# <span id="page-0-0"></span>Dynamical systems-based structured networks

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 $m4$ :

- Introduction to dynamical systems-based neural networks.
- Time-dependent symplectic networks.
- $\blacktriangleright$  1-Lipschitz and  $\alpha$  averaged networks.

## ResNets as dynamical systems

Residual Neural Networks (ResNets) are networks of the form  $\mathcal{N}_\theta=f_{\theta_L}\circ...\circ f_{\theta_1}$  with

$$
f_{\theta_i}(\mathbf{x}) = \mathbf{x} + B_i^{\top} \sigma (A_i \mathbf{x} + \mathbf{b}_i) \in \mathbb{R}^d, \ \mathbf{x} \in \mathbb{R}^d,
$$
  

$$
A_i, B_i \in \mathbb{R}^{h \times d}, \ \mathbf{b}_i \in \mathbb{R}^h, \ \theta_i = \{A_i, B_i, \mathbf{b}_i\}.
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#### The layer  $\blacktriangleright$

$$
f_{\theta_i}(\mathbf{x}) = \mathbf{x} + B_i^{\top} \sigma (A_i \mathbf{x} + \mathbf{b}_i) = \mathbf{x} + \mathcal{F}_{\theta_i}(\mathbf{x}) \in \mathbb{R}^d
$$

is an explicit Euler step of size 1 for the initial value problem

$$
\begin{cases} \dot{\mathbf{y}}(t) = B_i^\top \sigma(A_i \mathbf{y}(t) + \mathbf{b}_i) = \mathcal{F}_{\theta_i}(\mathbf{y}(t)), \\ \mathbf{y}(0) = \mathbf{x} \end{cases}
$$

.

▶ We can define ResNet-like neural networks by choosing a family of parametric functions  $\mathcal{S}_\Theta=\left\{\mathcal{F}_\theta:\mathbb{R}^d\to\mathbb{R}^d:\ \theta\in\Theta\right\}$  and a numerical method  $\Psi_\mathcal{F}^h$  like explicit Euler defined as  $\Psi^h_{\mathcal{F}}(\mathsf{x}) = \mathsf{x} + h\mathcal{F}(\mathsf{x})$ , and set

$$
\mathcal{N}_{\theta}(\mathbf{x}) = \Psi_{\mathcal{F}_{\theta_L}}^{h_L} \circ \cdots \circ \Psi_{\mathcal{F}_{\theta_1}}^{h_1}(\mathbf{x}), \ \mathcal{F}_{\theta_1}, ..., \mathcal{F}_{\theta_L} \in \mathcal{S}_{\Theta}.
$$

 $\triangleright$  We could also combine these residual blocks with lifting and projection layers, as for usual neural networks.

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 $\triangleright$  Choose a property  $P$  that the network has to satisfy, e.g. volume preservation.

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- **Choose a family of parametric vector fields**  $S_{\Theta}$  **whose solutions satisfy P, e.g.**

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\mathcal{F}_{\theta}(\mathbf{x}) = \begin{bmatrix} \sigma (A_1 \mathbf{x}_2 + \mathbf{b}_1) \\ \sigma (A_2 \mathbf{x}_1 + \mathbf{b}_2) \end{bmatrix}, \ \mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}
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## Structured networks based on dynamical systems<sup>1</sup>

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$$
\mathcal{F}_{\theta}(\mathbf{x}) = \begin{bmatrix} \sigma (A_1 \mathbf{x}_2 + \mathbf{b}_1) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \sigma (A_2 \mathbf{x}_1 + \mathbf{b}_2) \end{bmatrix}, \ \mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}.
$$

Choose a numerical method  $\Psi_{\mathcal{F}_{\theta}}^{h}$  that preserves the property  $\mathcal P$  at a discrete level, e.g.

$$
\Psi_{\mathcal{F}_{\theta}}^{h}(\mathbf{x}) = \begin{bmatrix} \mathbf{x}_1 + h\sigma \left( A_1\mathbf{x}_2 + \mathbf{b}_1 \right) =: \widetilde{\mathbf{x}}_1 \\ \mathbf{x}_2 + h\sigma \left( A_2\widetilde{\mathbf{x}}_1 + \mathbf{b}_2 \right) \end{bmatrix}.
$$

• The resulting network 
$$
\mathcal{N}_{\theta} = \Psi_{\mathcal{F}_{\theta_L}}^{h_L} \circ \cdots \circ \Psi_{\mathcal{F}_{\theta_1}}^{h_1}
$$
 will preserve  $\mathcal{P}$ .

<sup>1</sup>Elena Celledoni et al. "Dynamical Systems-Based Neural Networks". In: SIAM Journal on Scientific Computing 45.6 (2023), A3071–A3094.

# Time-dependent Symplectic Neural **Networks**

In collaboration with Priscilla Canizares, Carola-Bibiane Schönlieb, Ferdia Sherry, Zakhar Shumaylov<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>Priscilla Canizares et al. "Hamiltonian Matching for Symplectic Neural Integrators". In: arXiv preprint arXiv:2410.18262 (2024).

## Canonical Hamiltonian equations

▶ The equations of motion of canonical Hamiltonian systems write

<span id="page-9-0"></span>
$$
\dot{\mathbf{x}} = \mathbb{J}\nabla H(\mathbf{x}) = X_H(\mathbf{x}) \in \mathbb{R}^{2n}, \quad \mathbb{J} = \begin{bmatrix} 0 & I_n \\ -I_n & 0_n \end{bmatrix} \in \mathbb{R}^{2n \times 2n}.
$$
 (1)

Denoted with  $\phi_{H,t}:\mathbb{R}^{2n}\to\mathbb{R}^{2n}$  the exact flow of [\(1\)](#page-9-0), we have that

$$
\frac{d}{dt}H(\phi_{H,t}(\mathbf{x}_0)) = \nabla H(\phi_{H,t}(\mathbf{x}_0))^{\top} \mathbb{J} \nabla H(\phi_{H,t}(\mathbf{x}_0)) = 0,
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\left(\frac{\partial \phi_{H,t}(\mathbf{x}_0)}{\partial \mathbf{x}_0}\right)^{\top} \mathbb{J} \left(\frac{\partial \phi_{H,t}(\mathbf{x}_0)}{\partial \mathbf{x}_0}\right) = \mathbb{J},
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$$

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

## 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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 $\triangleright$  By the group property of the flow map, we know that

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

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

## 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  $\{(\mathbf{x}_0^n, \mathbf{y}_1^n,..., \mathbf{y}_M^n)\}_{n=1}^N$ ,  $\mathbf{y}_m^n\approx \phi_{H,t_m^n}(\mathbf{x}_0^n).$ 

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**Remark:** Given the several known qualitative properties of  $\phi_{H, t}$ , we want to exploit 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:

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

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\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}.
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$$

▶ The SympFlow architecture is defined as

$$
\mathcal{N}_{\theta}\left(t, \left(\mathbf{q}_0, \mathbf{p}_0\right)\right) = \phi_{\mathbf{p},t}^L \circ \phi_{\mathbf{q},t}^L \circ \cdots \circ \phi_{\mathbf{p},t}^1 \circ \phi_{\mathbf{q},t}^1((\mathbf{q}_0, \mathbf{p}_0)).
$$

## 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:

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

$$
= \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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with  $\tilde{V}^i(t, (\mathbf{q}, \mathbf{p})) = \partial_t V^i(t, \mathbf{q}).$ 

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with  $\tilde{V}^i(t, (\mathbf{q}, \mathbf{p})) = \partial_t V^i(t, \mathbf{q}).$ 

- The SympFlow is volume preserving. Þ.
- The SympFlow is the exact solution of a time-dependent Hamiltonian system. Ы

## 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  $\phi_{H^2,t}\circ \phi_{H^1,t}:\R^{2n}\to \R^{2n}$  is the exact flow of the time-dependent Hamiltonian system defined by the Hamiltonian function

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

This theorem implies that there is a Hamiltonian function  $\mathcal{H}(\mathcal{N}_{\theta}) : \mathbb{R} \times \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  such that

$$
\mathcal{N} _\theta\left(t, \textbf{x}\right) = \phi_{\mathcal{H}\left(\mathcal{N}_\theta\right), t}(\textbf{x})
$$

for every  $t \geq 0$  and  $\mathbf{x} \in \mathbb{R}^{2n}$ .

<sup>3</sup> 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.

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

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

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

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

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

$$
\mathcal{L}(\theta) = \frac{1}{N M} \sum_{n=1}^{N} \sum_{m=1}^{M} \left\| \mathcal{N}_{\theta} \left( t_{m}^{n}, \mathbf{x}_{0}^{n} \right) - \mathbf{y}_{m}^{n} \right\|_{2}^{2},
$$

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



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# Simple Harmonic Oscillator (unsupervised)

Equations of motion

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





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# Simple Harmonic Oscillator (supervised)



# 1-Lipschitz and  $\alpha$  – averaged neural networks

In collaboration with Elena Celledoni, Matthias J. Ehrhardt, Brynjulf Owren, Carola-Bibiane Schönlieb, Ferdia Sherry<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>Ferdia Sherry et al. "Designing stable neural networks using convex analysis and odes". In: *Physica D:* Nonlinear Phenomena 463 (2024), p. 134159.

## Adversarial robustness

Constraining the Lipschitz constant allows the reduction/control of the sensitivity of the network to perturbations in the input space.

## Convergent Plug-and-Play algorithms

They can help in Plug-and-Play algorithms to ensure the convergence of the iteration

$$
\mathbf{x}_{k+1} = \mathcal{N}_{\theta}(\mathbf{x}_k - \tau \nabla F(\mathbf{x}_k)).
$$

This iteration converges if  $\mathcal{N}_{\theta}$  is  $\alpha-$ averaged and the sequence has a fixed point<sup>a</sup>.

<sup>a</sup>Pravin Nair, Ruturaj G Gavaskar, and Kunal Narayan Chaudhury. "Fixed-Point and Objective Convergence of Plug-and-Play Algorithms". In: IEEE Transactions on Computational Imaging 7 (2021), pp. 337–348.

## Non-expansive dynamical systems

Dynamic	Dynamic
Explicit Euler approximation: $\dot{\mathbf{v}} = \mathcal{F}_{\theta}(\mathbf{x}) = -A^{\top} \sigma (A\mathbf{x} + \mathbf{b})$ .	
Explicit Euler approximation: $\Psi_{\mathcal{F}_{\theta}}^{h}(\mathbf{x}) = \mathbf{x} - hA^{\top} \sigma (A\mathbf{x} + \mathbf{b})$ .	
1-Lipschitz map: $\left\  \Psi_{\mathcal{F}_{\theta}}^{h}(\mathbf{y}) - \Psi_{\mathcal{F}_{\theta}}^{h}(\mathbf{x}) \right\ _{2} \leq \left\  \mathbf{y} - \mathbf{x} \right\ _{2}$ ,	

if  $h \leq 2/||A||_2^2$  and  $\sigma$  is 1-Lipschitz.

We define the 1–Lipschitz neural network

$$
\mathcal{N}_{\theta} = \Psi_{\mathcal{F}_{\theta_L}}^{h_L} \circ ... \circ \Psi_{\mathcal{F}_{\theta_L}}^{h_L} : \mathbb{R}^d \to \mathbb{R}^d,
$$

where  $h_1,...,h_L$  are adjusted during training to ensure  $h_i \leq 2/\|A_i\|_2^2.$ 

### $\alpha$ −averaged maps

A map  $F: \mathbb{R}^d \to \mathbb{R}^d$  is  $\alpha-$ averaged,  $\alpha \in (0,1)$ , if there is a  $1-$ Lipschitz map  $\, \in \mathbb{R}^d \to \,$  $\mathbb{R}^d$  such that

$$
F = (1 - \alpha)\mathrm{id} + \alpha T.
$$

If F is continuously differentiable and has symmetric Jacobian, then it is  $\alpha$  –averaged if and only if  $\operatorname{spectrum}(F'(\mathbf{x})) \subset [1-2\alpha, 1]$ . Composition of averaged maps is averaged.

The map

$$
\Psi_{\mathcal{F}_{\theta}}^{h}(\mathbf{x}) = \mathbf{x} - h A^{\top} \sigma \left( A \mathbf{x} + \mathbf{b} \right) = \nabla \left( \frac{\|\mathbf{x}\|_2^2}{2} - h \mathbf{1}^{\top} \gamma \left( A \mathbf{x} + b \right) \right), \ \gamma' = \sigma,
$$

is averaged if  $h \leq 2/\Vert A \Vert_2^2$ .

## Comparison of learned denoisers

$$
\Gamma_{\text{Euler}} := \mathcal{P} \circ \mathcal{N}_{\theta} \circ \mathcal{L},
$$
  

$$
\mathcal{L}(x_1, x_2, x_3) = (x_1, x_3, x_3, 0, ..., 0) \in \mathbb{R}^{64}, \ \mathcal{P}(x_1, ..., x_{64}) = (x_1, x_2, x_3) \in \mathbb{R}^3.
$$



Figure 2: Repeated application of the unconstrained denoiser DnCNN<sup>5</sup> and the constrained denoiser  $\Gamma_{\text{Euler}}$  to a given input image.

<sup>5</sup>Kai Zhang et al. "Beyond a Gaussian Denoiser: Residual Learning of Deep CNN for Image Denoising". In: IEEE transactions on image processing 26.7 (2017), pp. 3142–3155. Davide Murari (DAMTP) [Dynamical systems-based structured networks](#page-0-0) 21 / 22

# Plug-and-Play for a deblurring task



Figure 3: Using the learned Euler denoiser to solve an ill-posed inverse problem (deblurring) in a PnP fashion, with convergence guarantee. The numbers in the top right corner of each image are the PSNRs (in  $dB$ ) relative to the ground truth  $x$ .

- Canizares, Priscilla et al. "Hamiltonian Matching for Symplectic Neural Integrators". In: arXiv preprint arXiv:2410.18262 (2024).
- Celledoni, Elena et al. "Dynamical Systems—Based Neural Networks". In: SIAM Journal on Scientific Computing 45.6 (2023), A3071–A3094.
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# THANK YOU FOR THE ATTENTION

## Physics-informed neural networks

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

$$
\mathcal{L}(\theta) := \frac{1}{C} \sum_{c=1}^{C} \left\| \frac{d}{dt} \mathcal{N}_{\theta}(t, \mathbf{x}_{0}) \right\|_{t=t_{c}} - \mathcal{F} \left( \mathcal{N}_{\theta}(t_{c}, \mathbf{x}_{0}) \right) \right\|_{2}^{2} \rightarrow \min
$$

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

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

$$
\mathcal{L}(\theta) := \frac{1}{C} \sum_{c=1}^{C} \left\| \frac{d}{dt} \mathcal{N}_{\theta}(t, \mathbf{x}_{0}) \right\|_{t=t_{c}} - \mathcal{F} \left( \mathcal{N}_{\theta}(t_{c}, \mathbf{x}_{0}) \right) \right\|_{2}^{2} \rightarrow \min
$$

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

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

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

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

## Training issues with neural network

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



Figure 4: Solution comparison after reaching a loss value of 10<sup>-5</sup>. 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.



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

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

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

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

$$
\bar{\psi}_{s}(\mathbf{x}_{0}):=\mathcal{N}_{\theta}\left(s,\mathbf{x}_{0}\right), s\in[0,\Delta t),
$$

$$
\left(\bar{\psi}_{\Delta t}\right)^{k}:=\underbrace{\bar{\psi}_{\Delta t}\circ\cdots\circ\bar{\psi}_{\Delta t}}_{k \text{ times}}, k\in\mathbb{N}.
$$

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$$
\bar{\psi}_{\mathsf{s}}(\mathbf{x}_0) := \mathcal{N}_{\theta}(\mathsf{s}, \mathbf{x}_0), \ \mathsf{s} \in [0, \Delta t), \n(\bar{\psi}_{\Delta t})^k := \underbrace{\bar{\psi}_{\Delta t} \circ \cdots \circ \bar{\psi}_{\Delta t}}_{k \text{ times}}, \ k \in \mathbb{N}.
$$

 $\psi(t, \cdot) = \phi_{H,t}(\cdot)$  for the piecewise continuous Hamiltonian

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

## Hénon-Heiles (unsupervised)

## Equations of motion

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

0 20 40  $\begin{array}{ccc} t & t \\ \hline p_1 \text{ ODE45} & -- & p_1 \text{ SympFlow} \end{array}$ −0.5 0.0 0.5  $q_1$  ODE45  $\longrightarrow$   $q_1$  SympFlow  $0\qquad \qquad 20\qquad \quad \ \, 40$ t −0.50  $-0.25$ 0.00 0.25 0 20 40  $\frac{t}{p_2 \text{ ODE45}} \qquad \qquad - \qquad p_2 \text{ SympFlow}$ 0.0 0.5  $q_2$  ODE45  $-q_2$  SympFlow  $0\qquad \quad \ \ 20\qquad \quad \ \ \, 40$ t  $-0.5$ 0.0 0.5

Solution predicted using SympFlow with Hamiltonian Matching



## Imposing structure over a neural network

 $\triangleright$  To build networks satisfying a desired property, we can either restrict the parametrisation  $\mathcal{N}_{\theta}$  or modify the loss function.

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- $\blacktriangleright$  Restrict the architecture:

$$
\mathcal{N}_{\theta}(\mathbf{x}) = \frac{\widetilde{\mathcal{N}}_{\theta}(\mathbf{x})}{\left\|\widetilde{\mathcal{N}}_{\theta}(\mathbf{x})\right\|_2} \left\|\mathbf{x}\right\|_2.
$$

 $\triangleright$  Modify the loss function:

$$
\widetilde{\mathcal{L}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \|\mathcal{N}_{\theta}(\mathbf{x}_i) - \mathbf{y}_i\|_2^2 + \underbrace{\frac{1}{N} \sum_{i=1}^{N} (\|\mathbf{x}_i\|_2 - \|\mathcal{N}_{\theta}(\mathbf{x}_i)\|_2)^2}_{\text{regulariser}}.
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$$

Not all restrictions are equally effective, e.g.  $\mathcal{N}_R(\mathsf{x})=R\mathsf{x}$ ,  $R^\top R=l_d$ , is norm-preserving but probably not expressive enough.

 $\triangleright$  The inductive bias provided by modelling the network starting from dynamical systems, allows us to study these models using the theory of numerical analysis and dynamical systems.

### Universal approximation theorem

Let  $F: \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$  be a continuous function, with  $\Omega \subset \mathbb{R}^d$  a compact set. Then, for every  $\varepsilon > 0$ , there exists a finite set of gradient vector fields  $\nabla V^1,\cdots,\nabla V^L$ , spherepreserving vector fields  $X_5^1, \dots, X_5^L$ , and time steps  $h_1, \dots, h_L \in \mathbb{R}$  such that

$$
\left\|F - \Psi_{\nabla V^L}^{h_L} \circ \Psi_{X_S^L}^{h_L} \circ \ldots \circ \Psi_{\nabla V^1}^{h_1} \circ \Psi_{X_S^1}^{h_1} \right\|_{L^p(\Omega)} < \varepsilon.
$$

## <span id="page-46-0"></span>Idea of the proof

Let  $F: \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$  be a continuous function, with  $\Omega \subset \mathbb{R}^d$  a compact set. Then, for every  $\varepsilon > 0$ , there exists a finite set of  $C^1$  vector fields  $X^1,...,X^L$ , and time steps  $h_1, \dots, h_l \in \mathbb{R}$  such that<sup>a</sup>

$$
\left\|F-\Psi_{X^L}^{h_L}\circ\ldots\circ\Psi_{X^1}^{h_1}\right\|_{L^p(\Omega)}<\varepsilon.
$$

<sup>a</sup>Qianxiao Li, Ting Lin, and Zuowei Shen. "Deep learning via dynamical systems: An approximation perspective". In: Journal of the European Mathematical Society 25.5 (2022), pp. 1671–1709

### Presnov decomposition

For any  $X\in\mathcal{C}^1(\mathbb{R}^d,\mathbb{R}^d)$  there is a unique function  $U:\mathbb{R}^d\to\mathbb{R}$  with  $U(0)=0$ , and a unique sphere-preserving vector field  $X_S: \mathbb{R}^d \rightarrow \mathbb{R}^d$  such that

$$
X(\mathbf{x}) = \nabla U(\mathbf{x}) + X_{\mathcal{S}}(\mathbf{x}), \ \forall \mathbf{x} \in \mathbb{R}^d.
$$