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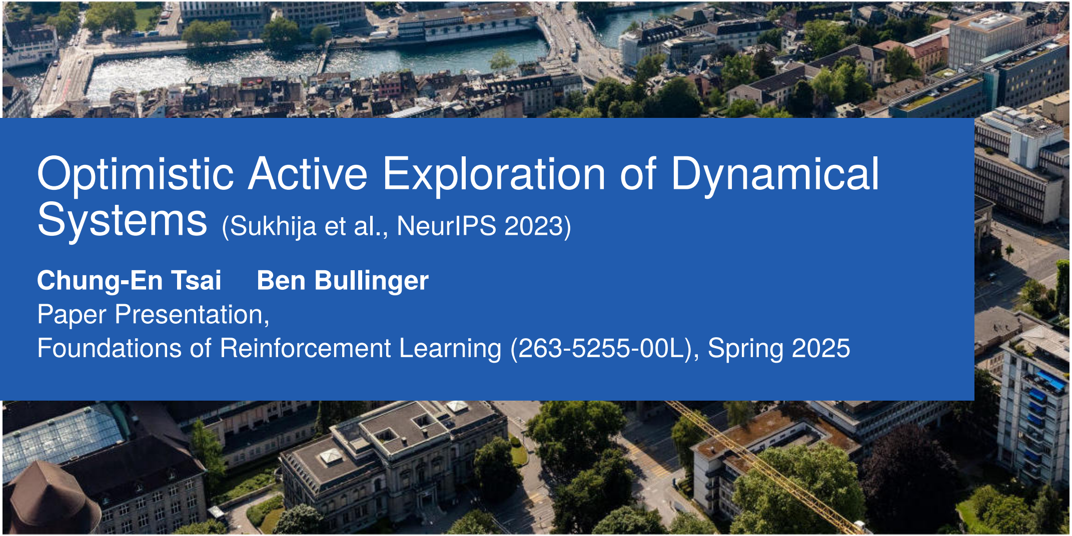
Department of Computer Science



Optimistic Active Exploration of Dynamical Systems (Sukhija et al., NeurIPS 2023)

Chung-En Tsai **Ben Bullinger**

Paper Presentation,
Foundations of Reinforcement Learning (263-5255-00L), Spring 2025

Outline

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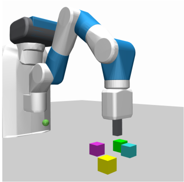
Motivation: Beyond Task-Specific Models



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- Learn a model for one specific reward
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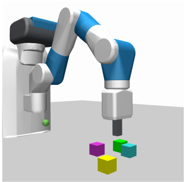

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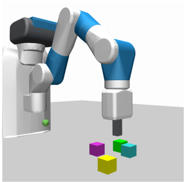

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Can we ***efficiently*** *learn accurate models that generalize to* ***any*** *downstream task?*

Outline

Problem Formulation (1/2)

Given an unknown discrete-time dynamical system $\boldsymbol{f}^\star : \mathcal{S} \times \mathcal{A} \to \mathcal{S} \subseteq \mathbb{R}^d$:

$$\boldsymbol{s}_{t+1} = \boldsymbol{f}^\star(\boldsymbol{s}_t, \boldsymbol{a}_t) + \boldsymbol{w}_t, \quad \boldsymbol{w}_t \sim \mathcal{N}(0, I).$$

Goal: Design algorithms for learning $\hat{\boldsymbol{f}} \approx \boldsymbol{f}^\star$ in episodic setting that is good for any reward functions.

Introduction video by Bhavya Sukhija. NeurIPS 2023.

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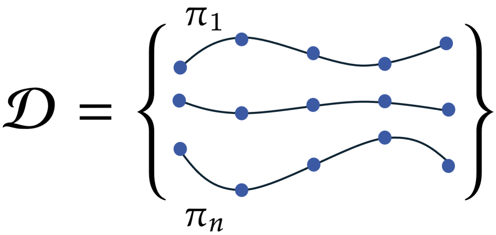

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Our problem can be divided into two parts:

- Exploration (our focus!): Collecting data by executing policies.
- Estimation: Building model from data.

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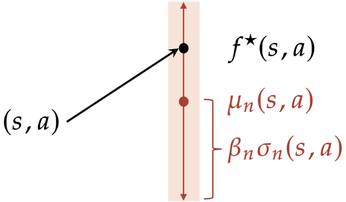
Well-Calibration Assumption

Given n data, we can construct confidence intervals:

$$|\boldsymbol{f}_i^\star(\boldsymbol{s}, \boldsymbol{a}) - \boldsymbol{\mu}_{n,i}(\boldsymbol{s}, \boldsymbol{a})| \leqslant \beta_n \boldsymbol{\sigma}_{n,i}(\boldsymbol{s}, \boldsymbol{a}) \quad \forall i \in [d], \text{ w.h.p.,}$$



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Related Work: Active Learning

	Bandit Optimization	Our Problem
Goal	$\max_x f^\star(x)$	Find $\hat{f} \approx f^\star$
$f^\star$	Objective	Dynamics
State space	No	Continuous
Planning	No	Yes

N. Srinivas et al. "Gaussian process optimization in the bandit setting: No regret and experimental design." ICML 2010. (The 1st presentation today!)

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Technique	Optimism in the face of uncertainty	

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Related Work: Maximum Entropy RL

What about collecting data by maximum entropy or entropy-regularized RL?

$$\max_{\boldsymbol{\pi}} \mathsf{H}\left(d_{\mu}^{\boldsymbol{\pi}}\right), \quad \max_{\boldsymbol{\pi}} \mathsf{E}\left[\sum_{t=0}^{\infty} \gamma^{t}\left(r(\boldsymbol{s}_t, \boldsymbol{a}_t) - \beta \log \pi(\boldsymbol{a}_t|\boldsymbol{s}_t)\right) \middle| \boldsymbol{s}_0 \sim \mu, \boldsymbol{\pi}\right].$$

- No guarantee for arbitrary reward functions in downstream tasks.

E. Hazan et al. "Provably efficient maximum entropy exploration." ICML 2019. (Previous presentation.)
B. Eysenbach and S. Levine. "Maximum entropy RL (provably) solves some robust RL problems." ICLR 2022.

Related Work: Reward-Free RL

- Study this problem in tabular settings or impose structural assumptions on values function and transitions.
- No practical algorithms.

C. Jin et al. "Reward-free exploration for reinforcement learning." ICML 2020.
R. Wang et al. "On reward-free reinforcement learning with linear function approximation." NeurIPS 2020.
J. Chen et al. "On the statistical efficiency of reward-free exploration in non-linear RL." NeurIPS 2022.

Contributions

- Propose OpAX, a practical algorithm for learning non-linear dynamics with continuous state-action spaces and without structural assumptions.
- In this setting, OpAX is the first algorithm to have a theoretical guarantee for a rich family of nonlinear dynamics.

Outline

OpAX: Overview

*Learn dynamics by **maximizing information gain**, not rewards*

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	Traditional Model-Based RL	OpAX
Objective	$\max_\pi \mathbb{E}[R(\pi)]$	$\max_\pi I(f^*; \mathcal{D})$
Exploration	Reward-driven	Uncertainty-driven
Convergence to $f^\star$	No guarantees	$\boldsymbol{\sigma}_n(\boldsymbol{s}, \boldsymbol{a}) \to 0$ (GP)
Generalization	No guarantees	Zero-shot (GP)

OpAX (1/4): Information-Theoretic Objective

Ideal Goal: Maximize mutual information between dynamics $\boldsymbol{f}^{\star}$ and collected data

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Greedy Episodic Approximation: At episode n, choose policy maximizing expected information gain:

$$\boldsymbol{\pi}_n^* = \underset{\boldsymbol{\pi} \in \Pi}{\arg\max}\, \mathsf{E}_{\tau^{\boldsymbol{\pi}}} \left[\mathrm{I}\left(\boldsymbol{f}^\star_{\tau^{\boldsymbol{\pi}}} ; \tau^{\boldsymbol{\pi}} \mid \mathcal{D}_{1:n-1} \right) \right]$$

where:

- $\boldsymbol{f}^\star_{\tau^{\boldsymbol{\pi}}} = (\boldsymbol{f}^\star(\boldsymbol{s}_0, \boldsymbol{a}_0), \ldots, \boldsymbol{f}^\star(\boldsymbol{s}_{T-1}, \boldsymbol{a}_{T-1}))$: true dynamics along trajectory
- $\mathcal{D}_{1:n-1}$: data from previous episodes

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Challenge

This objective is intractable in general. Need tractable approximation.

OpAX (2/4): Tractable Upper Bound

Lemma (Information Gain Upper Bound)

For Gaussian noise $\boldsymbol{w}_t \sim \mathcal{N}(0, I)$ *and epistemic uncertainty* $\boldsymbol{\sigma}_{n-1}$*:*

$$I\left(\boldsymbol{f}^{\star}_{\boldsymbol{\tau}^{\pi}}; \boldsymbol{\tau}^{\pi} \mid \mathcal{D}_{1:n-1}\right) \leqslant \frac{1}{2} \sum_{t=0}^{T-1} \sum_{j=1}^{d} \log\left(1 + \boldsymbol{\sigma}^2_{n-1,j}(\boldsymbol{s}_t, \boldsymbol{a}_t)\right)$$

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Tractable Exploration Objective: Maximize the upper bound

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Collect data where model is most uncertain $\Rightarrow$ maximal information gain

OpAX (3/4): Hallucination Policy

Problem: The planning objective requires knowing $\boldsymbol{f}^{\star}$, but $\boldsymbol{f}^{\star}$ is unknown!

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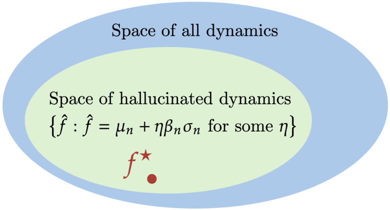
OpAX Solution:

Optimism in the face of uncertainty

Use a **hallucination policy** $\boldsymbol{\eta}$ to select optimistic dynamics

$$\hat{\boldsymbol{f}}_j(\boldsymbol{s}, \boldsymbol{a}) = \boldsymbol{\mu}_{n-1,j}(\boldsymbol{s}, \boldsymbol{a}) + \beta_{n-1}\boldsymbol{\sigma}_{n-1,j}(\boldsymbol{s}, \boldsymbol{a}) \cdot \boldsymbol{\eta}_j(\boldsymbol{s})$$

where $\boldsymbol{\eta} : \mathcal{S} \to [-1, 1]^d$.



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OpAX (4/4): Optimistic Planning

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subject to:

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where $\Xi = \{\boldsymbol{\eta} : \mathcal{S} \to [-1, 1]^d\}$ is the space of **hallucination policies**.

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Implementation

Solve as optimal control with extended action space $(\boldsymbol{\pi}, \boldsymbol{\eta})$.

Algorithm

OpAX: Optimistic Active Exploration

Init: Statistical model $(\boldsymbol{\mu}_0, \boldsymbol{\sigma}_0, \beta_0)$

for episode $n = 1, \ldots, N$ **do**

$$\boldsymbol{\pi}_n = \arg\max_{\pi \in \Pi} \max_{\eta \in \Xi} \mathbb{E}\left[\sum_{t=0}^{T-1} \sum_{j=1}^{d} \log\left(1 + \boldsymbol{\sigma}^2_{n-1,j}(\boldsymbol{s}_t, \boldsymbol{a}_t)\right)\right]$$ ➤ Prepare policy

$\mathcal{D}_n \leftarrow \textsc{Rollout}(\boldsymbol{\pi}_n)$ ➤ Measure

Update $(\boldsymbol{\mu}_n, \boldsymbol{\sigma}_n, \beta_n) \leftarrow \mathcal{D}_{1:n}$ ➤ Update model

end for

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Key Components:

- **Information reward**: $\log(1 + \boldsymbol{\sigma}^2)$
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Implementation:

- MPC for short horizons
- SAC for long horizons

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Assumptions

Regularity of the Dynamics

$f^\star$ lies in a RKHS with kernel k and $\|f^\star\| \leqslant 1$.

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Lemma

GP$(0, k)$ *is well-calibrated.*

Recall

$$\gamma_n(k) = \max_{\mathcal{D}_1, \dots, \mathcal{D}_n} \log\det(I + K_n).$$

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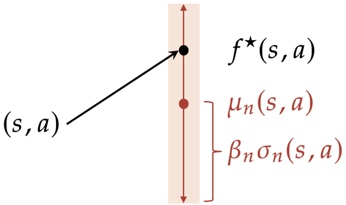
Main Guarantee

Theorem (Informal)

With high probability,

$$\max_{\pi} \mathbb{E}_{\pi}\left[\underbrace{\max_{t} \|\boldsymbol{\sigma}_n(\boldsymbol{s}_t, \boldsymbol{a}_t)\|_2^2}_{\text{maximum uncertainty along the trajectory}}\right] \leqslant \textit{poly}(T) \cdot \frac{\gamma_n(k)}{\sqrt{n}}, \quad \forall n \in \mathbb{N}.$$



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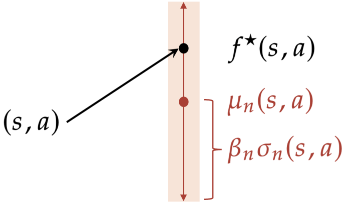


For linear and RBF kernels, $\gamma_n \approx \mathrm{polylog}(nT)$ and $\lim_{n\to\infty} \boldsymbol{\sigma}_n(s,a) \to 0$.

Zero-Shot Performance

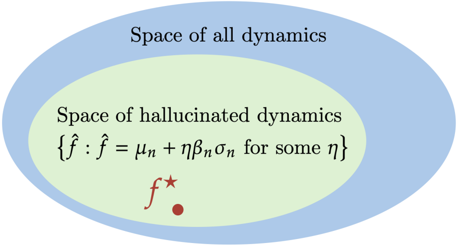
Theorem (Informal)

Consider an RL problem with a known bounded reward:

$$\arg\max_{\pi} R(\pi), \quad \boldsymbol{s}_{t+1} = \boldsymbol{f}^{\star}(\boldsymbol{s}_t, \boldsymbol{a}_t) + \boldsymbol{w}_t.$$

If $n \gtrsim \text{poly}(d, T, \varepsilon^{-1}, \gamma_n(k))$*, then* $\hat{\pi}$ *is* ε*-optimal, where*

$$\hat{\pi} \in \arg\max_{\boldsymbol{\pi}} \min_{\boldsymbol{\eta}} R(\boldsymbol{\pi}, \boldsymbol{\eta}), \quad \boldsymbol{s}_{t+1} = \boldsymbol{\mu}_n(\boldsymbol{s}_t, \boldsymbol{a}_t) + \boldsymbol{\eta}(s_t)\beta_n \boldsymbol{\sigma}_n(s_t, a_t) + \boldsymbol{w}_t.$$



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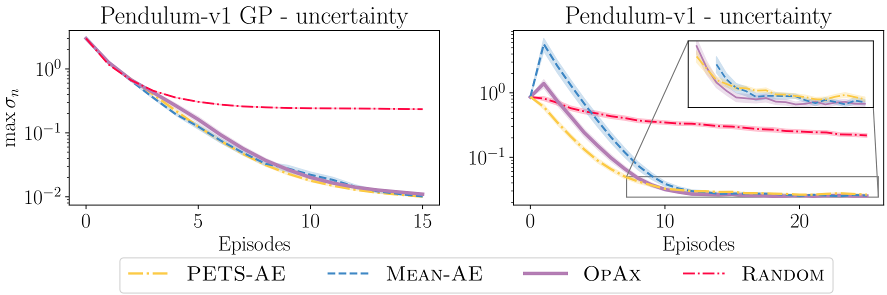
Experiments: Epistemic Uncertainty Reduction



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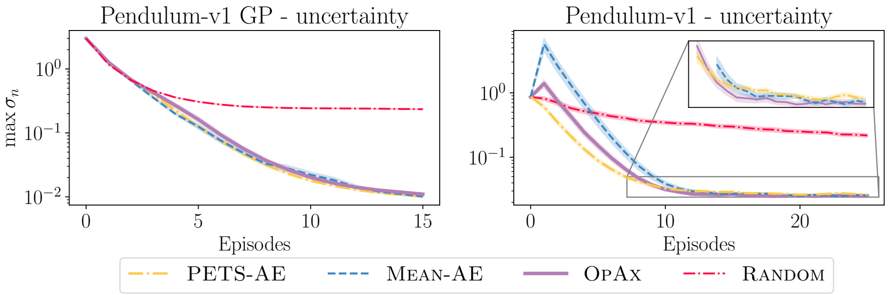

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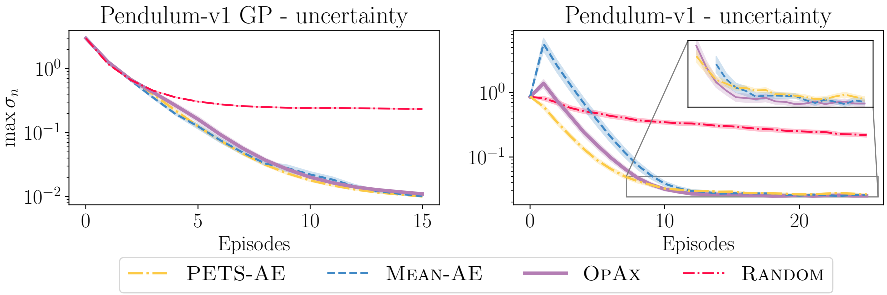

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Experiments validate theoretical results

Experiments: Downstream Tasks

- `OpAX` performs **on par** with `H-UCRL`[1] on trained tasks
- `OpAX` **outperforms** `H-UCRL` on some unseen tasks

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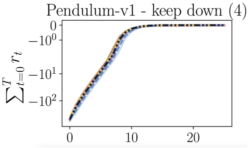

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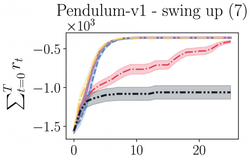

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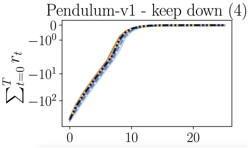

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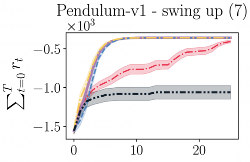

(b) Zero-shot task

Zero-shot swing up task:

(play)

(c) `H-UCRL`

(play)

(d) `OpAx`

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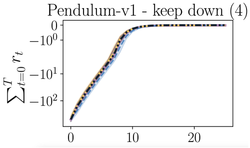
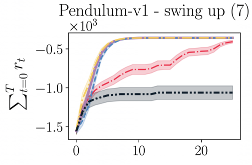
- `OpAX` performs **on par** with `H-UCRL`[1] on trained tasks
- `OpAX` **outperforms** `H-UCRL` on some unseen tasks

Evaluation (■: `H-UCRL`, ■: `OpAX`, ■: Random):



(a) Trained task



(b) Zero-shot task

Zero-shot swing up task:

(play)

(c) `H-UCRL`

(play)

(d) `OpAx`

More experiments in the paper.

[1] S. Curi et al. "Efficient model-based reinforcement learning through optimistic policy search and planning." NeurIPS 2020.

Outline

Conclusions

	Traditional Model-Based RL	**OpAX**
Objective	$\max_\pi \mathrm{E}[R(\pi)]$	$\max_\pi I(f^*; \mathcal{D})$
Exploration	Reward-driven	Uncertainty-driven
Convergence to $f^\star$	No guarantees	$\boldsymbol{\sigma}_n(\boldsymbol{s}, \boldsymbol{a}) \to 0$ (GP)
Generalization	No guarantees	Zero-shot (GP)

OpAX

Combines **active learning** with RL and achieves theoretical guarantees for learning many continuous nonlinear systems.

Open Challenges and Future Work

Key Limitations:

- **Computational cost:** Solving (π_n, η_n) is expensive
- **Model requirements:** Needs well-calibrated uncertainty
- **Known noise:** Guarantees only hold for (sub-)Gaussian noise.

Promising Directions:

- **Robust models:** Handle model misspecification
- **Beyond MDPs:** POMDPs, continuous time
- **Practical deployment:** Real-world robotics