t)\right) = 0$.

Indeed,

$$\frac{d}{dt}\left(\Psi(t)^T J \Psi(t)\right) = \Psi'(t)^T J \, \Psi(t) + \Psi(t)^T J \, \Psi'(t)$$

$$= \Psi(t)^T \nabla^2 H(\varphi_t(y_0)) \overbrace{J^{-T} J}^{=-I} \Psi(t)$$

$$+ \Psi(t)^T \underbrace{J J^{-1}}_{=I} \nabla^2 H(\varphi_t(y_0)) \Psi(t)$$

$$= 0 .$$

J is antisym.
$\Rightarrow J^T = -J$
$\Rightarrow J^{-T} \cdot J = -I$.

(we used that $\nabla^2 H(y) = (\nabla^2 H(y))^T$ since H is twice $\overset{\text{cont.}}{\text{diff.}}$

Thus, $\Psi(t)^T J \, \Psi(t) = \Psi(0)^T J \, \Psi(0) = J$.
(hence, the flow is symplectic).

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Rem.: If we take $f(y) = J^{-1} \nabla H(y)$

$$\begin{cases} y' = f(y) \\ \Psi' = f'(y)\Psi \end{cases} \Rightarrow \Psi^T J \Psi \text{ is a quadratic first integral.}$$

Goal 2: If an ODE has a symplectic flow, then it is Hamiltonian (true only locally).

Defn.: (locally Hamiltonian)

An ODE $y' = f(y)$, $f: U \to \mathbb{R}^{2d}$ is called locally Hamiltonian,

if $\forall y_0 \in U$ $\exists$ a neighbourhood V of y_0 and a function $H: V \to \mathbb{R}$ s.t.

$$f(y) = J^{-1} \nabla H(y) \quad \forall y \in V.$$

Theorem: let $f: U \to \mathbb{R}^{2d}$ be cont. differentiable with $U \subset \mathbb{R}^{2d}$.

Then $y' = f(y)$ is locally Hamiltonian

$\Leftrightarrow$ Its flow φ_t is symplectic for any initial condition and t small enough.

Preparation for the proof:

Lemma: (Euler - Lagrange)

With the notation above, assume that $f'(y)$ is symmetric $\forall y \in U$. Then $\forall y_0 \in U$, $\exists$ a neighbourhood V of y_0 and a function $H: V \to \mathbb{R}$ s.t.

$$f(y) = \nabla H(y) \quad \forall y \in V.$$

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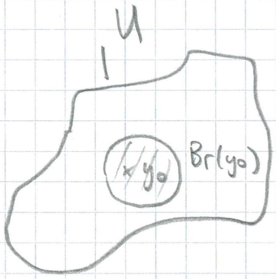
Proof: (of the lemma)

Assume WLOG $y_0 = 0$ and

ball $\to$ $B_r(0) = \{ y \in U : \|y\| < r \} \subset U$



Define for any $y \in B_r(0)$

$$H(y) = \int_0^1 y^T f(ty)\,dt .$$

Then, for all $k = 1, 2, \dots, d$,

$$\frac{\partial H}{\partial y_k}(y) = \int_0^1 \frac{\partial}{\partial y_k}\left(\sum_{i=1}^d y_i f_i(ty)\right) dt$$

$$= \int_0^1 \left(f_k(ty) + \sum_{i=1}^d t y_i \frac{\partial f_i}{\partial y_k}(ty)\right) dt$$

$$\overset{f' \text{ symm.}}{=} \int_0^1 \left(f_k(ty) + \sum_{i=1}^d t y_i \frac{\partial f_k}{\partial y_i}(ty)\right) dt$$

$$= \int_0^1 \frac{d}{dt}\left(t f_k(ty)\right) dt$$

$$= f_k(y) .$$

Hence, $f(y) = \nabla H(y)$. #

<u>Proof:</u> (of the theorem)

$\Longrightarrow$: follows from the Poincaré theorem.

$\Longleftarrow$: let φ_t be the flow of $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$

and assume that φ_t is symplectic for any $y_0 \in U$, t small enough.

Introduce $\Psi(t) = \frac{\partial}{\partial y_0} \varphi_t(y_0)$ so that

$$\begin{cases} \Psi'(t) = f'(\varphi_t(y_0))\Psi(t) \\ \Psi(0) = I \end{cases}$$

Then, φ_t symplectic $\Rightarrow \Psi^T J \Psi = J$,

hence,

$$0 = \frac{d}{dt}(\Psi(t)^T J \Psi(t)) = \Psi'(t)^T J \Psi(t) + \Psi(t)^T J \Psi'(t)$$

$$= \Psi(t)^T f'(\varphi_t(y_0))^T J \Psi(t) + \Psi(t)^T J f'(\varphi_t(y_0))\Psi(t)$$

$$= \Psi(t)^T \left(f'(\varphi_t(y_0))^T J + J f'(\varphi_t(y_0)) \right) \Psi(t)$$

Take $t = 0$, so that $\Psi(0) = I$, $\varphi_0(y_0) = y_0$ and

$\Rightarrow f'(y_0)^T J + J f'(y_0) = 0$

$\Rightarrow J f'(y_0) = -f'(y_0)^T J \overset{J \text{ anti-sym.}}{=} (J f'(y_0))^T$

$\Rightarrow \forall y_0 \in U$, $J f'(y_0)$ is symmetric.

$\Rightarrow \forall y_0 \in U$, $\exists\, V \subset U$, $H: V \to \mathbb{R}$ s.t.

Jacobian

$\forall y \in V \quad J f(y) = \nabla H(y)$

$\Rightarrow f(y) = J^{-1} \nabla H(y) \quad \forall y \in V.$ #

4. Symplectic numerical methods

Defn: (Symplectic method)

Let $\Phi_h : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be the numerical flow of a one-step method. We call the method symplectic, if Φ_h is a symplectic map whenever the method is applied to a smooth Hamiltonian ODE.

Proposition: The symplectic Euler method is symplectic.

Recall:
$$\begin{cases} p = -\dfrac{\partial H}{\partial q}(p,q) \\ q = \dfrac{\partial H}{\partial p}(p,q) \end{cases}$$

Symplectic Euler:
$$\begin{cases} p_1 = p_0 - h \dfrac{\partial H}{\partial q}(p_1, q_0) \\ q_1 = q_0 + h \dfrac{\partial H}{\partial p}(p_1, q_0). \end{cases}$$

Proof: Exercises.

How to study symplecticity for RK methods systematically?

Lemma: (Bochev & Scovel 1994)
For a RK method the following diagram commutes:

$$\begin{tikzcd}
y' = f(y),\ y(0) = y_0 \arrow[r, "\frac{\partial}{\partial y_0}"] \arrow[d, "RK"] & \begin{cases} y' = f(y),\ y(0) = y_0 \\ \Psi' = f'(y)\Psi,\ \Psi(0) = I \end{cases} \arrow[d, "RK"] \\
\{y_n\}_{n\geq 0} \arrow[r, "\frac{\partial}{\partial y_0}"] & \{y_n, \Psi_n\}_{n \geq 0}
\end{tikzcd}$$

① ②

Ex: Euler explicit

① $y_1 = y_0 + h f(y_0)$

$\dfrac{\partial y_1}{\partial y_0} = I + h \dfrac{\partial f}{\partial y_0}(y_0) I$

② $y_1 = y_0 + h f(y_0)$

$\Psi_1 = I + h \dfrac{\partial f}{\partial y}(y_0) I$

$\Rightarrow$ ① = ②

Proof: Consider $y' = f(y)$, $\Psi' = f'(y)\Psi$, apply RK:

$$g_i = y_n + h \sum_{j=1}^{s} a_{ij} f(g_j) \qquad k_i = f(g_i)$$

$$G_i = \Psi_n + h \sum_{j=1}^{s} a_{ij} f'(g_j) G_j \qquad K_i = f'(g_i) G_i$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(g_i)$$

$$\Psi_{n+1} = \Psi_n + h \sum_{i=1}^{s} b_i f'(g_i) G_i$$

(the desired result holds, if $\Psi_{n+1} = \frac{\partial}{\partial y_0} y_{n+1}$)

For $n=0$: $\frac{\partial}{\partial y_0} y_0 = I = \Psi_0$ ✓

Suppose $\frac{\partial y_n}{\partial y_0} = \Psi_n$ (*)

Then
$$\frac{\partial g_i}{\partial y_0} \overset{\text{chain rule}}{=} \frac{\partial y_n}{\partial y_0} + h \sum_{j=1}^{s} a_{ij} f'(g_j) \frac{\partial g_j}{\partial y_0}$$

$$\overset{(*)}{=} \Psi_n + h \sum_{j=1}^{s} a_{ij} f'(g_j) \frac{\partial g_j}{\partial y_0}$$

$\Rightarrow \frac{\partial g_i}{\partial y_0} = G_i$ (they solve the same matrix equation)

$$\Rightarrow \frac{\partial y_{n+1}}{\partial y_0} \overset{(*)}{=} \Psi_n + h \sum_{i=1}^{s} b_i f'(g_i) \frac{\partial g_i}{\partial y_0}$$

$$= \Psi_n + h \sum_{i=1}^{s} b_i f'(g_i) G_i$$

$$= \Psi_{n+1}.$$

Hence, by induction, the result holds.

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