NTNU
Norwegian University of Science and Technology

Neural Networks, Differential Equations, and Structure Preservation

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PhD thesis defence,
Trondheim, September 25, 2024

Supervisory Committee: Elena Celledoni, and Brynjulf Owren
Assessment Committee: Virginie Ehrlacher, Matthew Colbrook, and Jo Eidsvik

Papers in my thesis

PART 1: Structure preserving deep learning

- Dynamical Systems–Based Neural Networks

  Celledoni, E., Murari, D., Owren, B., Schönlieb, C. B., & Sherry, F., SIAM Journal of Scientific Computing
- Resilient Graph Neural Networks: A Coupled Dynamical Systems Approach

  Eliasof, M., Murari, D., Sherry, F., & Schönlieb, C. B., 27TH European Conference on Artificial Intelligence
- Predictions Based on Pixel Data: Insights from PDEs and Finite Differences

  Celledoni, E., Jackaman, J., Murari, D., & Owren, B., Submitted

Papers in my thesis

PART 2: Solving and discovering differential equations

- Lie Group integrators for mechanical systems

  Celledoni, E., Çokaj, E., Leone, A., Murari, D., & Owren, B., International Journal of Computer Mathematics

- Learning Hamiltonians of constrained mechanical systems

  Celledoni, E., Leone, A., Murari, D., & Owren, B., Journal of Computational and Applied Mathematics

- Neural networks for the approximation of Euler's elastica

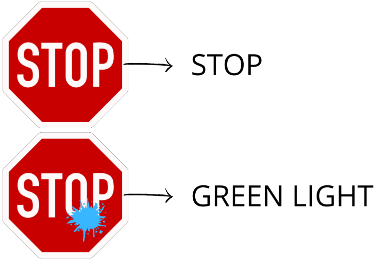
  Celledoni, E., Çokaj, E., Leone, A., Leyendecker, S., Murari, D., Owren, B., Sato Martín de Almagro, R.T. & Stavole, M., Submitted

- Parallel-in-Time Solutions with Extreme Learning Machines

  Betcke, M., Kreusser, L.M., & Murari, D., Submitted

Motivation

(a) ChatGPT: "Generate a picture of a monkey winning a marathon"



(b) Misclassification of an image that could harm self-driving cars.

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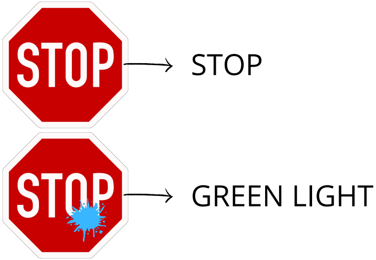


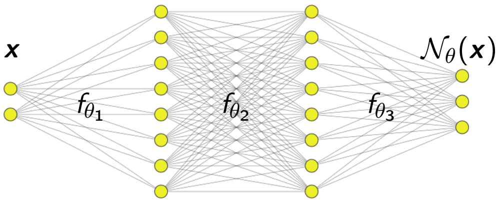
(b) Misclassification of an image that could harm self-driving cars.

- Neural networks can find accurate solutions to many problems but tend not to be interpretable or reproduce desired properties.
- We will see how to deal with some of these issues by applying the theory of dynamical systems and geometric integration.

What is a neural network?

- A neural network is a parametric map usually composed of building blocks called *layers of the network*:

$$\mathcal{N}_\theta(\boldsymbol{x}) = f_{\theta_L} \circ \cdots \circ f_{\theta_1}(\boldsymbol{x}), \;\; \theta = \{\theta_1, \cdots, \theta_L\}\,.$$



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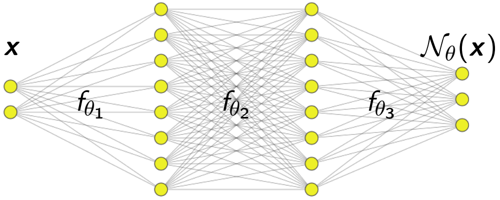
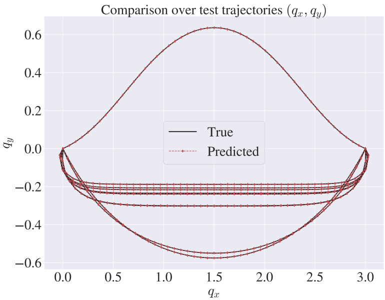


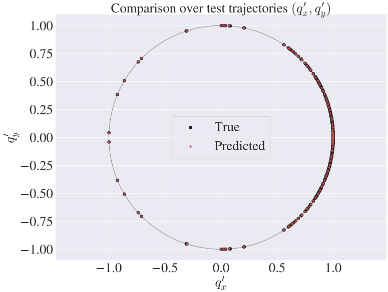
- Example: Residual Neural Networks (ResNets)

$$f_{\theta_i}(\boldsymbol{x}) = \boldsymbol{x} + B_i^\top \sigma\left(A_i\boldsymbol{x} + \boldsymbol{b}_i\right) \in \mathbb{R}^d, \;\; \boldsymbol{x} \in \mathbb{R}^d,$$
$$A_i, B_i \in \mathbb{R}^{h\times d}, \;\; \boldsymbol{b}_i \in \mathbb{R}^h, \;\; \theta_i = \{A_i, B_i, \boldsymbol{b}_i\}\,.$$

Example of the Euler's elastica

- **Goal**: Build an efficient approximate solver of the Euler's elastica
- **Dataset**: A set of boundary data $\boldsymbol{x}_i = \left(\boldsymbol{q}_i^0, \left(\boldsymbol{q}_i^0\right)', \boldsymbol{q}_i^N, \left(\boldsymbol{q}_i^N\right)'\right)$ and the respective approximate solutions $\boldsymbol{y}_i$ at some grid nodes.
- **Loss function**: $\mathcal{L}(\theta) := \frac{1}{M}\sum_{i=1}^{M} \|\mathcal{N}_\theta(\boldsymbol{x}_i) - \boldsymbol{y}_i\|_2^2 \rightarrow \min$.





Neural networks based on dynamical systems

- The layer

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

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

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

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- 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 $\Psi^h_{\mathcal{F}}$, like explicit Euler defined as $\Psi^h_{\mathcal{F}}(\boldsymbol{x}) = \boldsymbol{x} + h\mathcal{F}(\boldsymbol{x})$, and set

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

Imposing structure over a neural network

- 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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- **Restrict the architecture**:

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

- **Modify the loss function**:

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

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

Structured networks based on dynamical systems

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

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

Structured networks based on dynamical systems

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

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

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

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

Approximation properties

- 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.

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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 $\nabla V^1, \cdots, \nabla V^L$, sphere-preserving vector fields $X_S^1, \cdots, X_S^L$, and time steps $h_1, \cdots, h_L \in \mathbb{R}$ such that

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

Adversarial robustness for classification tasks

Description of the problem

Classification problem

Let $\Omega \subset \mathbb{R}^d$ be a set whose points are known to belong to C classes. Given part of their labels, we want to label the remaining points with a function $\mathcal{N}_\theta : \mathbb{R}^d \to \mathbb{R}^C$ where we set

$$\text{predicted class of } \boldsymbol{x} = \underset{c=1,\dots,C}{\arg\max} \left(\mathcal{N}_\theta(\boldsymbol{x})^\top \boldsymbol{e}_c \right).$$

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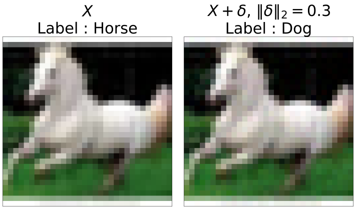
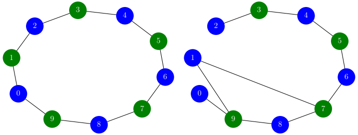
Adversarial examples





How to have guaranteed robustness

- Not all correct predictions are equivalent.
- Let $\ell(\boldsymbol{x}) = 2$ be the correct label for the point $\boldsymbol{x} \in \Omega$.
- $\mathcal{N}_{\theta_1}(\boldsymbol{x}) = \begin{bmatrix} 0.49 & 0.51 & 0 \end{bmatrix}$ is not so certain as a prediction.
- $\mathcal{N}_{\theta_2}(\boldsymbol{x}) = \begin{bmatrix} 0.05 & 0.9 & 0.05 \end{bmatrix}$ there is a higher gap here.

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Margin: $\mathcal{M}_{\mathcal{N}_\theta}(\boldsymbol{x}) := \mathcal{N}_\theta(\boldsymbol{x})^\top \boldsymbol{e}_{\ell(\boldsymbol{x})} - \max_{j \neq \ell(\boldsymbol{x})} \mathcal{N}_\theta(\boldsymbol{x})^\top \boldsymbol{e}_j.$

$\mathcal{M}_{\mathcal{N}_\theta}(\boldsymbol{x}) > 0 \implies \mathcal{N}_\theta$ correctly classifies $\boldsymbol{x}$.

$$\mathcal{M}_{\mathcal{N}_\theta}(\boldsymbol{x}) > \sqrt{2}\mathrm{Lip}(\mathcal{N}_\theta)\varepsilon \implies \mathcal{M}_{\mathcal{N}_\theta}(\boldsymbol{x} + \boldsymbol{\eta}) > 0 \, \forall \|\boldsymbol{\eta}\|_2 \leq \varepsilon.$$

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- We constrain the Lipschitz constant of $\mathcal{N}_\theta$ (and train the network so it maximises the margin).

Lipschitz-constrained networks

Contractive maps

$$\mathcal{F}_\theta^c(\boldsymbol{x}) = -A_c^\top \sigma\left(A_c \boldsymbol{x} + \boldsymbol{b}_c\right), \; A_c^\top A_c = I,$$

$$\Psi_{\mathcal{F}_\theta^c}^{h_c}(\boldsymbol{x}) = \boldsymbol{x} - h_c A_c^\top \sigma\left(A_c \boldsymbol{x} + \boldsymbol{b}_c\right)$$

$$\left\|\Psi_{\mathcal{F}_\theta^c}^{h_c}(\boldsymbol{y}) - \Psi_{\mathcal{F}_\theta^c}^{h_c}(\boldsymbol{x})\right\|_2 \leq \sqrt{1 - h_c + h_c^2}\,\|\boldsymbol{y} - \boldsymbol{x}\|_2$$

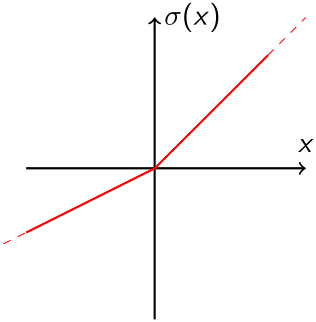

Figure: $\sigma(x) = \max\left\{x, \frac{x}{2}\right\}$

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Expansive maps

$$\mathcal{F}_\theta^e(\boldsymbol{x}) = A_e^\top \sigma\left(A_e\boldsymbol{x} + \boldsymbol{b}_e\right), \; A_e^\top A_e = I,$$

$$\Psi_{\mathcal{F}_\theta^e}^{h_e}(\boldsymbol{x}) = \boldsymbol{x} + h_e A_e^\top \sigma\left(A_e\boldsymbol{x} + \boldsymbol{b}_e\right)$$

$$\left\|\Psi_{\mathcal{F}_\theta^e}^{h_e}(\boldsymbol{y}) - \Psi_{\mathcal{F}_\theta^e}^{h_e}(\boldsymbol{x})\right\|_2 \leq (1 + h_e)\,\|\boldsymbol{y} - \boldsymbol{x}\|_2$$

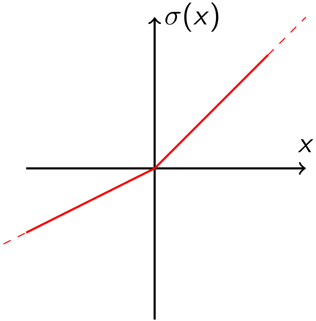


Figure: $\sigma(x) = \max\left\{x, \frac{x}{2}\right\}$

Lipschitz-constrained networks

- To get a $1-$Lipschitz neural network we alternate the one-step methods and restrict the step sizes suitably:

$$\mathcal{N}_\theta = \Psi^{h_{2L}}_{\mathcal{F}^c_{\theta_{2L}}} \circ \Psi^{h_{2L-1}}_{\mathcal{F}^e_{\theta_{2L-1}}} \circ \cdots \circ \Psi^{h_2}_{\mathcal{F}^c_{\theta_2}} \circ \Psi^{h_1}_{\mathcal{F}^e_{\theta_1}}$$

$$\sqrt{1 - h_{2k} + h_{2k}^2}\,(1 + h_{2k-1}) \leq 1, \;\; k = 1, \cdots, L.$$

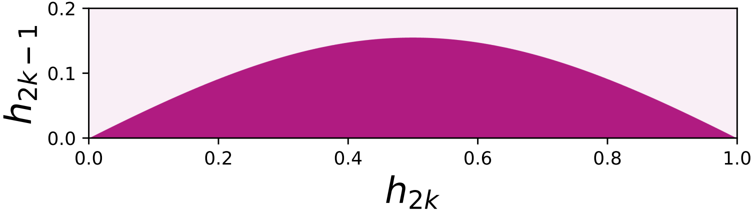
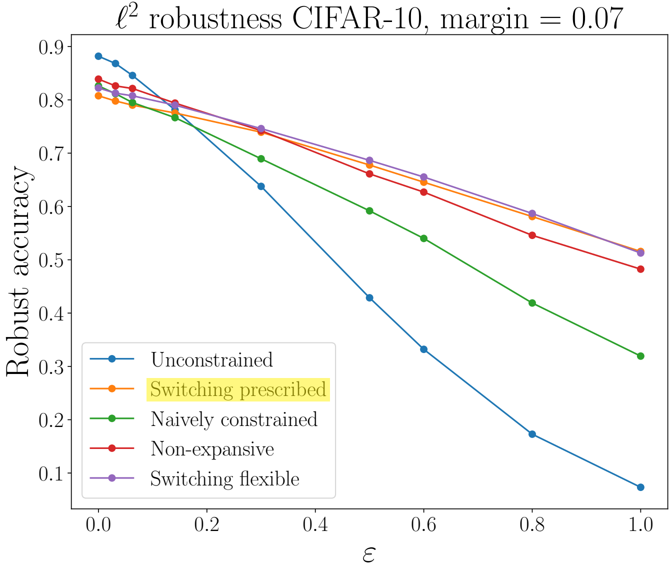


Figure: Admissible time steps to get a $1-$Lipschitz neural network

Numerical experiment with CIFAR-10



Learning tasks involving dynamical systems

Definition of the problem

- **Data**: $\left\{\left(\boldsymbol{x}_i^0, \boldsymbol{x}_i^1, \cdots, \boldsymbol{x}_i^M\right)\right\}_{i=1,\ldots,N}$, $\boldsymbol{x}_i^j = \phi_{\mathcal{F}}^{jh}\left(\boldsymbol{x}_i^0\right) + \boldsymbol{\delta}_i^j$, $j = 0, \cdots, M$, for an unknown $\mathcal{F} : \mathbb{R}^d \to \mathbb{R}^d$.

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- **Goal 1**: Approximate the vector field $\mathcal{F}$
- **Goal 2**: Approximate the map $\boldsymbol{x}_i^j \mapsto \boldsymbol{x}_i^{j+1}$, i.e., one step with the exact flow map $\phi_{\mathcal{F}}^h$.

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- **Generic solution strategy**: Introduce a parametric model $\mathcal{F}_\theta : \mathbb{R}^d \to \mathbb{R}^d$, choose a one-step method $\Psi_{\mathcal{F}_\theta}^h : \mathbb{R}^d \to \mathbb{R}^d$, and solve

$$\mathcal{L}(\theta) = \frac{1}{NM} \sum_{i=1}^N \sum_{j=1}^M \left\| \left(\Psi_{\mathcal{F}_\theta}^h\right)^j \left(\boldsymbol{x}_i^0\right) - \boldsymbol{x}_i^j \right\|_2^2 \to \min .$$

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- If we know more about $\mathcal{F}$ or the geometric properties of the flow $\phi_{\mathcal{F}}^h$ we might want to constrain this procedure.

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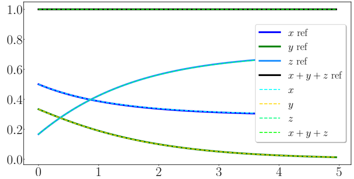
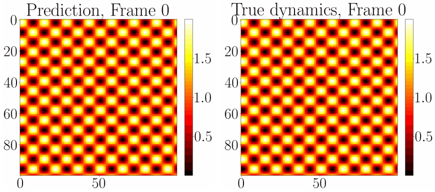
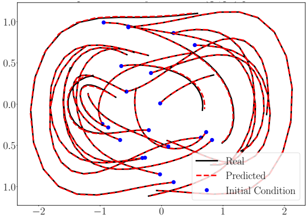
Problems we have considered



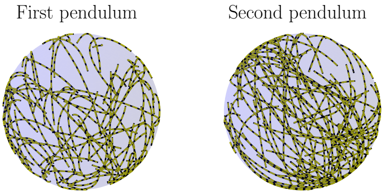
(a) Learning the mass preserving flow map of the SIR model.



(b) Learning the norm-preserving flow map of the linear advection PDE.



(c) Learning the Hamiltonian of unconstrained systems.



(d) Learning the Hamiltonian of constrained systems.

Constrained Hamiltonian systems

- Holonomically constrained Hamiltonian systems can be described by the differential algebraic equation

$$\begin{cases} \dot{\boldsymbol{y}}(t) = \mathbb{J}\nabla H(\boldsymbol{y}(t)), \quad \boldsymbol{y} = (\boldsymbol{q}, \boldsymbol{p}) \\ g(\boldsymbol{q}) = 0, \quad g : \mathbb{R}^d \to \mathbb{R}^c \end{cases}, \quad \mathbb{J} = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}.$$

- Its configuration manifold and associated tangent space are

$$\mathcal{Q} = \left\{ \boldsymbol{q} \in \mathbb{R}^d : \; g(\boldsymbol{q}) = 0 \right\} \subset \mathbb{R}^d, \; \dim(\mathcal{Q}) = d - c,$$
$$T_{\boldsymbol{q}}\mathcal{Q} = \left\{ \boldsymbol{v} \in \mathbb{R}^d : \; G(\boldsymbol{q})\boldsymbol{v} = 0 \right\}.$$

Parametrisation of $\mathcal{F}_\theta$

- The constrained dynamics can be reformulated in the more geometric way[1]

$$\begin{cases} \dot{\boldsymbol{q}} = P(\boldsymbol{q})\partial_{\boldsymbol{p}} H(\boldsymbol{q}, \boldsymbol{p}) \\ \dot{\boldsymbol{p}} = -P(\boldsymbol{q})^\top \partial_{\boldsymbol{q}} H(\boldsymbol{q}, \boldsymbol{p}) + W(\boldsymbol{q}, \boldsymbol{p})\partial_{\boldsymbol{p}} H(\boldsymbol{q}, \boldsymbol{p}), \end{cases}$$

where $P(\boldsymbol{q}) : \mathbb{R}^d \to T_{\boldsymbol{q}}\mathcal{Q}$.

[1] T. Lee, M. Leok, and N H. McClamroch. *Global formulations of Lagrangian and Hamiltonian Dynamics on Manifolds*. Vol. 13. Springer, 2017.

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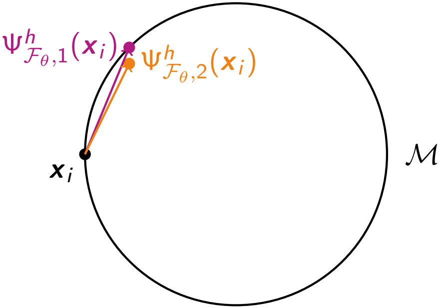
- We thus set

$$\mathcal{F}_\theta(\boldsymbol{q},\boldsymbol{p}) = \begin{bmatrix} P(\boldsymbol{q})\partial_{\boldsymbol{p}} H_\theta(\boldsymbol{q},\boldsymbol{p}) \\ -P(\boldsymbol{q})^\top \partial_{\boldsymbol{q}} H_\theta(\boldsymbol{q},\boldsymbol{p}) + W(\boldsymbol{q},\boldsymbol{p})\partial_{\boldsymbol{p}} H_\theta(\boldsymbol{q},\boldsymbol{p}) \end{bmatrix},$$

$$H_\theta(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}^\top M_{\theta_1}^{-1}(\boldsymbol{q})\boldsymbol{p} + \mathcal{N}_{\theta_2}(\boldsymbol{q}),\ \theta = (\theta_1,\theta_2)$$

[1] Lee, Leok, and McClamroch, *Global formulations of Lagrangian and Hamiltonian Dynamics on Manifolds*.

Choice of $\Psi^h_{\mathcal{F}_\theta}$



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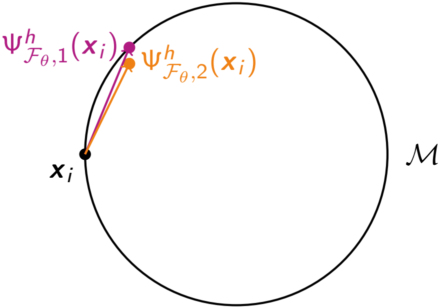

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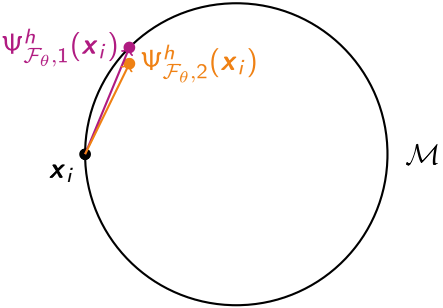

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- We consider the transitive Lie group action $\varphi : \mathcal{G} \times \mathcal{M} \to \mathcal{M}$, i.e., for every $m_1, m_2 \in \mathcal{M}$ there is $g \in \mathcal{G}$ with $\varphi(g, m_1) = m_2$.

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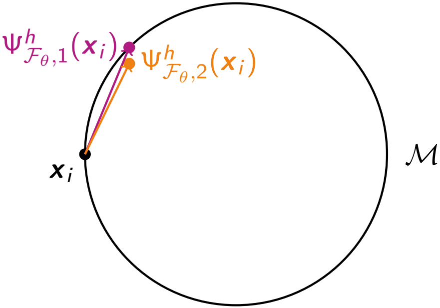

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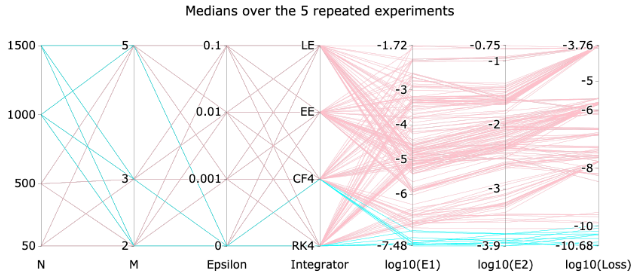
- For $\Psi_{\mathcal{F}_\theta,1}$ we choose a Lie group method, i.e., a method of the form $\Psi^h_{\mathcal{F}_\theta,1}(\mathbf{x}) = \varphi(g(\mathcal{F}_\theta, h, \mathbf{x}), \mathbf{x})$, $g(\mathcal{F}_\theta, h, \mathbf{x}) \in \mathcal{G}$.

Experimental results



$$\mathcal{E}_1 = \frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M}\left\| \left(\Psi^h_{\mathcal{F}}\right)^j\left(\boldsymbol{x}_i^0\right) - \left(\Psi^h_{\mathcal{F}_\theta}\right)^j\left(\boldsymbol{x}_i^0\right)\right\|_2^2$$

$$\mathcal{E}_2 = \frac{1}{N}\sum_{i=1}^{N}\left| H\left(\boldsymbol{x}_i\right) - H_\theta\left(\boldsymbol{x}_i\right) - \frac{1}{N}\sum_{l=1}^{N}\left(H\left(\boldsymbol{x}_l\right) - H_\theta\left(\boldsymbol{x}_l\right)\right)\right|$$

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THANK YOU FOR THE ATTENTION