Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index

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

INFORMS'24 Data Mining Best General Paper Competition

Coauthors

Raul Astudillo

Peter Frazier

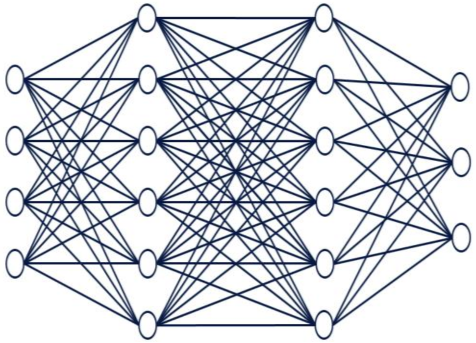
Ziv Scully

Alexander Terenin

World of Parameter Optimization

Hyperparameter tuning:

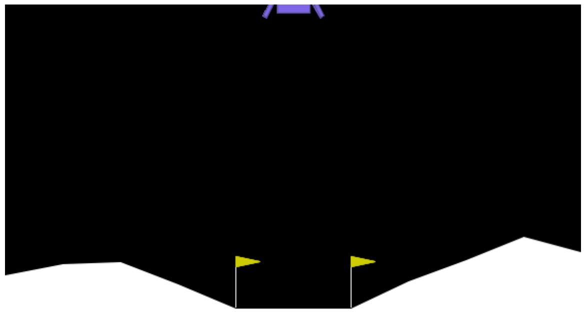
Training parameters →



→ Accuracy

Control optimization:

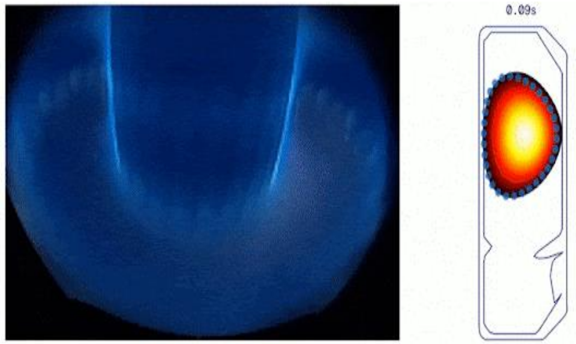
Control parameters →



→ Reward

Plasma physics:

Reactor parameters →



→ Stability

World of Parameter Optimization

Black-box optimization:

Input parameters ⟶  ⟶ Performance metrics

World of Parameter Optimization

Black-box optimization:

$x \longrightarrow$

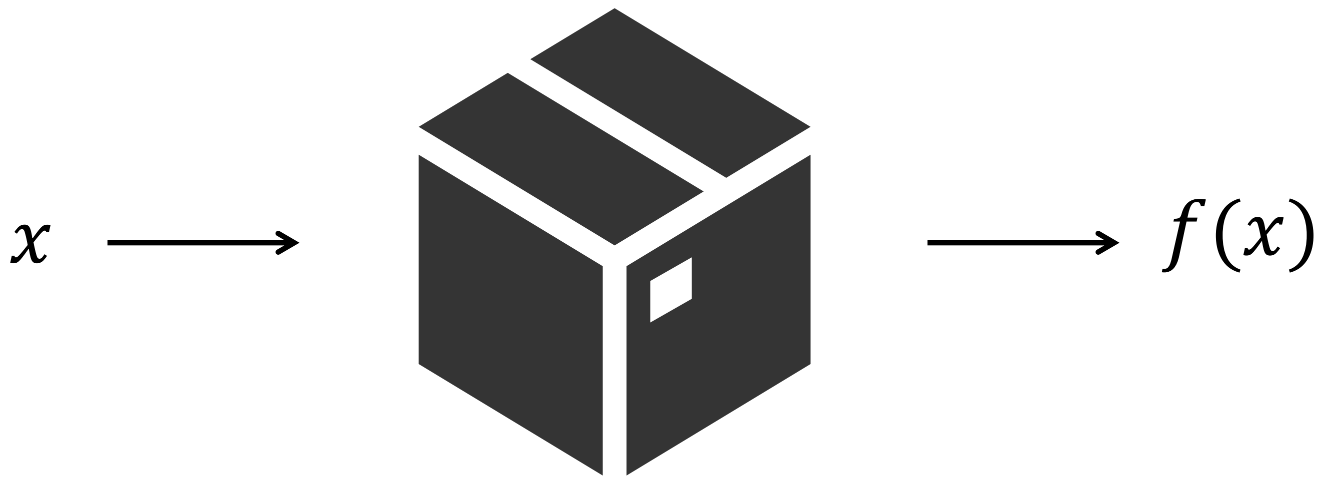
$\longrightarrow f(x)$

Optimizing Black-box Functions

$x \longrightarrow$  $\longrightarrow f(x)$

Goal: $\mathbf{max}_{x\in\mathcal{X}}\, f(x)$

Optimizing Black-box Functions



Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

$f \sim$Stochastic Process

Optimizing Black-box Functions

$x \longrightarrow$  $\longrightarrow f(x)$

expensive-to-evaluate

Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

Optimizing Black-box Functions

$x \longrightarrow$

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Goal: $\mathbf{max}\ \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

Optimizing Black-box Functions

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$f \sim$Gaussian Process

Bayesian Optimization

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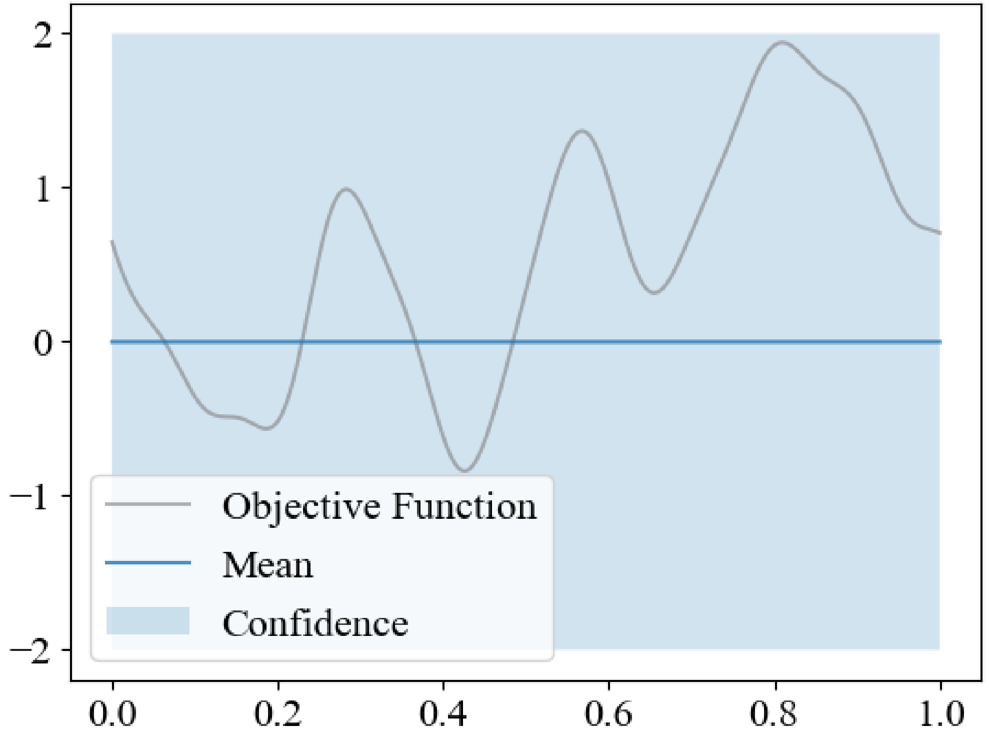
Bayesian Optimization



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Bayesian Optimization

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Bayesian Optimization

What to evaluate next?

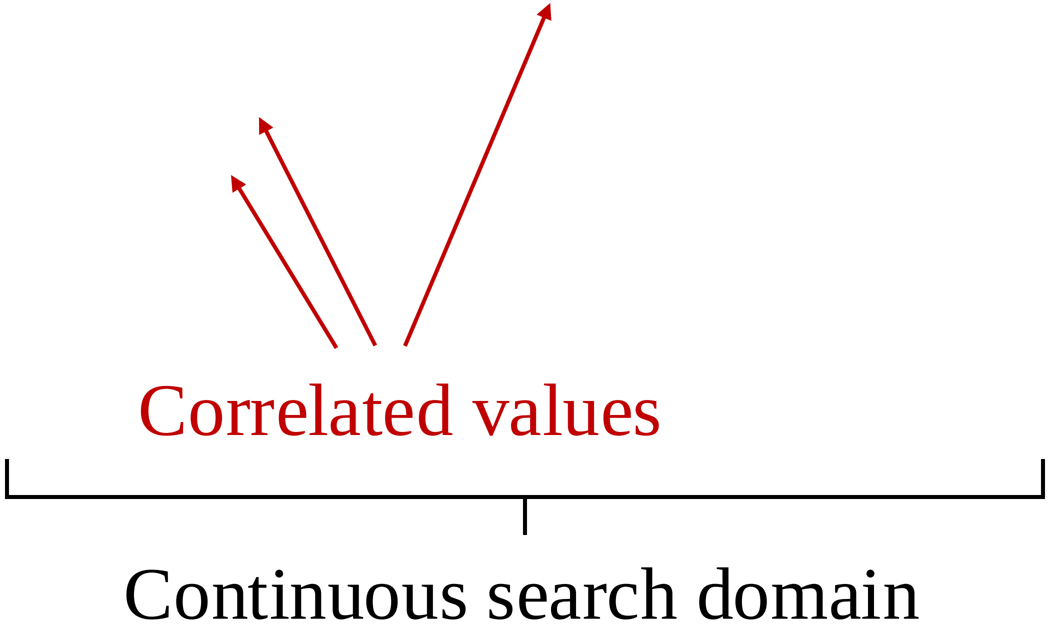
Bayesian Optimization

Optimal policy?

Bayesian optimization

Continuous search domain

Bayesian optimization



Bayesian Optimization

Correlation & continuity $\Longrightarrow$ Intractable MDP

Bayesian Optimization

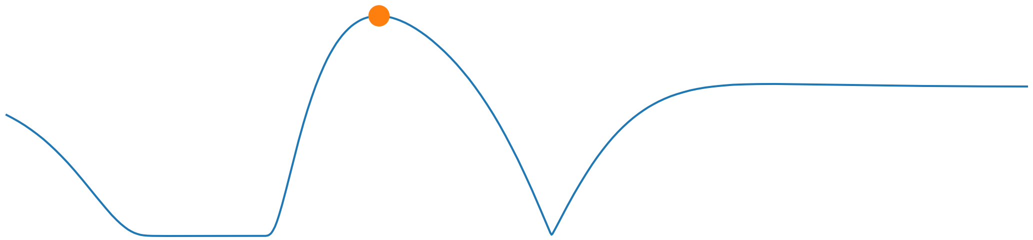
Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement

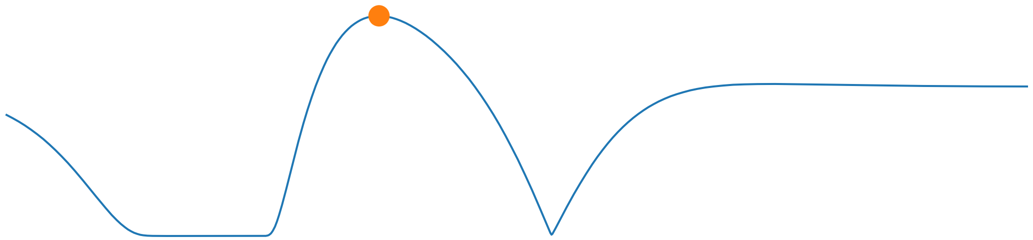
current best observed

data

$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{“improvement”}} \mid D]$$



Popular Policy: Expected Improvement



$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - \overset{\text{current best observed}}{y_{\text{best}}}, 0)}_{\text{“improvement”}} \mid \overset{\text{data}}{D}]$$

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

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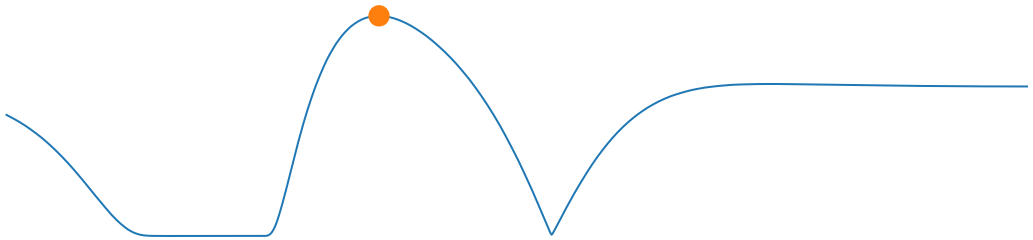
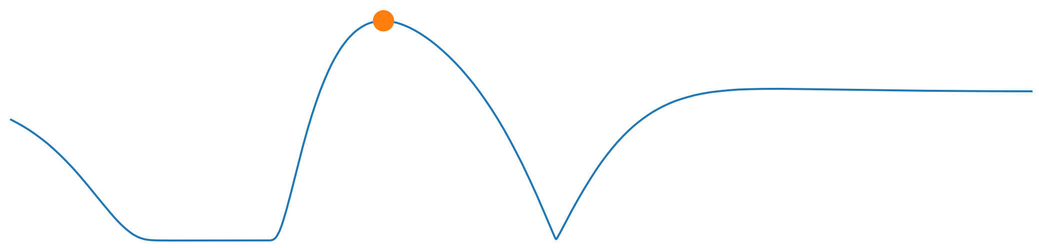


$$\max_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$$

One-step approximation to MDP

Popular Policy: Expected Improvement



Other improvement-based policy:

- Probability of Improvement
- Knowledge Gradient
- Multi-step Lookahead EI
- …

Approaches to Bayesian Optimization

- Improvement-based:
  - Expected Improvement
  - Probability of Improvement
  - Knowledge Gradient
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- Our work: Gittins Index

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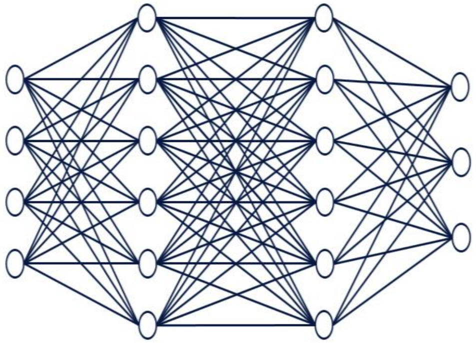
Why another approach?

Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters



Accuracy

Control optimization:

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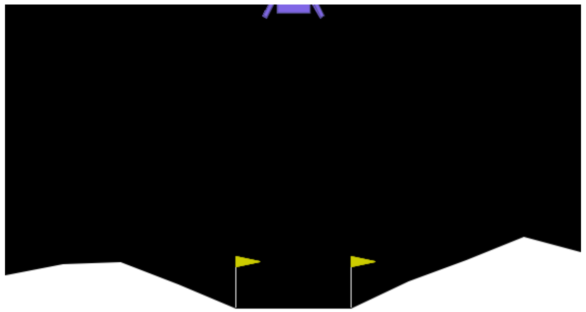

Reward

Plasma physics:

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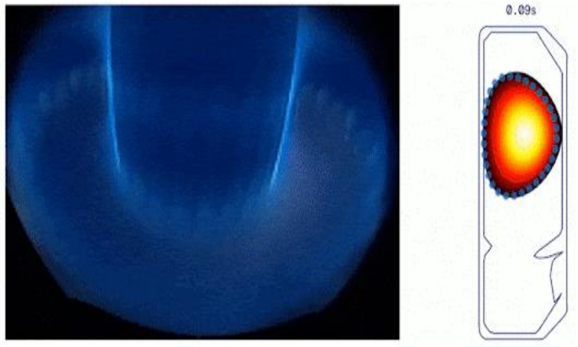
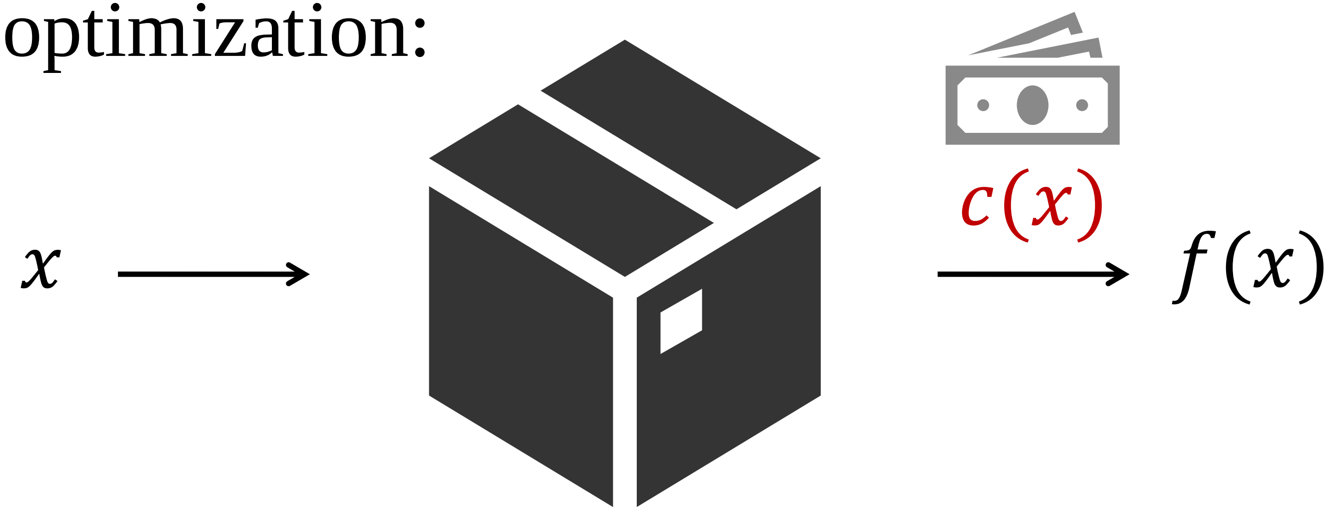


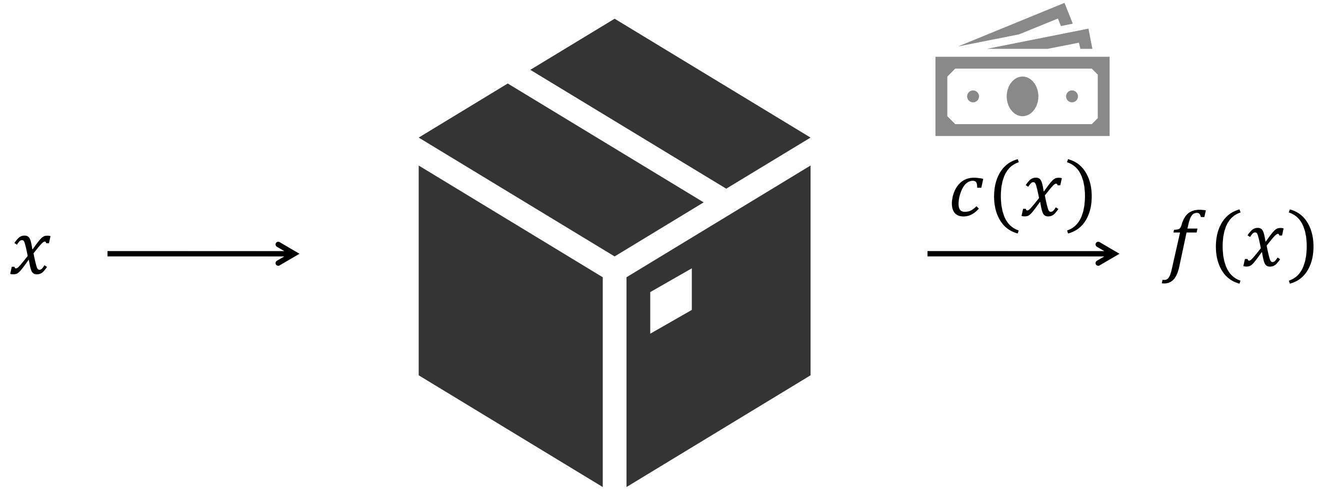
Stability

Challenge: Varying Evaluation Costs

Black-box optimization:



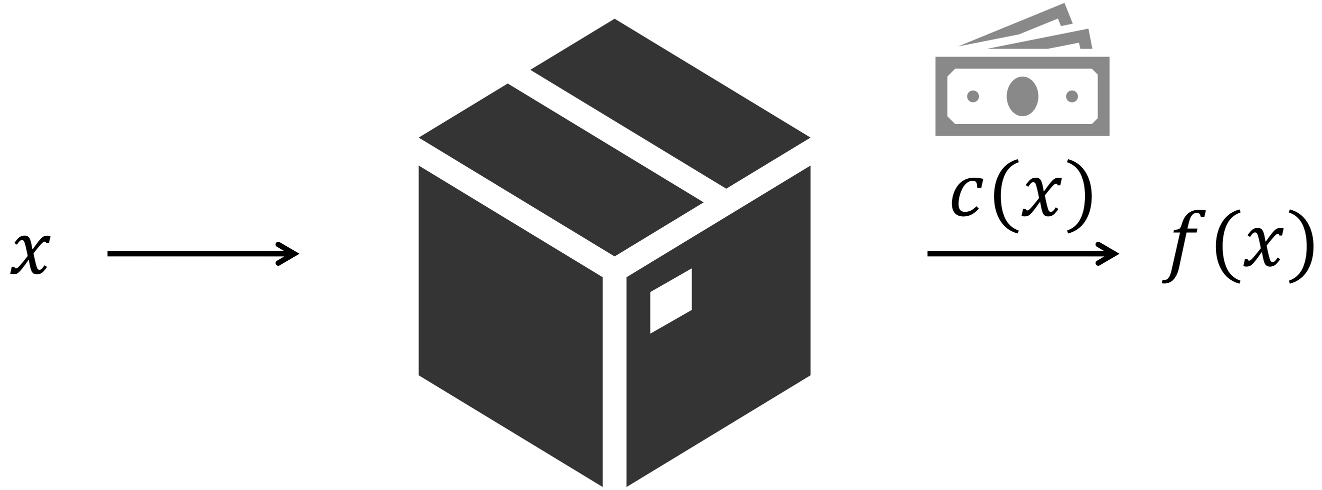
Challenge: Varying Evaluation Costs



Goal: **max** $\mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

s.t. $\mathbb{E} \sum_{t=1}^{T} c(x_t) \leq B$

Cost-aware Bayesian Optimization



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$$\text{s.t. } \mathbb{E} \sum_{t=1}^{T} c(x_t) \leq B$$

[Lee, Perrone, Archambeau, Seeger’21]

[Astudillo, Jiang, Balandat, Bakshy, Frazier’21]

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Expected improvement per cost

$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})/c(x)$

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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Why divide?

Cost-aware Bayesian Optimization

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Why divide?

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

Uniform costs

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Varying costs

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EI and EIPC policy can be arbitrarily bad under varying costs!

[Astudillo, Jiang, Balandat, Bakshy, Frazier’21]

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
Expected improvement	Expected improvement per cost
Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	slow

Cost-aware Bayesian Optimization

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Upper Confidence Bound	?
Thompson Sampling	?

Cost-aware Bayesian Optimization

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⋮	⋮

New design principle: Gittins Index

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
Expected improvement	Expected improvement per cost
Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
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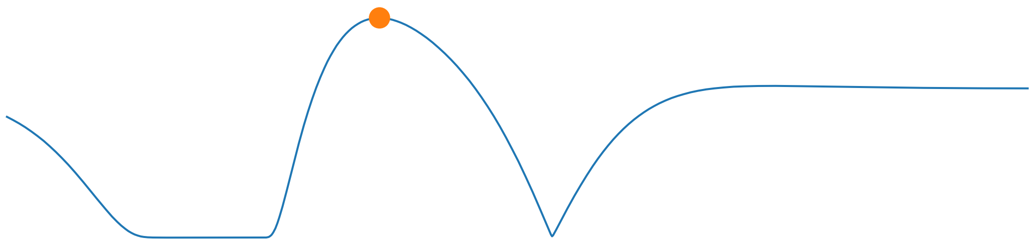
$\vdots$	$\vdots$

New design principle: Gittins Index

Cost-aware

Expected Improvement

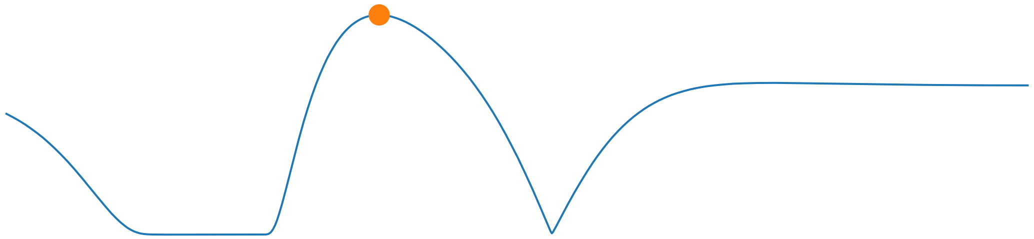


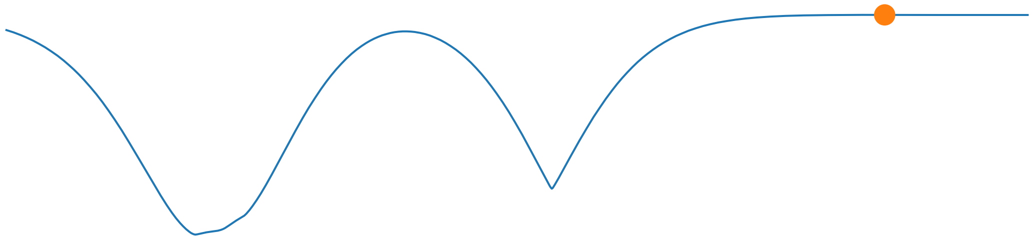
$$\mathrm{EI}(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

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

Expected Improvement

Gittins Index





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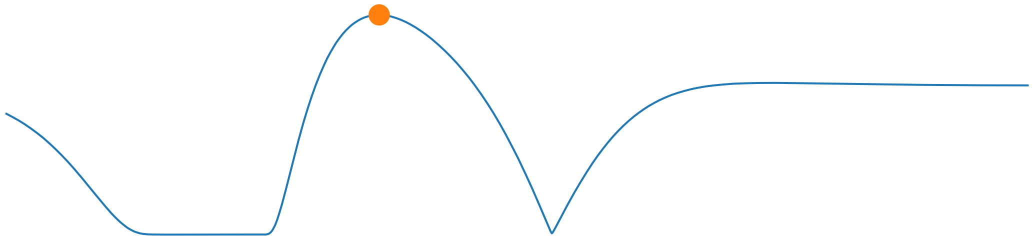
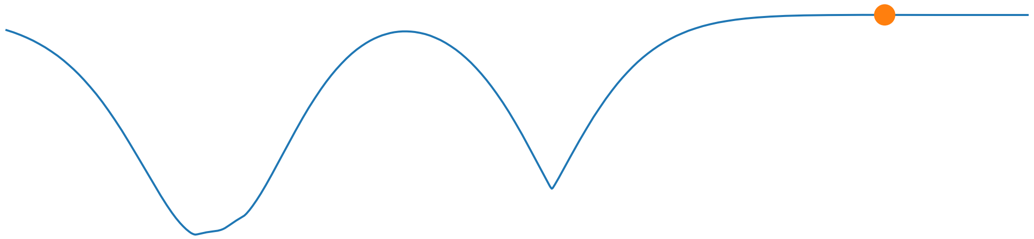
Expected Improvement

Gittins Index





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One-step approximation to MDP

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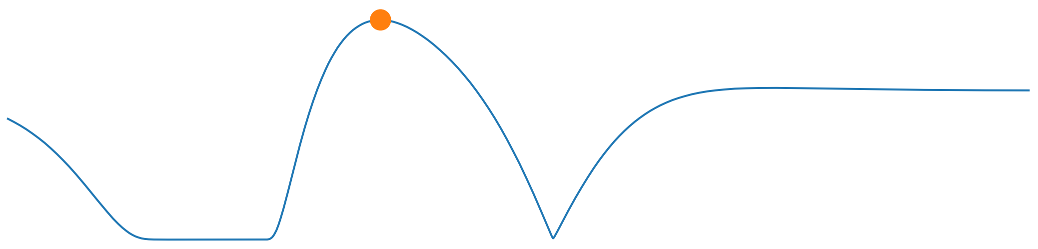

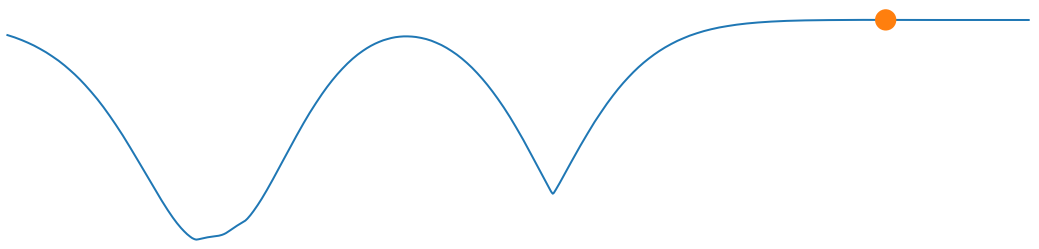

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Temporal simplification to MDP

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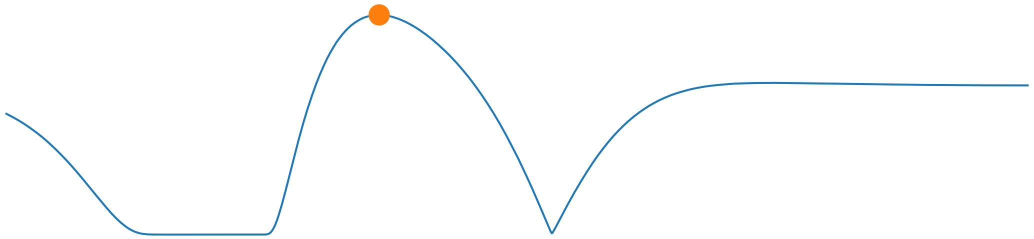
Expected Improvement



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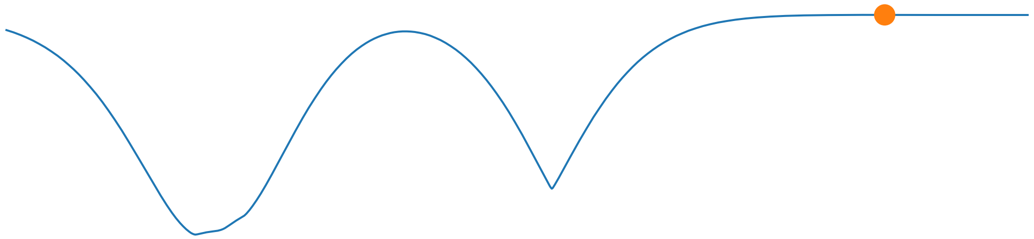

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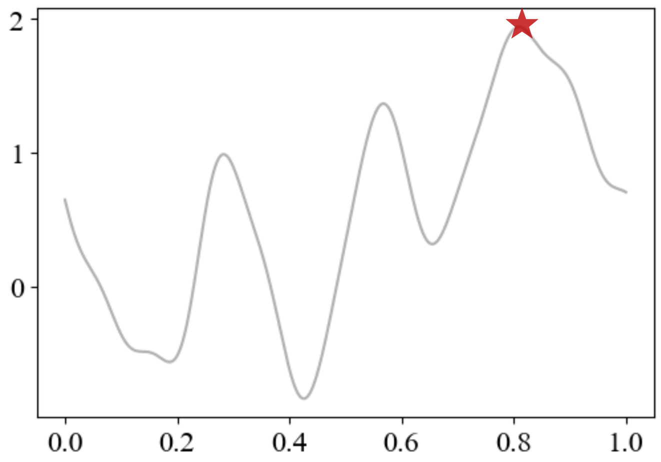
Spatial simplification to MDP

Our Approach: Spatial Simplification

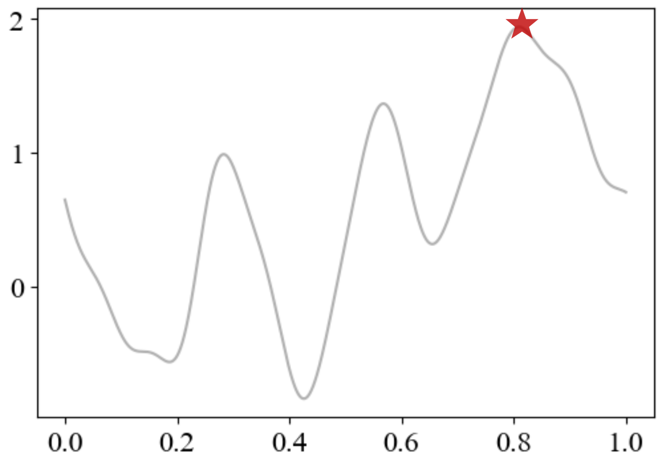


Bayesian Optimization

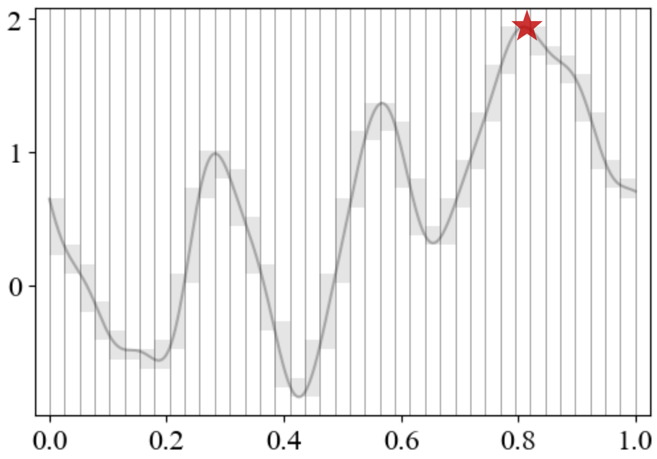
Continuous

Correlated

Our Approach: Spatial Simplification



$\Longrightarrow$

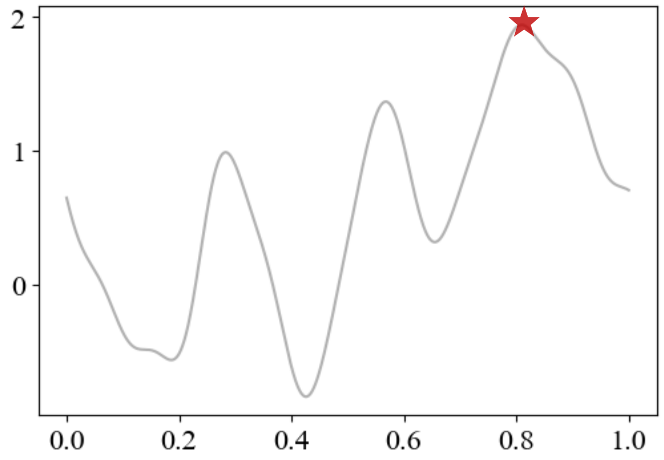


Bayesian Optimization

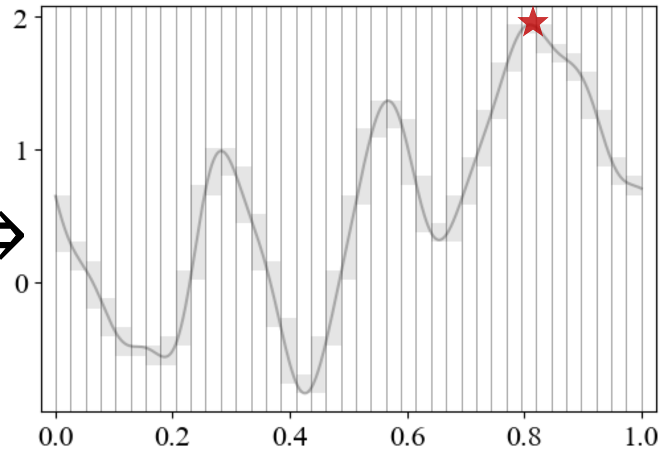
Continuous $\Longrightarrow$ Discrete

Correlated

Our Approach: Spatial Simplification



⟹

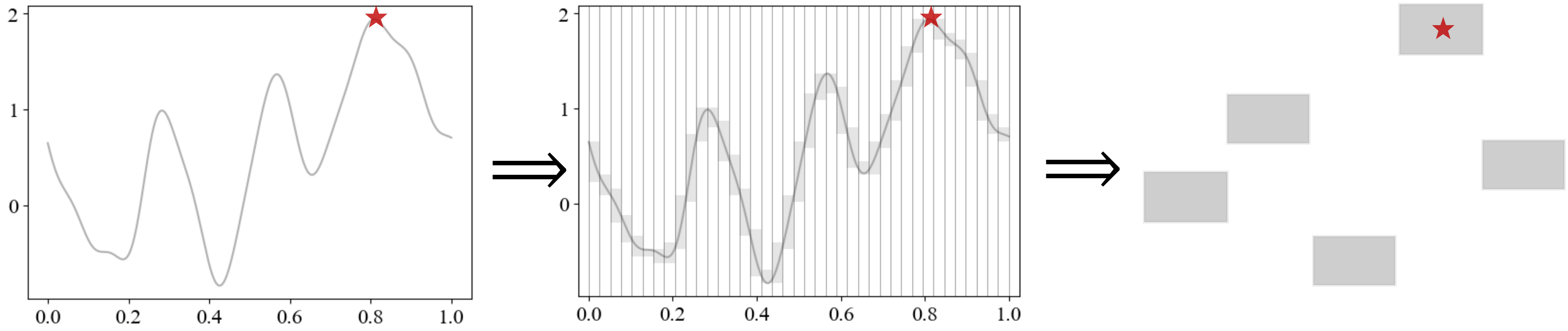


Bayesian Optimization

Continuous ⟹ Discrete

Correlated

Our Approach: Spatial Simplification

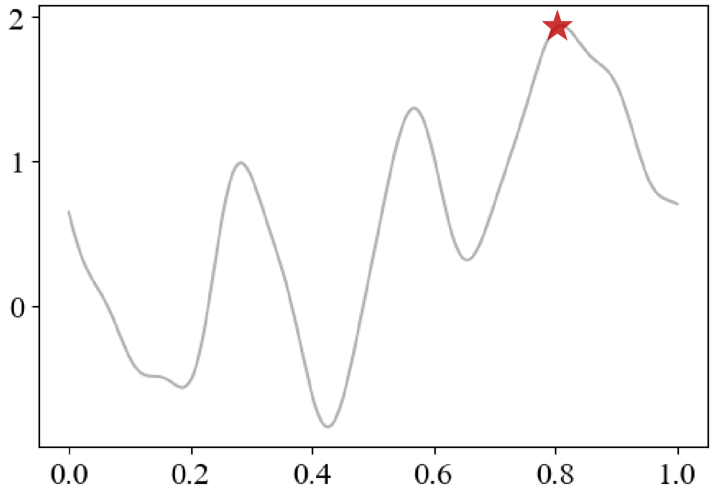


Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Our Approach: Spatial Simplification



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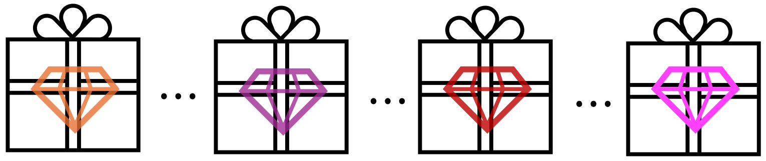
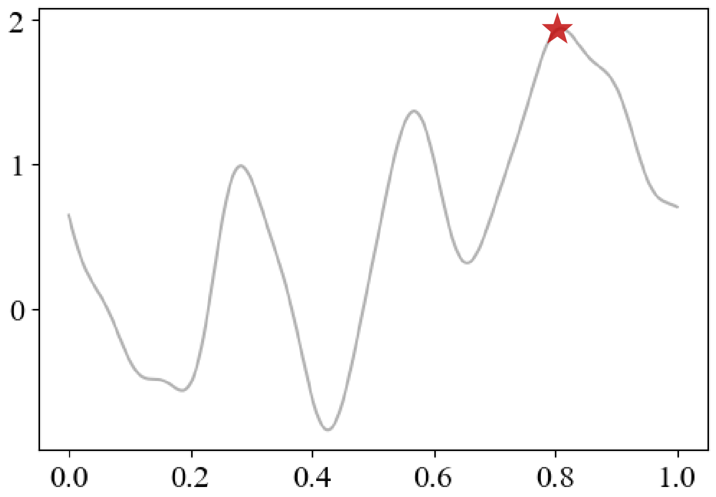


Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

Our Approach: Spatial Simplification



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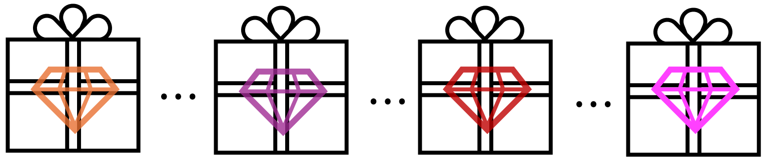


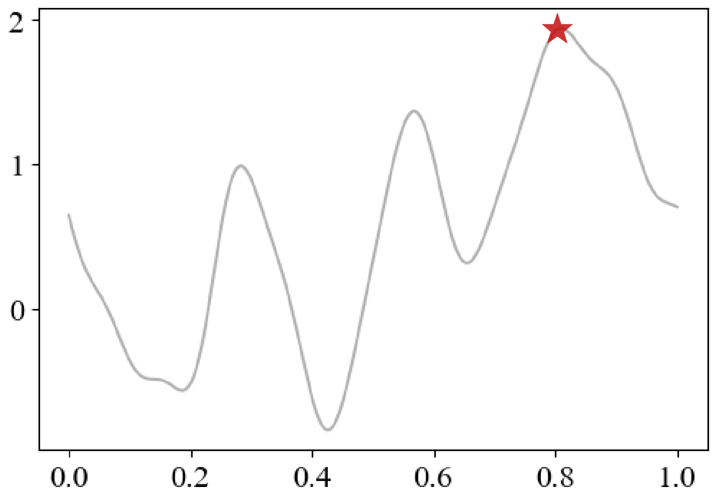
Bayesian Optimization | Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification



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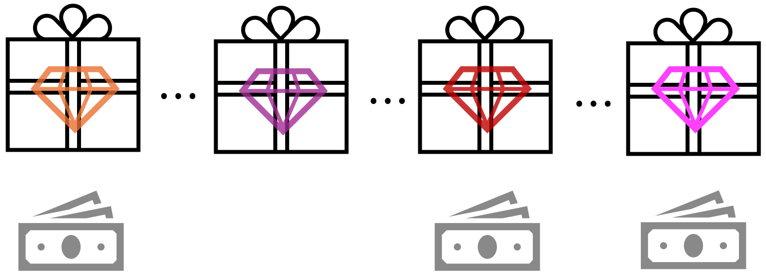


Bayesian Optimization | Pandora's Box

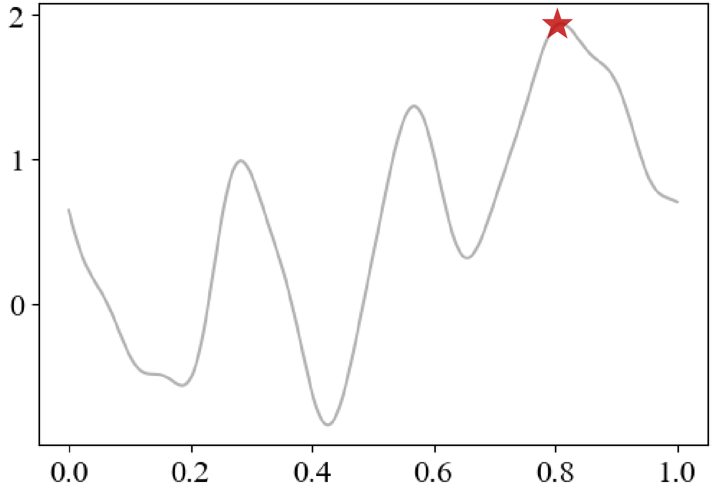
Continuous $\Longrightarrow$ Discrete

allow varying costs

Correlated $\Longrightarrow$ Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification



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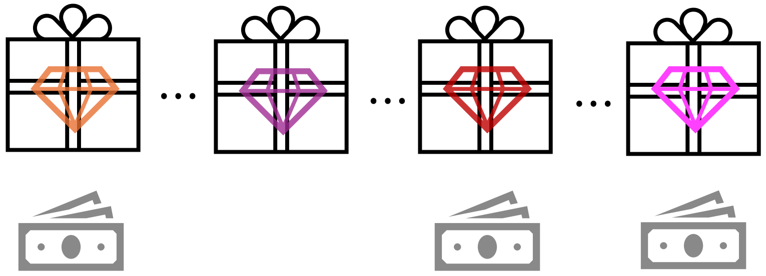


Bayesian Optimization		Pandora's Box [Weitzman'79]
Continuous	⟹	Discrete
Correlated	⟹	Independent
Is Gittins index good?		Optimal policy: Gittins index

Experiment Setup: Objective Functions

Samples from prior

Synthetic

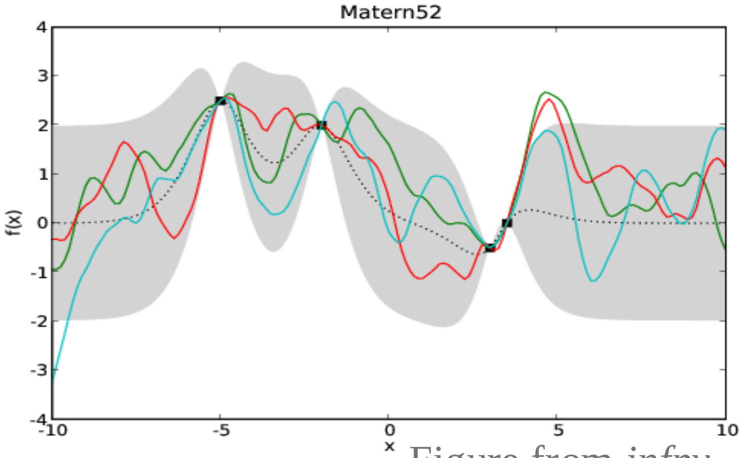


Figure from *infpy*

Ackley function

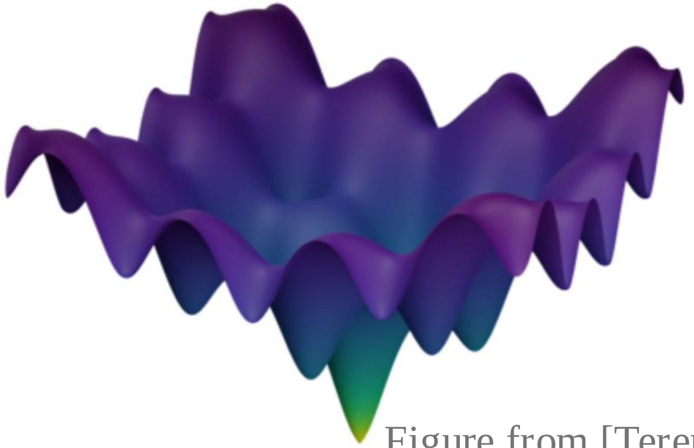


Figure from [Terenin'22]

Pest Control

Empirical

Figure from ChatGPT

Lunar Lander

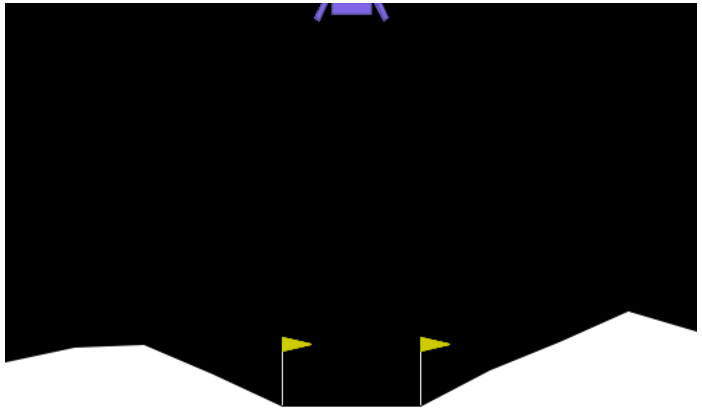
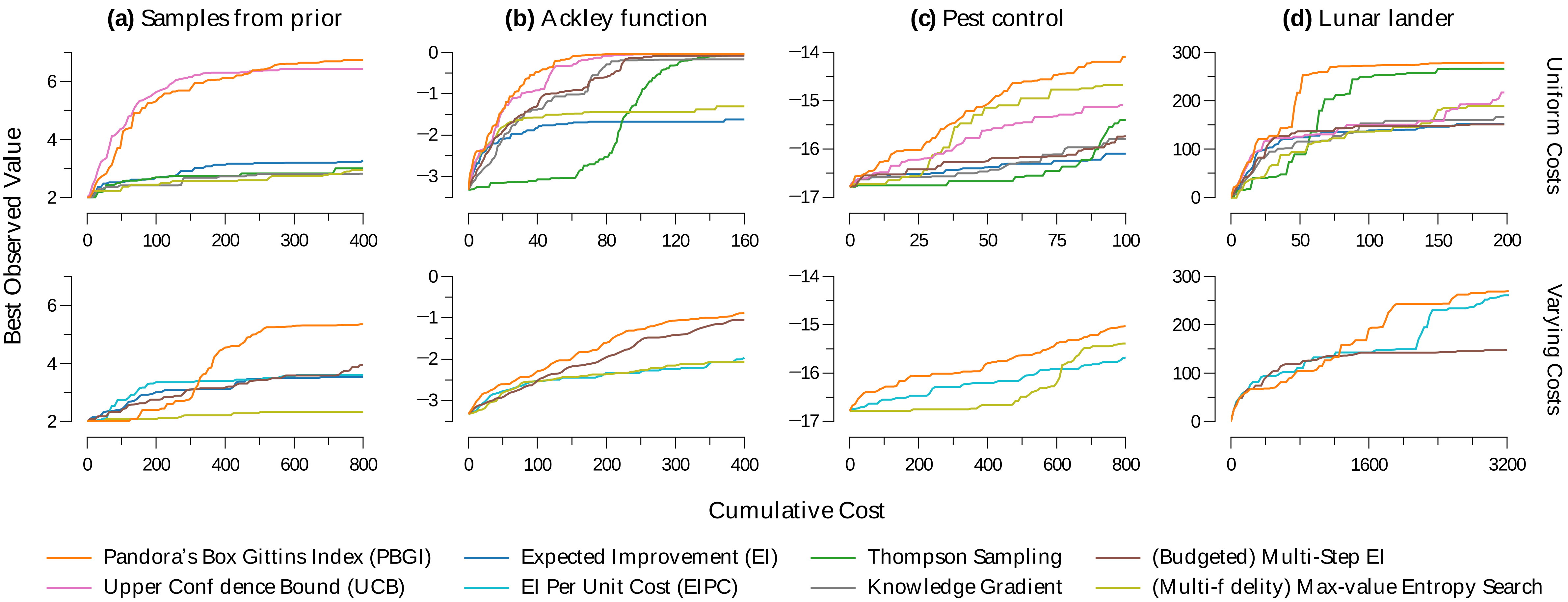


Figure from OpenAI Gym

Experiment results

Synthetic

Empirical



FAQ

- Easy-to-compute?

FAQ

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  Yes, EI + bisection

FAQ

- Easy-to-compute?

    Yes, EI + bisection

- Any theoretical results?

FAQ

- Easy-to-compute?

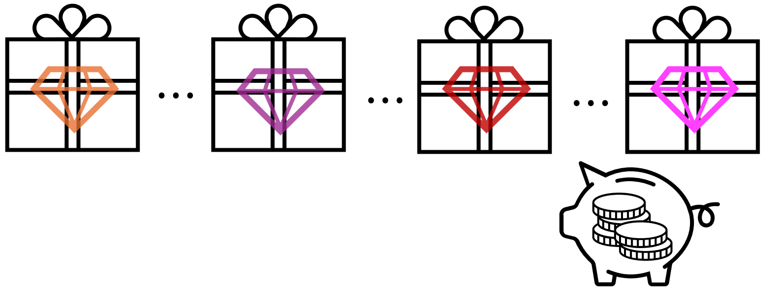
  Yes, EI + bisection

- Any theoretical results?

  Yes, expected-budget-constrained ≅ cost-per-sample

Theoretical Result

max best observed under budget

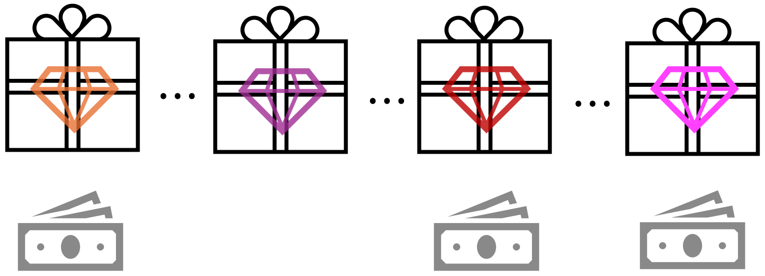


Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

max (best observed – costs)



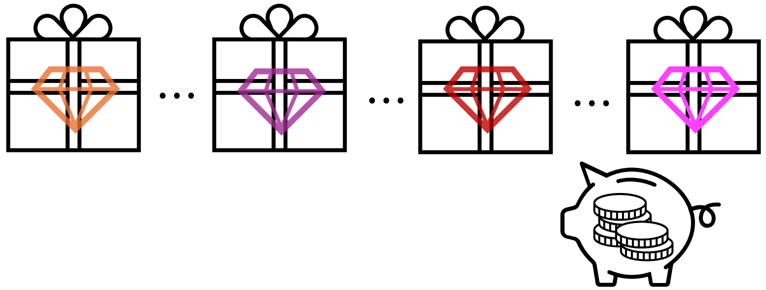
Pandora's Box

Cost per sample

Optimal policy: Gittins index

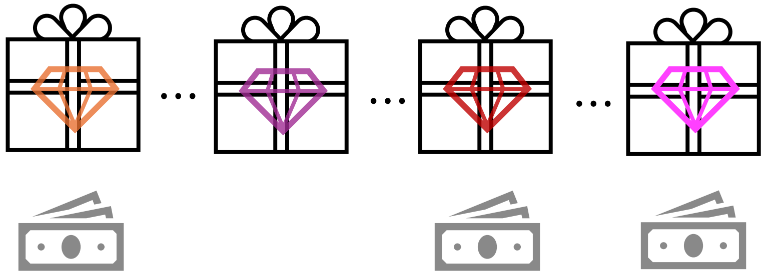
Theoretical Result

max best observed under budget



$\Leftarrow$

max (best observed – scaled costs)



Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh'24]

Pandora's Box

Cost per sample

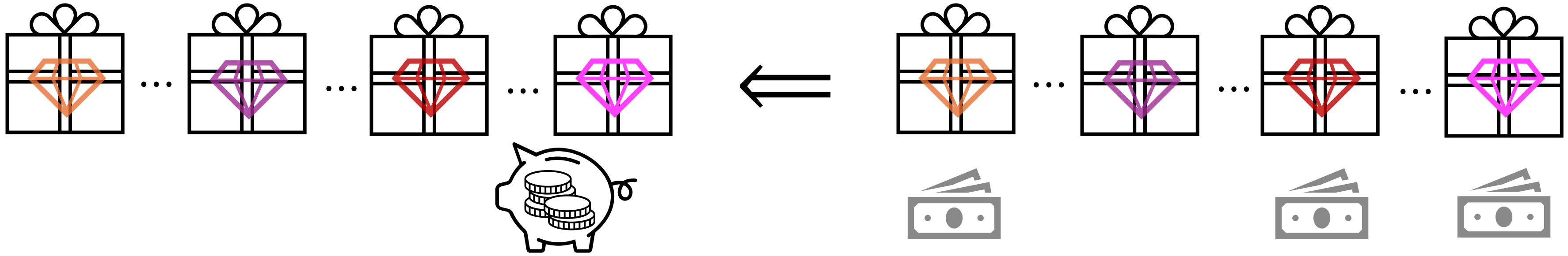
Optimal policy: Gittins index

Theoretical Result

budget-dependent

max best observed under budget

max (best observed – scaled costs)



Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh'24]

Pandora's Box

Cost per sample

Optimal policy: Gittins index

FAQ

- Easy-to-compute?

  Yes, EI + bisection
- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample
- Tuning parameters?

FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample

- Tuning parameters?

  Yes, control unit conversion

New Design Principle: Gittins Index

- Problem

    Bayesian optimization with varying costs

- Key idea

    linked to Pandora's box and Gittins index theory

- Impact

    competitive performance

- Future potential

    multi-stage optimization with partial feedback

Check our NeurIPS'24 paper on ArXiv!