



# PACSBO: Probably approximately correct safe Bayesian optimization

AI Day 2024

Abdullah Tokmak<sup>1,2</sup>

<sup>1</sup> Aalto University, Espoo, Finland

<sup>2</sup> Uppsala University, Uppsala, Sweden

October 21, 2024



Aalto University  
School of Electrical  
Engineering



UPPSALA  
UNIVERSITET

# Motivational example



# Introduction

## Goal

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



# Introduction

## Goal

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

- Unknown reward function  $f: \mathcal{A} \rightarrow \mathbb{R}$
- Control policy parameters  $a \in \mathcal{A}$
- We require **sample efficiency** and **safety guarantees**



# Introduction

## Goal

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

- Unknown reward function  $f: \mathcal{A} \rightarrow \mathbb{R}$
- Control policy parameters  $a \in \mathcal{A}$
- We require **sample efficiency** and **safety guarantees**



## 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**  $\mu_t$ , **standard deviation**  $\sigma_t$

# Gaussian process (GP) regression

- GPs to model unknown reward function  $f$  from samples
- GP characterized by **kernel**  $k$ : **Mean prediction**  $\mu_t$ , **standard deviation**  $\sigma_t$

## Regularity assumption

The reward function  $f$  is a member of the **reproducing kernel Hilbert space (RKHS)** of the chosen kernel  $k$ .

# Gaussian process (GP) regression

- GPs to model unknown reward function  $f$  from samples
- GP characterized by **kernel**  $k$ : **Mean prediction**  $\mu_t$ , **standard deviation**  $\sigma_t$

## Regularity assumption

The reward function  $f$  is a member of the **reproducing kernel Hilbert space (RKHS)** of the chosen kernel  $k$ .

## Regularity assumption

An upper bound  $B$  on the RKHS norm  $\|f\|_k$ ,  
i.e.,  $B \geq \|f\|_k$ , is known a priori.



# Gaussian process (GP) regression

- GPs to model unknown reward function  $f$  from samples
- GP characterized by **kernel**  $k$ : **Mean prediction**  $\mu_t$ , **standard deviation**  $\sigma_t$

## Regularity assumption

The reward function  $f$  is a member of the **reproducing kernel Hilbert space (RKHS)** of the chosen kernel  $k$ .

## Regularity assumption

An upper bound  $B$  on the RKHS norm  $\|f\|_k$ , i.e.,  $B \geq \|f\|_k$ , is known a priori.

## 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

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

## GP confidence intervals

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

---

<sup>1</sup>Y. Sui, A. Gotovos, J. W. Burdick, A. Krause, “Safe exploration for optimization with Gaussian processes,” 2015.

# Safe Bayesian optimization (BO) with GPs

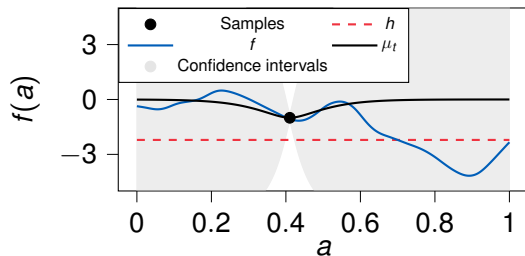
## Control policy optimization problem

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

## GP confidence intervals

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

$$\text{SAFEOPT}^1 (t = 0, B = \|f\|_k)$$



<sup>1</sup>Y. Sui, A. Gotovos, J. W. Burdick, A. Krause, “Safe exploration for optimization with Gaussian processes,” 2015.

# Safe Bayesian optimization (BO) with GPs

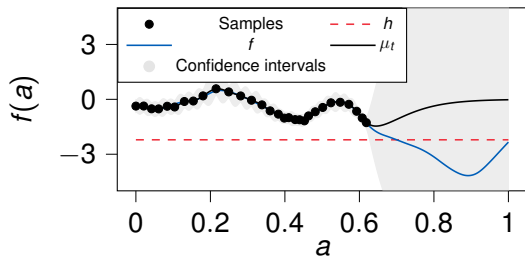
## Control policy optimization problem

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

## GP confidence intervals

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

SAFEOPT<sup>1</sup> ( $t = 30$ ,  $B = \|f\|_k$ )



<sup>1</sup>Y. Sui, A. Gotovos, J. W. Burdick, A. Krause, "Safe exploration for optimization with Gaussian processes," 2015.

# Safe Bayesian optimization (BO) with GPs

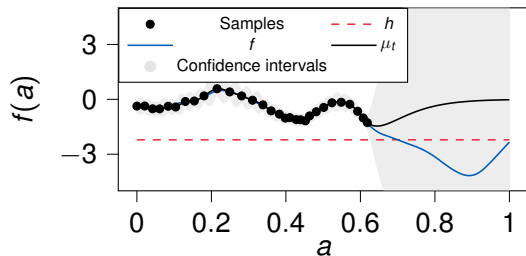
## Control policy optimization problem

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

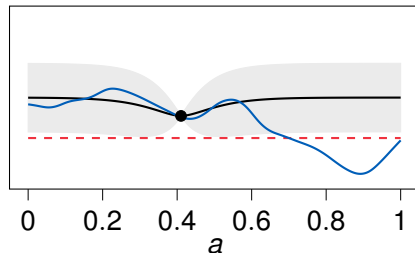
## GP confidence intervals

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

SAFEOPT<sup>1</sup> ( $t = 30$ ,  $B = \|f\|_k$ )



SAFEOPT<sup>1</sup> ( $t = 0$ ,  $B < \|f\|_k$ )



<sup>1</sup>Y. Sui, A. Gotovos, J. W. Burdick, A. Krause, "Safe exploration for optimization with Gaussian processes," 2015.

# Safe Bayesian optimization (BO) with GPs

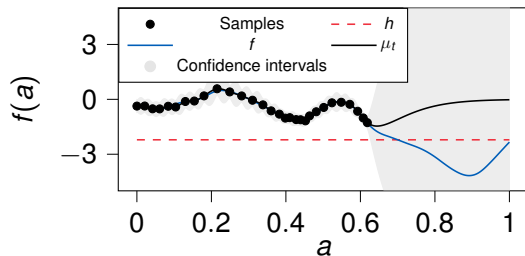
## Control policy optimization problem

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

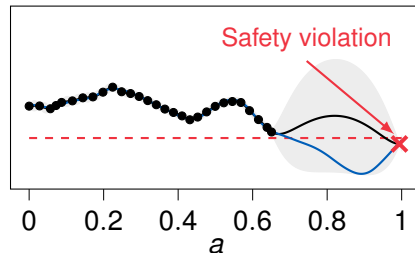
## GP confidence intervals

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

SAFEOPT<sup>1</sup> ( $t = 30$ ,  $B = \|f\|_k$ )



SAFEOPT<sup>1</sup> ( $t = 30$ ,  $B < \|f\|_k$ )



<sup>1</sup>Y. Sui, A. Gotovos, J. W. Burdick, A. Krause, "Safe exploration for optimization with Gaussian processes," 2015.

# RKHS norm assumption in safe BO

## Regularity assumption

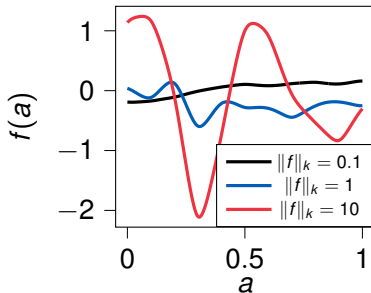
Most safe BO algorithms require an upper bound  $B$  on the RKHS norm ( $B \geq \|f\|_k$ ) a priori.

# 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.

- RKHS norm  $\|f\|_k$  characterizes “smoothness” of function  $f$



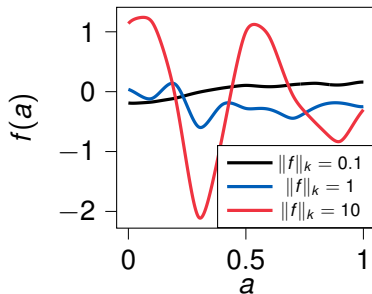


# RKHS norm assumption in safe BO

## Regularity assumption

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

- RKHS norm  $\|f\|_k$  characterizes “smoothness” of function  $f$
- Tight upper bound for **practicality**

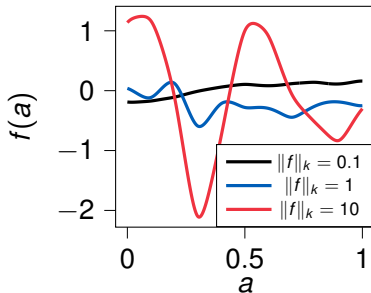


# RKHS norm assumption in safe BO

## Regularity assumption

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

- RKHS norm  $\|f\|_k$  characterizes “smoothness” of function  $f$
- Tight upper bound for **practicality**
- It is **unclear how to upper bound the RKHS norm** of unknown functions



# RKHS norm assumption in safe BO

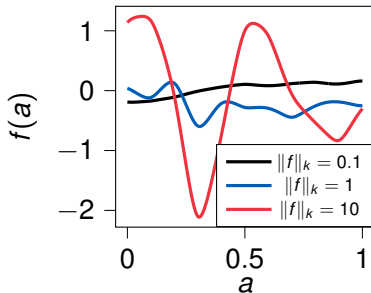
## Regularity assumption

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

- RKHS norm  $\|f\|_k$  characterizes “smoothness” of function  $f$
- Tight upper bound for **practicality**
- It is **unclear how to upper bound the RKHS norm** of unknown functions

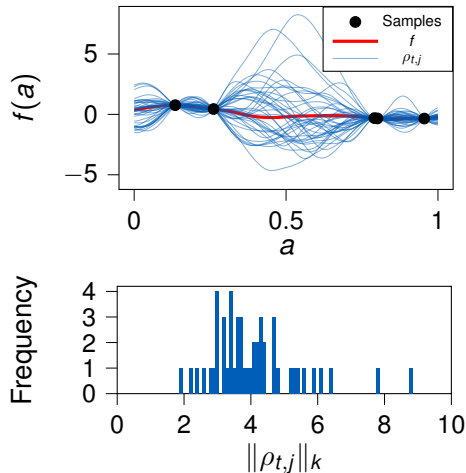
## Problem definition

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



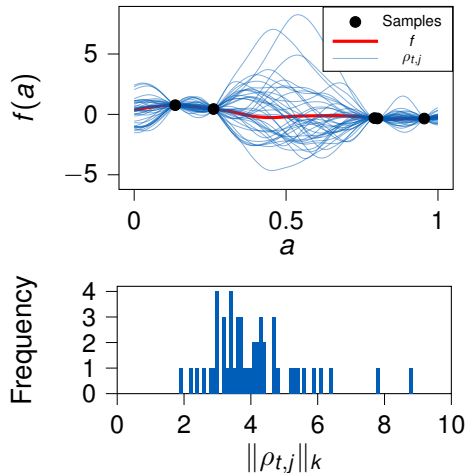
# Random RKHS functions

- 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  $f$



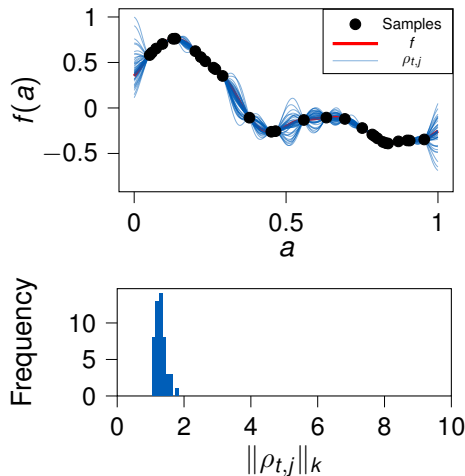
# Random RKHS functions

- 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  $f$
- Increasing sampling density:  
 $\rho_{t,j}, \|\rho_{t,j}\|_k \rightarrow f, \|f\|_k$



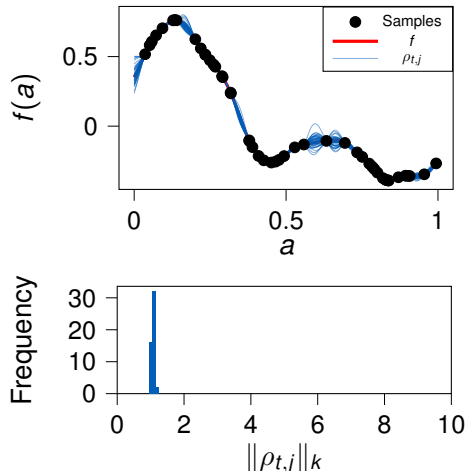
# Random RKHS functions

- 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  $f$
- Increasing sampling density:  
 $\rho_{t,j}, \|\rho_{t,j}\|_k \rightarrow f, \|f\|_k$



# 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  $f$
- Increasing sampling density:  
 $\rho_{t,j}, \|\rho_{t,j}\|_k \rightarrow f, \|f\|_k$



# Statistical guarantees

## Regularity assumptions

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

<sup>2</sup>W. Hoeffding, "Probability inequalities for sums of bounded random variables," The Annals of Statistics, 1962



# Statistical guarantees

## Regularity assumptions

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

## Theorem

Over-estimation of RKHS norm  $B_t \geq \|f\|_k$  is probably approximate correct (PAC)  $\forall t \geq 1$ .

<sup>2</sup>W. Hoeffding, "Probability inequalities for sums of bounded random variables," The Annals of Statistics, 1962

# Statistical guarantees

## Regularity assumptions

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

## Theorem

Over-estimation of RKHS norm  $B_t \geq \|f\|_k$  is probably approximate correct (PAC)  $\forall t \geq 1$ .

## Proof sketch

- $B_t \leftarrow \frac{1}{m} \sum_{j=1}^m \|\rho_{t,j}\|_k + \text{“safety-term”}$
- Statistical guarantees through Hoeffding's inequality<sup>3</sup>

<sup>2</sup>W. Hoeffding, “Probability inequalities for sums of bounded random variables,” The Annals of Statistics, 1962

# Local interpretation of the RKHS norm

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

## GP confidence intervals

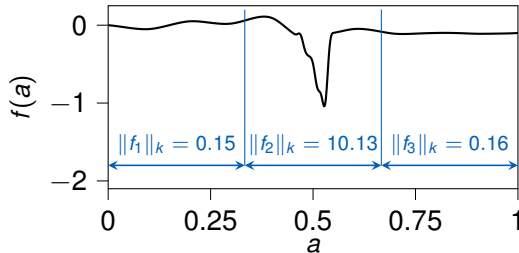
$$|f(a) - \mu_t(a)| \leq (B_t + \text{"data-term"}) \sigma_t(a)$$

# 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**

## GP confidence intervals

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

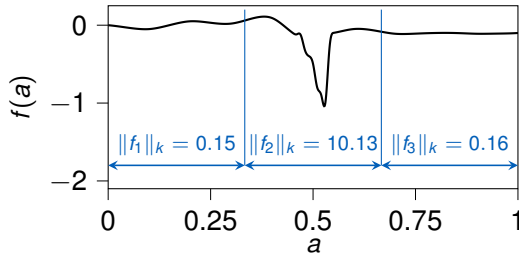


# Local interpretation of the RKHS norm

- Safe exploration for optimization:  
Restricted to **sub-space** of domain
- Exploit **local “smoothness”** to allow  
for more **optimistic exploration**
- Implementation: Three sub-domains  
around the convex hull of samples

## GP confidence intervals

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



## Problem definition

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

## Problem definition

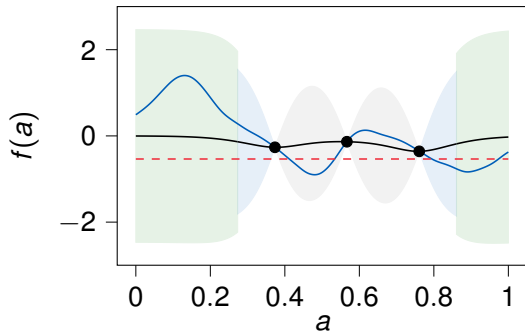
Develop a safe BO algorithm that estimates the RKHS norm  $\|f\|_k$  with guarantees.

PACSBO: **P**robably **a**pproximately **c**orrect **s**afe **B**ayesian **o**ptimization

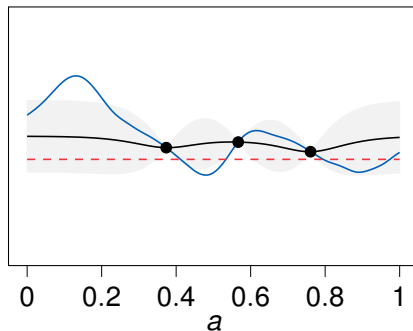
- Data-driven RKHS norm over-estimation with PAC bounds
- Local interpretation of the RKHS norm

# Numerical experiments

PACSBO ( $t = 0$ )



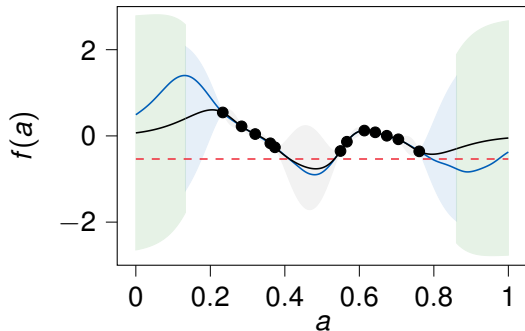
SAFEOPT ( $t = 0$ )



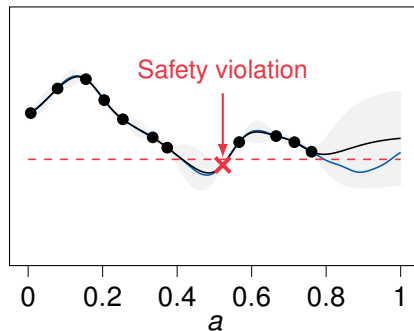


# Numerical experiments

PACCSBO ( $t = 10$ )



SAFEOPT ( $t = 10$ )



# Hardware experiment



# Conclusions

## Goal

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

## Problem definition

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

# Conclusions

## Goal

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

## Problem definition

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

## Contributions

1. Abdullah Tokmak, Thomas B. Schön, Dominik Baumann, "**PACSBO: Probably approximately correct safe Bayesian optimization**," In *Symposium on Systems Theory in Data and Optimization*, 2024.
2. Abdullah Tokmak, Kiran G. Krishnan, Thomas B. Schön, Dominik Baumann, "**Safe exploration in reproducing kernel Hilbert spaces**," submitted to *AISTATS 2025*.

# Conclusions

## Goal

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

## Problem definition

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

## Contributions

1. Abdullah Tokmak, Thomas B. Schön, Dominik Baumann, "**PACSBO: Probably approximately correct safe Bayesian optimization**," In *Symposium on Systems Theory in Data and Optimization*, 2024.
2. Abdullah Tokmak, Kiran G. Krishnan, Thomas B. Schön, Dominik Baumann, "**Safe exploration in reproducing kernel Hilbert spaces**," submitted to *AISTATS 2025*.



Preprints