Safe control parameter tuning with Bayesian optimization

Research talk

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March 25, 2025

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Motivational example

Introduction

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Optimize control parameters of safety-critical real-world systems.

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- Unknown reward function *f*: $\mathcal{A} \to \mathbb{R}$
- Control policy parameters $a \in \mathcal{A}$
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Solvable using classic reinforcement learning (RL)?

Classic RL struggles with both sample efficiency and safety guarantees.

Gaussian process (GP) regression

- GPs to model unknown reward function f from samples
- GP characterized by **kernel** k: **Mean prediction** μ_t, **standard deviation** σ_t

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GP confidence intervals

$|f(a) - \mu_t(a)| \leq (B + \text{"data-term"})\, \sigma_t(a)$

Safe Bayesian optimization (BO) with GPs

Control policy optimization problem

$\max_{a \in \mathcal{A}} f(a) \quad \text{subject to } f(a) \geq h$

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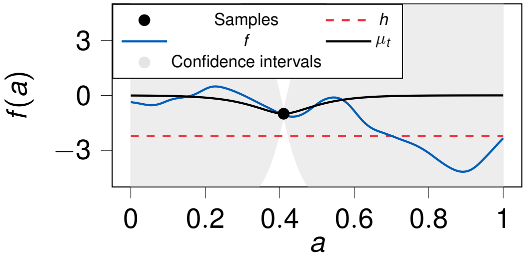

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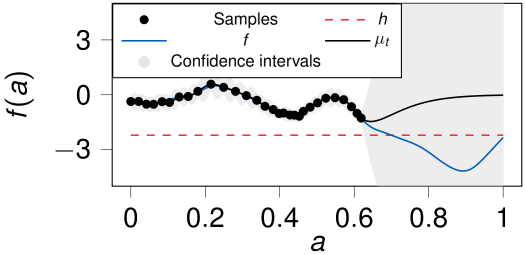

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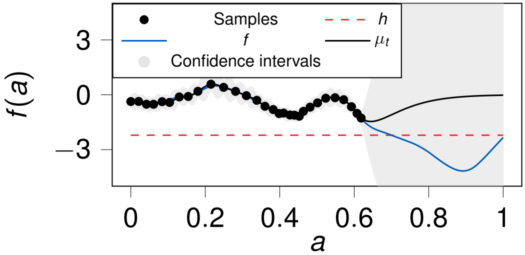

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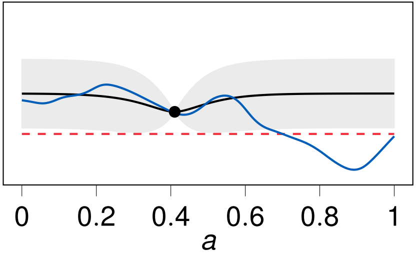

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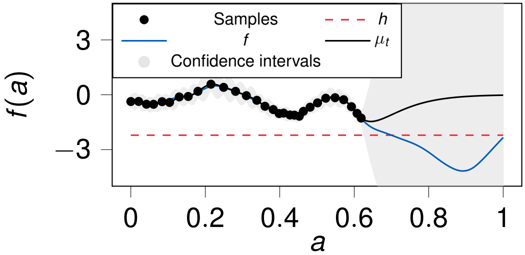

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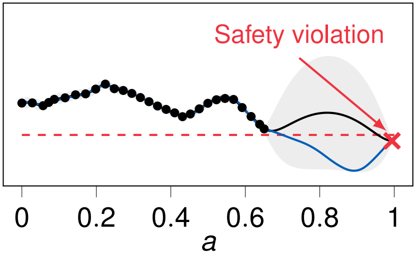

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RKHS norm assumption in safe BO

Regularity assumption

Most safe BO algorithms require an upper bound B on the RKHS norm ($B \geq \|f\|_k$) a priori.

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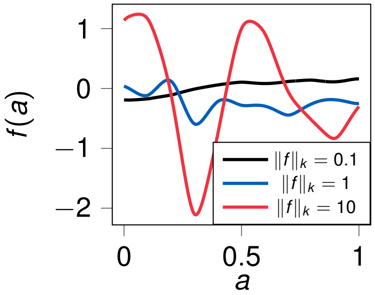

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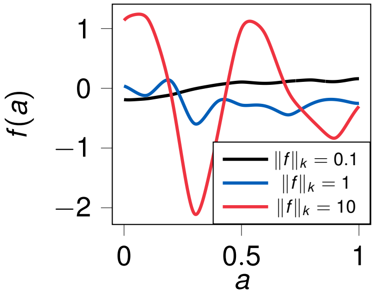

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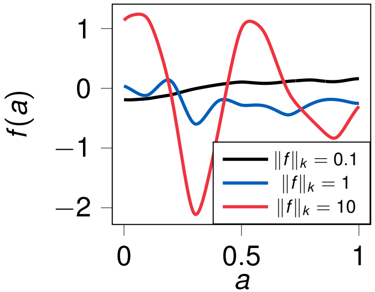

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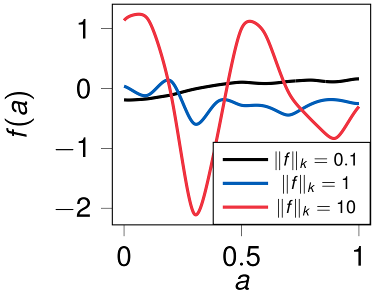

Problem definition

Develop a safe BO algorithm that over-estimates the RKHS norm $\|f\|_k$ with statistical guarantees.

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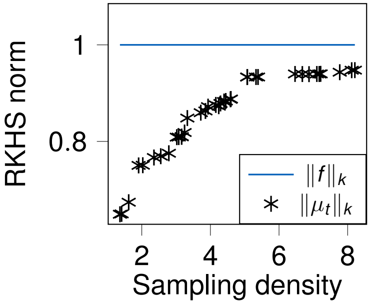
Predicting RKHS norms

- Increasing sampling density: $\mu_t \to f$ and $\|\mu_t\|_k \to \|f\|_k$ **from below**



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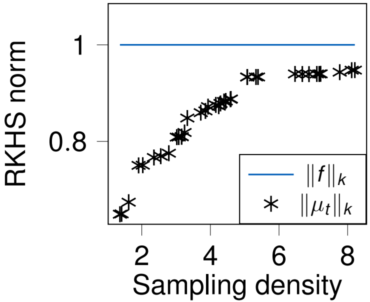

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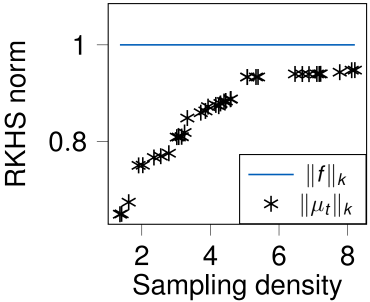
- **Training data** from toy examples
- Extrapolation: RNNs to exploit **sequential** nature of inputs



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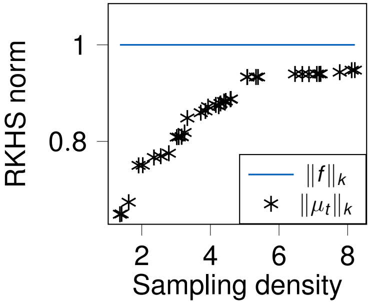
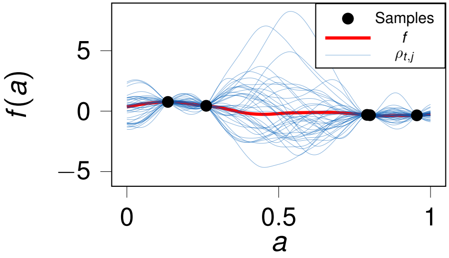


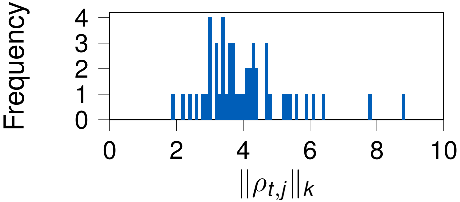
Theoretical guarantees instead of only heuristics

How do we get theoretical guarantees on the RKHS norm over-estimation?

Random RKHS functions

- Compute random RKHS functions $\rho_{t,j},\ j \in \{1, \ldots, \mathrm{m}\}$ with kernel k
- Random RKHS functions $\rho_{t,j}$ capture the behavior of reward function f





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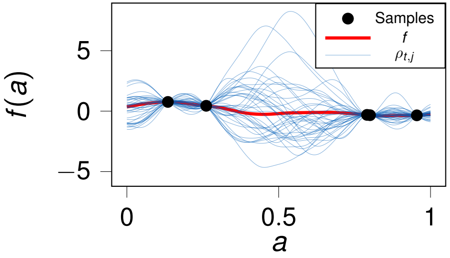

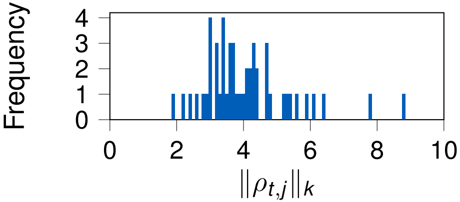

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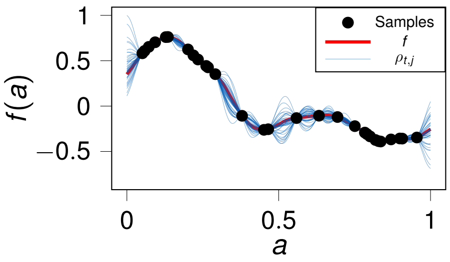

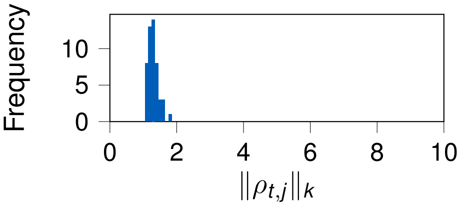

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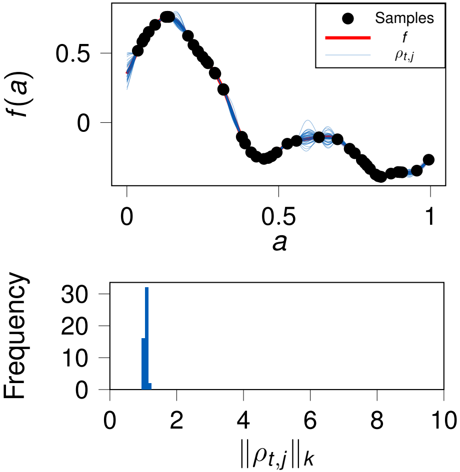

Statistical guarantees

Regularity assumptions

- Reward function f is a member of the RKHS of kernel k
- $\|f\|_k \leq \lim_{s\to\infty} \frac{1}{s} \sum_{j=1}^{s} \|\rho_{t,j}\|_k$

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Proof sketch

- $B_t \leftarrow \max\{\text{RNN prediction}, \frac{1}{m} \sum_{j=1}^{m} \|\rho_{t,j}\|_k + \text{“safety-term”}\}$
- Statistical guarantees through Hoeffding’s inequality[3]

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RKHS norm over-estimation as optimization problem

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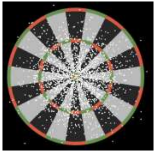

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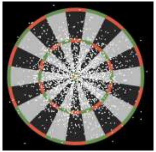
- **Analogy**: Minimum radius on darts board that contains all points
- Can we get better performance with **statistical guarantees**?



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RKHS norm over-estimation as optimization problem (2)

Chance-constrained optimization problem

Minimize $B_t \in \mathbb{R}_+$ subject to $B_t \geq \|f\|_k$ with high probability.

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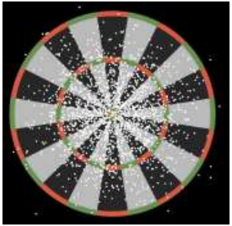

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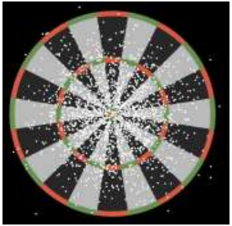

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- Some random RKHS functions might be **outliers**, i.e., $\|\rho_{t,j}\|_k \gg \|f\|_k$
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Sampling-and-discarding scenario approach

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Sampling-and-discarding scenario approach

Min. $B_t \in \mathbb{R}_+$ s.t. $B_t \geq \|\rho_{t,j}\|_k,\ j \in \{1, \ldots, m-r\} \wedge B_t < \|\rho_{t,j}\|_k,\ j \in \{m-r+1, \ldots, m\}$.

Theorem

Over-estimation of RKHS norm $B_t \geq \|f\|_k$ is PAC $\forall t \geq 1$.

Proof sketch

- Sampling-and-discarding scenario approach: $B_t \leftarrow \|\rho_{t,m-r}\|_k$
- RNN introduces lower bound: $B_t \leftarrow \max\{\text{RNN prediction}, \|\rho_{t,m-r}\|_k\}$

[5] M. C. Campi, S. Garatti, "A sampling-and-discarding approach to chance-constrained optimization: Feasibility and optimality," Springer, 2011.

Contrasting both approaches

Assumption (Scenario approach)

RKHS norms $\|\rho_{t,j}\|_k$, $j \in \{1, \dots, \mathrm{m}\}$ and $\|f\|_k$ are i.i.d. samples from the same (potentially unknown) probability space.

Assumption (Hoeffding's inequality)

$\|f\|_k \leq \lim_{s\to\infty} \frac{1}{s} \sum_{j=1}^{s} \|\rho_{t,j}\|_k$

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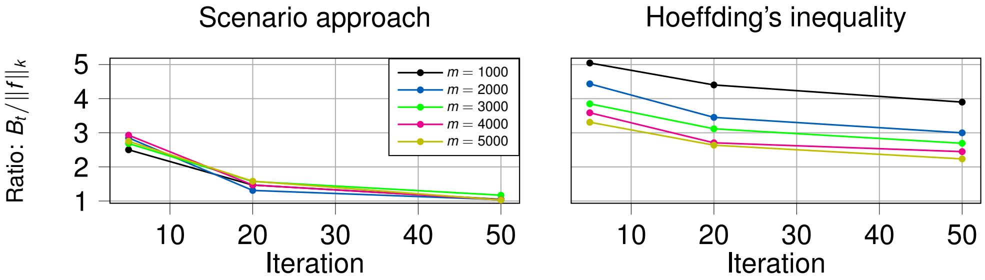

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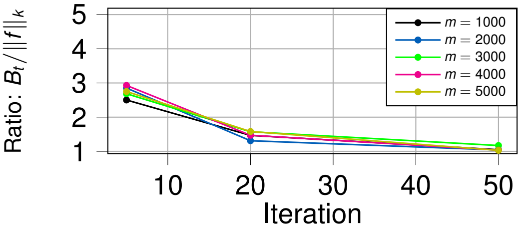
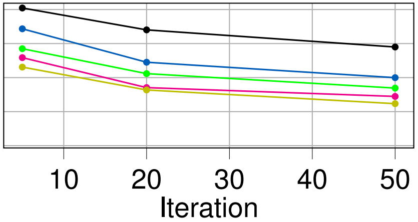
$\Rightarrow$ Hoeffding assumption **interpretability**?

Scenario approach



Hoeffding's inequality



Safe BO with RKHS norm over-estimation

Problem definition

Develop a safe BO algorithm that estimates the RKHS norm $\|f\|_k$ with guarantees.

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Theorem *(Safety)*

Safe BO algorithm with RKHS norm over-estimation ensures safety with high probability.

Proof sketch *(Safety)*

Combine safety proof of SafeOpt with RKHS norm over-estimation.

Local interpretation of the RKHS norm

- Safe exploration for optimization:
  Restricted to **sub-space** of domain

GP confidence intervals

$$|f(a) - \mu_t(a)| \leq (B_t + \text{“data-term”})\, \sigma_t(a)$$

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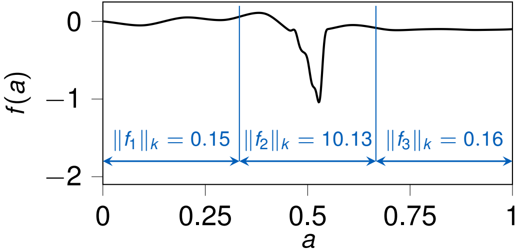

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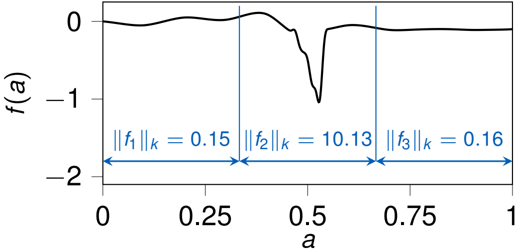
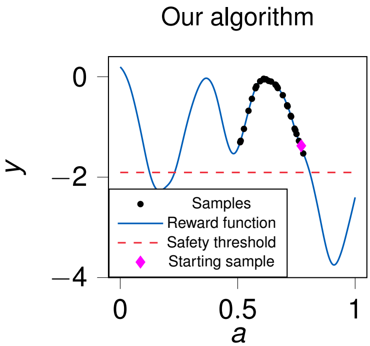
- **Adaptive** interpretation of locality: sub-domains around each sample
- **Significantly more scalable** through separate discretization in sub-domains



Numerical experiments



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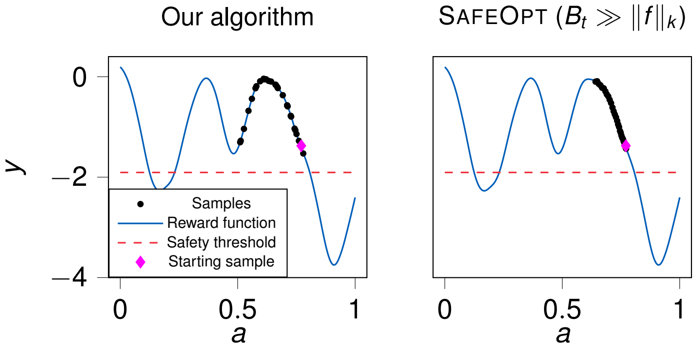

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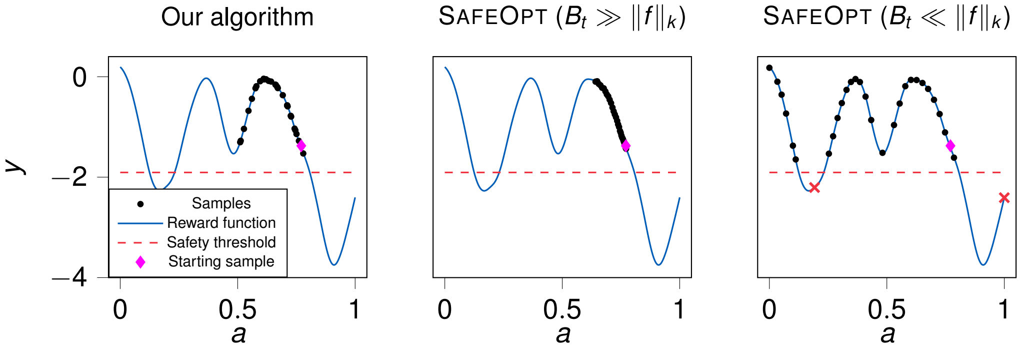

Safely fine-tuning RL policies

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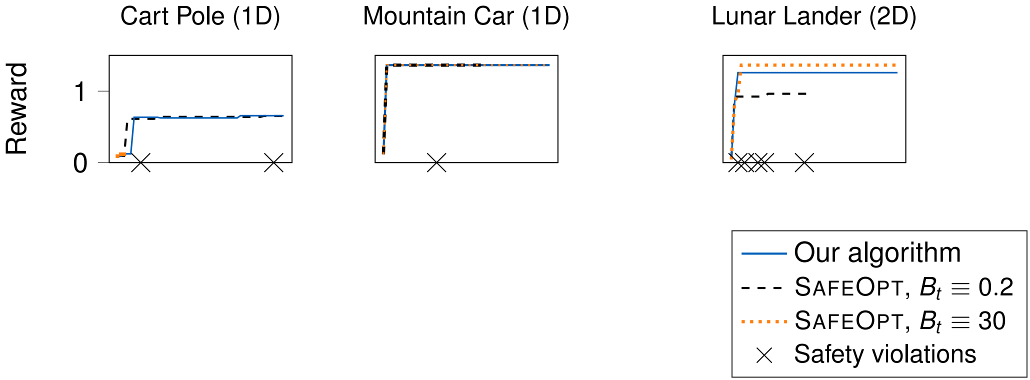

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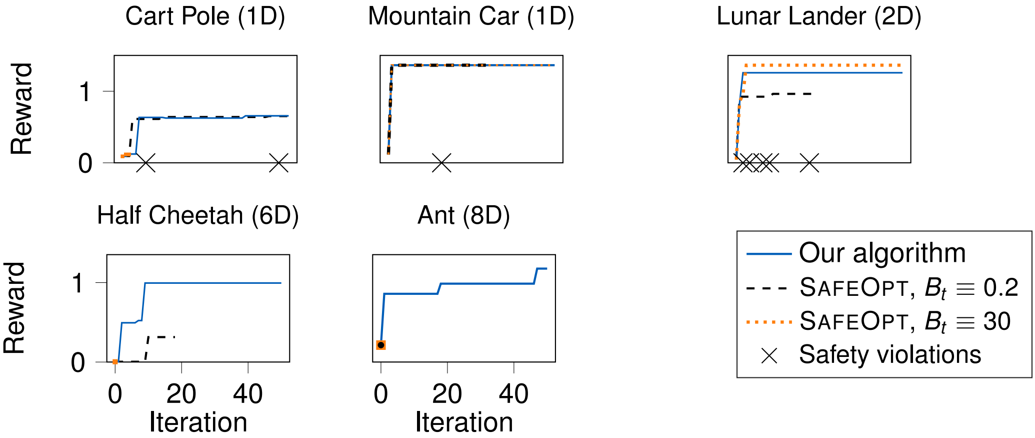

Hardware experiment

Limitations

Regularity assumption (Our approach)

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Regularity assumption (SafeOpt)

Most safe BO algorithms require an upper bound B on the RKHS norm ($B \geq \|f\|_k$) a priori.

- In contrast to SafeOpt, we systematically **integrate data, adapt bounds** and cover a **rich set of functions**

Outlook: Safe BO with scenario approach in Bayesian setting

- We used **frequentist confidence intervals**
- **Bayesian RKHS norm estimation**s with samples (scenario approach)

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- With more iterations, restrict probability space to interpolate gathered points

Outlook: Safe BO for distributed multi-agent systems (MASs)[6]

- Many safety-critical real-world problems are **distributed MASs** (e.g., factory robots)

[6] A. Tokmak, T. B. Schön, D. Baumann, "Toward safe control parameter tuning for distributed multi-agent systems," in preperation for CDC 2025.

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- Example $f \equiv f(a_1, a_2, a_3, a_4)$: If a_1 remains constant, corresponding y-value $f(a_1, a_2, a_3, a_4)$ may change, causing "discontinuities"

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Approach:

- Use **time** as a "latent" variable: static global function $f \approx$ time-varying dynamic function $f_{j,t}$
- One-step time-series prediction in the time domain to extrapolate other agents

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Conclusions

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2. Abdullah Tokmak, Kiran G. Krishnan, Thomas B. Schön, Dominik Baumann, "**Safe exploration in reproducing kernel Hilbert spaces**," accepted to AISTATS 2025.
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