



Safe exploration in reproducing kernel Hilbert spaces

Research talk

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Aalto University
School of Electrical
Engineering



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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 $f: \mathcal{A} \rightarrow \mathbb{R}$
- 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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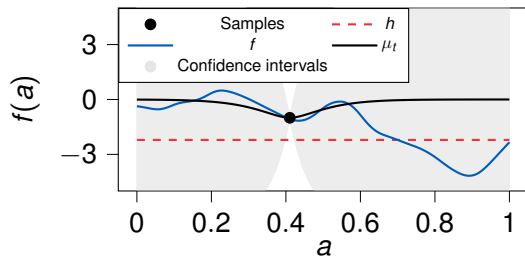
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$$\text{SAFEOPT}^1 (t = 0, B = \|f\|_k)$$



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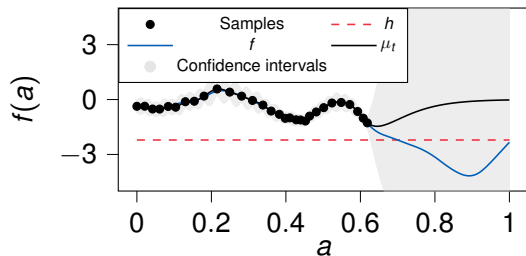
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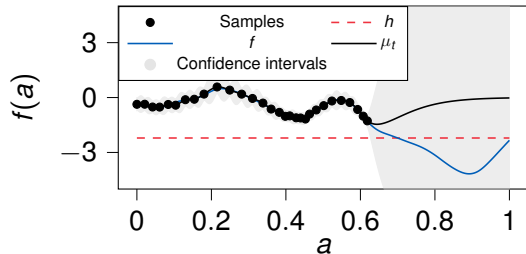
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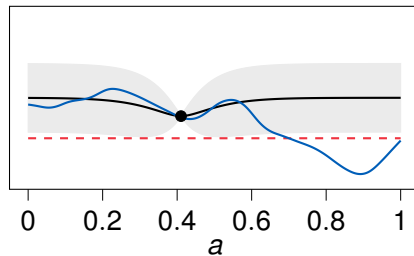
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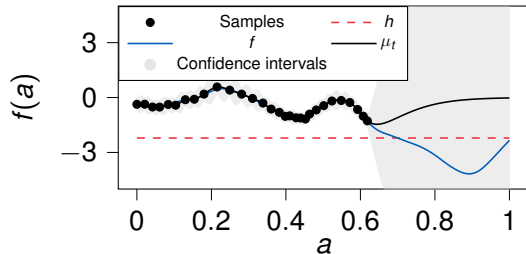
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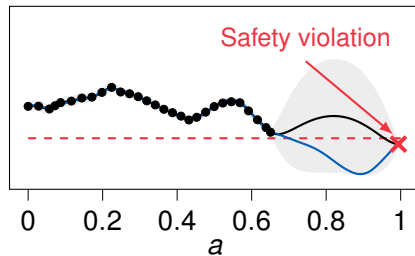
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RKHS norm assumption in safe BO

Regularity assumption

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

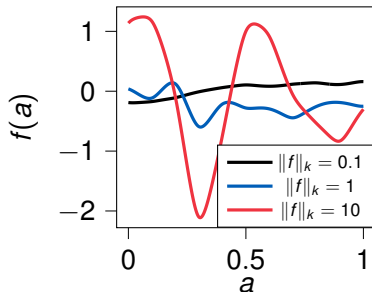
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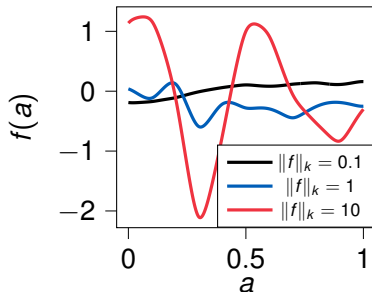
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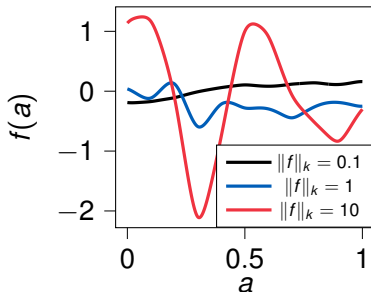
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- It is **unclear how to upper bound the RKHS norm** of unknown functions²



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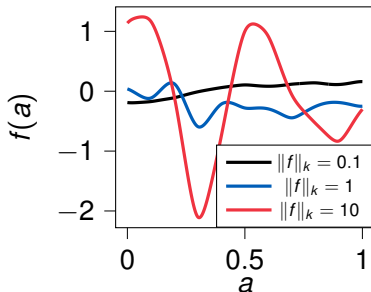
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Problem definition

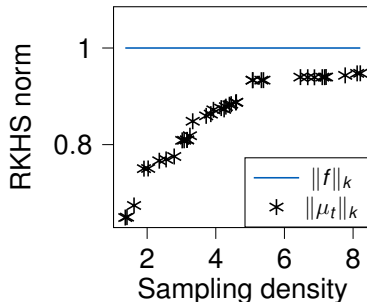
Develop a safe BO algorithm that over-estimates the RKHS norm $\|f\|_k$ with statistical guarantees.



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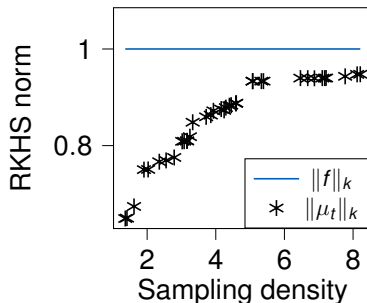
Predicting RKHS norms

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



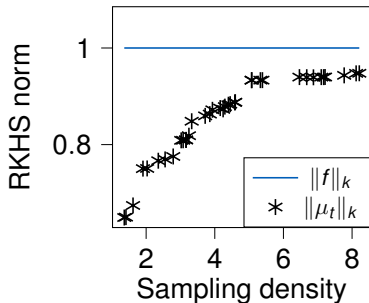
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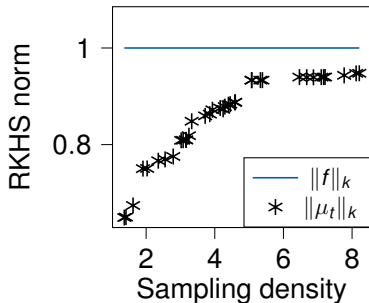
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- **Extrapolate** B_t from inputs $\|\mu_t\|_k$ and sampling density
- **Training data** from toy examples
- Extrapolation: RNNs to exploit **sequential** nature of inputs



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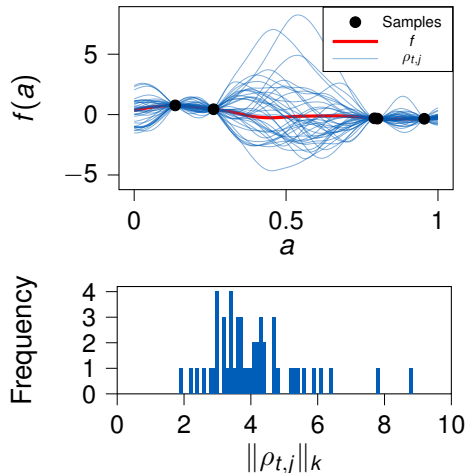


Theoretical guarantees instead of only heuristics

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

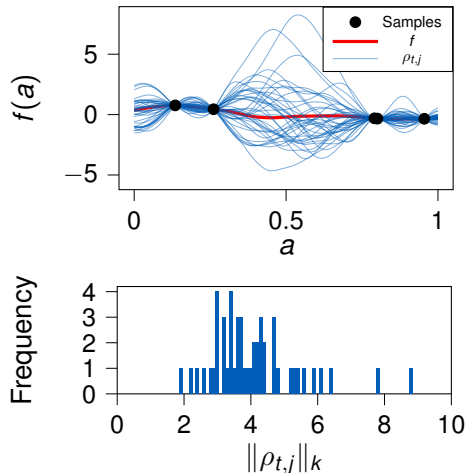
Random RKHS functions

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



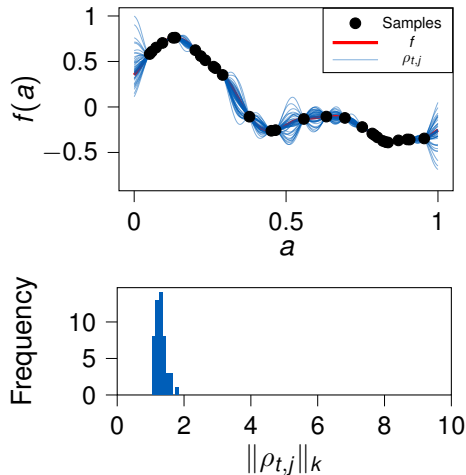
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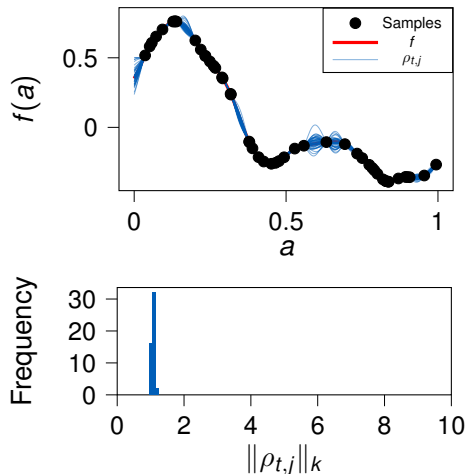
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Statistical guarantees

Regularity assumptions

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

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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 inequality³

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RKHS norm over-estimation as optimization problem

Nontrivial optimization problem

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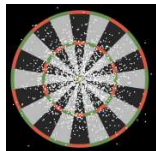
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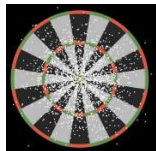
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- Can we get better performance with **statistical guarantees?**



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

- Solve chance-constrained optimization problem using scenario approach⁴ by fixing m i.i.d. scenarios
- Scenarios: random RKHS functions $\rho_{t,j}$, $j \in \{1, \dots, m\}$

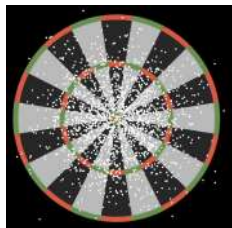
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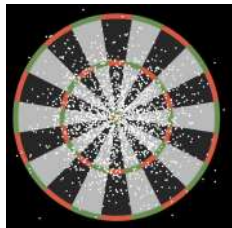
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Scenario approach

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- Some random RKHS functions might be **outliers**, i.e., $\|\rho_{t,j}\|_k \gg \|f\|_k$
- Sampling-and-discarding scenario approach:⁵ Trade **feasibility** for **performance**

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Sampling-and-discarding scenario approach

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Proof sketch

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

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Contrasting both approaches

Assumption (Scenario approach)

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

Assumption (Hoeffding's inequality)

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

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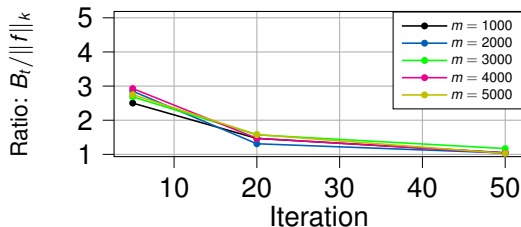
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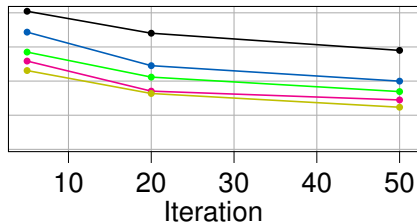
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Hoeffding's inequality



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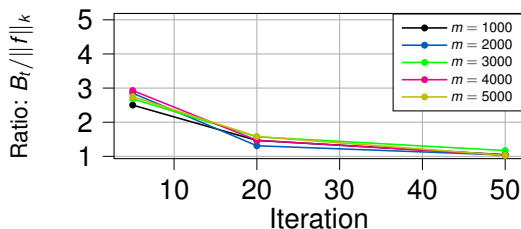
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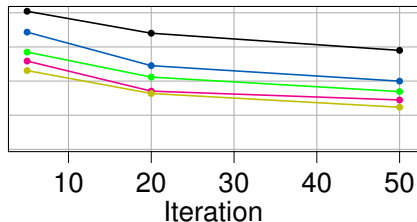
$$\|f\|_k \leq \lim_{s \rightarrow \infty} \frac{1}{s} \sum_{j=1}^s \|\rho_{t,j}\|_k$$

\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

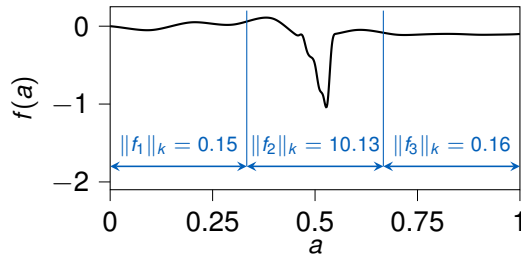
$$|f(a) - \mu_t(a)| \leq (B_t + \text{"data-term"}) \sigma_t(a)$$

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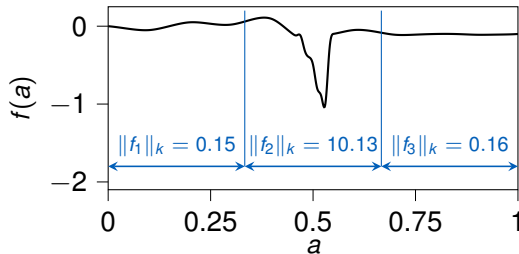


Local interpretation of the RKHS norm

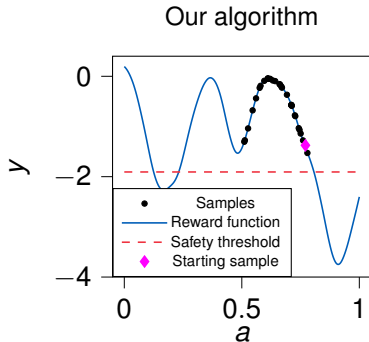
- Safe exploration for optimization:
Restricted to **sub-space** of domain
- Exploit **local “smoothness”** to allow
for more **optimistic exploration**
- **Adaptive** interpretation of locality:
sub-domains around each sample
- **Significantly more scalable** through
separate discretization in sub-domains

GP confidence intervals

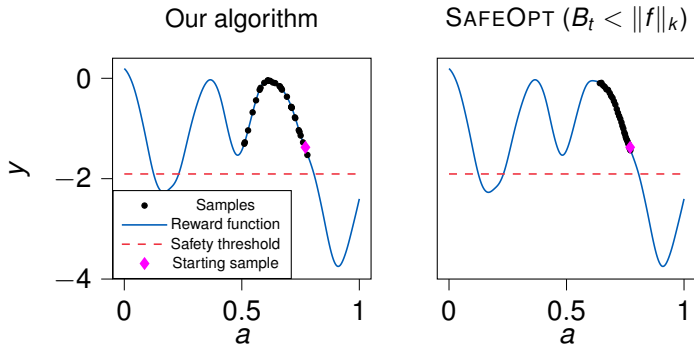
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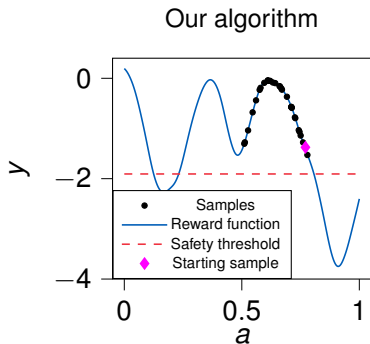
Numerical experiments



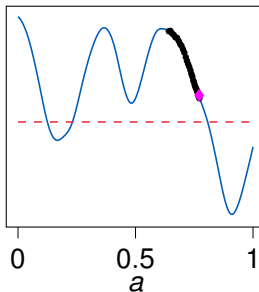
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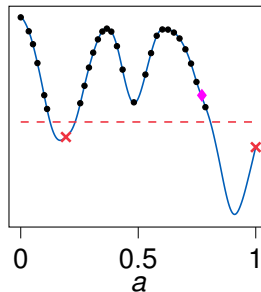
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SAFEOPT ($B_t < \|f\|_k$)

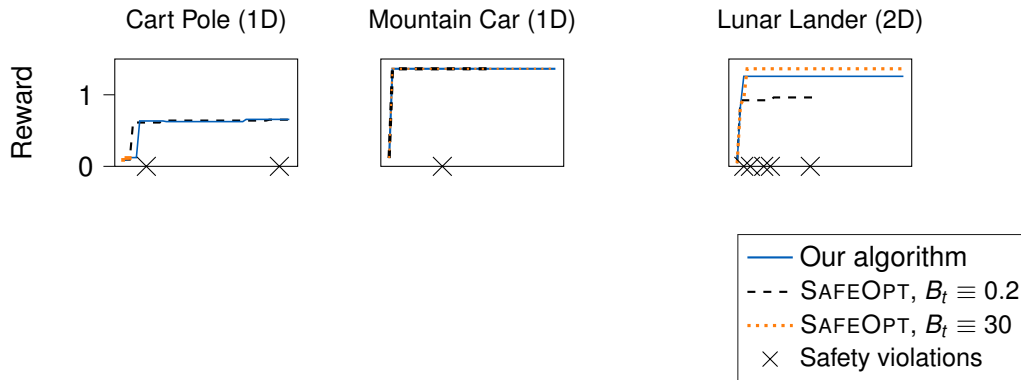


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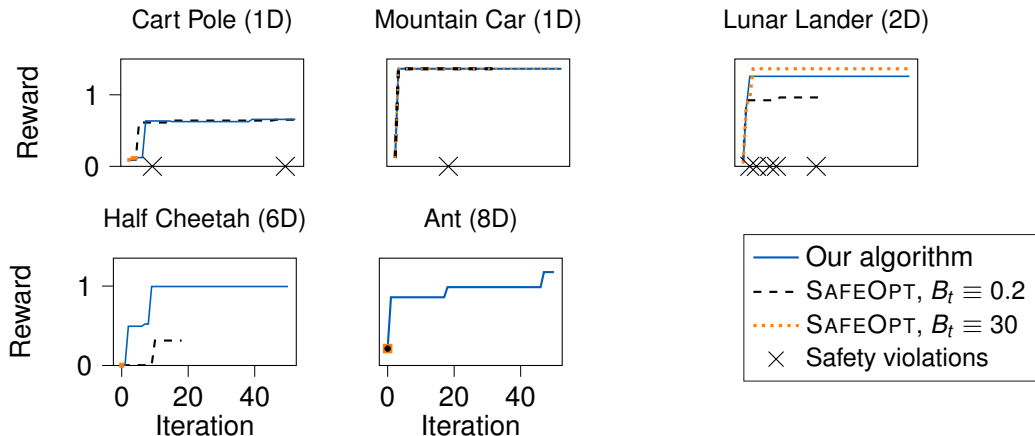


Safely fine-tuning RL policies

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Safely fine-tuning RL policies



Hardware experiment



Limitations

Regularity assumption (Our approach)

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

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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**

Conclusions

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

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Contributions

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