Towards physically structured probabilistic reinforcement learning

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Joint work with Steindór Sæmundsson, James T. Wilson, Viacheslav Borovitskiy, Peter Mostowsky, Katja Hoffmann, and Marc Deisenroth

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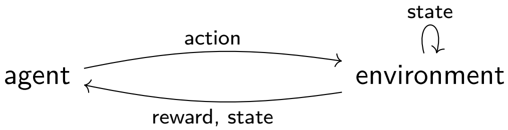
Reinforcement learning

An agent interacts with an environment in discrete time

At each time step

- Agent chooses action
- Environment changes to a new state
- Agent receives reward from environment



Goal: maximize reward

Continuous control

Continuous-time: controlled differential equations

$$\dot{x}(t) = f(x(t), u(x))$$

Goal: find control map $u : X \to U$ minimizing the path integral

$$\int_0^T c(x(t), u(t)) \mathrm{d}t + c(x(T))$$

f: unknown

Model-based RL: learn a model of f and act accordingly

(possibly taking uncertainty into account via Bayesian methods)

Geometric control and reinforcement learning

Robots are mechanical systems satisfying the laws of physics

Hence, letting $x = (q, p)$, the CDE

$$\dot{x}(t) = f(x(t), u(x))$$

carries the structure of Hamilton's equations

$$\dot{q}(t) = \frac{\partial H}{\partial p} \qquad \dot{p}(t) = -\frac{\partial H}{\partial q} + F$$

Our program: use this structure to make RL more data-efficient

- Formulate theory in the language of *geometry and mechanics*
- Motivates Bayesian theory on *Riemannian manifolds*

Variational integrator networks for physically structured embeddings

Steindór Sæmundsson, Alexander Terenin,
Katja Hoffmann, and Marc Deisenroth

Neural ODEs for embedding dynamical systems

Goal: learn an embedding of a dynamical system observed as pixels

Neural ODEs: view RNNs and ResNets as discretizations of ODEs

$$\dot{x}(t) = f(x(t), t)$$

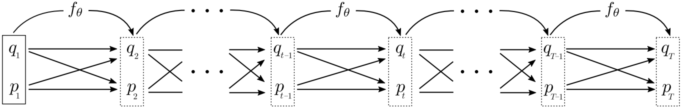
Idea: rather than a free-form ODE, work with Hamilton's equations

$$\dot{q}(t) = \frac{\partial H}{\partial p} \qquad\qquad \dot{p}(t) = -\frac{\partial H}{\partial q}$$

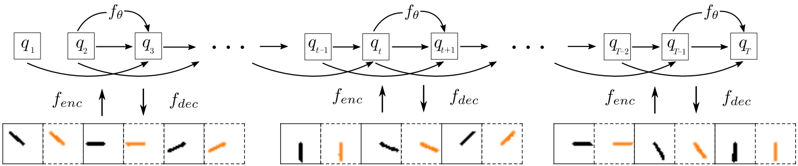
Variational integrator networks

Discretize the variational principle

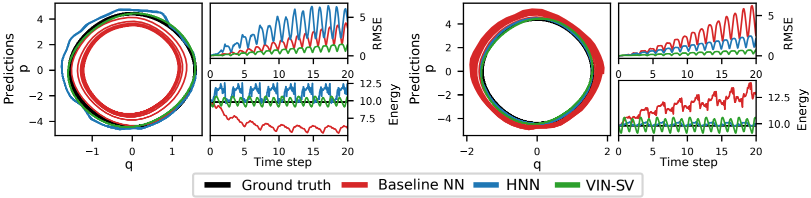
$\implies$ new network architectures!



Learn from pixels using a VAE

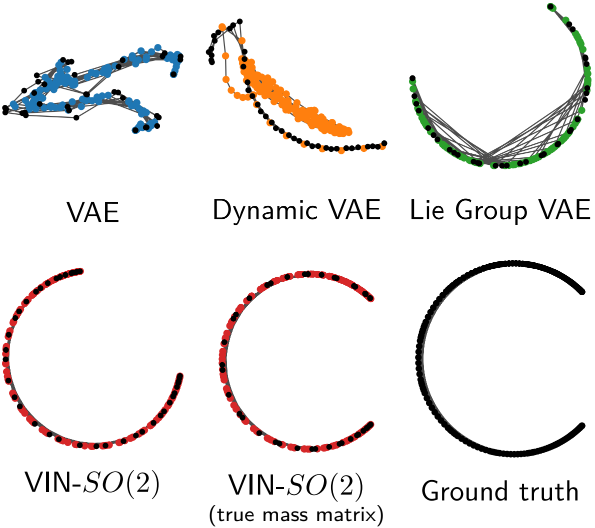


Conservation laws



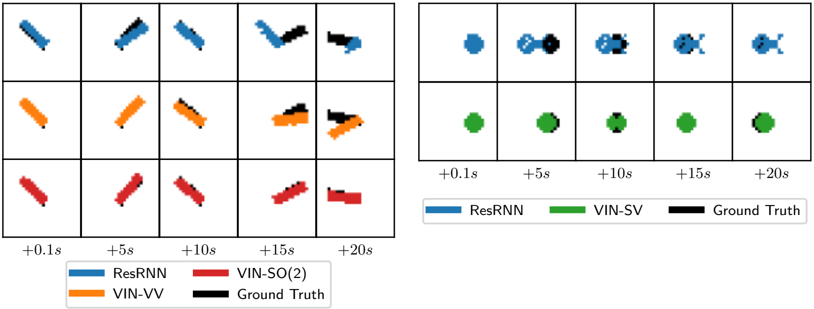
VINs conserve phase volume and momentum *exactly*
and conserve energy much better than free-form RNNs

Latent state space



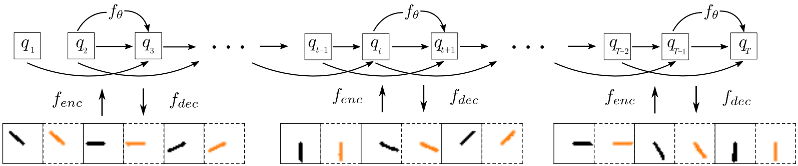
Continuous latent state space in space and time

Long-term forecasting



Better long-term accuracy in small-data settings

A physically structured architecture



✓ data-efficiency
✓ interpretability
✓ latent space behavior
✓ long-term generalization
✓ well-understood mathematics

☒ can be slightly less expressive
☒ external forces are tricky (working on this now)

Efficiently sampling functions from Gaussian process posteriors

James T. Wilson,[*] Viacheslav Borovitskiy,[*] Alexander Terenin,[*]
Peter Mostowsky,[*] and Marc Deisenroth




[*]Equal contribution

Probabilistic models for reinforcement learning

Controlled differential equations

$$\dot{x}(t) = f(x(t), u(x))$$

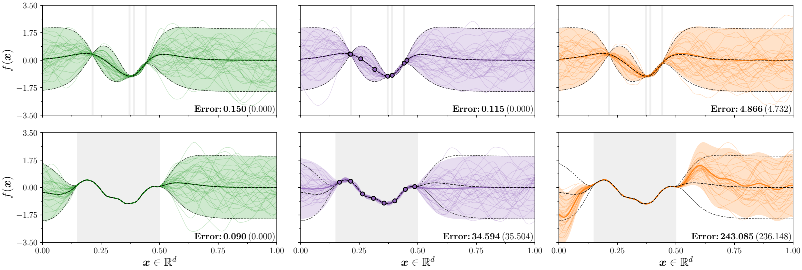
Time-discretization $\implies$ rollouts

$$x_{t+1} = x_t + \Delta f(x_t, u(x_t))$$
$$x_{t+2} = x_{t+1} + \Delta f(x_{t+1}, u(x_{t+1}))$$

✓ Gaussian processes: excellent data-efficiency (PILCO)

☒ Gaussian process rollouts: $O(T^3)$

This work: address this without sacrificing accuracy


Error: 0.150 (0.000)
Error: 0.115 (0.000)
Error: 4.866 (4.732)
Error: 0.090 (0.000)
Error: 34.594 (35.504)
Error: 243.085 (236.148)
$f(\boldsymbol{x})$
$\boldsymbol{x} \in \mathbb{R}^d$

Key idea: Matheron's update rule

$$(f \mid \boldsymbol{y})(\cdot) \overset{\mathrm{d}}{=} f(\cdot) + \mathbf{K}_{(\cdot)\boldsymbol{x}}\mathbf{K}_{\boldsymbol{x}\boldsymbol{x}}^{-1}(\boldsymbol{y} - \boldsymbol{f}_{\boldsymbol{x}})$$

Why? For $\begin{bmatrix}\boldsymbol{x}_1 \\ \boldsymbol{x}_2\end{bmatrix} \sim \mathrm{N}\left(\begin{bmatrix}\boldsymbol{\mu}_2 \\ \boldsymbol{\mu}_2\end{bmatrix}, \begin{bmatrix}\mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22}\end{bmatrix}\right)$ we have

$$(\boldsymbol{x}_1 \mid \boldsymbol{x}_2 = \boldsymbol{u}) \overset{\mathrm{d}}{=} \boldsymbol{x}_1 + \mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}^{-1}(\boldsymbol{u} - \boldsymbol{x}_2)$$

Path-wise sampling with sparse GPs

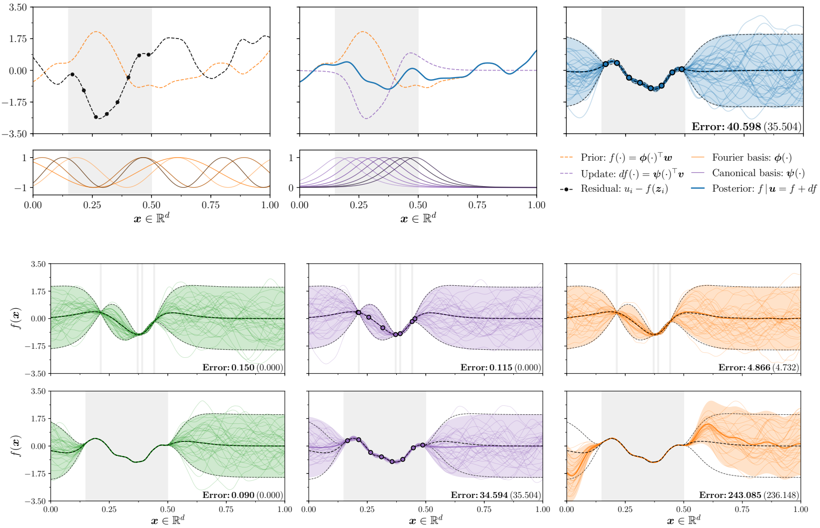
$$\underbrace{(f \mid \boldsymbol{y})(\cdot)}_{\text{posterior}} \overset{\mathrm{d}}{=} \underbrace{f(\cdot)}_{\text{prior}} + \underbrace{\mathbf{K}_{(\cdot)\boldsymbol{x}}\mathbf{K}_{\boldsymbol{x}\boldsymbol{x}}^{-1}(\boldsymbol{y} - \boldsymbol{f}_{\boldsymbol{x}})}_{\text{update}}$$

Prior term: discretize with random Fourier features

Data term: approximate with sparse GPs

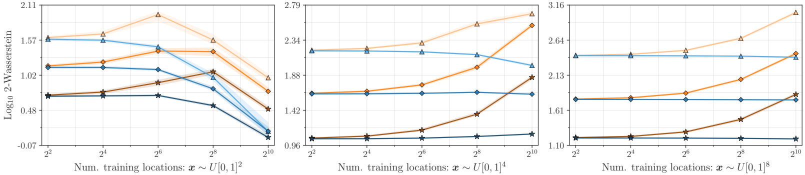
$$\underbrace{(f \mid \boldsymbol{y})(\cdot)}_{\substack{\text{approximate}\\\text{posterior}}} \overset{\mathrm{d}}{\approx} \underbrace{\sum_{i=1}^{\ell} w_i \phi_i(\cdot)}_{\substack{\text{RFF basis for}\\\text{stationary prior}}} + \underbrace{\sum_{i=1}^{m} v_i k(\cdot, z_i)}_{\substack{\text{canonical basis}\\\text{for sparse update}}} \qquad \boldsymbol{v} = \mathbf{K}_{\boldsymbol{z}\boldsymbol{z}}^{-1}(\boldsymbol{u} - \boldsymbol{\Phi}^\top \boldsymbol{w})$$

Visualizing decoupled sample paths



Error analysis

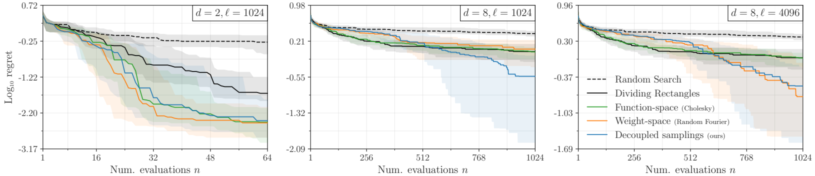
$$\underbrace{W_{2,L^2(\mathcal{X})}(f^{(d)}, f \mid \boldsymbol{y})}_{\text{total approximation error}} \leq \underbrace{W_{2,L^2(\mathcal{X})}(f^{(s)}, f \mid \boldsymbol{y})}_{\text{error in sparse posterior}} + \underbrace{C\, W_{2,L^2(\mathcal{X})}(f^{(w)}, f)}_{\text{error in approximate prior}}$$



Empirical Wasserstein error smaller than in RFF

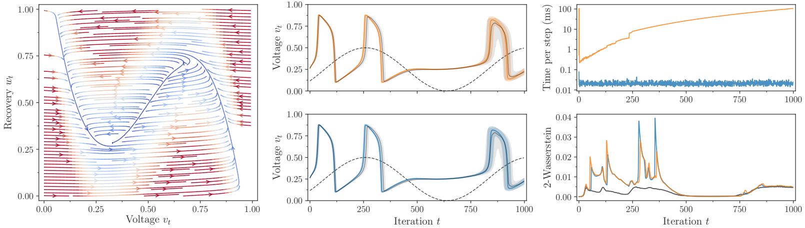
$$C = \sqrt{2\,\mathrm{diam}(\mathcal{X})^d \left(1 + \|k\|_\infty^2 \|\mathbf{K}_{\boldsymbol{zz}}^{-1}\|_{L(\ell^\infty;\ell^2)}^2\right)}$$

Thompson sampling



Improved performance owing to smaller error

FitzHugh-Nagumo model neuron dynamical system



Significantly more efficient time-stepping

Towards geometric PILCO: concluding remarks

Controlled Hamilton's equations

$$\dot{q}(t) = \frac{\partial H}{\partial p} \qquad \dot{p}(t) = -\frac{\partial H}{\partial q} + F_u$$

✓ time-step using VINs (or other symplectic residual RNNs)

✓ use path-wise formula for discretizing GP

- how to properly handle external and contact forces?
- how to define GPs on Riemannian manifolds? (current idea: SPDEs)
- does geometry and mechanics help on the policy side?

Concluding remarks

Thank you for your attention!

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S. Sæmundsson, A. Terenin, K. Hofmann, M. P. Deisenroth. Variational integrator networks for physically structured embeddings. Artificial Intelligence and Statistics, 2020. Available at: HTTPS://ARXIV.ORG/ABS/1910.09349

J. T. Wilson,* V. Borovitskiy,* A. Terenin,* P. Mostowsky,* M. P. Deisenroth. Efficiently sampling functions from Gaussian process posteriors, 2020. *Equal contribution. Available at: HTTPS://ARXIV.ORG/ABS/2002.09309.