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

Qian Xie (Cornell ORIE)
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

Bayesian Optimization

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

$\in$ decision-making under uncertainty

Applications:
Hyperparameter tuning
Drug discovery
Control design

Bayesian Optimization

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

∈ decision-making under uncertainty

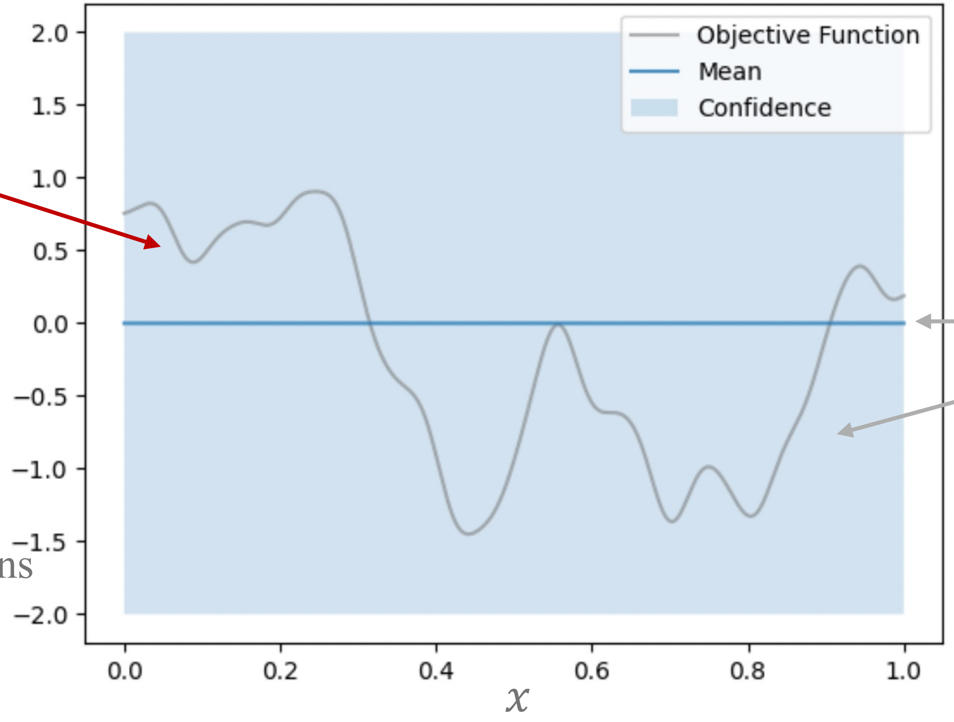
Applications:
Hyperparameter tuning
Drug discovery
Control design

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

mean: prediction

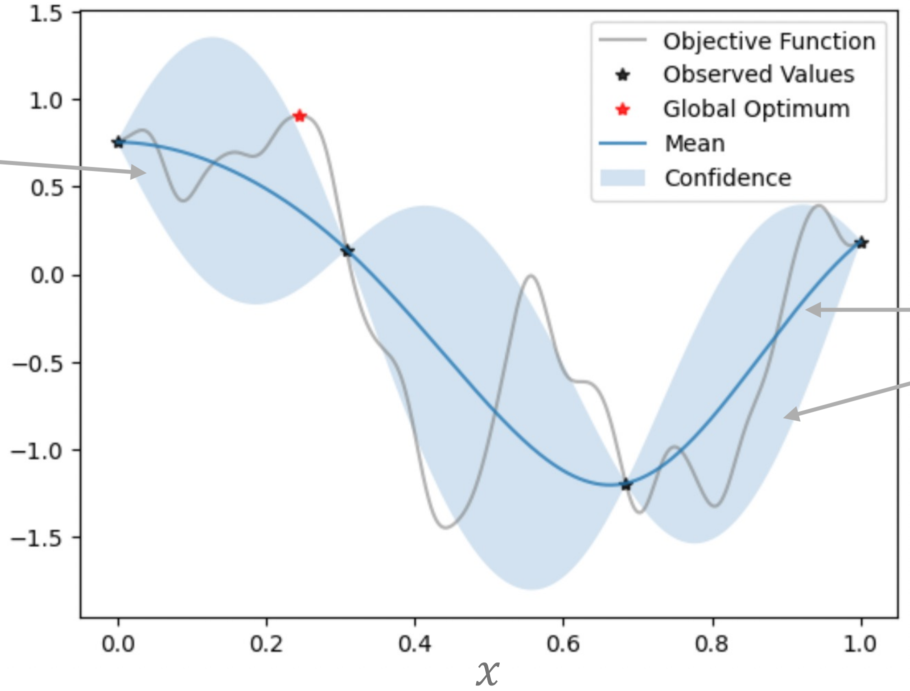
variance: confidence/uncertainty

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

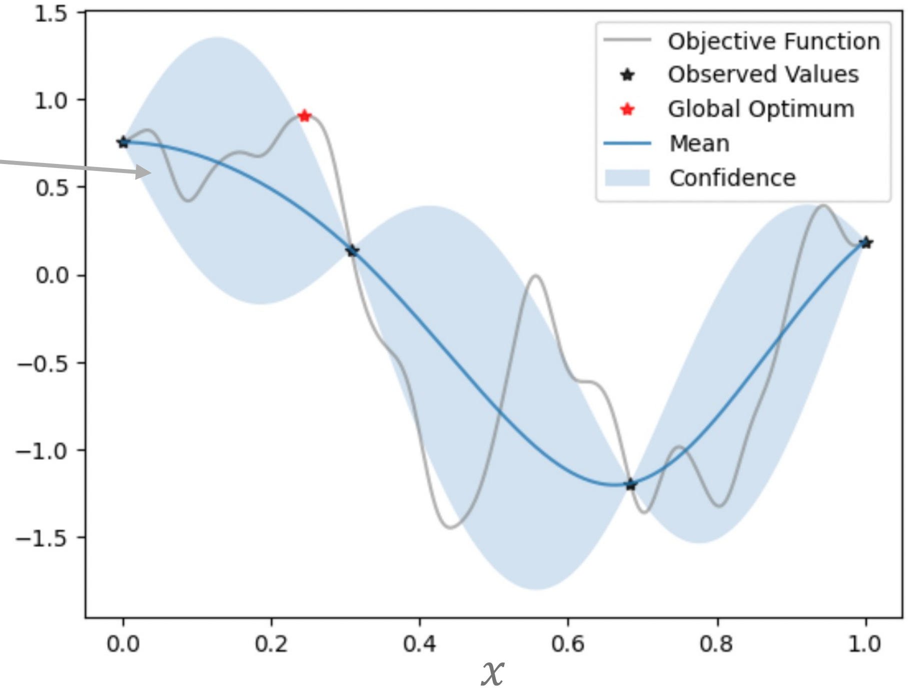
Objective: find global optimum $x^* = \mathrm{argmax}_{x \in \mathcal{X}}\, f(x)$

Decision: evaluate a set of points

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

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

Decision: evaluate a set of points

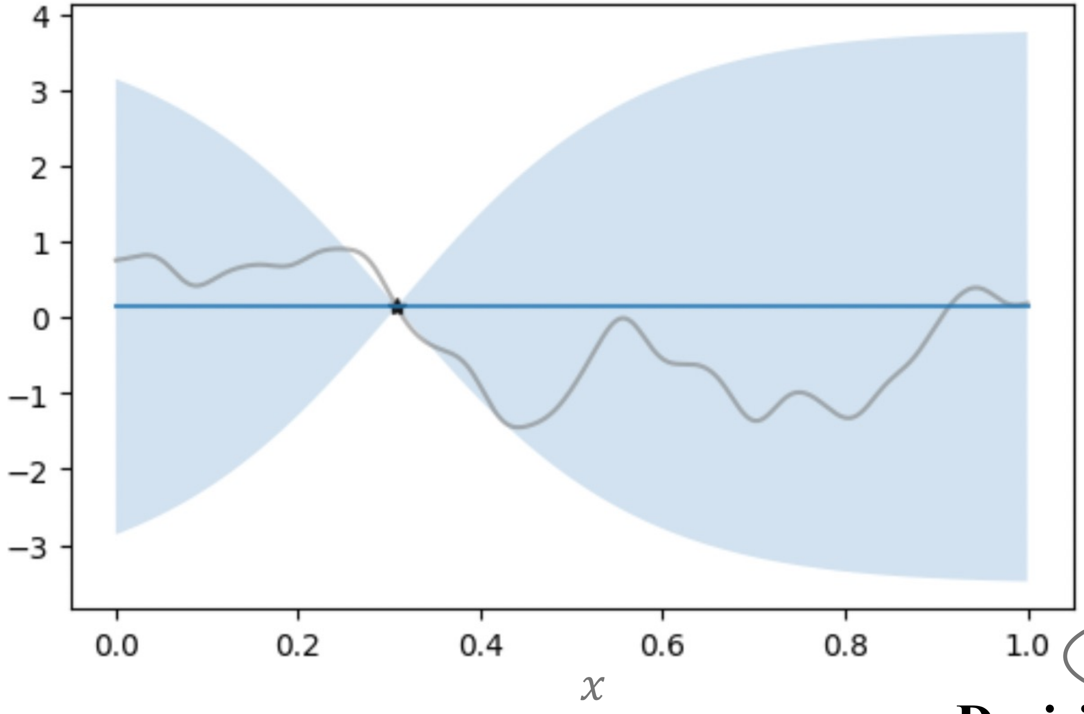
Bayesian Optimization

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

Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

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



adaptively

Decision: evaluate a set of points

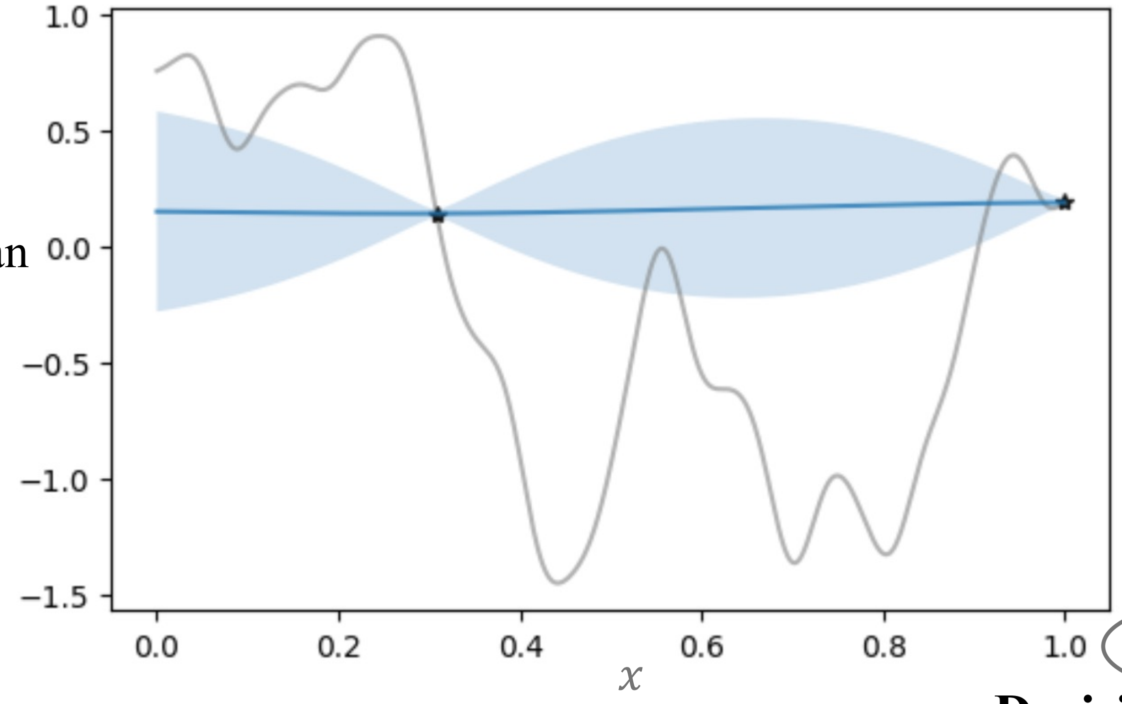
Bayesian Optimization

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

Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

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



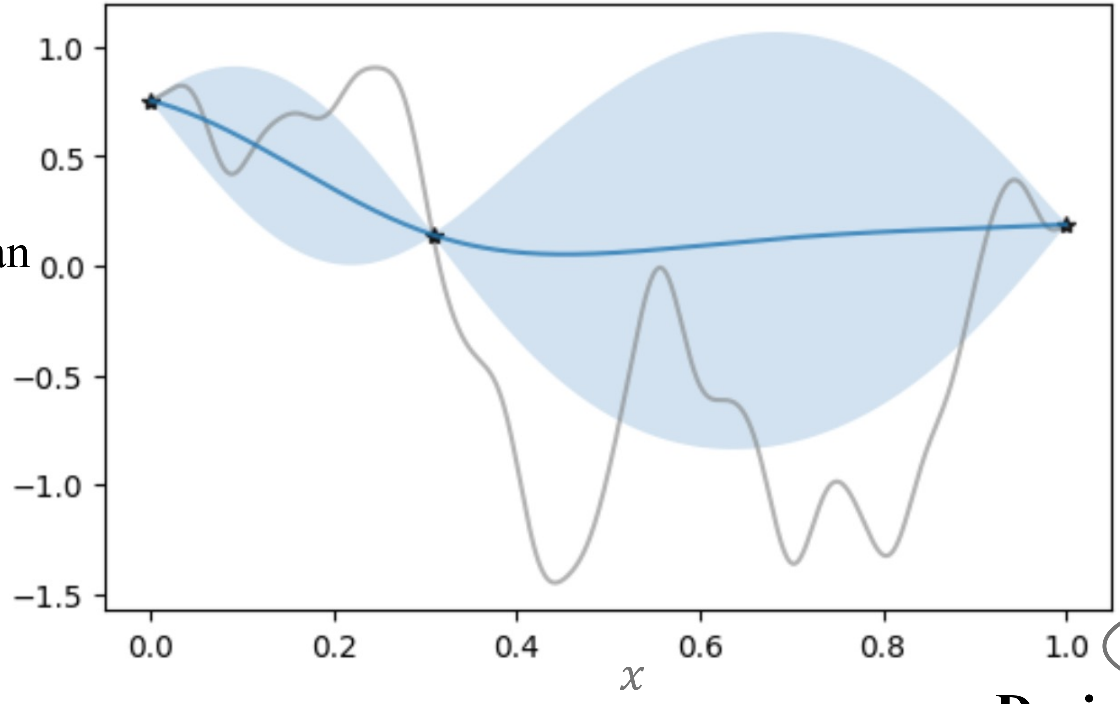
adaptively

Decision: evaluate a set of points

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

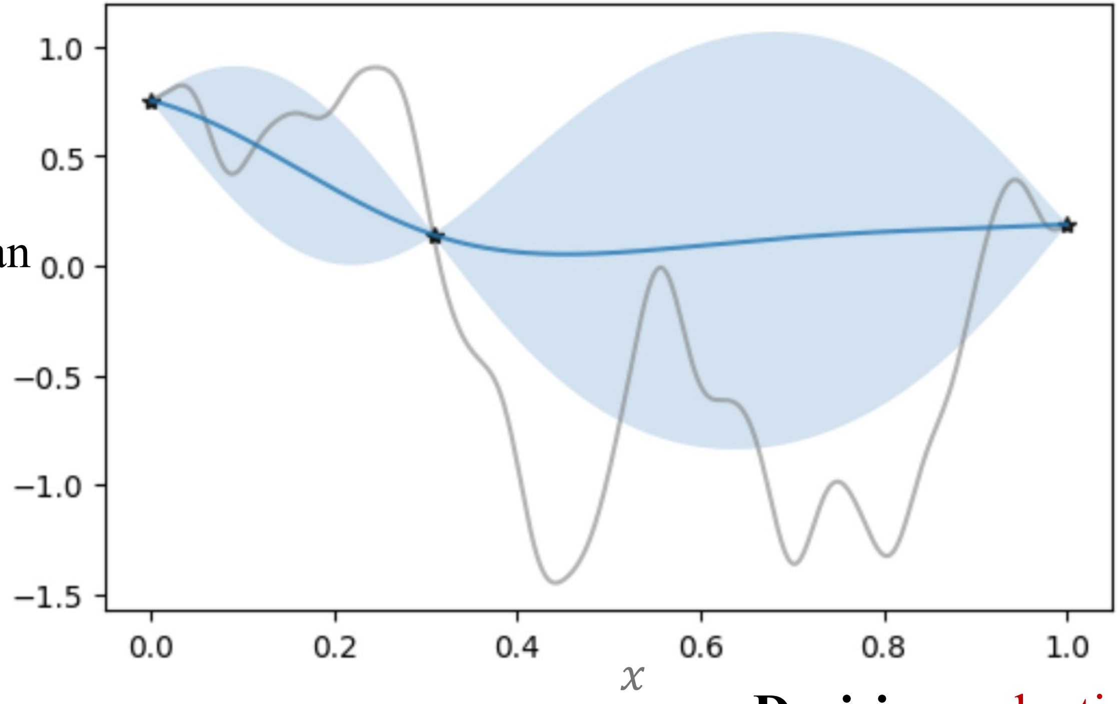
adaptively

Decision: evaluate a set of points

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

Decision: adaptively evaluate a set of points

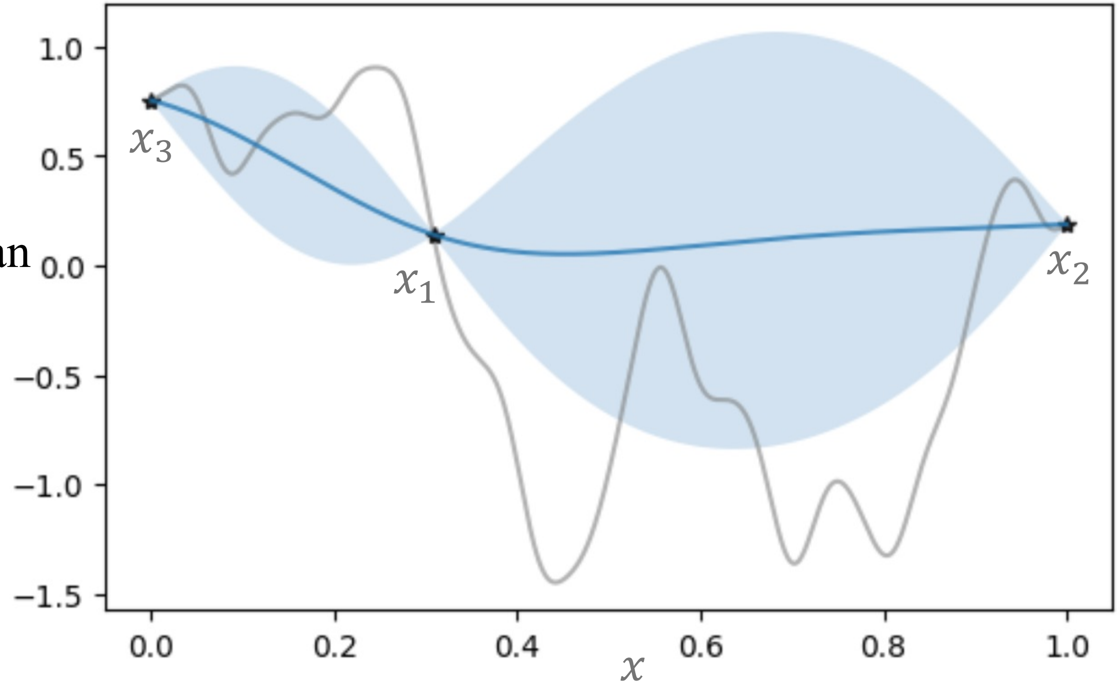
$$x_1, x_2, \ldots, x_T \in \mathcal{X}$$

T: time budget

Bayesian Optimization

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

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



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

Objective: optimize best observed value at time T

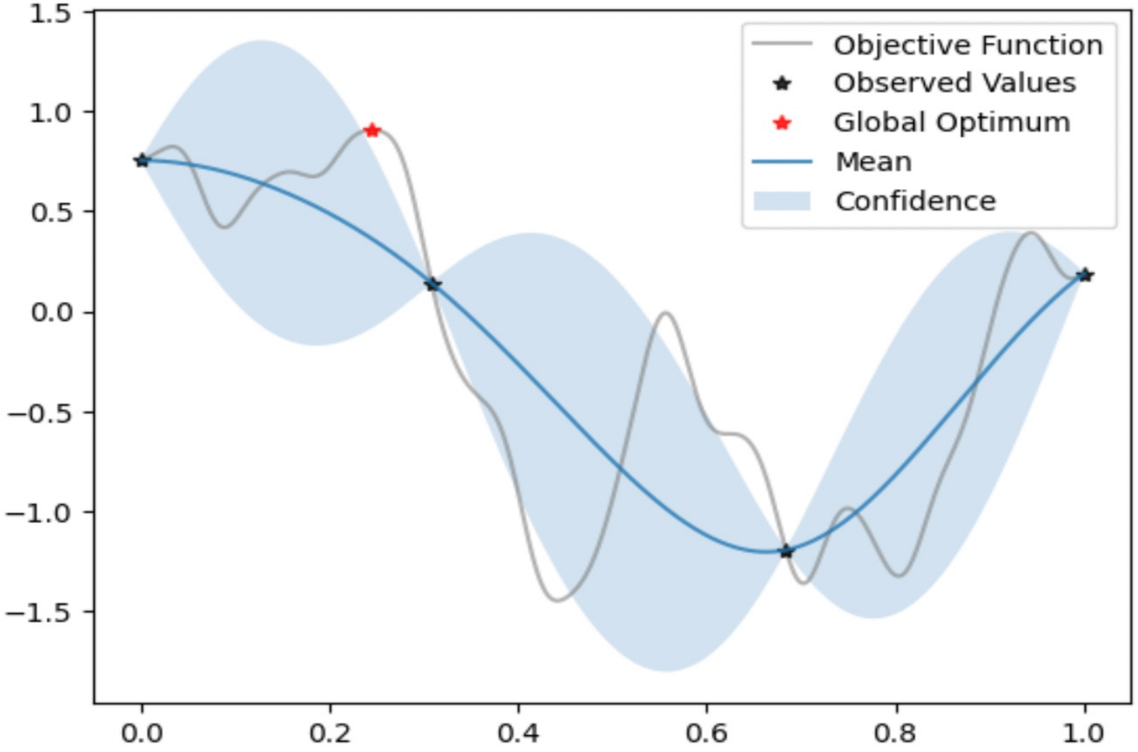
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

Decision: adaptively evaluate a set of points

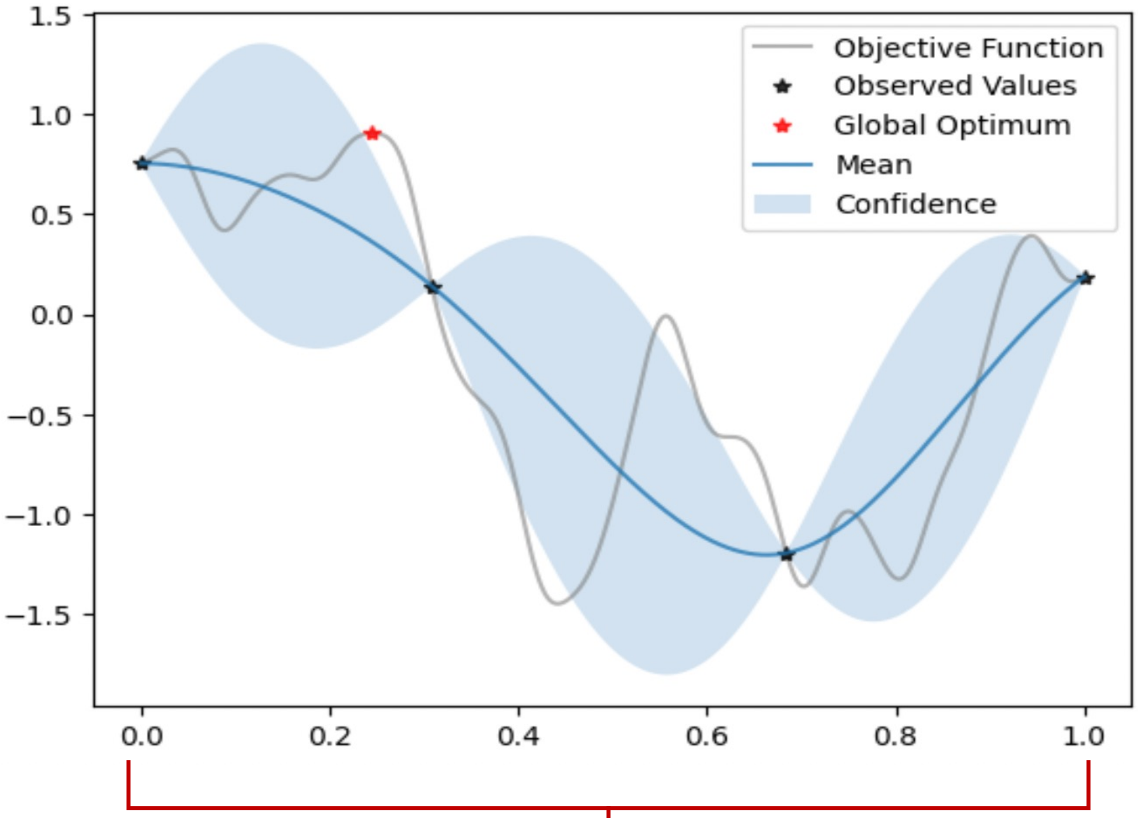
$$x_1, x_2, \ldots, x_T \in \mathcal{X}$$

T: time budget

Why is it hard?



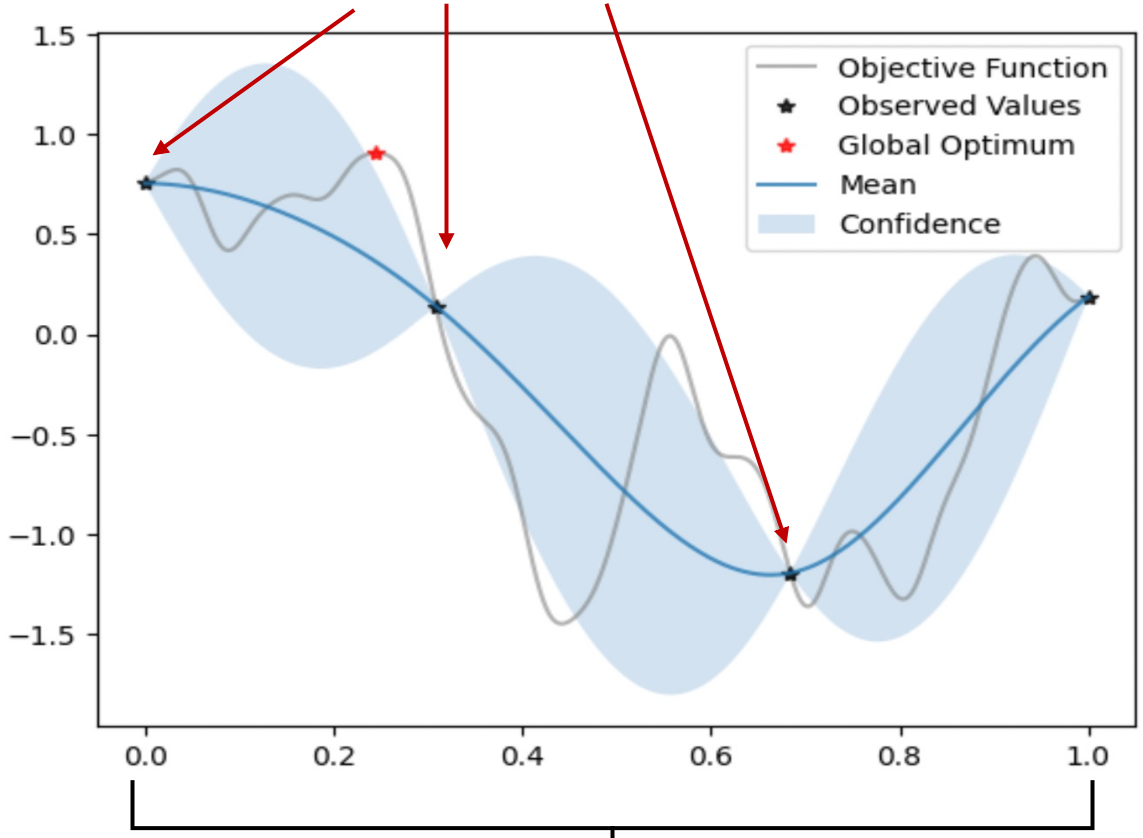
Why is it hard?



Continuous search domain

Why is it hard?

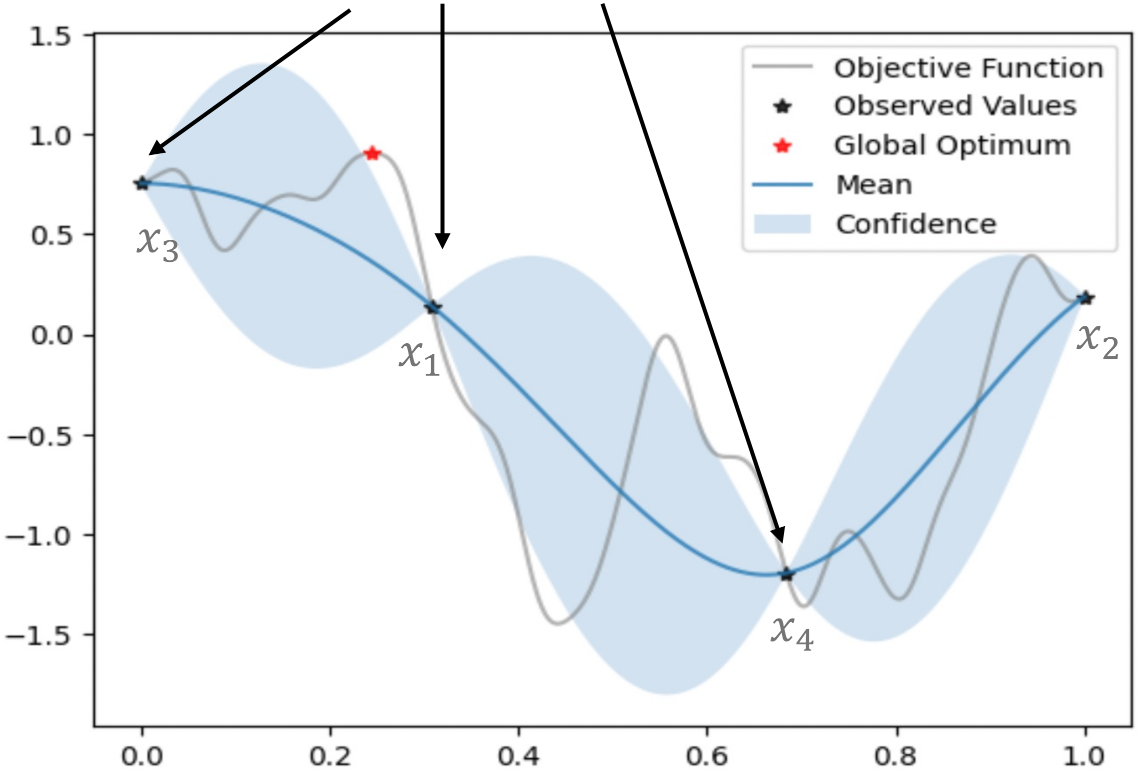
Correlated values



Continuous search domain

Why is it hard?

Correlated values



Continuous search domain

Hard budget constraint

~~$t = 1$~~

~~$t = 2$~~

~~$t = 3$~~

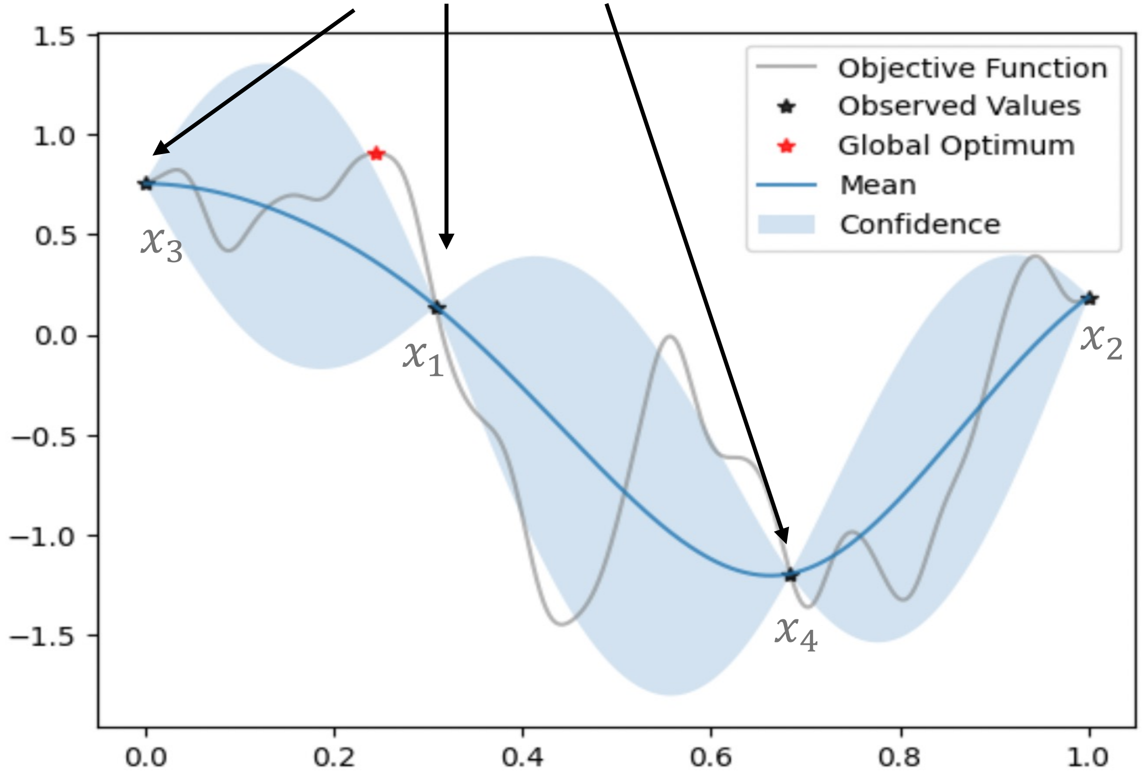
~~$t = 4$~~

⋮

$t = T$

Why is it hard?

Correlated values



Continuous search domain

Hard budget constraint

~~$t = 1$~~

~~$t = 2$~~

~~$t = 3$~~

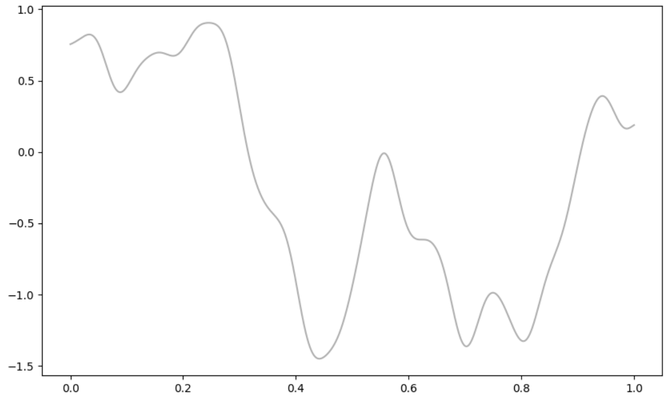
~~$t = 4$~~

⋮

$t = T$

$\Longrightarrow$ Optimal policy unknown!

Bayesian Optimization

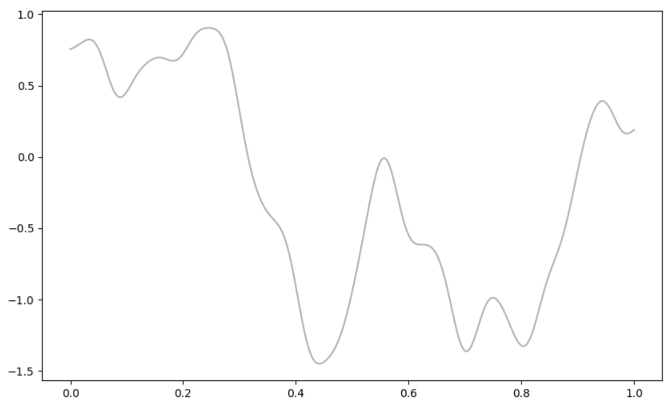


Continuous

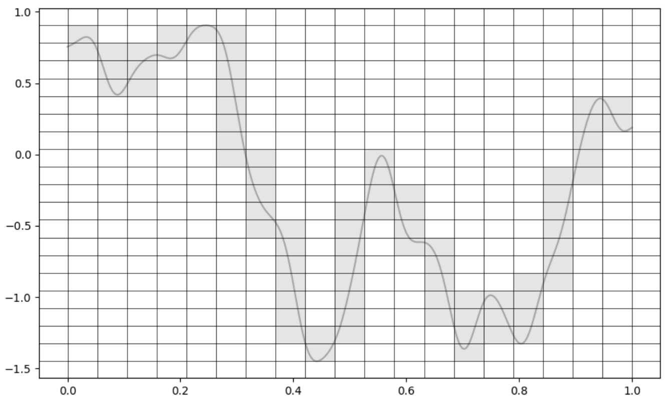
Correlated

Hard budget constraint

Bayesian Optimization



⟹

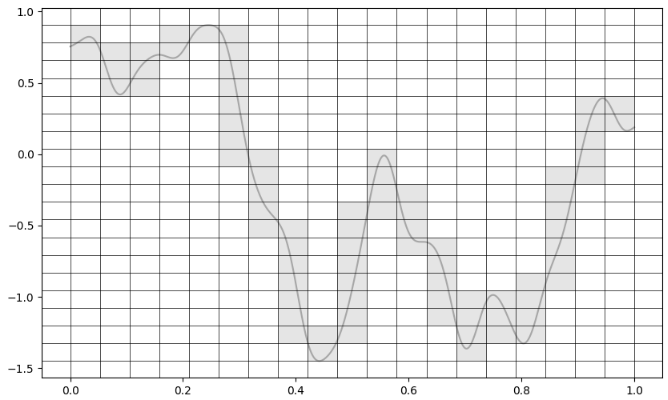


Continuous ⟹ Discrete

Correlated

Hard budget constraint

Bayesian Optimization

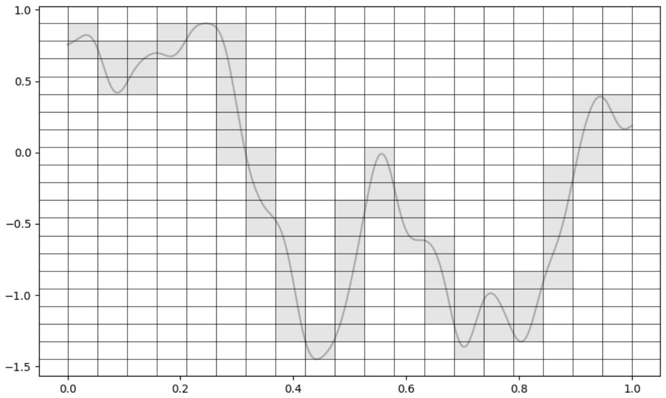


Continuous $\Longrightarrow$ Discrete

Correlated

Hard budget constraint

Bayesian Optimization



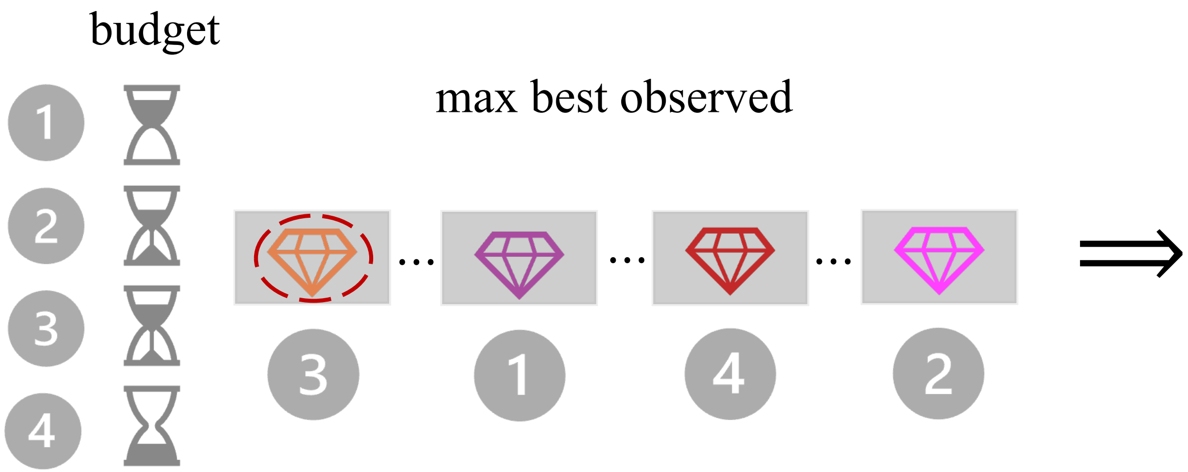
$\Longrightarrow$

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint

Bayesian Optimization

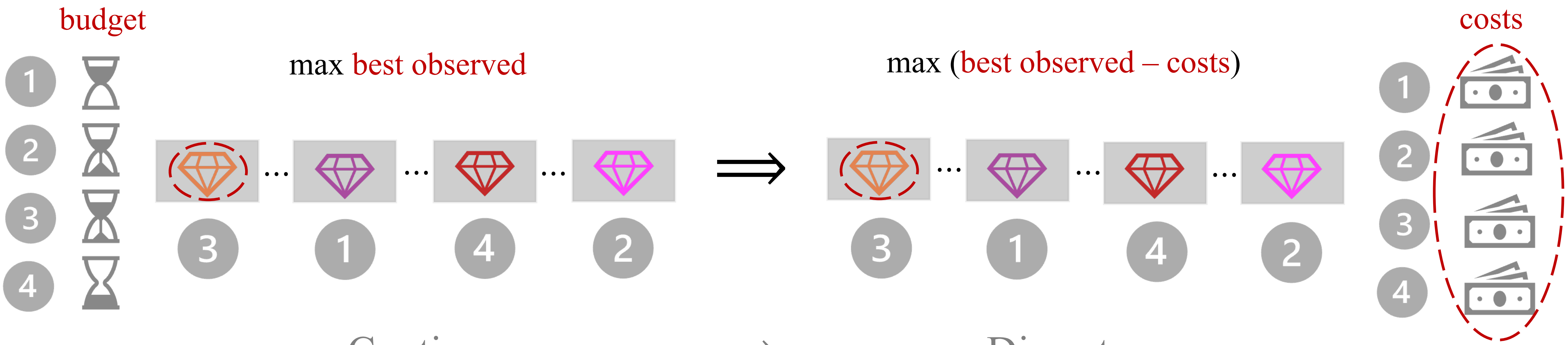


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint

Bayesian Optimization



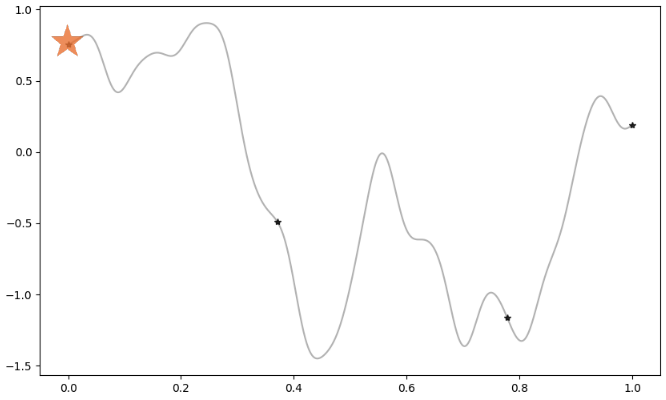
Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

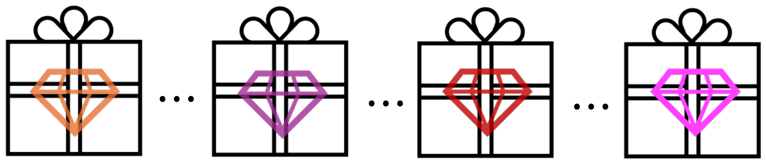
Hard budget constraint $\xRightarrow{\text{Lagrangian relaxation}}$ Cost per sample

Bayesian Optimization $\Longrightarrow$ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits



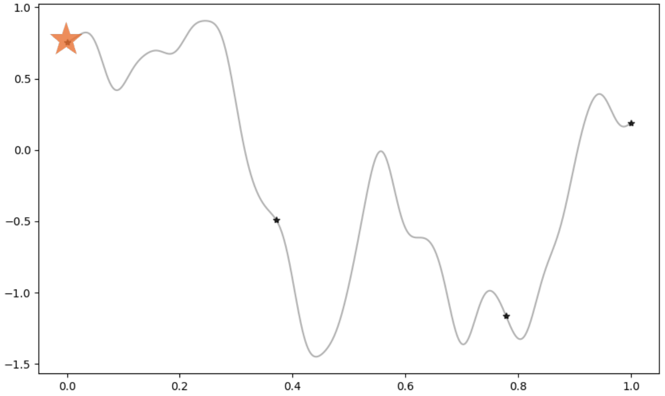
$\Longrightarrow$



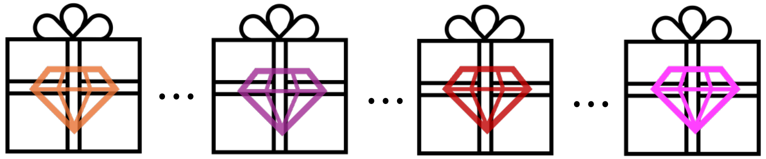
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample

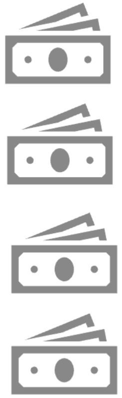
Bayesian Optimization ⟹ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits



⟹





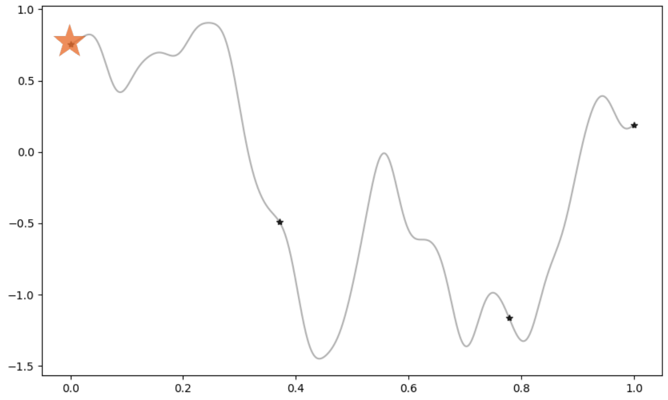
Continuous ⟹ Discrete

Correlated ⟹ Independent

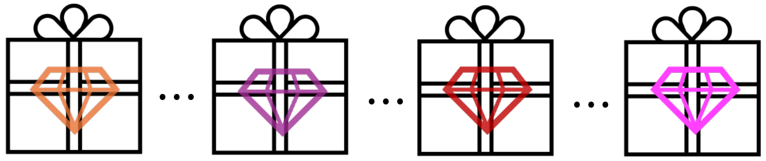
Hard budget constraint ⟹ Cost per sample

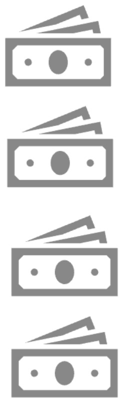
Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization $\Longrightarrow$ Pandora's Box



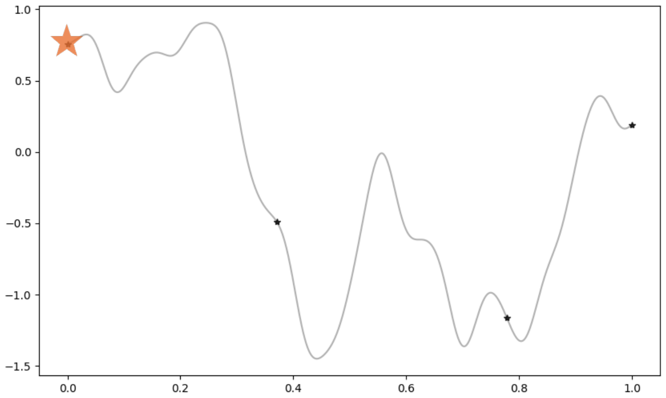
$\Longrightarrow$



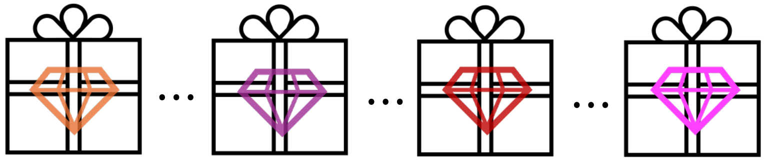


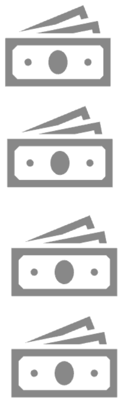
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	$\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



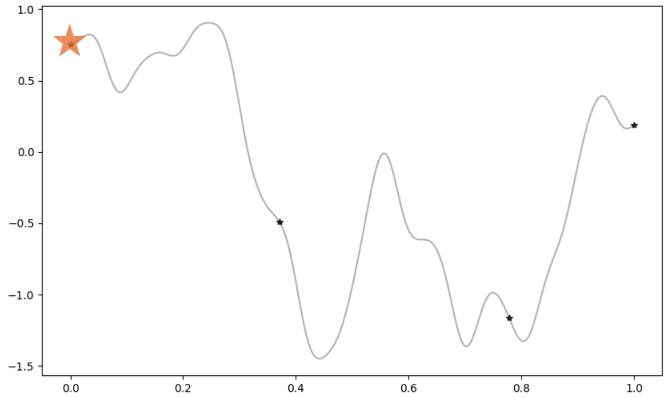
$\Longrightarrow$



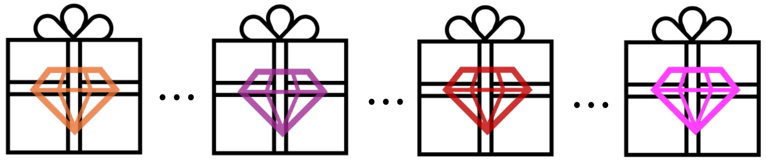


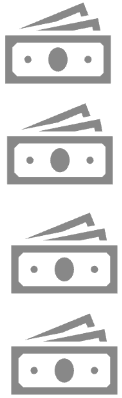
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	How to translate? $\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



$\Longrightarrow$





Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint $\Longrightarrow$ Cost per sample

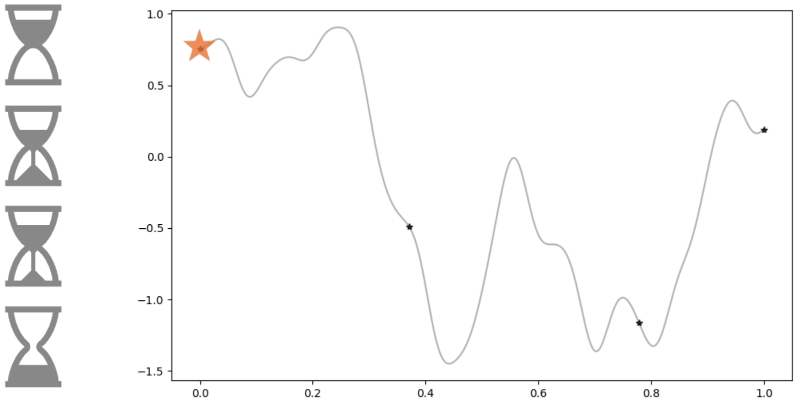
How to translate?

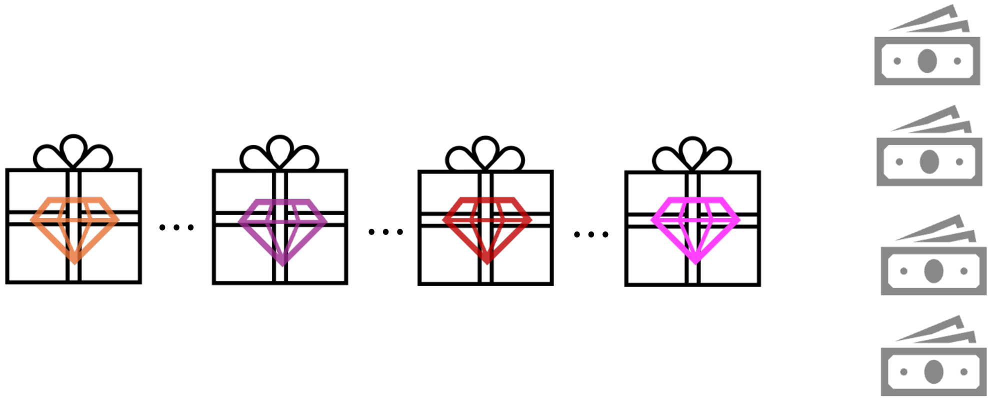
Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

Our contributions!

Our Contributions

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

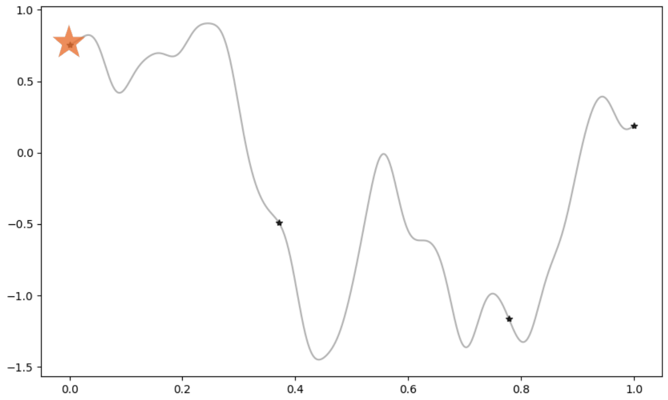


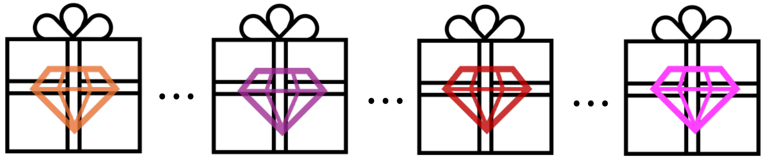


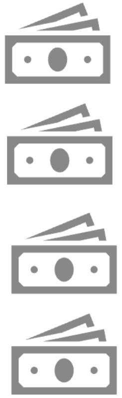
? $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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



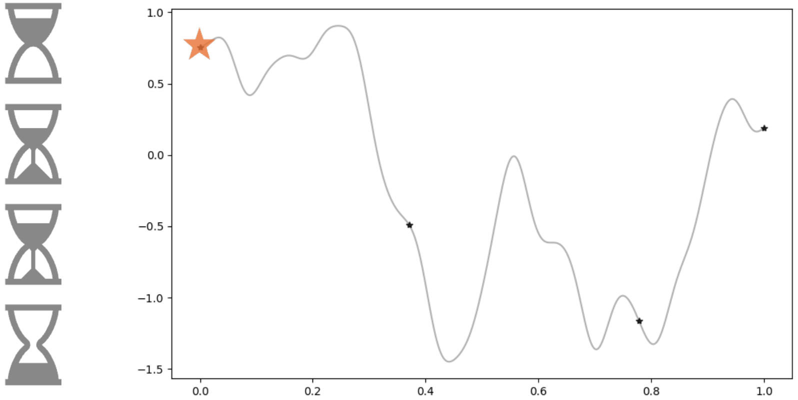


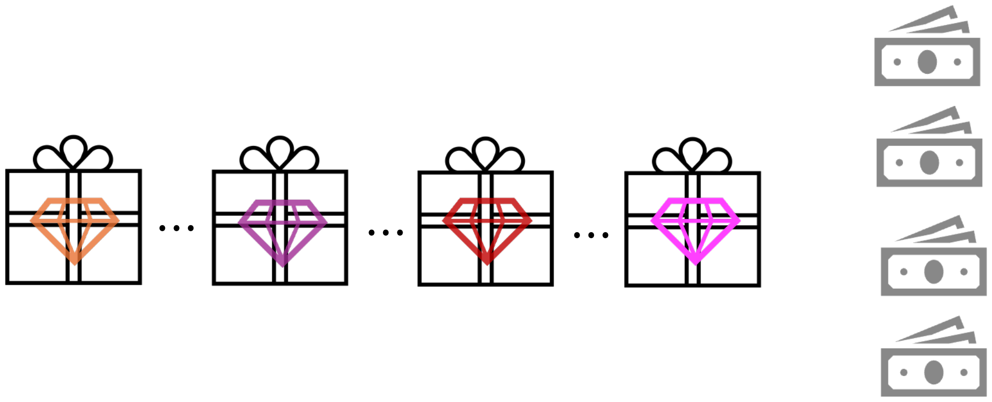


Our work $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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

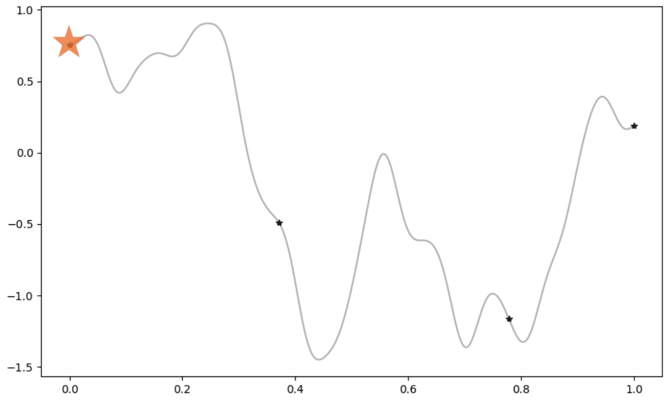


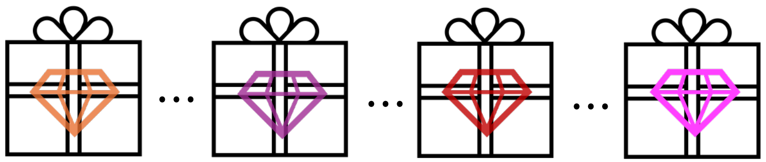


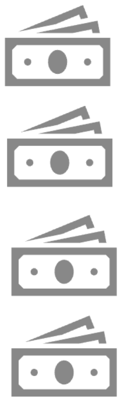
Our work $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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



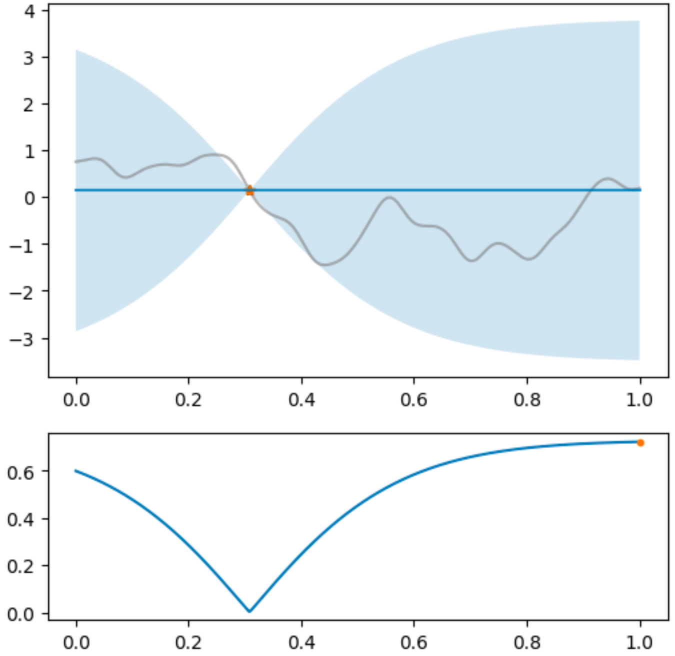




Our work $\Longleftarrow$ Pandora's Box Gittins index

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

mean: prediction

variance: confidence/uncertainty

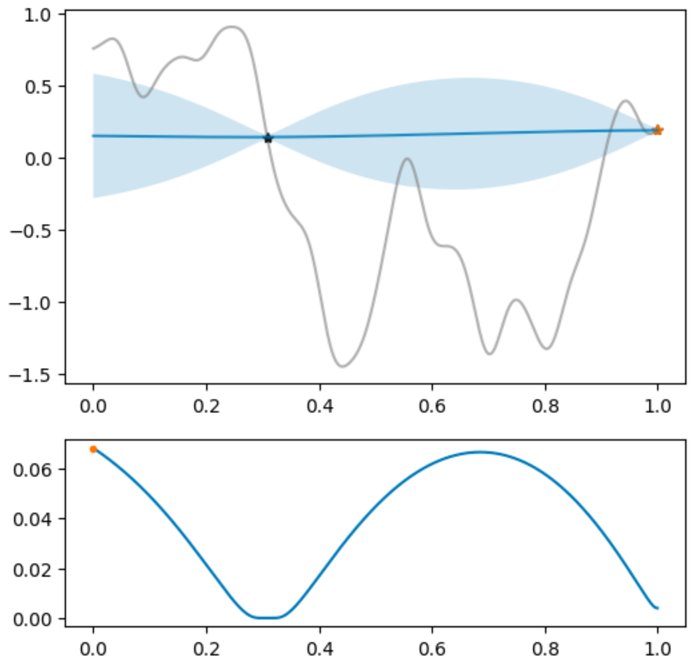
Trade-off between

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

D: observed data

y_{best}: current best observed value

Popular One-step Heuristic: EI



mean: prediction

variance: confidence/uncertainty

Trade-off between
- exploitation (high mean) and
- exploration (high uncertainty)

Expected improvement

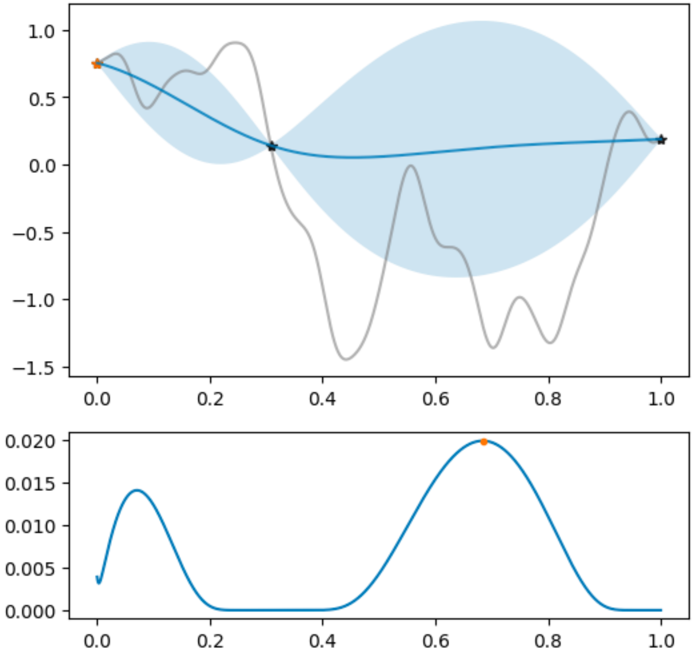
$$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^+]$$

D: observed data

y_{best}: current best observed value

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

Popular One-step Heuristic: EI



mean: prediction

variance: confidence/uncertainty

Trade-off between

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

Expected improvement

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

D: observed data

y_{best}: current best observed value

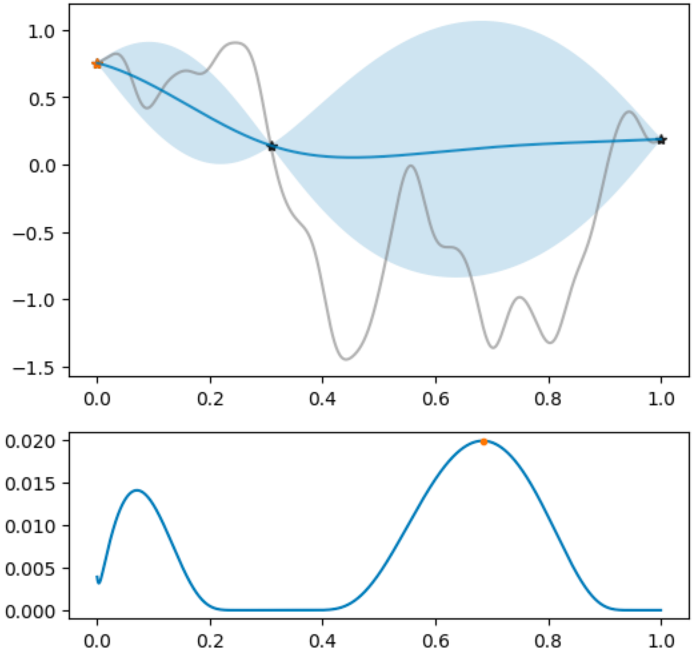
EI policy: evaluate $\mathrm{argmax}_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$

Popular One-step Heuristic: EI

Other heuristics:

simple
- Upper Confidence Bound
- Thompson Sampling

slow
- Predictive Entropy Search
- Knowledge Gradient
- Multi-step Lookahead EI



Expected improvement

mean: prediction

variance: confidence/uncertainty

Trade-off between
- exploitation (high mean) and
- exploration (high uncertainty)

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

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

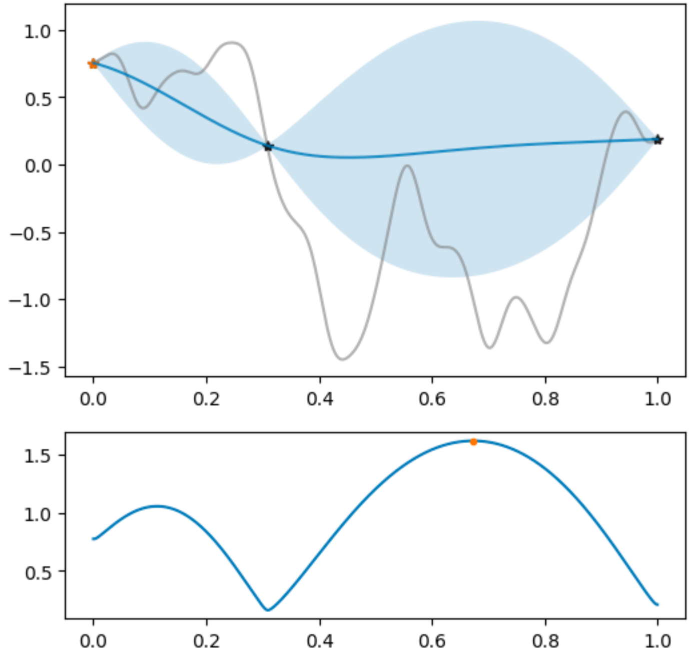
D: observed data

y_{best}: current best observed value

New One-step Heuristic: PBGI

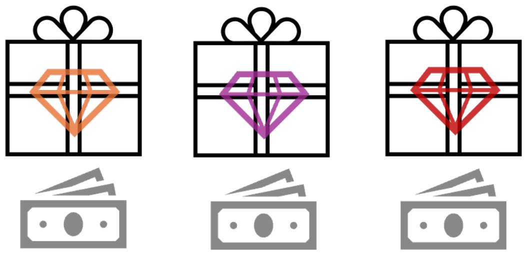
Other heuristics:

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



Pandora’s box Gittins index

Pandora’s box



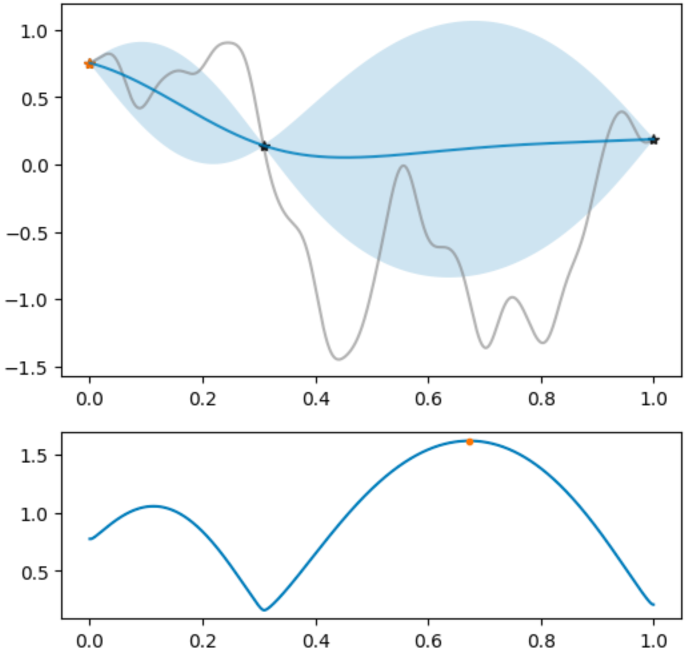
$\alpha^*(x)$: Gittins index function

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

New One-step Heuristic: PBGI

Other heuristics:

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



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

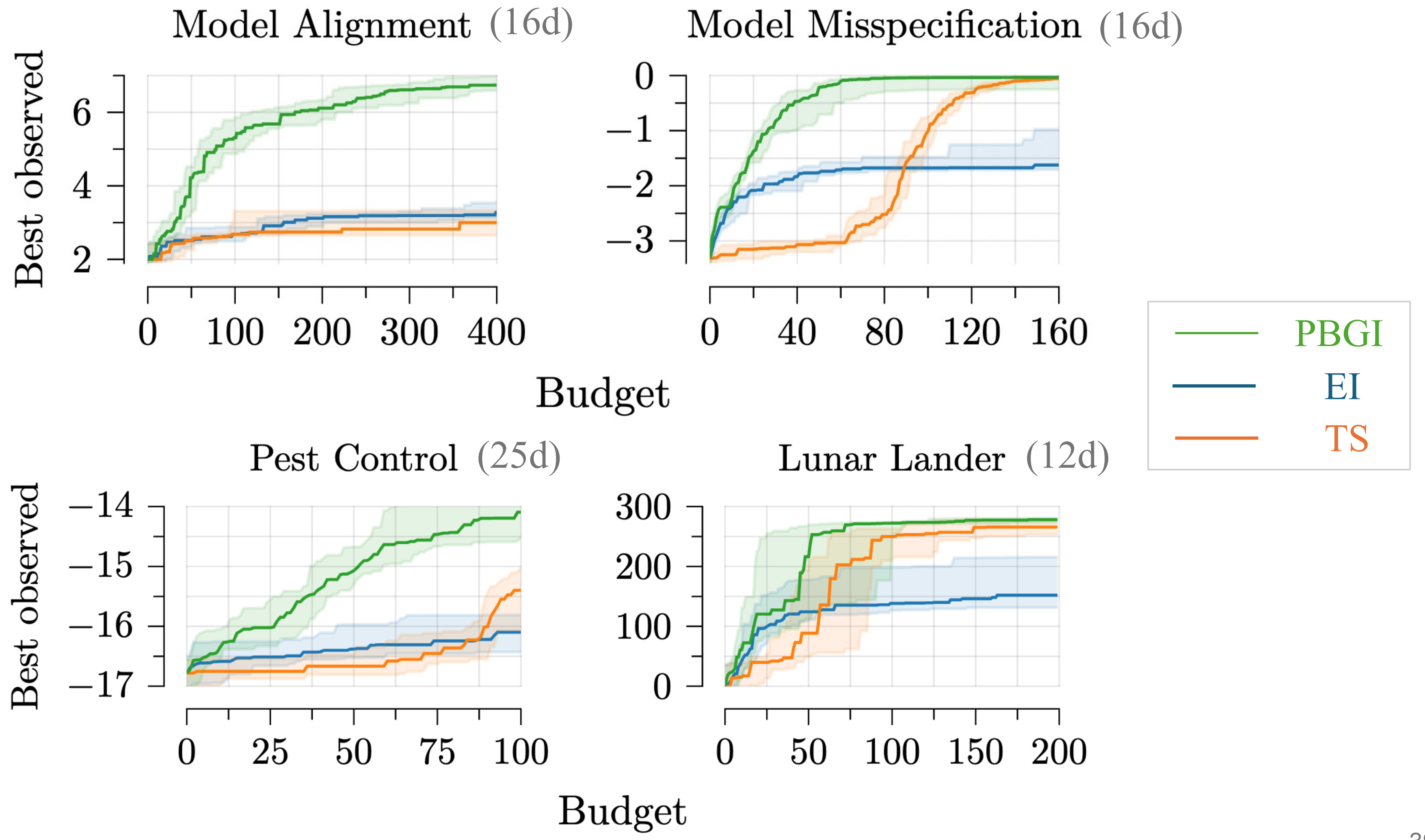
λ λ λ

λ: cost-per-sample
(Lagrange multiplier)

D: observed data

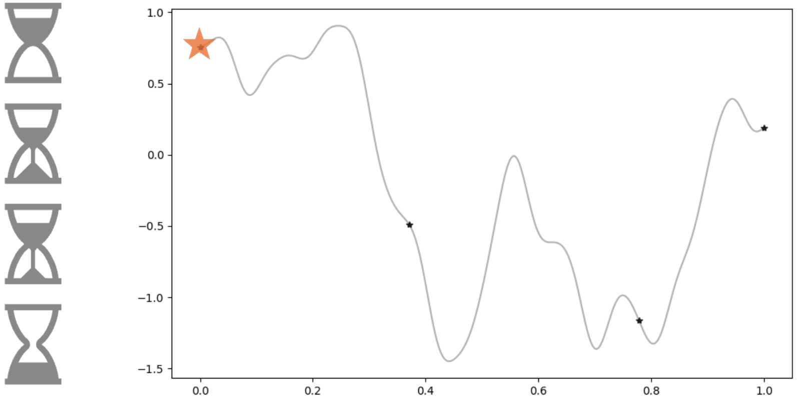
$\alpha^*(x)$: solution to $\mathrm{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

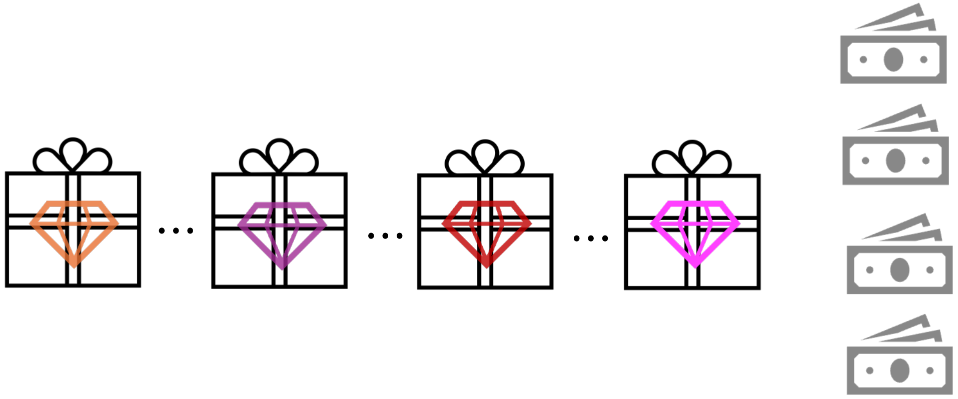
Experiment Results: PBGI vs EI vs TS



Conclusions

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





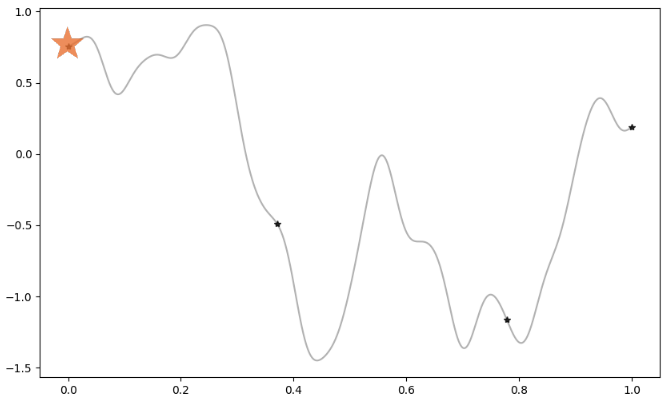
Our work ⟸ Pandora’s box Gittins index

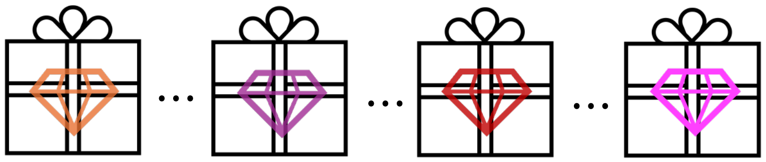
Check our preprint on arXiv!

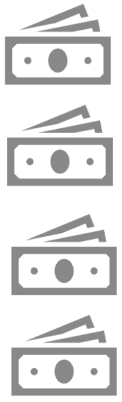
Conclusions

- 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!





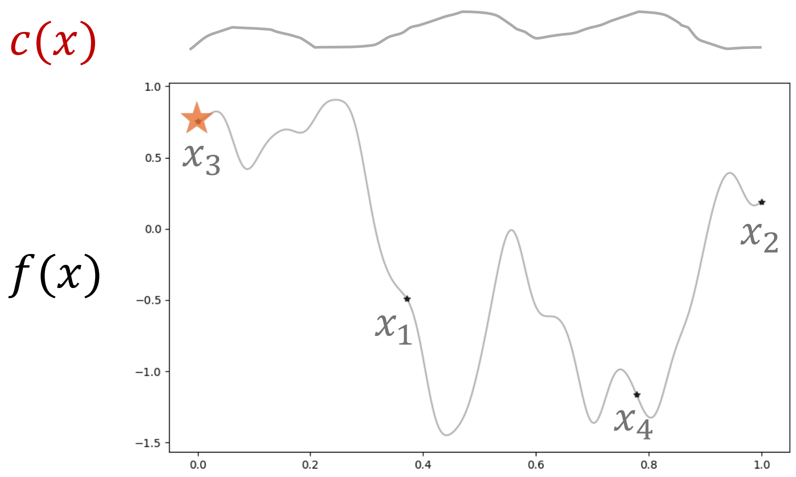


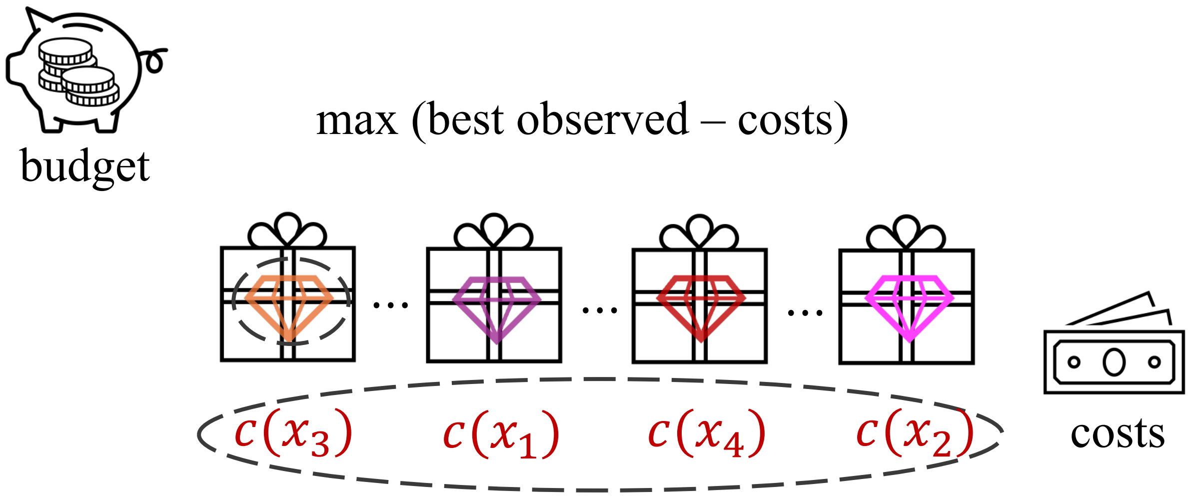
Our work ⟸ Pandora's box Gittins index

Check our preprint on arXiv!

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



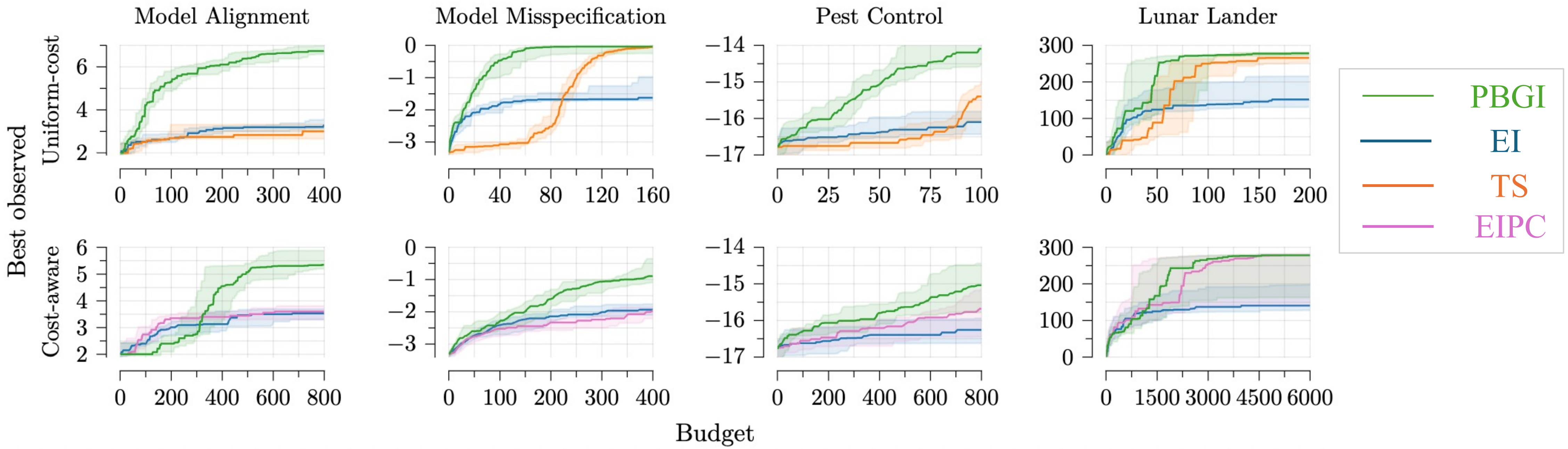


Our work $\Longleftarrow$ Pandora's Box Gittins index

Check our preprint on arXiv!

Heterogeneous-cost Experiment Results

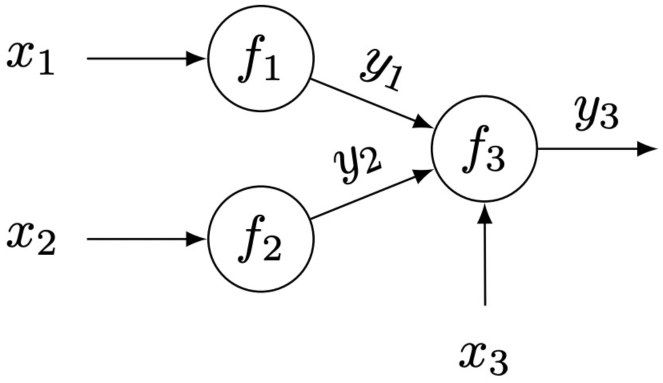
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs

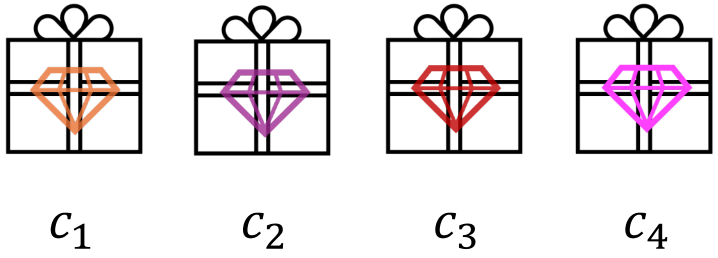


Check our preprint on arXiv!

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.)





? $\Longleftarrow$ Pandora's Box Gittins index

Check our preprint on arXiv!