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

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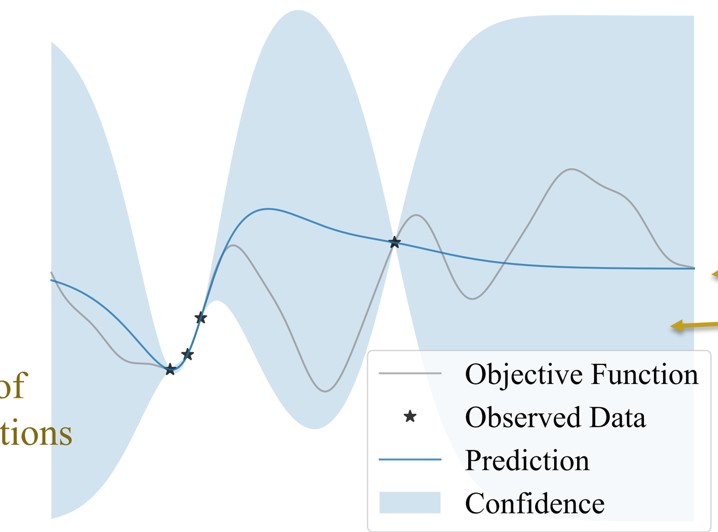
Introduction to Bayesian Optimization

Goal: optimize expensive-to-evaluate black-box function $\in$ decision-making under uncertainty

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

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

Objective: find global optimum $x^* = \arg\max_{x \in \mathcal{X}} f(x)$

$\Downarrow$

Objective: optimize best observed value at time T

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

Decision: evaluate a set of points

$\Downarrow$

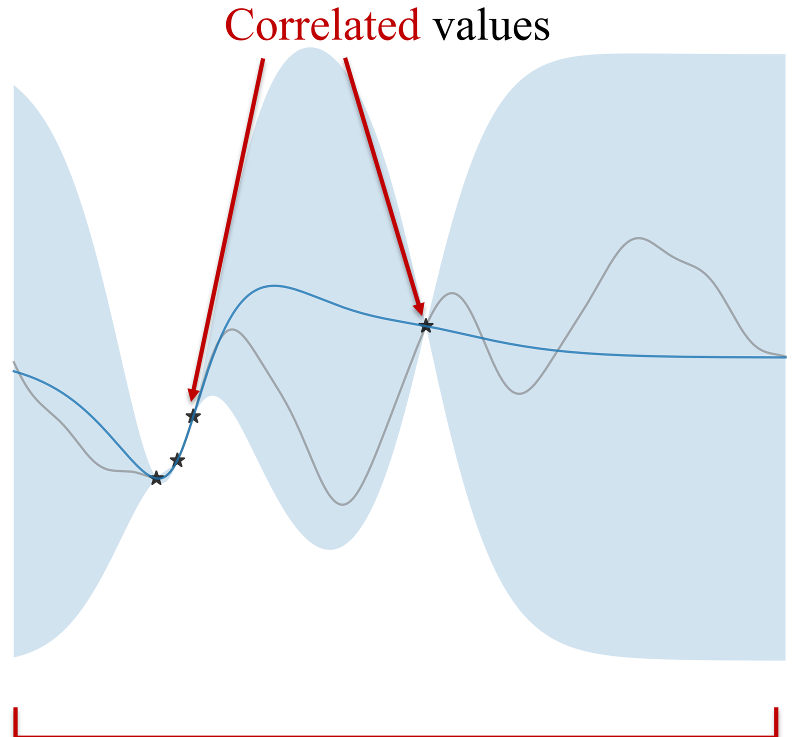
Decision: adaptively evaluate $x_1, x_2, \dots, x_T \in \mathcal{X}$ given time budget T

Why is Bayesian Optimization Hard?

Hard budget constraint

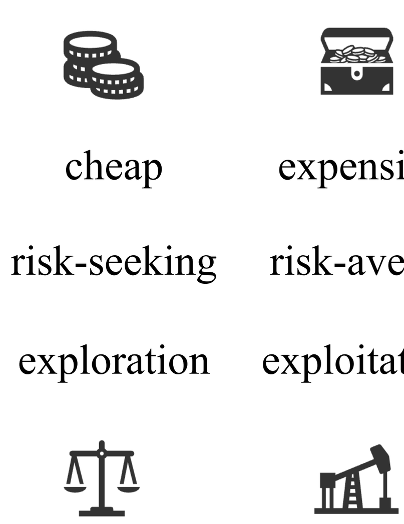
~~$t=1$~~
~~$t=2$~~
~~$t=3$~~
~~$t=4$~~
$\vdots$
$t=T$

Correlated values



Continuous search domain

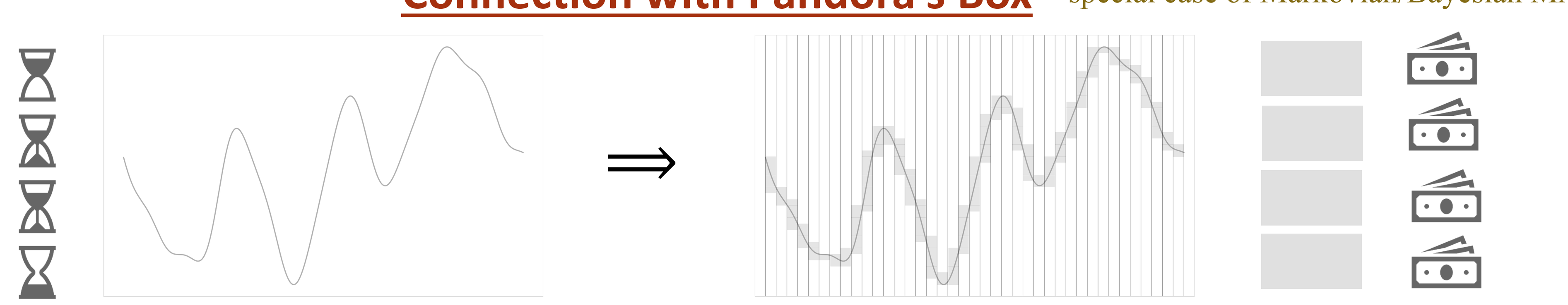
Evaluation costs handling



Optimal policy unknown!

Connection with Pandora's Box

special case of Markovian/Bayesian MAB



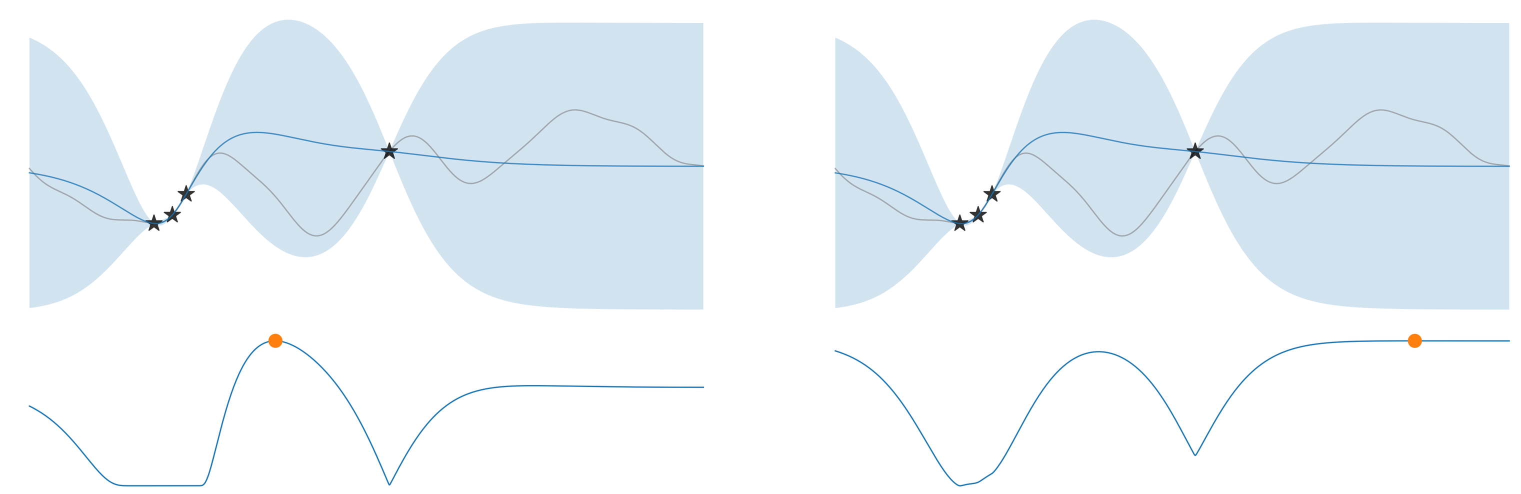
Continuous	$\Rightarrow$	Discrete
Correlated	$\Rightarrow$	Independent
Hard budget constraint	$\Rightarrow$ (Lagrangian relaxation)	Cost per sample
Is Gittins index good? (How to translate?)	$\Leftarrow$ (extension of [Aminian et al.'24])	Optimal policy: Gittins index [Weitzman'79]

Objective: maximize net utility

$$\max_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^{T} c(x_t)\right)$$

T: random stopping time

Acquisition Functions



Expected improvement (EI) popular

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

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

D: observed data, y_{best}: current best observed value

Pandora's box Gittins index (PBGI) new

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

PBGI policy: evaluate $\arg\max_x g(x)$

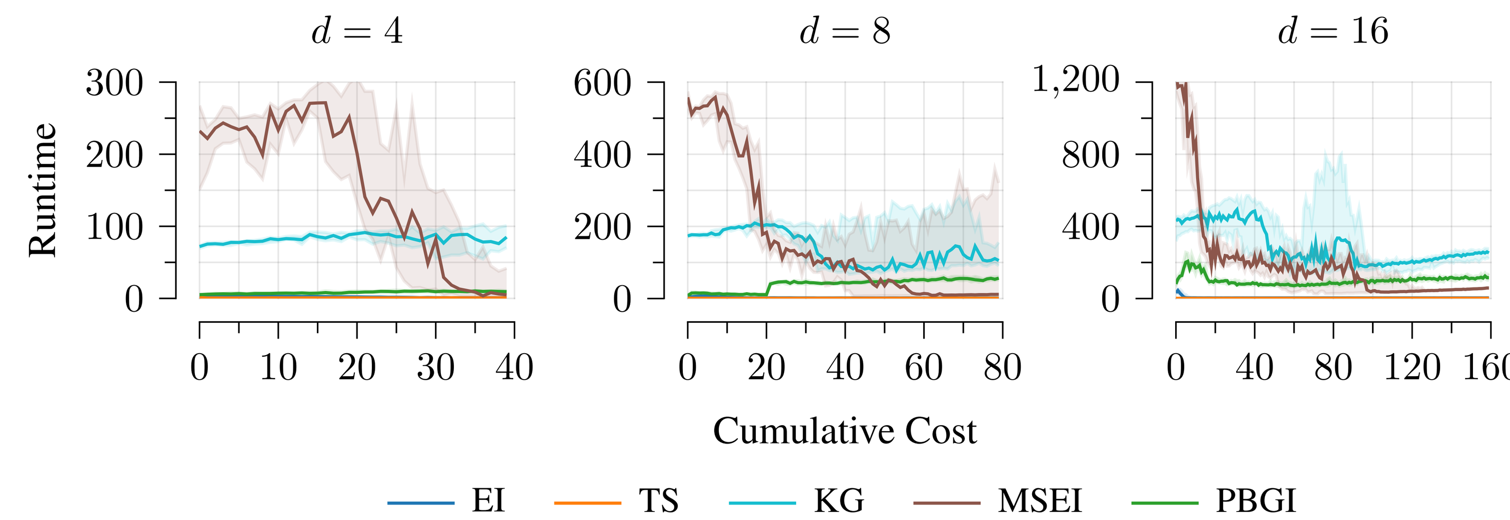
λ: cost-per-sample (Lagrange multiplier)

Other acquisition functions:

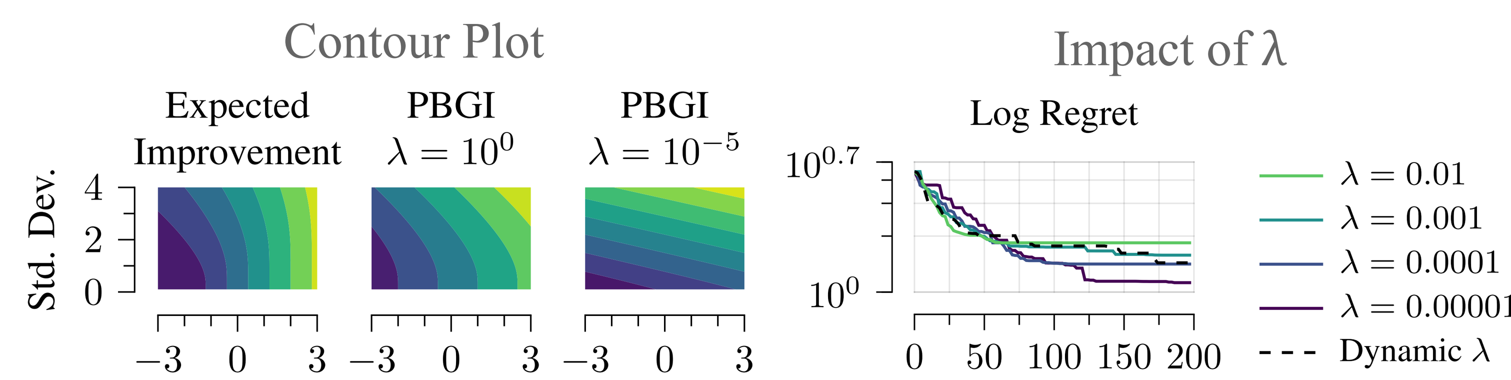
simple:
- Upper Confidence Bound (UCB)
- Thompson Sampling (TS)

- Predictive Entropy Search (unreliable)

slow:
- Knowledge Gradient (KG)
- Multi-step Lookahead EI (MSEI)



PBGI is easy to compute using bisection method!



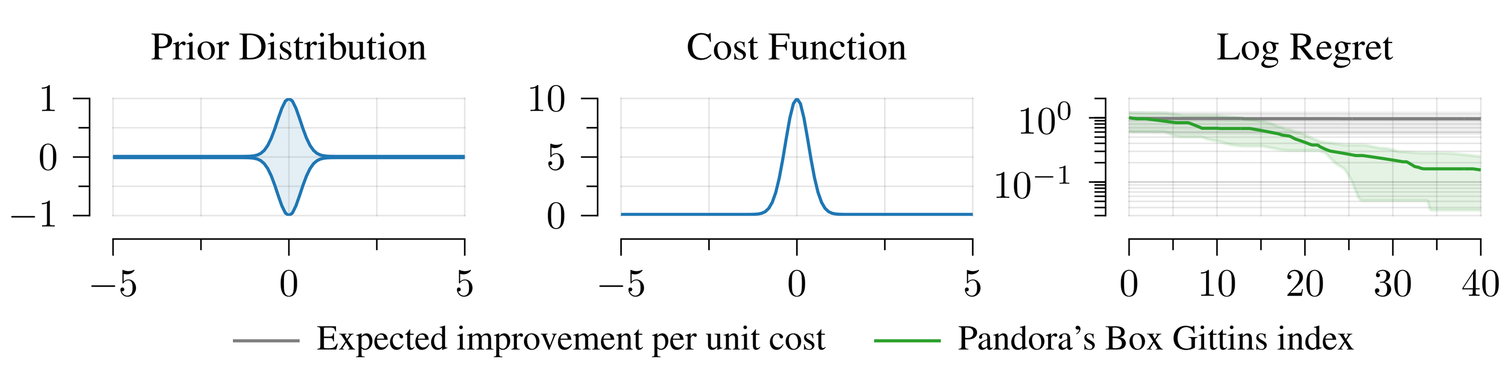
Connection with UCB?

Smaller λ, higher exploration

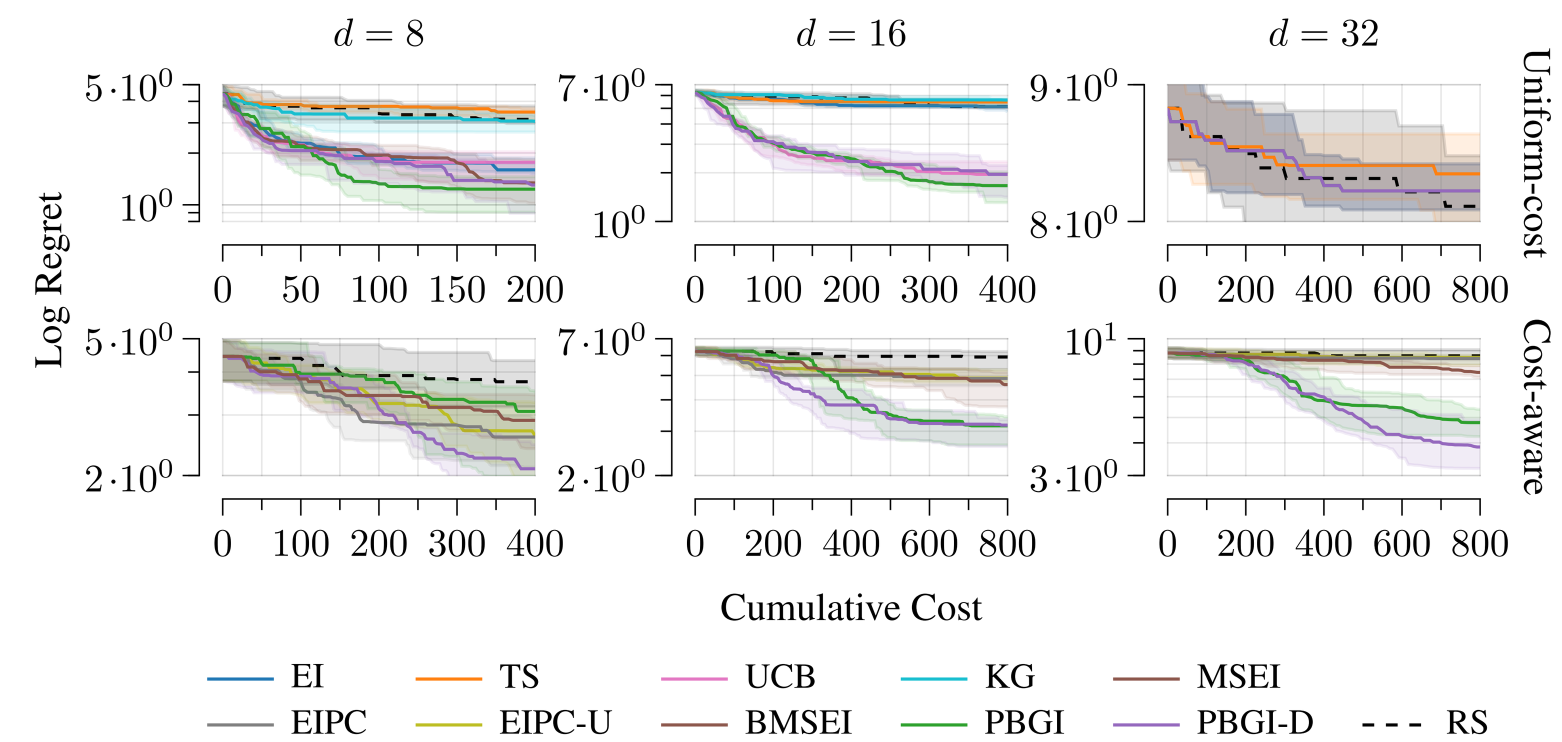
Heterogeneous Costs

- Given cost function $c: \mathcal{X} \to \mathbb{R}^+$ and budget B
- Replace λ with $\lambda c(x)$ to compute $g(x)$ as PBGI

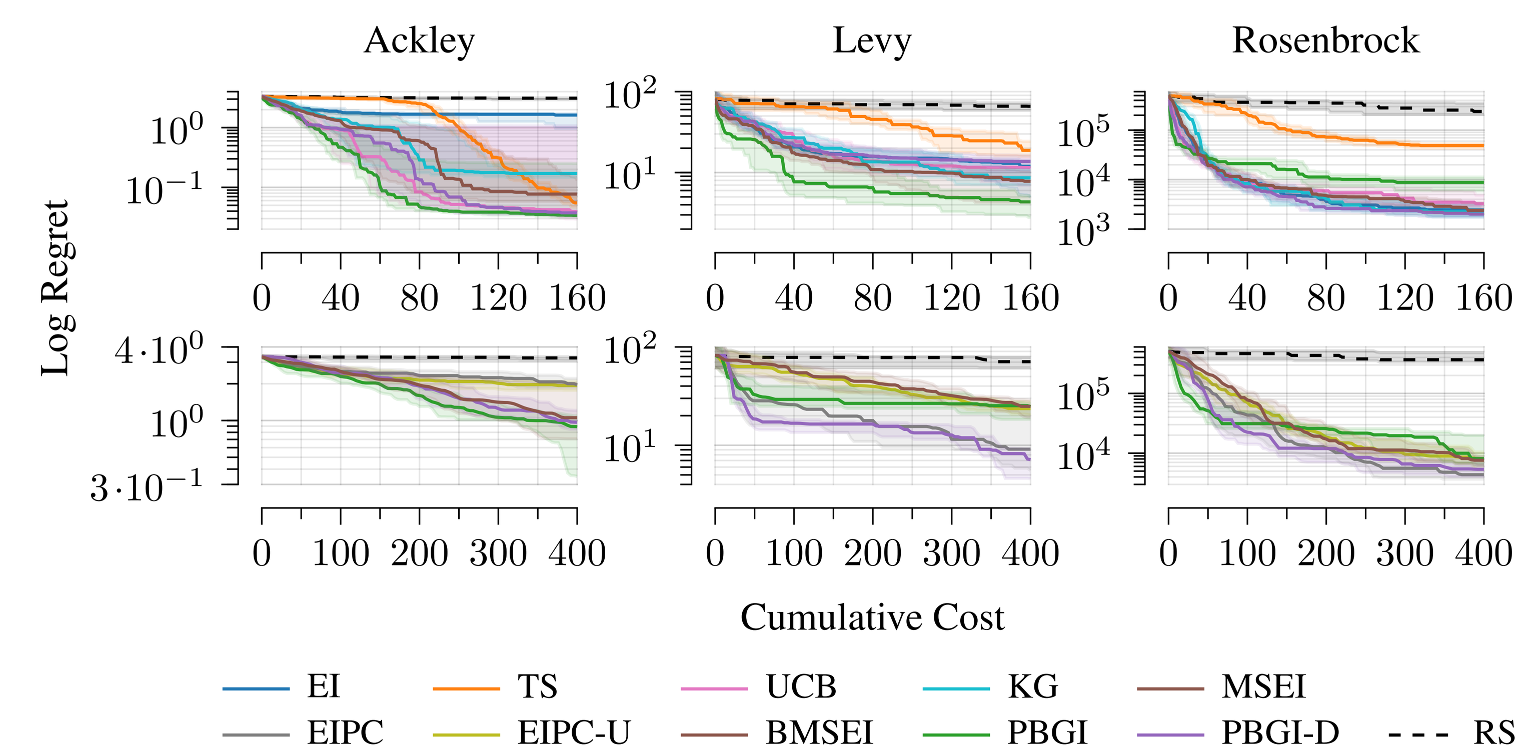
Baselines:
- EI Per Unit Cost (EIPC) — arbitrarily bad
- Budgeted MSEI (BMSEI) — slow



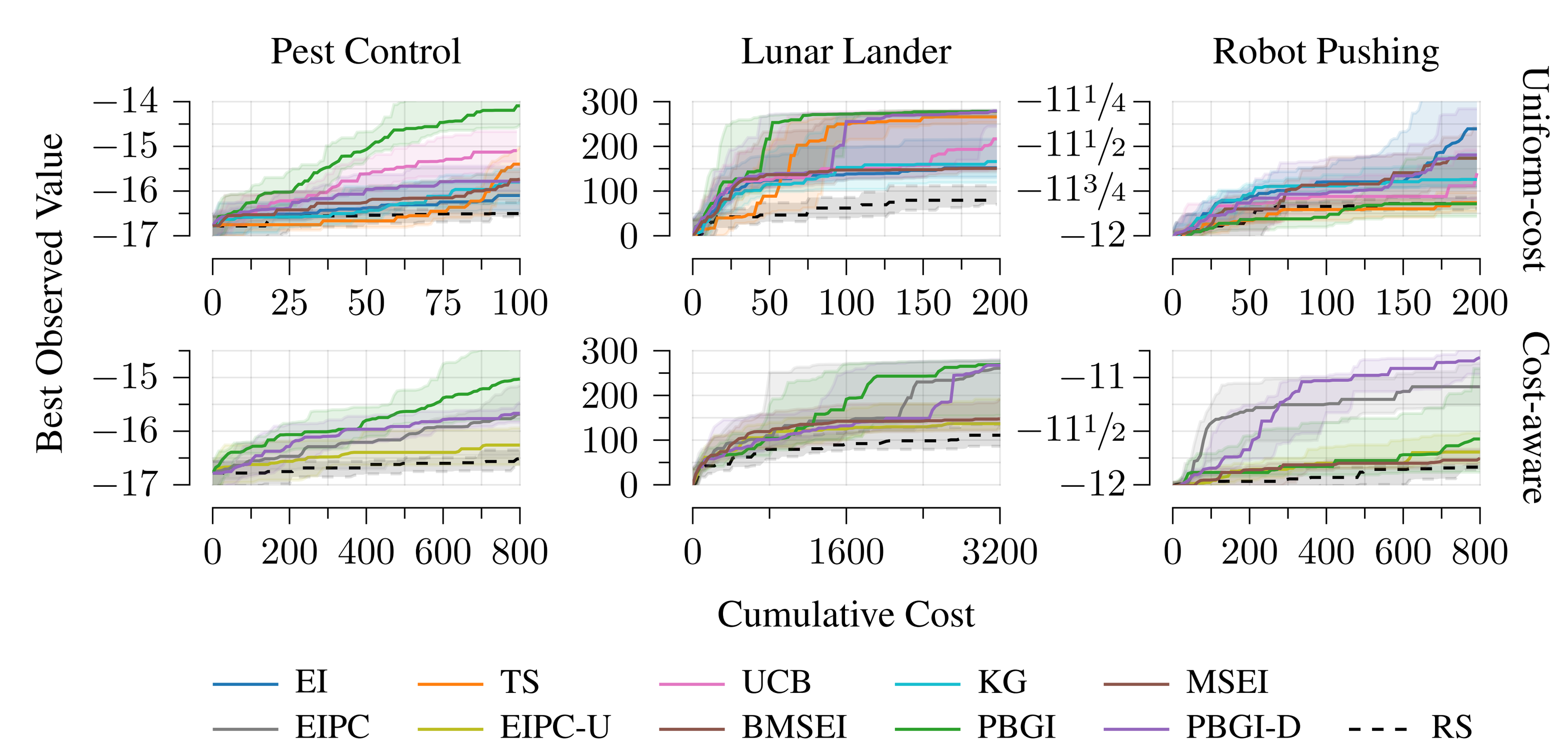
Experiment: Bayesian Regret



Experiment: Synthetic Benchmark



Experiment: Empirical



Future Work

Extension to complex BO (freeze-thaw, multi-fidelity, function network, etc.) via Gittins variants ("golf" Markovian MAB, optional inspection, etc.)