

A Machine Learning Approach to Optimal Control

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- **Vision:** Autonomous robots support humans in everyday activities ➤ Fast learning and automatic adaptation



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Fully **autonomous learning and decision making with little data** in real-life situations

Data-Efficient Reinforcement Learning

Ability to learn and make decisions in complex domains without requiring large quantities of data



1 Model-based RL

- ▶ Data-efficient decision making

2 Model predictive RL

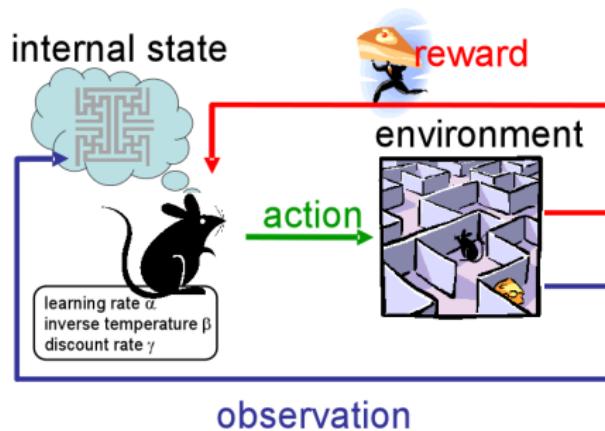
- ▶ Speed up learning further by online planning

3 Incorporation of structural prior knowledge

- ▶ Exploit physical and geometric properties to constrain the learning problem



Reinforcement Learning



- Learn to solve a task
- Trial-and-error interaction with the environment
- Feedback via reward/cost function

$$x_{t+1} = f(x_t, u_t) + w, \quad u_t = \pi(x_t, \theta)$$

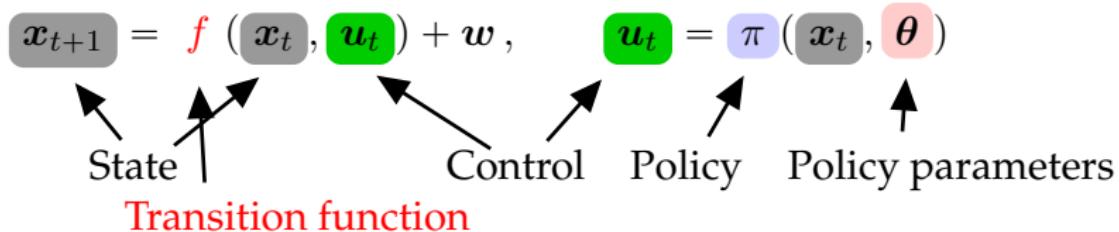
Diagram illustrating the Reinforcement Learning update rule:

- State**: Represented by x_t (grey box).
- Control**: Represented by u_t (green box).
- Policy**: Represented by π (purple box).
- Policy parameters**: Represented by θ (pink box).

Arrows indicate dependencies:

- A double-headed arrow connects State (x_t) and Control (u_t).
- A single-headed arrow points from State (x_t) to Transition function (f).
- A single-headed arrow points from Control (u_t) to Transition function (f).
- A single-headed arrow points from Policy (π) to Control (u_t).
- A single-headed arrow points from Policy parameters (θ) to Policy (π).

Transition function is written in red text below the arrows.



Objective (Controller Learning)

Find policy parameters $\boldsymbol{\theta}^*$ that minimize the expected long-term cost

$$J(\boldsymbol{\theta}) = \sum_{t=1}^T \mathbb{E}[c(\mathbf{x}_t) | \boldsymbol{\theta}], \quad p(\mathbf{x}_0) = \mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0).$$

Instantaneous cost $c(\mathbf{x}_t)$, e.g., $\|\mathbf{x}_t - \mathbf{x}_{\text{target}}\|^2$

- Typical objective in **optimal control** and **reinforcement learning** (Bertsekas, 2005; Sutton & Barto, 1998)

Objective

Minimize expected long-term cost $J(\theta) = \sum_t \mathbb{E}[c(x_t)|\theta]$

PILCO Framework: High-Level Steps

- 1 Probabilistic model for transition function f
 - System identification

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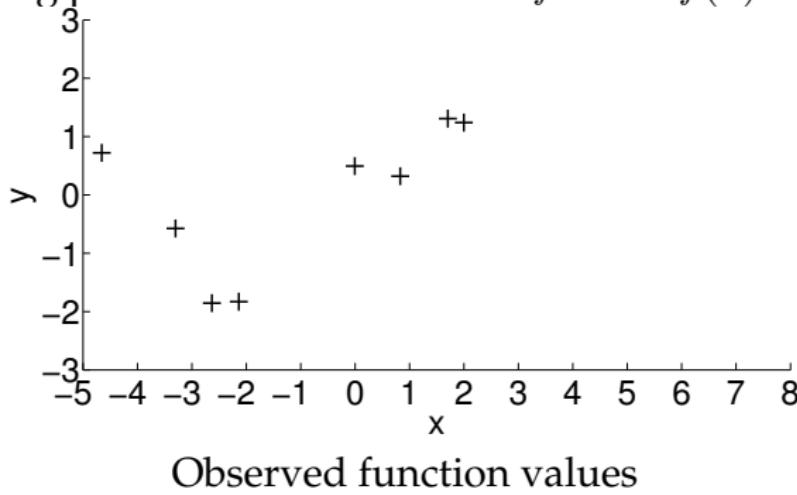
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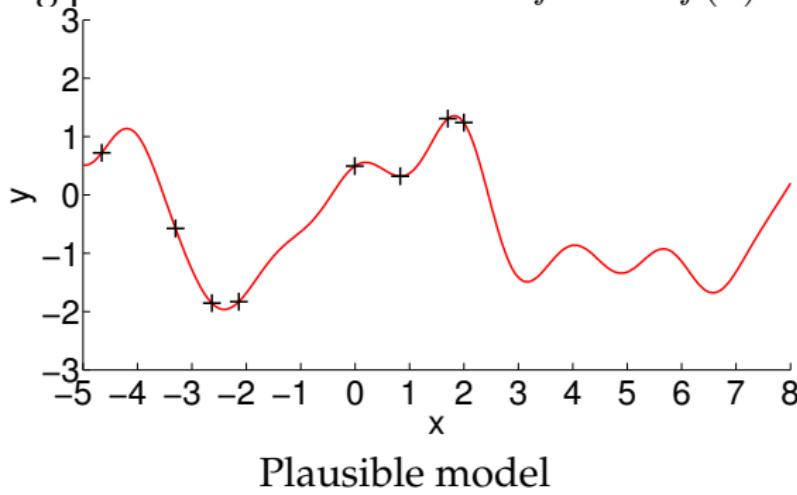
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Model learning problem: Find a function $f : x \mapsto f(x) = y$

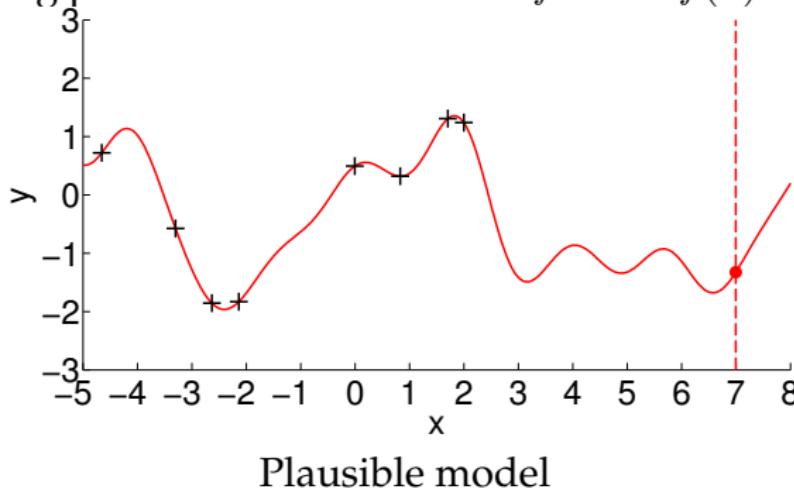


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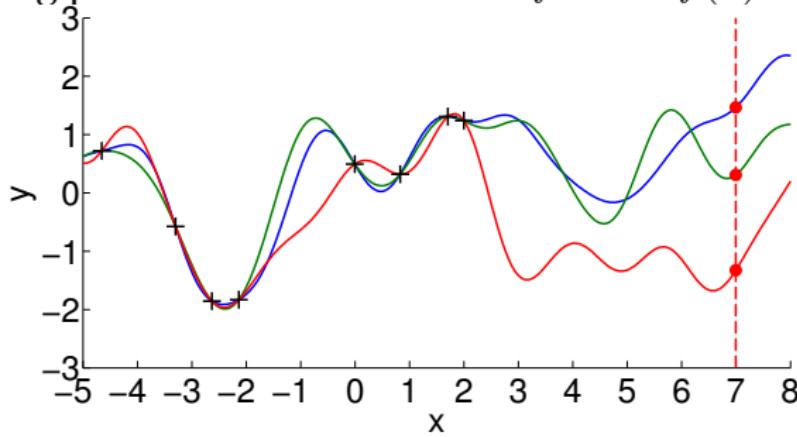
Plausible model

Model learning problem: Find a function $f : x \mapsto f(x) = y$



Predictions? Decision Making?

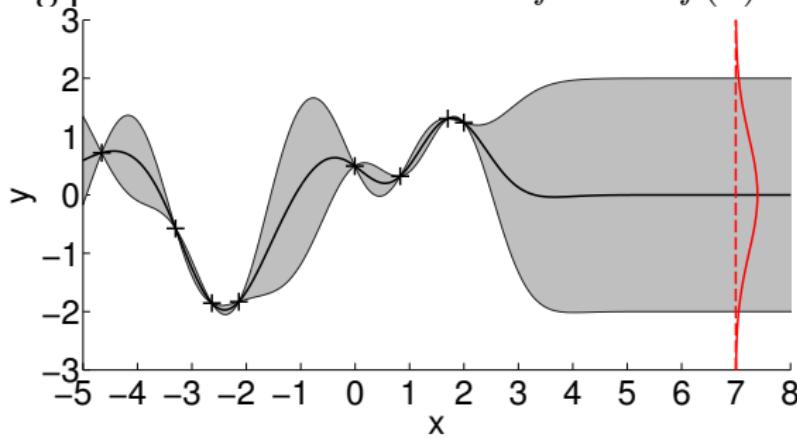
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More plausible models

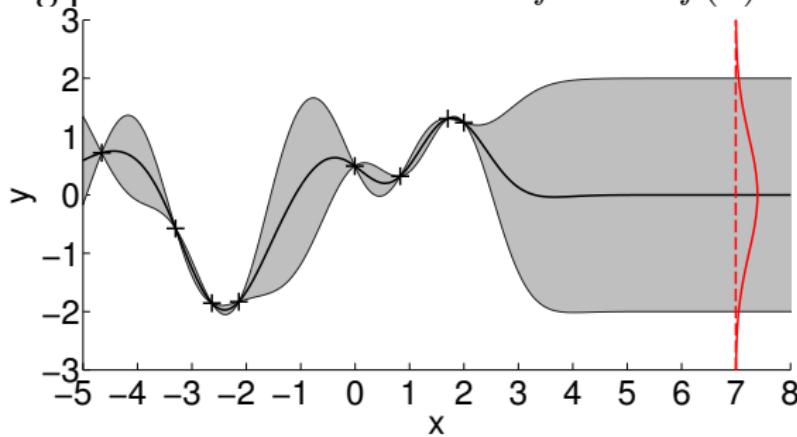
Predictions? Decision Making? Model Errors!

Model learning problem: Find a function $f : x \mapsto f(x) = y$



Distribution over plausible functions

Model learning problem: Find a function $f : x \mapsto f(x) = y$



Distribution over plausible functions

- ▶ Express **uncertainty** about the underlying function to be **robust to model errors**
- ▶ **Gaussian process** for model learning
(Rasmussen & Williams, 2006)

- Flexible Bayesian regression method
- Probability distribution over functions
- Fully specified by
 - Mean function m (average function)
 - Covariance function k (assumptions on structure)

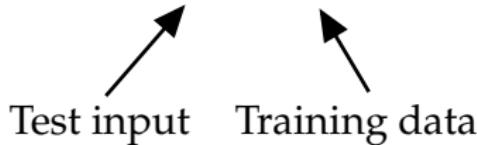
$$k(\boldsymbol{x}_p, \boldsymbol{x}_q) = \text{Cov}[f(\boldsymbol{x}_p), f(\boldsymbol{x}_q)]$$

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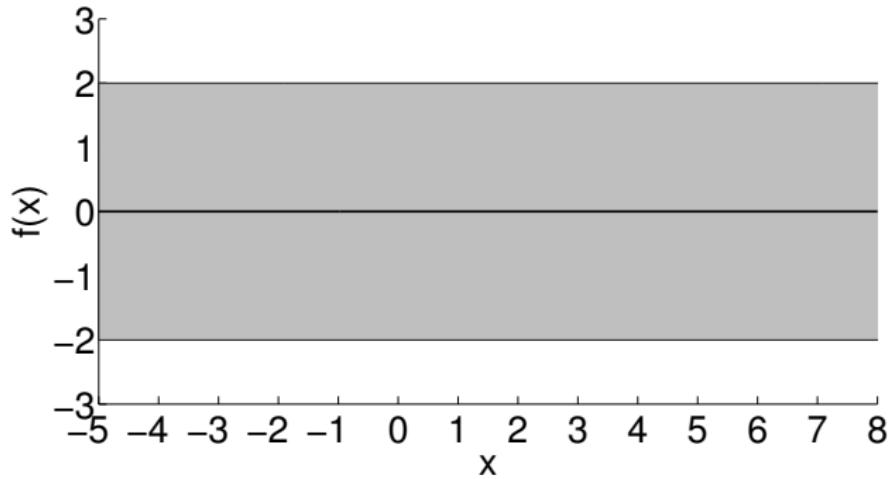
$$k(\mathbf{x}_p, \mathbf{x}_q) = \text{Cov}[f(\mathbf{x}_p), f(\mathbf{x}_q)]$$

- Posterior predictive distribution at \mathbf{x}_* is Gaussian (Bayes' theorem):

$$p(f(\mathbf{x}_*) | \mathbf{x}_*, \mathbf{X}, \mathbf{y}) = \mathcal{N}(f(\mathbf{x}_*) | m(\mathbf{x}_*), \sigma^2(\mathbf{x}_*))$$



Test input Training data

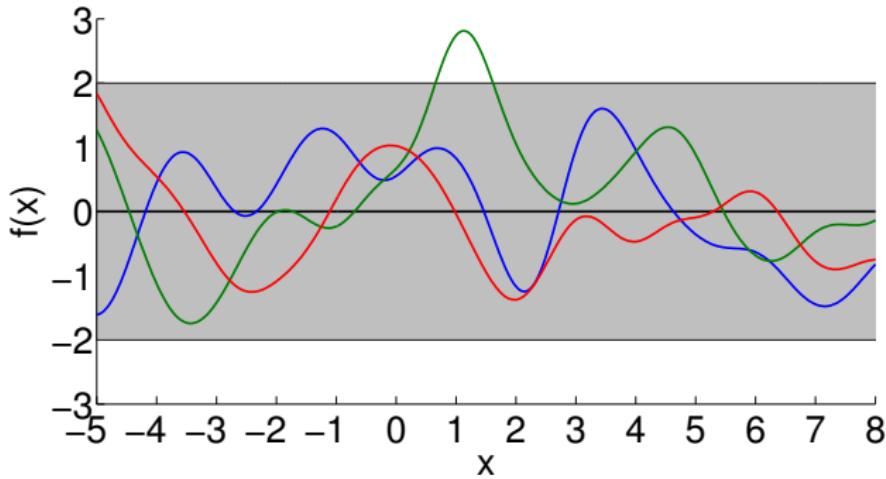


Prior belief about the function

Predictive (marginal) mean and variance:

$$\mathbb{E}[f(\mathbf{x}_*)|\mathbf{x}_*, \emptyset] = m(\mathbf{x}_*) = 0$$

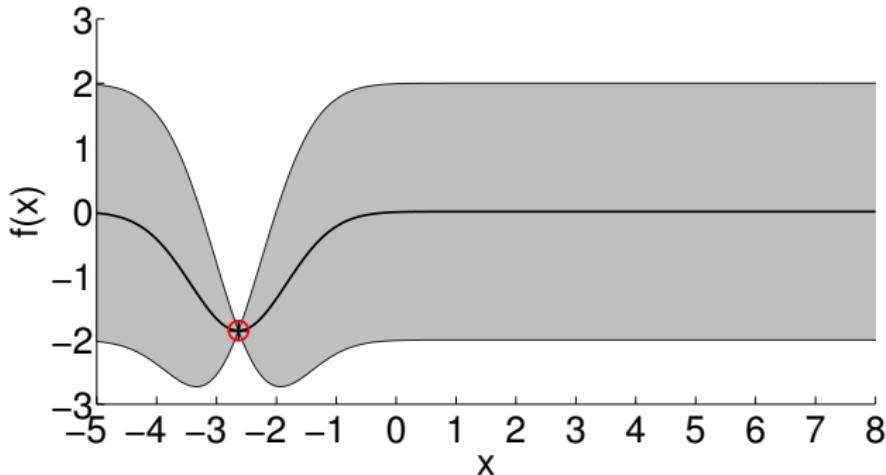
$$\mathbb{V}[f(\mathbf{x}_*)|\mathbf{x}_*, \emptyset] = \sigma^2(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x}_*)$$



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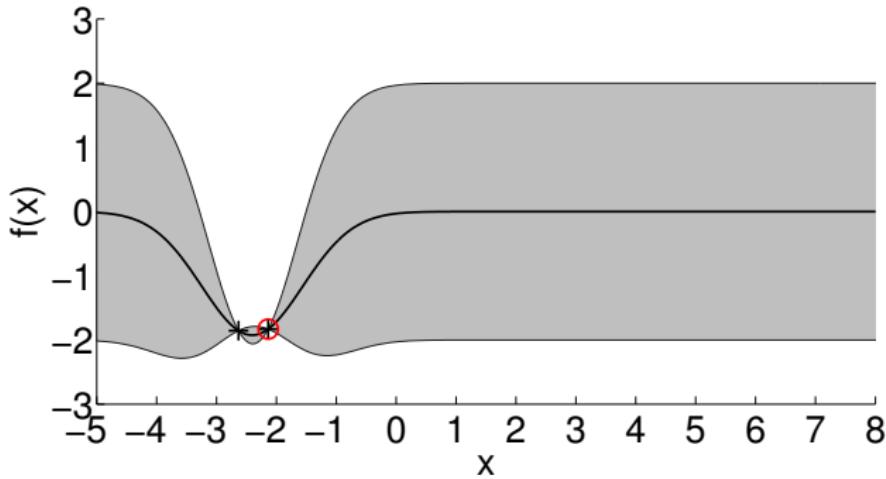


Posterior belief about the function

Predictive (marginal) mean and variance:

$$\mathbb{E}[f(\mathbf{x}_*)|\mathbf{x}_*, \mathbf{X}, \mathbf{y}] = m(\mathbf{x}_*) = \mathbf{k}(\mathbf{X}, \mathbf{x}_*)^\top \mathbf{k}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{y}$$

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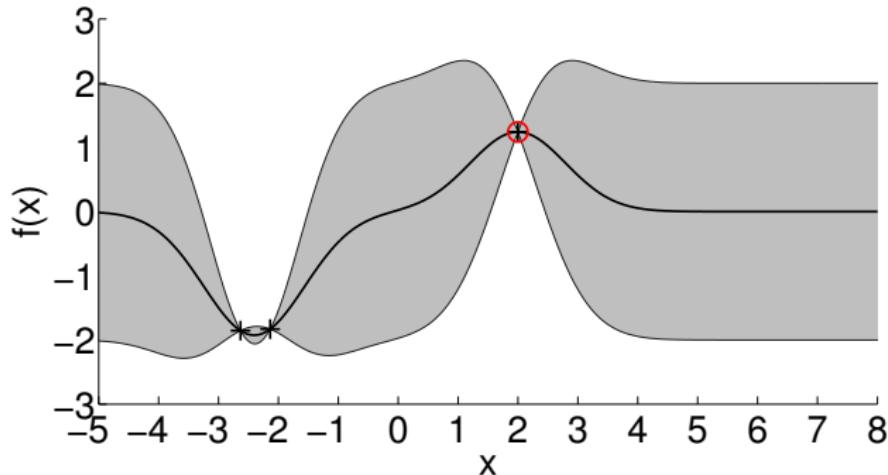


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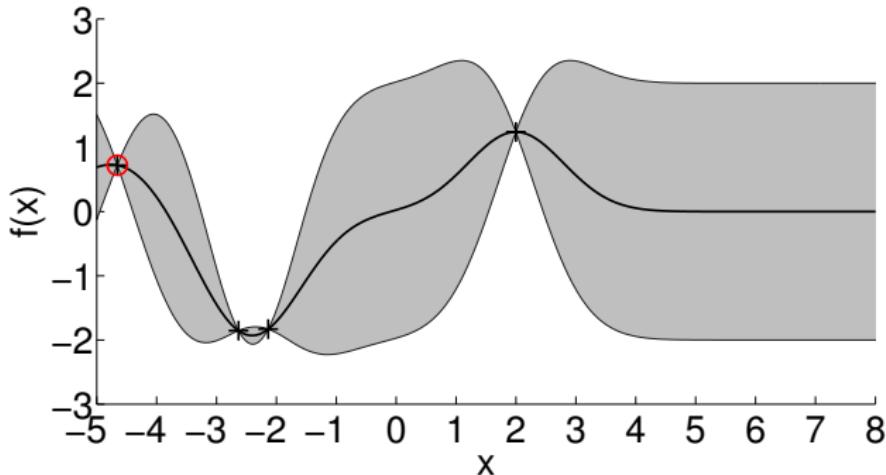


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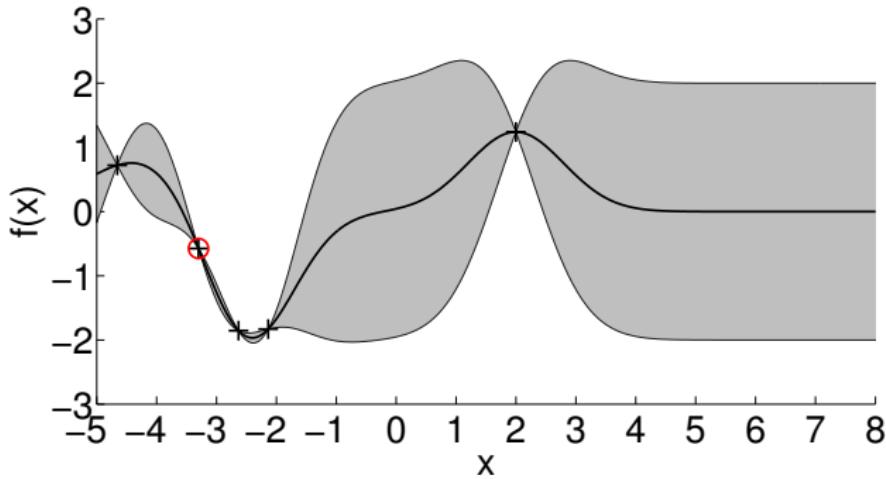


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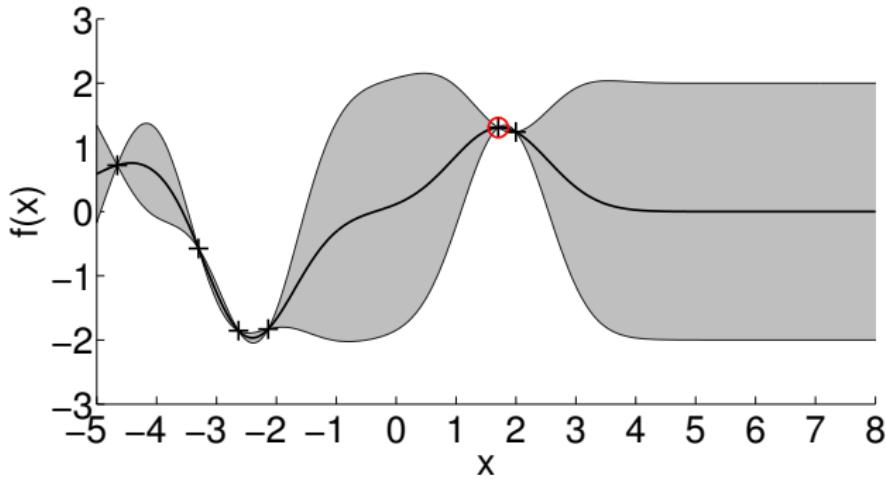


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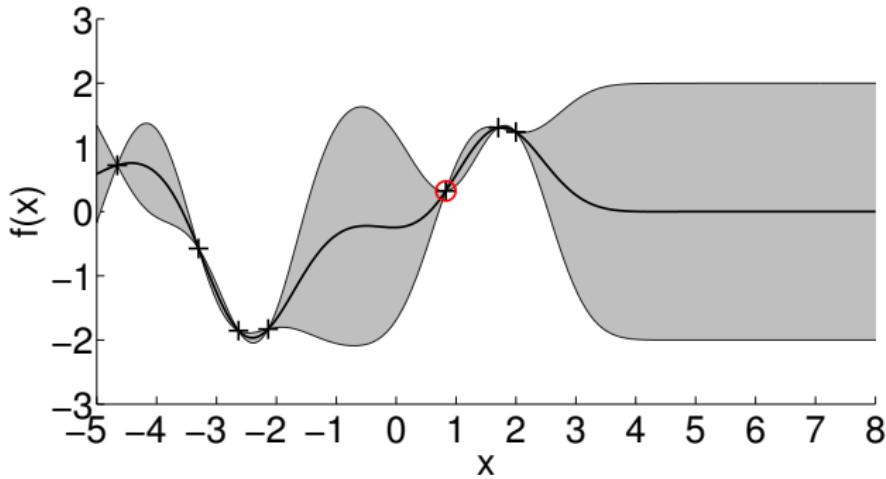


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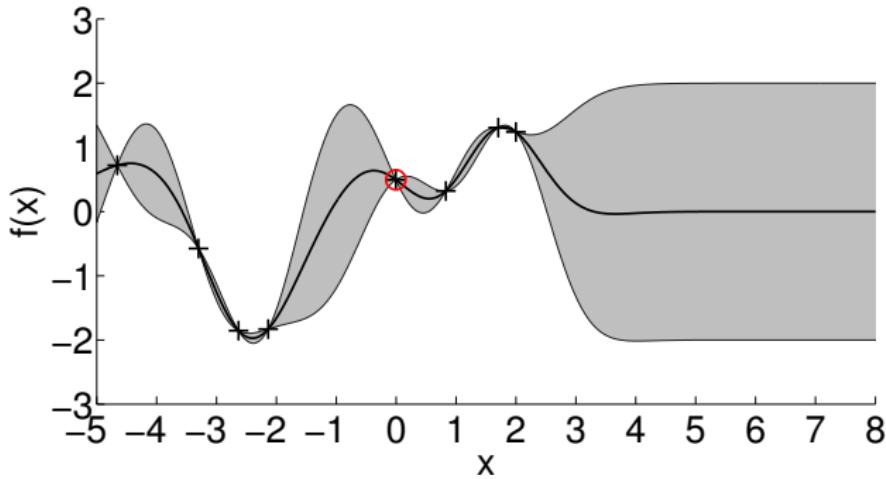


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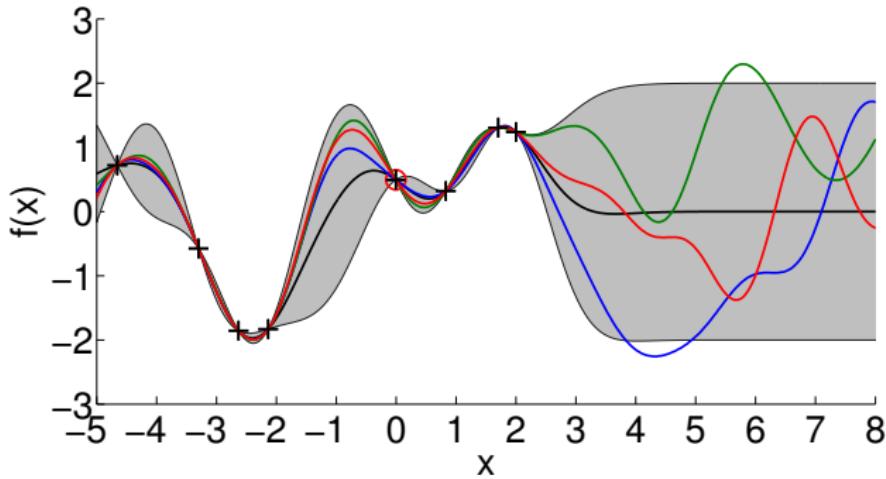


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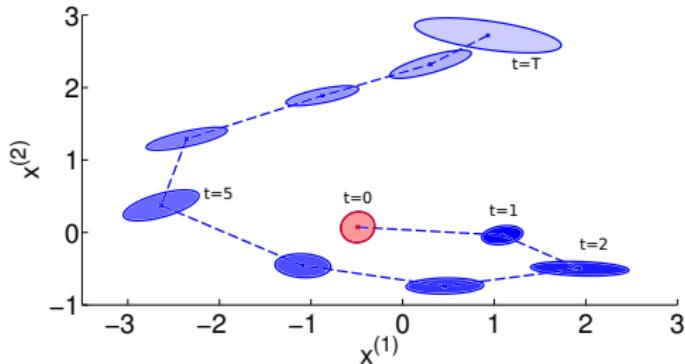
Objective

Minimize expected long-term cost $J(\theta) = \sum_t \mathbb{E}[c(x_t)|\theta]$

PILCO Framework: High-Level Steps

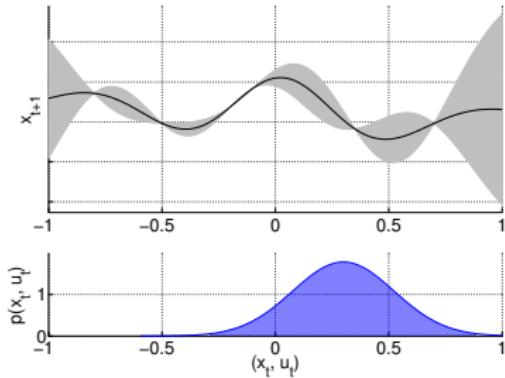
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Long-Term Predictions



- Iteratively compute $p(x_1|\theta), \dots, p(x_T|\theta)$

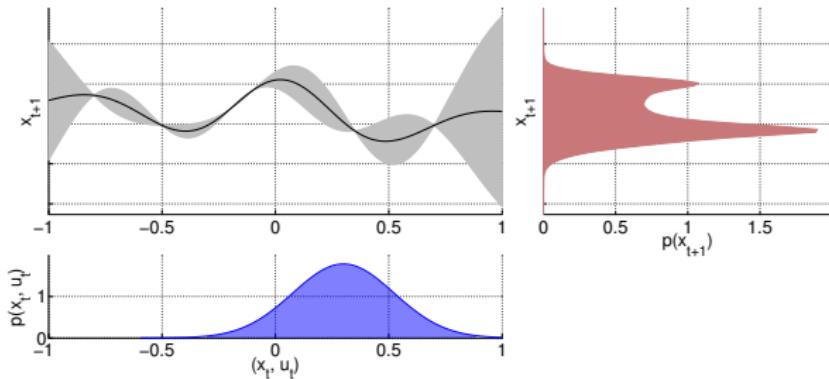
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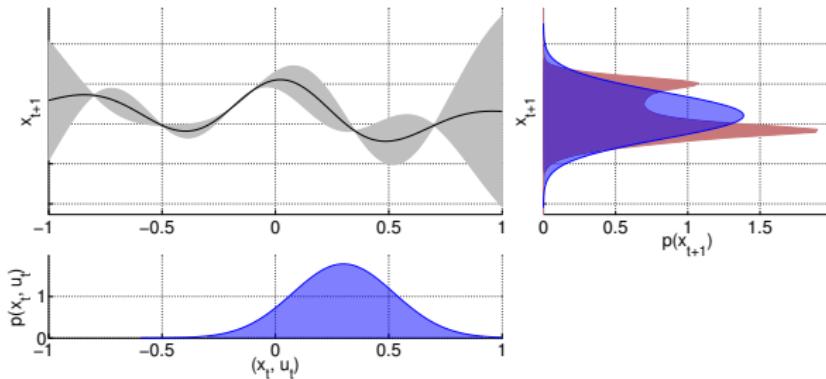
$$\underbrace{p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t, \boldsymbol{u}_t)}_{\text{GP prediction}} \quad \underbrace{p(\boldsymbol{x}_t, \boldsymbol{u}_t|\boldsymbol{\theta})}_{\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})}$$

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► GP moment matching

(Girard et al., 2002; Quiñonero-Candela et al., 2003)

Deisenroth et al. (IEEE-TPAMI, 2015): *Gaussian Processes for Data-Efficient Learning in Robotics and Control*

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Minimize expected long-term cost $J(\theta) = \sum_t \mathbb{E}[c(x_t)|\theta]$

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- 2 Compute long-term predictions $p(x_1|\theta), \dots, p(x_T|\theta)$
- 3 **Policy improvement**
 - Compute expected long-term cost $J(\theta)$
 - Find parameters θ that minimize $J(\theta)$
- 4 Apply controller

Objective

Minimize expected long-term cost $J(\theta) = \sum_t \mathbb{E}[c(x_t)|\theta]$

- Know how to predict $p(x_1|\theta), \dots, p(x_T|\theta)$

Objective

Minimize expected long-term cost $J(\boldsymbol{\theta}) = \sum_t \mathbb{E}[c(\mathbf{x}_t) | \boldsymbol{\theta}]$

- Know how to predict $p(\mathbf{x}_1 | \boldsymbol{\theta}), \dots, p(\mathbf{x}_T | \boldsymbol{\theta})$
- Compute

$$\mathbb{E}[c(\mathbf{x}_t) | \boldsymbol{\theta}] = \int c(\mathbf{x}_t) \mathcal{N}(\mathbf{x}_t | \boldsymbol{\mu}_t, \boldsymbol{\Sigma}_t) d\mathbf{x}_t, \quad t = 1, \dots, T,$$

and sum them up to obtain $J(\boldsymbol{\theta})$

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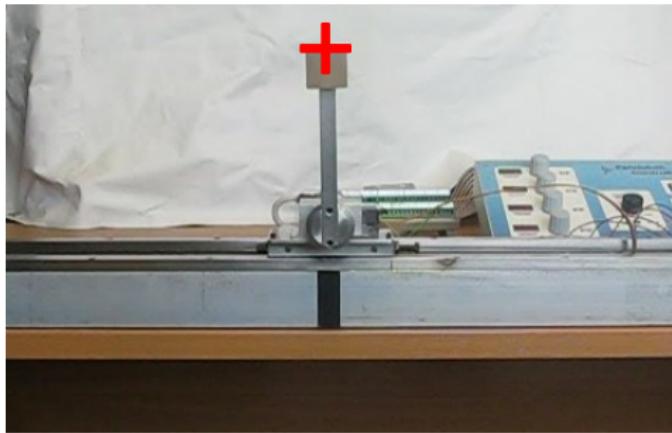
- Analytically compute gradient $dJ(\boldsymbol{\theta})/d\boldsymbol{\theta}$
- Standard gradient-based optimizer (e.g., BFGS) to find $\boldsymbol{\theta}^*$

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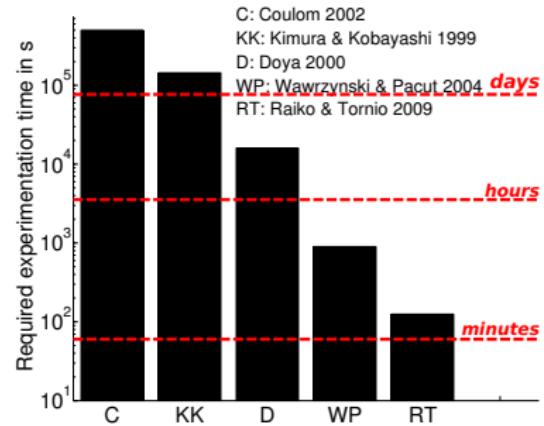
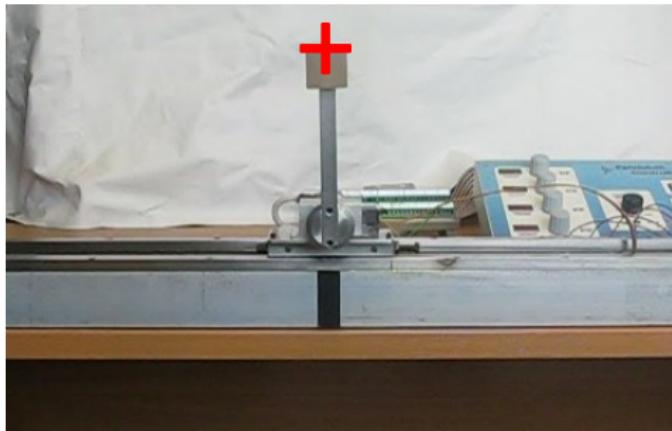
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- Swing up and balance a freely swinging pendulum on a cart
- No knowledge about nonlinear dynamics ➤ Learn from scratch
- Cost function $c(\mathbf{x}) = 1 - \exp(-\|\mathbf{x} - \mathbf{x}_{\text{target}}\|^2)$
- Code: <https://github.com/ICL-SML/pilco-matlab>

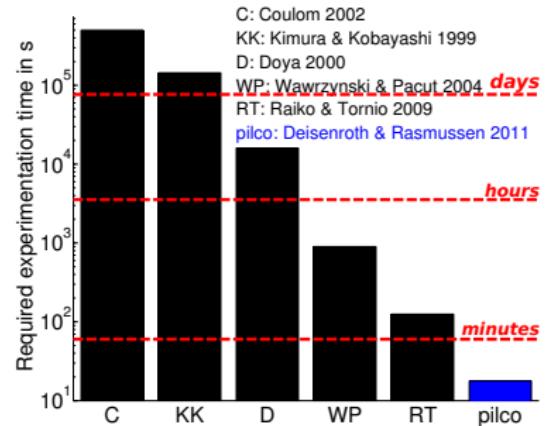
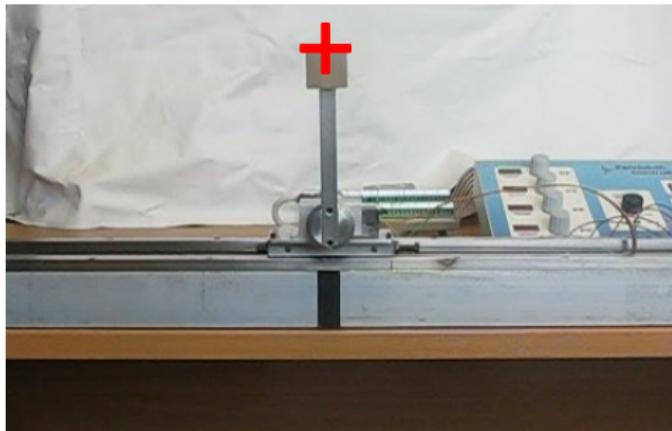
Standard Benchmark: Cart-Pole Swing-up



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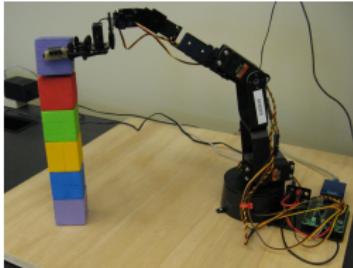
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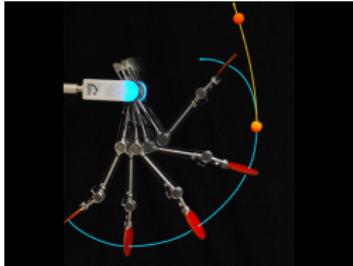
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- **Unprecedented learning speed** compared to state-of-the-art
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Deisenroth & Rasmussen (ICML, 2011): PILCO: A Model-based and Data-efficient Approach to Policy Search

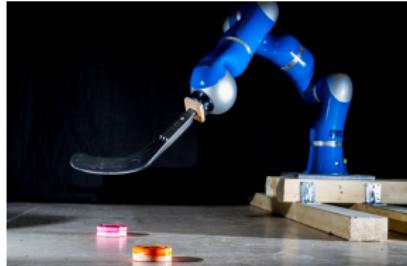
Wide Applicability



with D Fox



with P Englert, A Paraschos, J Peters



with A Kupcsik, J Peters, G Neumann



B Bischoff (Bosch), ESANN 2013



A McHutchon (U Cambridge)



B Bischoff (Bosch), ECML 2013

► Application to a wide range of robotic systems

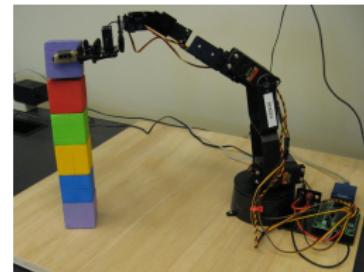
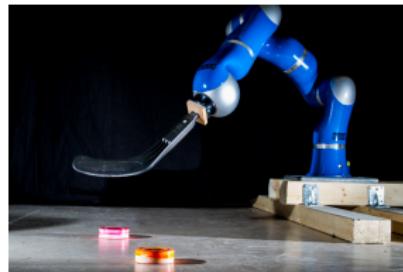
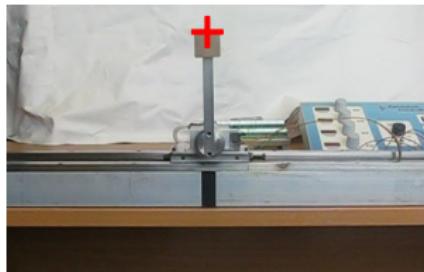
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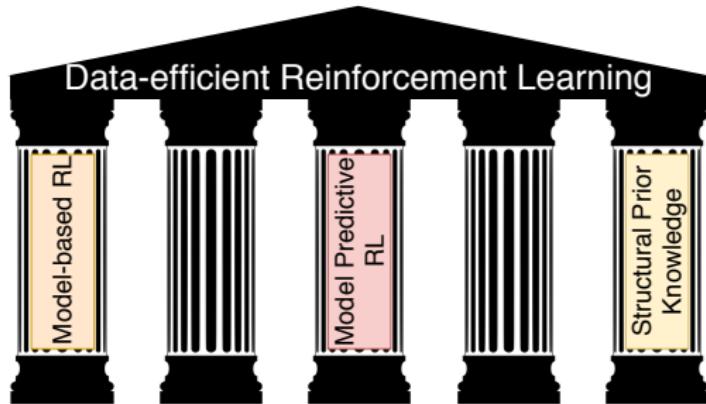
Deisenroth et al. (ICRA, 2014): *Multi-Task Policy Search for Robotics*

Kupcsik et al. (AIJ, 2017): *Model-based Contextual Policy Search for Data-Efficient Generalization of Robot Skills*

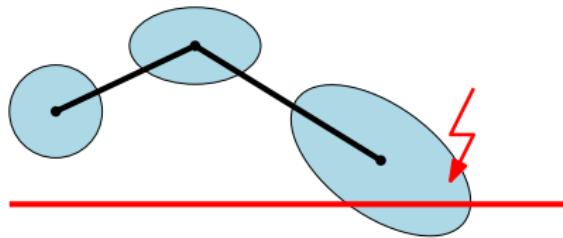
Summary (1)



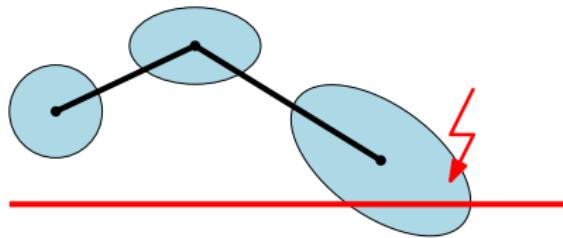
- In robotics, **data-efficient** learning is critical
- Probabilistic, model-based RL approach
 - Reduce model bias
 - Unprecedented learning speed
 - Wide applicability



Sanket Kamthe



- Deal with real-world **safety constraints** (states/controls)
- Use probabilistic model to predict whether state constraints are violated (e.g., Sui et al., 2015; Berkenkamp et al., 2017)
- Adjust policy if necessary (during policy learning)



- Deal with real-world **safety constraints** (states/controls)
- Use probabilistic model to predict whether state constraints are violated (e.g., Sui et al., 2015; Berkenkamp et al., 2017)
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- ▶ Safe exploration within an MPC-based RL setting
- ▶ Optimize control signals u_t directly (no policy parameters)

- Idea: Optimize control signals directly (instead of policy parameters)
- Few parameters to optimize ➤ Low-dimensional search space
- Open-loop control
➤ No chance of success (with minor model inaccuracies)

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- Few parameters to optimize ➤ Low-dimensional search space
- Open-loop control
 - No chance of success (with minor model inaccuracies)
- Model predictive control (MPC) turns this into a closed-loop control approach
- Use this within a trial-and-error RL setting

- Learned GP model for transition dynamics
- Repeat (while executing the policy):
 - 1 In current state x_t , determine optimal control sequence u_0^*, \dots, u_{H-1}^*
 - 2 Apply first control u_0^* in state x_t
 - 3 Transition to next state x_{t+1}
 - 4 Update GP transition model

- Uncertainty propagation is deterministic (GP moment matching)
 - Re-formulate system dynamics:

$$\mathbf{z}_{t+1} = f_{MM}(\mathbf{z}_t, \mathbf{u}_t)$$

$$\mathbf{z}_t = \{\boldsymbol{\mu}_t, \boldsymbol{\Sigma}_t\} \quad \text{► Collects moments}$$

Theoretical Results

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 - ▶ Re-formulate system dynamics:

$$z_{t+1} = f_{MM}(z_t, u_t)$$

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- Deterministic system function that propagates moments
- Lipschitz continuity (under mild assumptions) implies that we can apply Pontryagin's Minimum Principle
 - Control Hamiltonian $H(\lambda_{t+1}, z_t, u_t)$
 - Adjoint recursion for λ_t
 - Necessary optimality condition: $\partial H / \partial u_t = \mathbf{0}$
- ▶ Principled treatment of constraints on controls

Theoretical Results

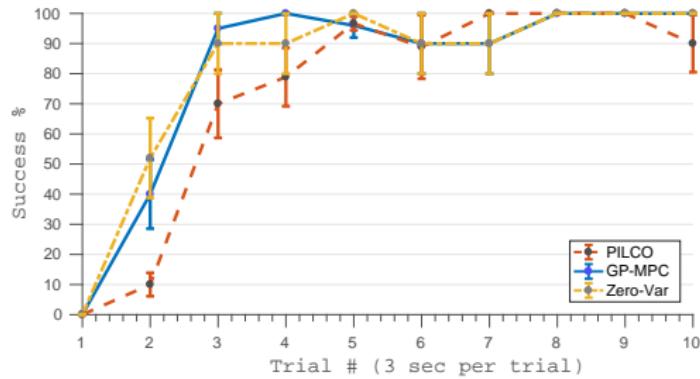
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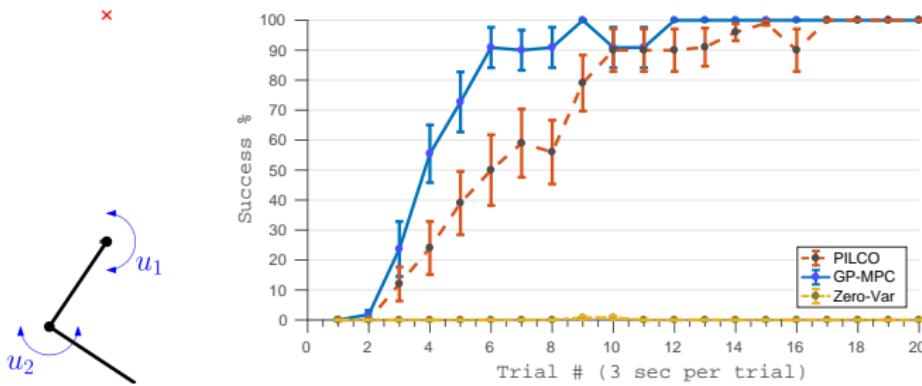
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- ▶ Principled treatment of constraints on controls
- Use predictive uncertainty to check violation of state constraints

Learning Speed (Cart Pole)



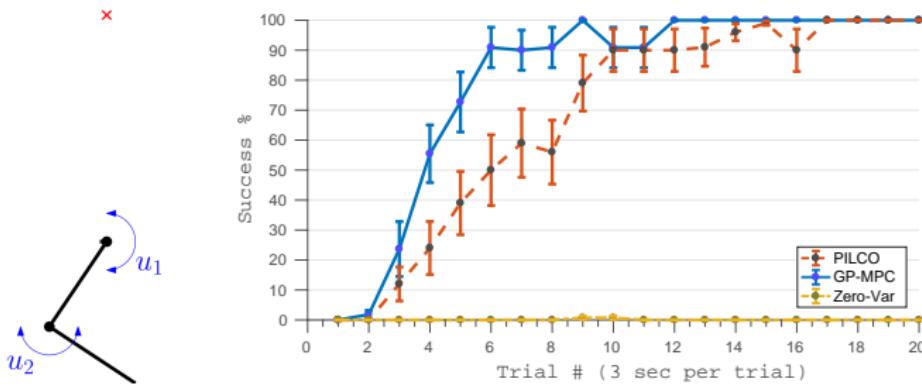
- Zero-Var: Only use the mean of the GP, discard variances for long-term predictions
- MPC: Increased data efficiency (40% less experience required than PILCO)
 - MPC more robust to model inaccuracies than a parametrized feedback controller

Learning Speed (Double Pendulum)



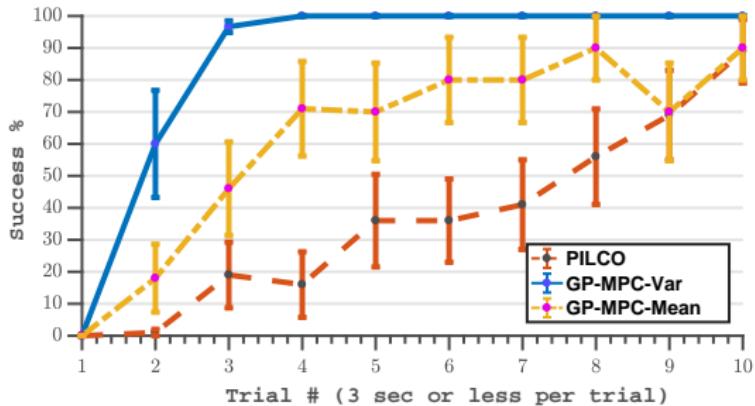
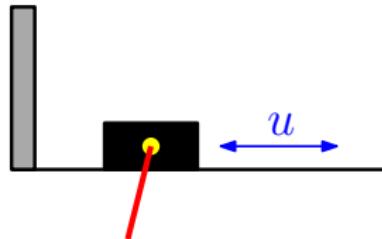
- GP-MPC maintains the same improvement in data efficiency
- Zero-Var fails:
 - Gets stuck in local optimum near start state
 - Insufficient exploration due to lack of uncertainty propagation

Learning Speed (Double Pendulum)



- GP-MPC maintains the same improvement in data efficiency
- Zero-Var fails:
 - Gets stuck in local optimum near start state
 - Insufficient exploration due to lack of uncertainty propagation
- Although MPC is fairly robust to model inaccuracies we cannot get away without uncertainty propagation

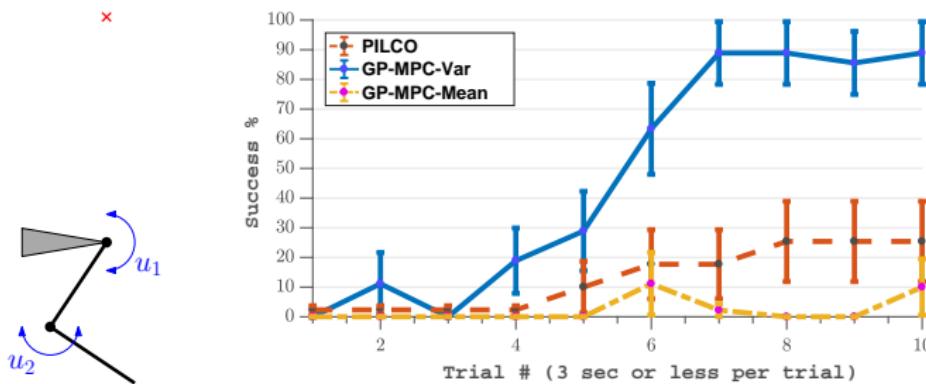
Safety Constraints (Cart Pole)



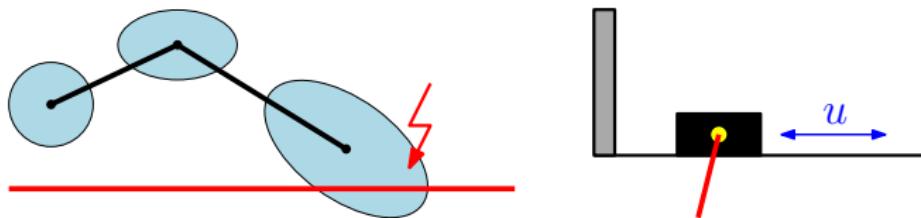
PILCO	16/100	constraint violations
GP-MPC-Mean	21/100	constraint violations
GP-MPC-Var	3/100	constraint violations

► Propagating model uncertainty important for safety

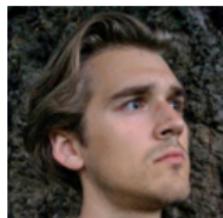
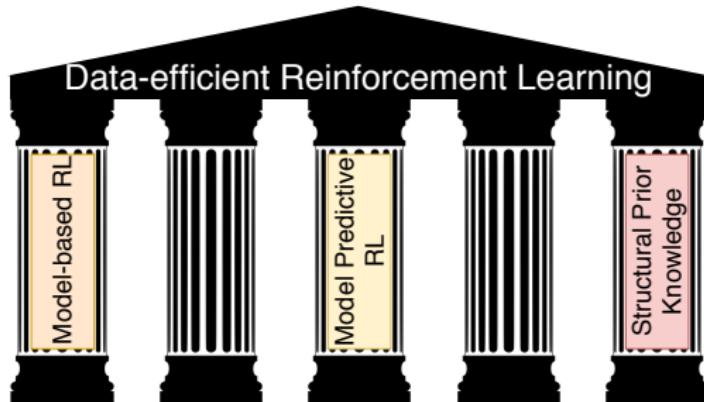
Safety Constraints (Double Pendulum)



Experiment	Double Pendulum
PILCO	23/100
GP-MPC-Mean	26/100
GP-MPC-Var	11/100



- Probabilistic prediction models for safe exploration
- Uncertainty propagation can be used to reduce violation of safety constraints
- MPC framework increases robustness to model errors
 - ▶ Increased data efficiency



Steindór Sæmundsson



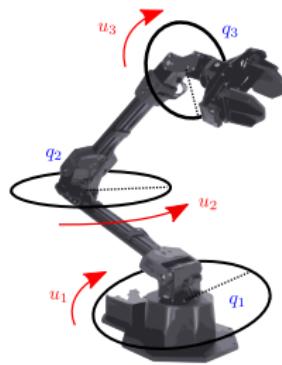
Alexander Terenin



Katja Hofmann

Structural Priors

High-level prior knowledge: e.g., laws of physics or configuration constraints



Equations of motion

$$u = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q}$$

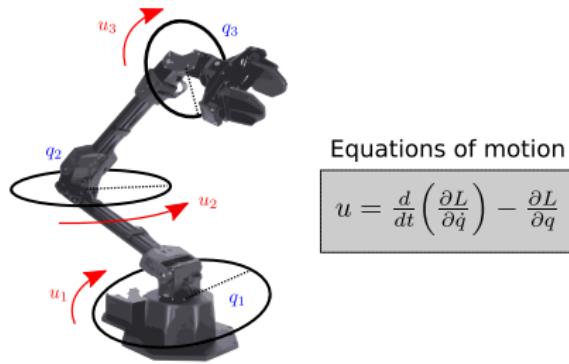
- ▶ Improve data efficiency and generalization

Variational Integrator Networks (VINs)

Network architectures with built-in physics and geometric structure

Outline:

- How we talk about physics
- How we think about neural networks
- How to encode physics and geometry into architecture



- General framework:
classical mechanics, quantum mechanics, relativity
- Global properties:
conservation laws, configuration manifold, etc.
- Solve differential equations

- Configuration space:

$$q \in \mathcal{Q}$$

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- Lagrangian (specifies physics):

$$L(q(t), \dot{q}(t)) = K - U = \text{kinetic energy} - \text{potential energy}$$

Physics: Key Objects

- Configuration space:

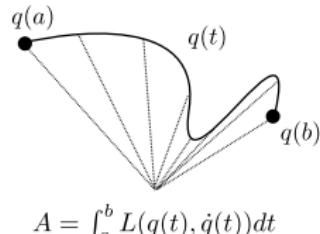
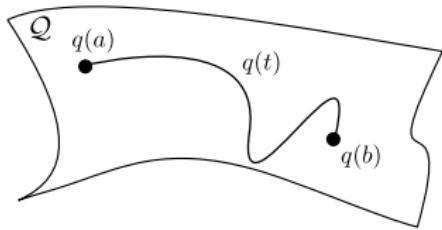
$$q \in \mathcal{Q}$$

- Lagrangian (specifies physics):

$$L(q(t), \dot{q}(t)) = K - U = \text{kinetic energy} - \text{potential energy}$$

- Action (maps trajectories to real numbers)

$$A = \int_a^b L(q(t), \dot{q}(t)) dt$$



Hamilton's Principle

Physical paths are stationary points of the action.

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Equations of motion (Euler-Lagrange equation):

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0$$

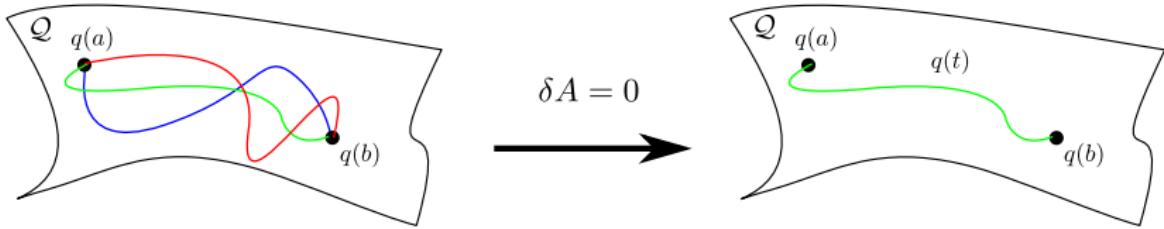
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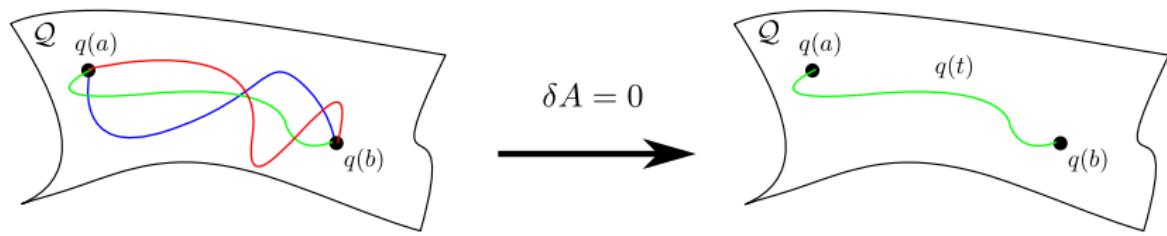
$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0$$

The **solution** $q(t)$ evolves according to the laws of physics.



Physics: Recap

- Lagrangian → Specifies the physics
- Hamilton's principle → Equations of motion
- Solution → Physical path



- Residual networks = Learnable approximate ODE solvers

$$\dot{\boldsymbol{x}}(t) = f(\boldsymbol{x}(t), t, \theta) \quad \longleftrightarrow \quad \boldsymbol{x}_{t+1} = \boldsymbol{x}_t + f(\boldsymbol{x}(t), \theta)$$

- Residual networks = Learnable approximate ODE solvers

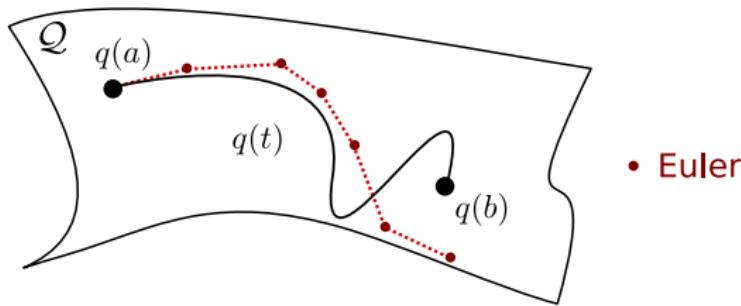
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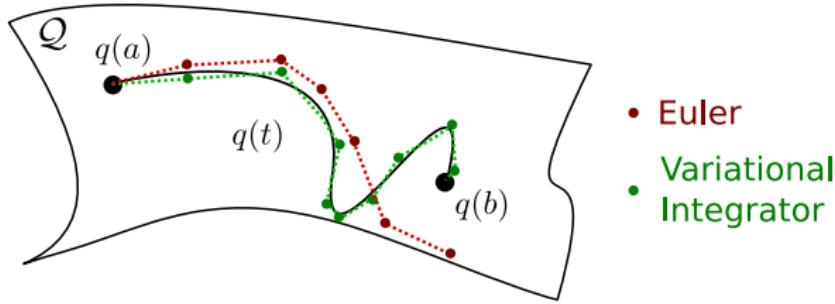
- **Intuition:** Physical networks = Learnable approximations to equations of motion
- **Problem:** Euler discretization leads to significant errors and physically implausible behavior



• Euler

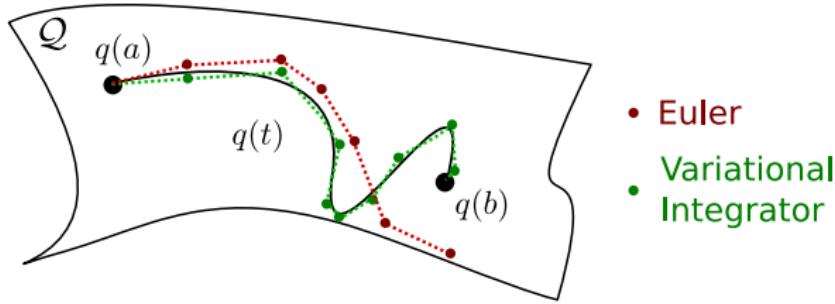
Variational Integrators

Geometric integrators that preserve global (physical) properties



Variational Integrators

Geometric integrators that preserve global (physical) properties



Properties:

- Symplectic (volume preserving)
- Momentum preserving
- Bounded energy behavior

1 Write down parameterized Lagrangian:

$$L_\theta(q(t), \dot{q}(t))$$

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Lagrangian: $q_{t+1} = f_\theta(q_t, q_{t-1})$

Hamiltonian: $[q_{t+1}, \dot{q}_{t+1}] = f_\theta(q_t, \dot{q}_t)$

Recipe for Variational Integrator Network

- 1 Write down parameterized Lagrangian:

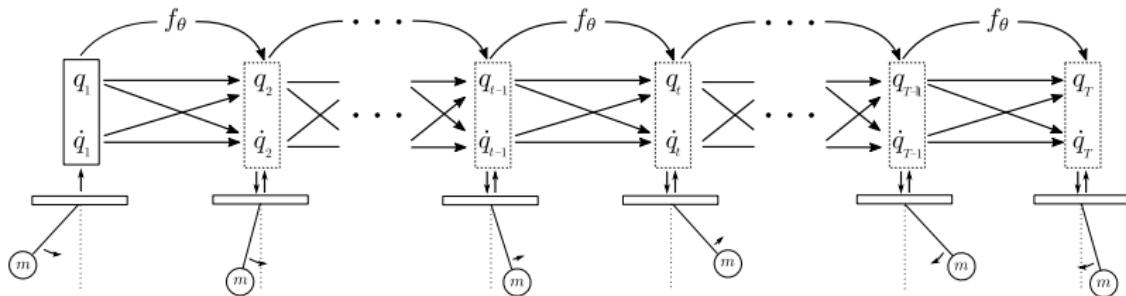
$$L_\theta(q(t), \dot{q}(t))$$

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- 3 f_θ defines the network architecture



Sæmundsson et al. (arXiv:1910.09349): *Variational Integrator Networks for Physically Meaningful Embeddings*

Newtonian Potential System:

$$L_\theta(q(t), \dot{q}(t)) = K_\theta(\dot{q}(t)) - U_\theta(q(t))$$

- Newtonian network on \mathbb{R}^D

$$q_{t+1} = 2q_t - q_{t-1} - h^2 f_\theta(q_t)$$

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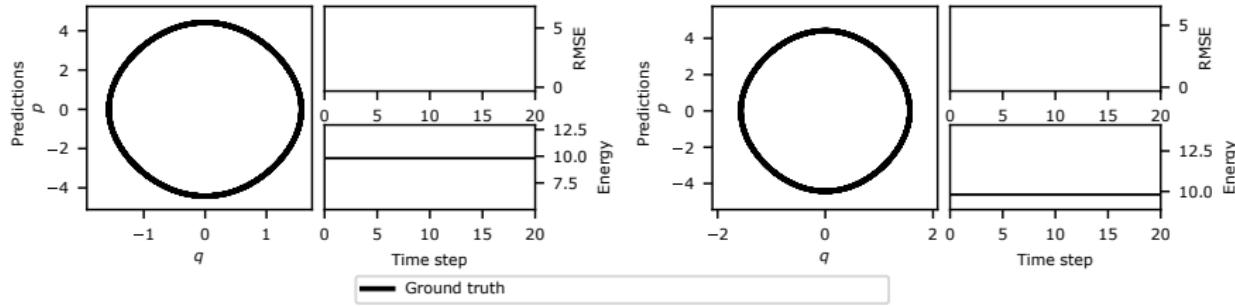
- Newtonian network on $SO(2)$

$$\sin \Delta q_t = \sin \Delta q_{t-1} + h^2 r_\theta(q_t)$$

$$q_{t+1} = q_t + \Delta q_t$$

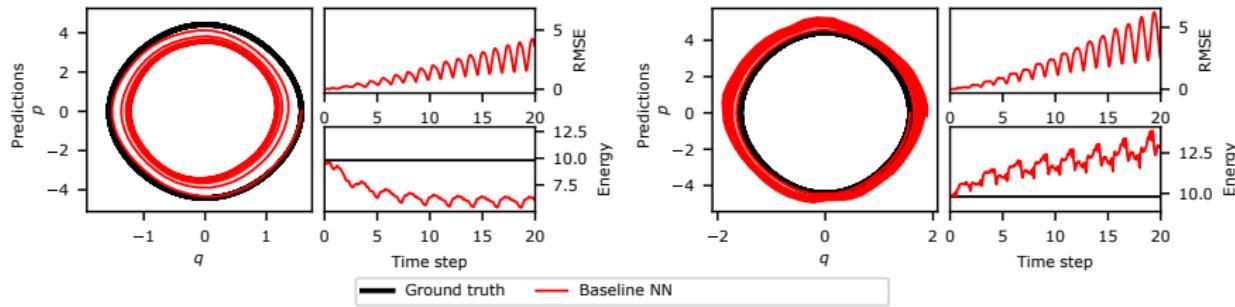
- ▶ Allows us to define dynamics on a manifold

Learning from Noisy Data: Pendulum



Pendulum System. **Left:** 150 observations; **Right:** 750 observations.

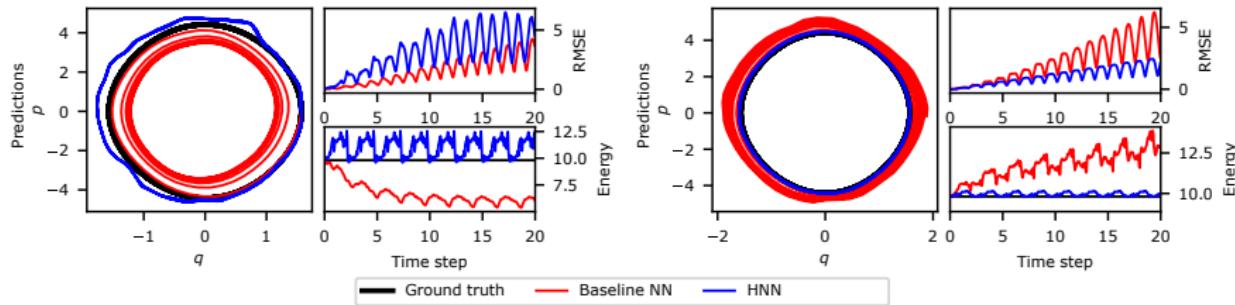
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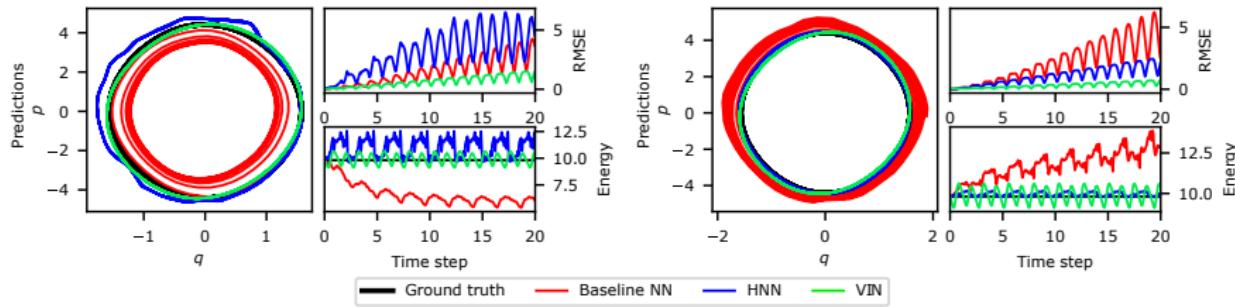
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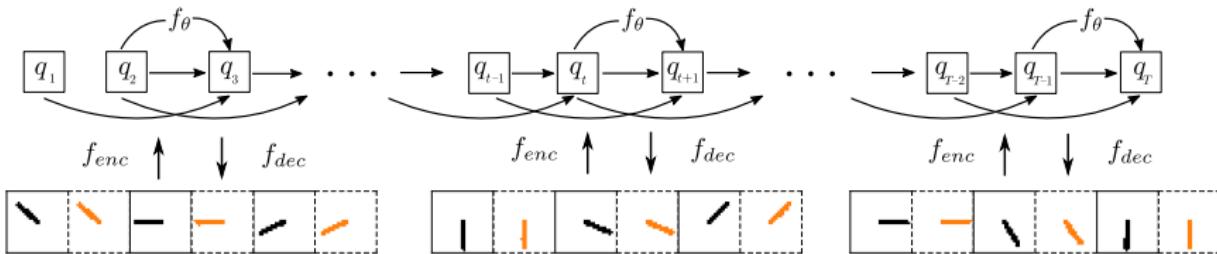
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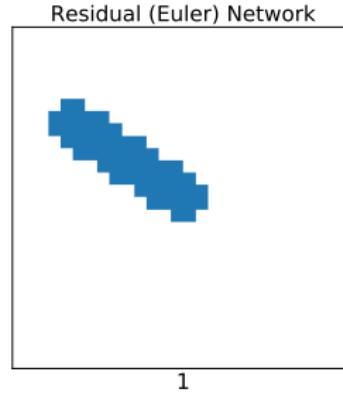
- **Baseline neural network:** Dissipates/adds energy for low and moderate data
- **Hamiltonian neural network (Greydanus et al., 2019):** Overfits in low-data regime
- **Variational integrator network:** Conserves energy and generalizes better in both regimes

Sæmundsson et al. (arXiv:1910.09349): *Variational Integrator Networks for Physically Meaningful Embeddings*



- VIN within variational auto-encoder (VAE) setup:
 - Learn physical system in lower-dimensional latent space
 - Use VIN for long-term forecasting
- ▶ Exploit geometry of the problem for system identification and forecasting

Learning from Pixel Data: Forecasting



- Observations: 28×28 pixel images of pendulum
- Training data: 40 images

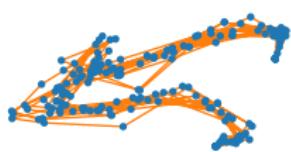
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- **DLG-VAE**: Physically meaningful long-term forecasts in latent and observation space

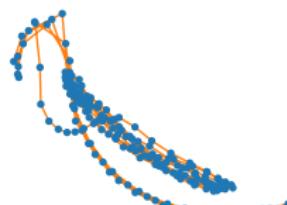
Learning from Pixel Data: Latent Embeddings



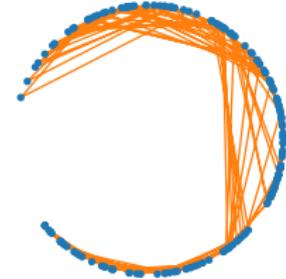
Vanilla VAE



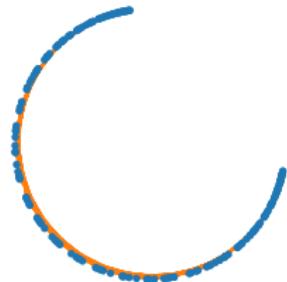
Dynamic VAE



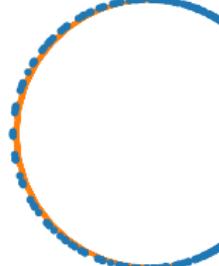
LG-VAE



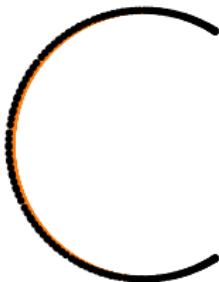
DLG-VAE



DLG-VAE (Fixed)

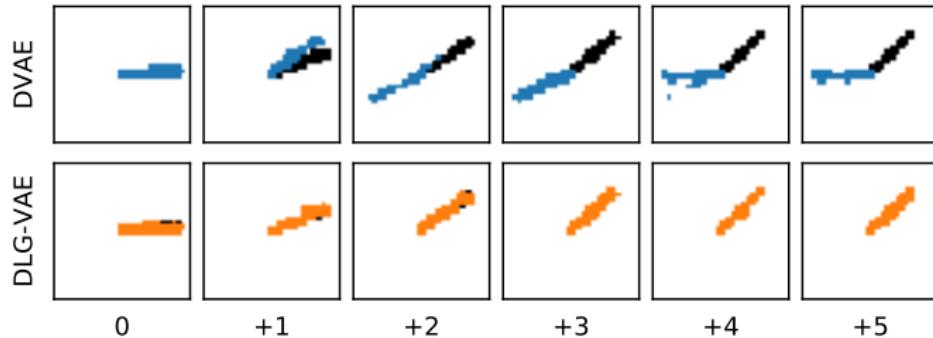


Ground truth



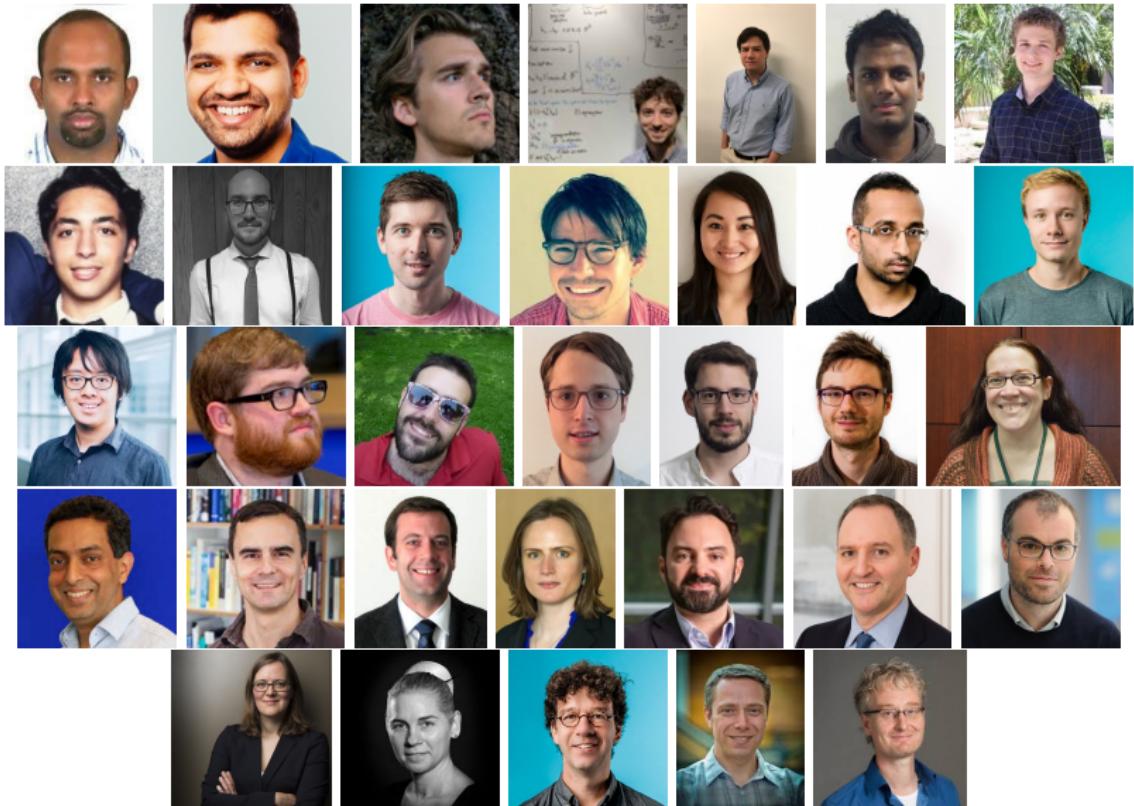
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Summary (3)

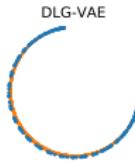
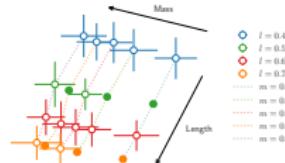
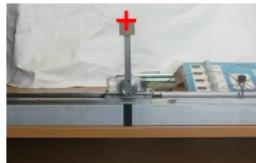


- Variational integrator networks to encode physics and geometric structure ➤ Interpretability
- Data-efficient learning and physically meaningful long-term forecasts

Team and Collaborators

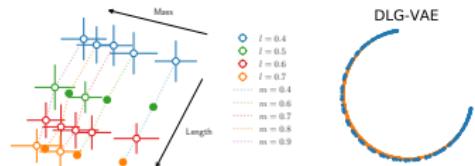
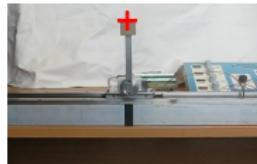


Wrap-up



- **Data efficiency** is a practical challenge for autonomous robots
- Three pillars of data-efficient machine learning
 - 1 **Model-based reinforcement learning** with learned probabilistic models for fast learning from scratch
 - 2 **Model predictive RL** for safe exploration and more robust models
 - 3 **Incorporation of structural priors** for learning physically meaningful predictive models

Wrap-up



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ありがとうございました

References I

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$$\begin{aligned}f &\sim GP(0, k), \quad \text{Training data: } \mathbf{X}, \mathbf{y} \\ \mathbf{x}_* &\sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})\end{aligned}$$

- Compute $\mathbb{E}[f(\mathbf{x}_*)]$

$$f \sim GP(0, k), \quad \text{Training data: } \mathbf{X}, \mathbf{y}$$
$$\mathbf{x}_* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Compute $\mathbb{E}[f(\mathbf{x}_*)]$

$$\mathbb{E}_{f, \mathbf{x}_*}[f(\mathbf{x}_*)] = \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_f[f(\mathbf{x}_*) | \mathbf{x}_*] \right] = \mathbb{E}_{\mathbf{x}_*} [m_f(\mathbf{x}_*)]$$

$$f \sim GP(0, k), \quad \text{Training data: } \mathbf{X}, \mathbf{y}$$
$$\mathbf{x}_* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Compute $\mathbb{E}[f(\mathbf{x}_*)]$

$$\begin{aligned}\mathbb{E}_{f, \mathbf{x}_*}[f(\mathbf{x}_*)] &= \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_f[f(\mathbf{x}_*) | \mathbf{x}_*] \right] = \mathbb{E}_{\mathbf{x}_*} [m_f(\mathbf{x}_*)] \\ &= \mathbb{E}_{\mathbf{x}_*} \left[k(\mathbf{x}_*, \mathbf{X})(\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y} \right]\end{aligned}$$

$$f \sim GP(0, k), \quad \text{Training data: } \mathbf{X}, \mathbf{y}$$

$$\mathbf{x}_* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Compute $\mathbb{E}[f(\mathbf{x}_*)]$

$$\begin{aligned}\mathbb{E}_{f, \mathbf{x}_*}[f(\mathbf{x}_*)] &= \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_f[f(\mathbf{x}_*) | \mathbf{x}_*] \right] = \mathbb{E}_{\mathbf{x}_*} [m_f(\mathbf{x}_*)] \\ &= \mathbb{E}_{\mathbf{x}_*} \left[k(\mathbf{x}_*, \mathbf{X})(\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y} \right] \\ &= \boldsymbol{\beta}^\top \int k(\mathbf{X}, \mathbf{x}_*) \mathcal{N}(\mathbf{x}_* | \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}_* \\ \boldsymbol{\beta} := (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y} \quad &\blacktriangleright \text{independent of } \mathbf{x}_*\end{aligned}$$

$$f \sim GP(0, k), \quad \text{Training data: } \mathbf{X}, \mathbf{y}$$

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- If k is a Gaussian (squared exponential) kernel, this integral can be solved analytically
- Variance of $f(\mathbf{x}_*)$ can be computed similarly