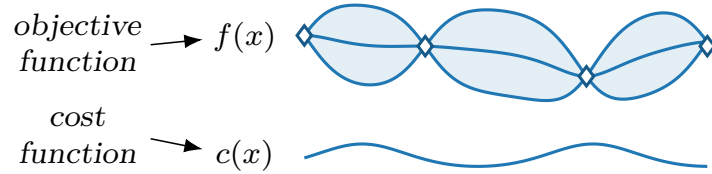


Cost-aware Stopping for Bayesian Optimization

Qian Xie^{*1}, Linda Cai^{*2}, Alexander Terenin¹, Peter Frazier¹, and Ziv Scully¹
¹Cornell University ²University of California, Berkeley



Cost-aware Bayesian Optimization with Adaptive Stopping



Cost-adjusted regret:
$$\underbrace{\min_{1 \leq t \leq \tau} f(x_t) - \inf_{x \in X} f(x)}_{\text{simple regret}} + \underbrace{\sum_{t=1}^{\tau} c(x_t)}_{\text{cumulative cost}}$$

Goal: Adaptively select inspections $x_1, x_2, \dots$ 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 $y_{1:t}^*$

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

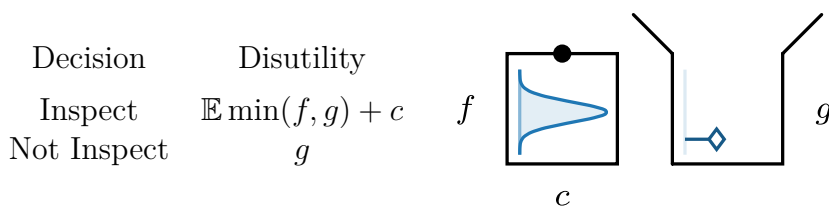
Expected Improvement per Cost (EIPC): Inspect the point with maximum expected improvement divided by cost

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

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

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

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



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 $\alpha_t^{\text{EI}}(x) \leq c$ where c is the unit cost.

Our PBGI/EIPC stopping rule:

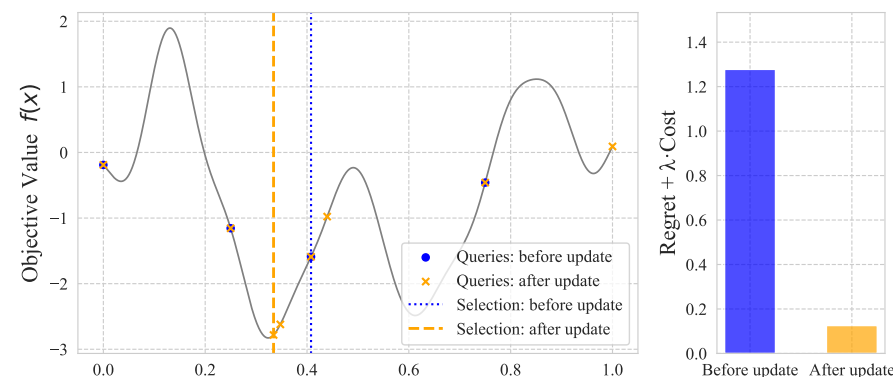
Independent-value setting: Stopping when the PBGI index at *every* unevaluated point is at least the current best observed value

$$\min_{x \in X \setminus \{x_1, \dots, x_t\}} \alpha^{\text{PBGI}}(x) \geq y_{1:t}^* \quad (1)$$

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

Correlated setting: Use $\alpha_{t-1}^{\text{PBGI}}$ (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 $\alpha_t^{\text{EIPC}}(x) \leq 1$.
- Yields tangible empirical gains in cost-adjusted regret.



Theoretical Guarantee

Theorem 1 (Upper Bound on Cost up to Stopping)

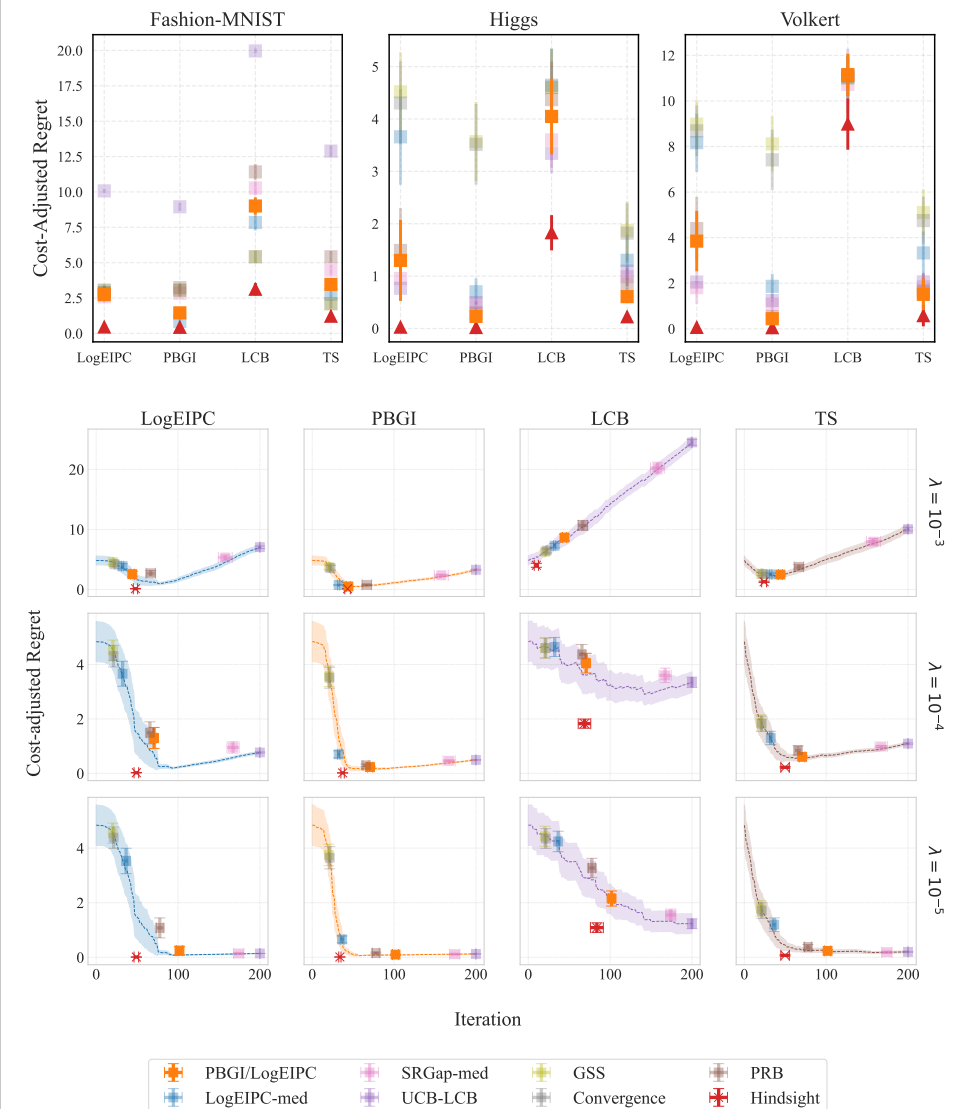
For f drawn from a stochastic process with constant-mean function μ , using PBGI or EIPC inspection rule with our stopping rule, the expected cumulative cost up to stopping is bounded by

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

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

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

Performance



Computation Time

