Gittins Indices for Bayesian Optimization: Insights from Pandora's Box

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Joint work with Raul Astudillo, Peter Frazier, Ziv Scully, and Alexander Terenin

NYC Ops Day’24 Joint PhD Colloquium

Bayesian Optimization

Goal: optimize expensive-to-evaluate black-box function

$\in$ decision-making under uncertainty

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Applications:
Hyperparameter tuning
Drug discovery
Control design

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∈ decision-making under uncertainty

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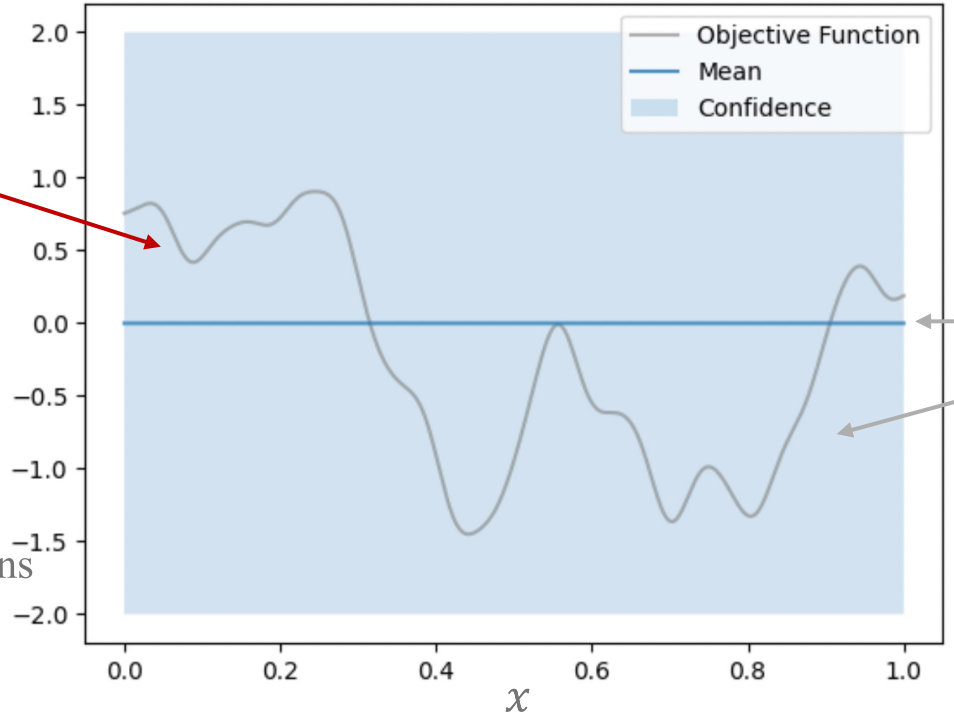
An unknown random function $f: \mathcal{X} \to \mathbb{R}$ drawn from a Gaussian process prior

Gaussian process: infinite-dimensional generalization of multivariate normal distributions



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Drug discovery
Control design

x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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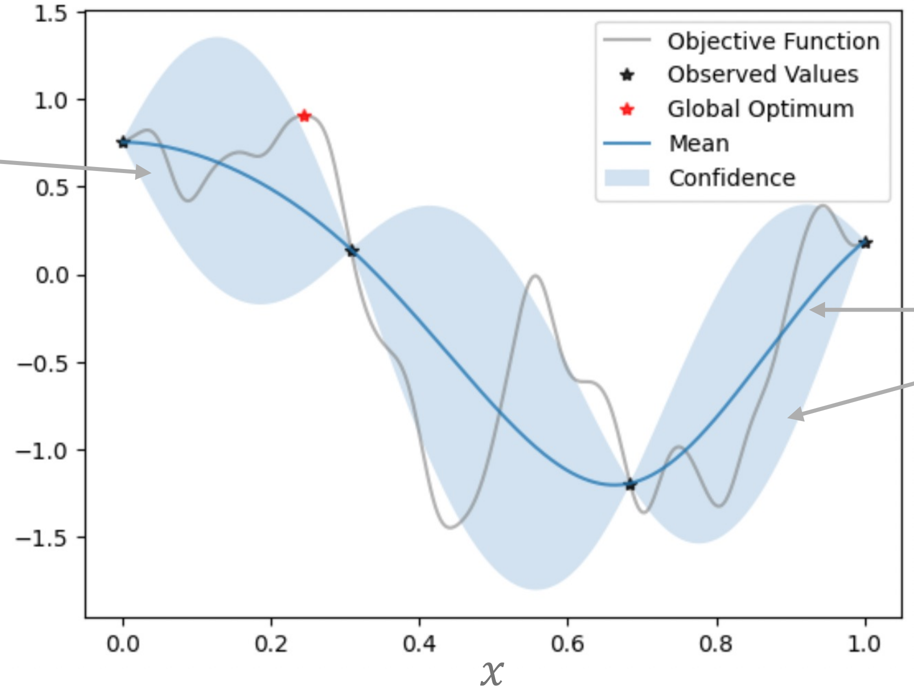

mean: prediction

variance: confidence/uncertainty

Objective: find global optimum $x^* = \mathrm{argmax}_{x \in \mathcal{X}}\, f(x)$

Decision: evaluate a set of points

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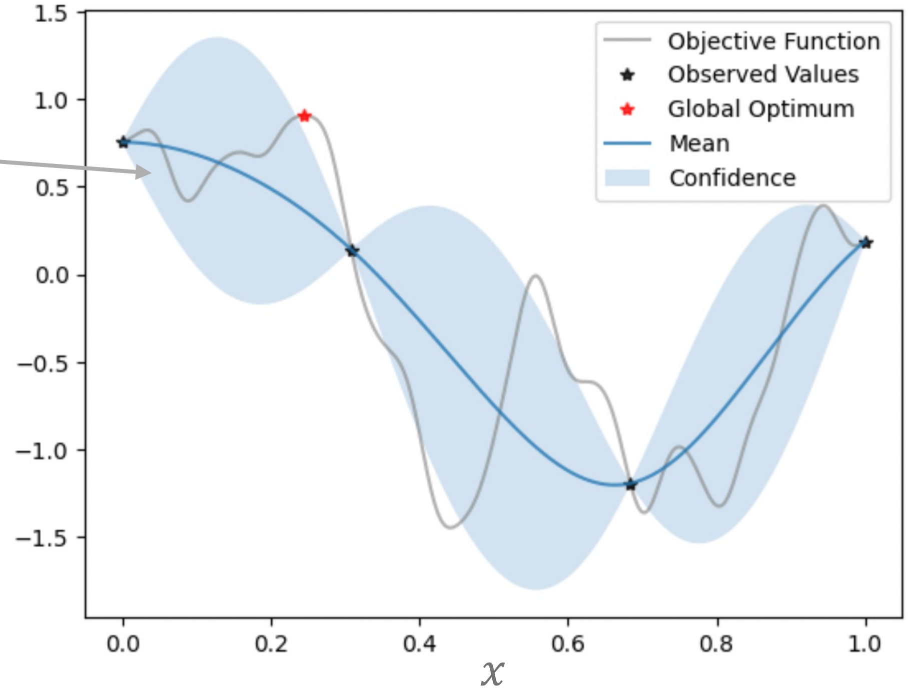

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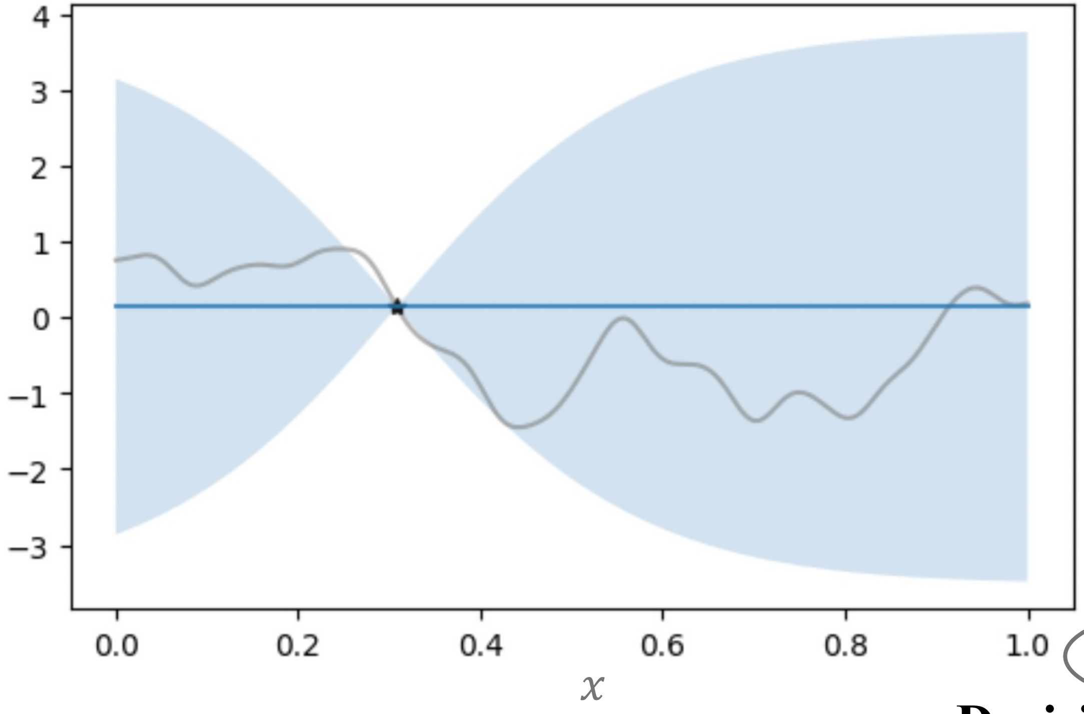

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adaptively

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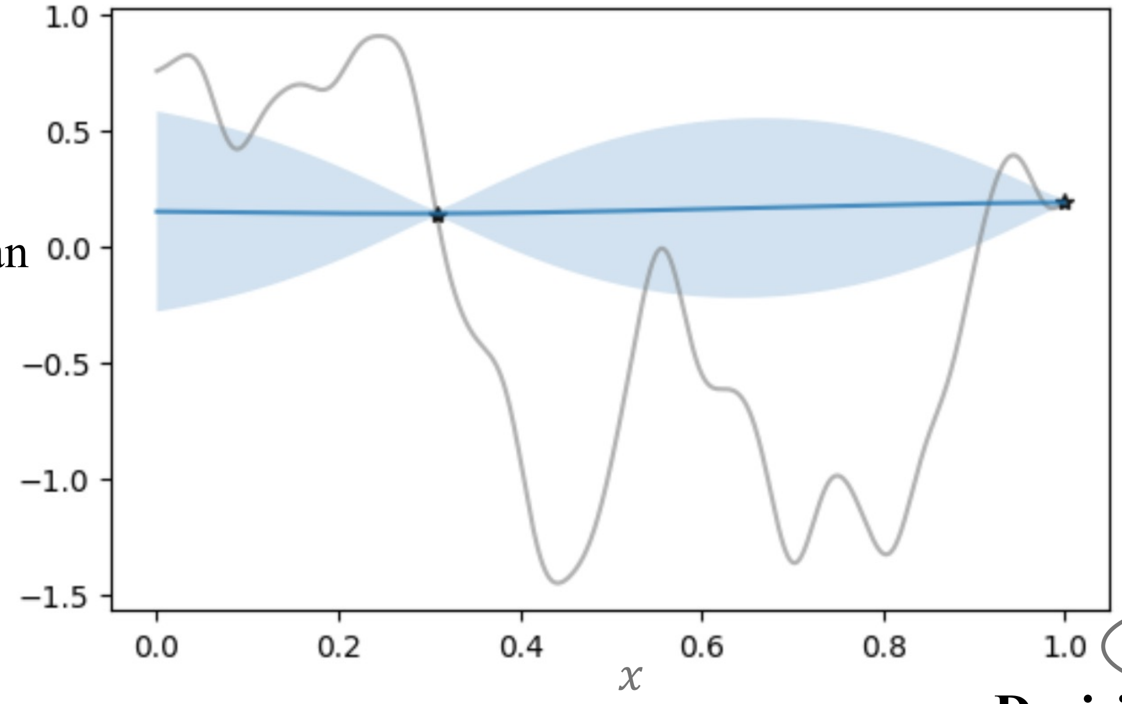

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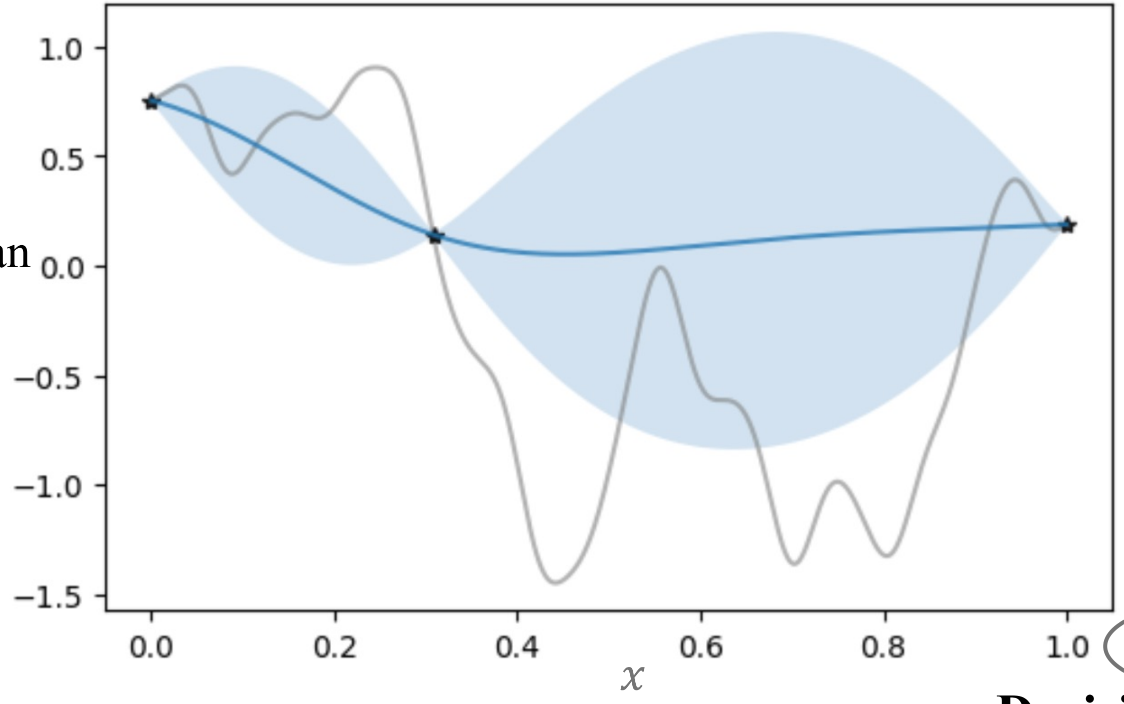

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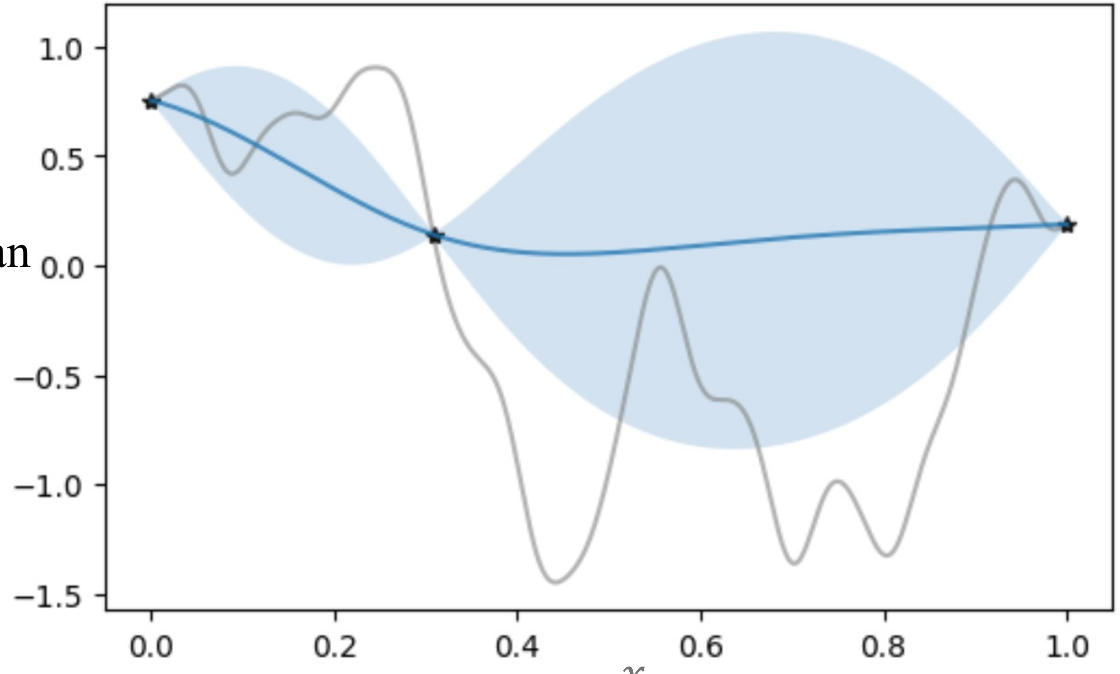

x

Decision: adaptively evaluate a set of points

$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

T: time budget

Bayesian Optimization

Goal: optimize expensive-to-evaluate black-box function

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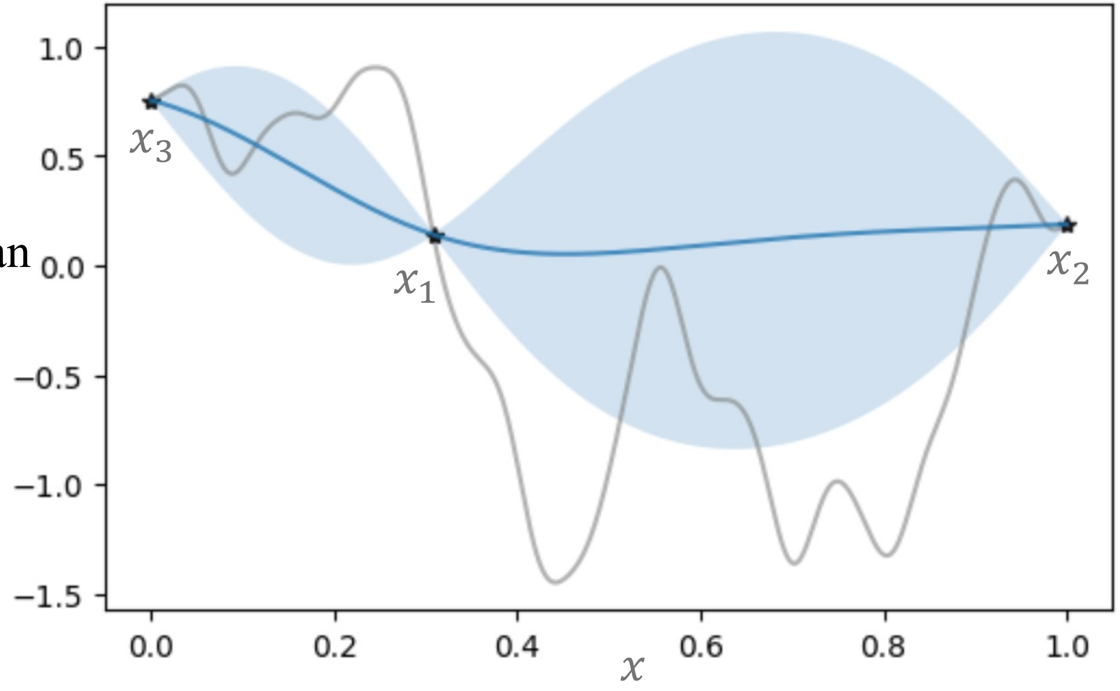

Applications:
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Drug discovery
Control design

x: hyperparameter/configuration

Objective: optimize best observed value at time T

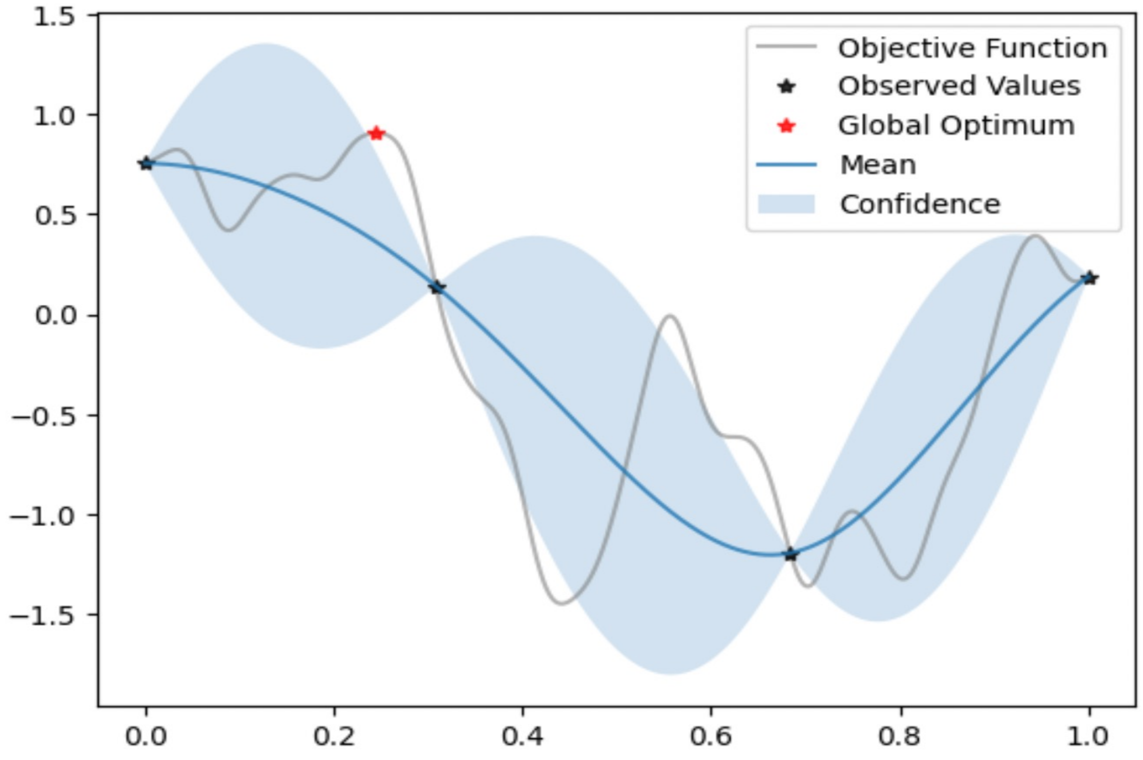
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

Decision: adaptively evaluate a set of points

$$x_1, x_2, \ldots, x_T \in \mathcal{X}$$

T: time budget

Why is it hard?



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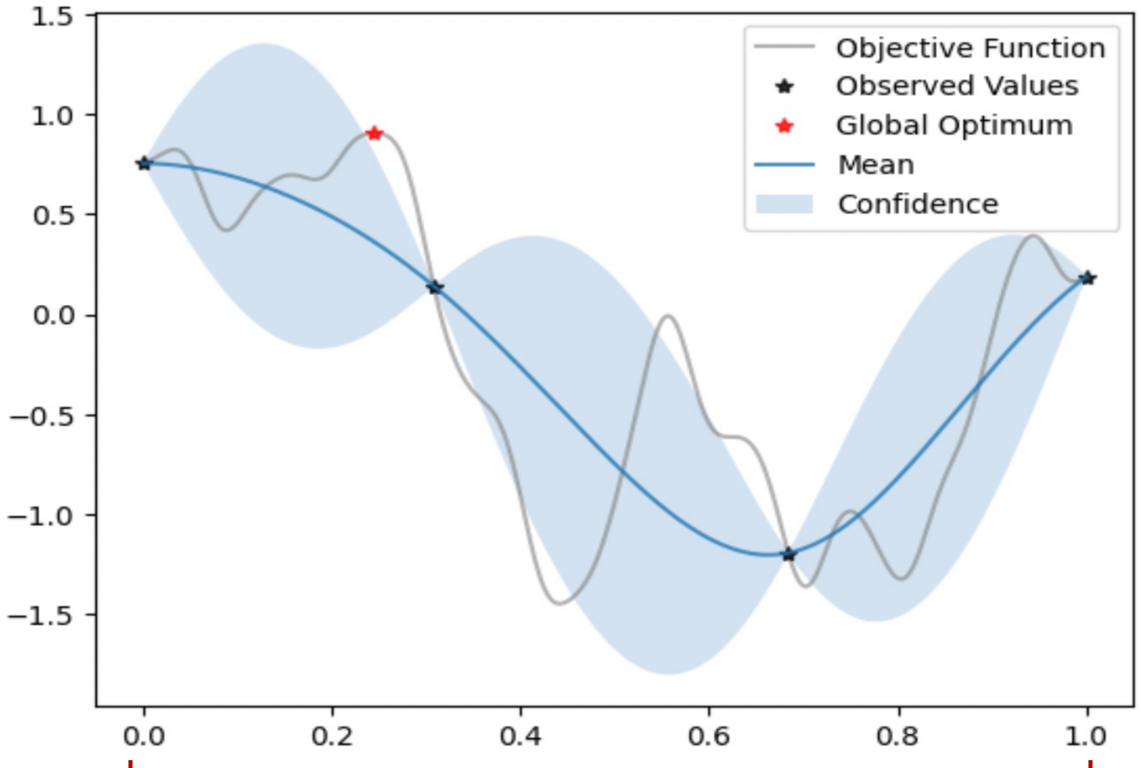
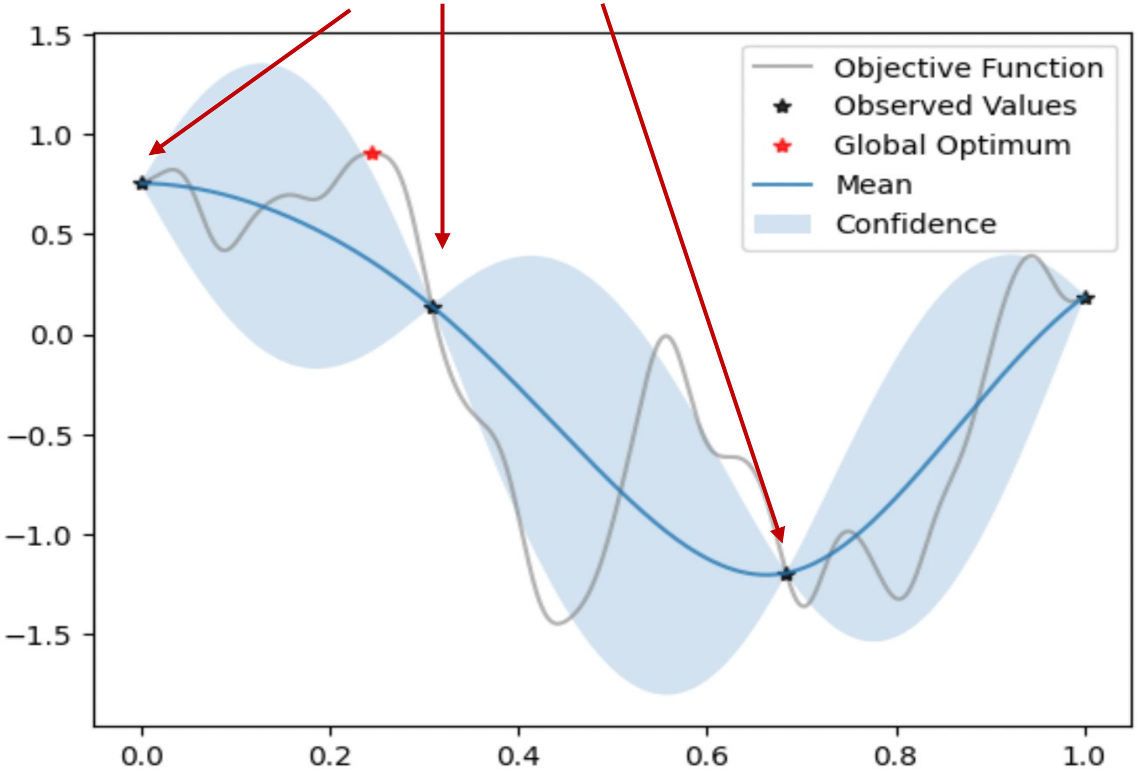


Continuous search domain

Why is it hard?

Correlated values



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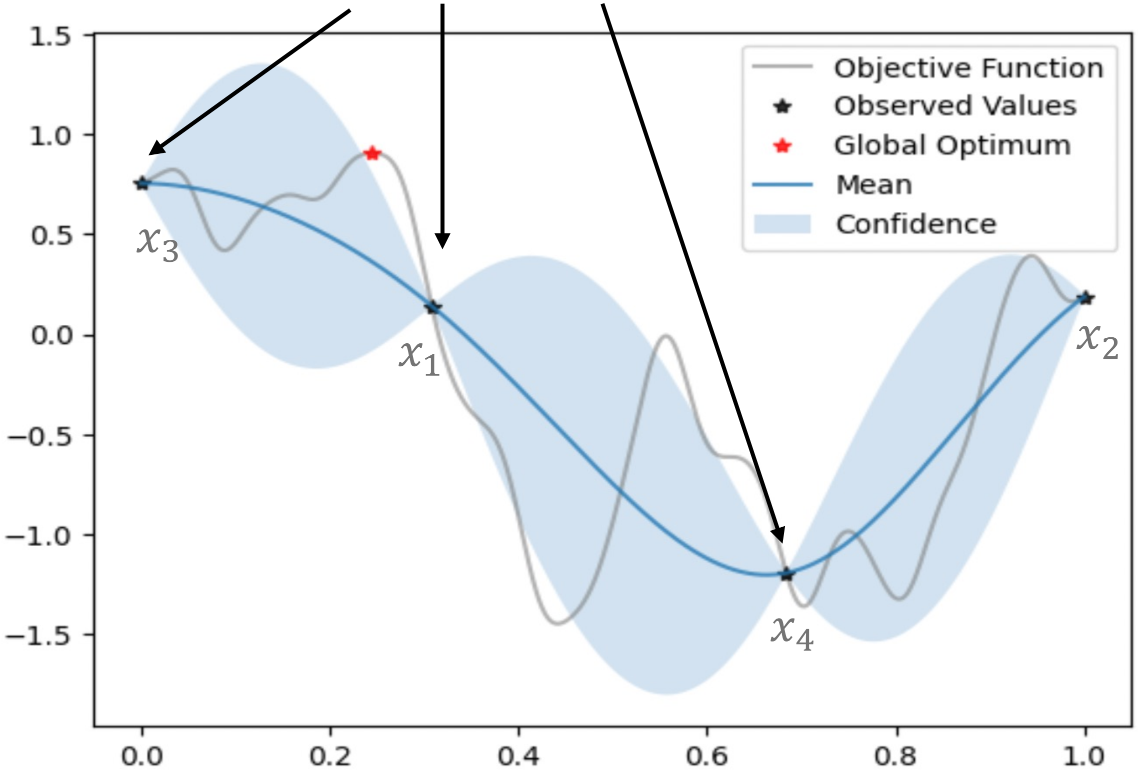

Continuous search domain

Hard budget constraint

~~$t = 1$~~

~~$t = 2$~~

~~$t = 3$~~

~~$t = 4$~~

⋮

$t = T$

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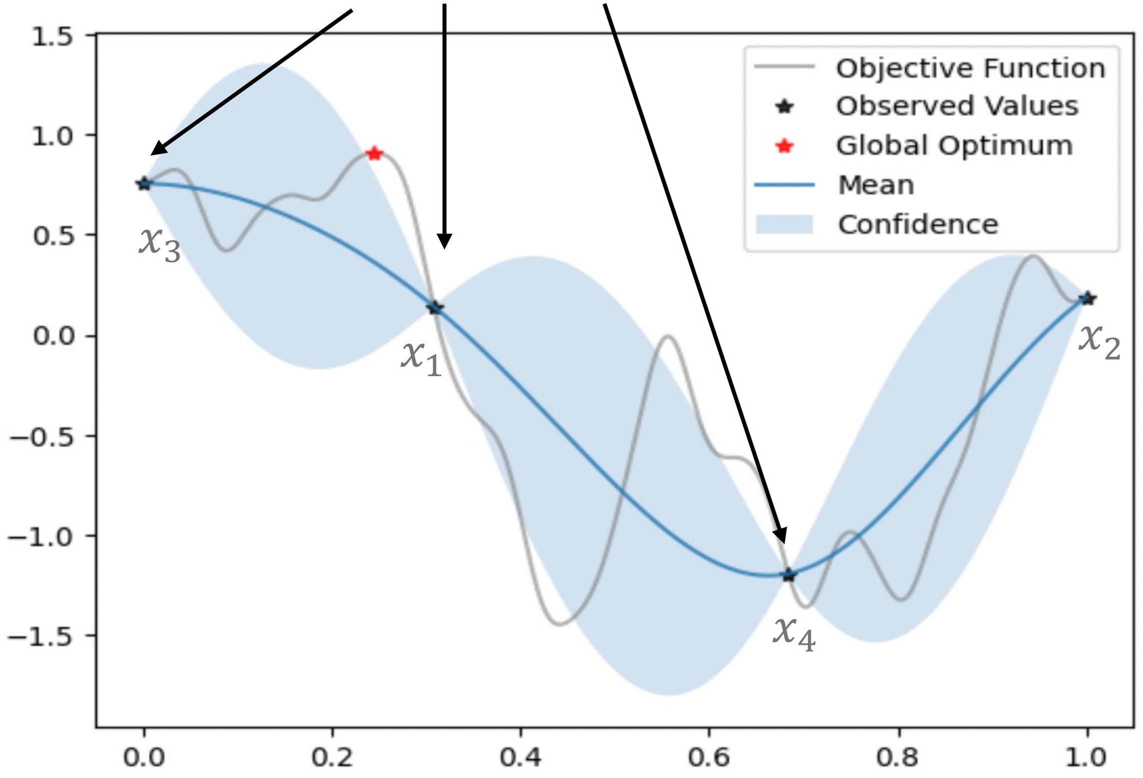
Correlated values



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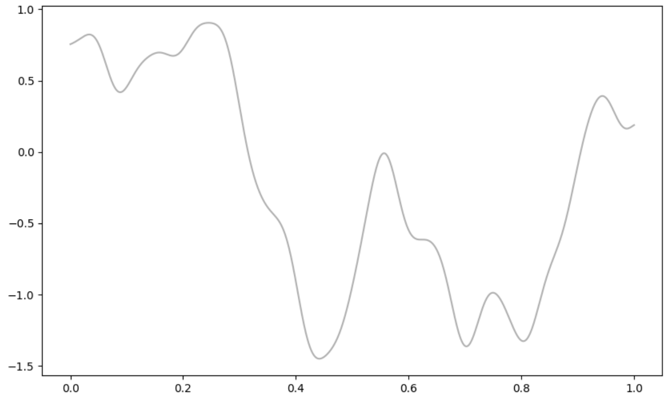
⋮

$t = T$

$\Longrightarrow$ Optimal policy unknown!

Bayesian Optimization

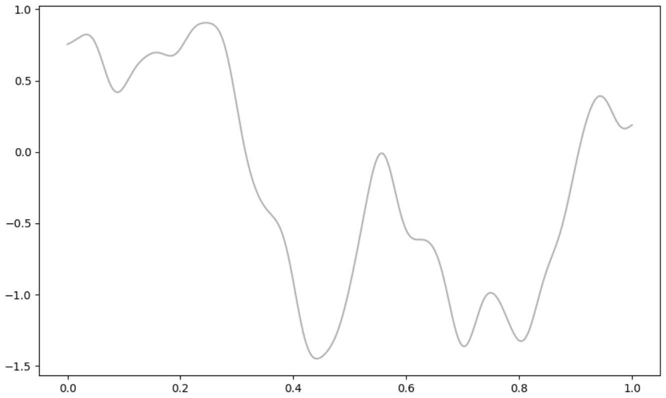


Continuous

Correlated

Hard budget constraint

Bayesian Optimization



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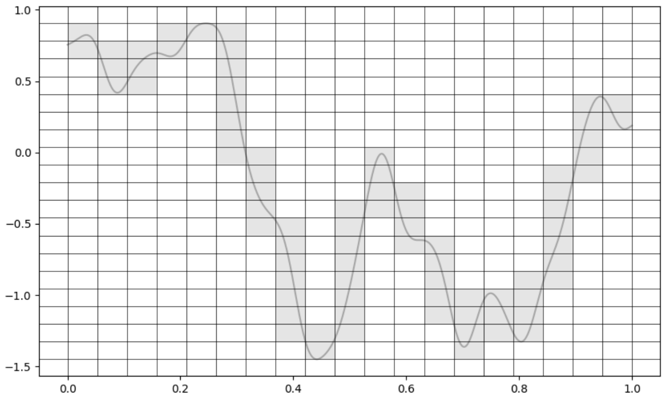
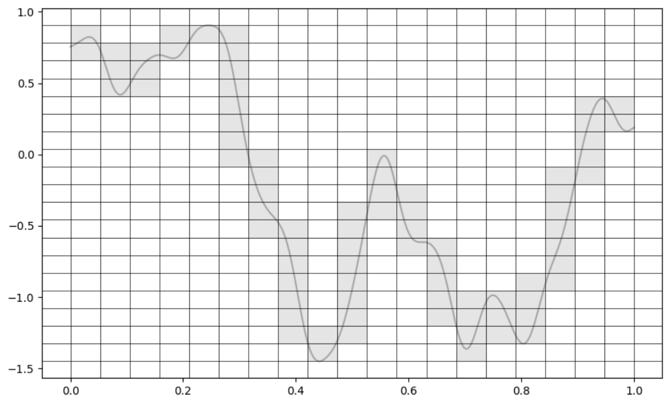


Continuous $\Longrightarrow$ Discrete

Correlated

Hard budget constraint

Bayesian Optimization



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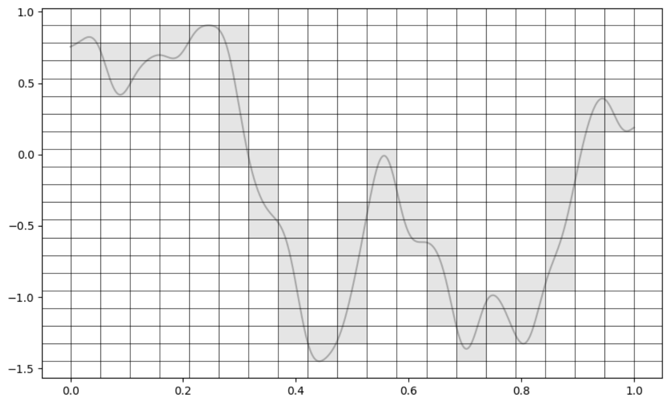

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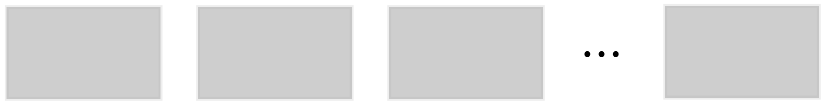
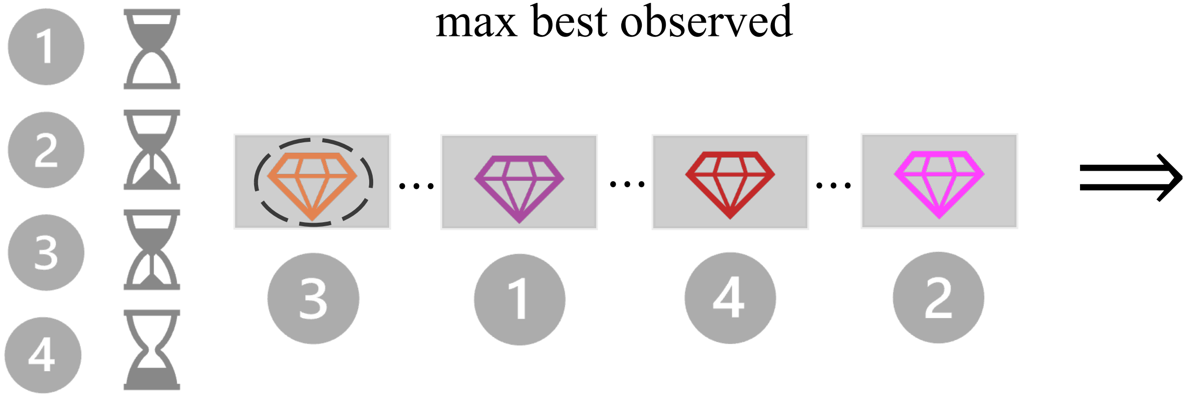


Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint		

Bayesian Optimization

budget

max best observed



Continuous $\Longrightarrow$ Discrete

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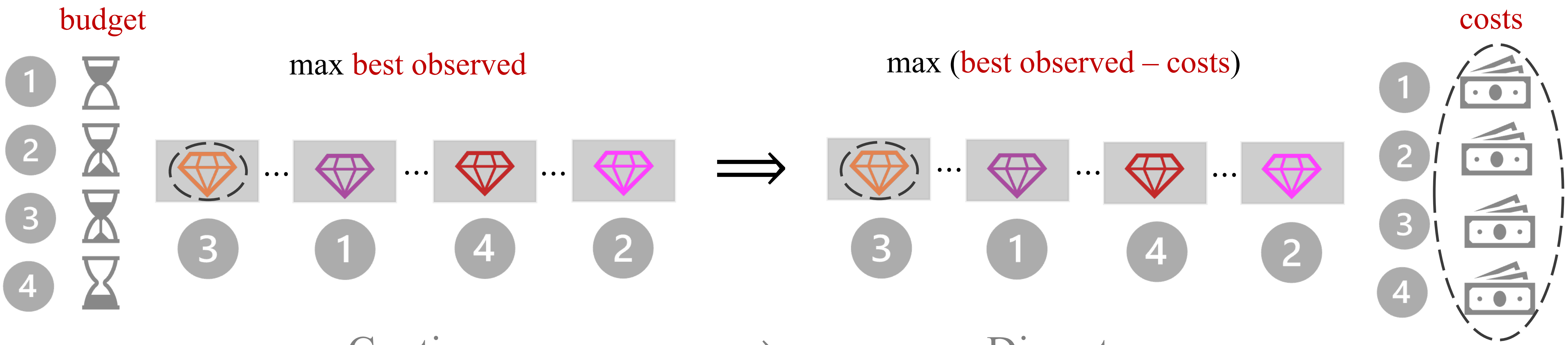
Hard budget constraint

Bayesian Optimization



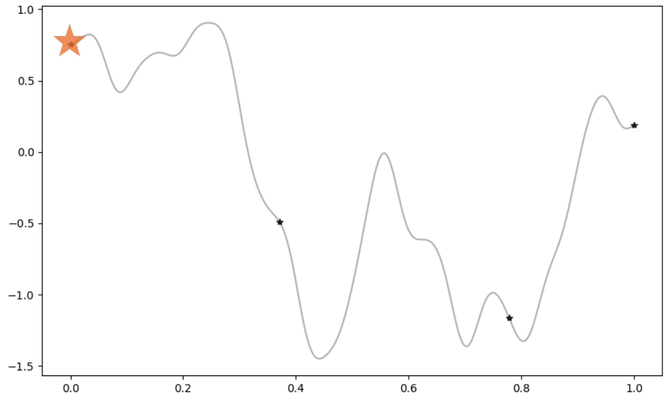
Continuous ⇒ Discrete

Correlated ⇒ Independent

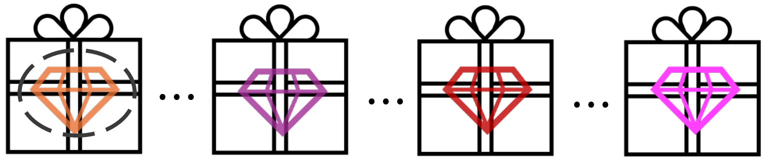
Hard budget constraint $\xRightarrow{\text{Lagrangian relaxation}}$ Cost per sample

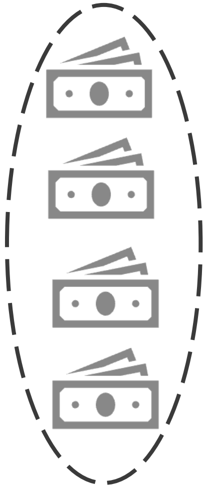
Bayesian Optimization ⟹ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits



⟹





Continuous	⟹	Discrete
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Hard budget constraint	⟹	Cost per sample

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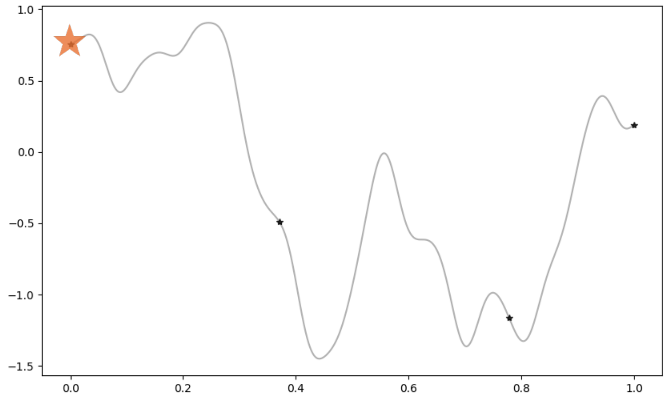

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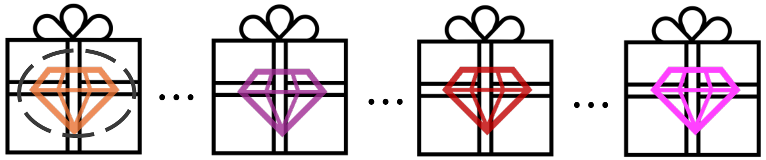
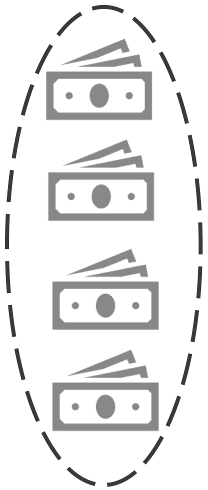




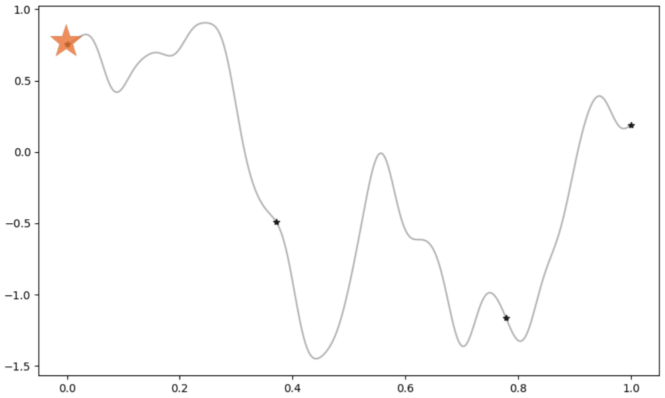
Continuous ⟹ Discrete

Correlated ⟹ Independent

Hard budget constraint ⟹ Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization $\Longrightarrow$ Pandora's Box



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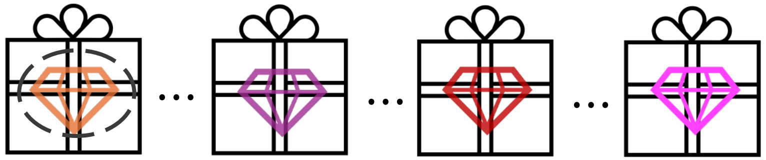

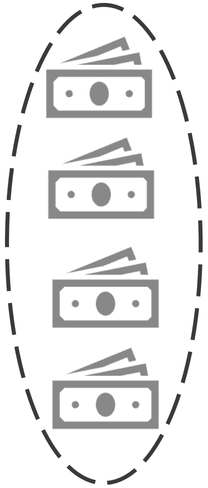

Continuous $\Longrightarrow$ Discrete

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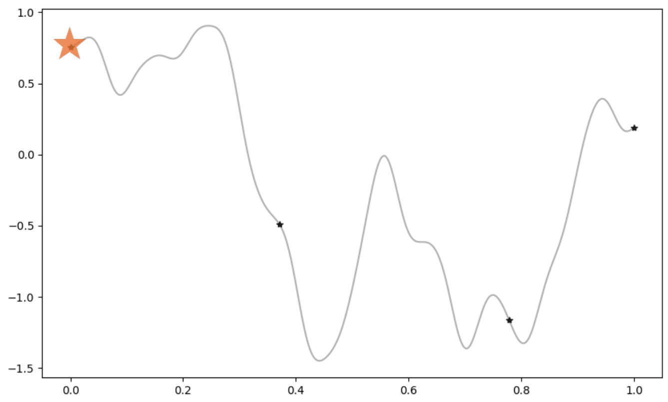
Hard budget constraint $\Longrightarrow$ Cost per sample

Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



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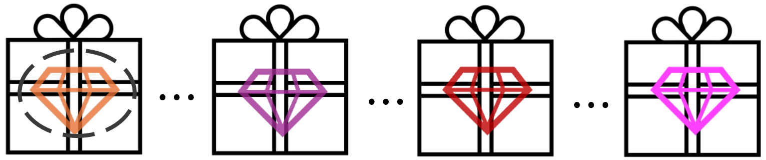

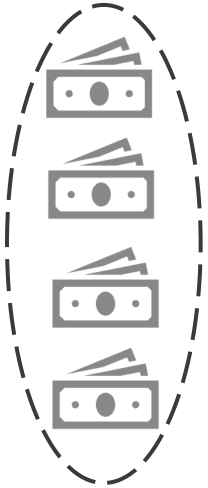

Continuous	$\Longrightarrow$	Discrete
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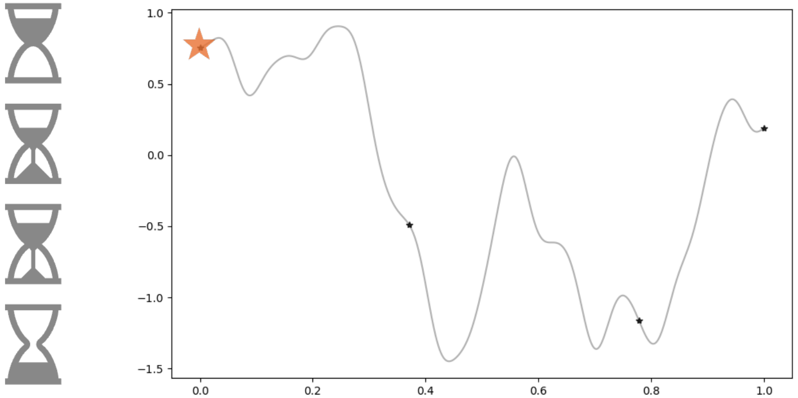
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	How to translate? $\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



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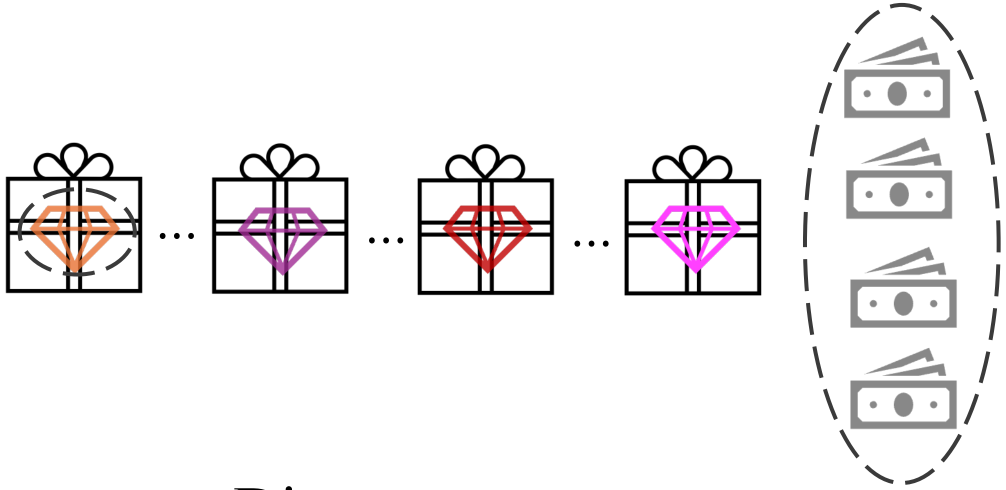


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint $\Longrightarrow$ Cost per sample

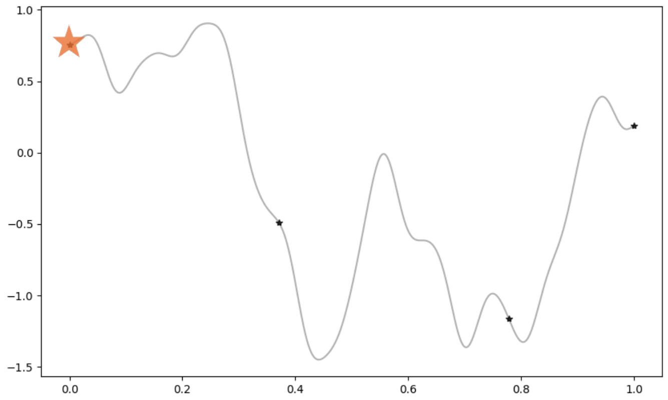
How to translate?

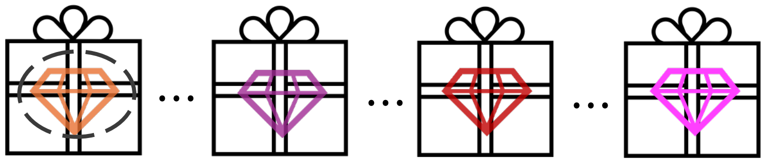
Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

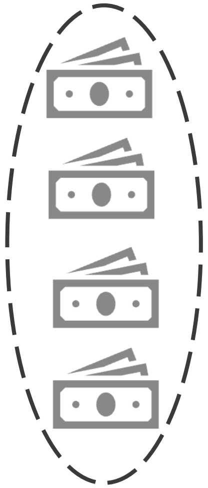
Our contributions!

Our Contributions

- How to translate?
- Is Pandora’s Box Gittins index (PBGI) good?



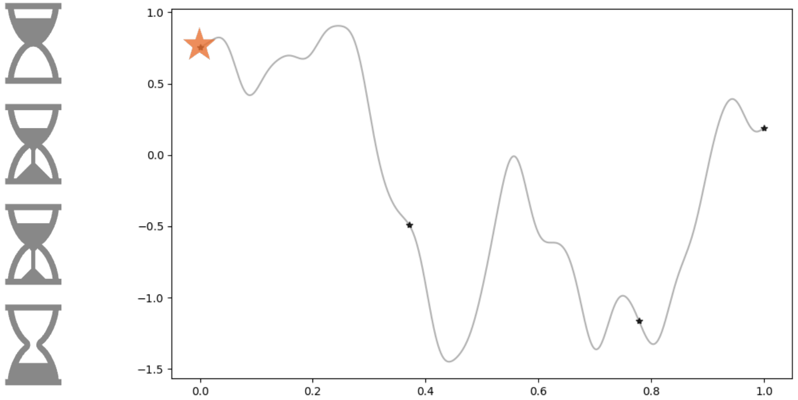


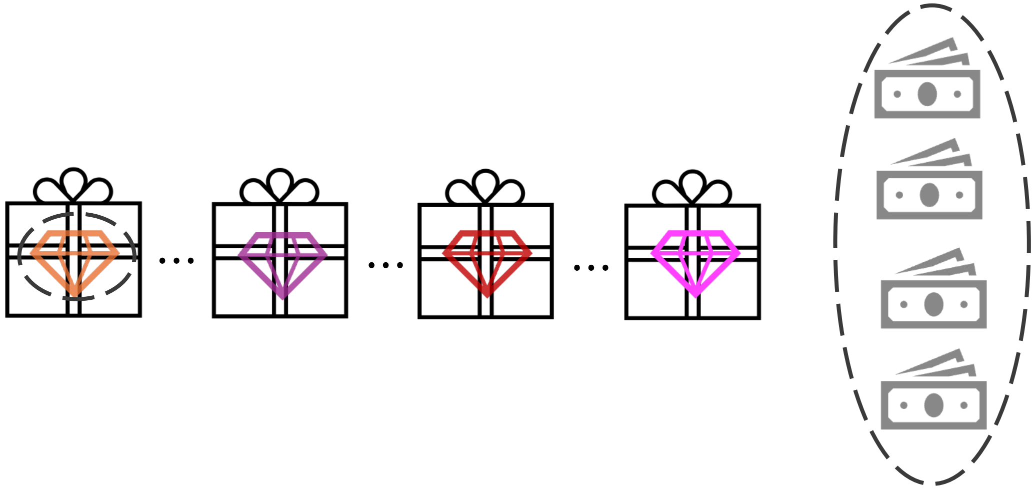


? $\Longleftarrow$ Pandora’s Box Gittins index

Our Contributions

- Develop PBGI policy for Bayesian optimization
- Is Pandora’s Box Gittins index (PBGI) good?

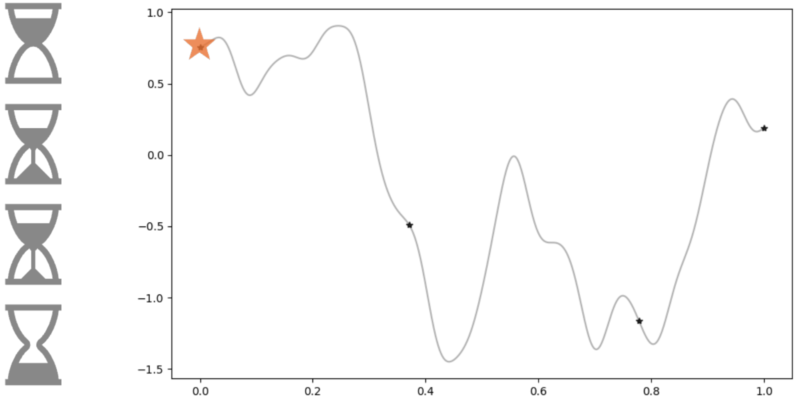


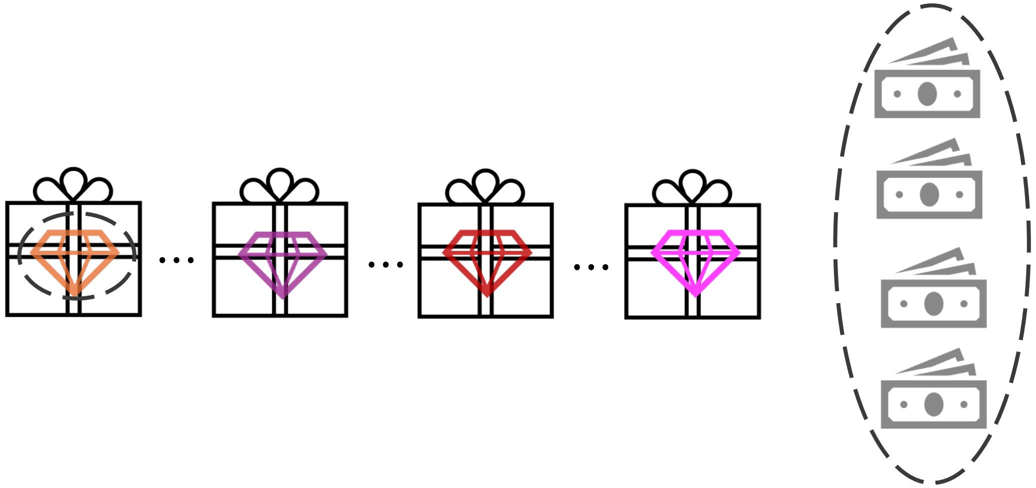


Our work $\Longleftarrow$ Pandora’s Box Gittins index

Our Contributions

- Develop PBGI policy for Bayesian optimization
- Show performance against baselines on synthetic & empirical experiments





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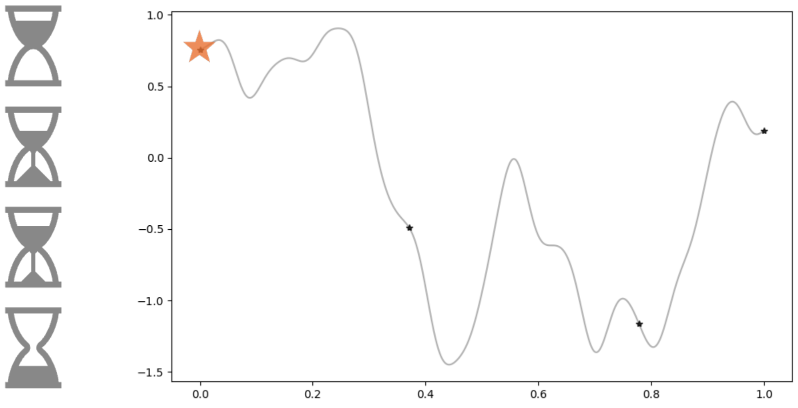
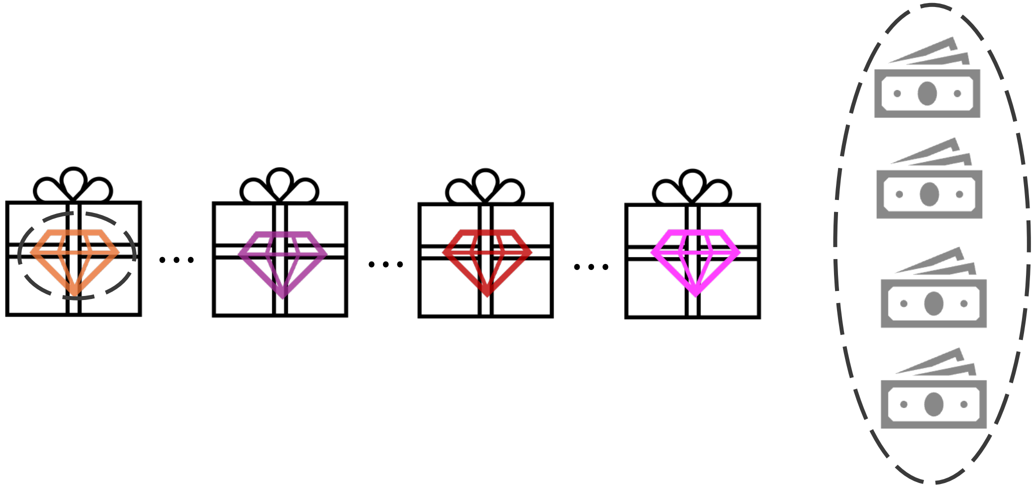
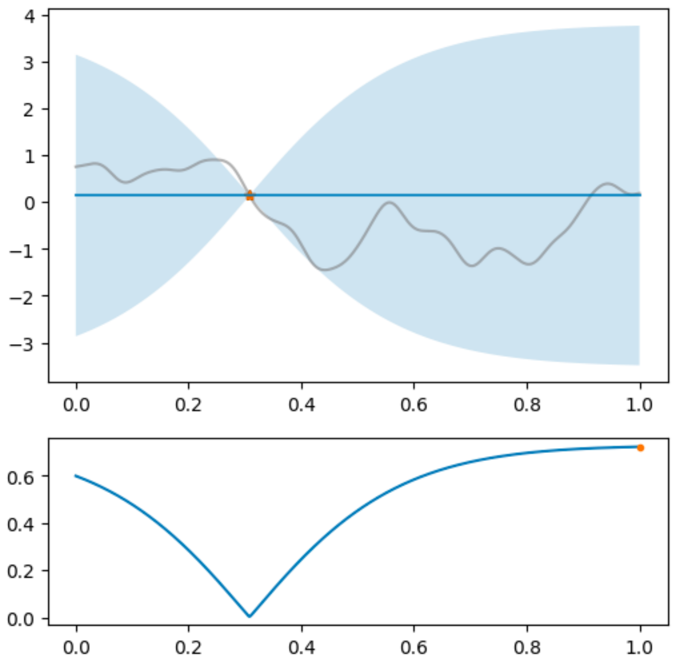




Our work ⟸ Pandora’s Box Gittins index

How is our PBGI policy different from baselines?

Popular One-step Heuristic: EI



Expected improvement

$$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^+]$$

EI policy: evaluate $\operatorname{argmax}_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$

mean: prediction

variance: confidence/uncertainty

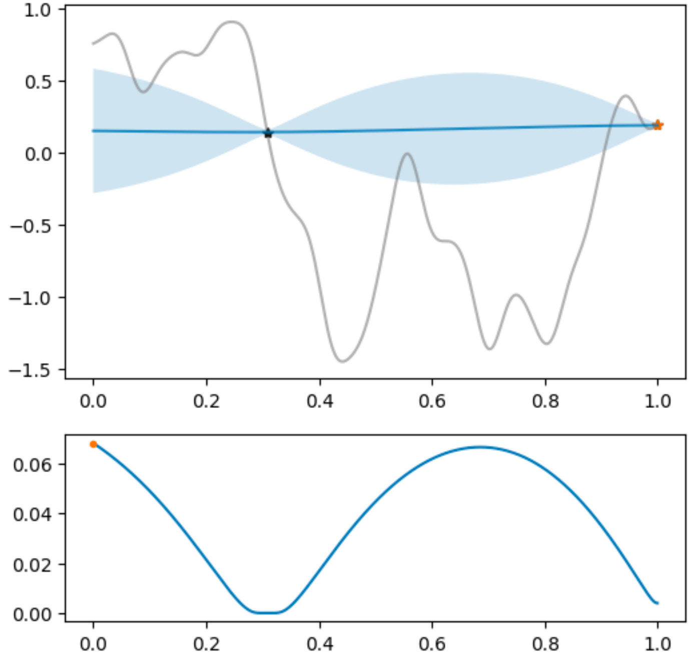
Trade-off between

- exploitation (high mean) and
- exploration (high uncertainty)

D: observed data

y_{best}: current best observed value

Popular One-step Heuristic: EI



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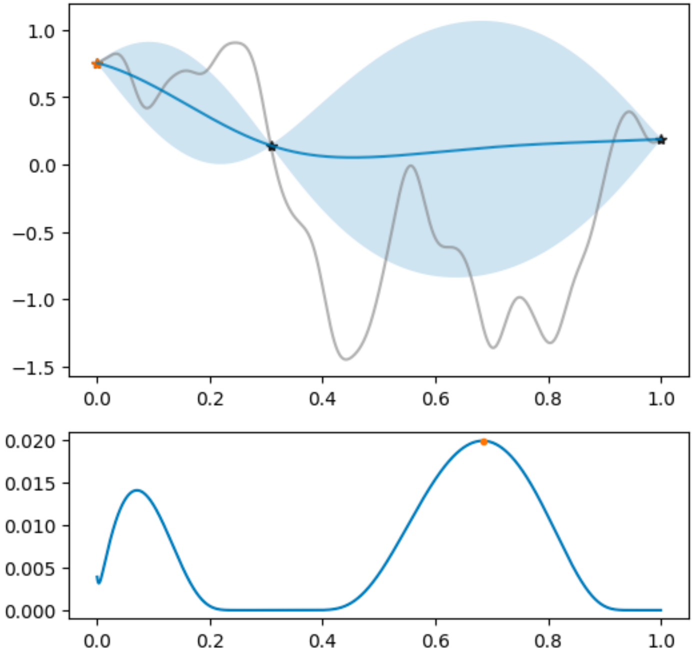

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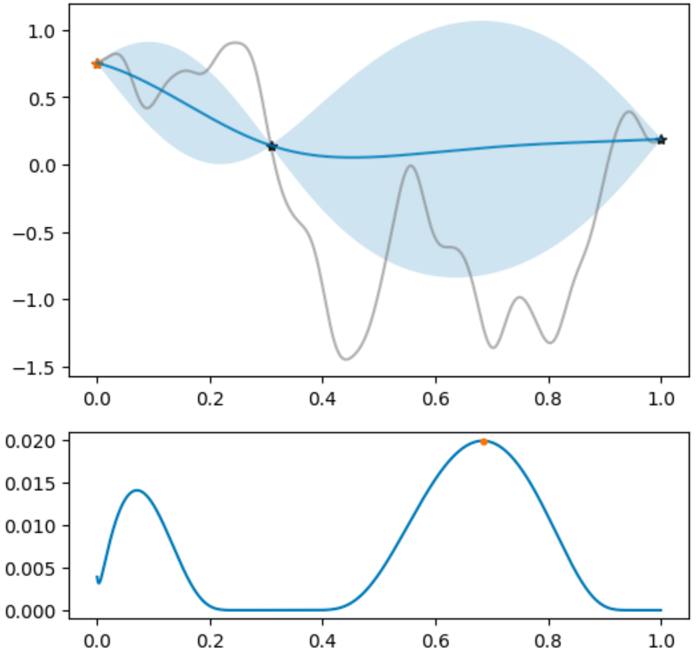
EI policy: evaluate $\operatorname{argmax}_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$

Popular One-step Heuristic: EI

Other heuristics:

simple
- Upper Confidence Bound
- Thompson Sampling (TS)
- Predictive Entropy Search
- Knowledge Gradient
- Multi-step Lookahead EI

slow



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EI policy: evaluate $\mathrm{argmax}_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$

New One-step Heuristic: PBGI

Other heuristics:
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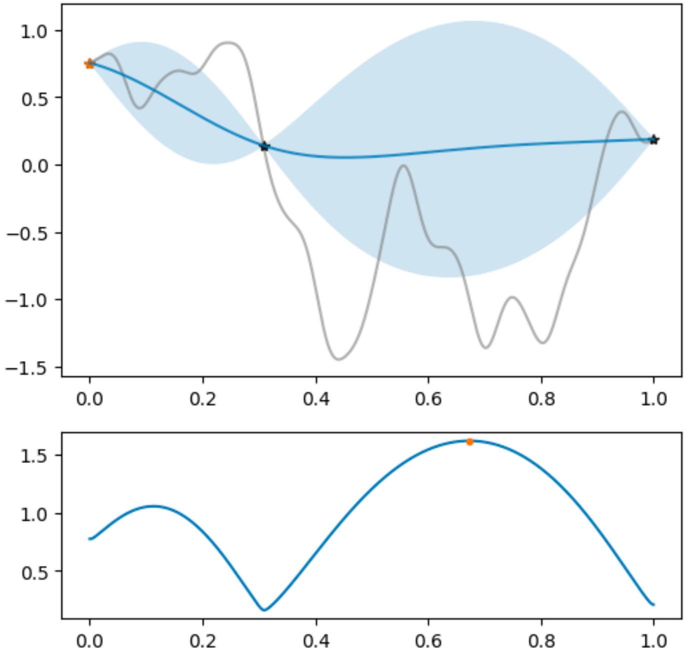
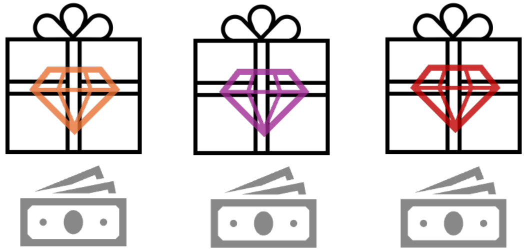
- Thompson Sampling (TS)
- Knowledge Gradient
- Predictive Entropy Search
- Multi-step Lookahead EI



Pandora's box Gittins index

Pandora's box



$\alpha^*(x)$: Gittins index function

PBGI policy: evaluate $\text{argmax}_x\, \alpha^*(x)$

New One-step Heuristic: PBGI

Other heuristics:
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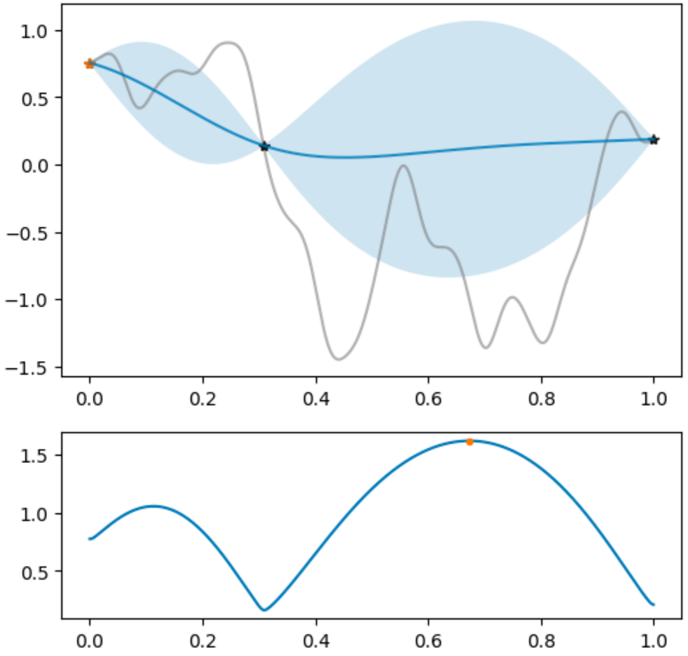


Pandora's box Gittins index

$$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^{+}]$$

PBGI policy: evaluate $\mathrm{argmax}_x\, \alpha^*(x)$

Pandora's box

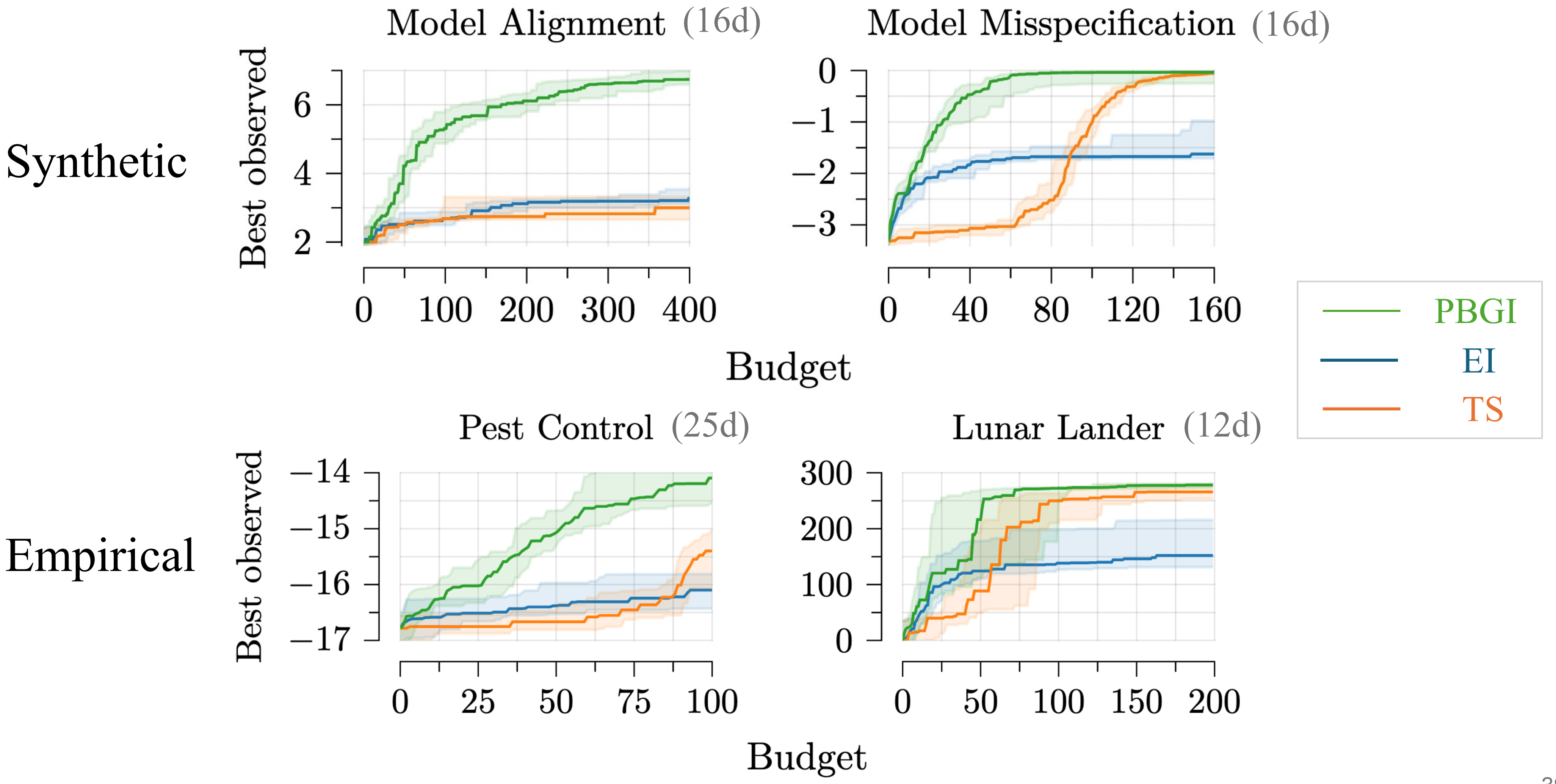
λ λ λ

λ: cost-per-sample
(Lagrange multiplier)

D: observed data

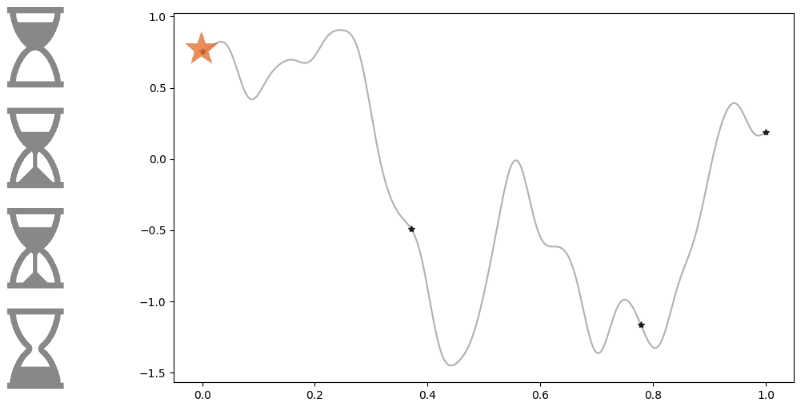
$\alpha^*(x)$: solution to $\mathrm{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

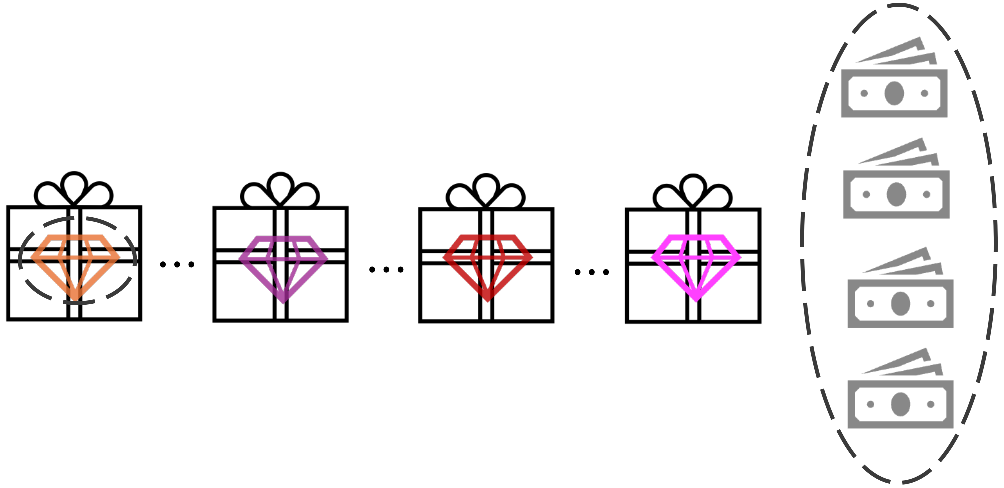
Experiment Results: PBGI vs EI vs TS



Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization





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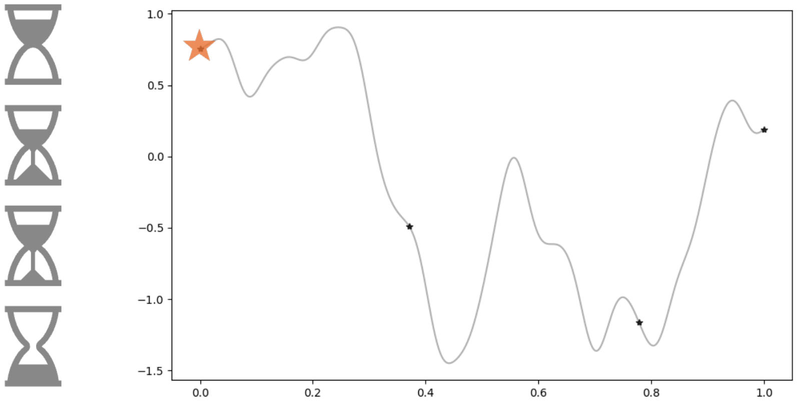
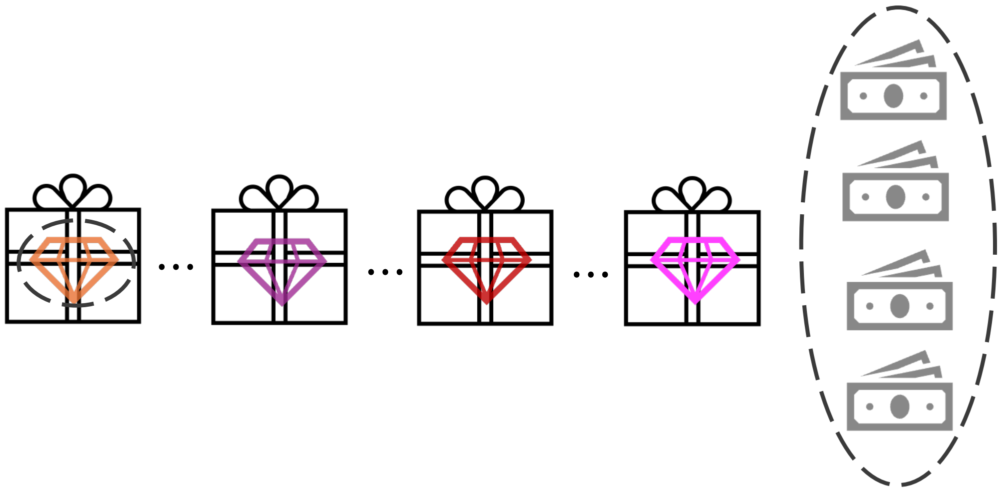
Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments

particularly on medium-high dimensions and relatively-large domains!





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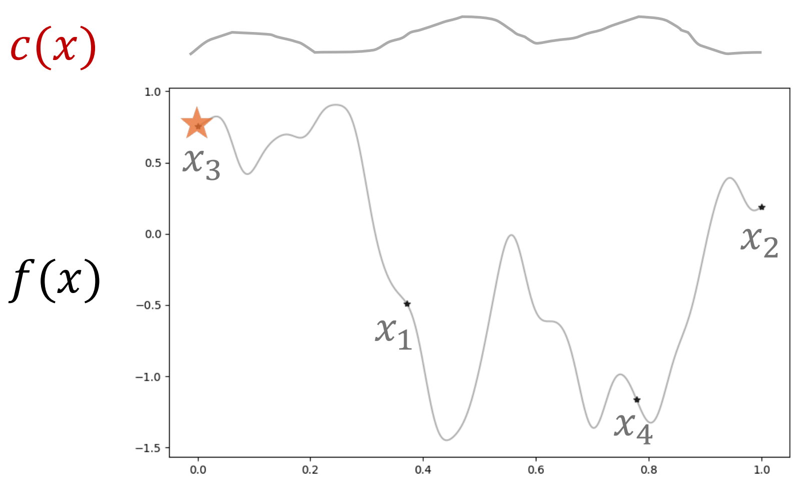
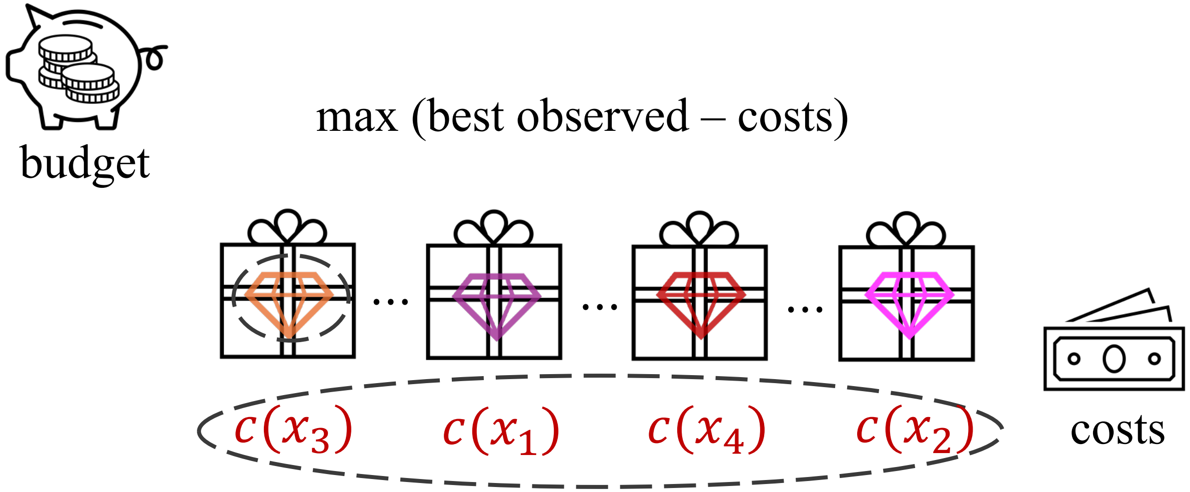
Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs





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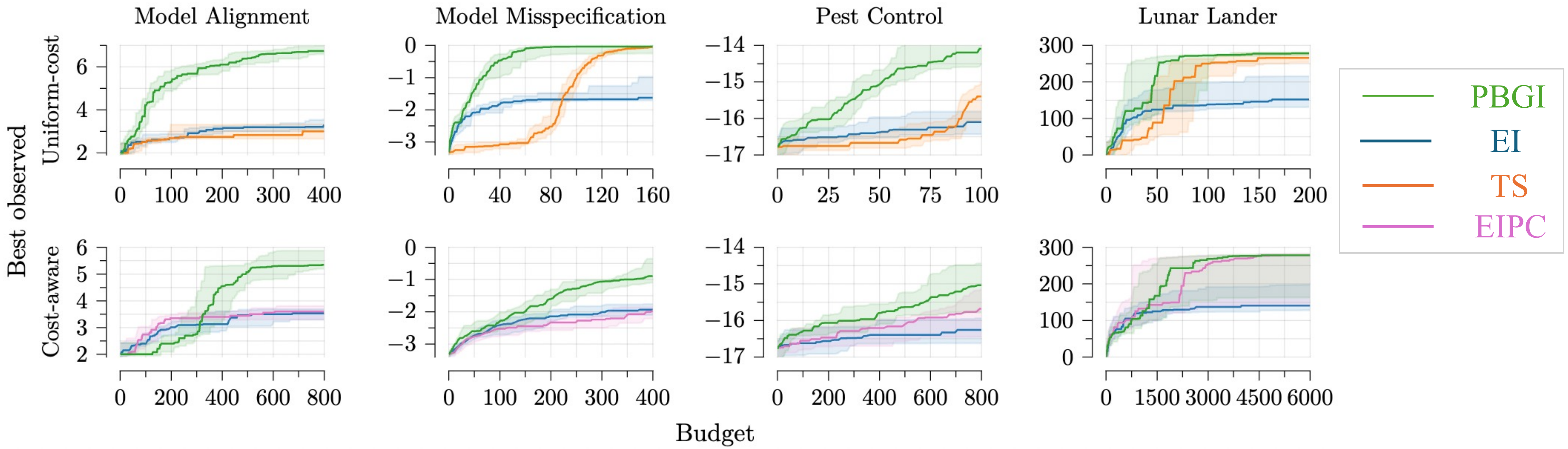
Heterogeneous-cost Experiment Results

- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs



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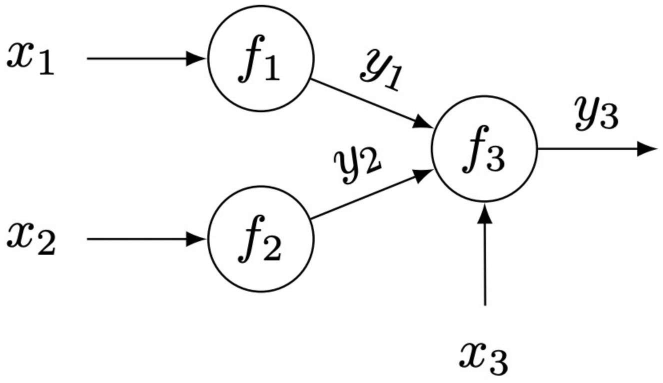
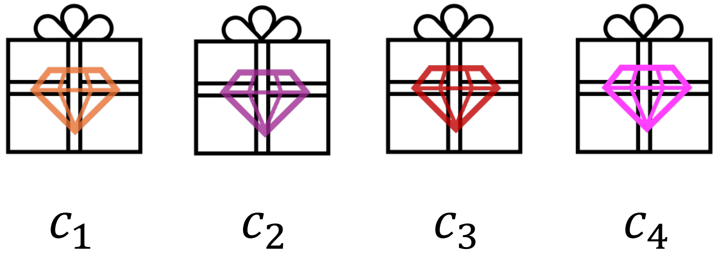
Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs
- Open door for complex BO (freeze-thaw, multi-fidelity, function network, etc.)





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