Probabilistic Models for Data-Efficient Reinforcement Learning

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Creative Machine Learning

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Autonomous Robots: Key Challenges



■ Three key challenges in autonomous robots: Modeling. Predicting. Decision making.



Robotics

Autonomous Robots: Key Challenges



- Three key challenges in autonomous robots:
 Modeling. Predicting. Decision making.
- No human in the loop ▶ "Learn" from data
- Automatically extract information
- Data-efficient (fast) learning
- Uncertainty: sensor noise, unknown processes, limited knowledge, ...

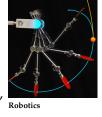


Robotics

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Reinforcement learning subject to data efficiency

Data-Efficient Reinforcement Learning



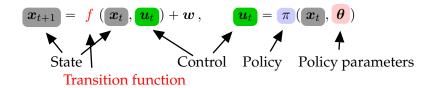


- 1 Model-based RL
 - ▶ Data-efficient decision making
- 2 Model predictive RL
 - ➤ Speed up learning further by online planning
- 3 Meta learning using latent variables
 - → Generalize knowledge to new situations

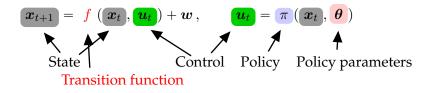




Reinforcement Learning and Optimal Control



Reinforcement Learning and Optimal Control



Objective (Controller Learning)

Find policy parameters θ^* that minimize the expected long-term cost

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

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

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



Objective

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

- \blacksquare Probabilistic model for transition function f
 - ▶ System identification



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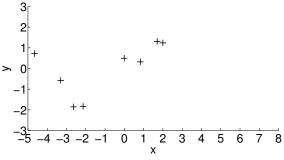
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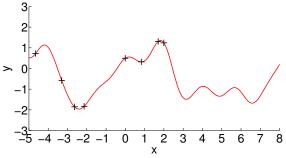
Model learning problem: Find a function $f: x \mapsto f(x) = y$



Observed function values



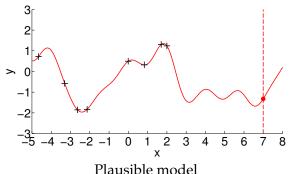
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Plausible model



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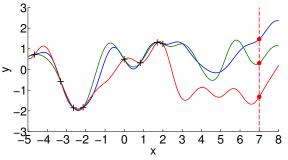


Plausible mode

Predictions? Decision Making?



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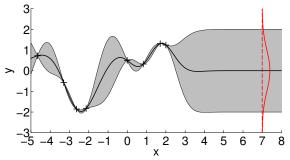


More plausible models

Predictions? Decision Making? Model Errors!



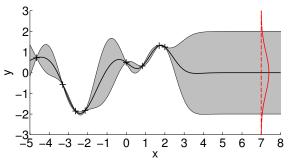
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Distribution over plausible functions



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)

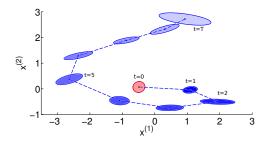


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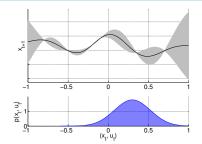
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■ Iteratively compute $p(x_1|\theta), \dots, p(x_T|\theta)$

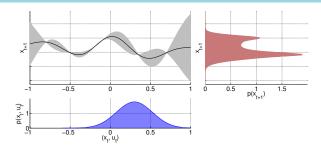




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$$\underbrace{p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t,\boldsymbol{u}_t)}_{\text{GP prediction}}\underbrace{p(\boldsymbol{x}_t,\boldsymbol{u}_t|\boldsymbol{\theta})}_{\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})}$$

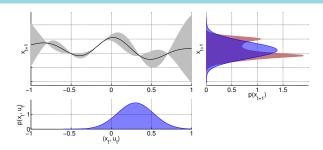




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▶ GP moment matching

(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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 - Compute expected long-term cost $J(\theta)$
 - Find parameters θ that minimize $J(\theta)$
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Policy Improvement



Objective

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

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

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

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

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

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

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

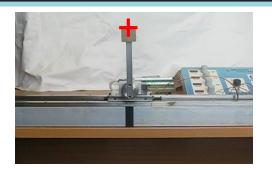


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Standard Benchmark: Cart-Pole Swing-up

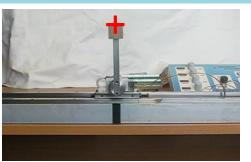


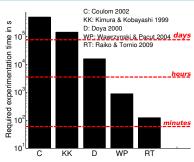


- Swing up and balance a freely swinging pendulum on a cart
- No knowledge about nonlinear dynamics ➤ Learn from scratch
- Cost function $c(\boldsymbol{x}) = 1 \exp(-\|\boldsymbol{x} \boldsymbol{x}_{\text{target}}\|^2)$
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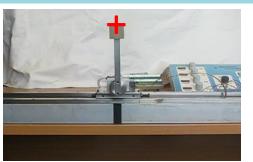


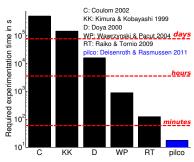


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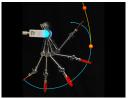




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- Unprecedented learning speed compared to state-of-the-art
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Wide Applicability







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



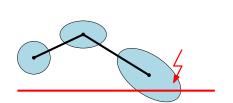




- In robotics, data-efficient learning is critical
- Probabilistic, model-based RL approach
 - Reduce model bias
 - Unprecedented learning speed
 - Wide applicability

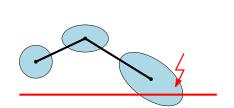








- Deal with real-world safety constraints (states/controls)
- Use probabilistic model to predict whether state constraints are violated (e.g., Sui et al., 2015; Berkenkamp et al., 2017)
- Adjust policy if necessary (during policy learning)





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- ➤ Safe exploration within an MPC-based RL setting
- ightharpoonup Optimize control signals u_t directly (no policy parameters)

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- 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):
 - 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

Theoretical Results



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

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- Deterministic system function that propagates moments
- Lipschitz continuity (under mild assumptions) implies that we can apply Pontryagin's Minimum Principle
 - ▶ Principled treatment of control constraints



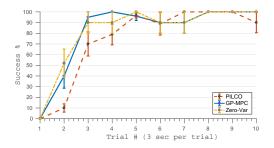
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 - ▶ Principled treatment of control constraints
- Use predictive uncertainty to check violation of state constraints

Learning Speed (Cart Pole)

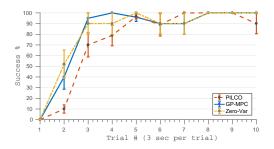




■ Zero-Var: Only use the mean of the GP, discard variances for long-term predictions

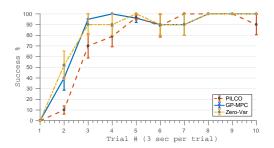
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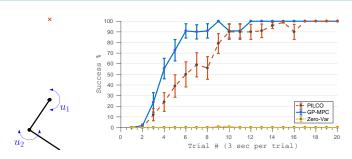


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- MPC more robust to model inaccuracies than a parametrized feedback controller

Kamthe & Deisenroth (AISTATS, 2018): Data-Efficient Reinforcement Learning with Probabilistic Model Predictive Control

Learning Speed (Double Pendulum)

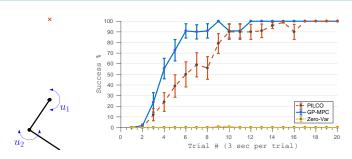




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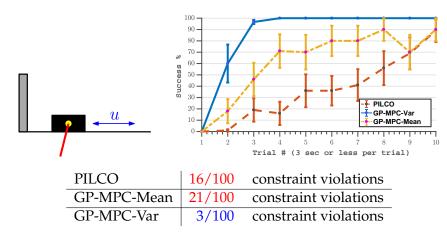




- GP-MPC maintains the same improvement in data efficiency
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 - Insufficient exploration due to lack of uncertainty propagation
- Although MPC is fairly robust to model inaccuracies we cannot get away without uncertainty propagation

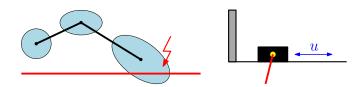
Safety Constraints (Cart Pole)





▶ Propagating model uncertainty important for safety

Kamthe & Deisenroth (AISTATS, 2018): Data-Efficient Reinforcement Learning with Probabilistic Model Predictive Control



- 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











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



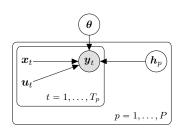


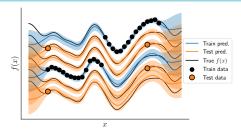




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- Shared global parameters describe general dynamics
- Describe task-specific (local) configurations with latent variable
- Online variational inference of (unseen) configurations

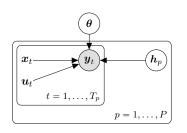


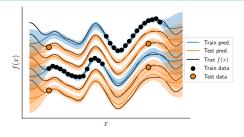




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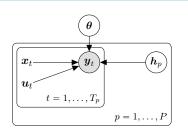


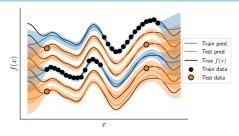


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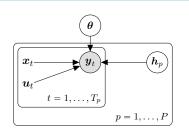


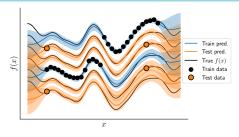


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 ▶ Variational inference to find a posterior on latent configuration





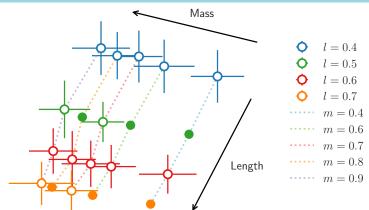


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- Latent variable h_p describes task-specific properties
 ▶ Variational inference to find a posterior on latent configuration
- Fast online inference of new configurations (no model re-training required)

Latent Embeddings





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

Meta-RL (Cart Pole): Training



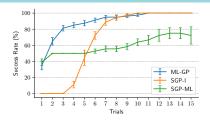


■ Pre-trained on 6 training configurations until solved

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

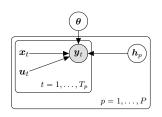
▶ Meta learning can help speeding up RL

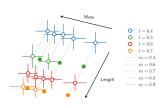
Meta-RL (Cart Pole): Few-Shot Generalization



- 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



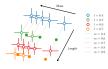


- Generalize knowledge from known situations to unseen ones ➤ Few-shot learning
- Latent variable can be used to infer task similarities
- Significant speed-up in model learning and model-based RL







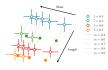


- **Data efficiency** is a practical challenge for autonomous robots
- Three pillars of data-efficient reinforcement learning for autonomous robots
 - Model-based reinforcement learning with learned probabilistic models for fast learning from scratch
 - 2 Model predictive reinforcement learning with learned dynamics models accelerates 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









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Thank you for your attention

References I



- F. Berkenkamp, M. Turchetta, A. P. Schoellig, and A. Krause. Safe Model-based Reinforcement Learning with Stability Guarantees. In Advances in Neural Information Processing Systems, 2017.
- [2] D. P. Bertsekas. Dynamic Programming and Optimal Control, volume 1 of Optimization and Computation Series. Athena Scientific, Belmont, MA, USA, 3rd edition, 2005.
- [3] D. P. Bertsekas. Dynamic Programming and Optimal Control, volume 2 of Optimization and Computation Series. Athena Scientific, Belmont, MA, USA, 3rd edition, 2007.
- [4] B. Bischoff, D. Nguyen-Tuong, T. Koller, H. Markert, and A. Knoll. Learning Throttle Valve Control Using Policy Search. In Proceedings of the European Conference on Machine Learning and Knowledge Discovery in Databases, 2013.
- [5] M. P. Deisenroth, P. Englert, J. Peters, and D. Fox. Multi-Task Policy Search for Robotics. In Proceedings of the International Conference on Robotics and Automation, 2014.
- [6] M. P. Deisenroth, D. Fox, and C. E. Rasmussen. Gaussian Processes for Data-Efficient Learning in Robotics and Control. IEEE Transactions on Pattern Analysis and Machine Intelligence, 37(2):408–423, 2015.
- [7] M. P. Deisenroth and C. E. Rasmussen. PILCO: A Model-Based and Data-Efficient Approach to Policy Search. In Proceedings of the International Conference on Machine Learning, 2011.
- [8] M. P. Deisenroth, C. E. Rasmussen, and D. Fox. Learning to Control a Low-Cost Manipulator using Data-Efficient Reinforcement Learning. In Proceedings of Robotics: Science and Systems, 2011.
- [9] P. Englert, A. Paraschos, J. Peters, and M. P. Deisenroth. Model-based Imitation Learning by Probabilistic Trajectory Matching. In Proceedings of the IEEE International Conference on Robotics and Automation, 2013.
- [10] P. Englert, A. Paraschos, J. Peters, and M. P. Deisenroth. Probabilistic Model-based Imitation Learning. Adaptive Behavior, 21:388–403, 2013.
- [11] A. Girard, C. E. Rasmussen, and R. Murray-Smith. Gaussian Process Priors with Uncertain Inputs: Multiple-Step Ahead Prediction. Technical Report TR-2002-119, University of Glasgow, 2002.
- [12] S. Kamthe and M. P. Deisenroth. Data-Efficient Reinforcement Learning with Probabilistic Model Predictive Control. In Proceedings of the International Conference on Artificial Intelligence and Statistics, 2018.

References II



- [13] A. Kupcsik, M. P. Deisenroth, J. Peters, L. A. Poha, P. Vadakkepata, and G. Neumann. Model-based Contextual Policy Search for Data-Efficient Generalization of Robot Skills. Artificial Intelligence, 2017.
- [14] T. X. Nghiem and C. N. Jones. Data-driven Demand Response Modeling and Control of Buildings with Gaussian Processes. In Proceedings of the American Control Conference, 2017.
- [15] J. Quiñonero-Candela, A. Girard, J. Larsen, and C. E. Rasmussen. Propagation of Uncertainty in Bayesian Kernel Models—Application to Multiple-Step Ahead Forecasting. In IEEE International Conference on Acoustics, Speech and Signal Processing, volume 2, pages 701–704, Apr. 2003.
- [16] C. E. Rasmussen and C. K. I. Williams. Gaussian Processes for Machine Learning. The MIT Press, 2006.
- [17] S. Sæmundsson, K. Hofmann, and M. P. Deisenroth. Meta Reinforcement Learning with Latent Variable Gaussian Processes. In Proceedings of the Conference on Uncertainty in Artificial Intelligence, 2018.
- [18] Y. Sui, A. Gotovos, J. W. Burdick, and A. Krause. Safe Exploration for Optimization with Gaussian Processes. In Proceedings of the International Conference on Machine Learning, 2015.
- [19] M. K. Titsias. Variational Learning of Inducing Variables in Sparse Gaussian Processes. In Proceedings of the International Conference on Artificial Intelligence and Statistics, 2009.

Controller Parametrization



■ Controller:

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

where σ is a squashing function.

Controller Parametrization



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$$\tilde{\pi}(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{k=1}^{K} w_k \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_k)^{\top} \boldsymbol{\Lambda}(\boldsymbol{x} - \boldsymbol{\mu}_k)\right)$$
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where σ is a squashing function.

■ Parameters:

$$\boldsymbol{\theta} := \{w_k, \boldsymbol{\mu}_k, \boldsymbol{\Lambda}\}$$

Controller Parametrization



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■ Parameters:

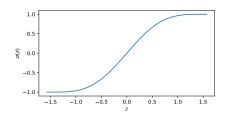
$$\boldsymbol{\theta} := \{w_k, \boldsymbol{\mu}_k, \boldsymbol{\Lambda}\}$$

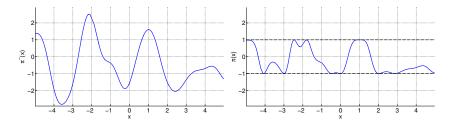
■ Squashing function:

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

Squashing Function



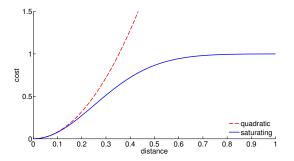




Cost Functions



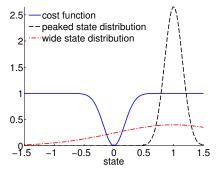
- Quadratic cost $c(\mathbf{x}) = (\mathbf{x} \mathbf{x}_{\text{target}})^{\top} \mathbf{W} (\mathbf{x} \mathbf{x}_{\text{target}})$
- Saturating cost $c(\boldsymbol{x}) = 1 \exp\left(-(\boldsymbol{x} \boldsymbol{x}_{\text{target}})^{\top} \boldsymbol{W} (\boldsymbol{x} \boldsymbol{x}_{\text{target}})\right)$



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



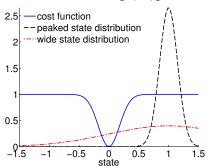
Task: Minimize $\mathbb{E}[c(\boldsymbol{x}_t)]$

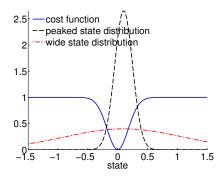


■ In the early stages of learning, state predictions are expected to be far away from the target



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

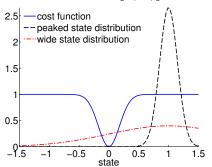


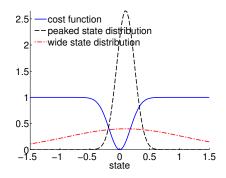


■ In the early stages of learning, state predictions are expected to be far away from the target ➤ Exploration favored



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

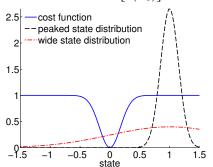


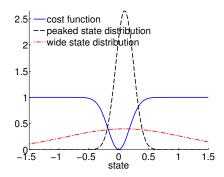


- In the early stages of learning, state predictions are expected to be far away from the target ➤ Exploration favored
- In the final stages of learning, state predictions are expected to be close to the target



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

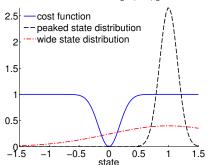


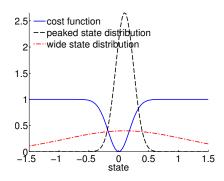


- In the early stages of learning, state predictions are expected to be far away from the target ➤ Exploration favored
- In the final stages of learning, state predictions are expected to be close to the target ➤ Exploitation favored



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





- 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



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

■ Compute $\mathbb{E}[f(x_*)]$



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

■ Compute $\mathbb{E}[f(x_*)]$

$$\mathbb{E}_{f,\boldsymbol{x}_*}[f(\boldsymbol{x}_*)] = \mathbb{E}_{\boldsymbol{x}}\big[\mathbb{E}_f[f(\boldsymbol{x}_*)|\boldsymbol{x}_*]\big] = \mathbb{E}_{\boldsymbol{x}_*}\big[\frac{m_f(\boldsymbol{x}_*)}{m_f(\boldsymbol{x}_*)}\big]$$



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

■ Compute $\mathbb{E}[f(x_*)]$

$$\mathbb{E}_{f,\boldsymbol{x}_*}[f(\boldsymbol{x}_*)] = \mathbb{E}_{\boldsymbol{x}}[\mathbb{E}_f[f(\boldsymbol{x}_*)|\boldsymbol{x}_*]] = \mathbb{E}_{\boldsymbol{x}_*}[m_f(\boldsymbol{x}_*)]$$
$$= \mathbb{E}_{\boldsymbol{x}_*}[k(\boldsymbol{x}_*,\boldsymbol{X})(\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1}\boldsymbol{y}]$$



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

lacksquare Compute $\mathbb{E}[f(\boldsymbol{x}_*)]$

$$\begin{split} \mathbb{E}_{f, \boldsymbol{x}_*}[f(\boldsymbol{x}_*)] &= \mathbb{E}_{\boldsymbol{x}} \Big[\mathbb{E}_{f} [f(\boldsymbol{x}_*) | \boldsymbol{x}_*] \Big] = \mathbb{E}_{\boldsymbol{x}_*} [m_f(\boldsymbol{x}_*)] \\ &= \mathbb{E}_{\boldsymbol{x}_*} \Big[k(\boldsymbol{x}_*, \boldsymbol{X}) (\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1} \boldsymbol{y} \Big] \\ &= \boldsymbol{\beta}^\top \int k(\boldsymbol{X}, \boldsymbol{x}_*) \mathcal{N} \big(\boldsymbol{x}_* \, | \, \boldsymbol{\mu}, \, \boldsymbol{\Sigma} \big) d\boldsymbol{x}_* \\ \boldsymbol{\beta} &:= (\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1} \boldsymbol{y} \quad \text{\ref{eq:proposition}} \quad \text{independent of } \boldsymbol{x}_* \end{split}$$



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

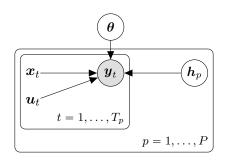
■ Compute $\mathbb{E}[f(\boldsymbol{x}_*)]$

$$\begin{split} \mathbb{E}_{f, \boldsymbol{x}_*}[f(\boldsymbol{x}_*)] &= \mathbb{E}_{\boldsymbol{x}} \left[\frac{\mathbb{E}_{f}[f(\boldsymbol{x}_*) | \boldsymbol{x}_*]}{\|\boldsymbol{x}_*\|} \right] = \mathbb{E}_{\boldsymbol{x}_*} \left[\frac{m_f(\boldsymbol{x}_*)}{\|\boldsymbol{x}_*\|} \right] \\ &= \mathbb{E}_{\boldsymbol{x}_*} \left[\frac{k(\boldsymbol{x}_*, \boldsymbol{X}) (\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1} \boldsymbol{y}}{\|\boldsymbol{y}\|} \right] \\ &= \boldsymbol{\beta}^\top \int k(\boldsymbol{X}, \boldsymbol{x}_*) \mathcal{N} \big(\boldsymbol{x}_* \, | \, \boldsymbol{\mu}, \, \boldsymbol{\Sigma} \big) d\boldsymbol{x}_* \\ \boldsymbol{\beta} &:= (\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1} \boldsymbol{y} \quad \text{\ref{eq:proposition}} \quad \text{\ref{eq:proposition}} \quad \boldsymbol{\alpha}_* \end{split}$$

- If k is a Gaussian (squared exponential) kernel, this integral can be solved analytically
- Variance of $f(x_*)$ can be computed similarly

Meta Learning Model

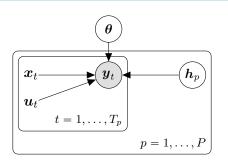




$$f(\cdot) \sim GP$$

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





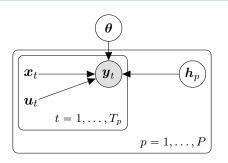
$$f(\cdot) \sim GP$$

$$p(\boldsymbol{H}) = \prod_{p} p(\boldsymbol{h}_{p}), \quad p(\boldsymbol{h}_{p}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

$$p(\boldsymbol{Y}, \boldsymbol{H}, \boldsymbol{f}(\cdot)|\boldsymbol{X}, \boldsymbol{U}) = \prod_{p=1}^{P} p(\boldsymbol{h}_{p}) \prod_{t=1}^{T_{p}} p(\boldsymbol{y}_{t}|\boldsymbol{x}_{t}, \boldsymbol{u}_{t}, \boldsymbol{h}_{p}, \boldsymbol{f}(\cdot)) p(\boldsymbol{f}(\cdot))$$

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

Variational Inference in Meta Learning Model



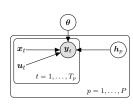
Mean-field variational family:

$$\begin{split} q(\boldsymbol{f}(\cdot), \boldsymbol{H}) &= q(\boldsymbol{f}(\cdot))q(\boldsymbol{H}) \\ q(\boldsymbol{H}) &= \prod_{p=1}^{P} \mathcal{N}(\boldsymbol{h}_{p}|\boldsymbol{n}_{p}, \boldsymbol{T}_{p}) \,, \\ q(\boldsymbol{f}(\cdot)) &= \int p(\boldsymbol{f}(\cdot)|\boldsymbol{f}_{Z})q(\boldsymbol{f}_{Z})d\boldsymbol{f}_{Z} \quad \Longrightarrow \text{SV-GP (Titsias, 2009)} \end{split}$$

Evidence Lower Bound



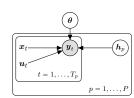
$$ELBO = \mathbb{E}_{q(\boldsymbol{f}(\cdot),\boldsymbol{H})} \Big[\log \frac{p(\boldsymbol{Y},\boldsymbol{H},\boldsymbol{f}(\cdot)|\boldsymbol{X},\boldsymbol{U})}{q(\boldsymbol{f}(\cdot),\boldsymbol{H})} \Big]$$



Evidence Lower Bound



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



Evidence Lower Bound



$$\begin{split} ELBO &= \mathbb{E}_{q(\boldsymbol{f}(\cdot),\boldsymbol{H})} \Big[\log \frac{p(\boldsymbol{Y},\boldsymbol{H},\boldsymbol{f}(\cdot)|\boldsymbol{X},\boldsymbol{U})}{q(\boldsymbol{f}(\cdot),\boldsymbol{H})} \Big] \\ &= \sum_{p=1}^{P} \sum_{t=1}^{T_p} \mathbb{E}_{q(\boldsymbol{f}_t|\boldsymbol{x}_t,\boldsymbol{u}_t,\boldsymbol{h}_p)q(\boldsymbol{h}_p)} \Big[\log p(\boldsymbol{y}_t|\boldsymbol{f}_t) \Big] \\ &- \mathrm{KL}(q(\boldsymbol{H})||p(\boldsymbol{H})) - \frac{\mathrm{KL}(q(\boldsymbol{f}(\cdot))||p(\boldsymbol{f}(\cdot)))}{\mathrm{Monte Carlo \ estimate}} \\ &= \sum_{p=1}^{P} \sum_{t=1}^{T_p} \widehat{\mathbb{E}}_{q(\boldsymbol{f}_t|\boldsymbol{x}_t,\boldsymbol{u}_t,\boldsymbol{h}_p)q(\boldsymbol{h}_p)} \Big[\log p(\boldsymbol{y}_t|\boldsymbol{f}_t) \Big] \\ &- \mathrm{KL}(q(\boldsymbol{H})||p(\boldsymbol{H})) - \frac{\mathrm{KL}(q(\boldsymbol{F}_Z)||p(\boldsymbol{F}_Z))}{\mathrm{KL}(q(\boldsymbol{F}_Z)||p(\boldsymbol{F}_Z))} \end{split}$$

closed-form solution

