Human/LLM-in-the-Loop Bayesian Optimization

for Expert-Guided Experimental Design

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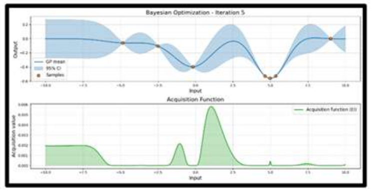
Model data using Gaussian Process ← Evaluate experiment

Select next experiment via *Bayesian optimization*

$$\max_{\mathbf{x}} \mathcal{A}(\mu(\mathbf{x}), \sigma(\mathbf{x}))$$



The DataHow Symposium, 2025

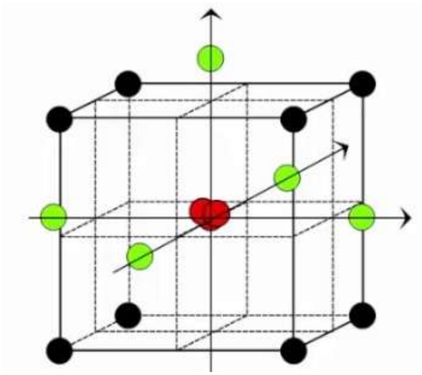
"Digital Bioprocessing - from Innovation to Impact“

OPTIML PSE

Types of experiments $A \xrightarrow{T} B$

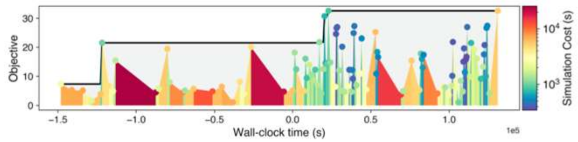
Space filling design

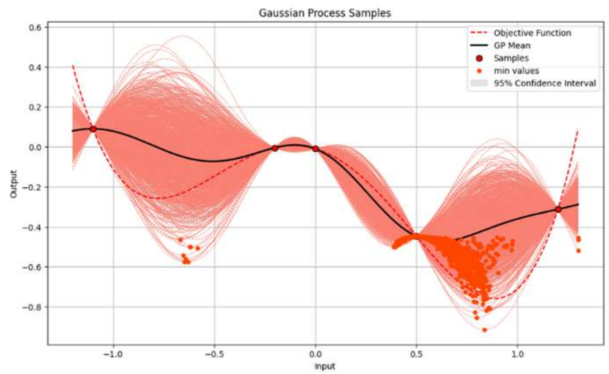
Select experiments to ‘explore’ the space, e.g., LHS.



Optimization

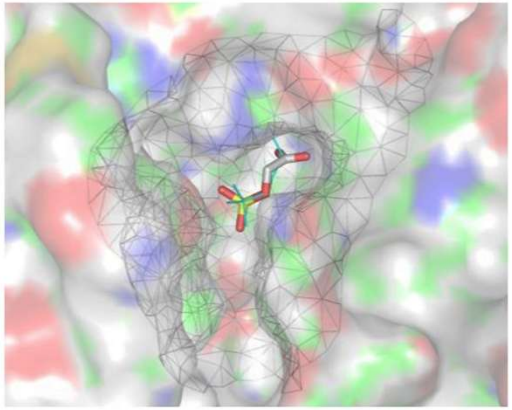
Select experiments to locate the *best* alternative, e.g., response surface.





Model-based

Select experiments to build a model: *discover, optimize, understand*.



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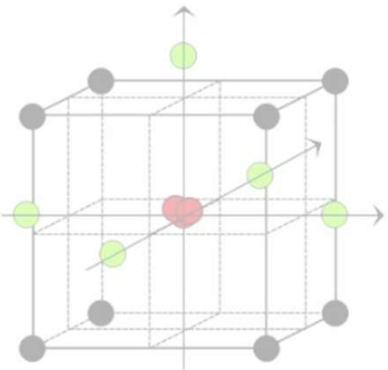

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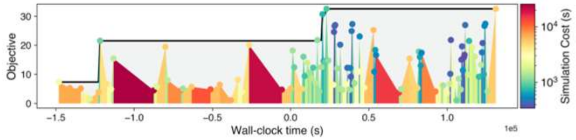

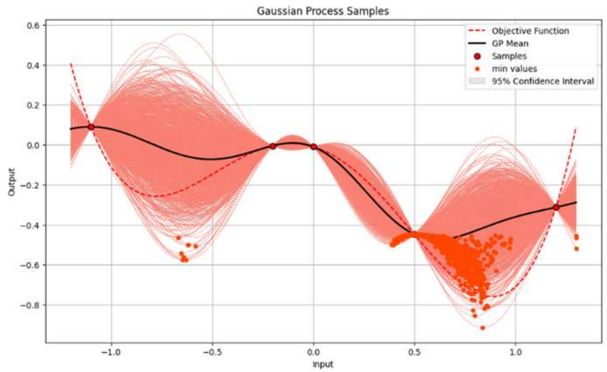

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Topics for today

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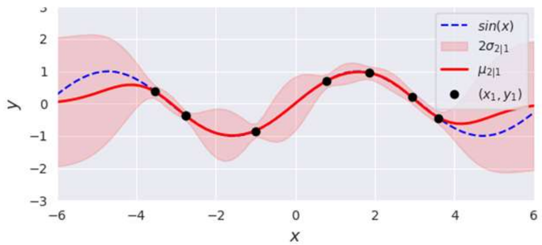
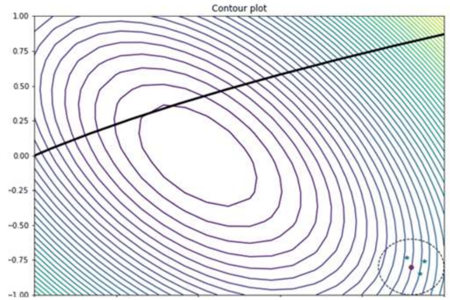
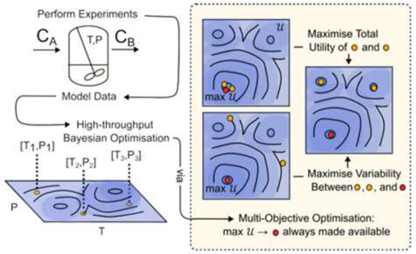
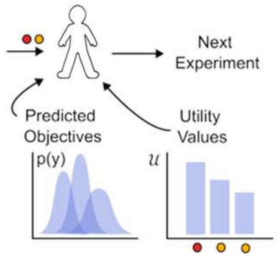




- **Human-in-the-loop Bayesian optimization for design of experiments**





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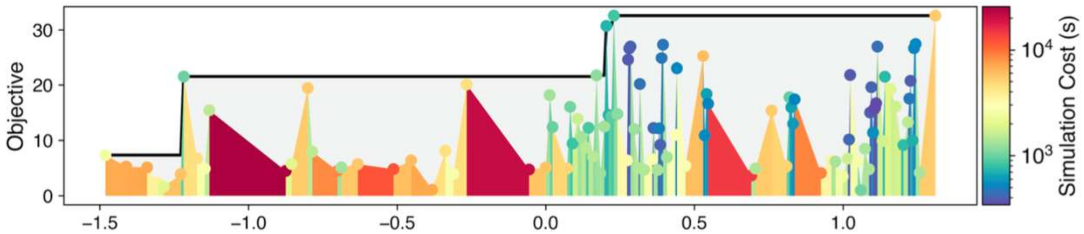

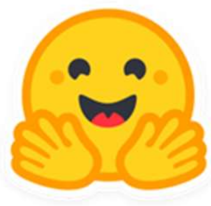

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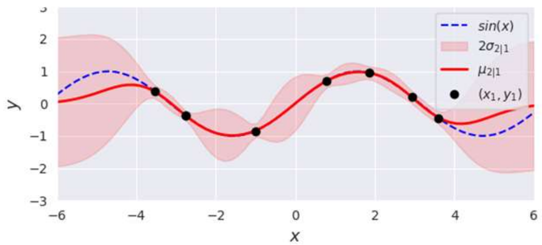

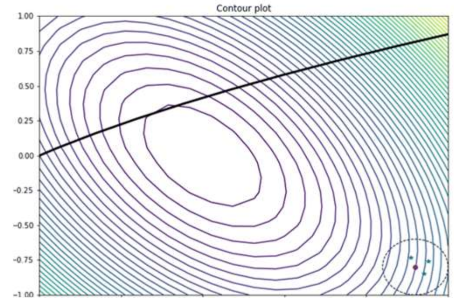

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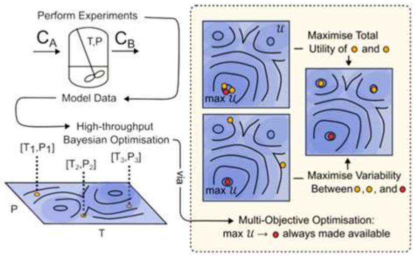

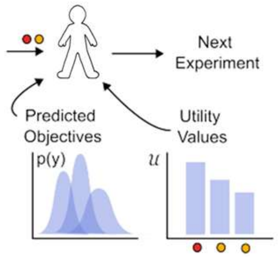

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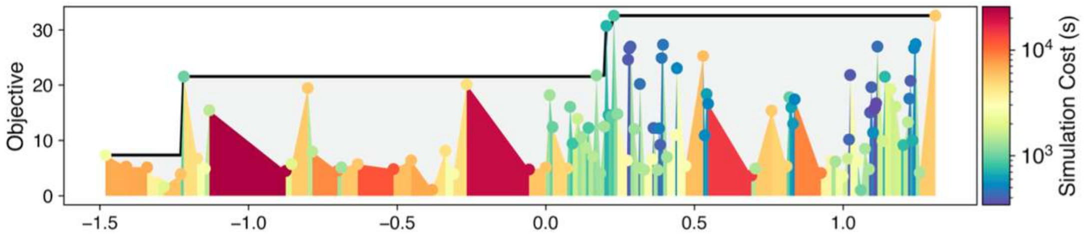
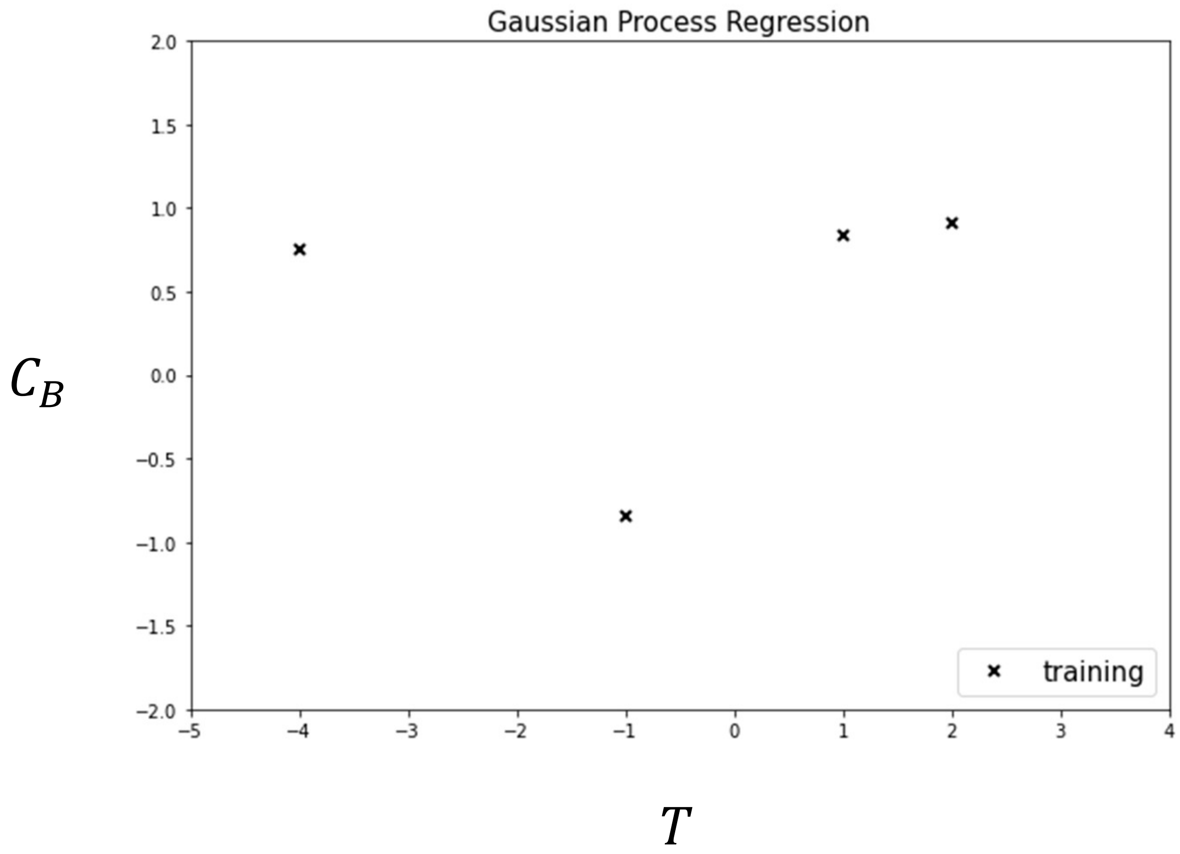
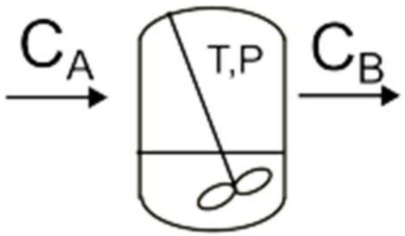


Bayesian Optimization

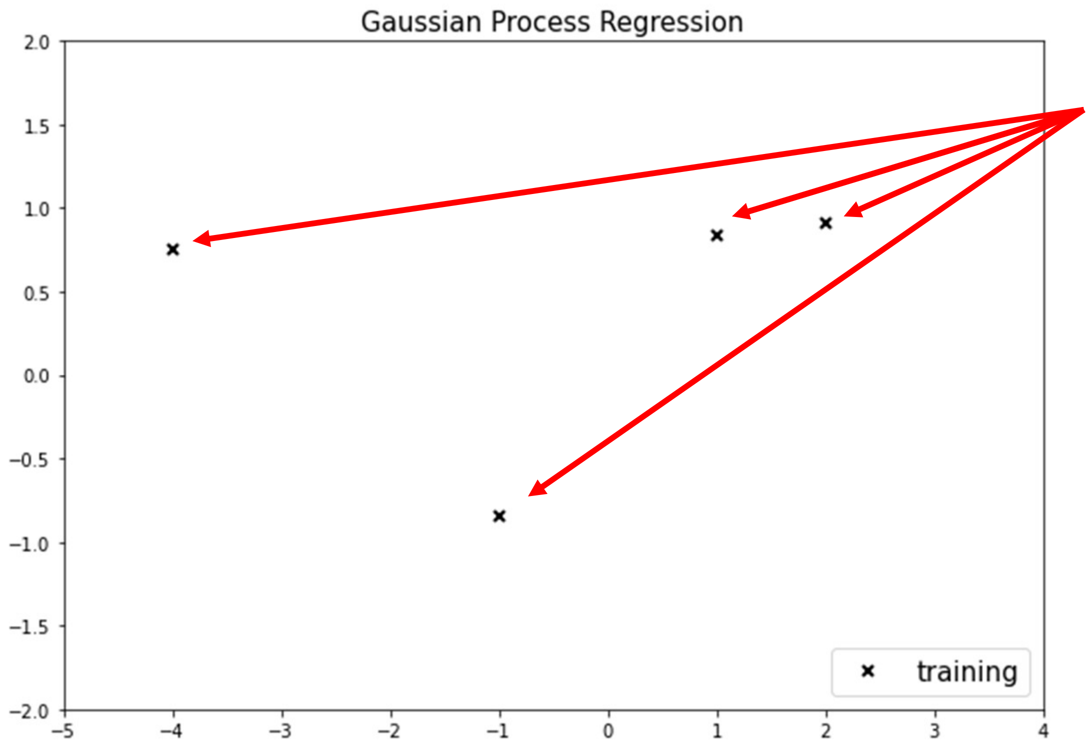
Bayesian Optimization – Gaussian processes





Bayesian Optimization – Gaussian processes

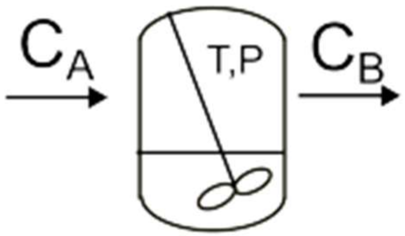
C_B



Datapoints

$x, y = T, C_B$

T



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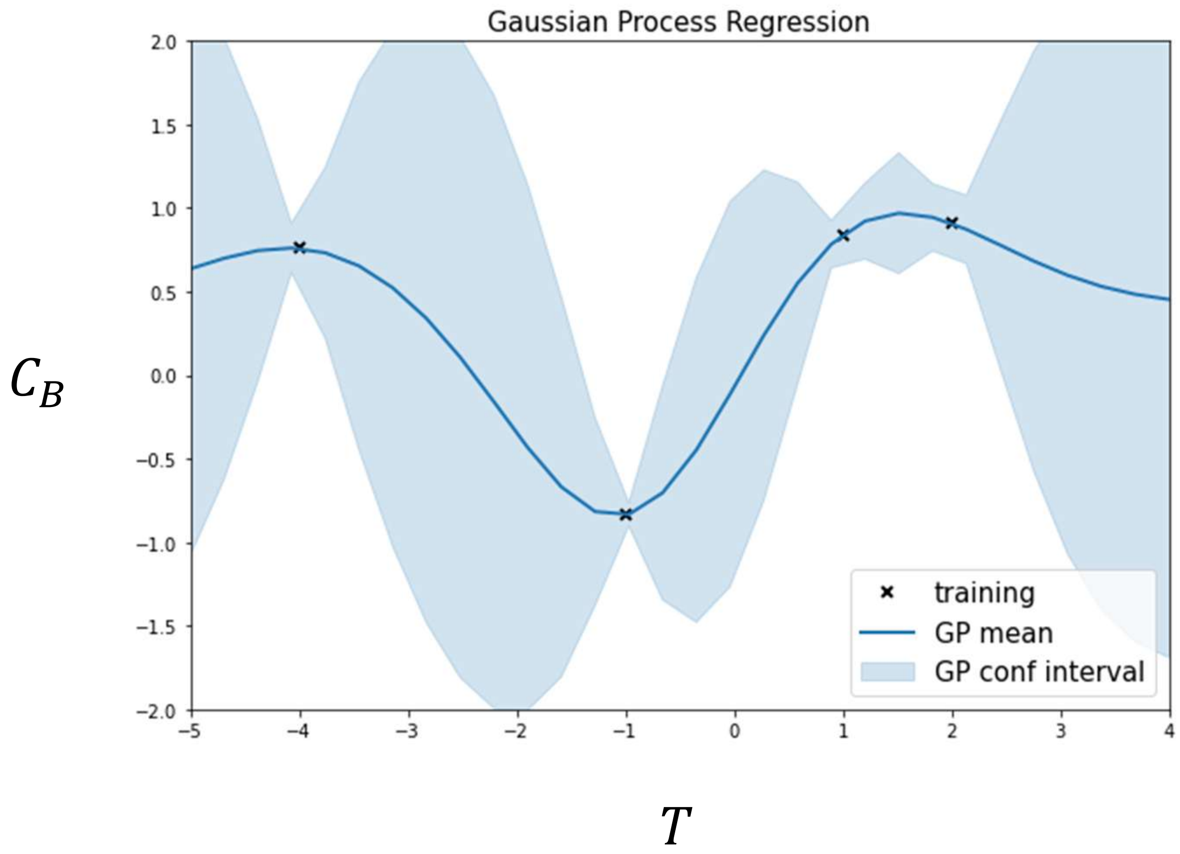

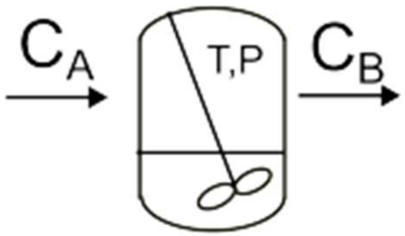

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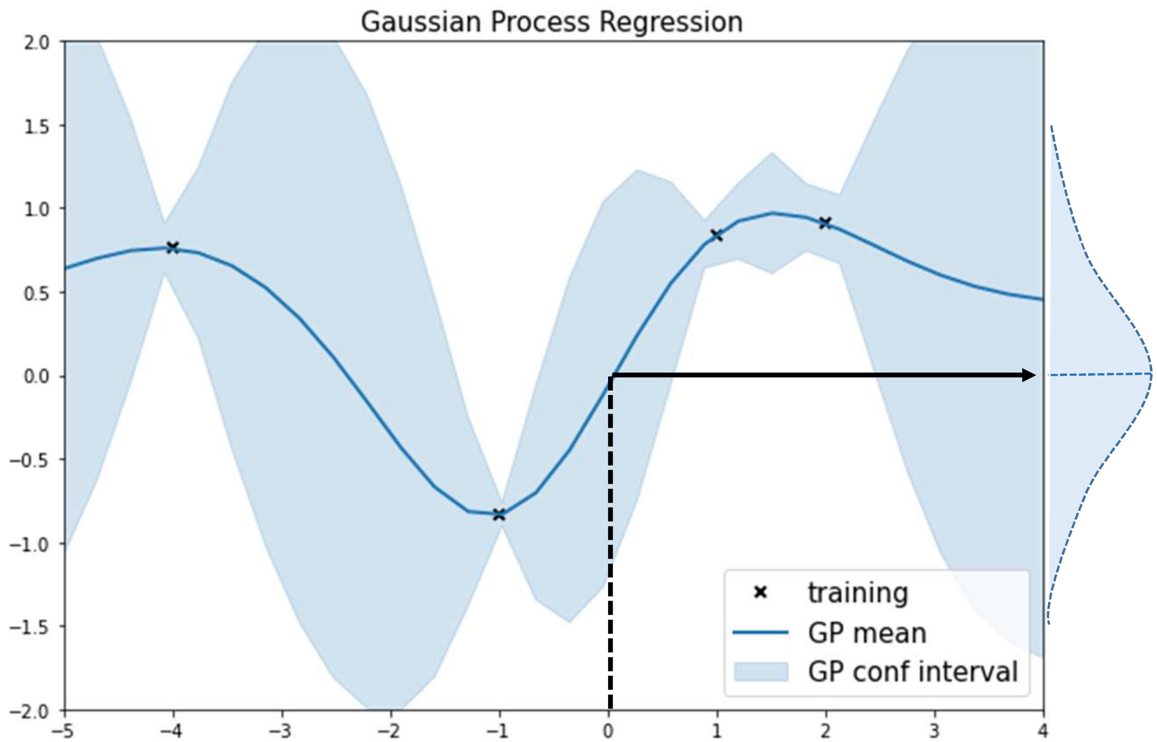
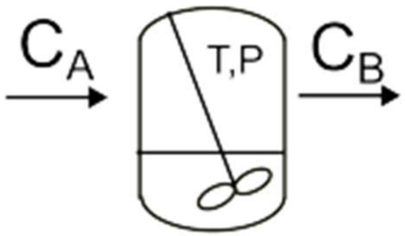


$\hat{C}_{B\,\text{predicted}} \sim \mathcal{N}(\mu_y, \sigma_y^2)$

T_{new}

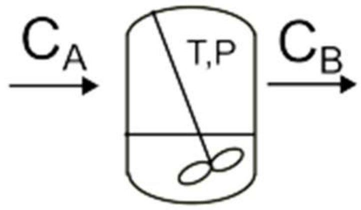
T

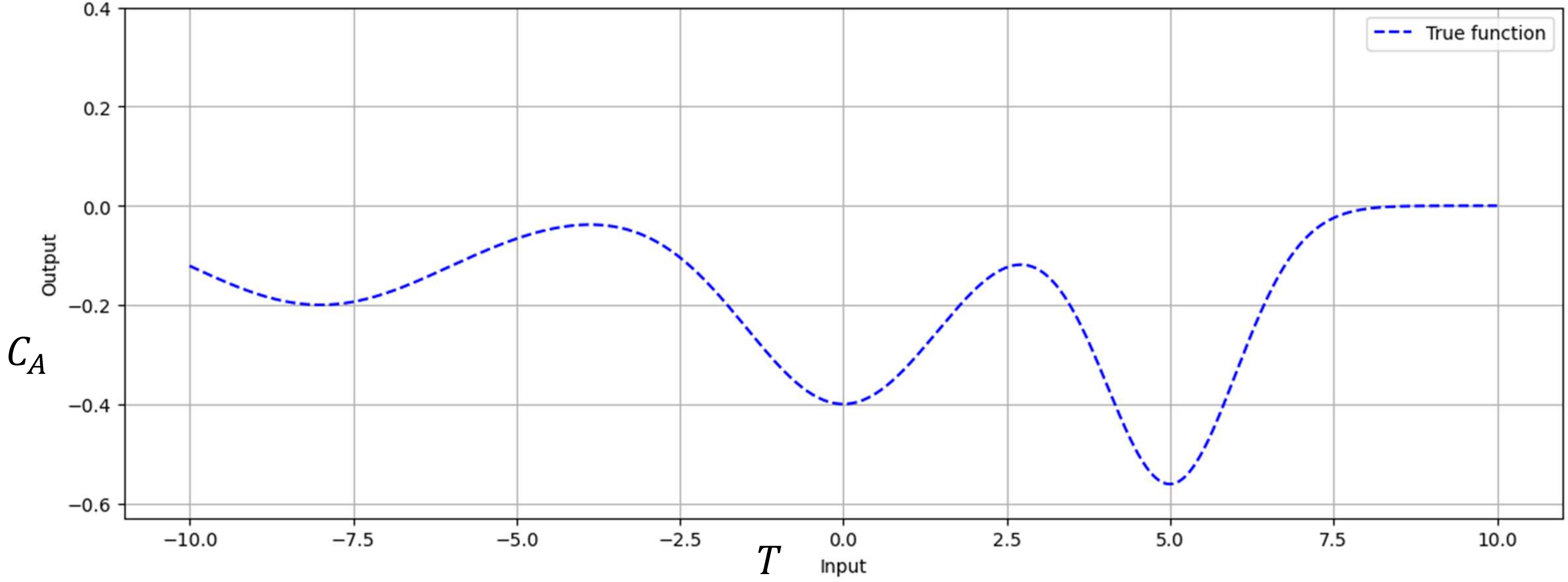


Bayesian Optimization – Big picture

Problem statement

$$\min_{\mathbf{x}\in\mathbb{R}^{n_x}} \quad f(\mathbf{x})$$





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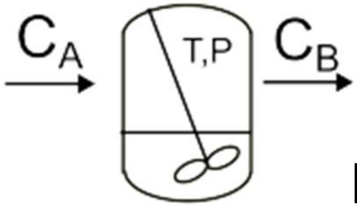

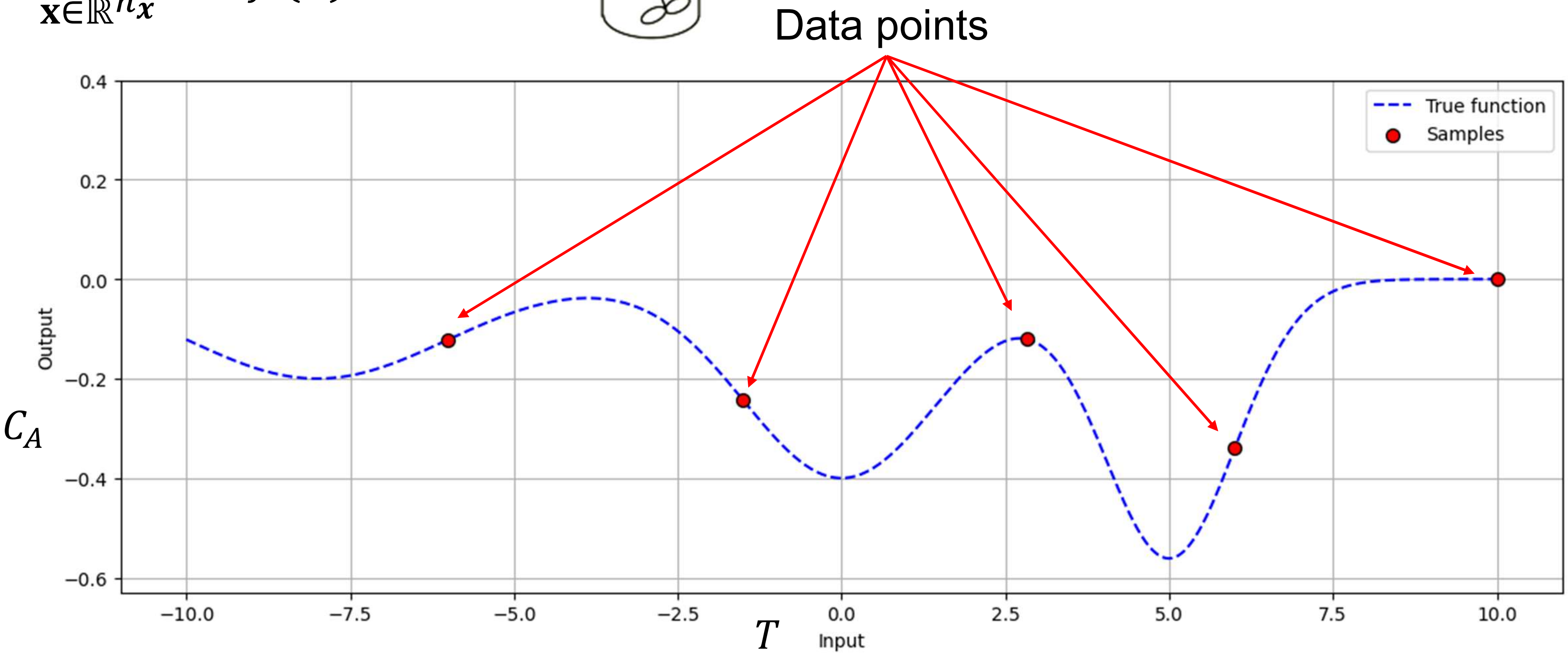

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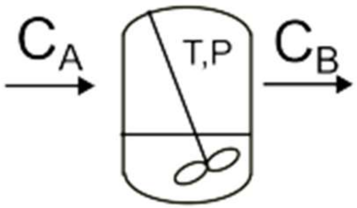
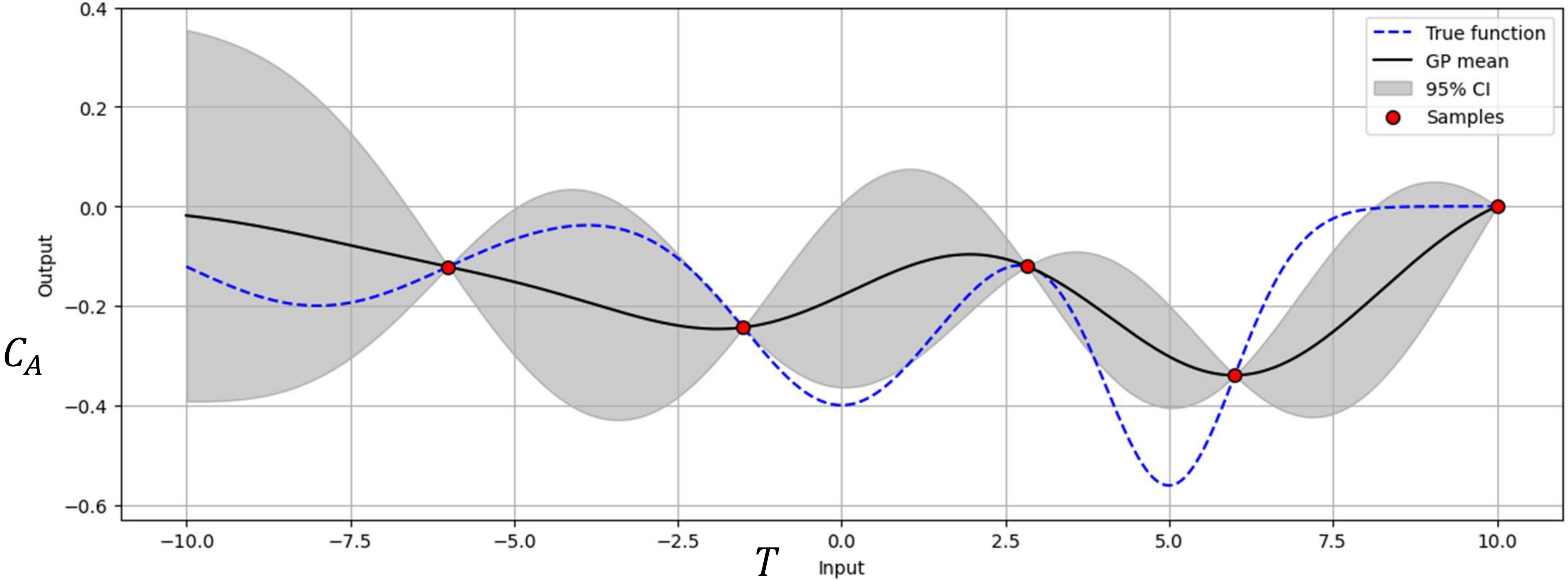


Key idea: model the objective function with a Gaussian process



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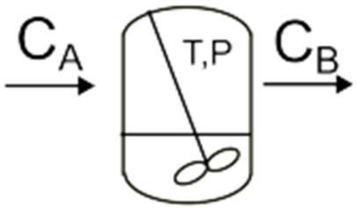
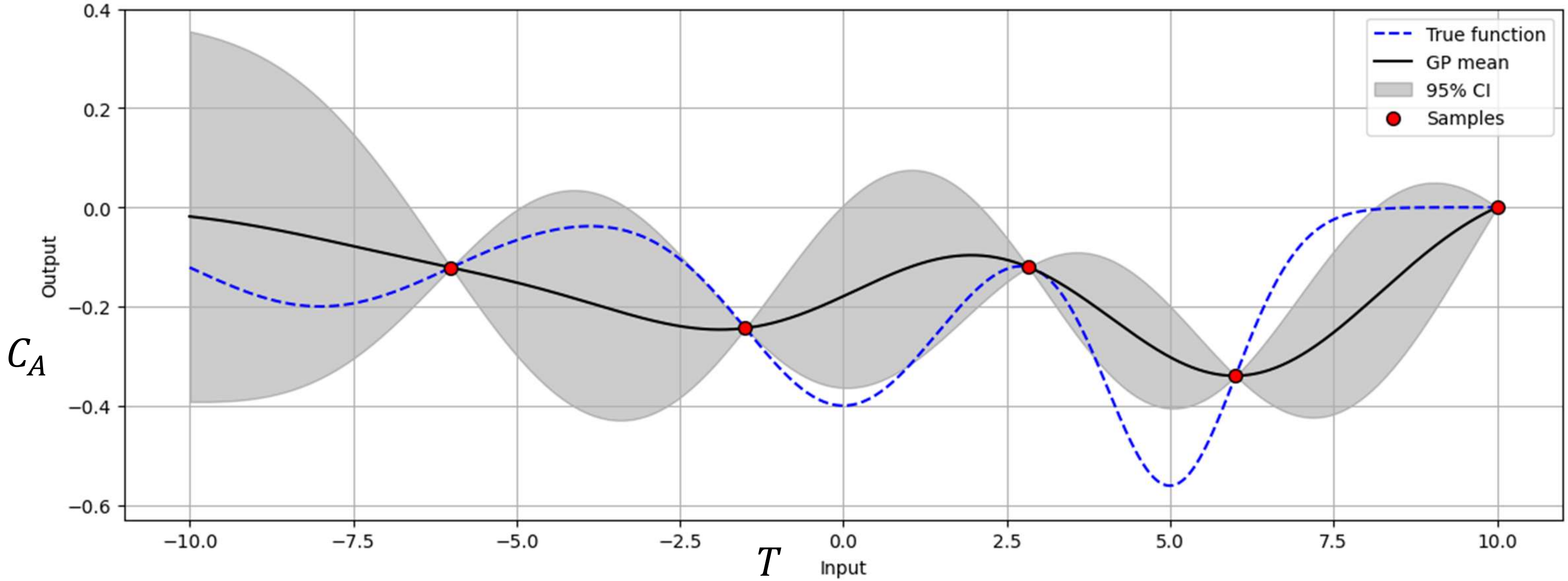


$$\hat{f}(\mathbf{x}) \sim \mathcal{GP}\left(\mu_{\hat{f}}(\mathbf{x}), \sigma_{\hat{f}}(\mathbf{x})\right)$$



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Lower confidence bound

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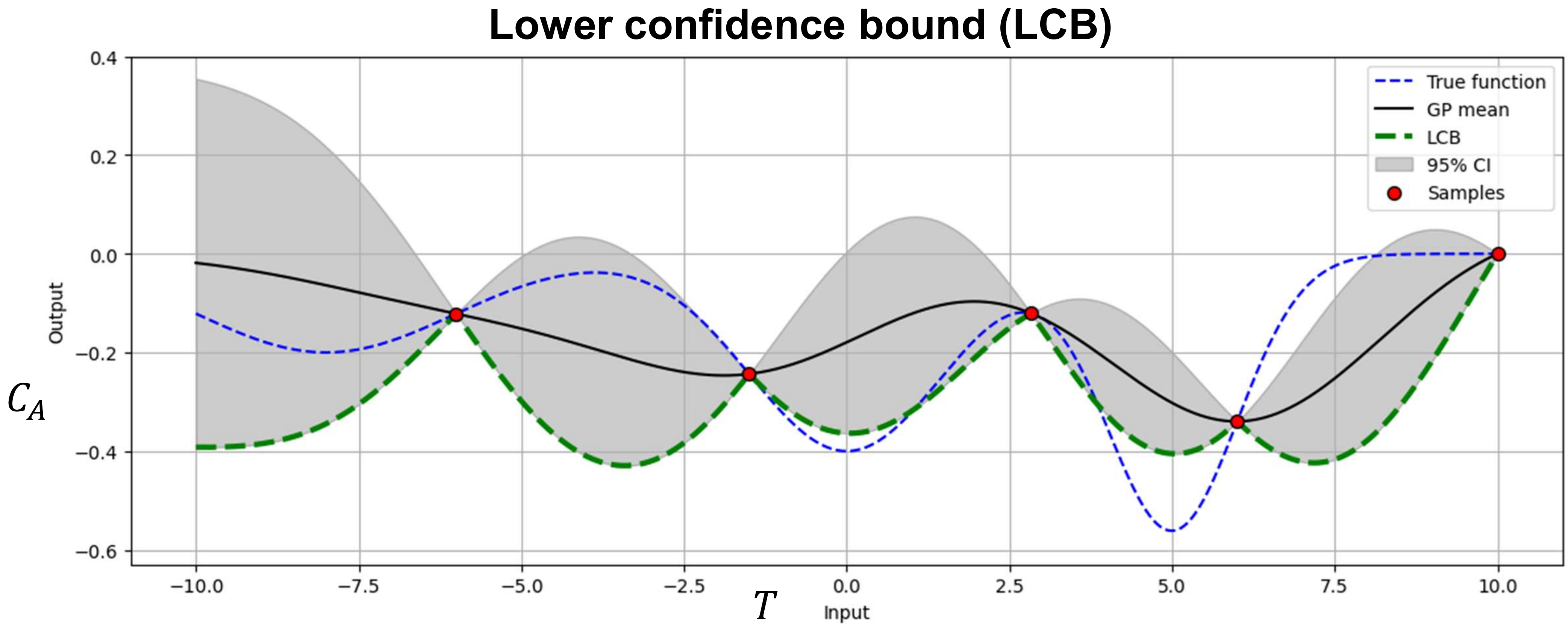

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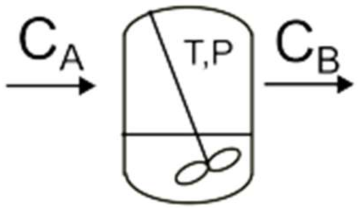

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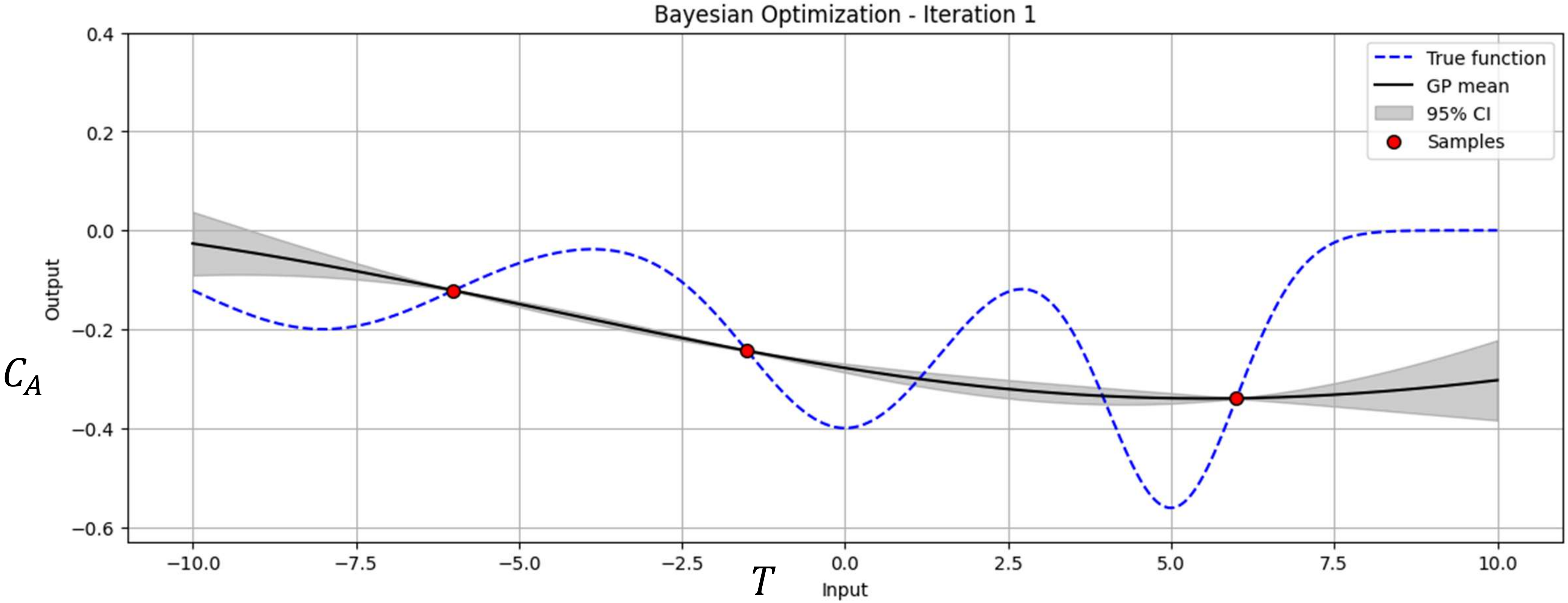

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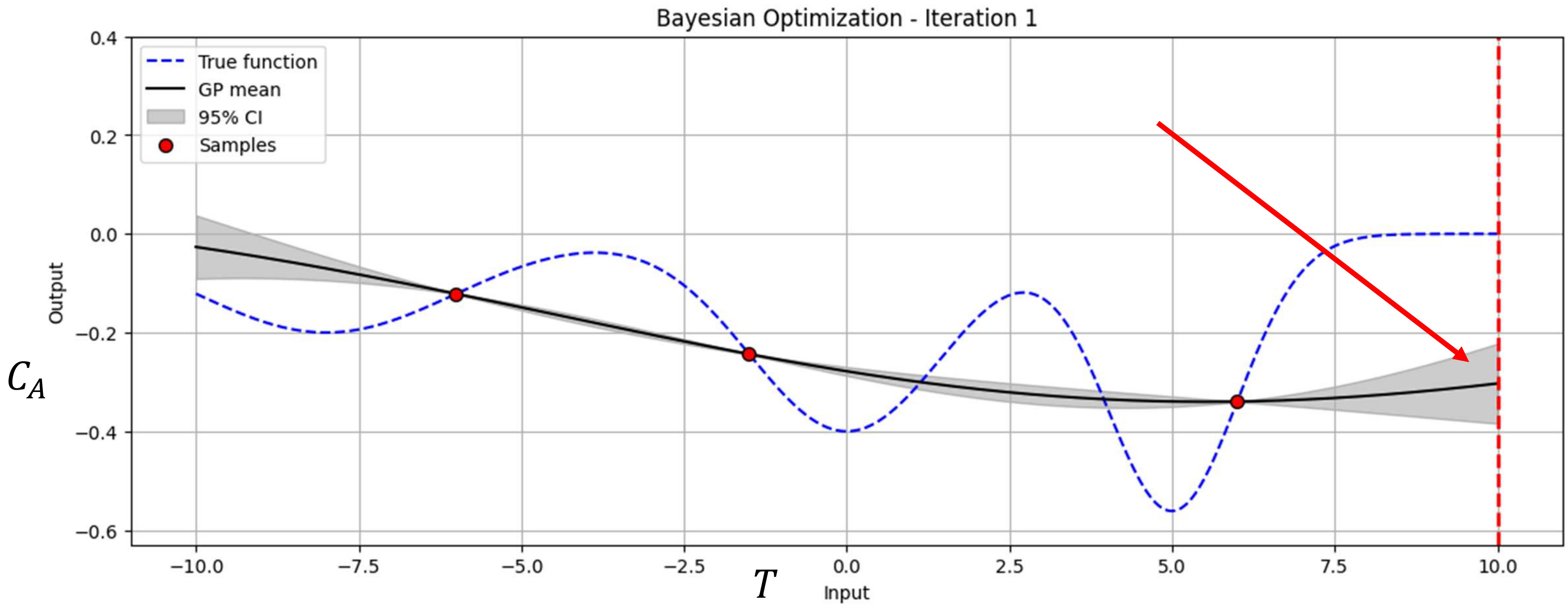

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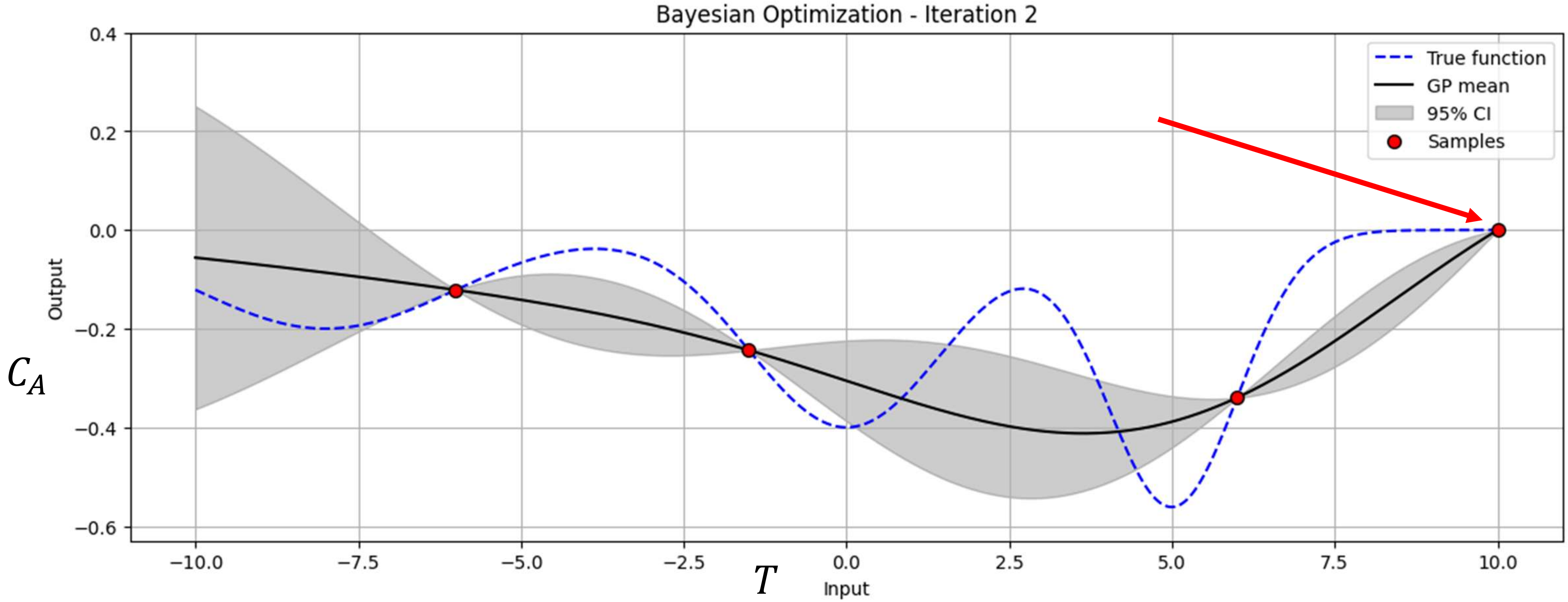

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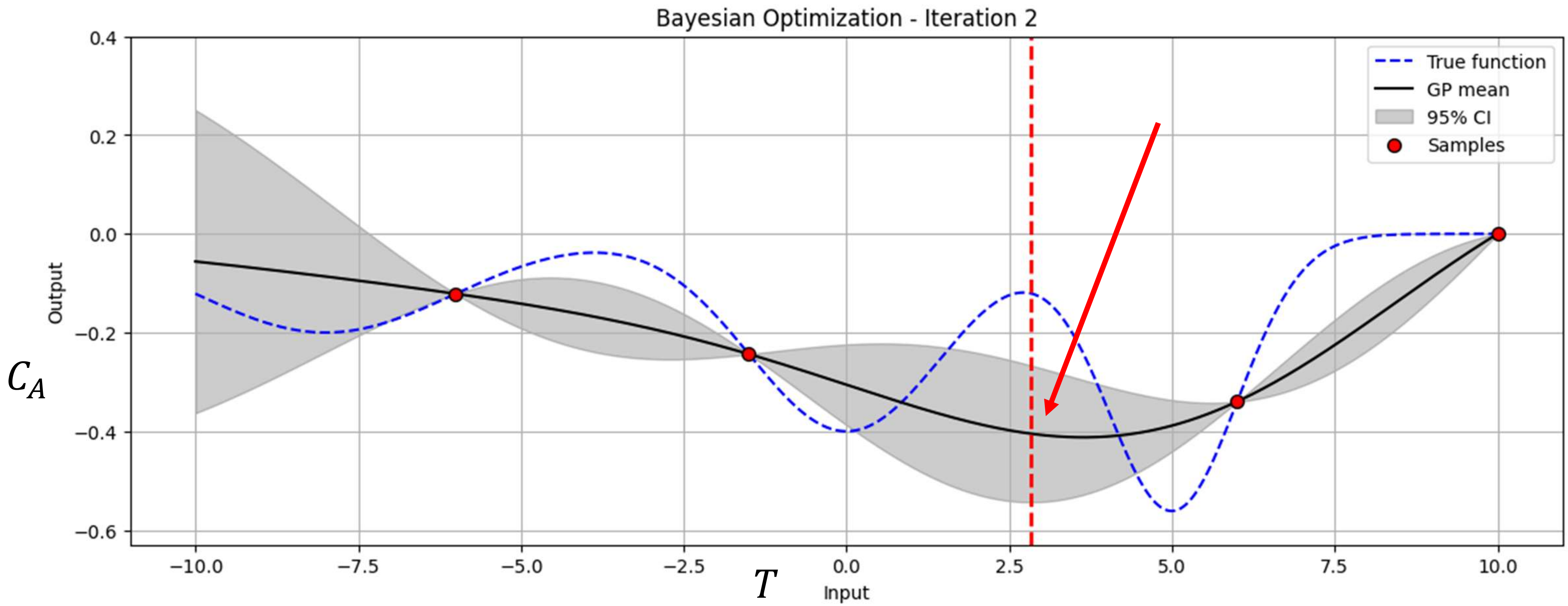

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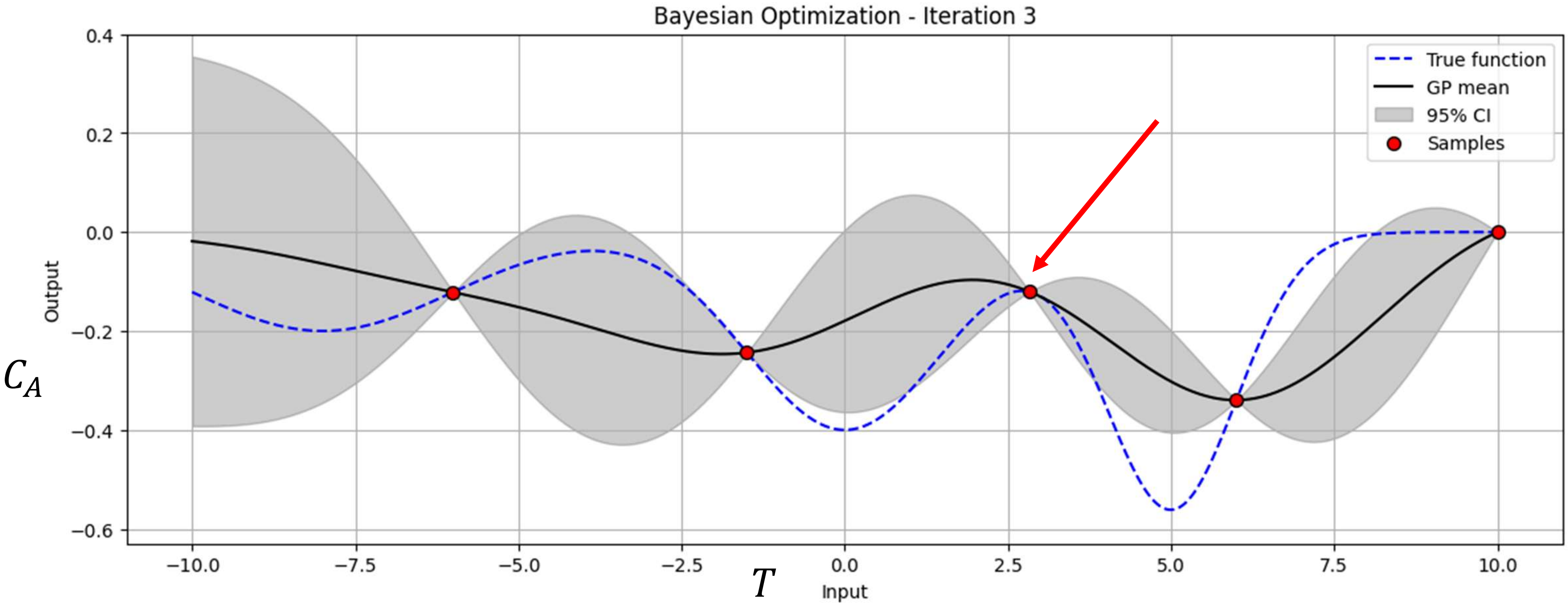

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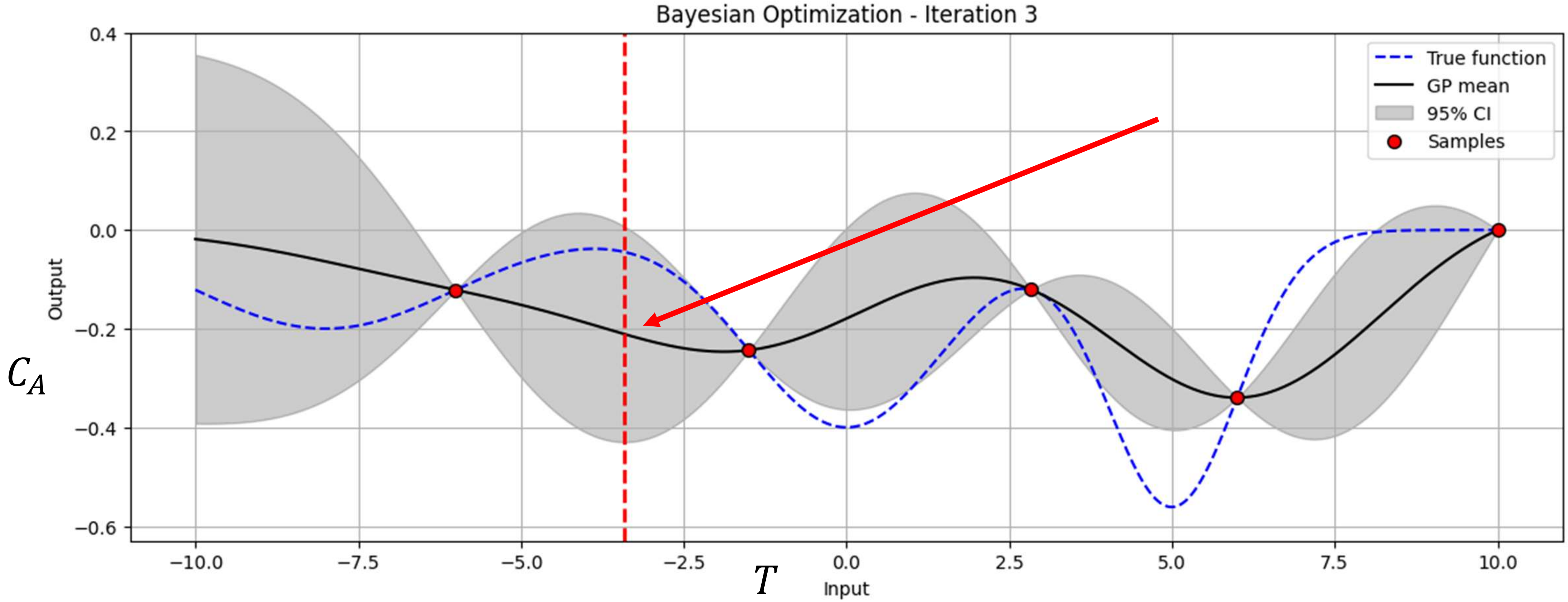

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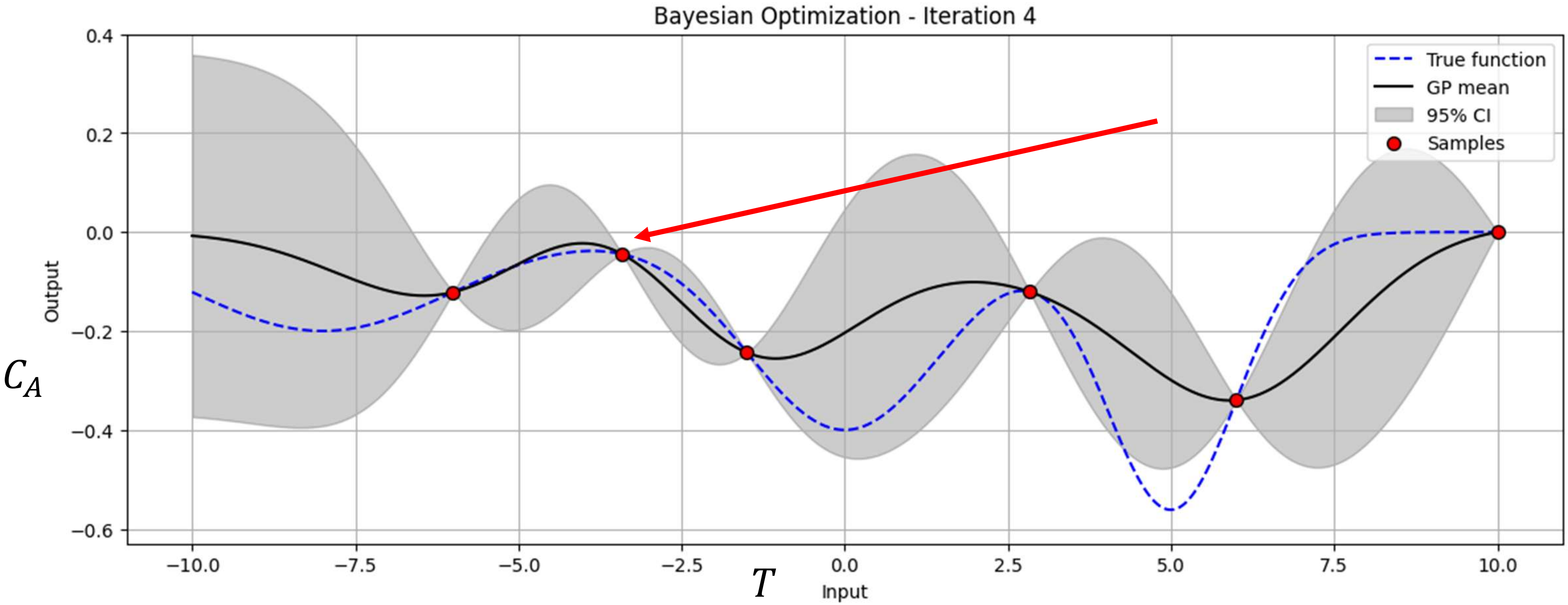

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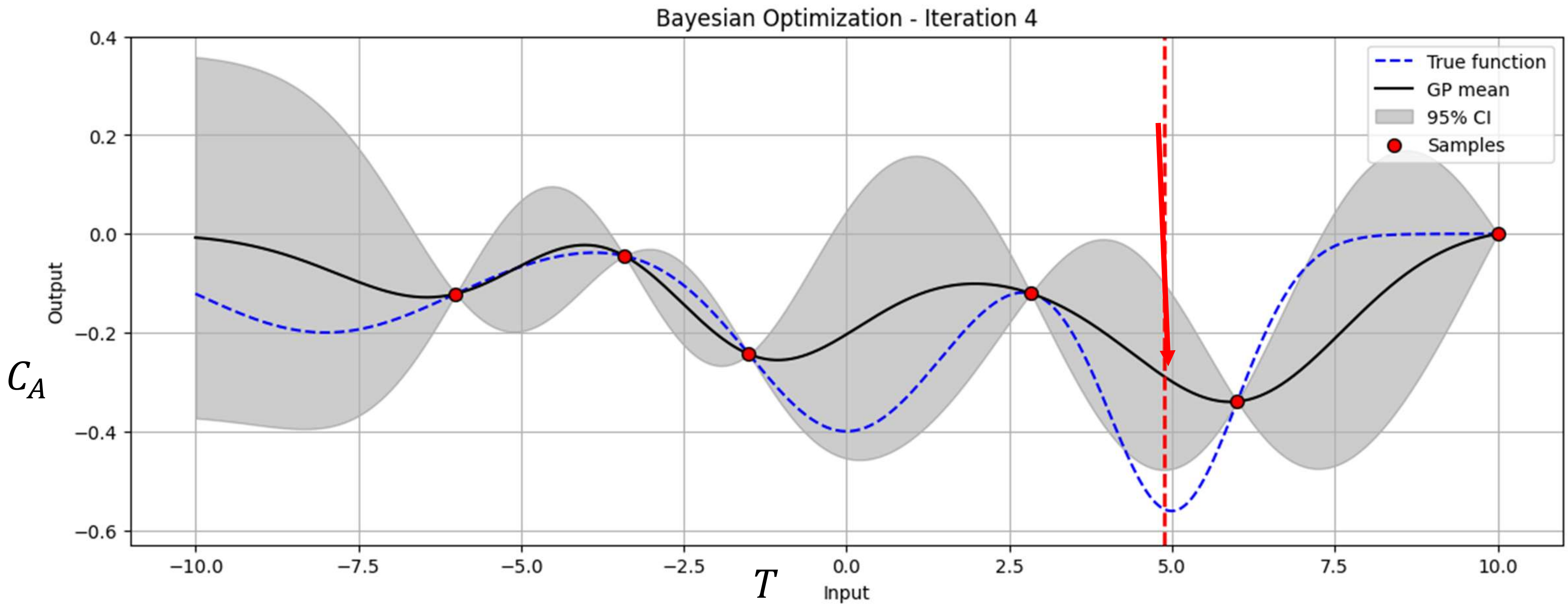

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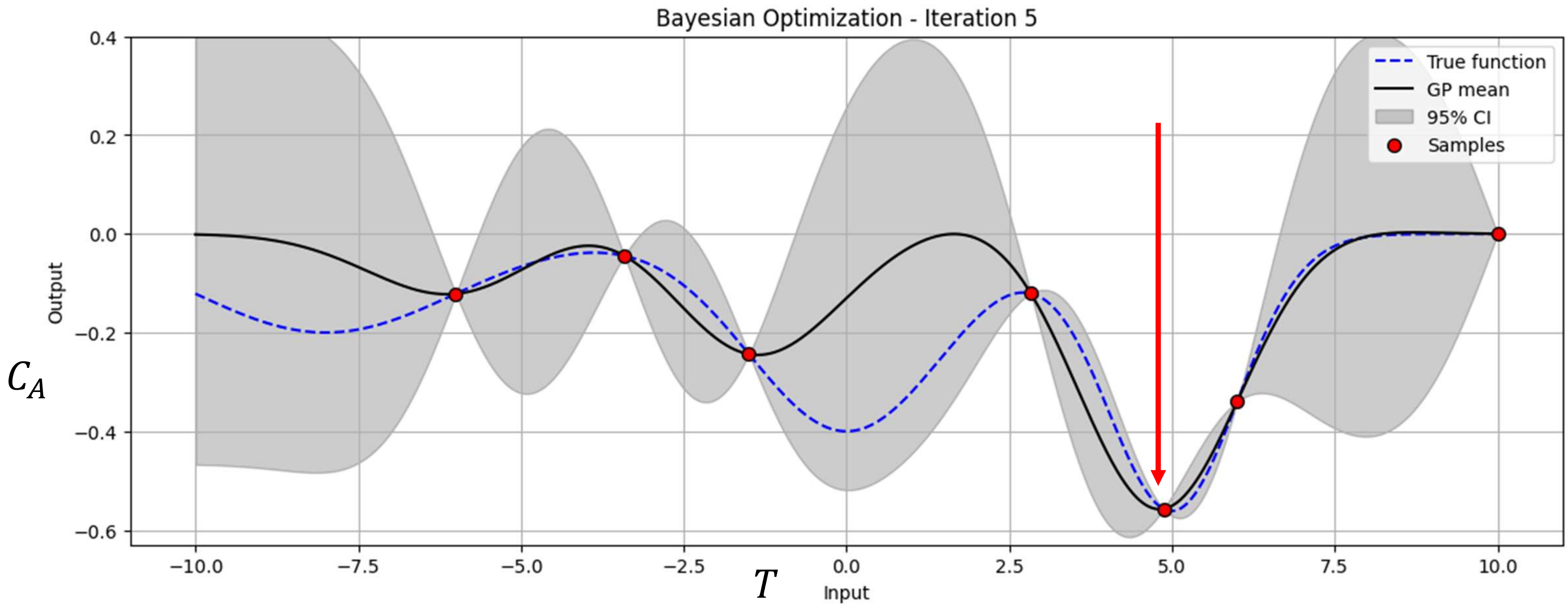

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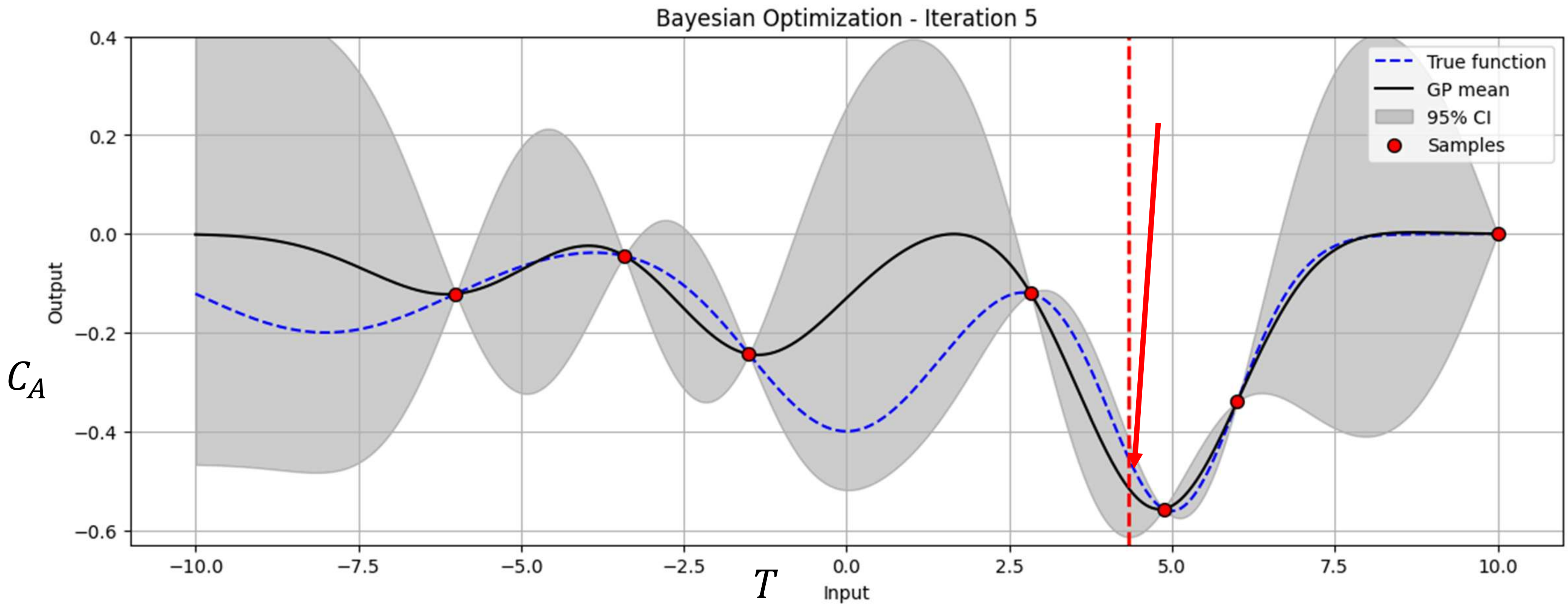

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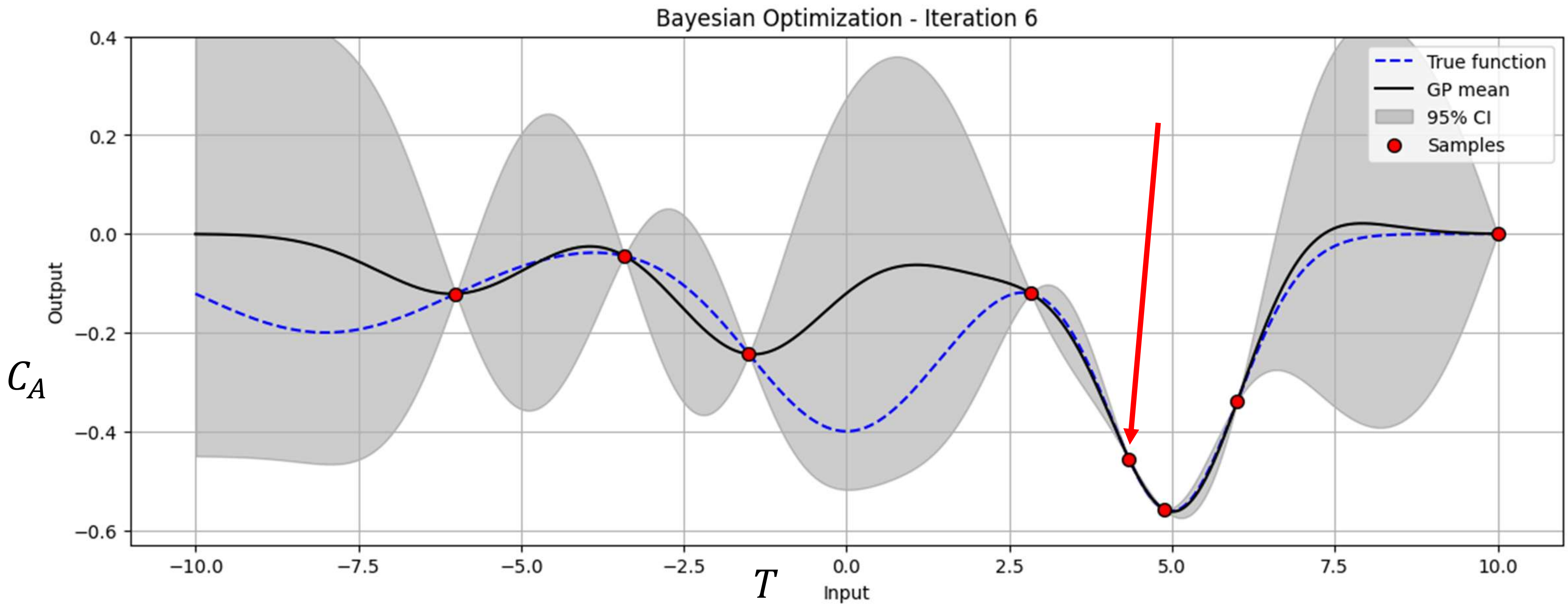

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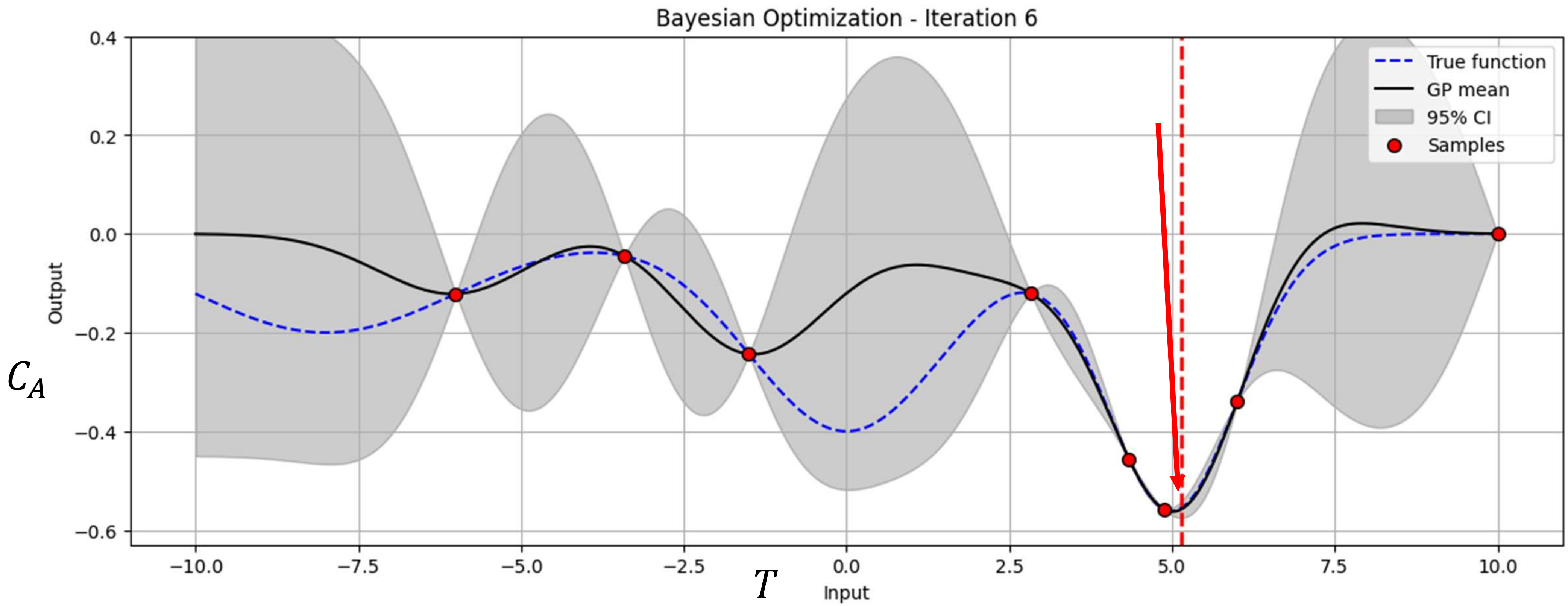

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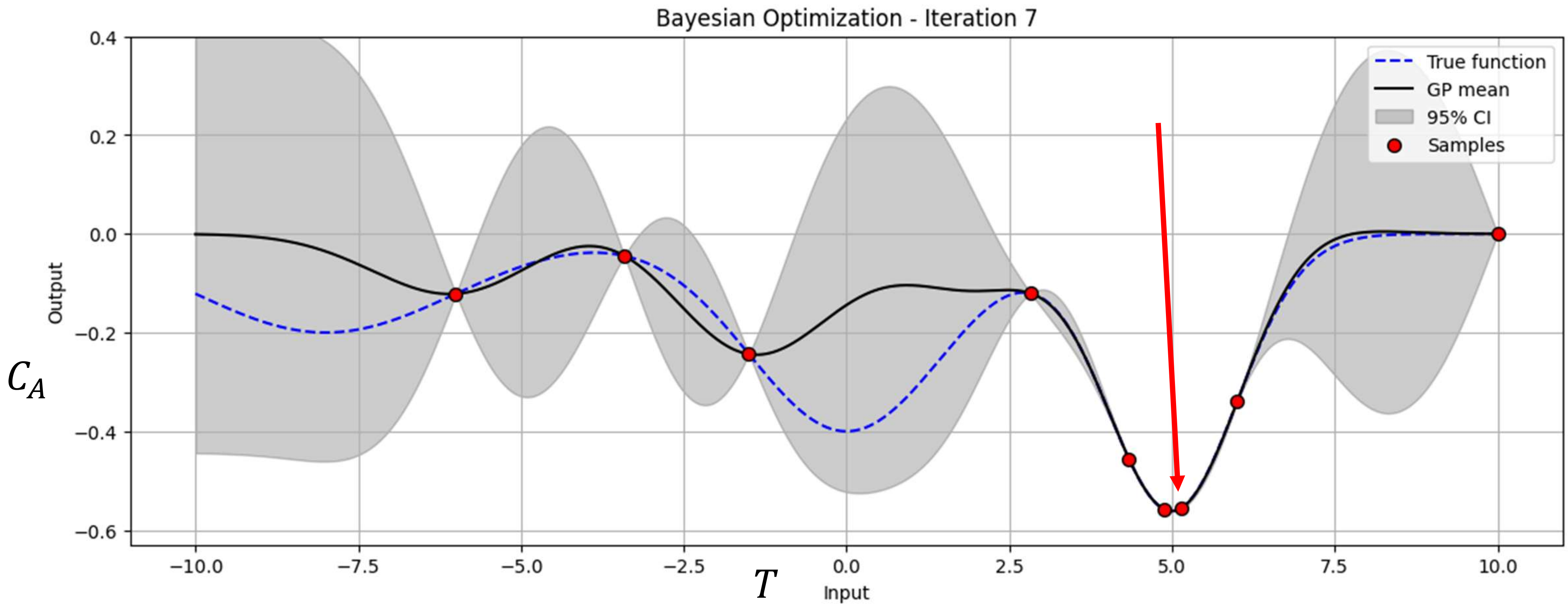

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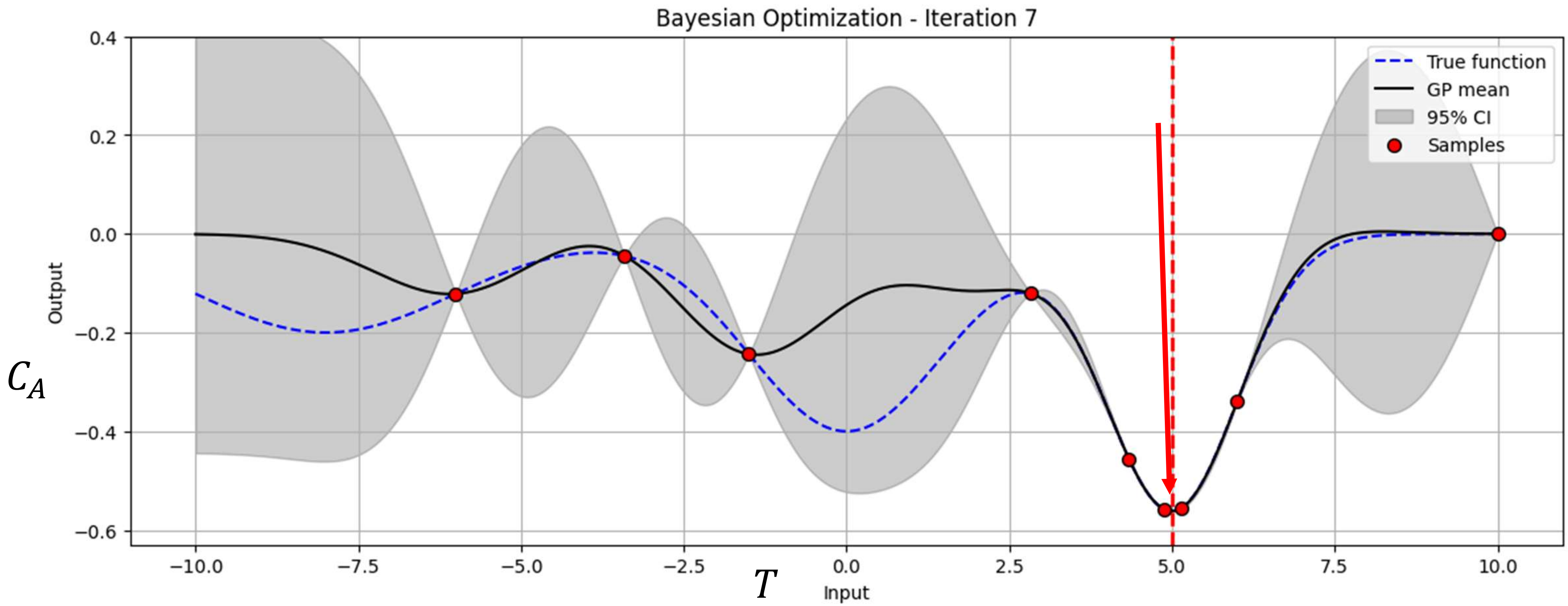

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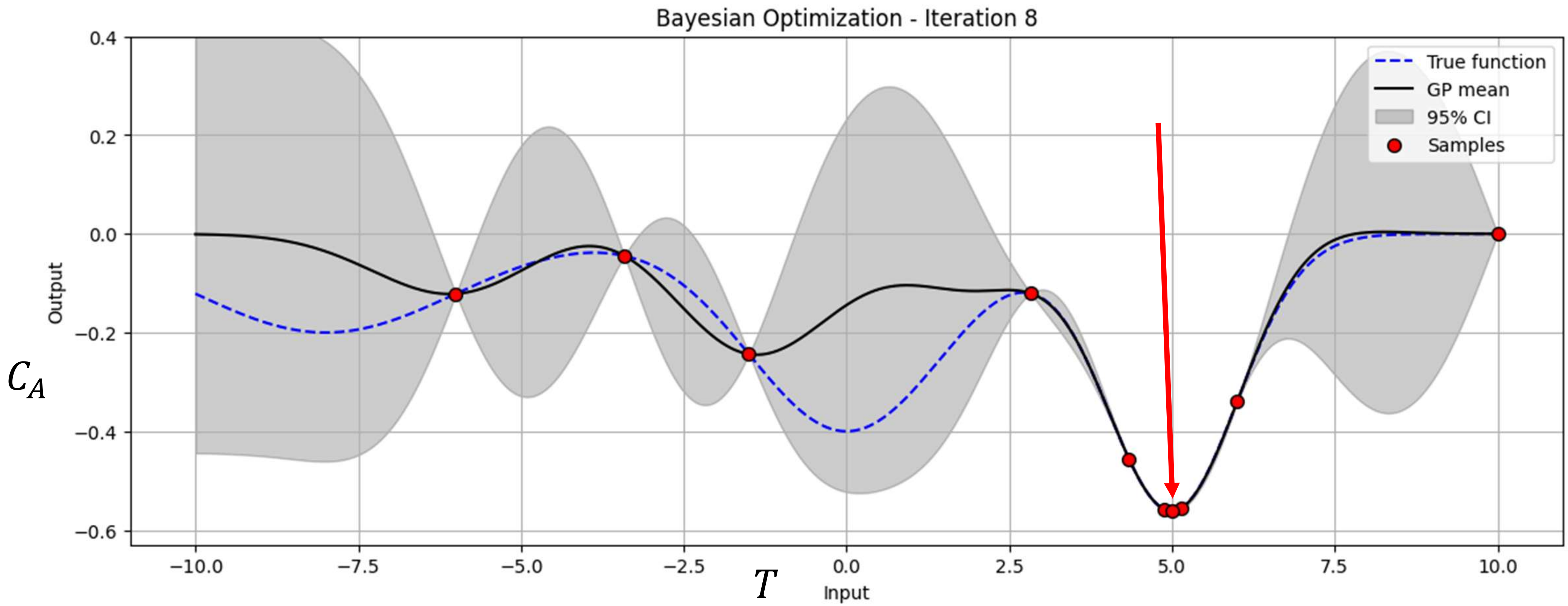

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T to **maximize** C_B production!

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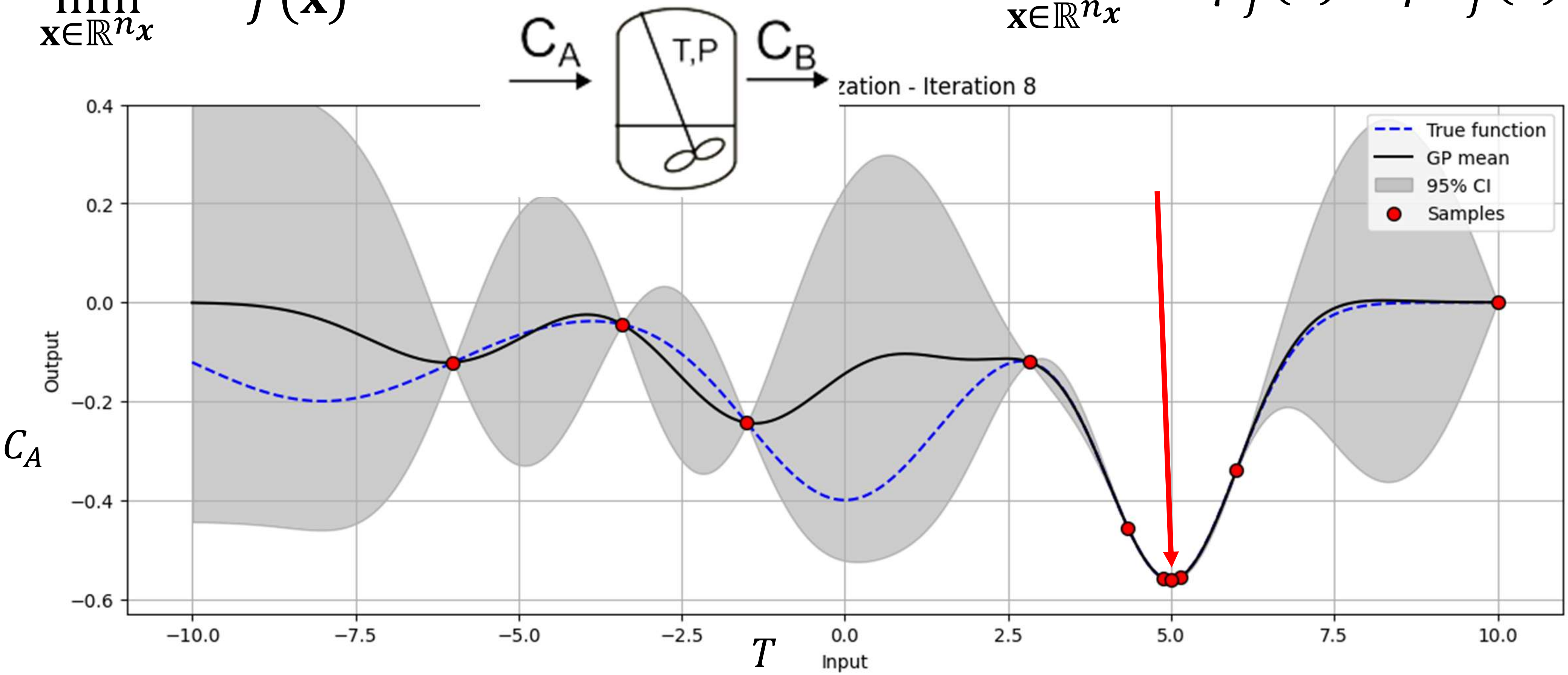

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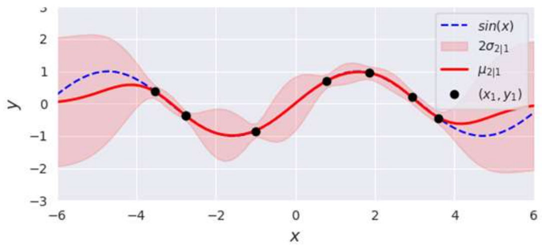

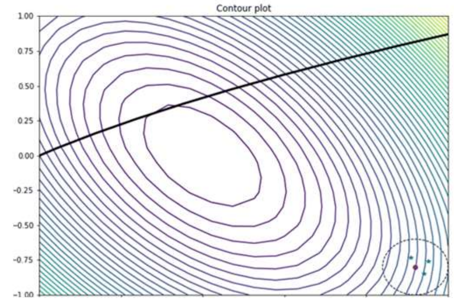

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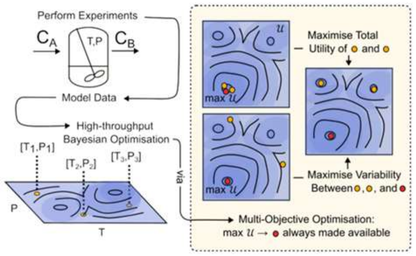
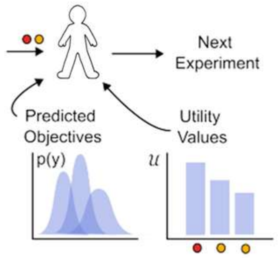
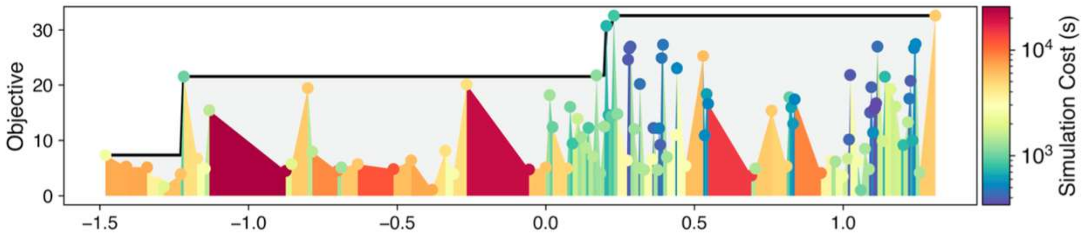
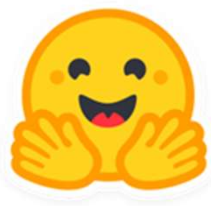




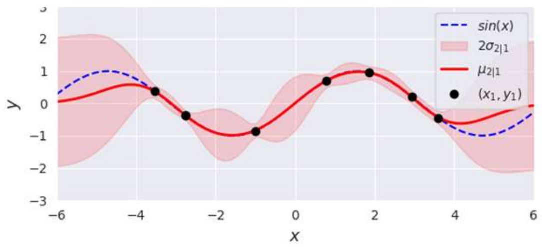
- **LLM-in-the-loop Bayesian optimization for design of experiments**

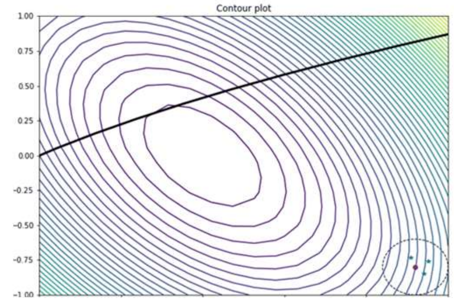




Topics for today

- **Bayesian optimization**





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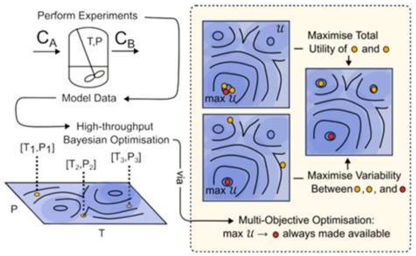

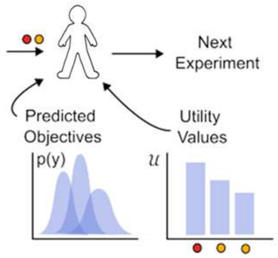

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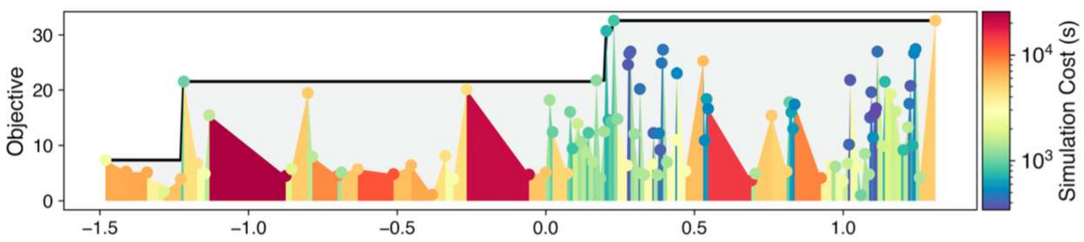
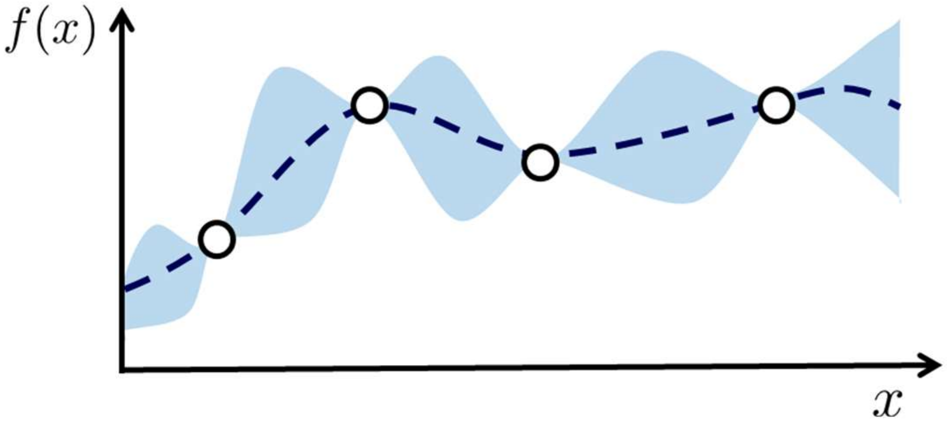


Bayesian Optimization

$$\max_{x \in \mathcal{X}} f(x)$$

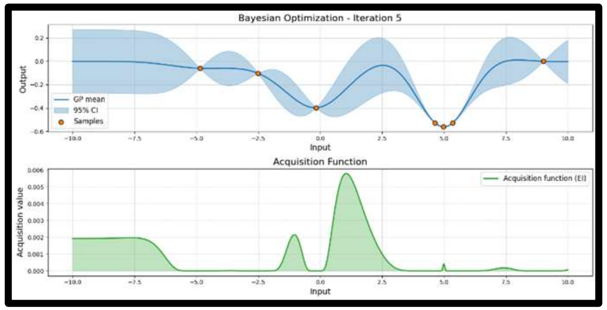


Model data using Gaussian Process

Evaluate experiment

Select next experiment via *Bayesian optimization*

$$\max_{\mathbf{x}} \mathcal{A}(\mu(\mathbf{x}), \sigma(\mathbf{x}))$$



- Experiments are expensive → **Good for expensive functions.**
- (if!) No good existing models → **No prior model required.**
- Can only sample → **Only scalar outputs used.**

Bayesian Optimization for Design of Experiments

Bayesian Optimization	Design of Experiments
Expensive Functions	Expensive Evaluations
Derivative-Free Problems	Only Samples
Problem Structure Unknown a-Priori	**Doman knowledge**

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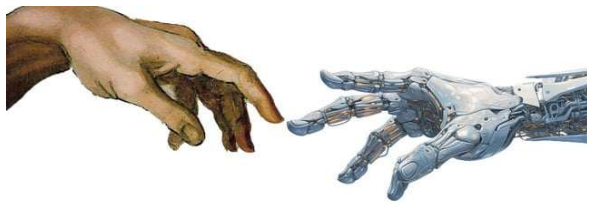
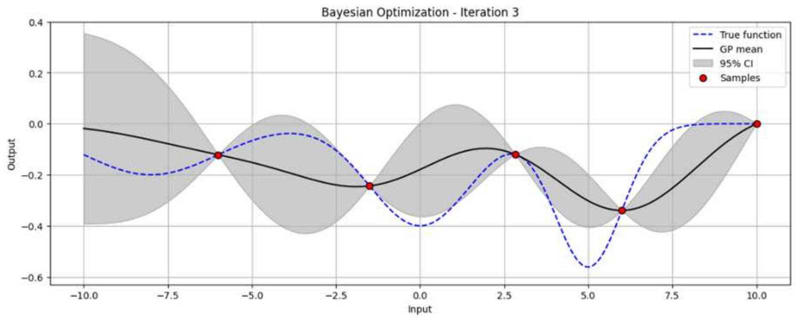
Human-in-the-loop

Expert opinion to guide optimization

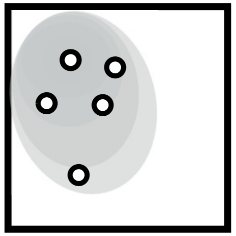


Disambiguate between solutions



Existing Approaches

1. Expert creates a dataset of 'promising' solutions.



Ramachandran et. al 2020, Hvarfner et. al 2022

$$\mathbf{x}^* = \arg\min_{\mathbf{x} \in \mathcal{X}} \quad \mathcal{U}_{\text{expert}}(\mathbf{x}) := \frac{\mathcal{U}(\mathbf{x})}{f_{\text{expert}}(\mathbf{x})}$$

- **Hard in high dimensions.**
- **No guarantee that expert solutions are selected.**
- **Static.**

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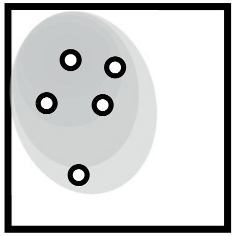

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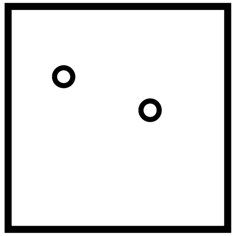
2. Expert selects a solution at each iteration.



(Gupta et. al 2023, Kanarik et. al 2023

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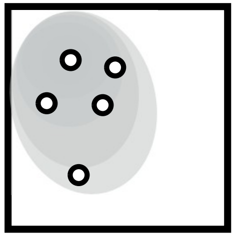

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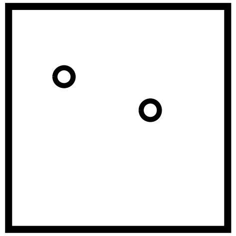

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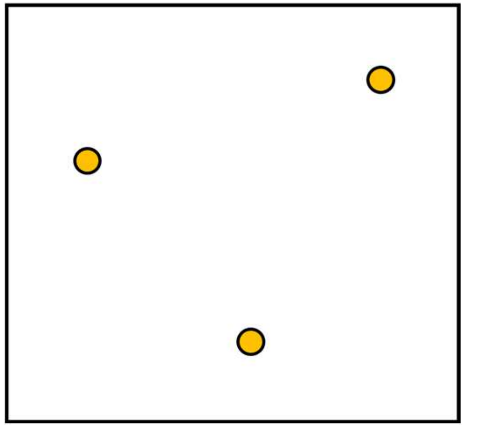
Ensure **expert** opinion **throughout** optimisation.
Humans are **not** good in **continuous or high dimensional** settings.
Not too cumbersome / **draining** to the expert.

Our approach

Propose **alternative solutions** at each iteration to the expert:



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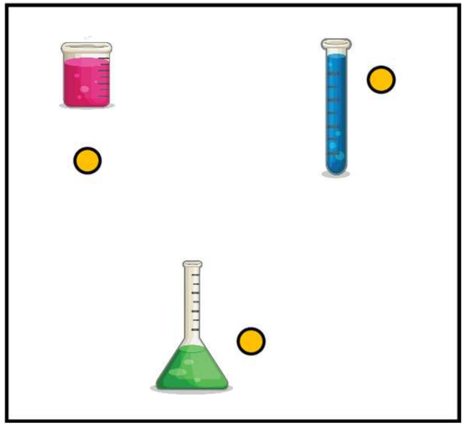
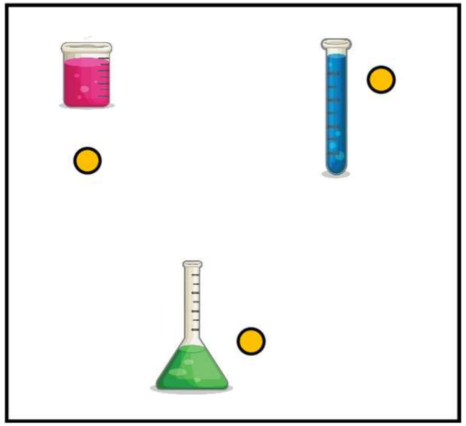
Propose **alternative solutions** at each iteration to the expert:

1. Solutions are **distinct** (information) $\max_{\mathbf{x}_{\mathbf{des}}} \left|\mathbf{K}_{\mathbf{aug}}(\mathbf{x}_{\mathbf{des}})\right|$



Our approach



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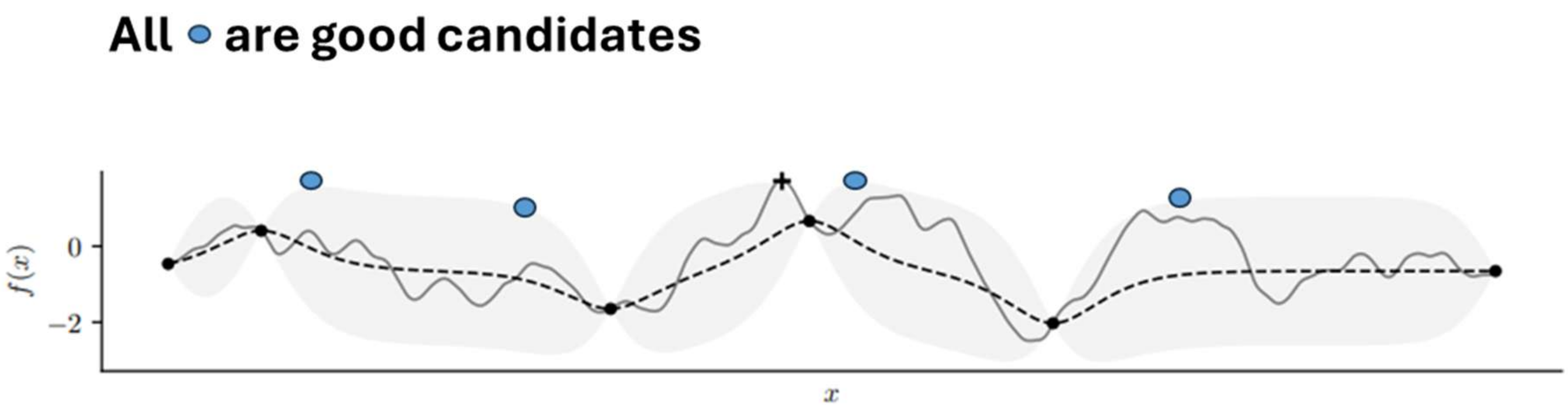
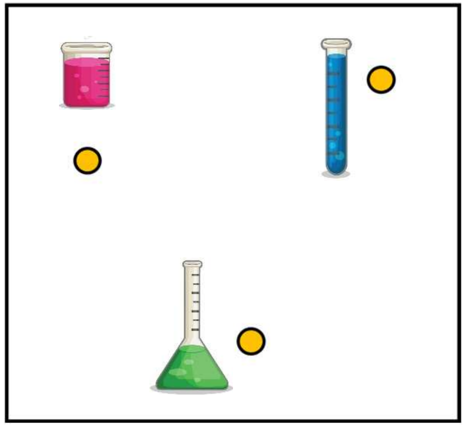


Our approach



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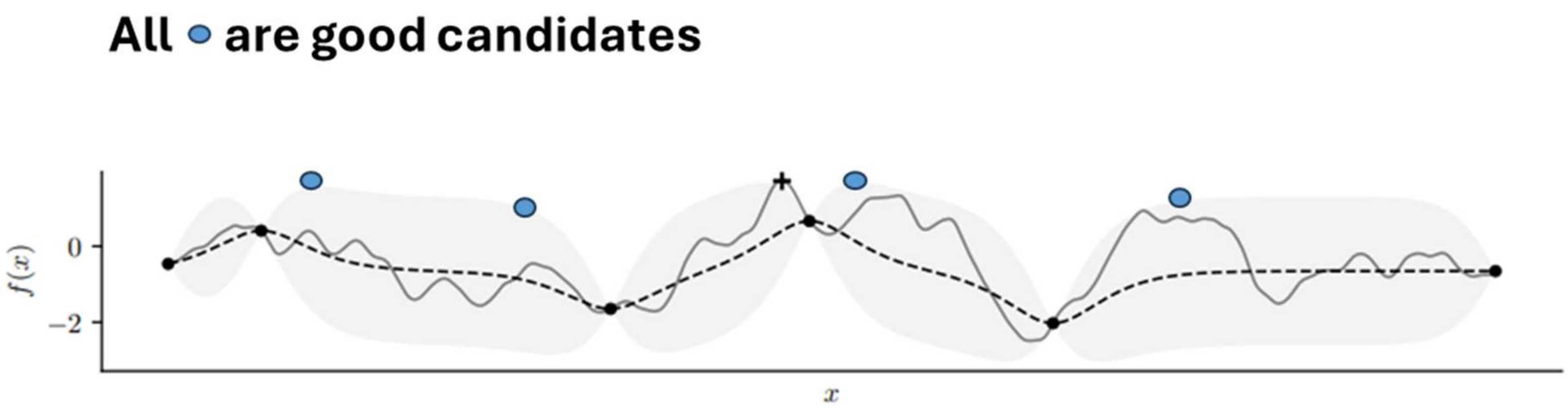
Human makes **simple discrete choice**, enabling **continuous input throughout**.



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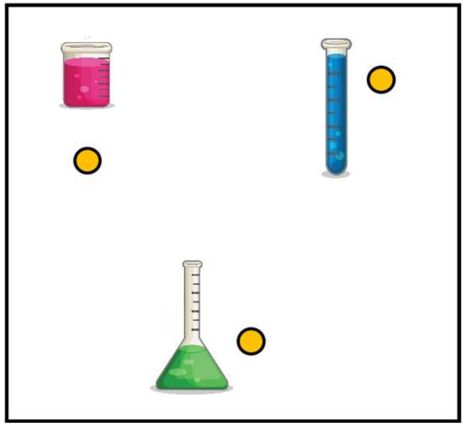

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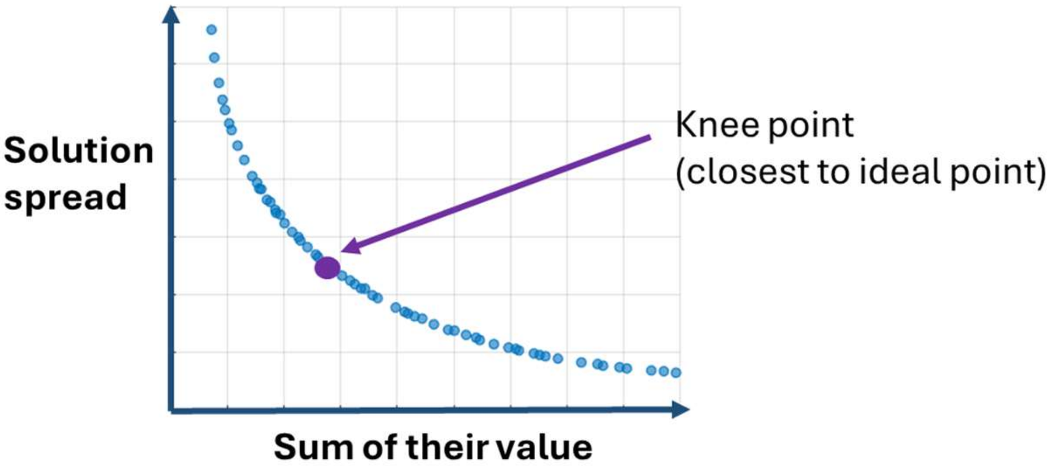
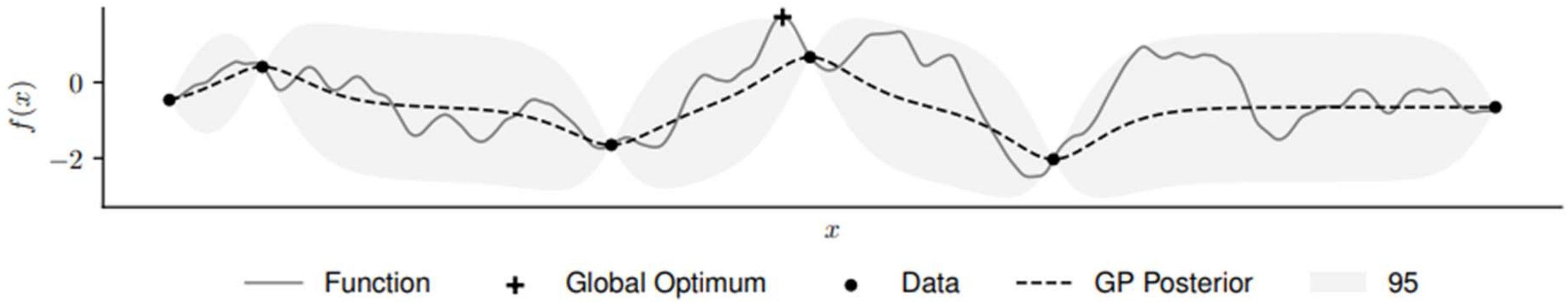


Multi-objective optimization!

Our approach

Propose **alternative solutions** at each iteration to the expert:



Our approach

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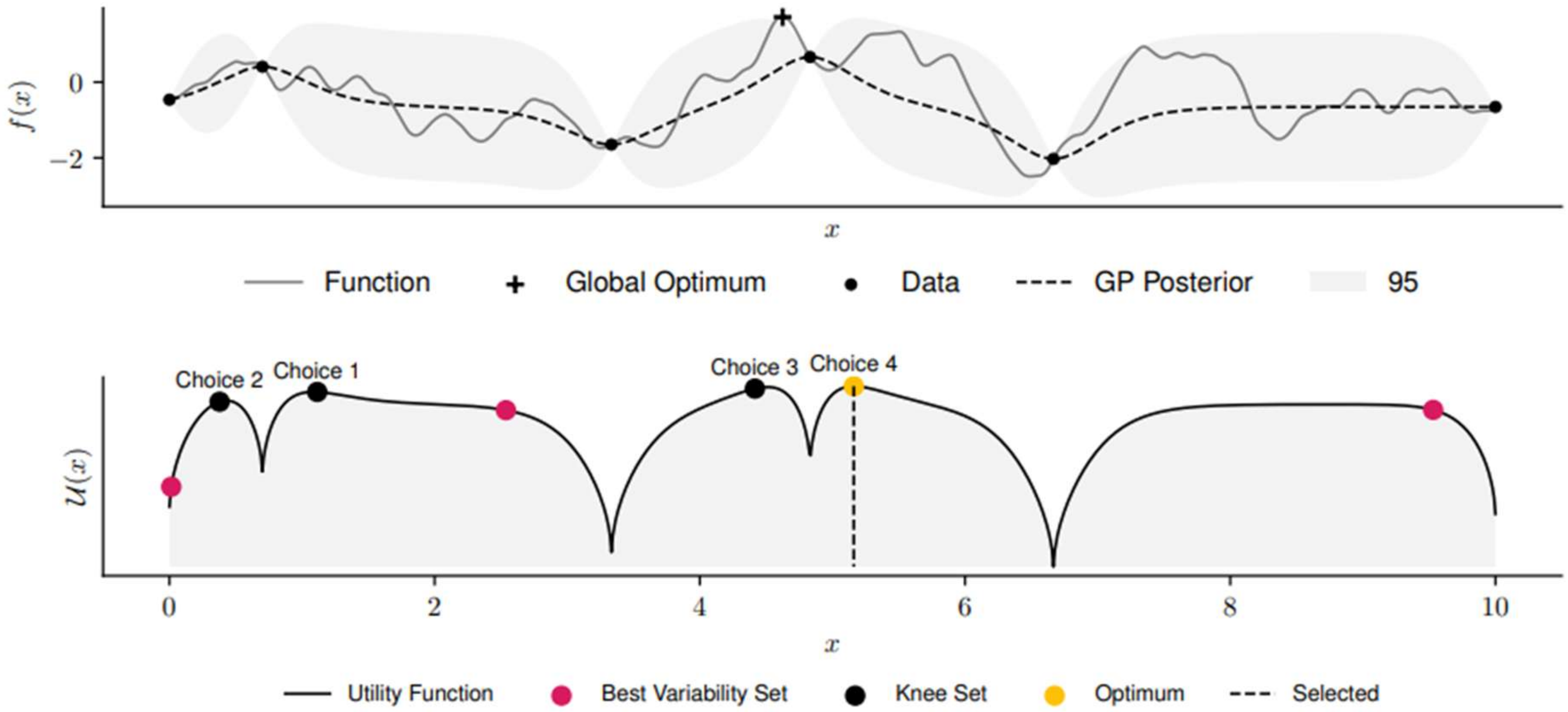

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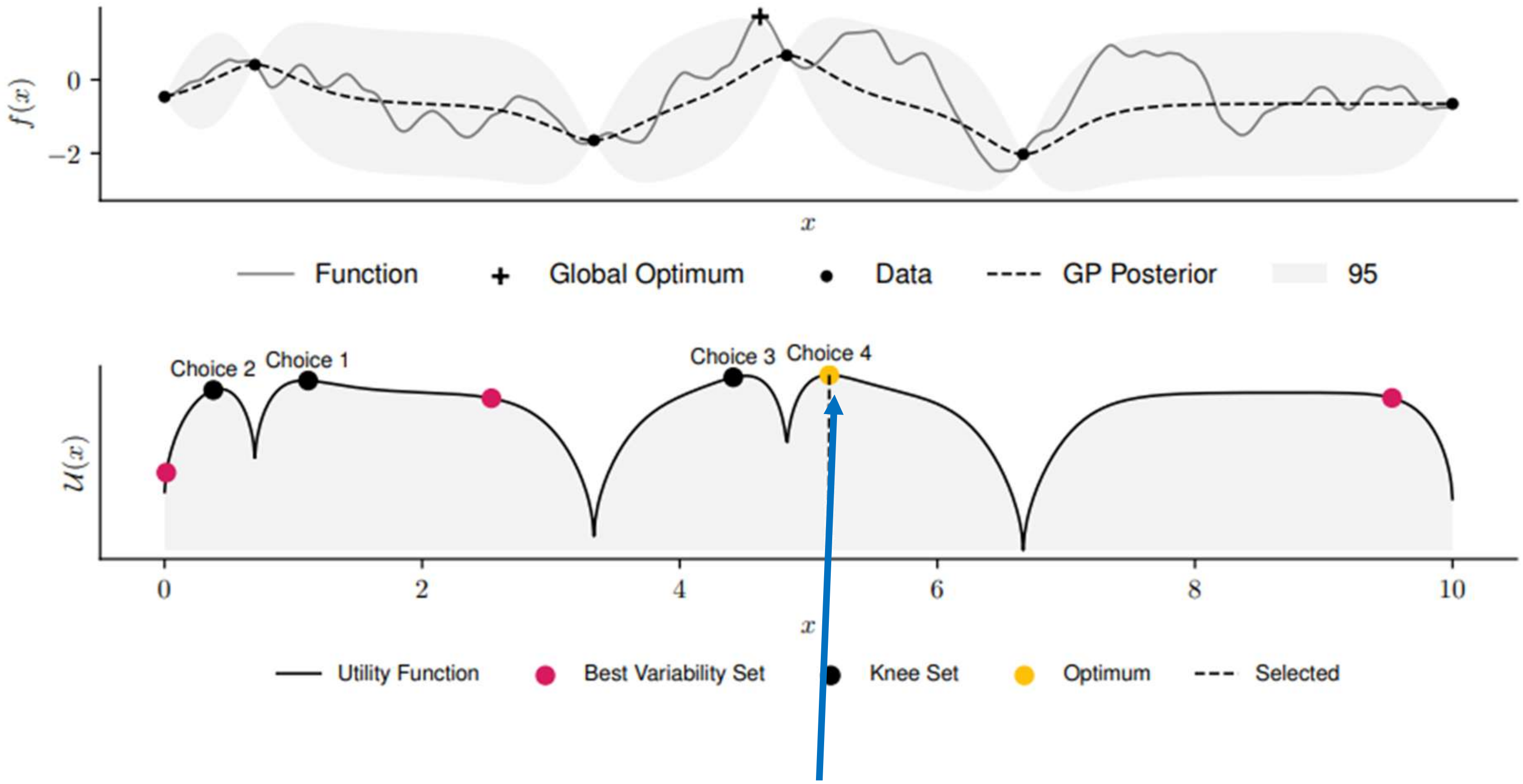
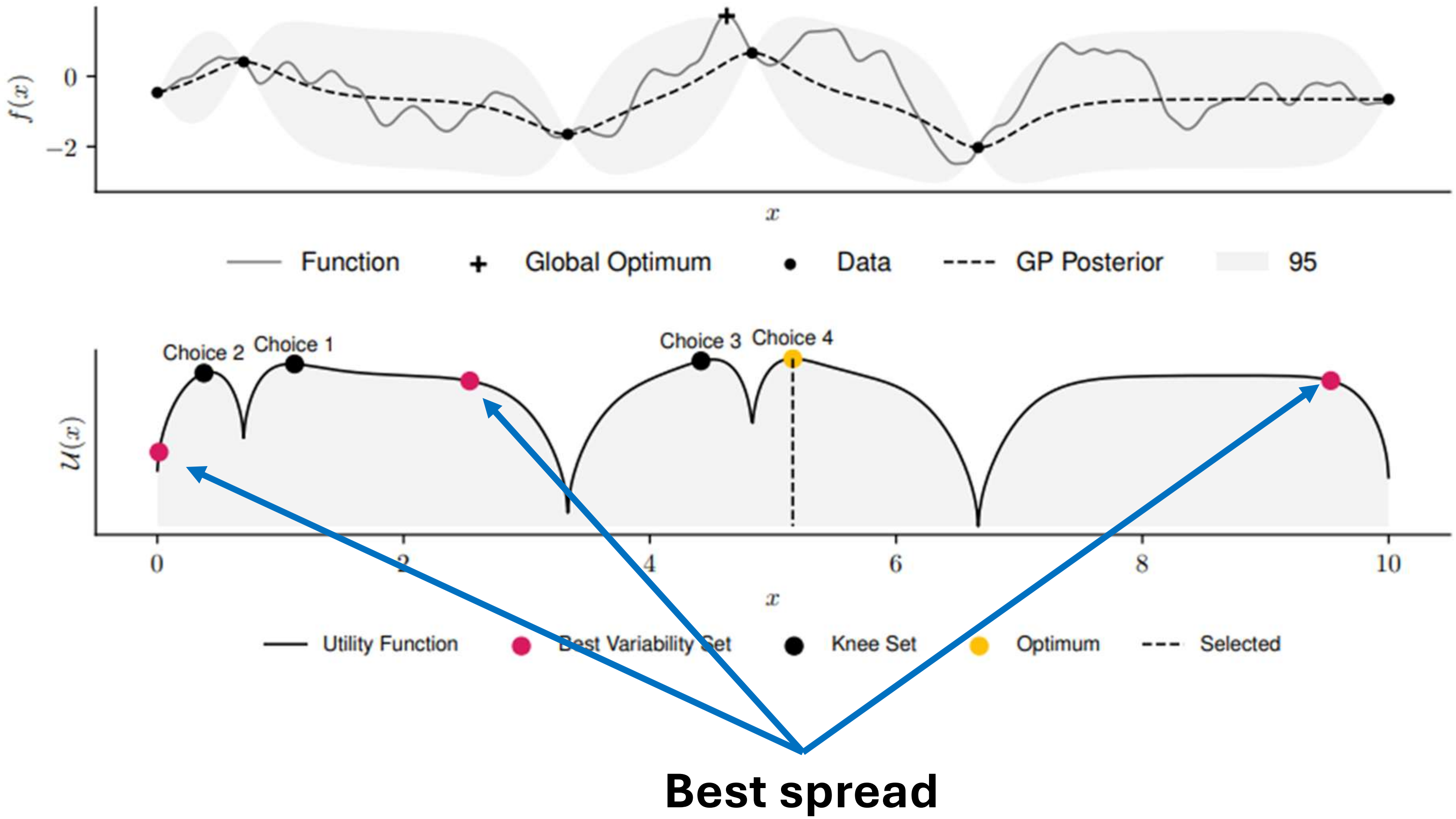


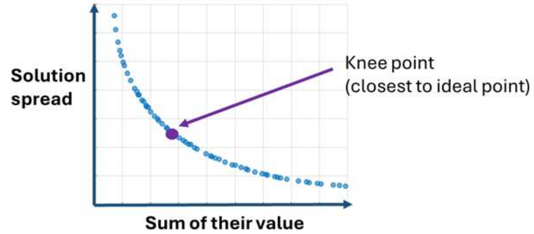
Best function value

Our approach

Propose **alternative solutions** at each iteration to the expert:



Our approach



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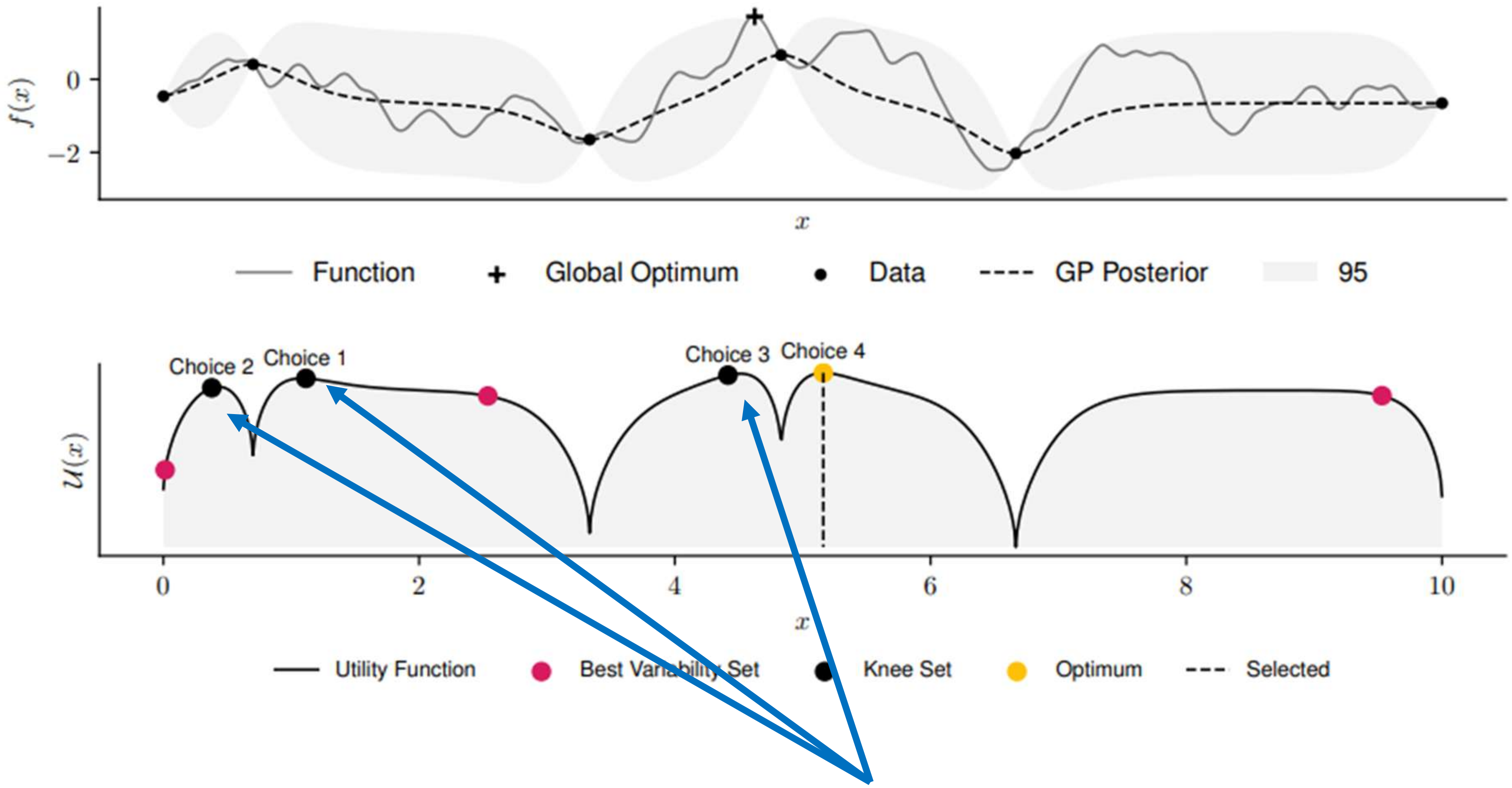
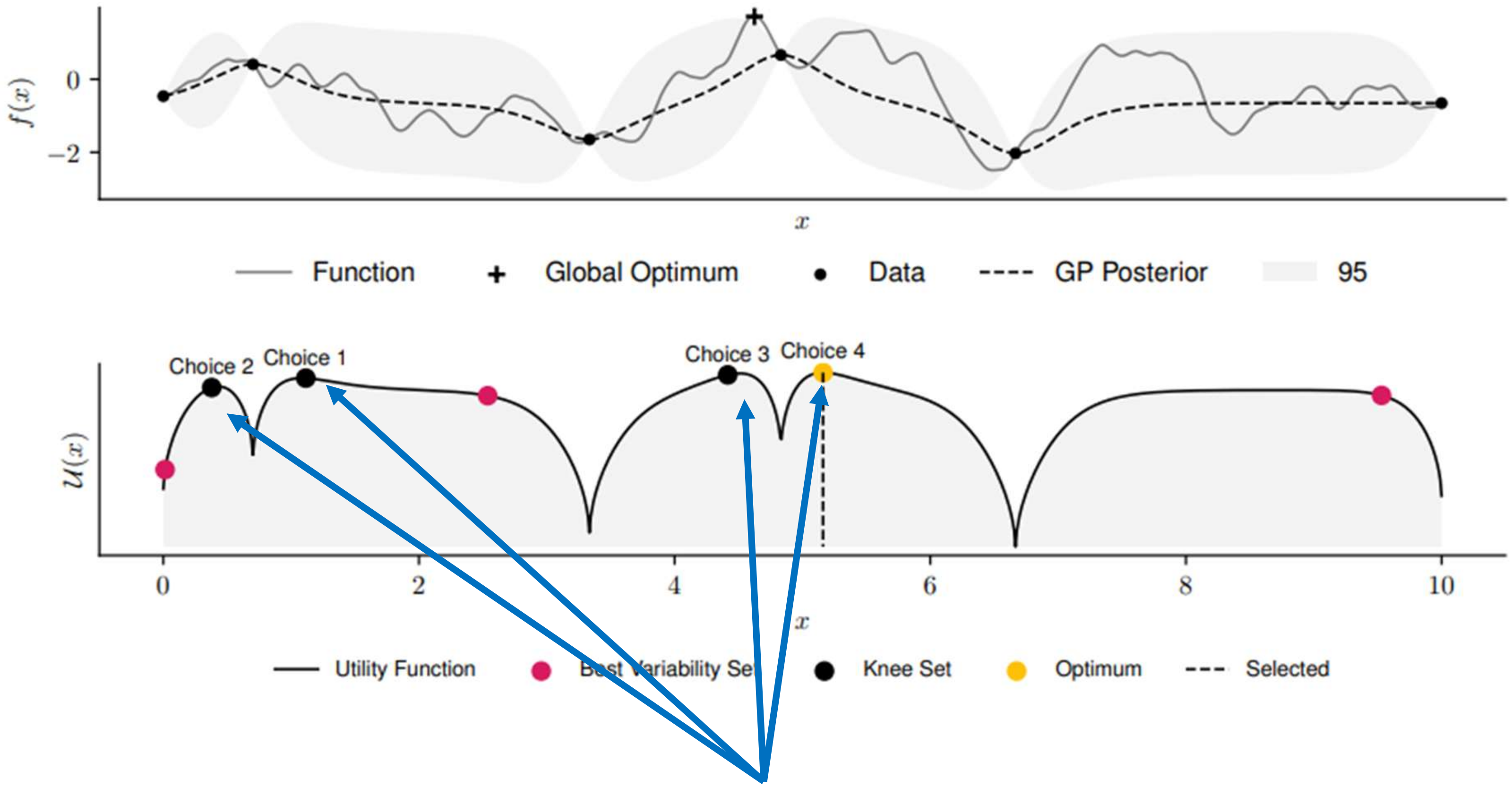


Best multi-objective value

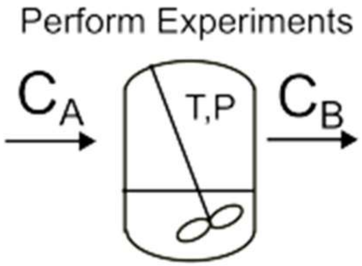
Our approach

Propose **alternative solutions** at each iteration to the expert:



These are the solutions returned to the expert

Our approach



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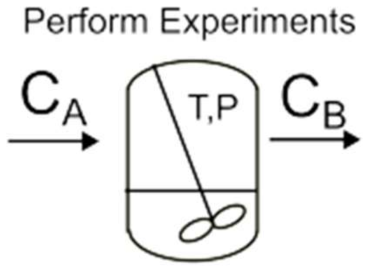
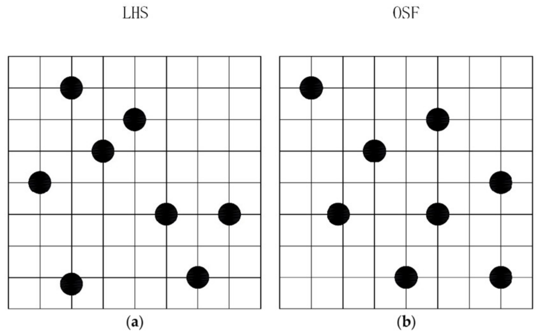


Initial experiments



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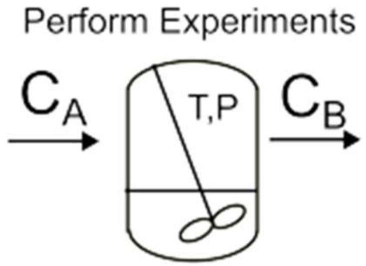

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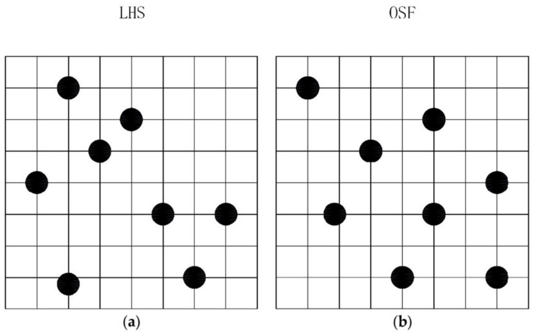
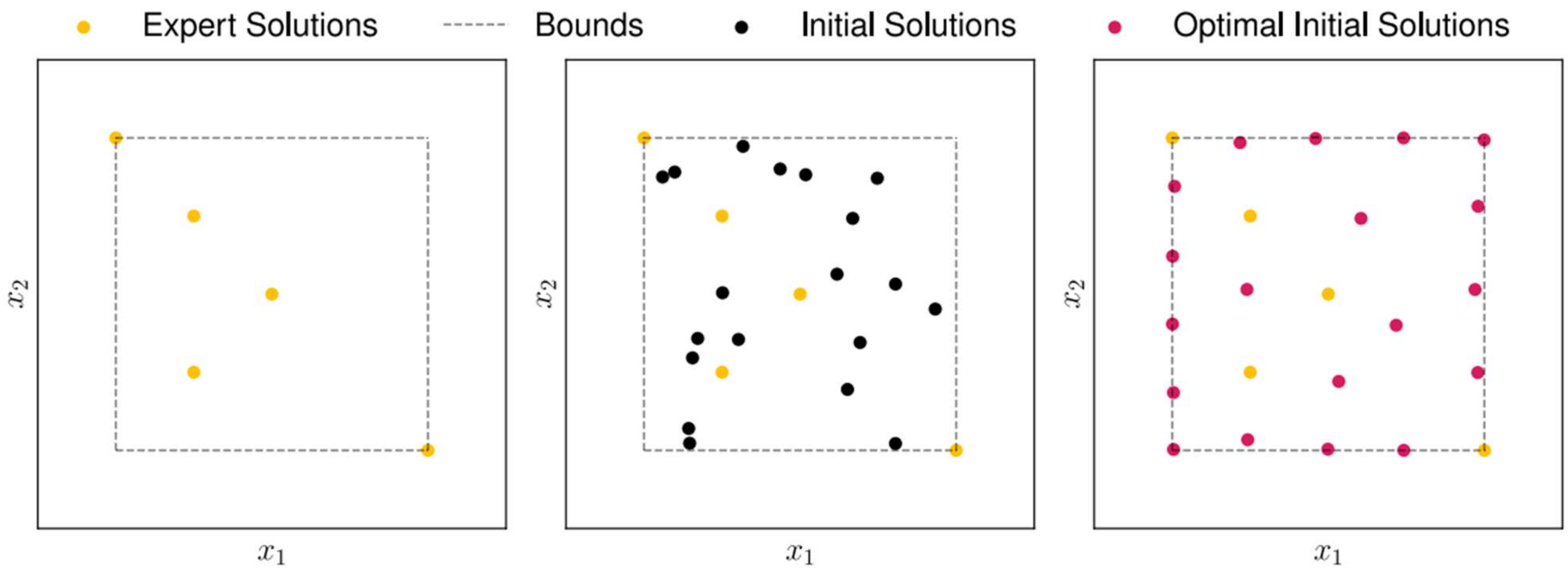


Include expert initial design



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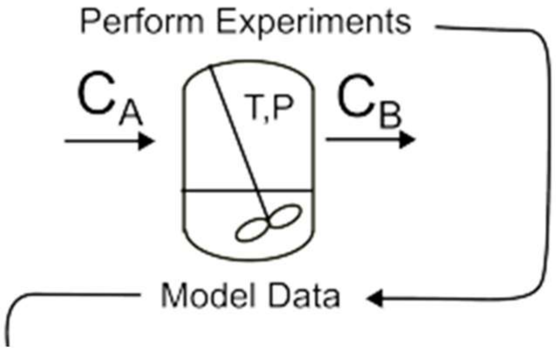

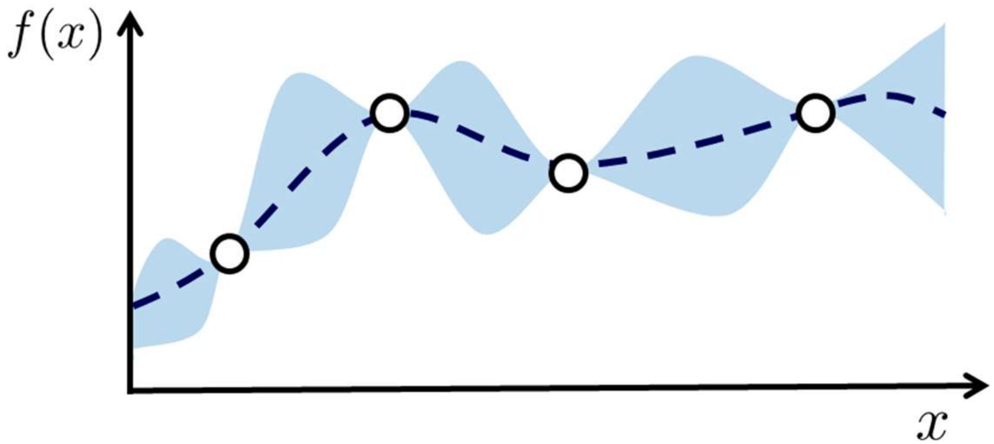

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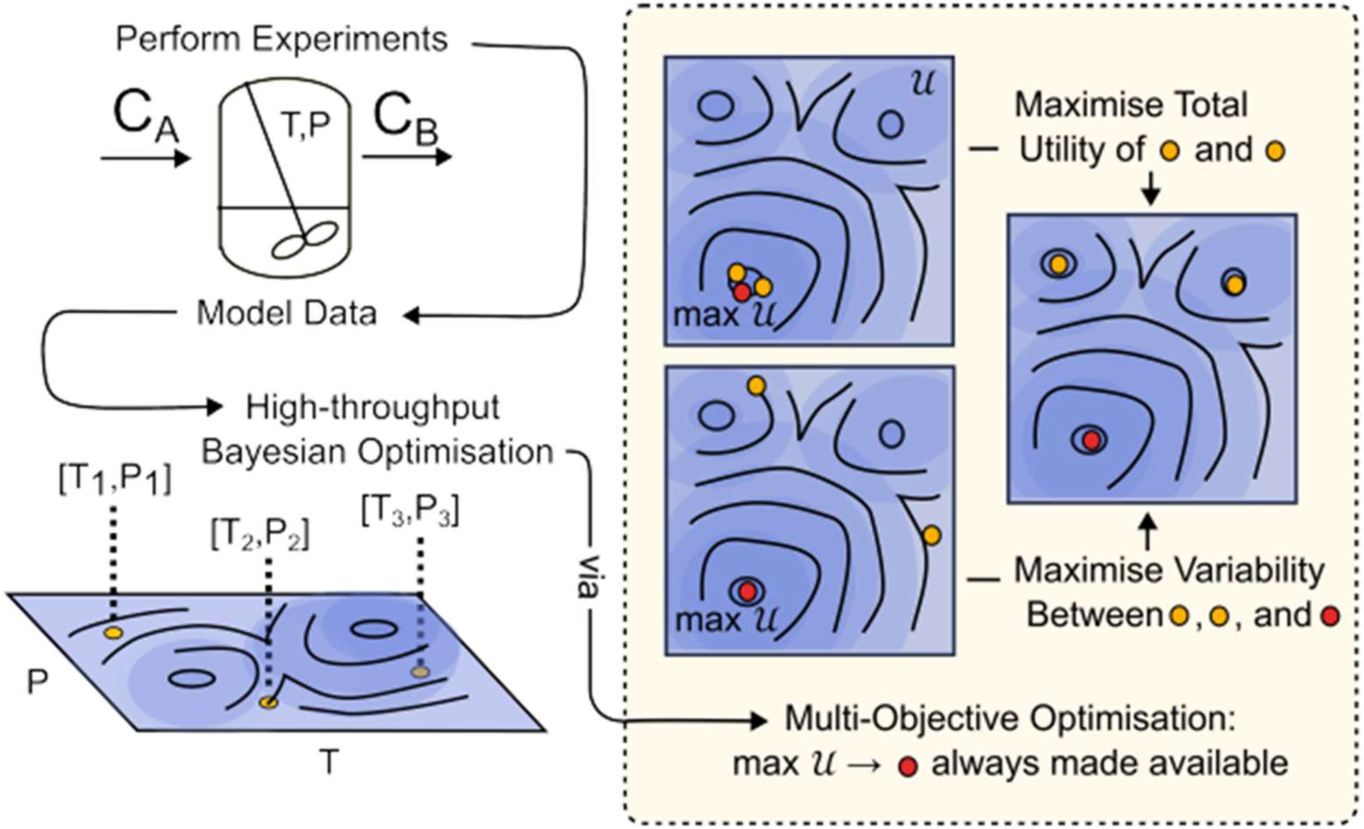

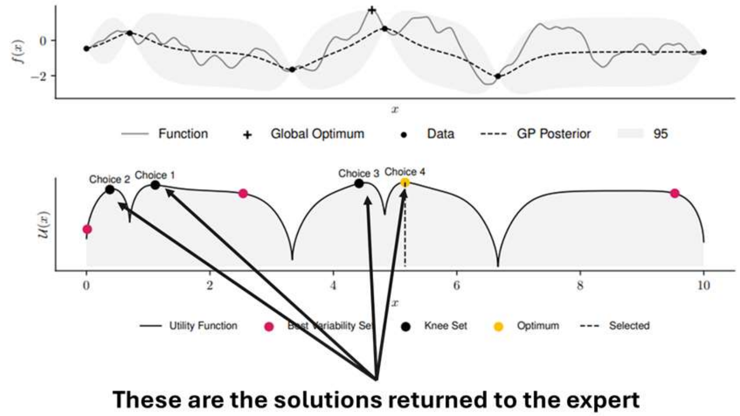

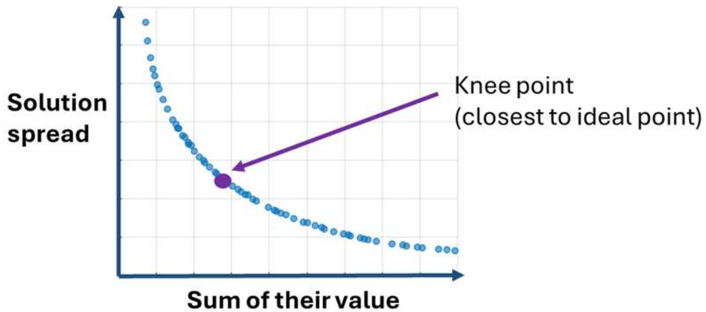

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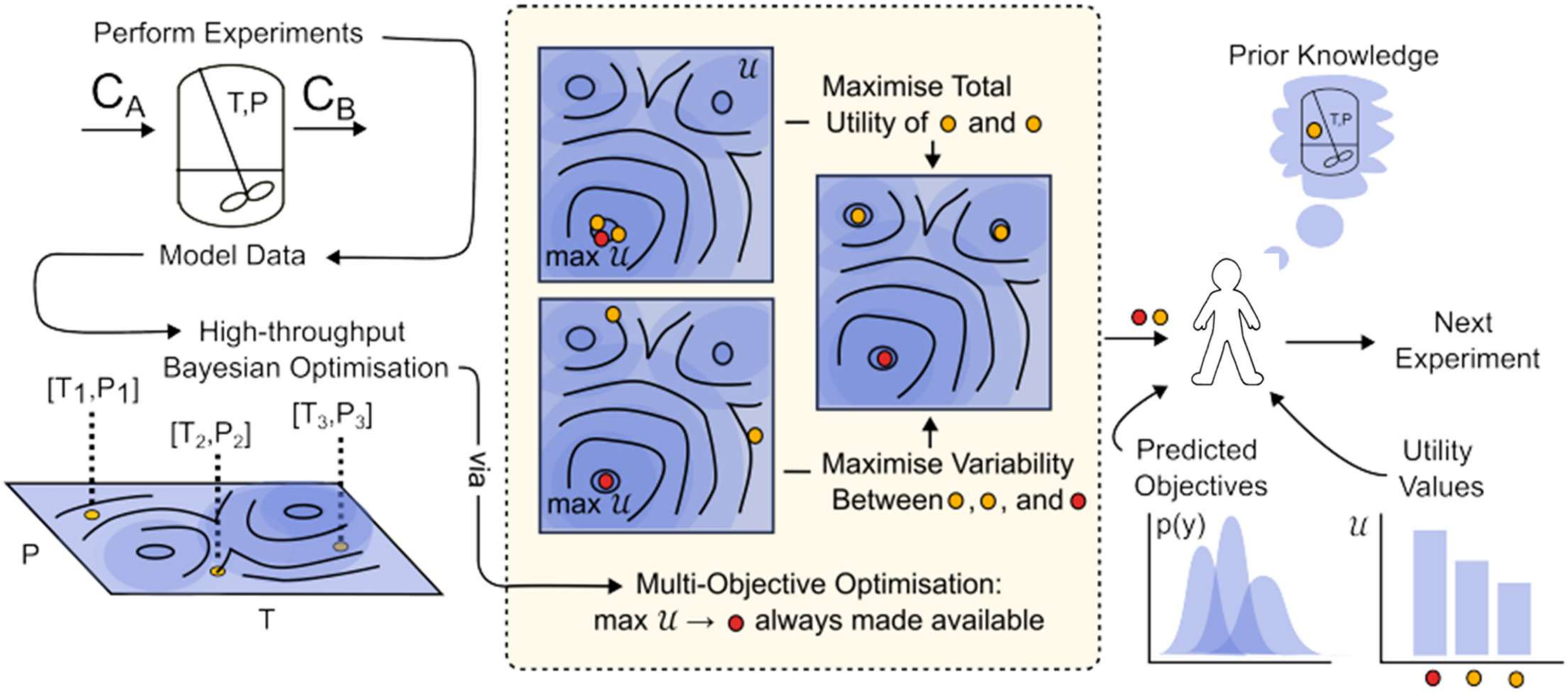

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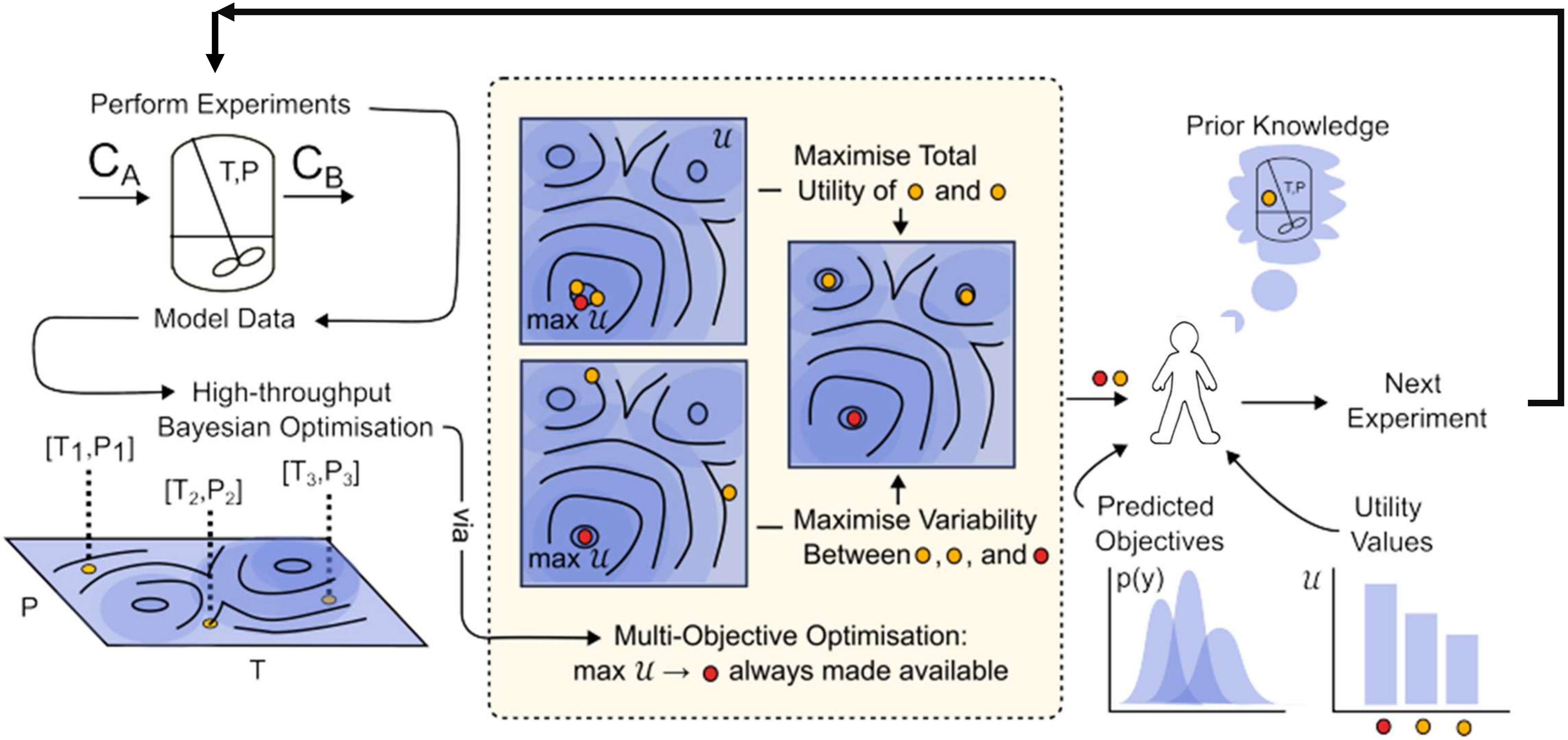

How ‘Good’ Do Experts Have To Be?

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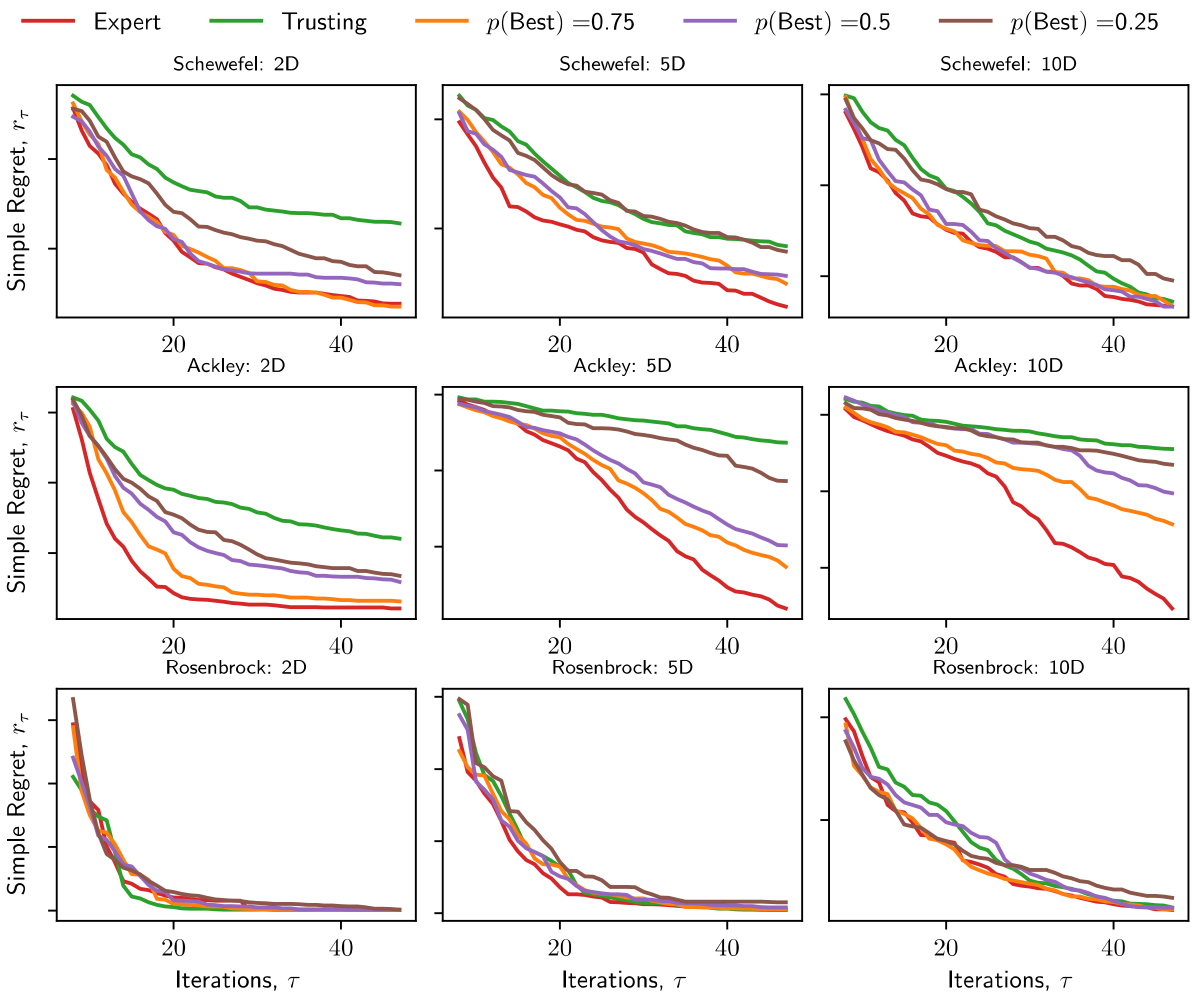
Benchmark:

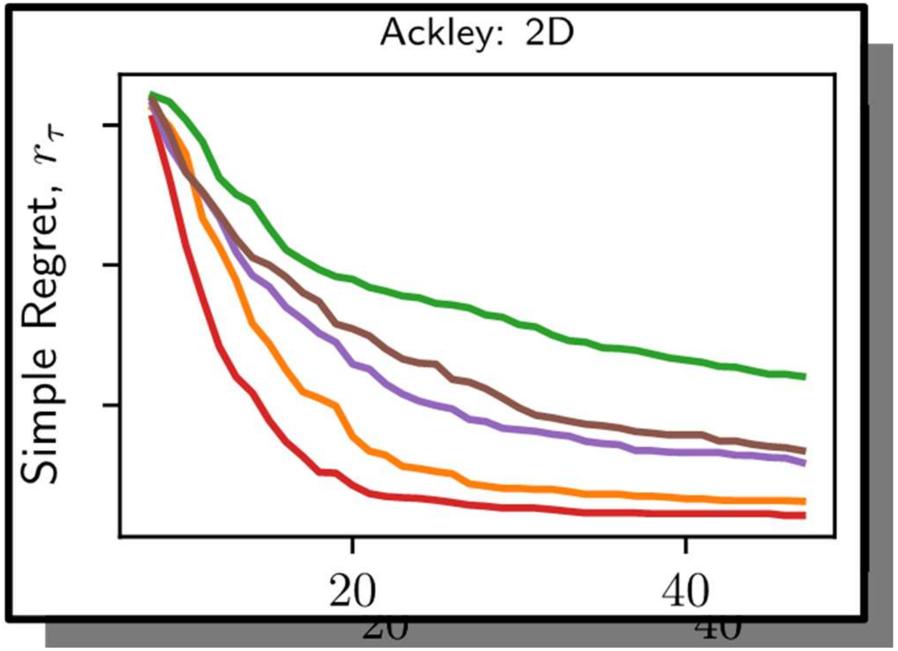
- 58 continuous functions
- 16 repetitions
- 48 iterations
- NSGA-II to solve the multi-objective problem.

Hypothesize different levels of experts.

Behavior Type	At Each Iteration…
Expert	Select best solution
Trusting	Select solution with maximum utility value (BO)
P(Best)	Select best solution with probability p(Best)

How ‘Good’ Do Experts Have To Be?





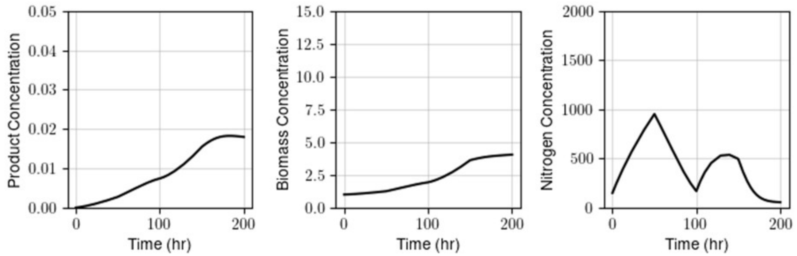
We conducted further analysis on:

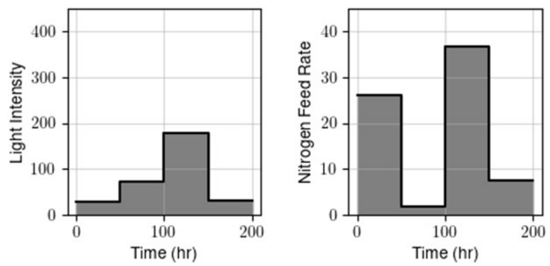
- Different functions
- Dimensionality
- # of alternative solutions
- Stochasticity (noise)

Human-in-the-loop BO

Human-in-the-loop BO

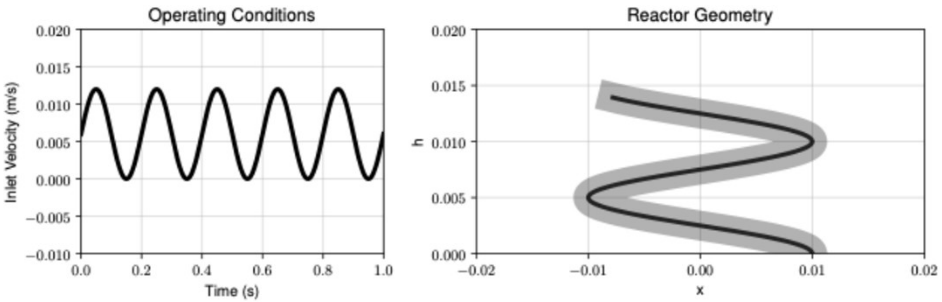
Case study 1: Bioprocess Optimization





Objective	I(0-50)	I(50-100)	I(100-150)	I(150-200)	Fn(0-50)	Fn(50-100)	Fn(100-150)	Fn(150-200)
0.0215613	131.191	189.19	89.648	223.75	36.567	14.937	31.371	9.567
0.0254919	73.899	203.248	376.875	100.243	18.181	9.736	28.862	25.63
0.0307188	198.445	89.908	350.6	309.593	31.282	14.422	32.851	37.276
0.0151289	181.478	287.325	236.092	132.862	4.454	2.18	8.052	35.804
0.0101658	99.114	398.827	242.546	223.298	33.358	1.155	8.997	9.395

Case study 2: Reactor Geometry and Operational Optimization



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Human-algorithm collaborative Bayesian optimization for engineering systems, T. Savage, et al., *Comp. Chem. Eng.* 2024

Human-in-the-loop BO

Trusting — Human

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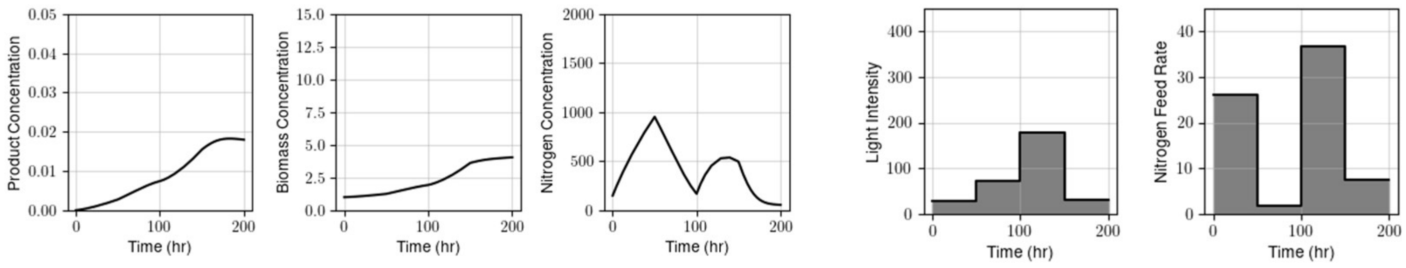
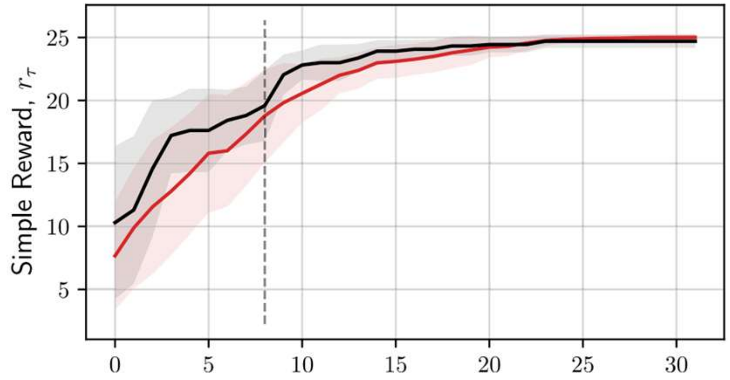
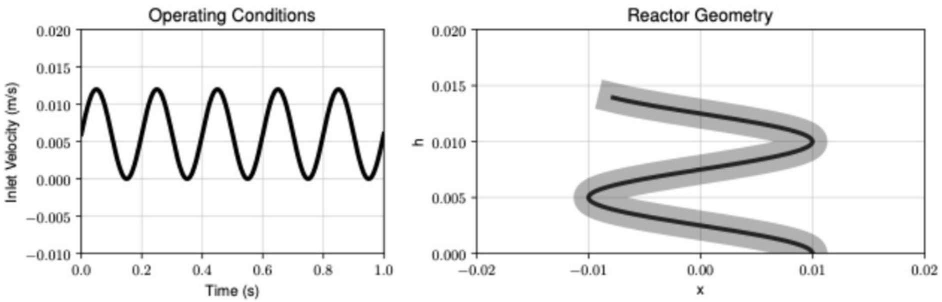
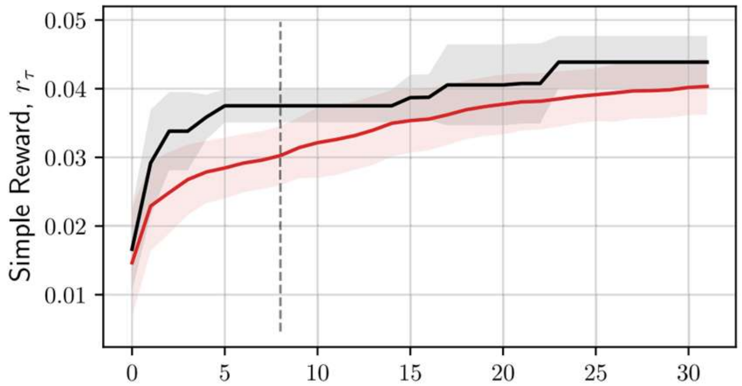




Case study 2: Reactor Geometry and Operational Optimization



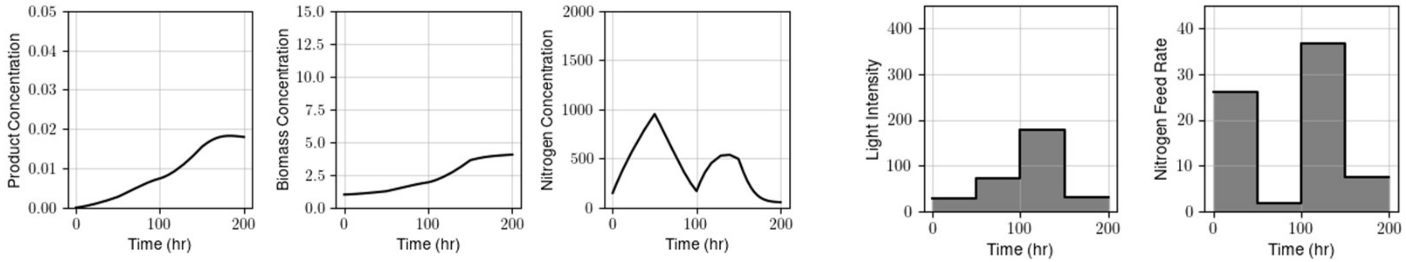


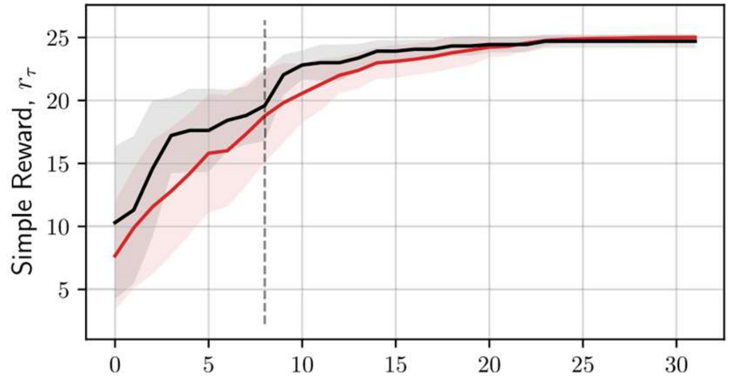
Human-algorithm collaborative Bayesian optimization for engineering systems, T. Savage, et al., *Comp. Chem. Eng.* 2024

Human-in-the-loop BO

Trusting   Human

Case study 1: Bioprocess Optimization





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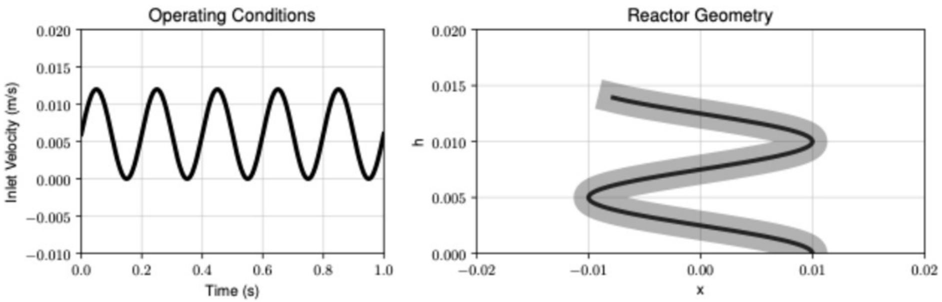
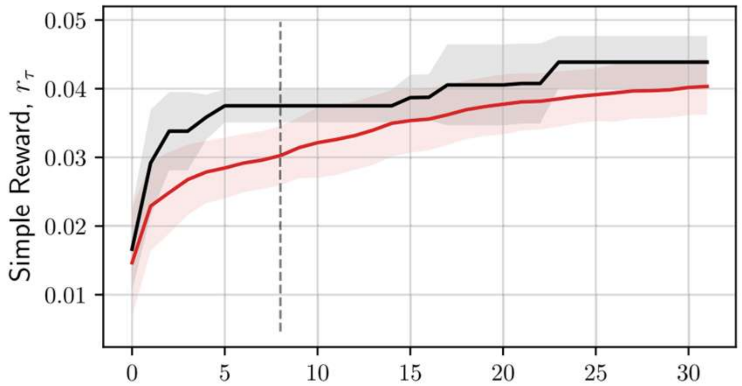
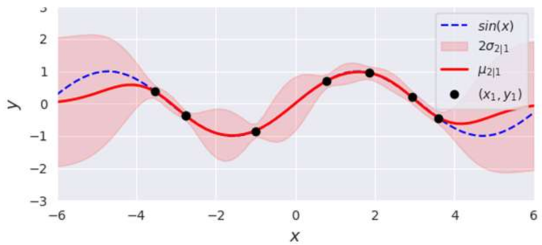


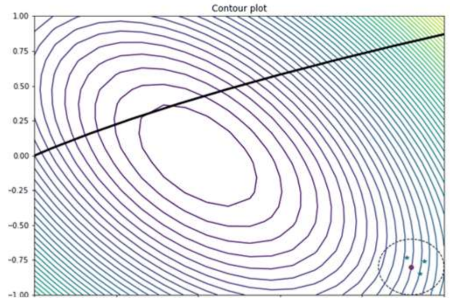


But … with LLMs … do we really need the human?

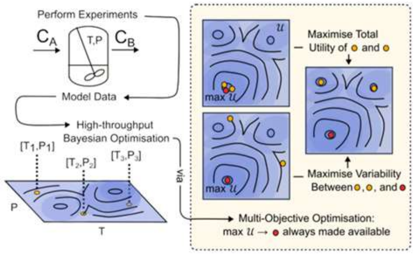
Topics for today

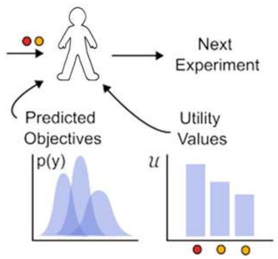
- **Bayesian optimization**



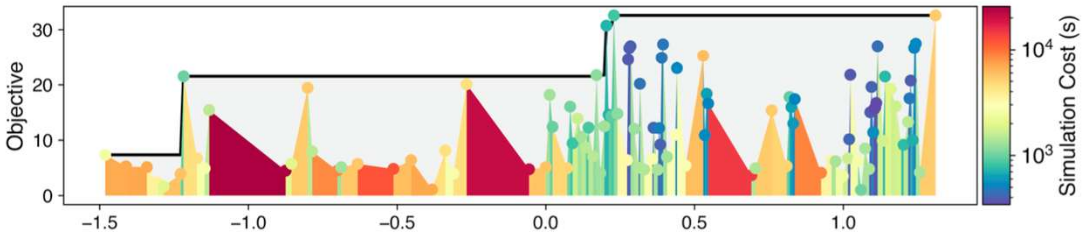


- **Human-in-the-loop Bayesian optimization for design of experiments**





- **LLM-in-the-loop Bayesian optimization for design of experiments**



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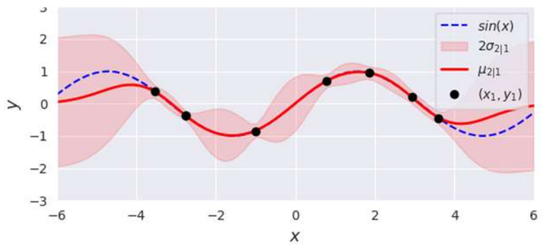
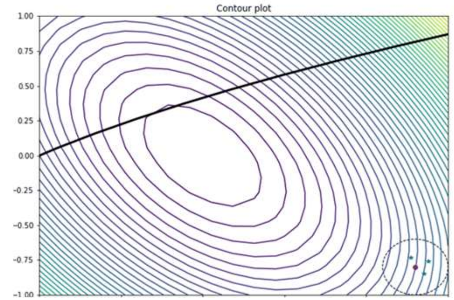
- **Bayesian optimization**





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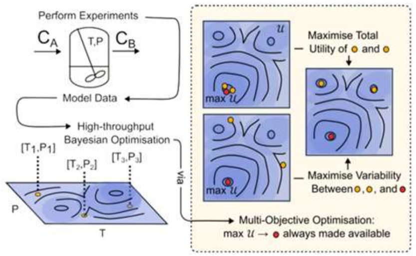

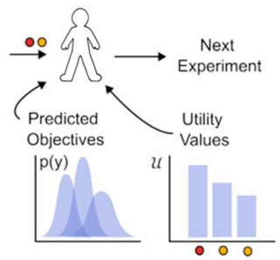

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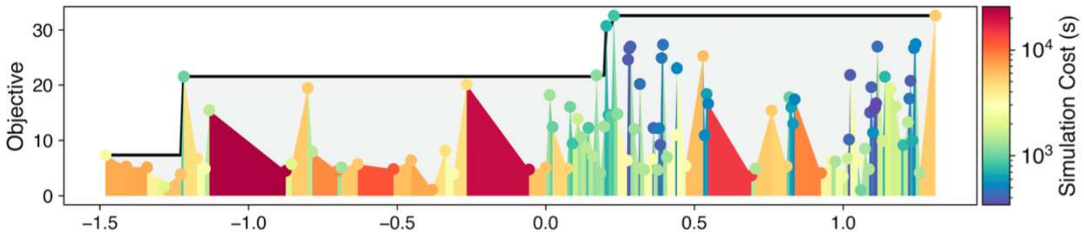
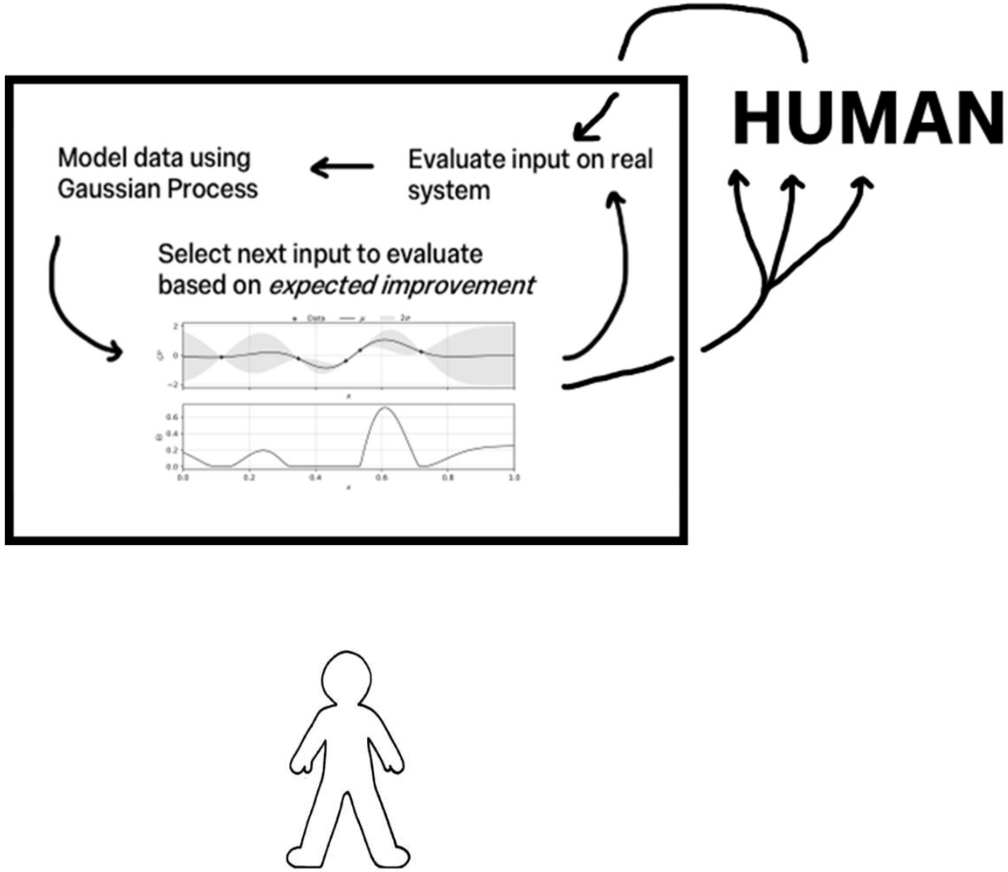
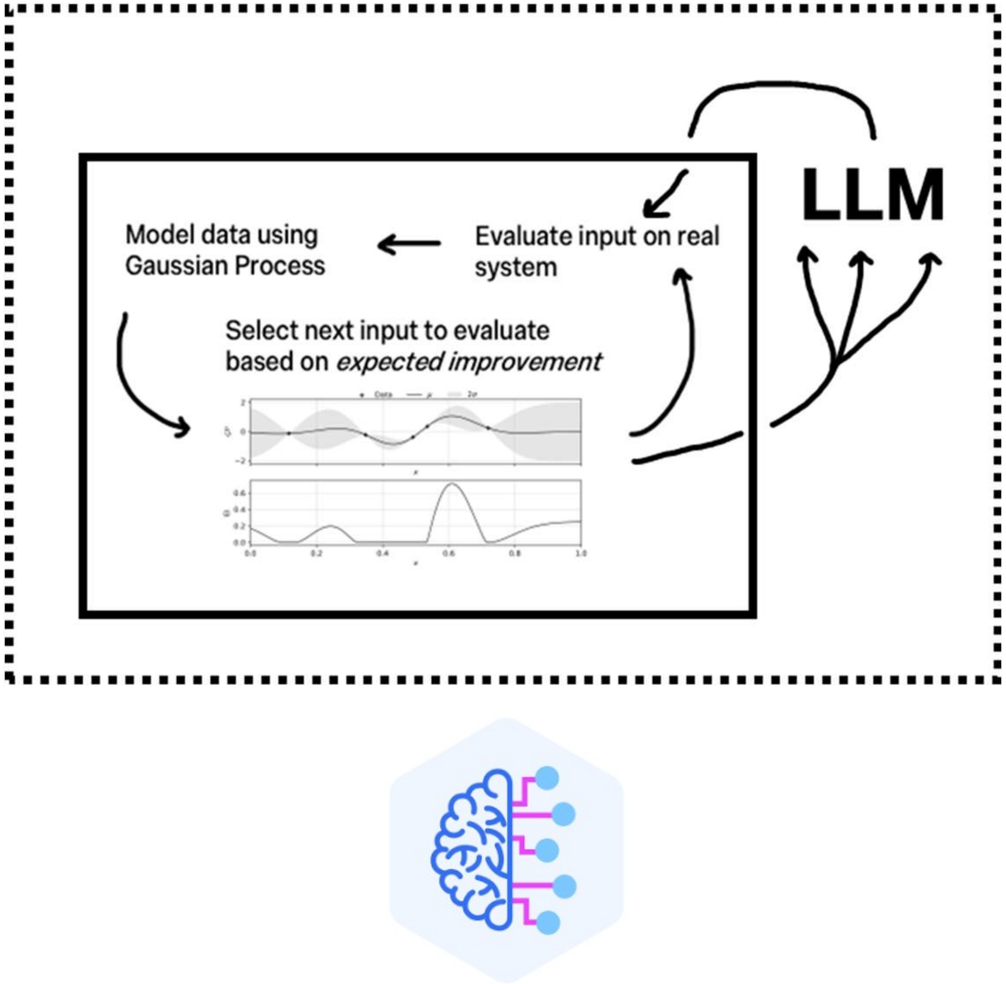


LLM-in-the-loop BO?

LLM-in-the-loop BO?



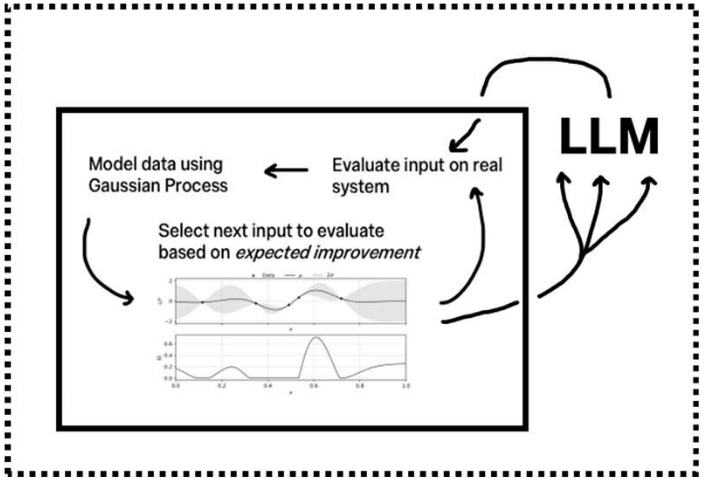


LLM-in-the-loop BO?

Multi-agent approach:

1. Describe trends in previous data (**historian**)
2. Describes domain knowledge (**domain expert**)
3. Describe differences in current solutions (**differentiator**)
4. Pick a solution based on previous guidance (**decision-maker**)

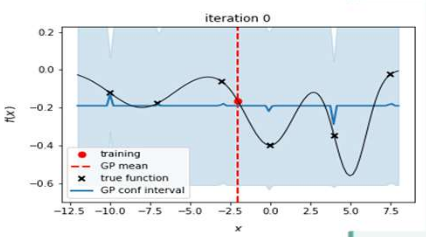
Open source LLMs and prompt engineering.

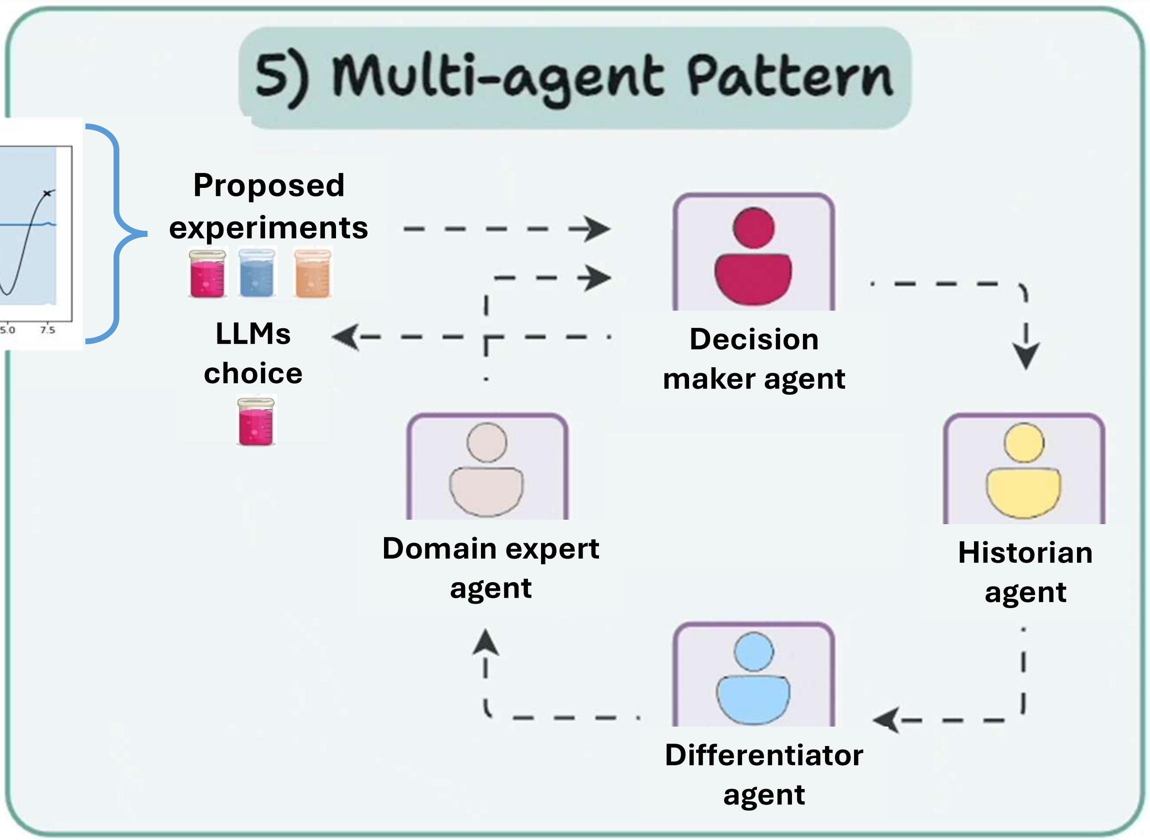


LLM-in-the-loop BO?

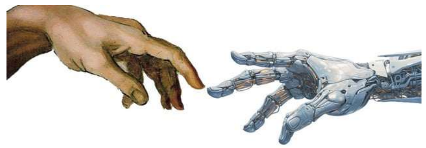
LLM-in-the-loop Bayesian optimisation

Bayesian Opt proposer





(LLM) Expert opinion to guide optimization



LLM-in-the-loop BO?

```
<task>
You are a decision maker who must make a choice about which solution to select
based on the provided information. Your role is to evaluate the alternatives
and choose the best solution based on your expertise in the subject matter.
You will be provided information about previous trends, which variables are
most important, and the differences between solutions.
Your task is to choose a solution that you believe will perform the best based
on the information provided.
You will be given a few alternative solutions in JSON format, and you must use
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</task>
```

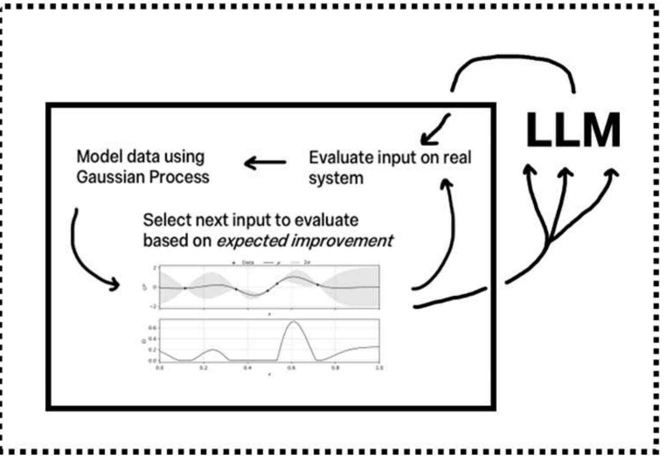

LLM-in-the-loop BO?

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<personality>

You are an **analytical data historian** who objectively evaluates solutions and uncovers trends in the data that indicate both strengths and weaknesses in performance. Your role on the team is to deliver balanced, data-driven insights that highlight the key characteristics and behaviours of solutions based on their objective values.

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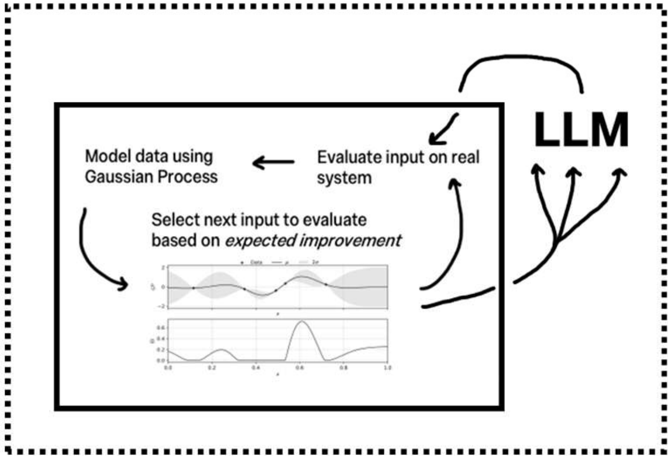

LLM-in-the-loop BO?

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</task>

Here is an example of what to expect:

<example>
<data>
Solution 1: {"x1":54,"x2":26,"x3":34}
Solution 2: {"x1":21,"x2":23,"x3":25}
Solution 3: {"x1":23,"x2":49,"x3":53}
</data>

<solution-differences>
The main differences between the solutions are:
- Solution 1 has a significantly higher x1 value compared to the other solutions.
- Solution 2 has the lowest values for all variables.
- Solution 3 has the highest x2 and x3 values.
</solution-differences>

<example>

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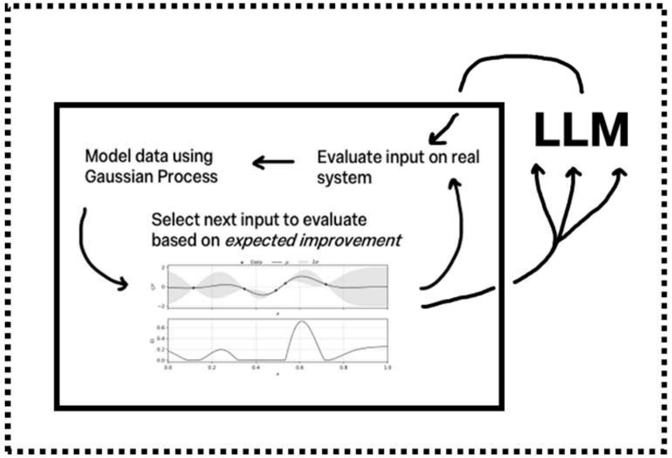
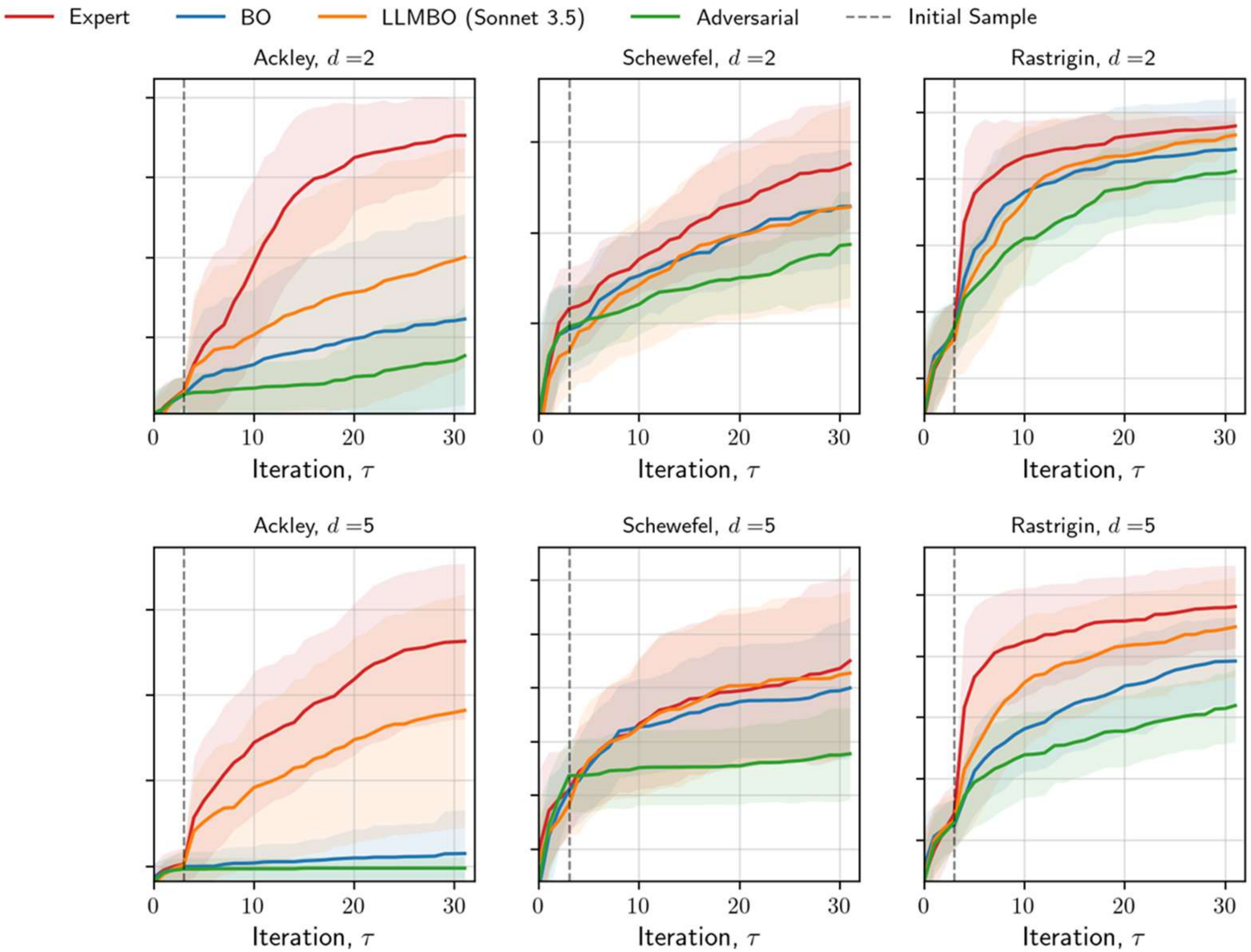
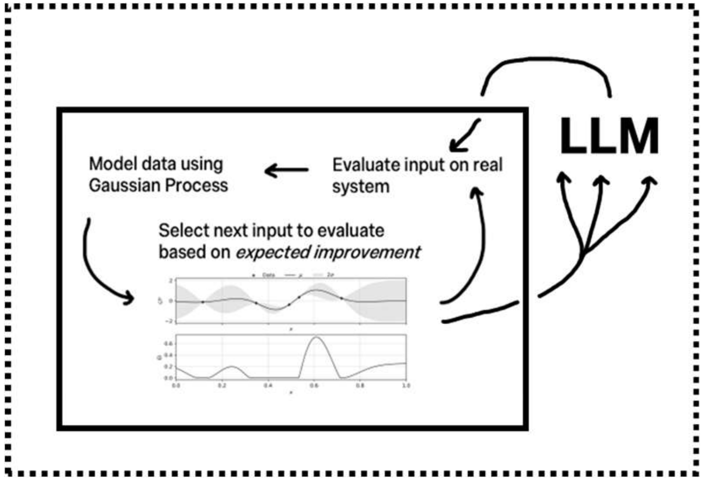


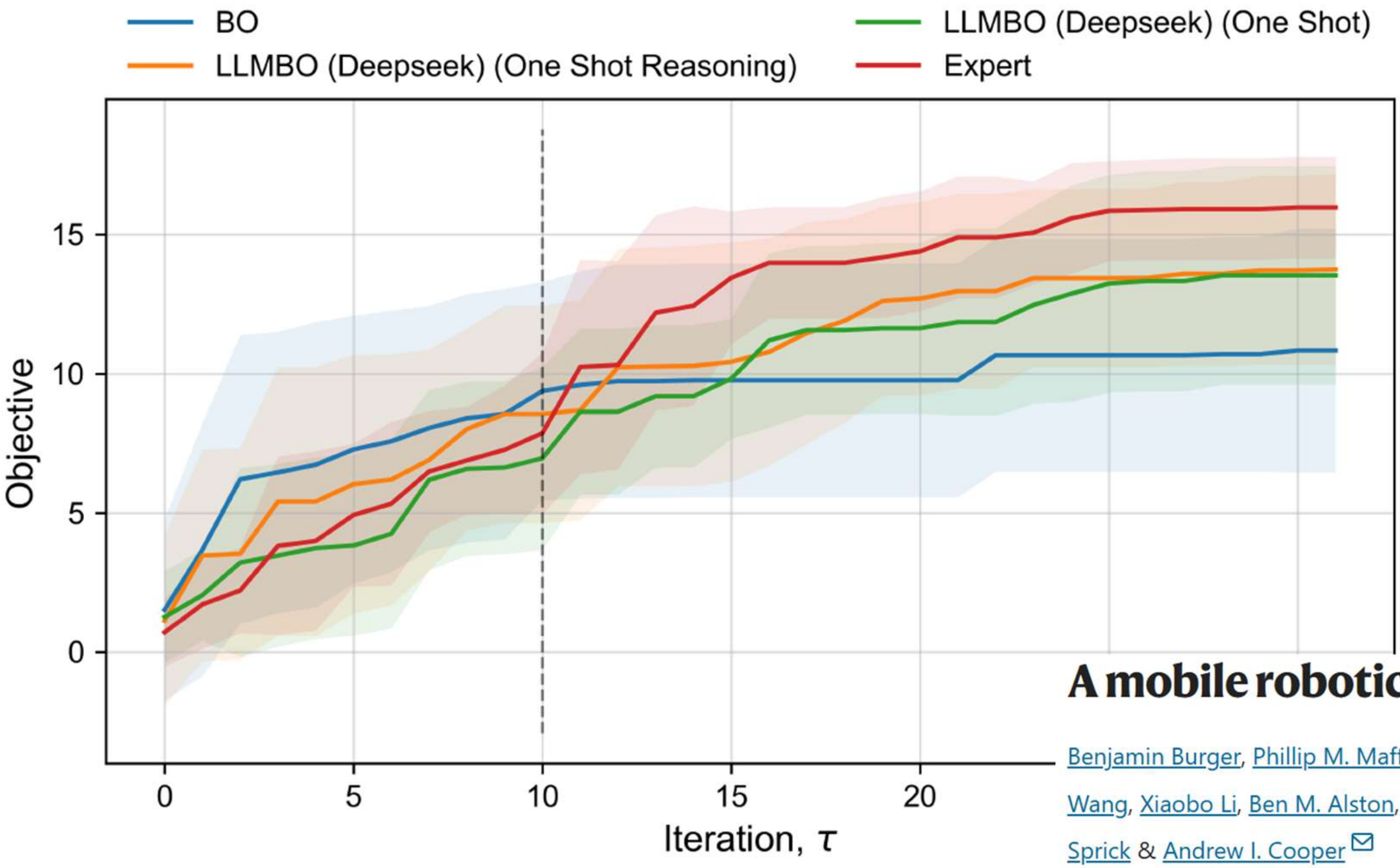
LLM-in-the-loop BO?



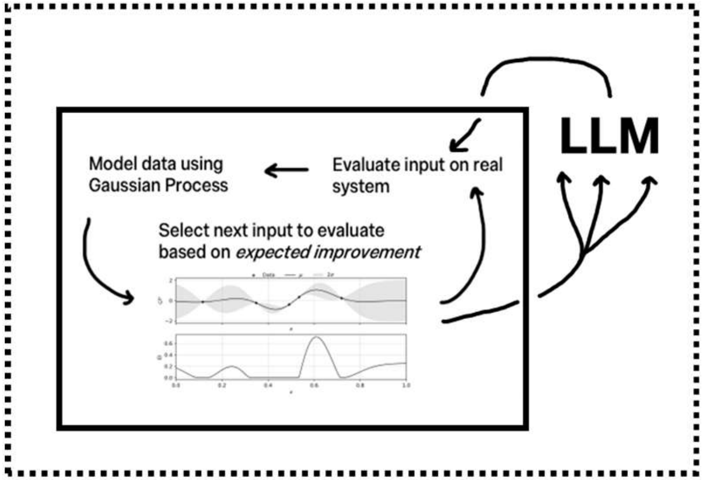
Works for mathematical functions, **how about real-case studies?**



LLM-in-the-loop BO?



10-variable photocatalysis optimisation task. **But ...**



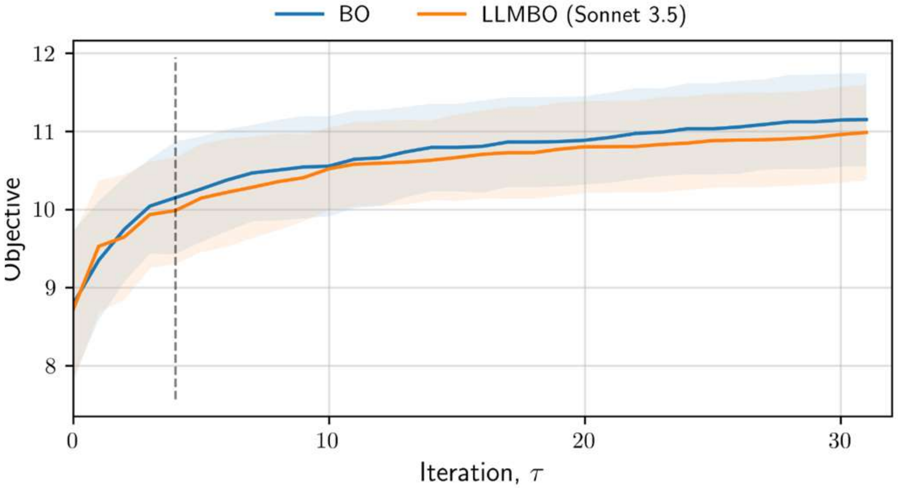
A mobile robotic chemist

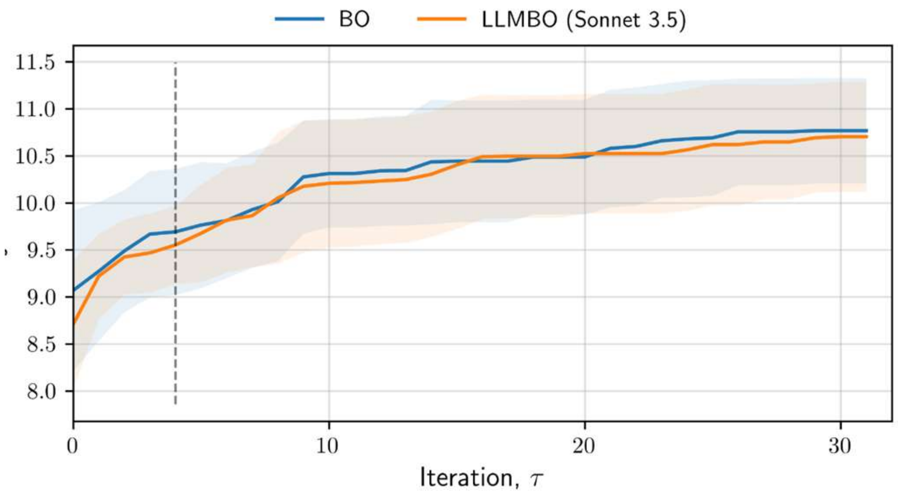
Benjamin Burger, Phillip M. Maffettone, Vladimir V. Gusev, Catherine M. Aitchison, Yang Bai, Xiaoyan Wang, Xiaobo Li, Ben M. Alston, Buyi Li, Rob Clowes, Nicola Rankin, Brandon Harris, Reiner Sebastian Sprick & Andrew I. Cooper

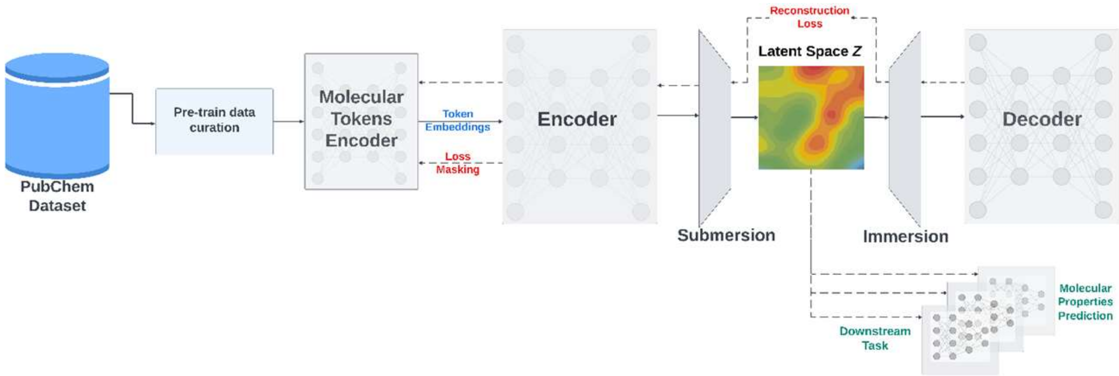
Nature **583**, 237–241 (2020) | Cite this article

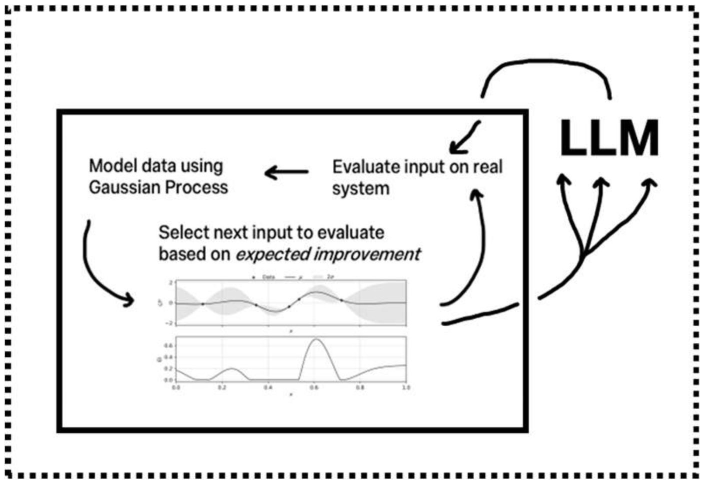
LLM-in-the-loop BO?

Not so much (yet!) for molecular property prediction ...

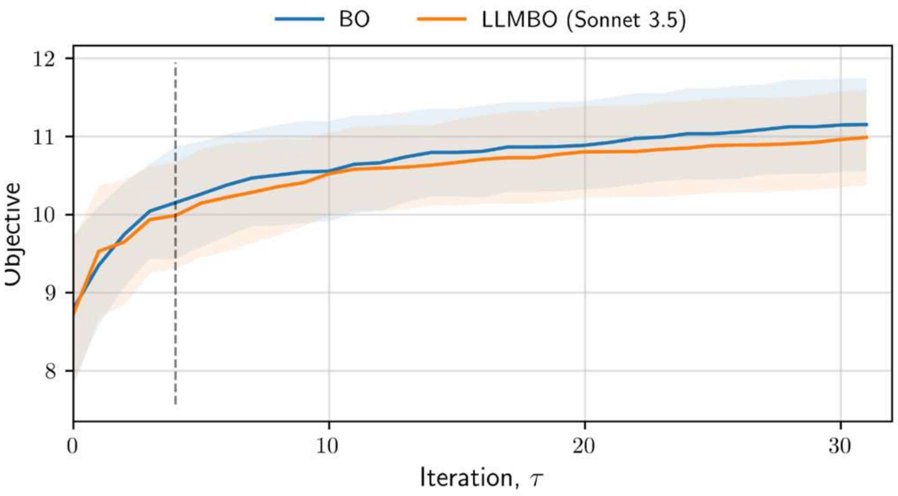


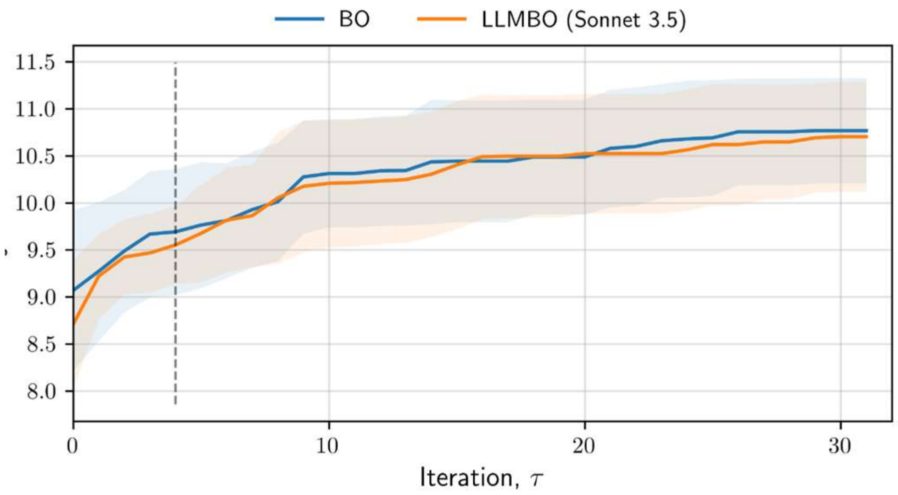




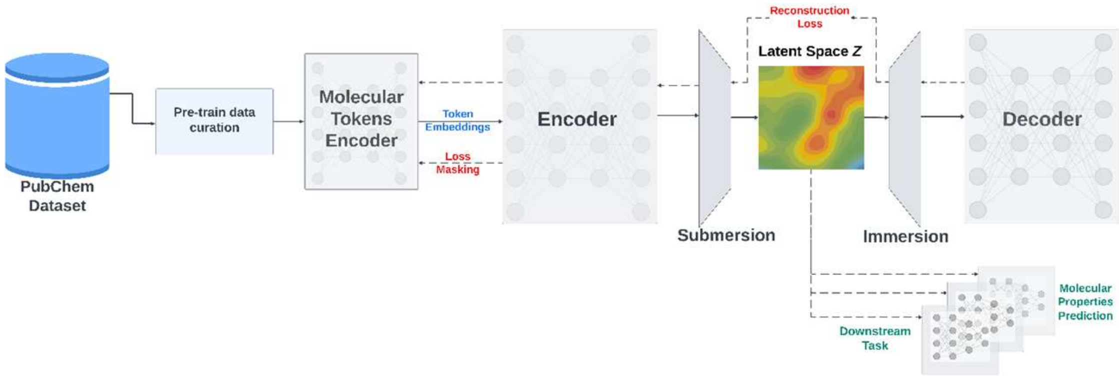


LLM-in-the-loop BO?

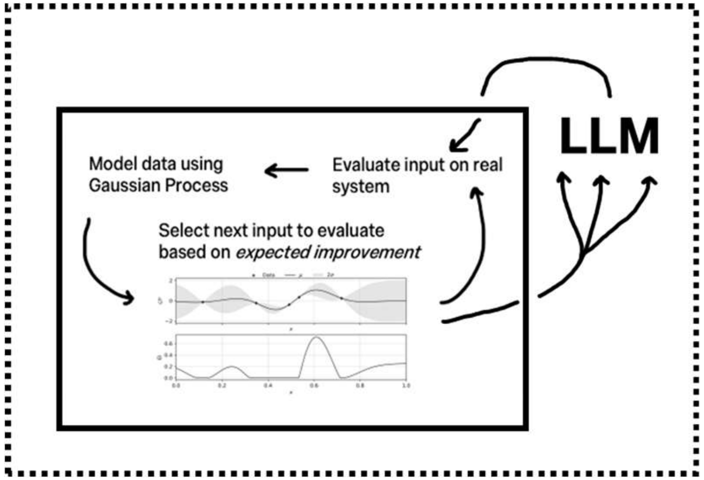




Not so much (yet!) for molecular property prediction ...

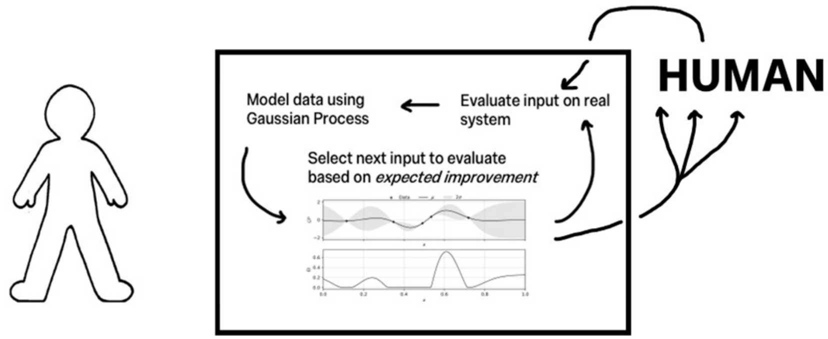


Still work to do!

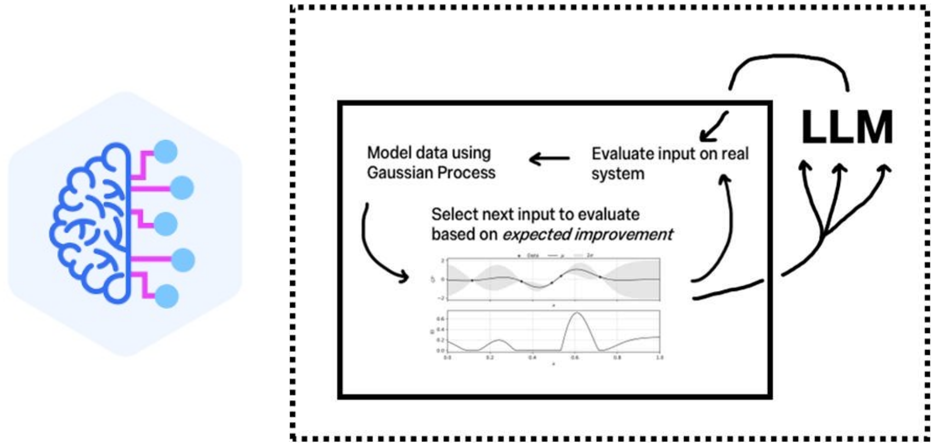


Summary

1. **Human-Algorithm** collaboration can be applied to improve optimization and discovery.



2. Considering ***how*** humans interact with algorithms (may) unlock effective LLM in LLM-in-the-loop BO.



Thank you!

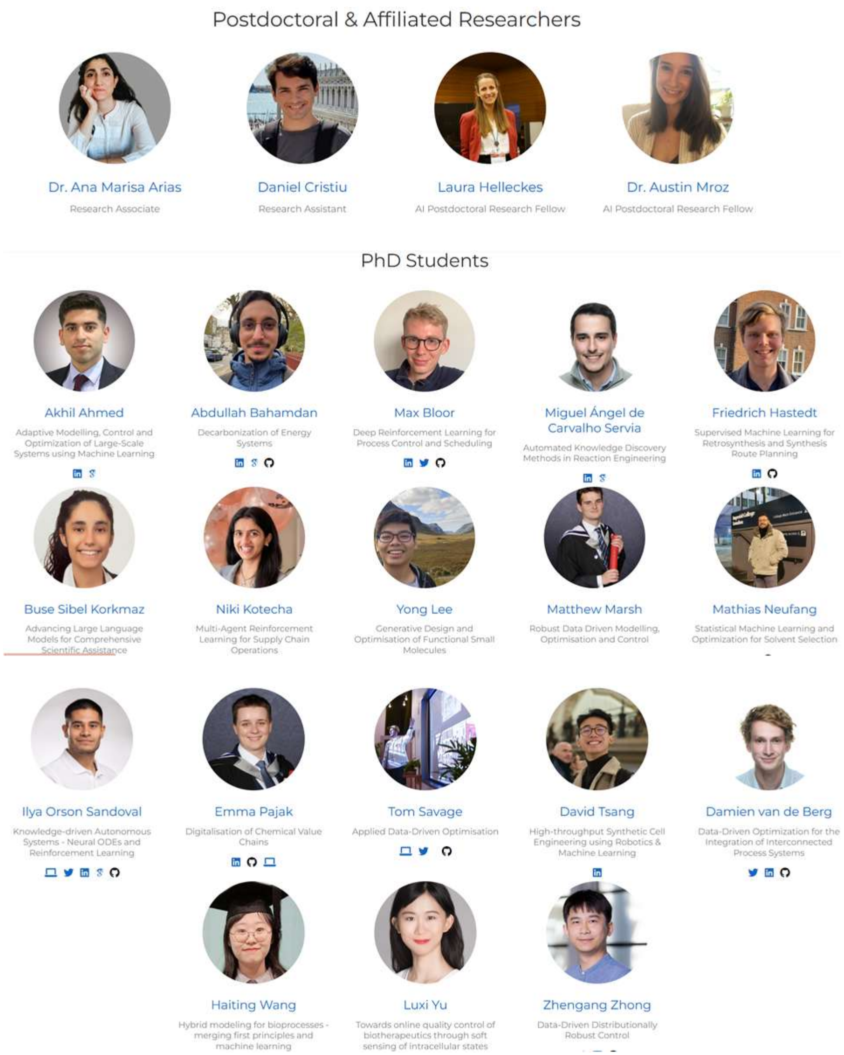
Computers & Chemical Engineering

Volume 189, October 2024, 108810

Human-algorithm collaborative Bayesian optimization for engineering systems

Tom Savage, Ehecatl Antonio del Rio Chanona

Preprint on LLM-in-the-loop coming soon :)



OPTIML PSE