

# Data-Efficient Reinforcement Learning with Probabilistic Models

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



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- Currently: Data-hungry learning or human guidance

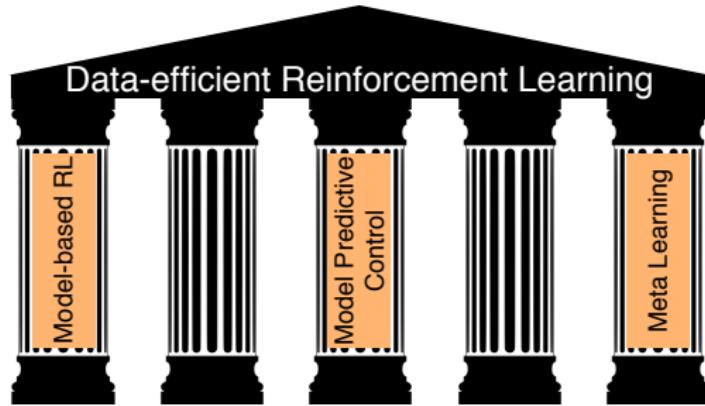


- **Vision:** Autonomous robots support humans in everyday activities ➤ Fast learning and automatic adaptation
- Currently: Data-hungry learning or human guidance

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

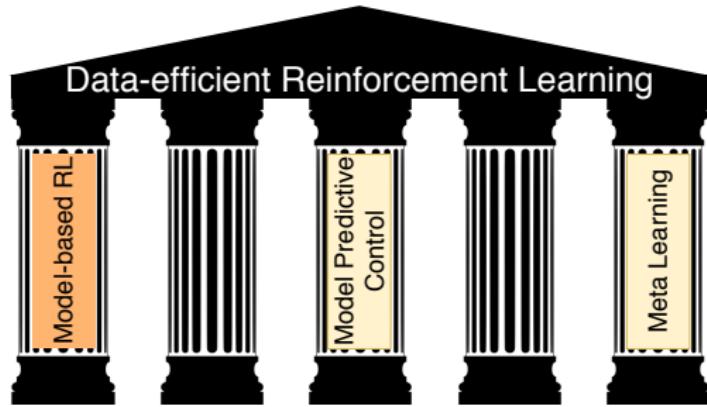
- ▶ Data-efficient decision making

## 2 Model predictive RL

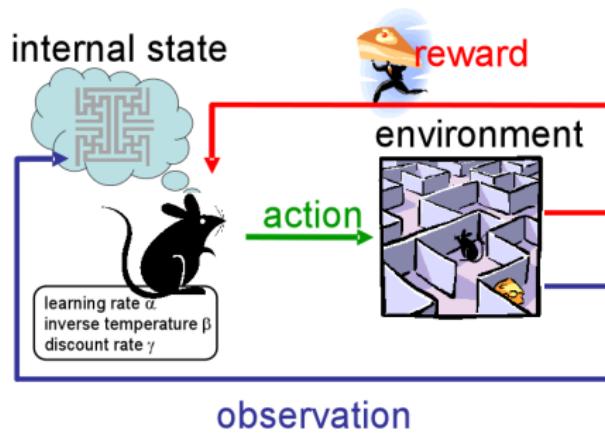
- ▶ Speed up learning further by online planning

## 3 Meta learning using latent variables

- ▶ Generalize knowledge to new situations



# Reinforcement Learning



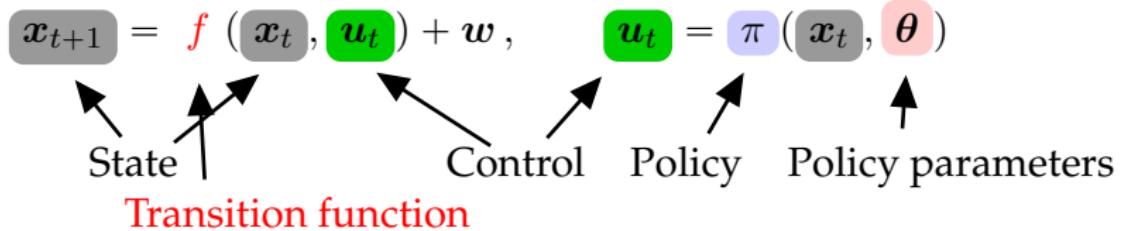
- Learn to solve a task
- Trial-and-error interaction with the environment
- Feedback via reward/cost function

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

Diagram illustrating the components of the equations:

- State**: Points to  $x_t$  in the first equation.
- Control**: Points to  $u_t$  in both equations.
- Policy**: Points to  $\pi$  in the second equation.
- Policy parameters**: Points to  $\theta$  in the second equation.

**Transition function**: Points to the term  $f(\cdot, \cdot)$  in the first equation.



## 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

## Objective

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

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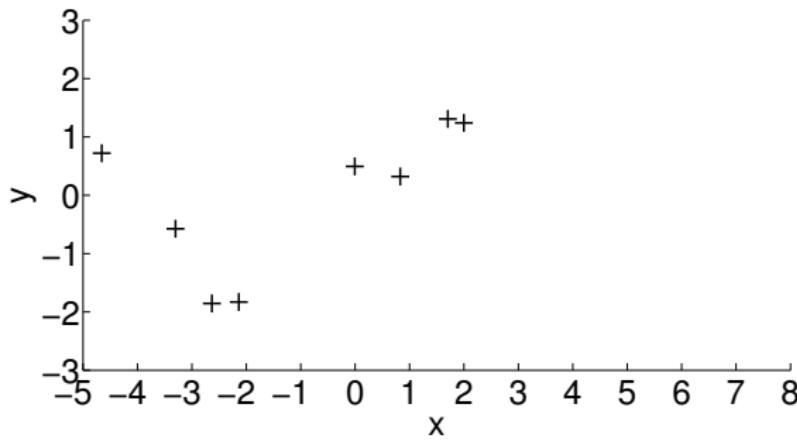
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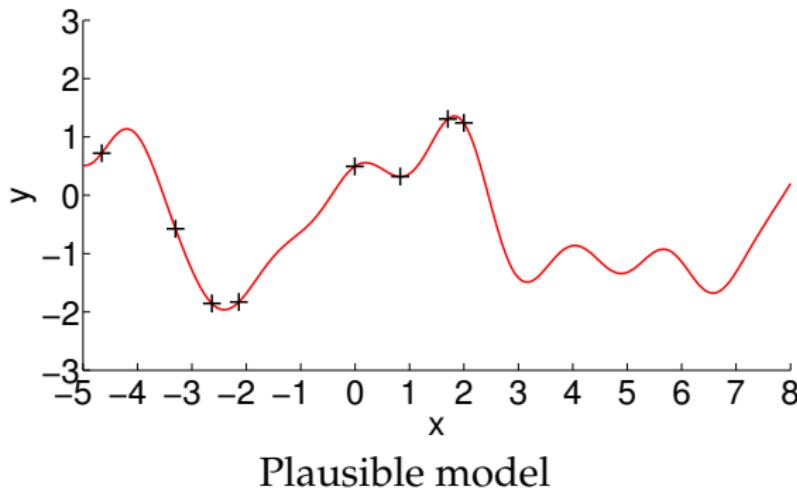
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Model learning problem: Find a function  $f : x \mapsto f(x) = y$

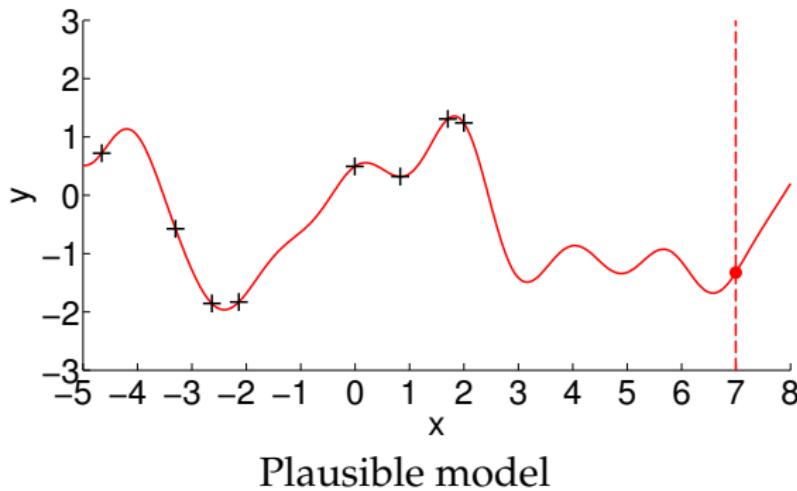


Observed function values

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

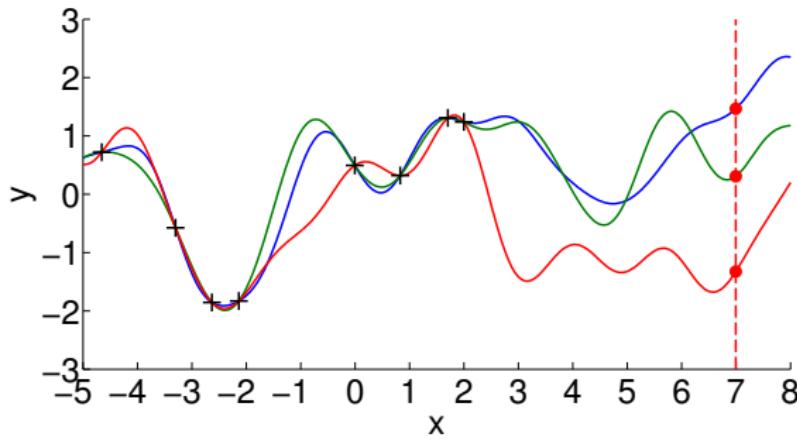


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Predictions? Decision Making?

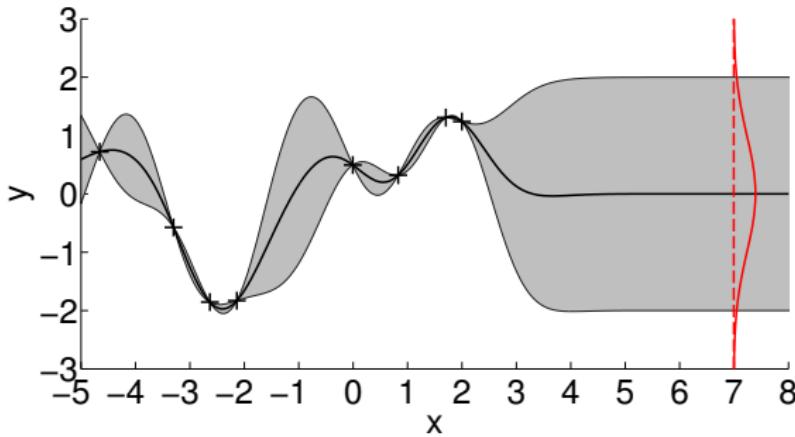
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More plausible models

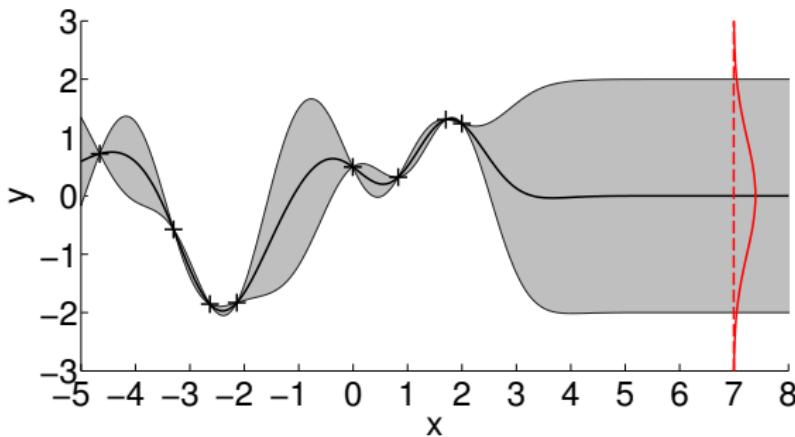
Predictions? Decision Making? Model Errors!

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)

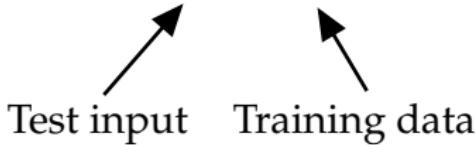
$$k(\boldsymbol{x}_p, \boldsymbol{x}_q) = \text{Cov}[f(\boldsymbol{x}_p), f(\boldsymbol{x}_q)]$$

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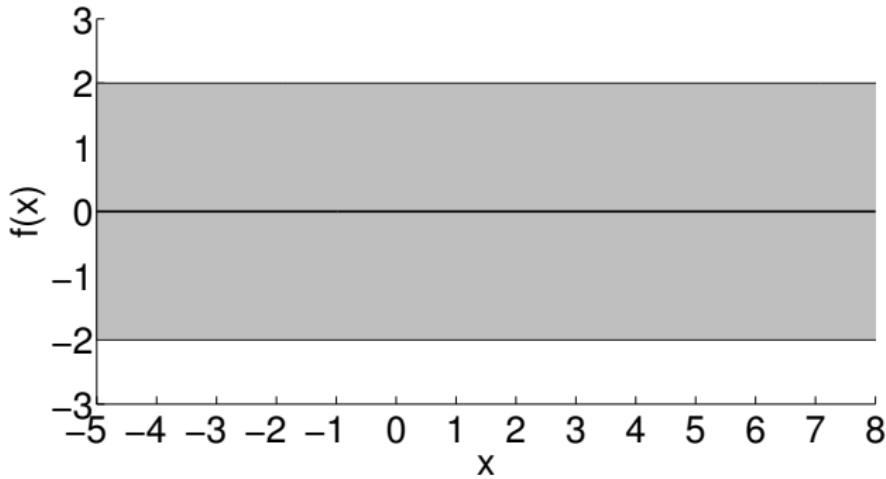
$$k(\mathbf{x}_p, \mathbf{x}_q) = \text{Cov}[f(\mathbf{x}_p), f(\mathbf{x}_q)]$$

- 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

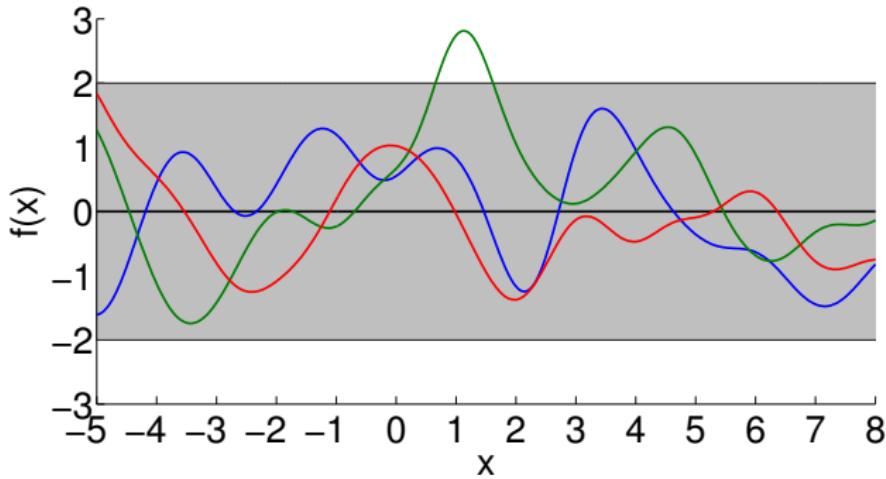


Prior belief about the function

Predictive (marginal) mean and variance:

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

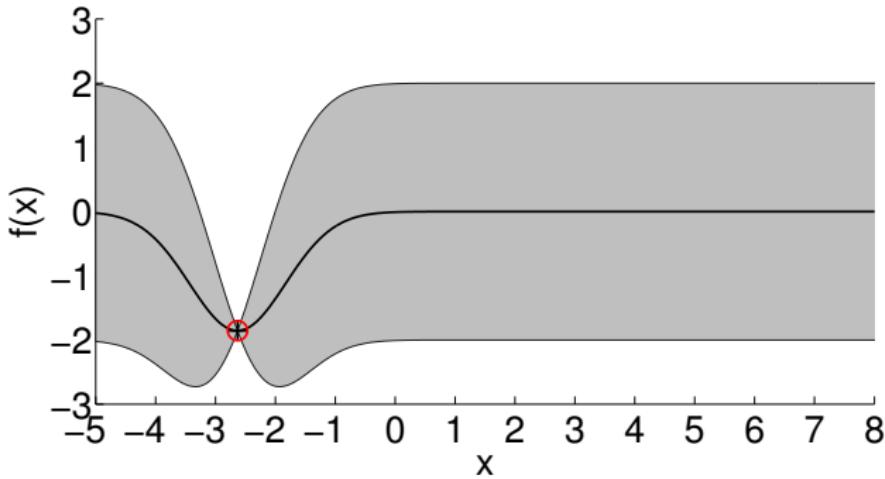
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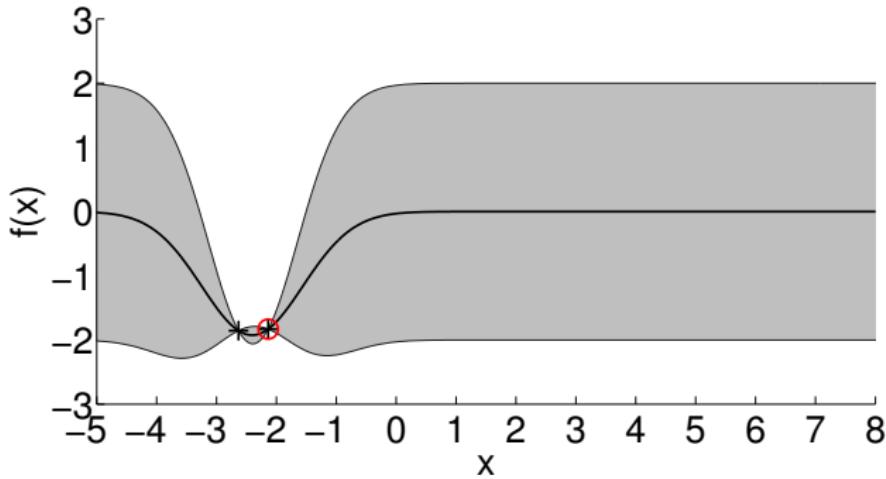


Posterior belief about the function

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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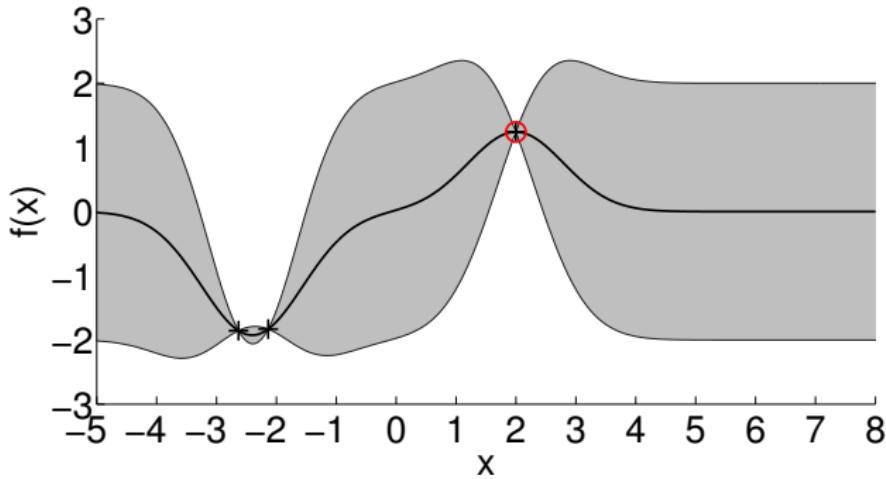


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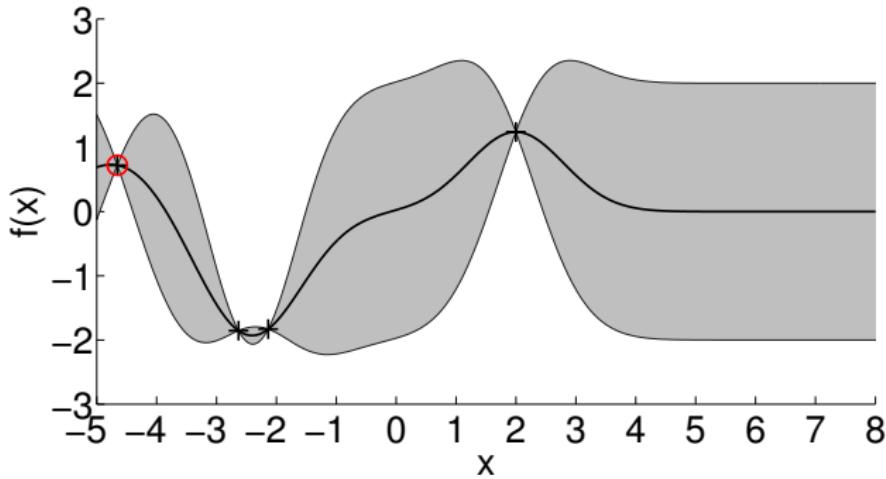


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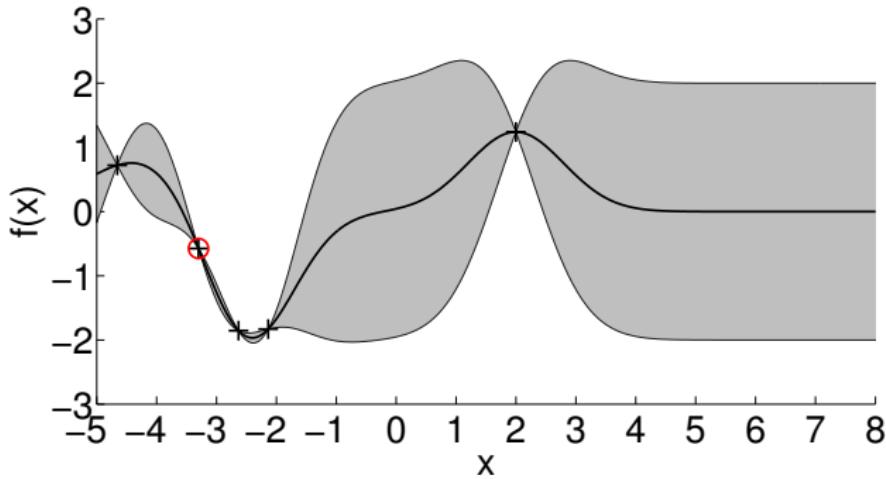


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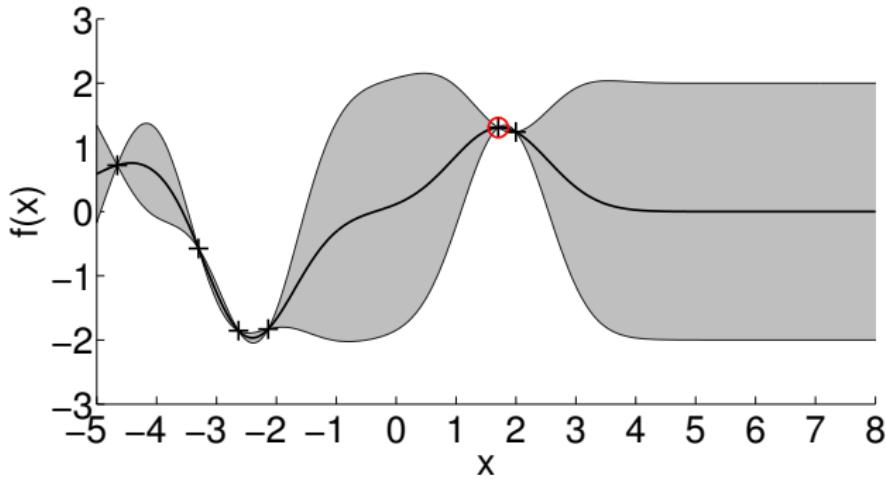


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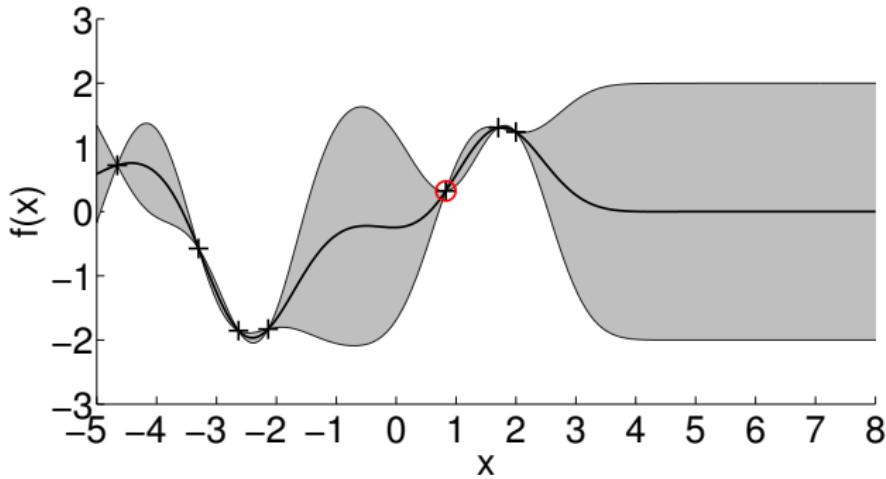


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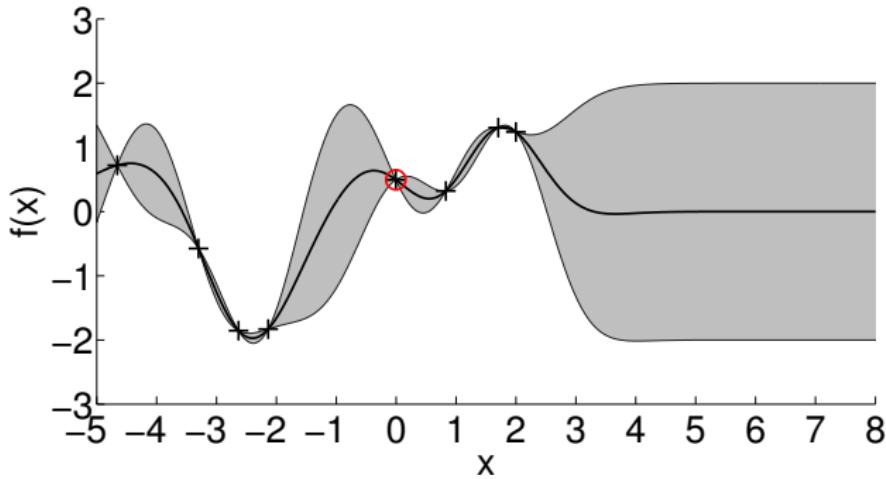


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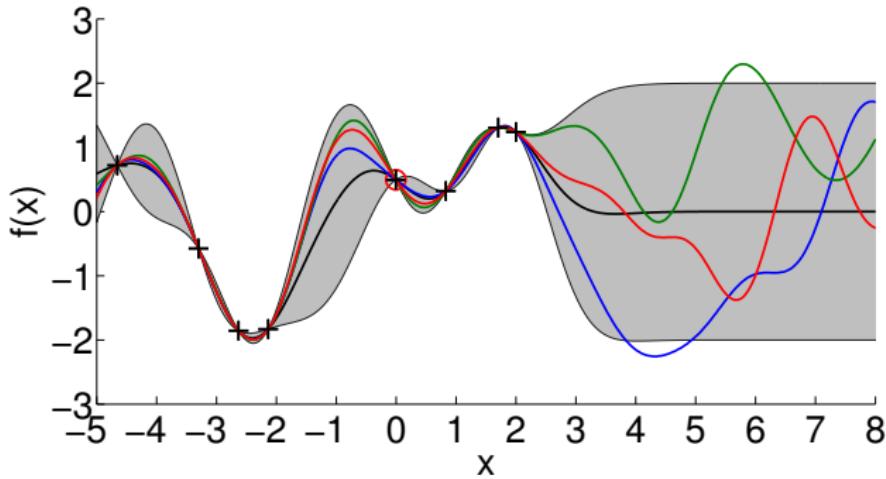


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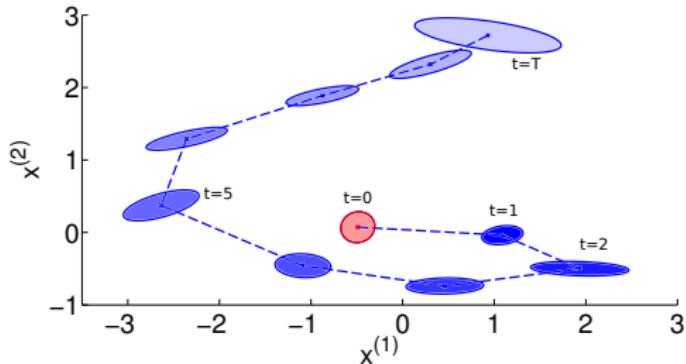
## Objective

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

## PILCO Framework: High-Level Steps

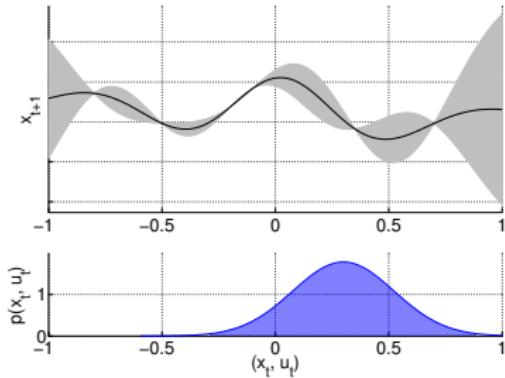
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# Long-Term Predictions



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

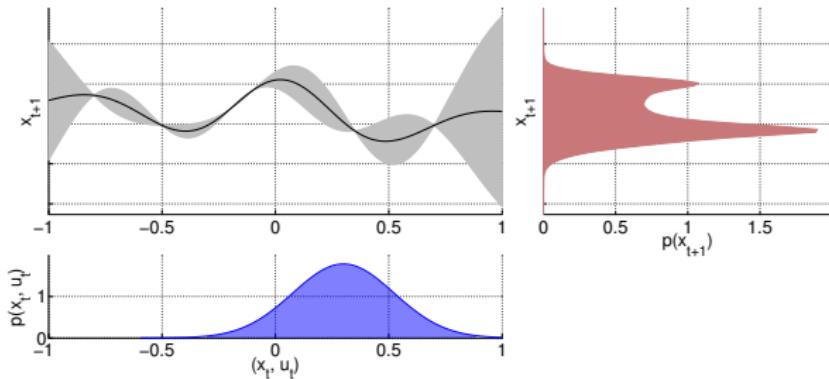
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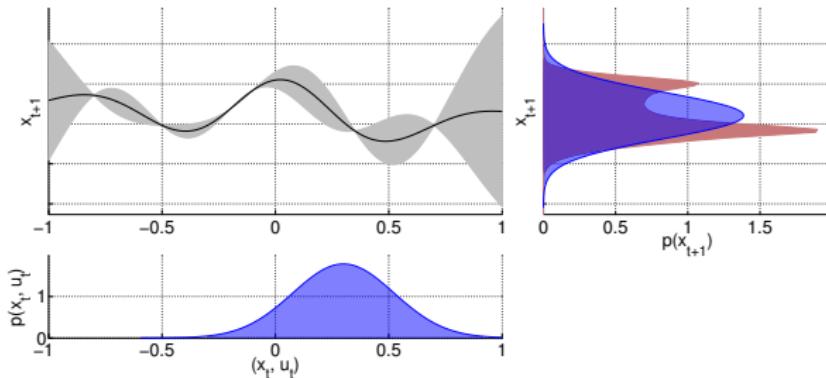
$$\underbrace{p(\mathbf{x}_{t+1}|\mathbf{x}_t, \mathbf{u}_t)}_{\text{GP prediction}} \quad \underbrace{p(\mathbf{x}_t, \mathbf{u}_t|\boldsymbol{\theta})}_{\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})}$$

# Long-Term Predictions



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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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  - Compute expected long-term cost  $J(\theta)$
  - Find parameters  $\theta$  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  $J(\boldsymbol{\theta})$

## Objective

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

- Know how to predict  $p(\mathbf{x}_1|\boldsymbol{\theta}), \dots, p(\mathbf{x}_T|\boldsymbol{\theta})$
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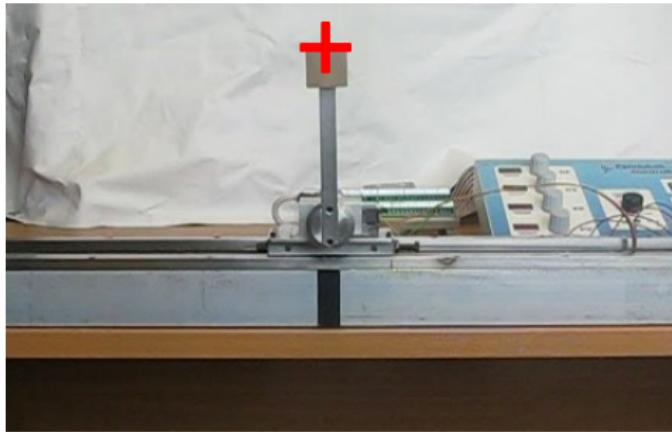
- Analytically compute gradient  $dJ(\boldsymbol{\theta})/d\boldsymbol{\theta}$
- Standard gradient-based optimizer (e.g., BFGS) to find  $\boldsymbol{\theta}^*$

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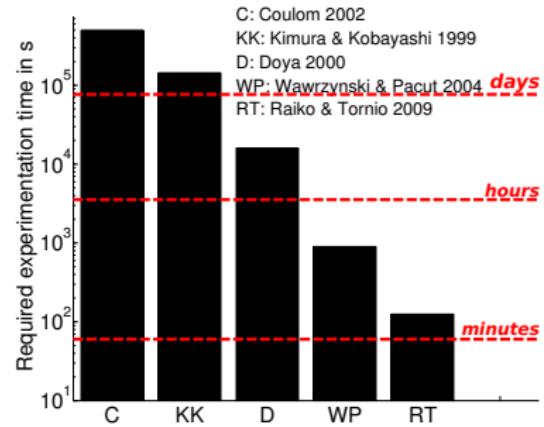
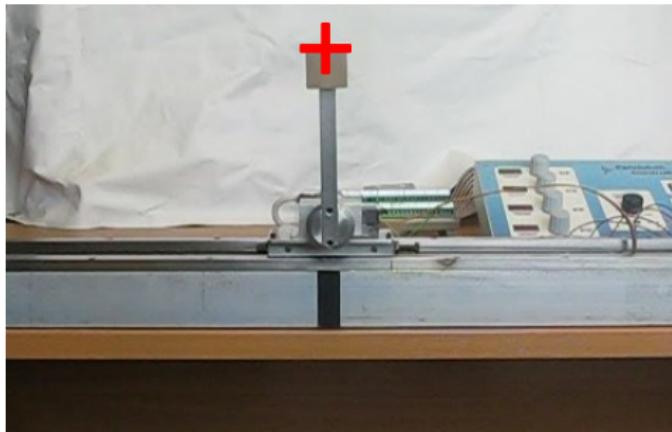


- Swing up and balance a freely swinging pendulum on a cart
- No knowledge about nonlinear dynamics ➤ Learn from scratch
- Cost function  $c(\mathbf{x}) = 1 - \exp(-\|\mathbf{x} - \mathbf{x}_{\text{target}}\|^2)$
- Code: <https://github.com/ICL-SML/pilco-matlab>

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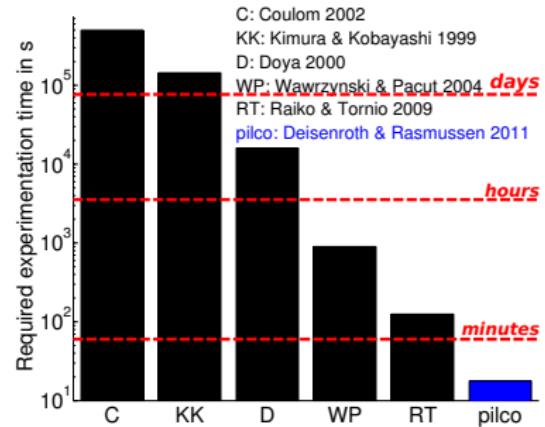
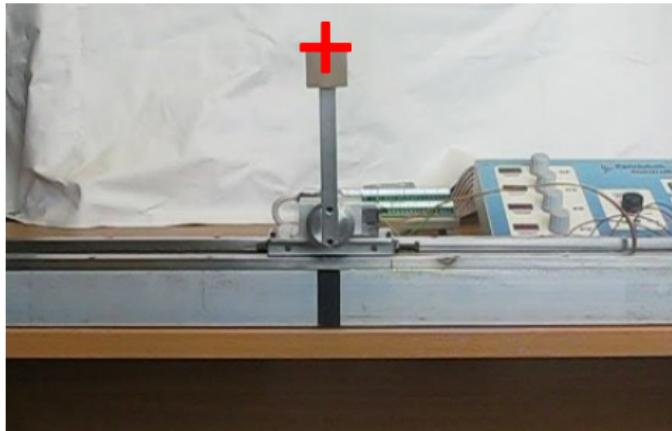
Deisenroth & Rasmussen (ICML, 2011): PILCO: A Model-based and Data-efficient Approach to Policy Search

# Standard Benchmark: Cart-Pole Swing-up



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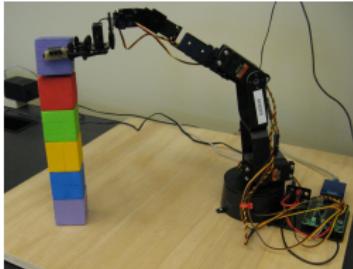
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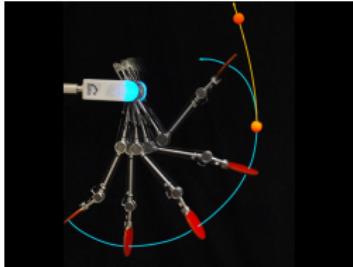
- Swing up and balance a freely swinging pendulum on a cart
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- Cost function  $c(\mathbf{x}) = 1 - \exp(-\|\mathbf{x} - \mathbf{x}_{\text{target}}\|^2)$
- **Unprecedented learning speed** compared to state-of-the-art
- Code: <https://github.com/ICL-SML/pilco-matlab>

Deisenroth & Rasmussen (ICML, 2011): PILCO: A Model-based and Data-efficient Approach to Policy Search

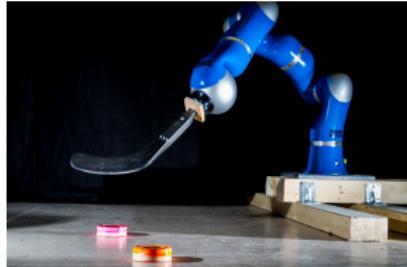
# Wide Applicability



with D Fox



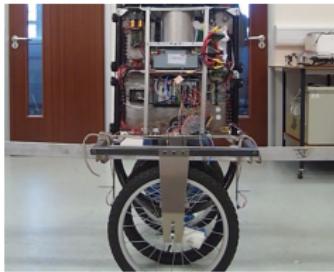
with P Englert, A Paraschos, J Peters



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

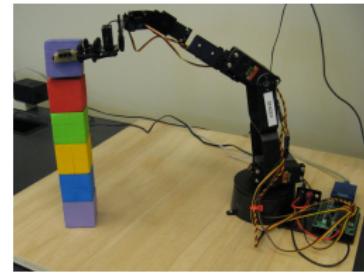
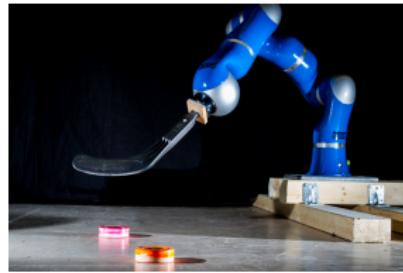
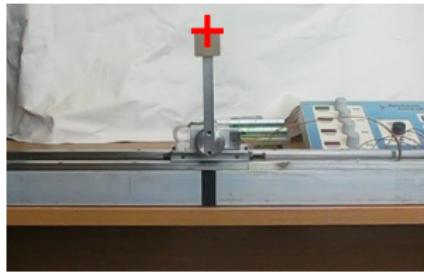
Deisenroth et al. (RSS, 2011): *Learning to Control a Low-Cost Manipulator using Data-efficient Reinforcement Learning*

Englert et al. (ICRA, 2013): *Model-based Imitation Learning by Probabilistic Trajectory Matching*

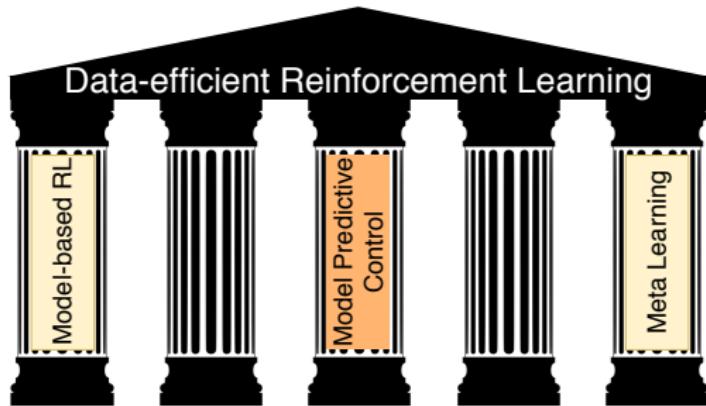
Deisenroth et al. (ICRA, 2014): *Multi-Task Policy Search for Robotics*

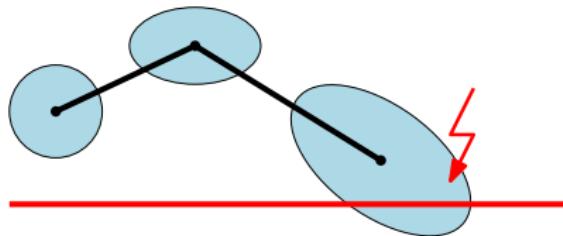
Kupcsik et al. (AIJ, 2017): *Model-based Contextual Policy Search for Data-Efficient Generalization of Robot Skills*

# Summary (1)

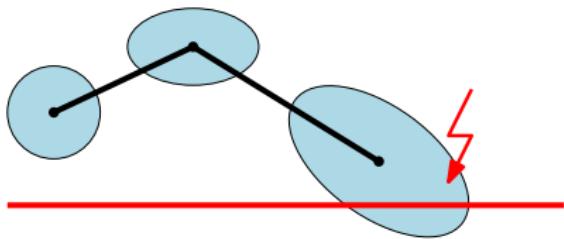


- In robotics, **data-efficient** learning is critical
- Probabilistic, model-based RL approach
  - Reduce model bias
  - Unprecedented learning speed
  - Wide applicability





- 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)
- Adjust policy if necessary (during policy learning)
- ▶ 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:

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

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

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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  $\lambda_t$
  - Necessary optimality condition:  $\partial H / \partial u_t = \mathbf{0}$
- Principled treatment of constraints on controls

# Theoretical Results

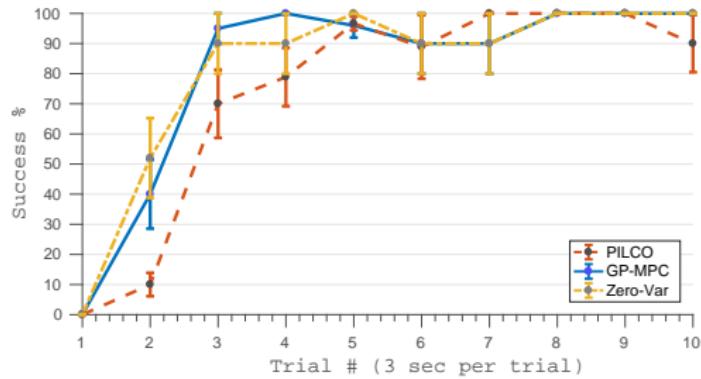
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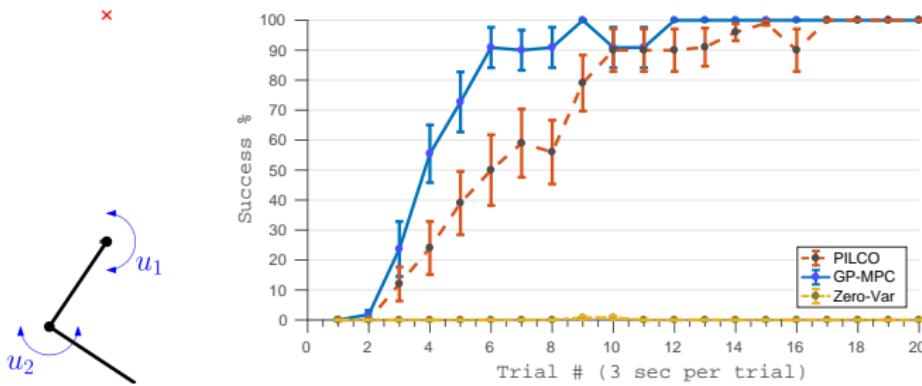
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- ▶ Principled treatment of constraints on controls
- Use predictive uncertainty to check violation of state constraints

# Learning Speed (Cart Pole)



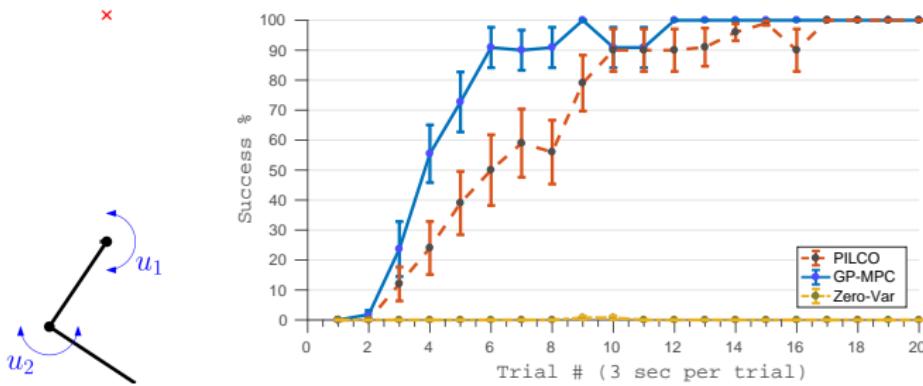
- Zero-Var: Only use the mean of the GP, discard variances for long-term predictions
- MPC: Increased data efficiency (40% less experience required than PILCO)
  - MPC more robust to model inaccuracies than a parametrized feedback controller

# Learning Speed (Double Pendulum)



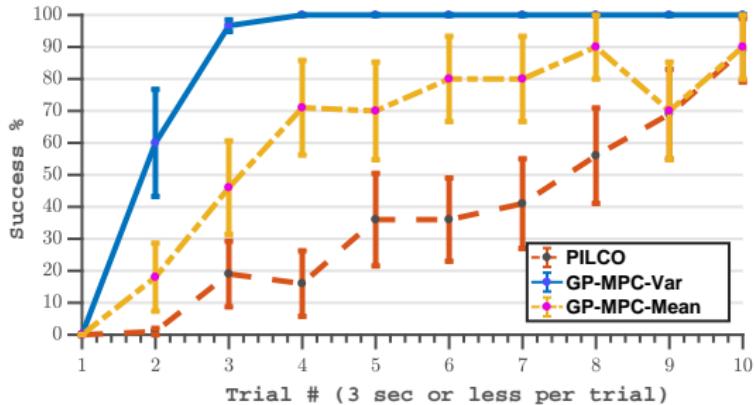
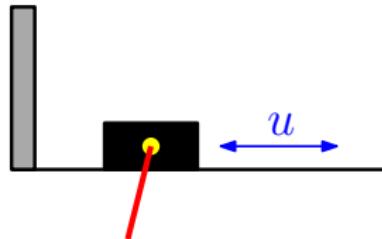
- GP-MPC maintains the same improvement in data efficiency
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  - Gets stuck in local optimum near start state
  - Insufficient exploration due to lack of uncertainty propagation

# 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

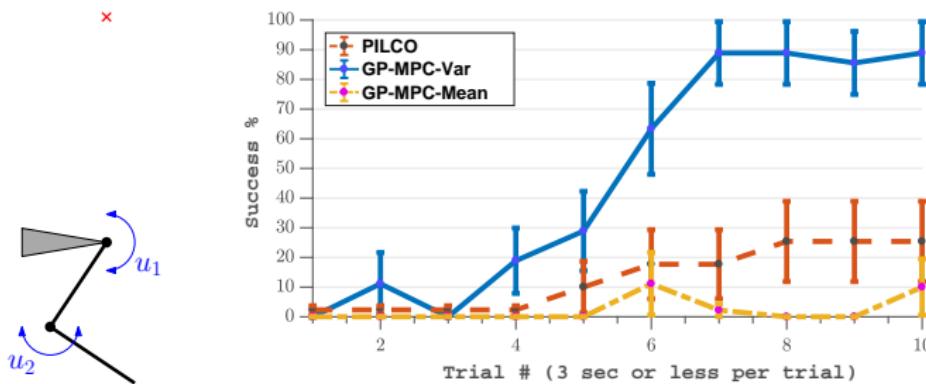
# Safety Constraints (Cart Pole)



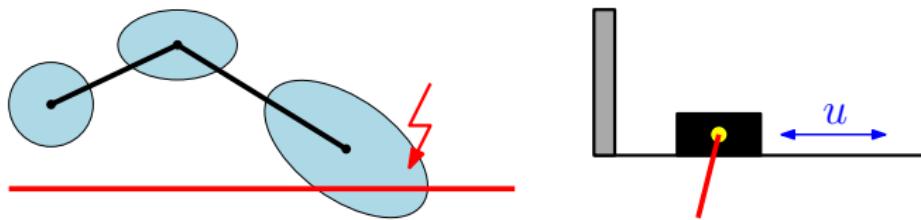
|             |        |                       |
|-------------|--------|-----------------------|
| PILCO       | 16/100 | constraint violations |
| GP-MPC-Mean | 21/100 | constraint violations |
| GP-MPC-Var  | 3/100  | constraint violations |

► Propagating model uncertainty important for safety

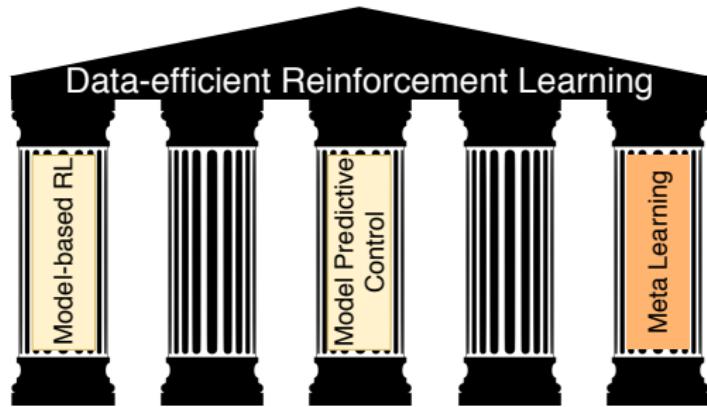
# Safety Constraints (Double Pendulum)



| 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





## Meta Learning

Generalize knowledge from known tasks to new (related) tasks



## Meta Learning

Generalize knowledge from known tasks to new (related) tasks

- Different robot configurations (link lengths, weights, ...)
- Re-use experience gathered so far generalize learning to new dynamics that are similar
  - ▶ Accelerated learning

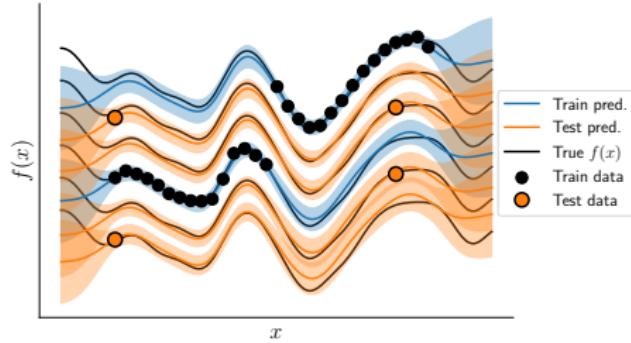
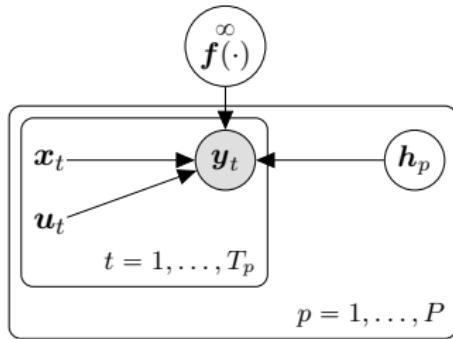


- Separate global and task-specific properties
- Shared global parameters describe general dynamics
- Describe task-specific (local) configurations with latent variable



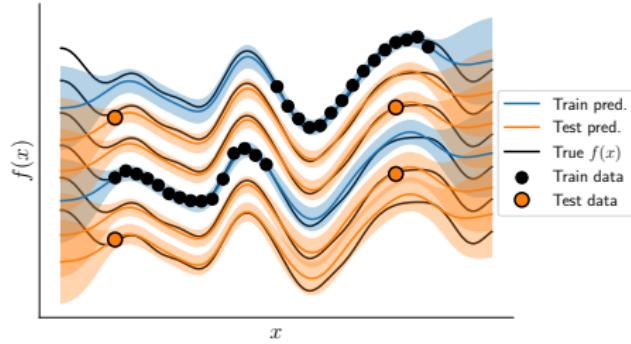
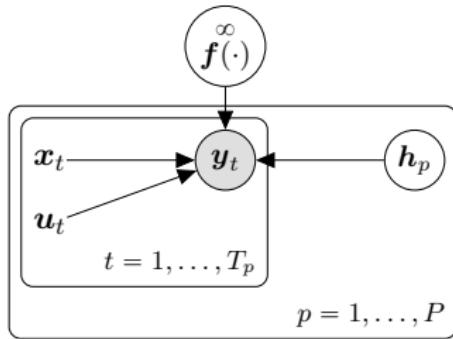
- Separate global and task-specific properties
- Shared global parameters describe general dynamics
- Describe task-specific (local) configurations with latent variable
- Online variational inference of (unseen) configurations

# Meta Model Learning with Latent Variables



$$\mathbf{y}_t = f(\mathbf{x}_t, \mathbf{u}_t, \mathbf{h}_p)$$

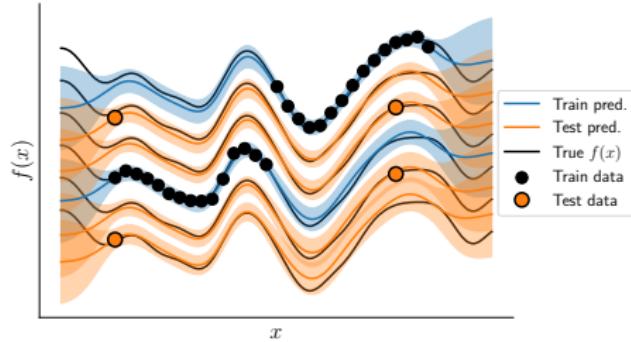
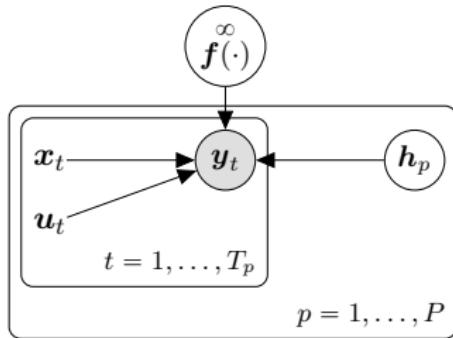
# Meta Model Learning with Latent Variables



$$y_t = f(x_t, u_t, h_p)$$

- GP captures global properties of the dynamics

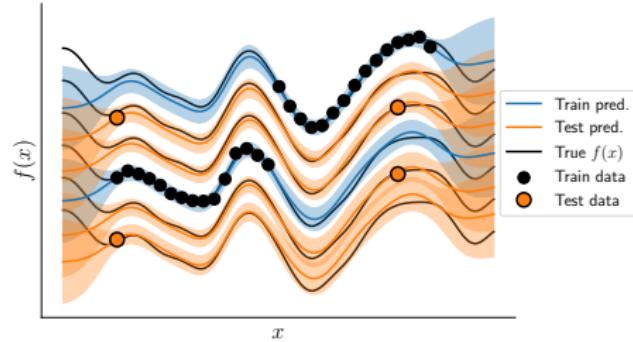
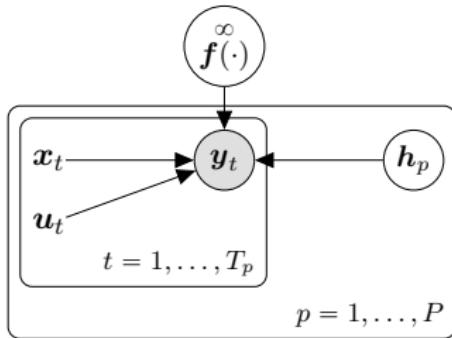
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$$y_t = f(x_t, u_t, h_p)$$

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  - ▶ Variational inference to find a posterior on latent configuration

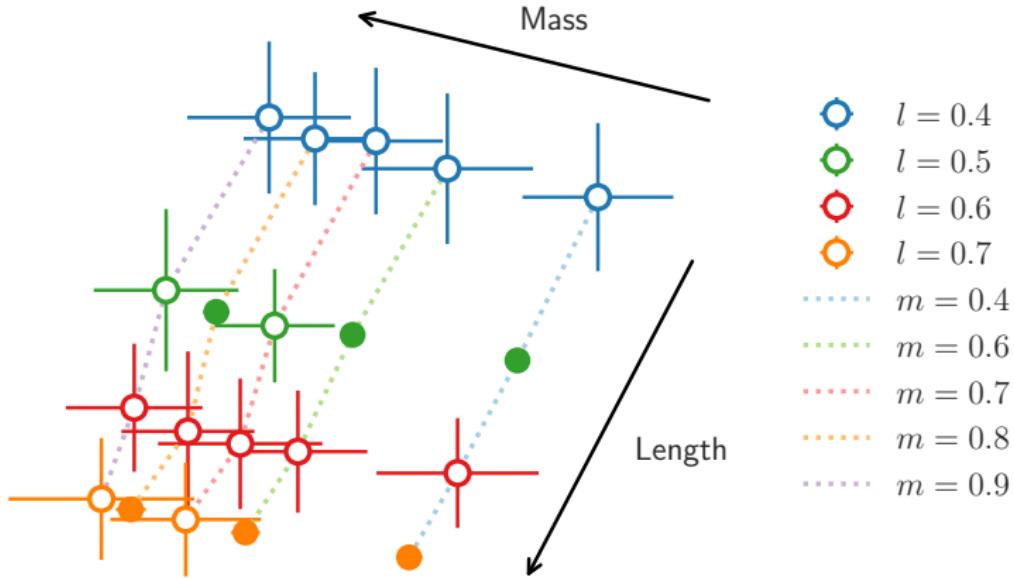
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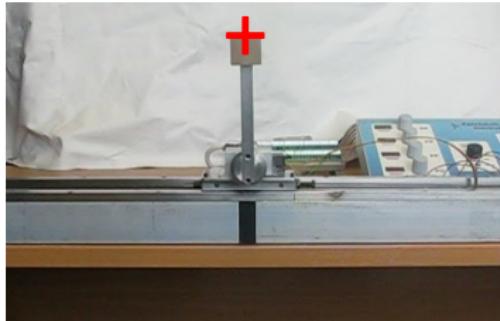
$$y_t = f(x_t, u_t, h_p)$$

- GP captures global properties of the dynamics
- Latent variable  $h_p$  describes local configuration
  - ▶ Variational inference to find a posterior on latent configuration
- Fast online inference of new configurations (no model re-training required)

# Latent Embeddings



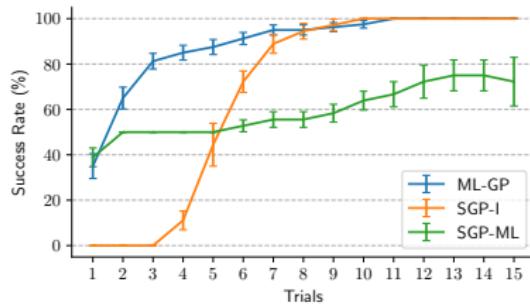
- Latent variable  $h$  encodes length  $l$  and mass  $m$  of the cart pole
- 6 training tasks, 14 held-out test tasks



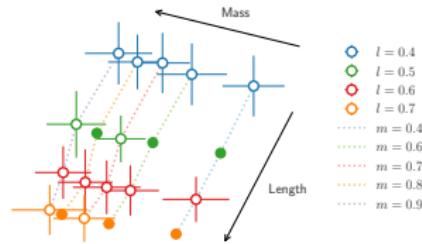
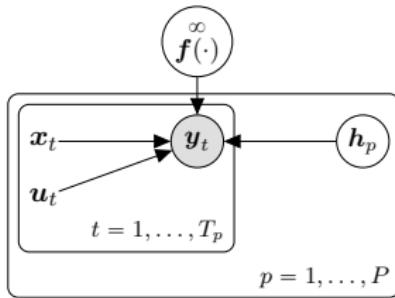
- Pre-trained on 6 training configurations until solved

| Model         | Training (s)   | Description                          |
|---------------|----------------|--------------------------------------|
| Independent   | $16.1 \pm 0.4$ | Independent GP-MPC                   |
| Aggregated    | $23.7 \pm 1.4$ | Aggregated experience (no latents)   |
| Meta learning | $15.1 \pm 0.5$ | Aggregated experience (with latents) |

► Meta learning can help speeding up RL

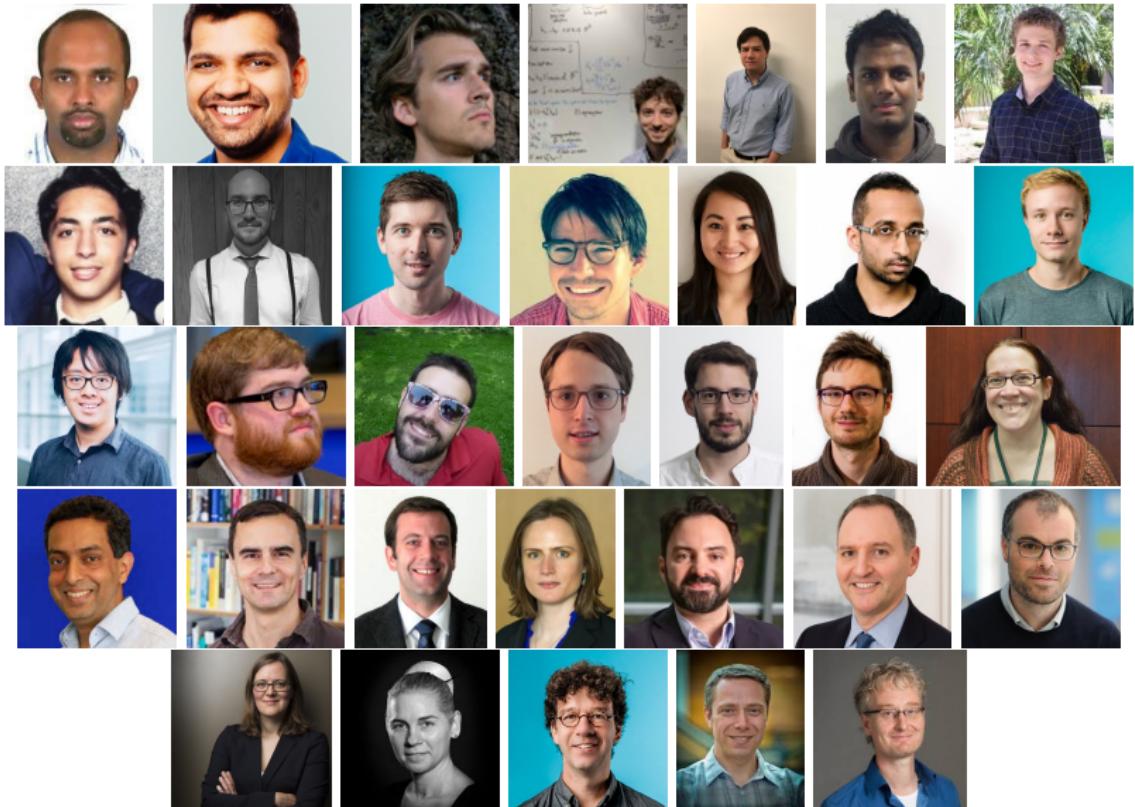


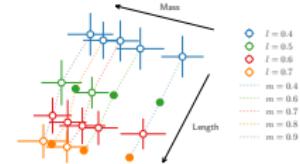
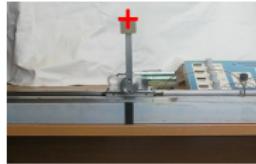
- Few-shot generalization on 4 unseen configurations
  - Success: solve all 10 (6 training + 4 test) tasks
  - Meta learning: blue
  - Independent (GP-MPC): orange
  - Aggregated experience model (no latents): green
- **Meta RL generalizes well to unseen tasks**



- Generalize knowledge from known situations to unseen ones
  - ▶ **Few-shot learning**
- Latent variable can be used to **infer task similarities**
- Significant speed-up in model learning and model-based RL

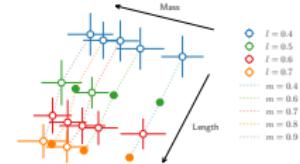
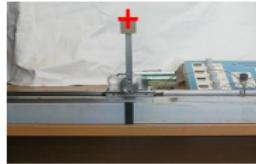
# Team and Collaborators





- **Data efficiency** is a practical challenge for autonomous robots
- Three pillars of data-efficient reinforcement learning for autonomous robots
  - 1 **Model-based reinforcement learning** with learned probabilistic models for fast learning from scratch
  - 2 **Model predictive control** with learned dynamics models accelerate learning and allow for safe exploration
  - 3 **Meta learning** using latent variables to generalize knowledge to new situations
- **Key to success:** Probabilistic modeling and Bayesian inference

# Wrap-Up



- **Data efficiency** is a practical challenge for autonomous robots
- Three pillars of data-efficient reinforcement learning for autonomous robots
  - 1 **Model-based reinforcement learning** with learned probabilistic models for fast learning from scratch
  - 2 **Model predictive control** with learned dynamics models accelerate learning and allow for safe exploration
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- **Key to success:** Probabilistic modeling and Bayesian inference

**Thank you for your attention**

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## ■ Controller:

$$\tilde{\pi}(\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^K w_k \exp \left( -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu}_k) \right)$$
$$u = \pi(\mathbf{x}, \boldsymbol{\theta}) = u_{\max} \sigma(\tilde{\pi}(\mathbf{x}, \boldsymbol{\theta})) \in [-u_{\max}, u_{\max}] ,$$

where  $\sigma$  is a squashing function.

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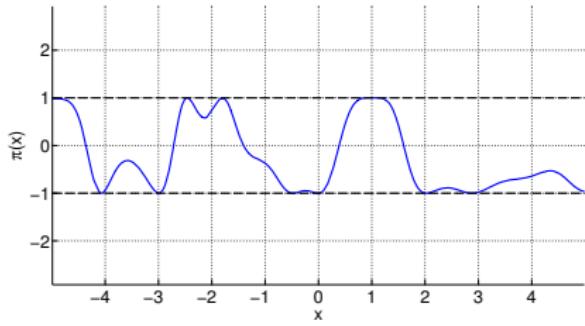
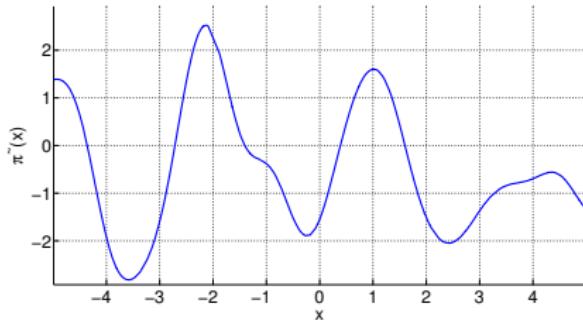
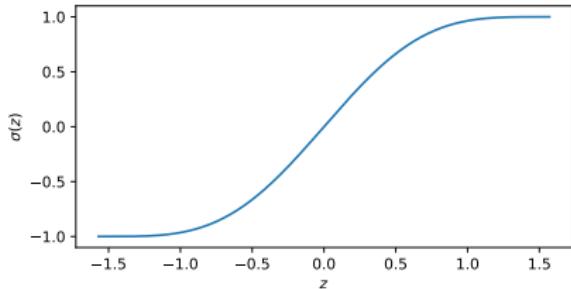
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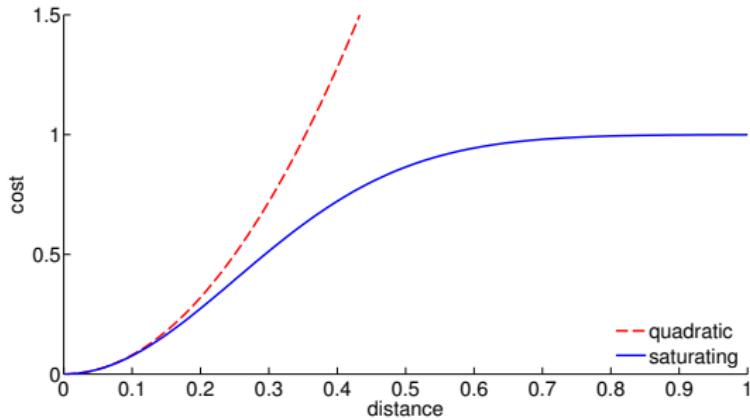
- Squashing function:

$$\sigma(z) = \frac{9}{8} \sin(z) + \frac{1}{8} \sin(3z)$$

# Squashing Function

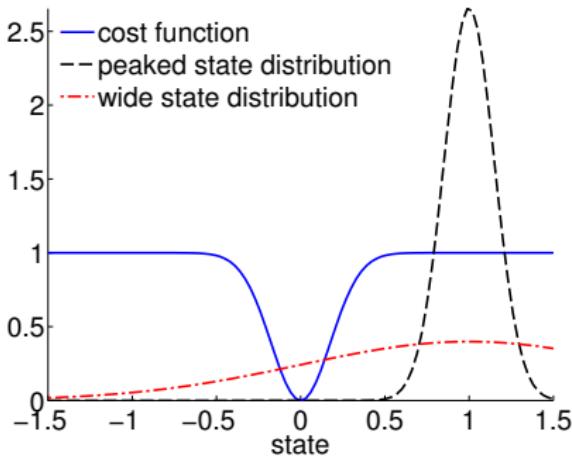


- **Quadratic cost**  $c(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_{\text{target}})^{\top} \mathbf{W} (\mathbf{x} - \mathbf{x}_{\text{target}})$
- **Saturating cost**  $c(\mathbf{x}) = 1 - \exp \left( - (\mathbf{x} - \mathbf{x}_{\text{target}})^{\top} \mathbf{W} (\mathbf{x} - \mathbf{x}_{\text{target}}) \right)$



- Quadratic cost pays a lot of attention to states “far away”
  - ▶ Bad idea for exploration

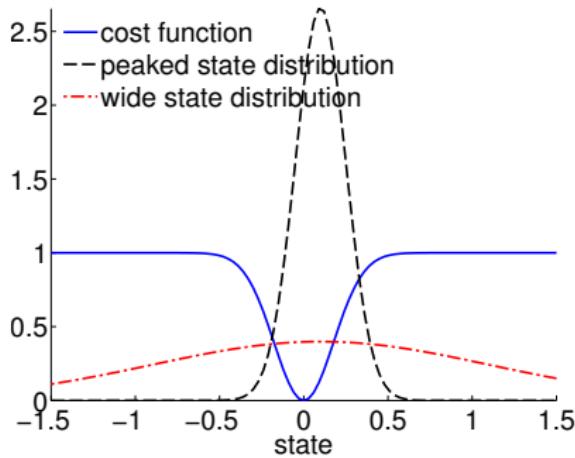
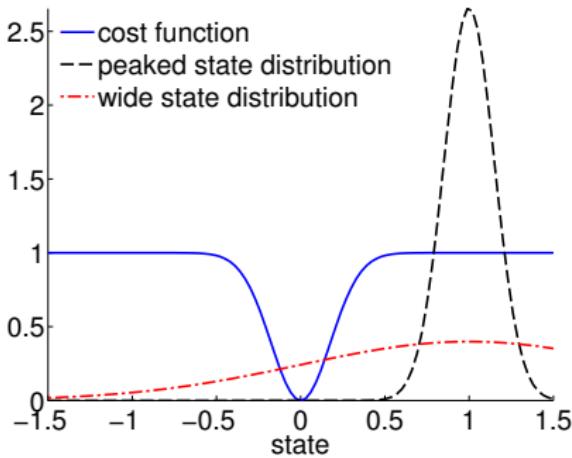
Task: Minimize  $\mathbb{E}[c(\mathbf{x}_t)]$



- In the **early stages of learning**, state predictions are expected to be far away from the target

# Natural Exploration with the Saturating Cost

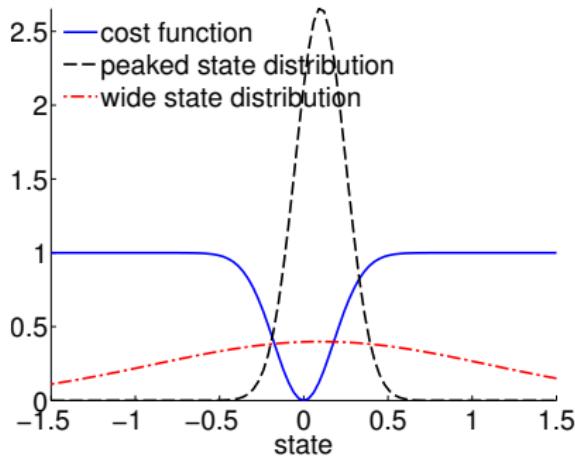
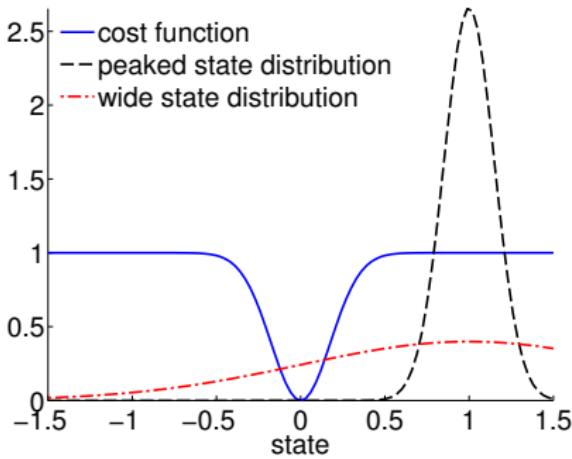
Task: Minimize  $\mathbb{E}[c(x_t)]$



- In the **early stages of learning**, state predictions are expected to be far away from the target ➤ **Exploration** favored

# Natural Exploration with the Saturating Cost

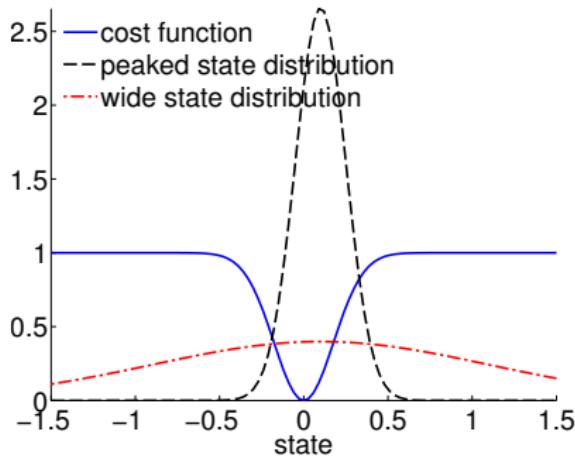
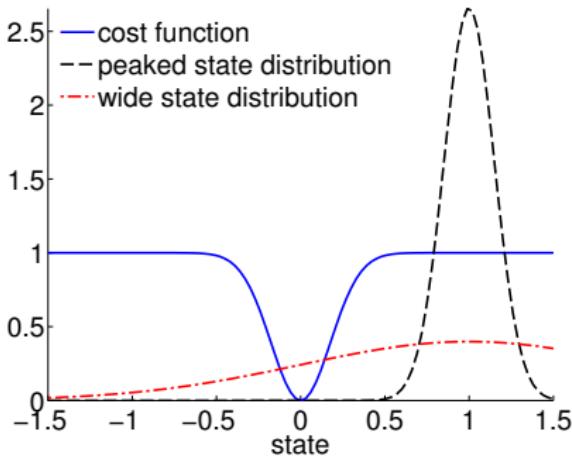
Task: Minimize  $\mathbb{E}[c(x_t)]$



- In the **early stages of learning**, state predictions are expected to be far away from the target ► **Exploration** favored
- In the **final stages of learning**, state predictions are expected to be close to the target

# Natural Exploration with the Saturating Cost

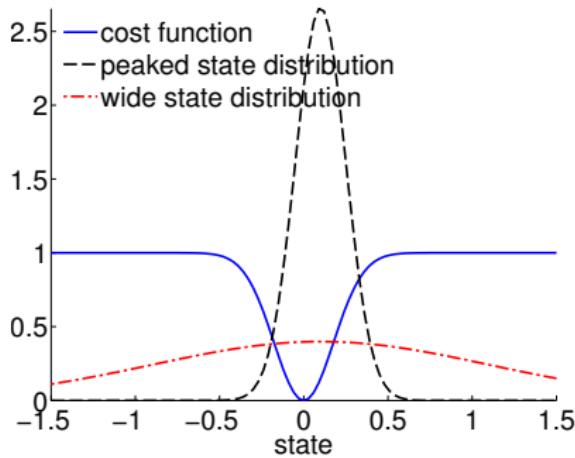
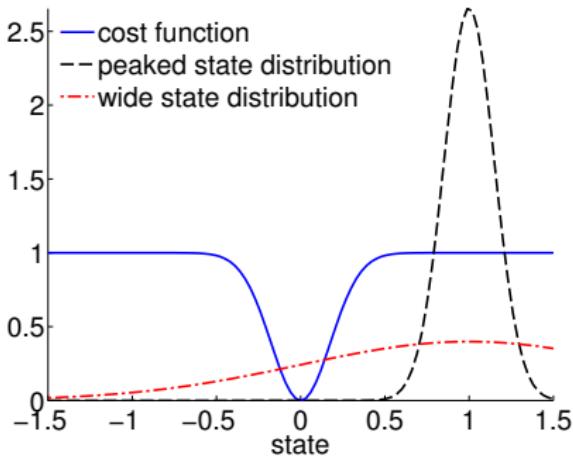
Task: Minimize  $\mathbb{E}[c(x_t)]$



- In the **early stages of learning**, state predictions are expected to be far away from the target ► **Exploration** favored
- In the **final stages of learning**, state predictions are expected to be close to the target ► **Exploitation** favored

# Natural Exploration with the Saturating Cost

Task: Minimize  $\mathbb{E}[c(x_t)]$



- In the **early stages of learning**, state predictions are expected to be far away from the target ► **Exploration** favored
- In the **final stages of learning**, state predictions are expected to be close to the target ► **Exploitation** favored
- Bayesian treatment: **Natural exploration/exploitation trade-off**

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

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

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

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

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

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

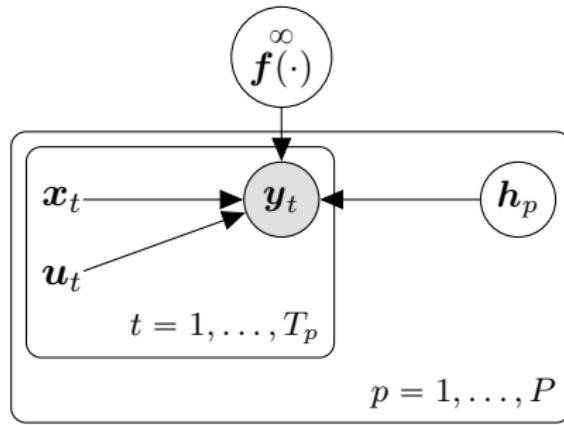
$$\mathbf{x}_* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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

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

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

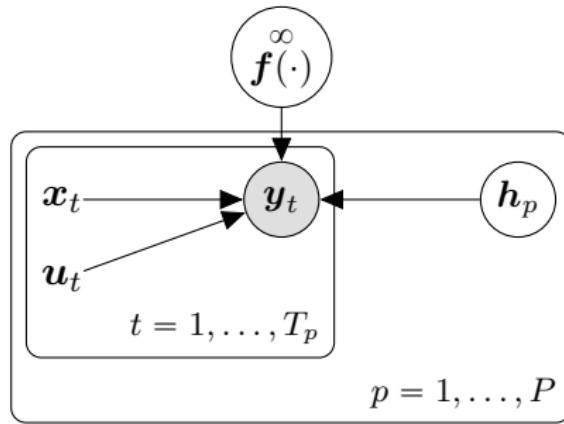
# Meta Learning Model



$$\mathbf{f}(\cdot) \sim GP$$

$$p(\mathbf{H}) = \prod_p p(\mathbf{h}_p), \quad p(\mathbf{h}_p) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$

# Meta Learning Model

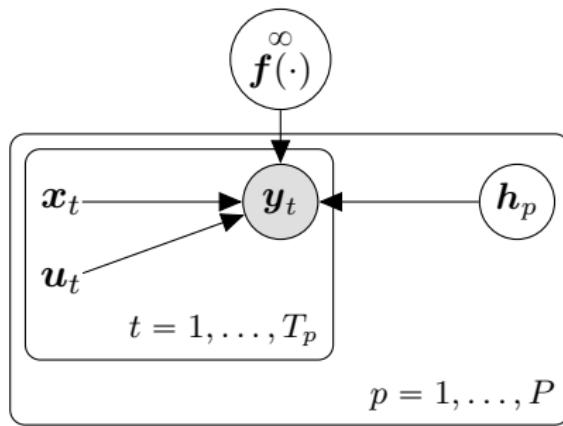


$$\mathbf{f}(\cdot) \sim GP$$

$$p(\mathbf{H}) = \prod_p p(\mathbf{h}_p), \quad p(\mathbf{h}_p) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$p(\mathbf{Y}, \mathbf{H}, \mathbf{f}(\cdot) | \mathbf{X}, \mathbf{U}) = \prod_{p=1}^P p(\mathbf{h}_p) \prod_{t=1}^{T_p} p(\mathbf{y}_t | \mathbf{x}_t, \mathbf{u}_t, \mathbf{h}_p, \mathbf{f}(\cdot)) p(\mathbf{f}(\cdot))$$

$$\mathbf{y}_t = \mathbf{x}_{t+1} - \mathbf{x}_t$$



Mean-field variational family:

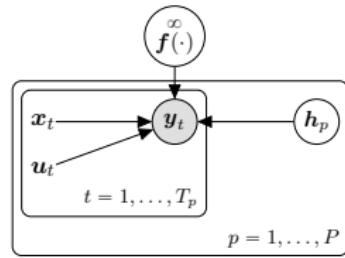
$$q(\mathbf{f}(\cdot), \mathbf{H}) = q(\mathbf{f}(\cdot))q(\mathbf{H})$$

$$q(\mathbf{H}) = \prod_{p=1}^P \mathcal{N}(\mathbf{h}_p | \mathbf{n}_p, \mathbf{T}_p),$$

$$q(\mathbf{f}(\cdot)) = \int p(\mathbf{f}(\cdot) | \mathbf{f}_Z) q(\mathbf{f}_Z) d\mathbf{f}_Z \quad \blacktriangleright \text{SV-GP (Titsias, 2009)}$$

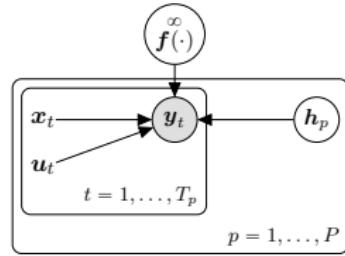
# Evidence Lower Bound

$$ELBO = \mathbb{E}_{q(\mathbf{f}(\cdot), \mathbf{H})} \left[ \log \frac{p(\mathbf{Y}, \mathbf{H}, \mathbf{f}(\cdot) | \mathbf{X}, \mathbf{U})}{q(\mathbf{f}(\cdot), \mathbf{H})} \right]$$



# Evidence Lower Bound

$$\begin{aligned} ELBO &= \mathbb{E}_{q(\mathbf{f}(\cdot), \mathbf{H})} \left[ \log \frac{p(\mathbf{Y}, \mathbf{H}, \mathbf{f}(\cdot) | \mathbf{X}, \mathbf{U})}{q(\mathbf{f}(\cdot), \mathbf{H})} \right] \\ &= \sum_{p=1}^P \sum_{t=1}^{T_p} \mathbb{E}_{q(\mathbf{f}_t | \mathbf{x}_t, \mathbf{u}_t, \mathbf{h}_p) q(\mathbf{h}_p)} \left[ \log p(\mathbf{y}_t | \mathbf{f}_t) \right] \\ &\quad - \text{KL}(q(\mathbf{H}) || p(\mathbf{H})) - \text{KL}(q(\mathbf{f}(\cdot)) || p(\mathbf{f}(\cdot))) \end{aligned}$$



# Evidence Lower Bound

$$\begin{aligned}
 ELBO &= \mathbb{E}_{q(\mathbf{f}(\cdot), \mathbf{H})} \left[ \log \frac{p(\mathbf{Y}, \mathbf{H}, \mathbf{f}(\cdot) | \mathbf{X}, \mathbf{U})}{q(\mathbf{f}(\cdot), \mathbf{H})} \right] \\
 &= \sum_{p=1}^P \sum_{t=1}^{T_p} \mathbb{E}_{q(\mathbf{f}_t | \mathbf{x}_t, \mathbf{u}_t, \mathbf{h}_p) q(\mathbf{h}_p)} \left[ \log p(\mathbf{y}_t | \mathbf{f}_t) \right] \\
 &\quad - \text{KL}(q(\mathbf{H}) || p(\mathbf{H})) - \text{KL}(q(\mathbf{f}(\cdot)) || p(\mathbf{f}(\cdot))) \\
 &\quad \underbrace{\quad \quad \quad \text{Monte Carlo estimate}}_{\text{closed-form solution}} \\
 &= \sum_{p=1}^P \sum_{t=1}^{T_p} \overbrace{\mathbb{E}_{q(\mathbf{f}_t | \mathbf{x}_t, \mathbf{u}_t, \mathbf{h}_p) q(\mathbf{h}_p)} \left[ \log p(\mathbf{y}_t | \mathbf{f}_t) \right]}^{\text{closed-form solution}} \\
 &\quad - \text{KL}(q(\mathbf{H}) || p(\mathbf{H})) - \text{KL}(q(\mathbf{F}_Z) || p(\mathbf{F}_Z))
 \end{aligned}$$

