Shape analysis and structure preservation

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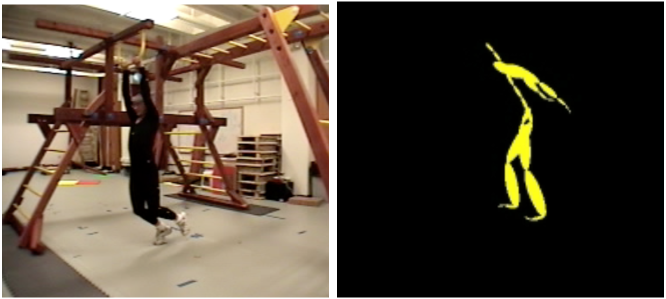
Outline

- Introduction: shape analysis for curves and surfaces, and for human motion data.
- Learning the equations of motion from data using a discrete Lagrange d'Alembert principle.
- Examples on synthetic data, pixel data and real-world data.
- Other ongoing and future work.

Given N *observation of previous values of a time series* $\{q_n\}_n$ *forecast future values:*

- Directly from the data.
- By learning (discrete) mechanical equations first.



CMU Graphics Lab Motion Capture Database

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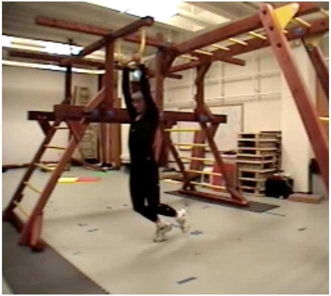

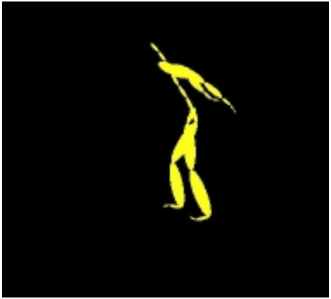

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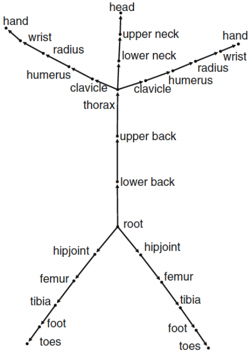
Some challenges:

- Find appropriate metrics.
- Deal with constraints.
- Learning Hamiltonians / Lagrangians for mechanical systems.
- Learn external forces.
- Provide enough data.

Skeletal animation

Skeleton consisting of bones connected by joints. One 3D rotation for each joint.

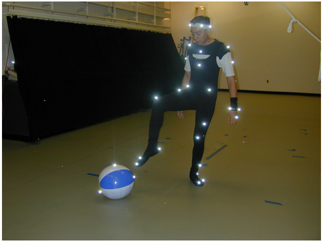


Human activity: $g : [0, T] \to \mathcal{J}$, $\mathcal{J} = \mathrm{SO}(3)^n$, where $[0, T]$ is a time interval.

- Data obtained by motion capturing.
- Motion manipulation is the processing of the data.
- CMU Motion Capturing Database.

Motion capturing: only data and one simple differential equation

Only data: $g : [0, T] \to SO(3)^n$



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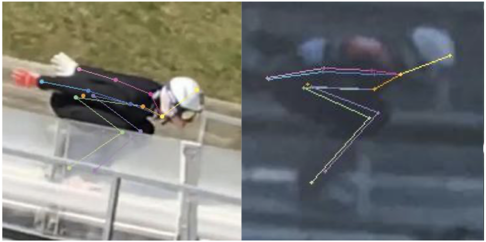

R. O. Hide, NTNU, master thesis

Motion capturing: only data and one simple differential equation

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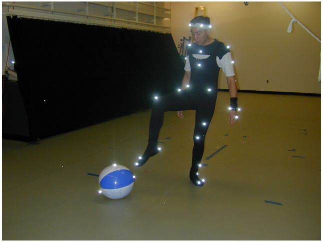
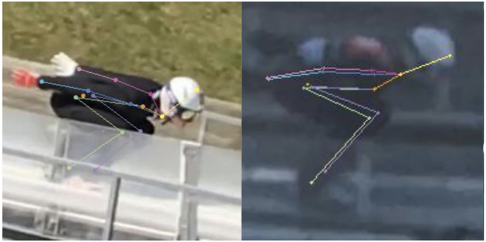


CMU Motion Capture Database



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Motion manipulation done via shape analysis

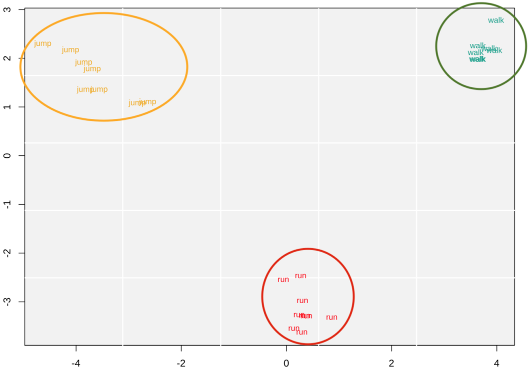
and we use one simple differential equation

$$\dot{g} = q(t)g(t), \qquad g(0) = e.$$

expressing the need of derivative information

- M. Eslitzbichler, *Modelling character motions on infinite-dimensional manifolds*, The Visual Computer, 2014.
- E. C., M. Eslitzbichler and A. Schmeding, *Shape analysis on Lie groups with applications in computer animation*, J Geometric Mechanics, 2016.
- E. C., S. Eidnes and A. Schmeding, *Shapes on homogeneous manifolds*, The Abel Symposium, 187-220, 2018.
- P. E. Lystad, *Signatures in Shape Analysis*, Master Thesis, NTNU, 2019.
- E. C., H. Glöckner, J. Riseth and A. Schmeding, *Deep learning of diffeomorphisms for optimal reparametrizations of shapes*, BIT, 2023.

Classifying running, walking, jumping animations as shapes (DP)



- $SO(3)^n$-valued time curves: the geometry of rotations is preserved.
- We treat time curves as shapes: use a reparametrisation invariant distance function: $d_{\mathcal{P}}$
- Dynamic programming, to find the optimal reparametrisation.
- Classical multidimensional scaling to visualize distances in a lower dimensional space.

- E. C., P.E. Lystad, N.Tapia, Signatures in Shape Analysis: an Efficient Approach to Motion Identification, Proceedings of the GSI conference 2019.

- Shapes are *unparametrized curves* (or surfaces) in a vector space or on a manifold.
- The use of shapes is natural in applications where one wants to compare curves or surfaces independently of their parametrisation.

Definition of **shapes** via an equivalence relation: let $\mathrm{I} \subset \mathbb{R}$ an interval, consider

$$\mathcal{P} := \mathrm{Imm}(\mathrm{I}, \mathbb{R}^n) = \{c \in C^\infty(\mathrm{I}, \mathbb{R}^n) \mid \dot{c}(t) \neq 0\},$$

$\mathcal{P}$ is called pre-shape space and is an **infinite dimensional manifold**. Let $c_0, c_1 \in \mathcal{P}$ then

$$c_0 \sim c_1 \Longleftrightarrow \exists\, \varphi : \quad c_0 = c_1 \circ \varphi$$

with $\varphi \in \mathrm{Diff}^+(\mathrm{I})$ a orientation preserving diffeomorphism on I

Shape space:

$$\mathcal{S} := \mathrm{Imm}(\mathrm{I}, \mathbb{R}^n)/\mathrm{Diff}^+(\mathrm{I})$$

Distance function on $\mathcal{S} = \mathcal{P}/\mathrm{Diff}^+(I)$

Definition of a **distance** function $d_{\mathcal{S}}$ to measure similarities between two shapes $[c_0]$ and $[c_1]$. The distance function on $\mathcal{S}$ should be independent of the choice of representatives.

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Let $d_{\mathcal{P}}$ be a reparametrization invariant distance function on $\mathcal{P}$ i.e.

$$d_{\mathcal{P}}(c_0, c_1) = d_{\mathcal{P}}(c_0 \circ \varphi, c_1 \circ \varphi) \quad \forall \varphi \in \mathrm{Diff}^+(\mathrm{I}).$$

Definition of distance on $\mathcal{S}$:

$$d_{\mathcal{S}}([c_0],[c_1]) := \inf_{\varphi \in \mathrm{Diff}^+(\mathrm{I})} d_{\mathcal{P}}(c_0, c_1 \circ \varphi).$$

Proposition

If $d_{\mathcal{P}}$ is a reparametrization invariant distance function on $\mathcal{P}$, then $d_{\mathcal{S}}([c_0],[c_1])$ is independent of the choice of representatives of $[c_0]$ and $[c_1]$.

Distance on $\mathcal{P}$ via **SRVT** *and Q-transform*

One can proceed first transforming the curves and then computing L_2 distances:

$$Q : \mathcal{P} \to C^\infty(I, \mathbb{R}^n), \quad c \mapsto q,$$

$$Q : \mathcal{P} \to C^\infty(I, \mathbb{R}^n), \quad c \mapsto q, \quad Q(c) := \begin{cases} \frac{\dot{c}}{\sqrt{\|\dot{c}\|}} & \text{SRVT} \\ \sqrt{\|\dot{c}(\cdot)\|}\, c(\cdot) & Q-\text{transform} \end{cases}$$

$$d_{\mathcal{P}}(c_0, c_1) = d_{L^2}(Q(c_0), Q(c_1)) = \|q_0 - q_1\|_{L_2}.$$

With this definition $d_{\mathcal{P}}$ is reparametrization invariant and $d_{\mathcal{S}}$ is well defined, because Q is equivariant wrt reparametrizations:

$$Q(c \circ \varphi)(t) = \sqrt{\dot{\varphi}(t)} \cdot (Q(c) \circ \varphi)(t)$$

- A. Srivastava, E. Klassen, S.H. Joshi, and I.H. Jermyn. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2011.
- M. Mani, S. Kurtek, C. Barillot, A. Srivastava, *IEEE Symposium on Biomedical Imaging*, 2010.

Optimal reparametrization problem

Optimal reparametrization problem: let $q_0 = Q(c_0)$, $q_1 = Q(c_1)$, given shapes $[c_0]$ and $[c_1]$

$$d_{\mathcal{S}}([c_0],[c_1]) = \inf_{\varphi \in \mathrm{Diff}^+(\mathrm{I})} E(\varphi), \qquad E(\varphi) = d_{\mathcal{P}}(c_0, c_1 \circ \varphi) = \|q_0 - \sqrt{\dot{\varphi}}\,(q_1 \circ \varphi)\|^2_{L_2}.$$

Optimisation problem on an infinite dimensional Lie group $\mathrm{Diff}^+(\mathrm{I})$, with "Lie algebra" $T_{\mathrm{id}}\mathrm{Diff}^+(\mathrm{I})$, $I = [0,1]$.
We parametrize the diffeomorphisms with deep neural networks as follows:

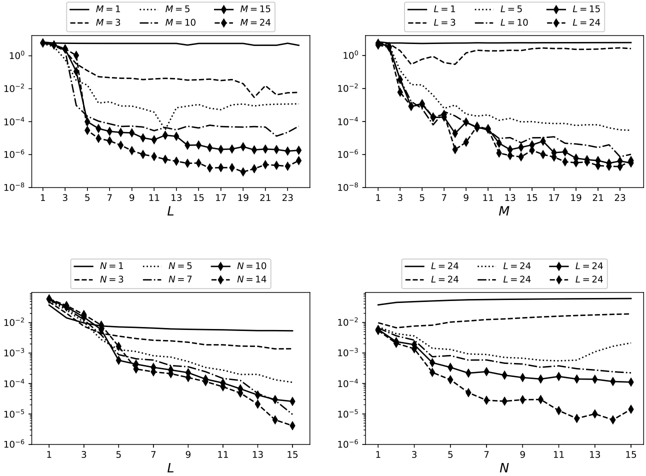
Consider a basis $v_1, v_2, \dots$ of $T_{\mathrm{id}}\mathrm{Diff}^+(\mathrm{I})$ write

$$\varphi_\theta = (\mathrm{id} + h_1 f_{\theta_1}) \circ \cdots \circ (\mathrm{id} + h_L f_{\theta_L}).$$

$$f_{\theta_\ell} = \sum_{j=1}^{M} \beta_j^\ell v_j, \qquad \theta_\ell = \{\beta_j^\ell\}_{j=1,\dots,M}^{\ell=1,\dots,L}$$

Optimise on these "approximate diffeomorphisms".

- E. Celledoni, H. Glöckner, J. Riseth and A. Schmeding, *Deep neural networks on diffeomorphism groups for optimal shape reparametrization*, BIT, 2023.


M = 1
M = 5
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N = 3
N = 7
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Parametric surfaces embedded in $\mathbb{R}^3$

Domain $\Omega = [0,1]^2$. Denoting by $f : \Omega \to \mathbb{R}^3$ the parametric surface, f_x and f_y the partial derivatives.

Normal vector and area scaling factor:

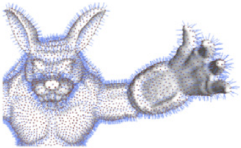
$$\mathrm{n}_f(x,y) = f_x \times f_y, \qquad a_f(x,y) = |f_x \times f_y|$$

then

$$\mathcal{P} = \{f \in C^\infty(\Omega,\mathbb{R}) \,|\, a_f(x,y) > 0, \forall (x,y) \in \Omega\}$$

Implicit neural representations: $g : \mathbb{R}^3 \to \mathbb{R}$, e.g. the *signed distance function* approximated by a neural network g_θ

$$\mathcal{M} = g^{-1}(0).$$

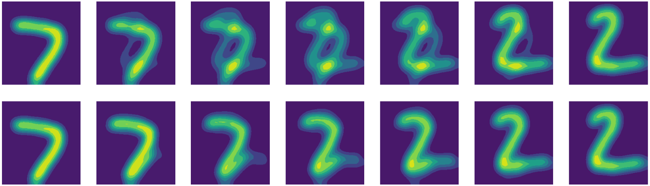


oriented point cloud

- I.H. Jermyn, et al., *Elastic shape matching of parameterized surfaces using square root normal fields.* In: A. Fitzgibbon, S. Lazebnik, P. Perona, Y. Sato, C. Schmid (eds.) Computer Vision, ECCV 2012, Springer, (2012).
- S. Kurtek, et al., *A novel Riemannian framework for shape analysis of 3d objects.* In: 2010 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, (2010).
- L. Schirmer et al., *Geometric implicit neural representations for signed distance functions*, Computers and Graphics, 2022.

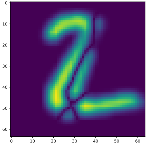
Data generation, optimal deformation

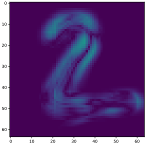
MNIST, matching of images, handwritten digits

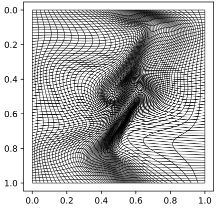


Top $\lambda(f_1, f_2, \tau) := \tau f_1 + (1-\tau) f_2$

Bottom $\gamma(f_1, f_2, \tau) := \tau f_1 + (1-\tau) f_2 \circ \varphi^*$, φ^* optimal reparametrization.







- E. C., H. Glöckner, J. Riseth and A. Schmeding, *Deep learning of diffeomorphisms for optimal reparametrizations of shapes*, BIT, 2023.

Learning Mechanical systems from data

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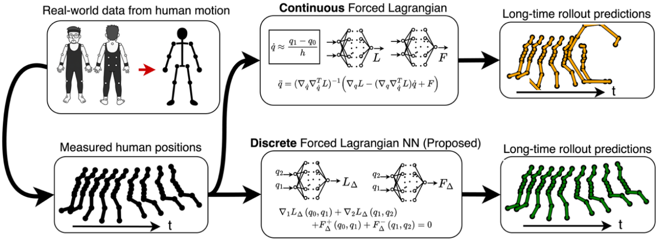

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- We assume to measure **only position data**.
- Necessary to take into account external forces and dissipative forces.
- We **use the laws of physics**.
- We want to learn separately the the **external forces** from the **conservative forces** (coming from the the Lagrangian).
- Optional: we learn separately kinetic energy (the mass matrix) and potential energy.

Joint work with M. D. Hansen and B.K. Tapley

Lagrange d'Alembert principle - Balance of forces

LdA principle

$$\delta\left(\int_{t_0}^{t_N} L\left(q(t),\dot{q}(t)\right)dt\right)+\int_{t_0}^{t_N} F\left(q(t),\dot{q}(t),u(t)\right)\cdot\delta q(t)\,dt=0,$$

where δ denotes variations that vanish at the endpoints

$q(t_0)=q_0$ and $q(t_N)=q_N$,

$L:TQ\to\mathbb{R}$ is the Lagrangian function

$F:TQ\to TQ^*$ is the Lagrangian force, a fiber preserving map
$F:(q,\dot{q})\mapsto(q,F(q,\dot{q}))$,

Lagrange d'Alembert principle - Balance of forces

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Forced Euler- Lagrange Equations (equivalent to LdA)

$$0=\mathcal{E}(L,F)(q,t):=\frac{\partial L}{\partial q}\left(q(t),\dot{q}(t)\right)-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\left(q(t),\dot{q}(t)\right)\right)+F\left(q(t),\dot{q}(t)\right).$$

LdA suggests that we should learn L separately from F.

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In the spirit of *Geometric Mechanics-Variational Integrators*, we use a **discrete LdA**.

- J E Marsden and M West, *Discrete variational integrators*, Acta Numerica, (2001);
- DM de Diego, R. Sato Martin de Almagro, *Variational order for forced Lagrangian systems*, Nonlinearity, 2018.

Discrete Lagrange d'Alembert principle: using only position data

$$L_\Delta(q_n, q_{n+1}) \approx \int_{t_n}^{t_n+h} L\big(q(t), \dot{q}(t)\big)\, dt,$$

$$F_\Delta^-(q_n, q_{n+1}, h)\cdot \delta q_n + F_\Delta^+(q_n, q_{n+1}, h)\cdot \delta q_{n+1} \approx \int_{t_n}^{t_n+h} F\big(q(t), \dot{q}(t)\big)\cdot \delta q(t)\, dt,$$

$L_\Delta : Q \times Q \to \mathbb{R}$ (discrete Lagrangian), $F_\Delta^\pm : Q \times Q \to T^*Q$ (discrete force)

$$\pi_Q^- = \pi_Q \circ F_\Delta^- \qquad \pi_Q^- : Q\times Q \to Q, \qquad \pi_Q^+ = \pi_Q \circ F_\Delta^+ \qquad \pi_Q^+ : Q\times Q \to Q,$$

with $\pi_Q : T^*Q \to Q$ the projection.

The discrete Lagrange-d'Alembert principle: find a discrete trajectory $\{q_n\}_{n=1}^N$ s.t.

$$\delta \sum_{n=0}^{N-1} L_\Delta(q_n, q_{n+1}) + \sum_{n=0}^{N-1} \left[F_\Delta^-(q_n, q_{n+1})\cdot \delta q_n + F_\Delta^+(q_n, q_{n+1})\cdot \delta q_{n+1}\right] = 0,$$

for all variations $\{\delta q_n\}_{n=0}^N$ vanishing at the endpoints $\delta q_0 = \delta q_N = 0$.

Discrete forced Euler-Lagrange equations:

$$0 = \mathcal{E}_\Delta(L_\Delta, F_\Delta)(q_{n-1}, q_n, q_{n+1}) := D_2\, L_\Delta(q_{n-1}, q_n) + D_1\, L_\Delta(q_n, q_{n+1}) \\ + F_\Delta^+(q_{n-1}, q_n) + F_\Delta^-(q_n, q_{n+1}), \quad n = 2, \ldots, N-1,$$

where D_1 and D_2 denote differentiation with respect to the first and second variable.

Goal: learn NNs $L_\theta \approx L$ and $F_\theta \approx F$ from the observed trajectories of the mechanical system

Direct Discrete Lagrange d'Alembert setting: Given L Lagrangian and F forces compute trajectories $\{q_n\}_{n=0}^N$ of the mechanical system satisfying Discrete LdA principle.

Inverse discrete LdA setting:
Given multiple observed (discrete) trajectories $\{q_n\}_{n=0}^N$ we seek approximations to the Lagrangian and forces (L, F).
We replace (L, F) with neural networks approximations

$$L_\theta \approx L, \qquad F_\theta \approx F$$

(L_θ, F_θ) are then the unknowns of our problem which we find minimizing the loss function

$$\mathcal{L} = \mathcal{L}_{\text{mech}}(L_\theta, F_\theta) + \mathcal{L}_{\text{reg}}$$

Example - discretization of the LdA - loss function to find the parameters

$$L_\Delta(q_n, q_{n+1}) := h\,L_\theta\left(\frac{q_n+q_{n+1}}{2}, \frac{q_{n+1}-q_n}{h}\right) = h\,L_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right)$$

$$F_\Delta^{+}(q_n, q_{n+1}, h) := \frac{h}{2}\,F_\theta\left(\frac{q_n+q_{n+1}}{2}, \frac{q_{n+1}-q_n}{h}\right) = \frac{h}{2}\,F_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right)$$

$$F_\Delta^{-}(q_n, q_{n+1}, h) := \frac{h}{2}\,F_\theta\left(\frac{q_n+q_{n+1}}{2}, \frac{q_{n+1}-q_n}{h}\right) = \frac{h}{2}\,F_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right)$$

where

$$\bar{q}_{n+\frac{1}{2}} = \frac{1}{2}(q_n + q_{n+1})$$
$$\bar{\dot{q}}_{n+\frac{1}{2}} = \frac{1}{h}(q_{n+1} - q_n).$$

Loss function is the residual of the discrete forced Euler- Lagrange equations:

$$\mathcal{L}_{\text{mech}}(L_\theta, F_\theta) = \frac{h}{2}\sum_{\mathcal{T}}\sum_{n=2}^{N-1}\Bigg\| D_1\,L_\theta\left(\bar{q}_{n-\frac{1}{2}}, \bar{\dot{q}}_{n-\frac{1}{2}}\right) + \frac{2}{h}\,D_2\,L_\theta\left(\bar{q}_{n-\frac{1}{2}}, \bar{\dot{q}}_{n-\frac{1}{2}}\right)$$
$$+ D_1\,L_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right) - \frac{2}{h}\,D_2\,L_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right)$$
$$+ F_\theta\left(\bar{q}_{n-\frac{1}{2}}, \bar{\dot{q}}_{n-\frac{1}{2}}\right) + F_\theta\left(\bar{q}_{n+\frac{1}{2}}, \bar{\dot{q}}_{n+\frac{1}{2}}\right)\Bigg\|_2$$

Structure of Lagrangians, Forces and Regularization

- **free**: $L_\theta = L_\theta(q,\dot{q})$, $F_\theta = F_\theta(q,\dot{q})$, feed forward NNs.
- **structured**:
  - a mechanical Lagrangian

    $$L_\theta(q,\dot{q}) = \frac{1}{2}\dot{q}^T M_\theta(q)\dot{q} - U_\theta(q),$$

    with $M_\theta(q)$ SPD:

    $$M_\theta(q) = \epsilon I + C_\theta^T(q)C_\theta(q)$$

    learn M_θ through the factors C_θ, and learn U_θ,
  - and dissipative force $F_\theta = -K_\theta\dot{q}$ with $K_\theta = K_\theta^T$ a symmetric positive definite matrix.

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Regularization: Impose L_θ to be a *regular Lagrangian*, i.e.

$$S := \left(\frac{\partial^2 L_\theta(q,\dot{q})}{\partial\dot{q}_i\partial\dot{q}_j}\right),$$

$$\mathcal{L}_{\text{reg}} = \frac{1}{N_r}\sum_{r=1}^{N_r}\left|\log\left(|\det(S_r)|\right)\right|, \qquad S_r = S(\bar{q}_{r+\frac{1}{2}},\bar{\dot{q}}_{r+\frac{1}{2}})$$

on N_r regularization points given from the training dataset.

Related work: by Offen and Ober-Blöbaum

- Propose to learn the Lagrangian of Euler-Lagrange dynamics, with no external forces. Approximate the Lagrangian using Gaussian Processes.
- Discuss the problem of non uniqueness of the Lagrangian and propose ways to learn regular Lagrangians.
- Introduce the concept of *inverse modified Lagrangian* $L_{invmod} \approx L$ and

$$L = L_{invmod} + \tilde{L}\, h^p + \mathcal{O}(h^{p+1})$$

- For more accurate approximations of L use *Lagrangian Backward Error Analysis* and L_{invmod}.
- Use only position data.
- Experiments on synthetic data.

- S Ober-Blöbaum, C. Offen, *Variational Learning of Euler-Lagrange Dynamics from Data*. Journal of Computational and Applied Mathematics, 421, 2023.
- C. Offen, S. Ober-Blöbaum, *Symplectic integration of learned Hamiltonian systems*, Chaos, 2022.
- C. Offen, S. Ober-Blöbaum, *Learning discrete Lagrangians for variational PDEs from data and detection of travelling waves*, 2023, arXiv preprint arXiv:2302.08232.

Higher order approximations of L and F

- We use a symmetric multi-step approach.
- Symmetric multi-step variational discretization have good geometric properties. (Hairer and Lubich)

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- Symmetric multi-step variational discretization have good geometric properties. (Hairer and Lubich)

Order 4:

$$L_\Delta(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = hL_\theta(\bar{q}_n, \bar{v}_n),$$
$$F^+_\Delta(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = \frac{h}{2}F_\theta(\bar{q}_n, \bar{v}_n),$$
$$F^-_\Delta(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = \frac{h}{2}F_\theta(\bar{q}_n, \bar{v}_n),$$

where

$$\bar{q}_n = \frac{1}{12}(-q_{n-2} + 8q_{n-1} + 4q_{n+1} + q_{n+2}), \qquad \bar{v}_n = \frac{1}{12h}(q_{n-2} - 8q_{n-1} + 8q_{n+1} - q_{n+2}).$$

- We use a symmetric multi-step approach.
- Symmetric multi-step variational discretization have good geometric properties. (Hairer and Lubich)

Order 4:

$$L_\Delta(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = hL_\theta(\bar{q}_n, \bar{v}_n),$$
$$F_\Delta^+(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = \frac{h}{2}F_\theta(\bar{q}_n, \bar{v}_n),$$
$$F_\Delta^-(q_{n-2}, q_{n-1}, q_{n+1}, q_{n+2}) = \frac{h}{2}F_\theta(\bar{q}_n, \bar{v}_n),$$

where

$$\bar{q}_n = \frac{1}{12}(-q_{n-2} + 8q_{n-1} + 4q_{n+1} + q_{n+2}), \qquad \bar{v}_n = \frac{1}{12h}(q_{n-2} - 8q_{n-1} + 8q_{n+1} - q_{n+2}).$$

Higher order: use coefficients δ_j ($j = -k, \ldots, k$), $\delta_j = -\delta_{-j}$, for a derivative approximation of order $2k$,

$$\bar{v}_n = \frac{1}{h}\sum_{j=-k}^{k}\delta_j q_{n-j}, \quad \bar{q}_n = (1-\delta_1)q_{n+1} - \sum_{j=-k, j\neq 0,1}^{k}\delta_j q_{n-j}, \quad \delta_j = \frac{(-1)^{j-1}}{j}\frac{k!^2}{(k-j)!(k+j)!},$$

for $j = 1, \ldots, k$ and where $\delta_0 = 0$.

- E. Hairer and C. Lubich, *Symmetric multistep methods over long times.* Numer. Math., 2004
- E. Hairer and C. Lubich, *Symmetric multistep methods for charged particle dynamics.* SMAI J. Comput. Math., 2017.

Related work: Lagrangian NN and Generalized Lagrangian NN

- Formulate their learning problem starting from the **(Forced) Euler-Lagrange Equations**:

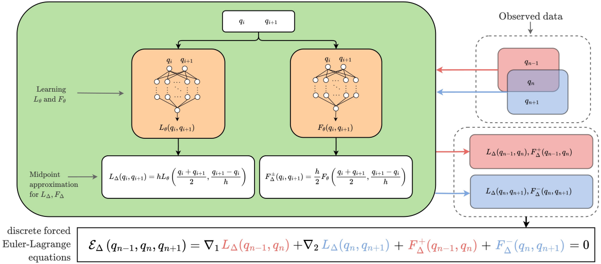
$$0 = \frac{\partial L}{\partial q}\left(q(t), \dot{q}(t)\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\left(q(t), \dot{q}(t)\right)\right) + F\left(q(t), \dot{q}(t)\right).$$

- By expanding $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\left(q(t), \dot{q}(t)\right)\right)$ and **assuming** $\frac{\partial^2 L}{\partial \dot{q}^2}$ **invertible** one obtains

$$\ddot{q} = \left(\frac{\partial^2 L}{\partial \dot{q}^2}\right)^{-1}\left(\frac{\partial L}{\partial q} - \dot{q} \cdot \frac{\partial^2 L}{\partial q \partial \dot{q}} + F\right)$$

  Then solve this equation numerically to obtain $\{\hat{q}_n, \dot{\hat{q}}_n\}_{n=0}^N$ to compare with the observed data $\{q_n, \dot{q}_n\}_{n=0}^N$ in a least squares loss function.
- Learn both L_θ and F_θ.
- Need both position and velocity data (or approximate velocity with finite differences).
- Experiments on synthetic data.

- Miles Cranmer, Sam Greydanus, Stephan Hoyer, Peter Battaglia, David Spergel, and Shirley Ho. *Lagrangian neural networks*, arXiv:2003.04630.
- Xiao, S., Zhang, J. and Tang, Y. *Generalized Lagrangian Neural Networks.* arXiv:2401.03728. Jan. 2024. http://arxiv.org/abs/2401.03728 (June 26, 2024).



Extrapolation error: is the error at the k-th step of a trajectory computed numerically, with $k \geq 2$ after L_θ and F_θ are learned.

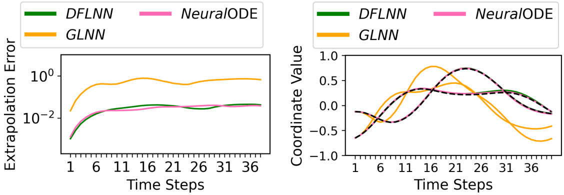
$$\text{Extrapolation Error}_k = \frac{1}{N_\mathcal{T}} \sum_{i=0}^{N_\mathcal{T}} \| q_k^{\{i\}} - \hat{q}_k^{\{i\}} \|_2^2 . \tag{1}$$

Mean square error associated to the k-th step of a predicted trajectory:

- q_k^i true trajectory at time step k given the initial condition for $\{q_0^i, q_1^i\}$;
- $\hat{q}_k^{\{i\}}$ is the solution of $\mathcal{E}_\Delta(\hat{q}_{k-2}^i, \hat{q}_{k-1}^i, \hat{q}_k^i) = 0$ for trajectory i, starting from $\mathcal{E}_\Delta(q_0^i, q_1^i, \hat{q}_2^i) = 0$.

Where $N_\mathcal{T}$ is the number of trajectories of N steps (segments of triplets $\{q_{n-1}, q_n, q_{n+1}\}$ are selected from each trajectory and used as input to the NNs during training).

Experiments (synthetic data): damped double pendulum



The model was trained on the damped dataset and evaluated on a test dataset with same damping.

Left: Extrapolation error given time step $h = C \cdot 10^{-2}$ and a training dataset containing 320 trajectories. Test dataset contains 10 trajectories.

Right: Prediction rollouts.

Experiments (synthetic data): damped double pendulum

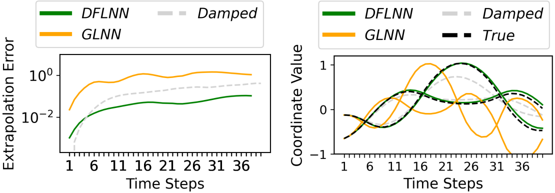
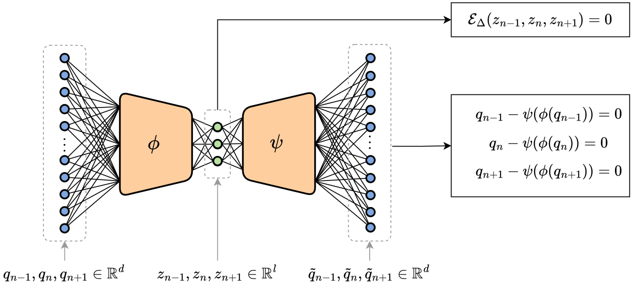


Figure: Evaluating the conservative part of the trained Lagrangian-based models on an undamped double pendulum dataset. The lightgray line is included as a reference to the damped system that the model is being trained on.

Dimensionality reduction for pixel data and human motion data

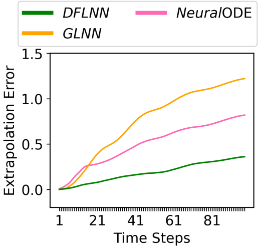


An autoencoder is applied to reduce the high-dimensional input dimension to a lower-dimensional latent space. The proposed model is applied to the dynamics in the latent space.

Experiments (synthetic data): pixel pendulum

Experiment inspired by:

- L. Mars Gao and J. Nathan Kutz, *Bayesian autoencoders for data-driven discovery of coordinates, governing equations and fundamental constants*, Prooceedings of the Royal Society A, 2024.



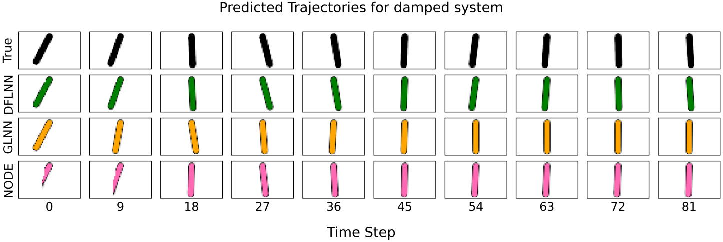
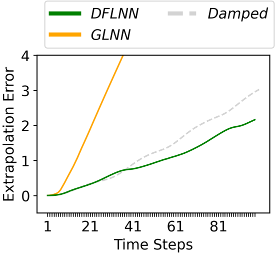


Figure: Results for a simple pendulum represented through pixel images. The models are trained on a damped dataset, and evaluated on a test dataset with the same damping.

Experiments (synthetic data): pixel pendulum



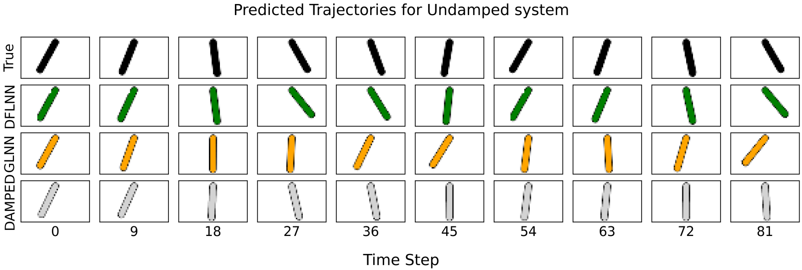
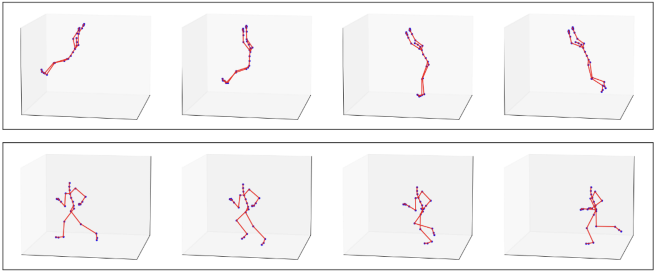
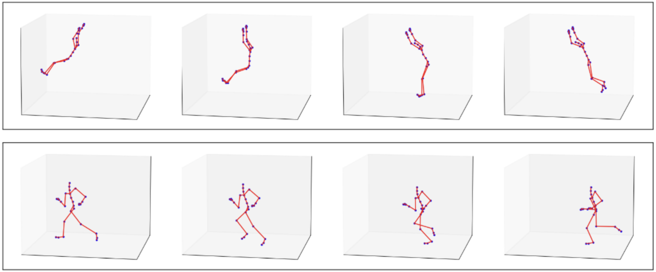


Figure: Results for a simple pendulum represented through pixel images. The models are trained on a damped dataset, the conservative part of the trained Lagrangian-based models is evaluated on an undamped simple pendulum system. The lightgray line and figures are included as a reference to the damped system that the model has been trained on.

Experiments (real-world data)

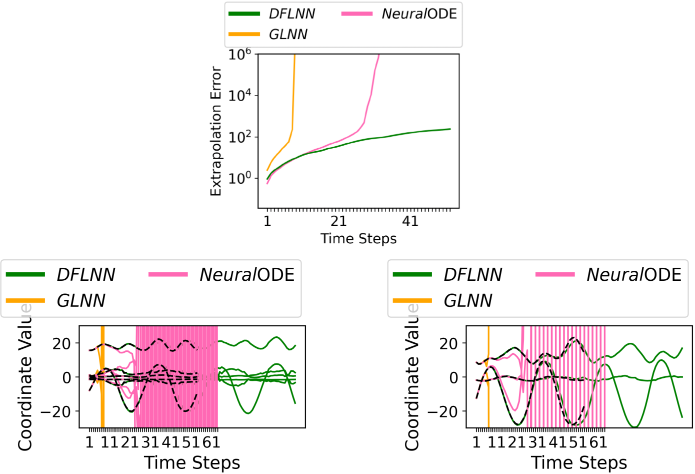


Experiments (real-world data)



- Too few trajectories for the same motion: need to augment the data-set.
- Use two trials of the same motion for the same person.
- Extract 10 trajectories per trial for a total of 20 trajectories.
- We track the motion of 10 joints: `rtibia`, `rfemur`, `rhipjoint`, `root`, `lowerback`, `upperback`, `thorax`, `rclavicle`, `rhumerus`, and `rradius`.
- Use a Savitzky-Golay filter to smoothen the data.
- Perform dimensionality reduction including the parameters of an autoencoder in the training.

Experiments (real-life data): swinging motion



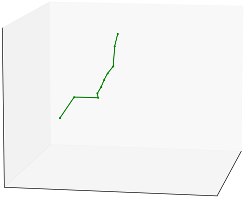
Reconstruction of human motion, capturing a swinging motion. (Black - recorded motion)

Top Extrapolation error.

Left Prediction rollouts in coordinate space for the root of the skeleton.

Right Prediction rollouts for the the right femur.

Animated skeletal movement



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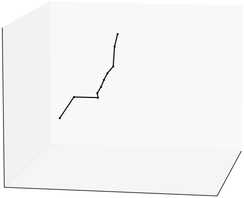

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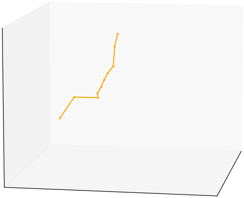
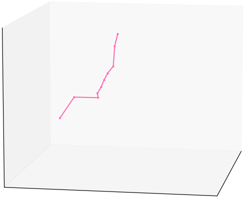
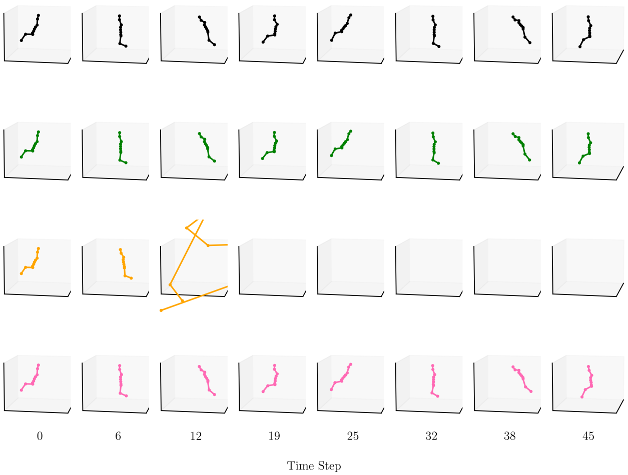




Skeletal movement snapshots



Green notation is DFLNN (proposed), yellow is the GLNN model, and pink lines a Neural ODE. The ground truth is indicated in black. Full movement represented as a skeletal sketch.

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