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

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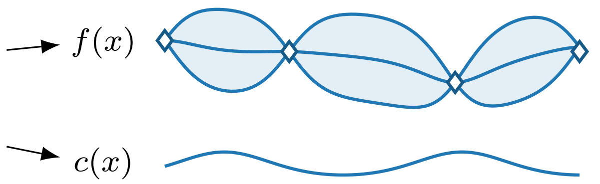
Abstract

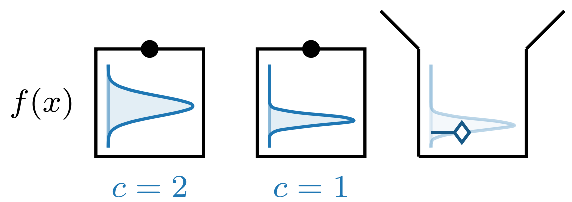
Bayesian optimization is a technique for efficient global optimization of black-box unknown functions. In many practical settings, it is desirable to explicitly incorporate function evaluation costs into acquisition functions used for Bayesian optimization. To do so, we develop a connection between cost-aware Bayesian optimization and *Pandora's Box*, a decision problem from economics. The Pandora's Box problem admits a Bayesian-optimal solution based on an expression called the *Gittins index*, which can be reinterpreted as an acquisition function. We demonstrate empirically that this acquisition function performs well on cost-aware Bayesian optimization, particularly in medium-high dimensions. We further show that this performance carries over to classical Bayesian optimization without explicit evaluation costs. Our work constitutes a first step towards integrating techniques from Gittins index theory into Bayesian optimization.

Cost-aware Bayesian Optimization



Expected-budget-constrained (EBC) Bayesian optimization: $\mathbb{E}\sup_{x\in X} f(x) - \mathbb{E}\max_{1\le t\le T} f(x_t)$ subject to $\mathbb{E}\sum_{t=1}^{T} c(x_t) \le B$

Pandora's Box



Cost-per-sample (CPS) objective: $\mathbb{E}\max_{1\le t\le T} f(x_t) - \mathbb{E}\sum_{t=1}^{T} c(x_t)$

Optimal policy (notation: $\mathrm{EI}_\psi(x;y) = \mathbb{E}\max(0,\psi(x)-y)$):

$\alpha^\star(x) = g$ where g solves $\mathrm{EI}_f(x;g) = c(x)$

Our work: EBC and CPS problems are equivalent
(extends prior work on generalized Pandora's boxes to continuous rewards)

Key difference from Bayesian optimization: no correlations

Pandora's Box Gittins Index: a new acquisition function

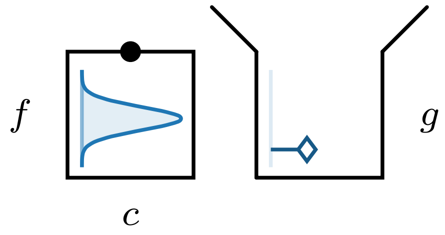
$\alpha_t^{\mathrm{PBGI}}(x) = g$ where g solves $\mathrm{EI}_{f|x_{1:t},y_{1:t}}(x;g) = \lambda c(x)$

Idea: extend $\alpha^\star$ by plugging posterior in for f
λ: cost scaling factor from budget-constraint Lagrangian duality
Computation: one-dimensional convex optimization

Where does α_t^{PBGI} come from?

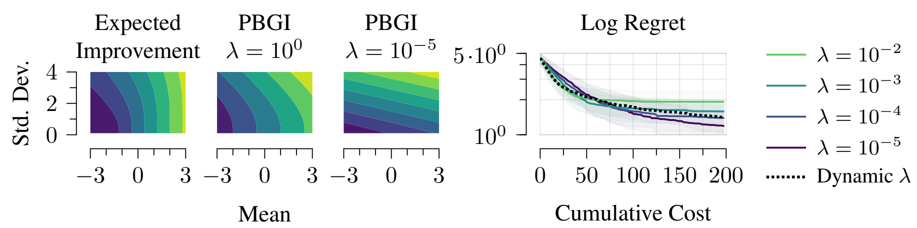
Simplified problem: one closed and one open box

Decision	Value
Open box	$\mathbb{E}\max(f,g) - c$
Don't open	g

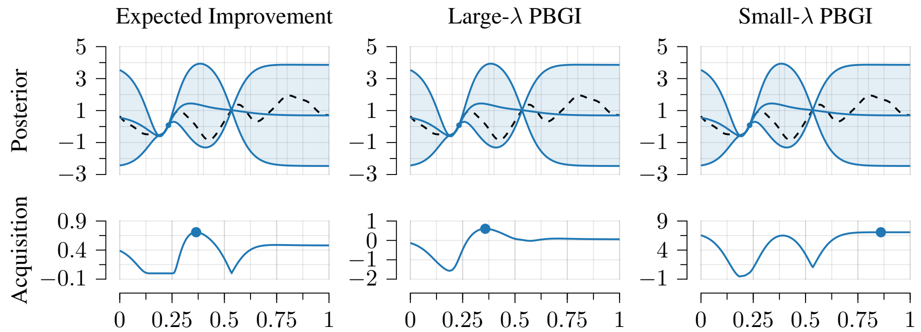


Should one open the closed box? Depends on the observed value g!
If *both* opening and not opening are optimal: g is a *fair value*
α_t^{PBGI}: pick points according to their fair values

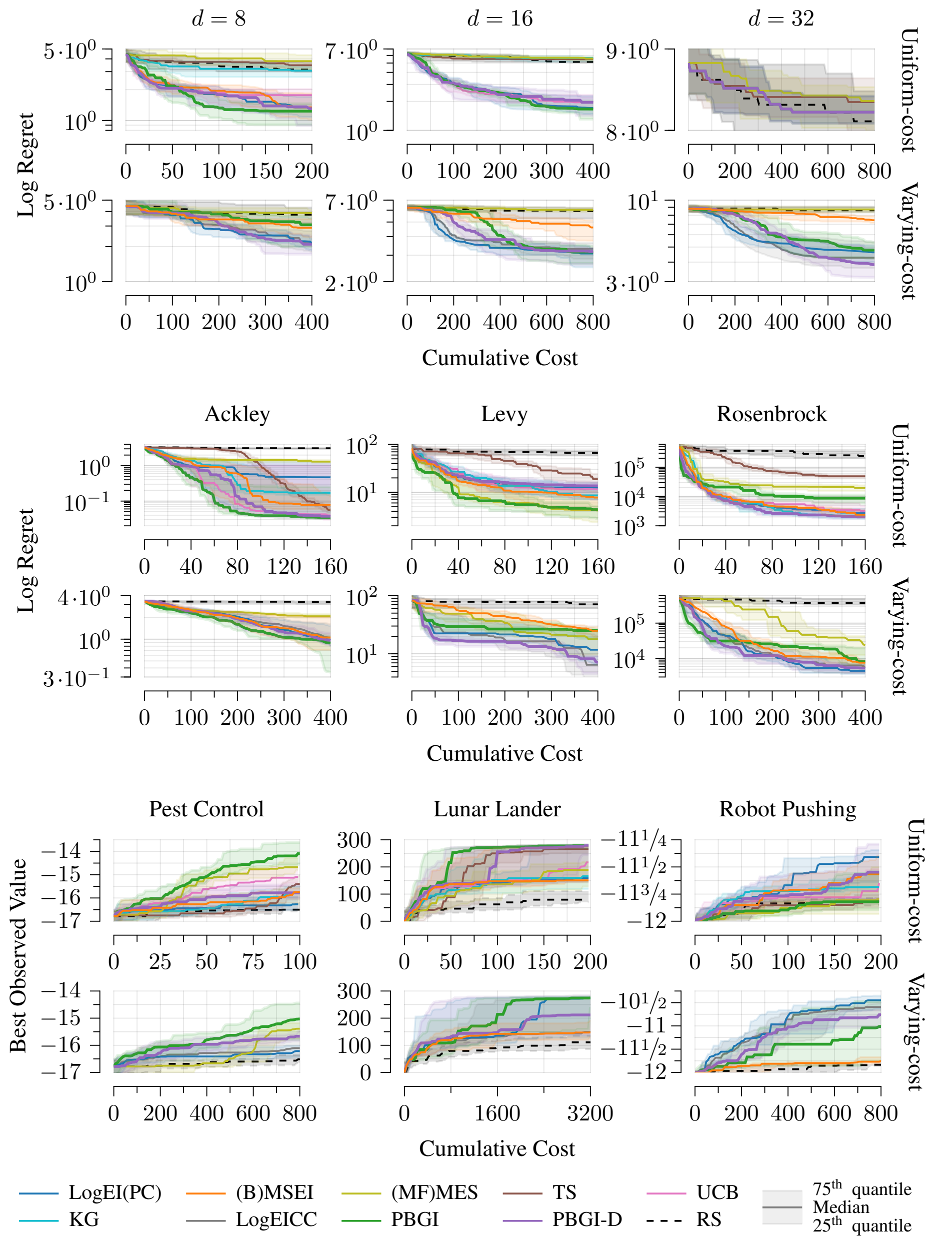
Behavior and Comparisons



Large λ: similar to α_t^{EI} Small λ: similar to α_t^{UCB}



Performance



Computation Time