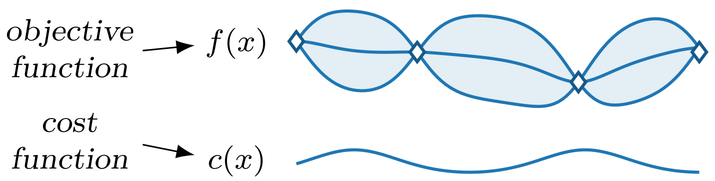
Cost-aware Stopping for Bayesian Optimization

Qian Xie*[1], Linda Cai*[2], Alexander Terenin[1], Peter Frazier[1], and Ziv Scully[1]
[1]Cornell University [2]University of California, Berkeley

Cost-aware Bayesian Optimization with Adaptive Stopping



Cost-adjusted regret: $\mathbb{E}\left[\underbrace{\min_{1\le t\le\tau} f(x_t) - \inf_{x\in X} f(x)}_{\text{simple regret}} + \underbrace{\sum_{t=1}^{\tau} c(x_t)}_{\text{total cost}}\right]$

Goal: Adaptively select inspections $x_1, x_2, \cdots$ and stop at time τ to minimize expected cost-adjusted regret.

Existing Inspection Rules

Expected Improvement (EI): Inspect the point with maximum expected improvement over the current best observed value $y^*_{1:t}$

$$\alpha_t^{\mathrm{EI}}(x) = \mathrm{EI}_{f|x_{1:t},y_{1:t}}(x; y^*_{1:t}) \quad \text{where} \quad \mathrm{EI}_\psi(x;y) = \mathbb{E}\left[(y-\psi(x))^+\right].$$

Expected Improvement per Cost (EIPC): Inspect the point with maximum expected improvement divided by cost

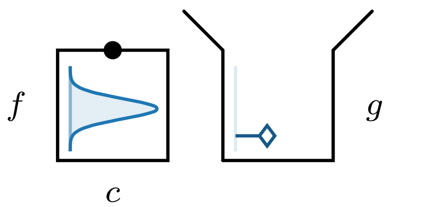
$$\alpha_t^{\mathrm{EIPC}}(x) = \alpha_t^{\mathrm{EI}}(x)/c(x).$$

Pandora's Box Gittins Index (PBGI): (Xie et al., 2024) Inspect the point with the minimum index given by

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

Intuition: (Weitzman, 1979) Is inspection worth the cost?

Decision	Disutility
Inspect	$\mathbb{E}\min(f,g)+c$
Not Inspect	g



Should one inspect the closed box? Depends on outside option g! If *both* inspection and no inspection are optimal: g is a *fair value*. α_t^{PBGI}: pick points according to their fair values.

Other inspection rules: lower confidence bound (LCB), Thompson sampling (TS), ...

PBGI/EIPC Stopping Rule

Existing EI stopping rule: (Nguyen et al., 2017) Under the *uniform-cost* setting, stop when $\alpha_t^{\mathrm{EI}}(x) \le c$ where c is the unit cost.

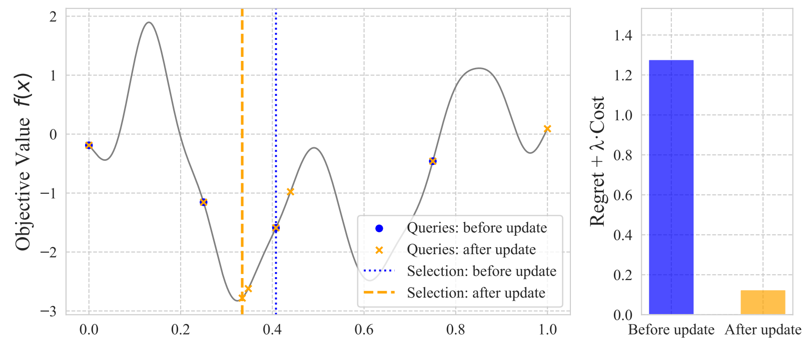
Our new PBGI/EIPC stopping rule:
Independent-value setting: Stopping when the PBGI index at *every* unevaluated point is at least the current best observed value

$$\min_{x\in X\setminus\{x_1,\ldots,x_t\}} \alpha^{\mathrm{PBGI}}(x) \ge y^*_{1:t} \tag{1}$$

is *Bayesian-optimal* when paired with the PBGI inspection rule.

Correlated setting: Use $\alpha_{t-1}^{\mathrm{PBGI}}$ (*before* posterior update) [Gergatsouli & Tzamos, 2023] or α_t^{PBGI} (*after* update) **[our work]** in (1)?

- More faithfully reflects Weitzman's fair value interpretation.
- Equivalent to an EIPC stopping rule: stop when the *expected improvement* at each point x is at most its inspection cost $c(x)$.
- Yields tangible empirical gains in cost-adjusted regret.



Theoretical Guarantee

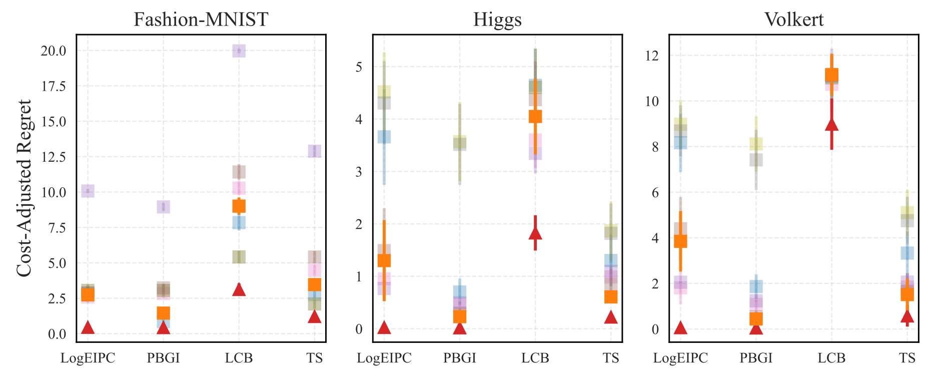
Theorem 1 (Upper Bound on Cost up to Stopping)
For f drawn from a stochastic process with constant-mean function μ, using PBGI or EIPC inspection rule with our stopping rule, the expected cumulative cost up to stopping is bounded by

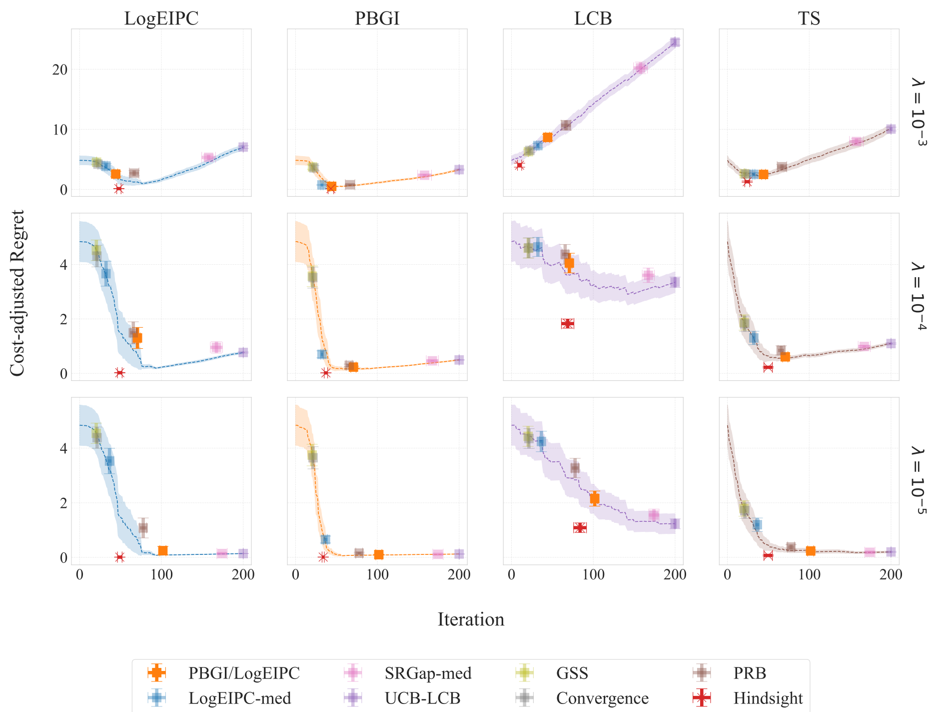
$$\mathbb{E}\left[\sum_{t=2}^{\tau} c(x_t)\right] \le \mu - \mathbb{E}\left[\min_{x\in X} f(x)\right]. \tag{2}$$

Key insight: Using our stopping rule, both PBGI and EIPC are guaranteed to inspect only points where their inspection cost $\le$ the one-step expected improvement before stopping.

Benefit: Avoid excessive cost spending, unlike many existing non-cost-aware stopping rules.

Performance





Computation Time