Symplectic Neural Flows for Modelling and Discovery

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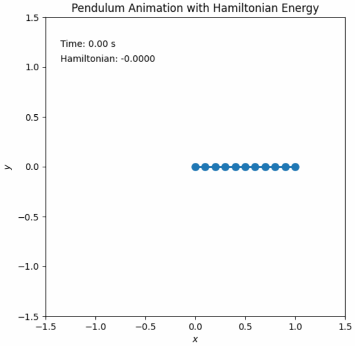
Motivation


Pendulum Animation with Hamiltonian Energy
Time: 0.00 s
Hamiltonian: -0.0000
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
y
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
x

Canonical Hamiltonian equations

- The equations of motion of canonical Hamiltonian systems write

$$\begin{cases} \dot{\mathbf{x}} = \mathbb{J}\nabla H(\mathbf{x}) = X_H(\mathbf{x}) \in \mathbb{R}^{2n} \\ \mathbf{x}(0) = \mathbf{x}_0 \end{cases}, \quad \mathbb{J} = \begin{bmatrix} 0 & I_n \\ -I_n & 0_n \end{bmatrix} \in \mathbb{R}^{2n\times 2n}. \tag{1}$$

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- Denoted with $\phi_{H,t} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ the exact flow of (1), $\phi_{H,t}(\mathbf{x}_0) = \mathbf{x}(t)$, we have that
  - $$\frac{d}{dt}H(\phi_{H,t}(\mathbf{x}_0)) = \nabla H(\phi_{H,t}(\mathbf{x}_0))^\top \mathbb{J}\nabla H(\phi_{H,t}(\mathbf{x}_0)) = 0,$$

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  - the flow preserves the canonical volume form of $\mathbb{R}^{2n}$.

Symplectic numerical methods

A one-step numerical method $\varphi^h : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is symplectic if and only if when applied to a Hamiltonian system the map φ^h is symplectic, i.e.,

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Symplectic and energy preserving methods

Let $\dot{\mathbf{x}} = \mathbb{J}\nabla H(\mathbf{x})$ be a Hamiltonian system with Hamiltonian H and no conserved quantities other than H. Let φ^h be a symplectic and energy-preserving method for the Hamiltonian system. Then φ^h reproduces the exact solution up to a time re-parametrisation.

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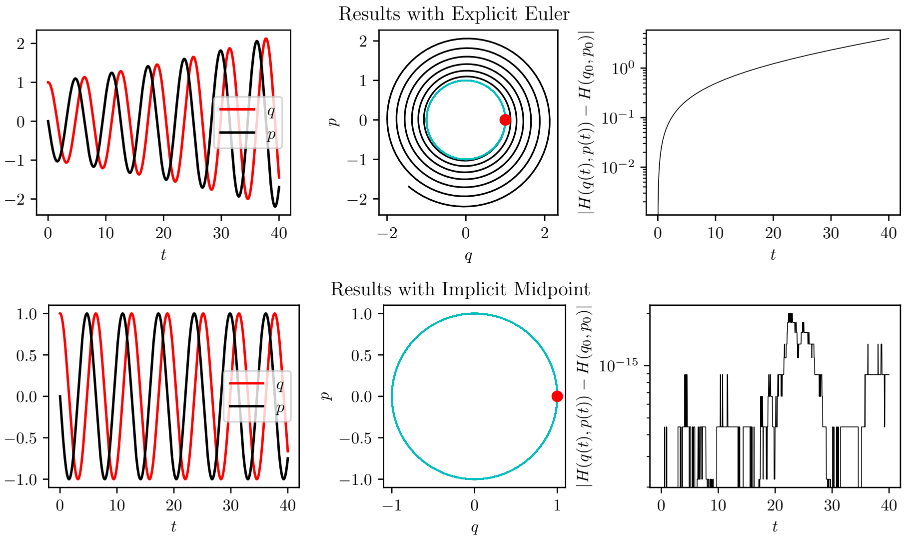
Informal theorem

A symplectic method almost conserves the Hamiltonian for an exponentially long time.

Example: simple harmonic oscillator



Forward invariant subset of the phase space

- Suppose $\mathbf{x}(t) \in \Omega \subset \mathbb{R}^{2n}$, whenever $\mathbf{x}(0) \in \Omega$, for any $t \geq 0$.

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- By the group property of the flow map, we know that

$$\phi_{H,n\Delta t+\delta t} = \phi_{H,\delta t} \circ \underbrace{\phi_{H,\Delta t} \circ \dots \circ \phi_{H,\Delta t}}_{n \text{ times}}, \quad n \in \mathbb{N},\ \delta t \in (0, \Delta t).$$

  As a consequence, to approximate $\phi_{H,t} : \Omega \to \Omega$ for any $t \geq 0$, we only have to approximate it for $t \in [0, \Delta t]$.

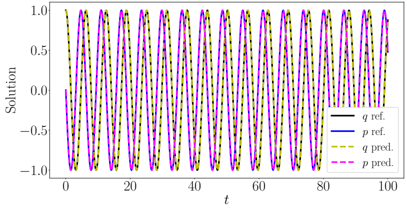

Figure 2: Neural network trained to approximate $\phi_{H,t}$ for $t \in [0, \Delta t = 1]$ and applied up to $T = 100$.

Two learning problems associated to Hamiltonian systems

Unsupervised solution of the Hamiltonian equations

Approximate the flow map $\phi_{H,t} : \Omega \to \Omega$, for any $t \geq 0$, on a compact forward invariant set $\Omega \subset \mathbb{R}^{2n}$, given the Hamiltonian energy $H : \mathbb{R}^{2n} \to \mathbb{R}$.

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Supervised approximation of an unknown Hamiltonian flow map

Approximate the flow map $\phi_{H,t} : \Omega \to \Omega$, for any $t \geq 0$, on a compact forward invariant set $\Omega \subset \mathbb{R}^{2n}$, given trajectory segments $\{(\mathbf{x}_0^n, \mathbf{y}_1^n, \dots, \mathbf{y}_M^n)\}_{n=1}^N$, $\mathbf{y}_m^n \approx \phi_{H,t_m^n}(\mathbf{x}_0^n)$.

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Remark: Given the several known qualitative properties of $\phi_{H,t}$, we want to leverage them when designing the approximating map.

The SympFlow

- We now build a neural network that approximates $\phi_{H,t} : \Omega \to \Omega$ for a forward invariant set $\Omega \subset \mathbb{R}^{2n}$, and $t \in [0, \Delta t]$, while reproducing the qualitative properties of $\phi_{H,t}$.

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- We rely on two building blocks, which applied to $(\mathbf{q},\mathbf{p})\in\mathbb{R}^{2n}$ write:

$$\phi_{\mathbf{p},t}((\mathbf{q},\mathbf{p}))=\begin{bmatrix}\mathbf{q}\\ \mathbf{p}-(\nabla_{\mathbf{q}}V(t,\mathbf{q})-\nabla_{\mathbf{q}}V(0,\mathbf{q}))\end{bmatrix},\ \phi_{\mathbf{q},t}((\mathbf{q},\mathbf{p}))=\begin{bmatrix}\mathbf{q}+(\nabla_{\mathbf{p}}K(t,\mathbf{p})-\nabla_{\mathbf{p}}K(0,\mathbf{p}))\\ \mathbf{p}\end{bmatrix}.$$

The `SympFlow`

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- The `SympFlow` architecture is defined as

$$\mathcal{N}_\theta\,(t, (\mathbf{q}_0, \mathbf{p}_0)) = \phi^L_{\mathbf{p},t} \circ \phi^L_{\mathbf{q},t} \circ \cdots \circ \phi^1_{\mathbf{p},t} \circ \phi^1_{\mathbf{q},t}((\mathbf{q}_0, \mathbf{p}_0)),$$

with

$$V^i(t,\mathbf{q}) = \ell_{\theta_3^i} \circ \sigma \circ \ell_{\theta_2^i} \circ \sigma \circ \ell_{\theta_1^i}\left(\begin{bmatrix} \mathbf{q} \\ t \end{bmatrix}\right), \quad K^i(t,\mathbf{p}) = \ell_{\rho_3^i} \circ \sigma \circ \ell_{\rho_2^i} \circ \sigma \circ \ell_{\rho_1^i}\left(\begin{bmatrix} \mathbf{p} \\ t \end{bmatrix}\right)$$

$$\ell_{\theta_k^i}(x) = A_k^i x + a_k^i, \;\; \ell_{\rho_k^i}(x) = B_k^i x + b_k^i, \;\; k = 1,2,3, \;\; i = 1, ..., L.$$

Properties of the SympFlow

- The SympFlow is symplectic for every time $t \in \mathbb{R}$. The building blocks we compose are exact flows of time-dependent Hamiltonian systems:

$$\phi^i_{\mathbf{p},t}((\mathbf{q},\mathbf{p})) = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} - \left(\nabla_{\mathbf{q}} V^i(t,\mathbf{q}) - \nabla_{\mathbf{q}} V^i(0,\mathbf{q})\right) \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{q} \\ \mathbf{p} - \nabla_{\mathbf{q}} \left(\int_0^t \partial_s V^i(s,\mathbf{q}) ds\right) \end{bmatrix} = \phi_{\widetilde{V}^i,t}((\mathbf{q},\mathbf{p})),$$

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- The `SympFlow` is the exact solution of a time-dependent Hamiltonian system.

Composition of Hamiltonian flows[1]

Theorem (The Hamiltonian flows are closed under composition)

Let $H^1, H^2 : \mathbb{R} \times \mathbb{R}^{2n} \to \mathbb{R}$ be continuously differentiable functions. Then, the map $\phi_{H^2,t} \circ \phi_{H^1,t} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is the exact flow of the time-dependent Hamiltonian system defined by the Hamiltonian function

$$H^3(t, \mathbf{x}) = H^2(t, \mathbf{x}) + H^1\left(t, \phi^{-1}_{H^2,t}(\mathbf{x})\right).$$

- This theorem implies that there is a Hamiltonian function $\mathcal{H}(\mathcal{N}_\theta) : \mathbb{R} \times \mathbb{R}^{2n} \to \mathbb{R}$ such that
$$\mathcal{N}_\theta\left(t, \mathbf{x}\right) = \phi_{\mathcal{H}(\mathcal{N}_\theta),t}(\mathbf{x})$$
for every $t \geq 0$ and $\mathbf{x} \in \mathbb{R}^{2n}$.

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[1] Leonid Polterovich. *The Geometry of the Group of Symplectic Diffeomorphisms*. Lectures in Mathematics ETH Zürich. Basel: Springer Basel AG, 2001. ISBN: 978-3-7643-6432-8.

Extension of the `SympFlow` outside of $[0, \Delta t]$

- Once we have trained $\mathcal{N}_\theta$ to be reliable for $t \in [0, \Delta t]$, we extend it for longer times as

$$\psi\left(t, \mathbf{x}_0\right) := \bar{\psi}_{t-\Delta t\lfloor t/\Delta t\rfloor} \circ \left(\bar{\psi}_{\Delta t}\right)^{\lfloor t/\Delta t\rfloor}\left(\mathbf{x}_0\right),$$

for $t \in [0, +\infty)$ and $\mathbf{x}_0 \in \Omega \subset \mathbb{R}^{2n}$, where

$$\begin{aligned}
\bar{\psi}_s\left(\mathbf{x}_0\right) &:= \mathcal{N}_\theta\left(s, \mathbf{x}_0\right), \; s \in [0, \Delta t), \\
\left(\bar{\psi}_{\Delta t}\right)^k &:= \underbrace{\bar{\psi}_{\Delta t} \circ \cdots \circ \bar{\psi}_{\Delta t}}_{k \text{ times}}, \; k \in \mathbb{N}.
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- $\psi(t, \cdot) = \phi_{\widetilde{H},t}$ for the piecewise continuous Hamiltonian

$$\widetilde{H}\left(t, \mathbf{x}\right) := \mathcal{H}\left(\mathcal{N}_\theta\right)\left(t - \Delta t\lfloor t/\Delta t\rfloor, \mathbf{x}\right).$$

Universal Approximation Theorem

Theorem

Let $H : \mathbb{R} \times \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}^{2n}$ compact, be a continuously differentiable function. For any $\varepsilon > 0$, there is a `SympFlow` $\bar{\psi}_t$ *such that*

$$\sup_{\substack{t \in [0, \Delta t] \\ \mathbf{x} \in \Omega}} \left\| \bar{\psi}_t(\mathbf{x}) - \phi_{H,t}(\mathbf{x}) \right\|_\infty < \varepsilon.$$

Training of the SympFlow to solve $\dot{\mathbf{x}}(t) = X_H(\mathbf{x}(t))$

- The SympFlow is based on modelling the scalar-valued potentials $\widetilde{V}^i, \widetilde{K}^i : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ with feed-forward neural networks.

- To train the overall model $\mathcal{N}_\theta$ we minimise the loss function

$$\mathcal{L}(\theta) = \underbrace{\frac{1}{N_r}\sum_{i=1}^{N_r}\left\| \frac{d}{dt}\mathcal{N}_\theta\left(t, \mathbf{x}_0^i\right)\Big|_{t=t_i} - \mathbb{J}\nabla H\left(\mathcal{N}_\theta\left(t_i, \mathbf{x}_0^i\right)\right)\right\|_2^2}_{\text{Residual term}}$$

$$+ \underbrace{\frac{1}{N_m}\sum_{j=1}^{N_m}\left(\mathcal{H}(\mathcal{N}_\theta)(t_j, \mathbf{x}^j) - H(\mathbf{x}^j)\right)^2}_{\text{Hamiltonian matching}},$$

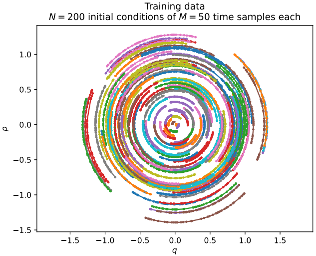
where we sample $t_i, t_j \in [0, \Delta t]$, and $\mathbf{x}_0^i, \mathbf{x}^i \in \Omega \subset \mathbb{R}^{2n}$.

Supervised training of the `SympFlow` to approximate $\phi_{H,t}$

- To train the overall model $\mathcal{N}_\theta$ we minimise the loss function

$$\mathcal{L}(\theta) = \frac{1}{NM} \sum_{n=1}^{N} \sum_{m=1}^{M} \left\| \mathcal{N}_\theta \left(t_m^n, \mathbf{x}_0^n \right) - \mathbf{y}_m^n \right\|_2^2 ,$$

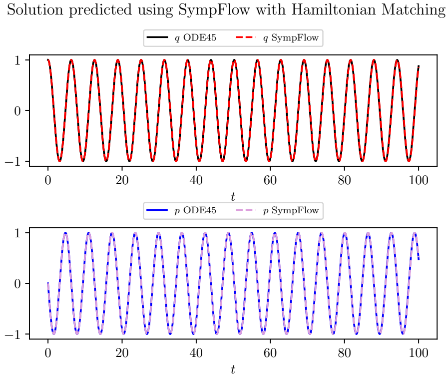
where $\mathbf{x}_0^n \in \Omega \subset \mathbb{R}^{2n}$, and $\mathbf{y}_m^n \approx \phi_{H,t_m^n}(\mathbf{x}_0^n)$.

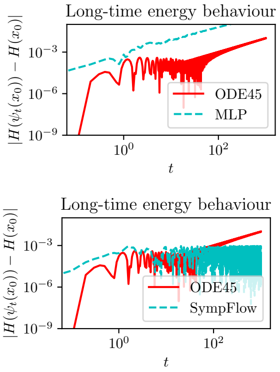


Simple Harmonic Oscillator (unsupervised)

Equations of motion

$$\dot{x} = p, \;\; \dot{p} = -x.$$





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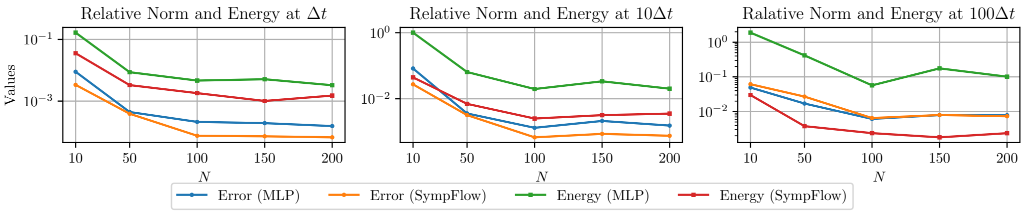
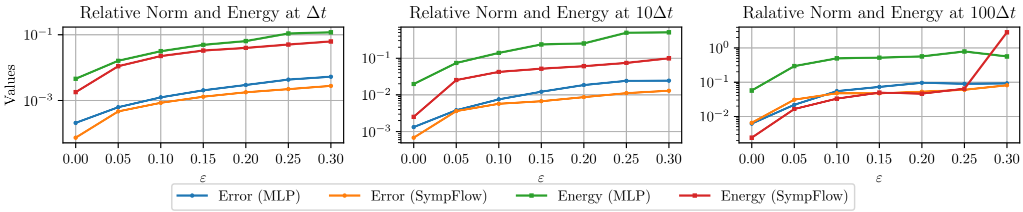


(a) Fixed $M = 50$ and $\varepsilon = 0$.



(b) Fixed $N = 100$ and $M = 50$.

Hénon–Heiles (unsupervised)

Equations of motion

$$\dot{x} = p_x, \ \dot{y} = p_y, \ \dot{p}_x = -x - 2xy, \ \dot{p}_y = -y - (x^2 - y^2).$$

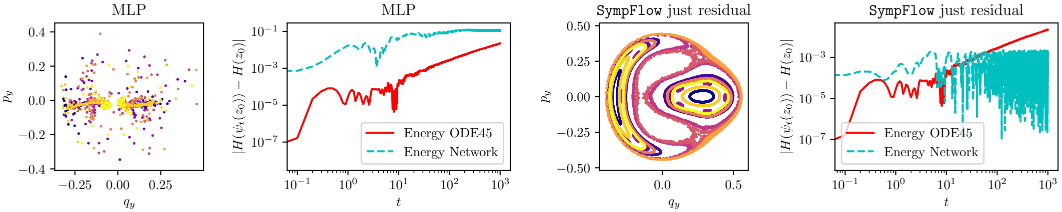


Figure 4: **Unsupervised experiment — Hénon–Heiles:** Comparison of the Poincaré sections and the energy behaviour up to time $T = 1000$.

Future extensions

- Improve the efficiency of the method by replacing gradients of MLPs with some other alternatives (Topic of a Summer Project in Cambridge that Zak and I proposed).
- Extend the approach to capture parametric dependencies, and apply this procedure for parameter identification.
- Improve our theoretical understanding of the dynamics exactly solved by the `SympFlow`.
- Apply the method to higher dimensional systems.

THANK YOU FOR THE ATTENTION

davidemurari.com/sympflow to read the paper

Physics-informed neural networks

- We introduce a parametric map $\mathcal{N}_\theta(\cdot, \mathbf{x}_0) : [0, T] \to \mathbb{R}^d$ such that $\mathcal{N}_\theta(0, \mathbf{x}_0) = \mathbf{x}_0$, and choose its weights so that

$$\mathcal{L}(\theta) := \frac{1}{C} \sum_{c=1}^{C} \left\| \frac{d}{dt} \mathcal{N}_\theta(t, \mathbf{x}_0) \Big|_{t=t_c} - \mathcal{F}\left(\mathcal{N}_\theta(t_c, \mathbf{x}_0)\right) \right\|_2^2 \to \min$$

for some collocation points $t_1, \ldots, t_C \in [0, T]$.

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  for some collocation points $t_1, \dots, t_C \in [0, T]$.

- Then, $t \mapsto \mathcal{N}_\theta(t, \mathbf{x}_0)$ will solve a different IVP

$$\begin{cases} \dot{\mathbf{y}}(t) = \mathcal{F}(\mathbf{y}(t)) + \left(\frac{d}{dt} \mathcal{N}_\theta(t, \mathbf{x}_0)\Big|_{t=t} - \mathcal{F}(\mathbf{y}(t)) \right) \in \mathbb{R}^d, \\ \mathbf{y}(0) = \mathbf{x}_0 \in \mathbb{R}^d, \end{cases}$$

  where hopefully the residual $\frac{d}{dt} \mathcal{N}_\theta(t, \mathbf{x}_0)\Big|_{t=t} - \mathcal{F}(\mathbf{y}(t))$ is small in some sense.

Training issues with neural network

- Solving a single IVP on $[0, T]$ with a neural network can take long training time.
- The obtained solution can not be used to solve the same ordinary differential equation with a different initial condition.

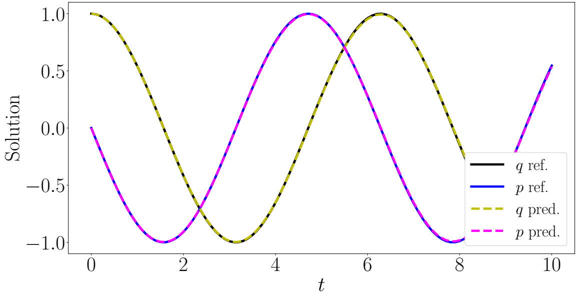

Figure 5: Solution comparison after reaching a loss value of 10^{-5}. The training time is of 87 seconds (7500 epochs with 1000 new collocation points randomly sampled at each of them).

Training issues with neural network

- It is hard to solve initial value problems over long time intervals.