Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

INFORMS Annual Meeting 2025 Job Market Showcase

Black-Box Optimization

Input x $\longrightarrow$  $\longrightarrow$ Performance metric $f(x)$

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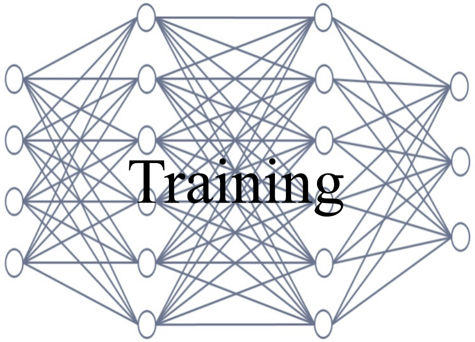
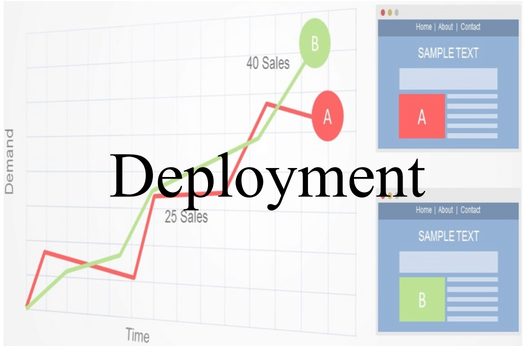
ML model training:

Training hyperparameters $\longrightarrow$ 

$\longrightarrow$ Accuracy

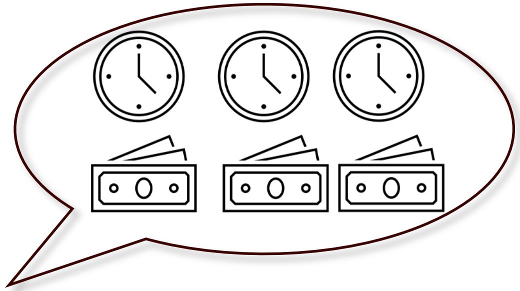
Adaptive experimentation:

Decision/design variables $\longrightarrow$ 

$\longrightarrow$ Revenue

Black-Box Optimization

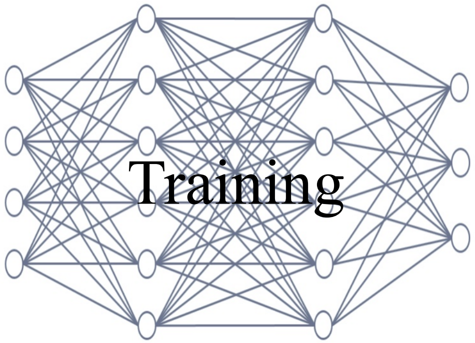
Input x →  → Performance metric $f(x)$



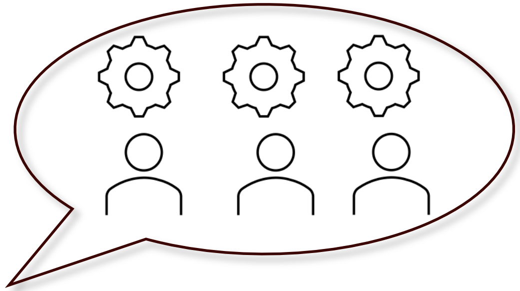
Training time

Compute credits

ML model training:

Training hyperparameters → 

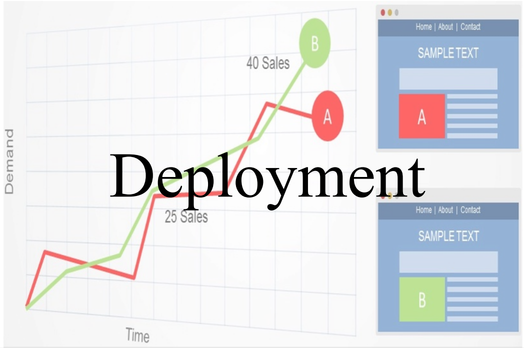
→ Accuracy



Operational cost

User experience

Adaptive experimentation:

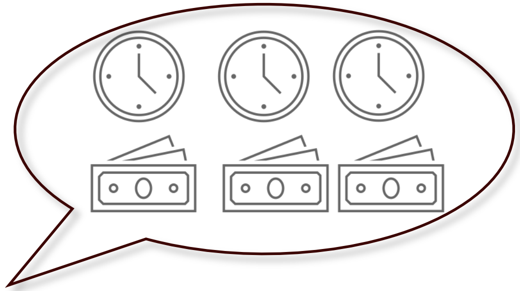
Decision/design variables → 

→ Revenue

Black-Box Optimization

expensive-to-evaluate

Input x →  → Performance metric $f(x)$



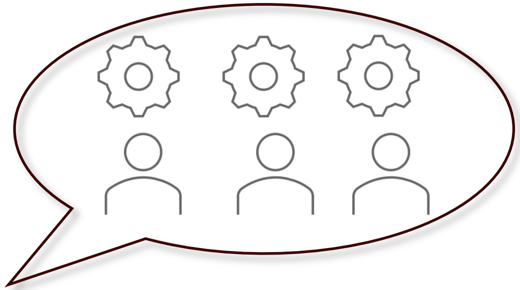
Training time

Compute credits

ML model training:

Training hyperparameters → 

→ Accuracy



Operational cost

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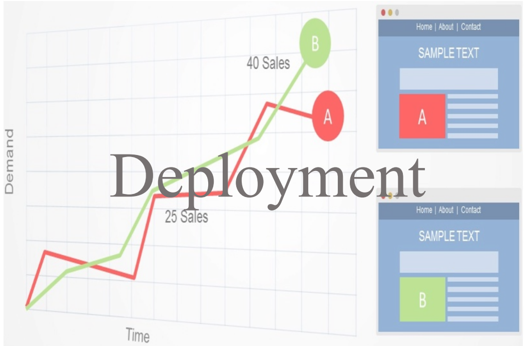
Decision/design variables → 

→ Revenue

Black-Box Optimization

Input x $\longrightarrow$  $\longrightarrow$ Performance metric $f(x)$

expensive-to-evaluate

High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected best observed value $\mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

Black-Box Optimization

expensive-to-evaluate

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adaptively

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Fewer #evaluations

Black-Box Optimization

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expensive-to-evaluate

adaptively

High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected best observed value $\mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization

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

Black-box function

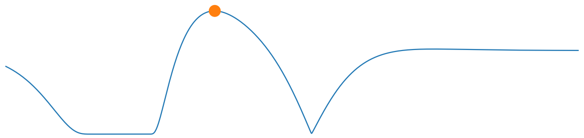
Bayesian Optimization

x →  → $f(x)$

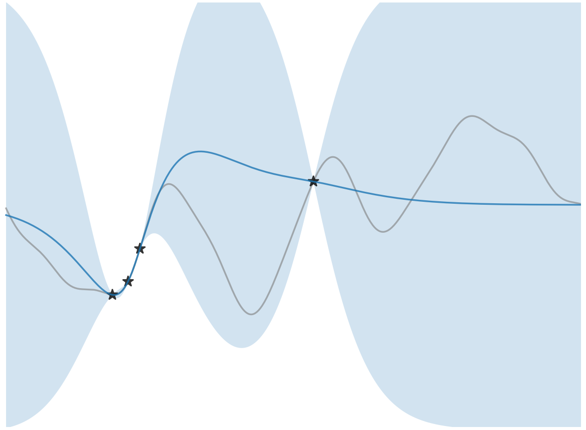
Select next input
(gradient-based optimization)

Black-box function

Update belief
(Bayes' rule)



Decision rule
(e.g., UCB, TS)



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

x →  → $f(x)$

Black-box function

Update belief
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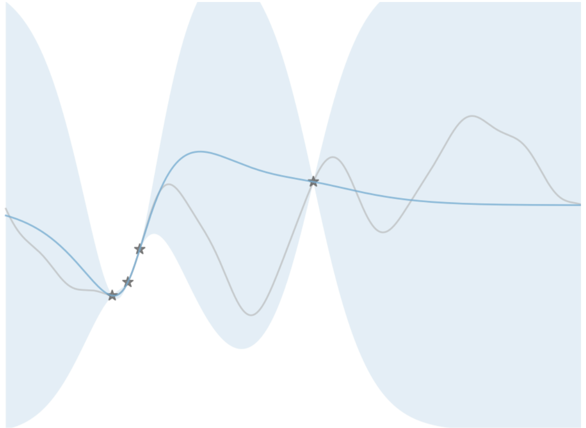

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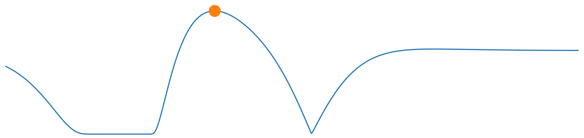

My focus

Decision rule
(e.g., UCB, TS)

Select next input
(gradient-based optimization)

Existing Design Principles

- Improvement-based
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling

New Design Principle: Gittins Index

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- **Gittins Index**

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? Why another principle?

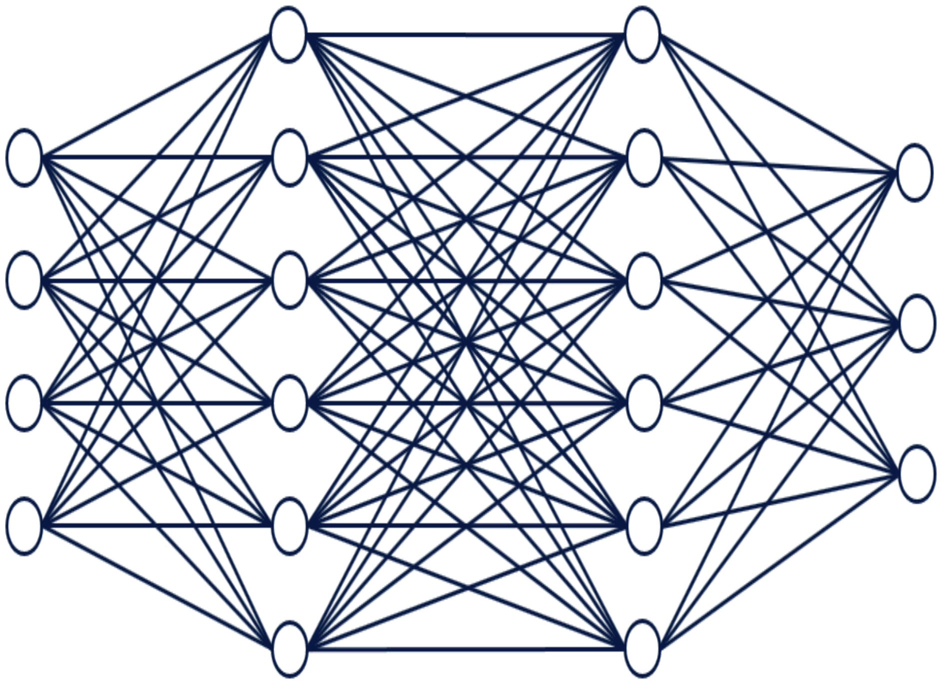
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Under-explored Practical Considerations

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback



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New design principle:
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Why Gittins index?

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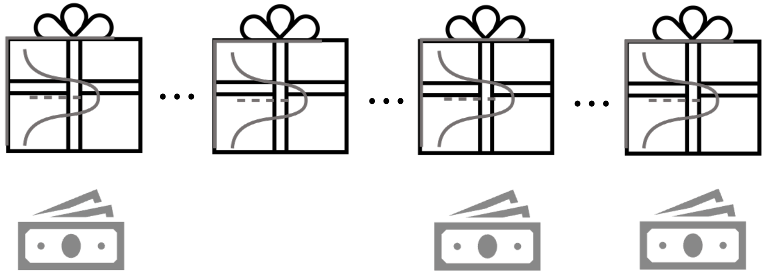
Optimal in related sequential decision problems



Why Gittins index?

Varying evaluation costs

Features in Pandora's box

Smart stopping time

Features in Pandora's box

Observable multi-stage feedback

New design principle:
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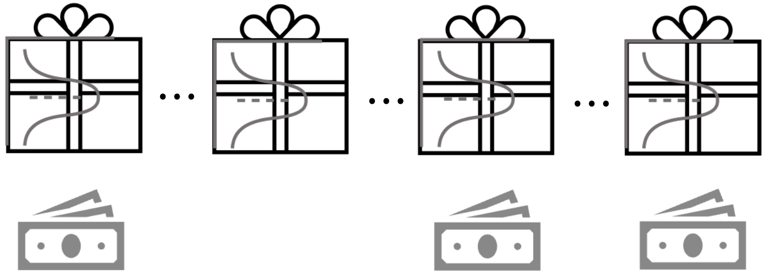

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Varying evaluation costs

Features in Pandora's box

Smart stopping time

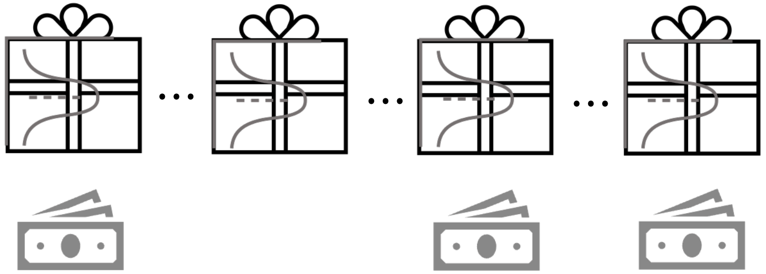
Features in Pandora's box

Observable multi-stage feedback

Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



New Design Principle: Gittins Index

- Improvement-based (e.g., LogEIPC)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index (PBGI)

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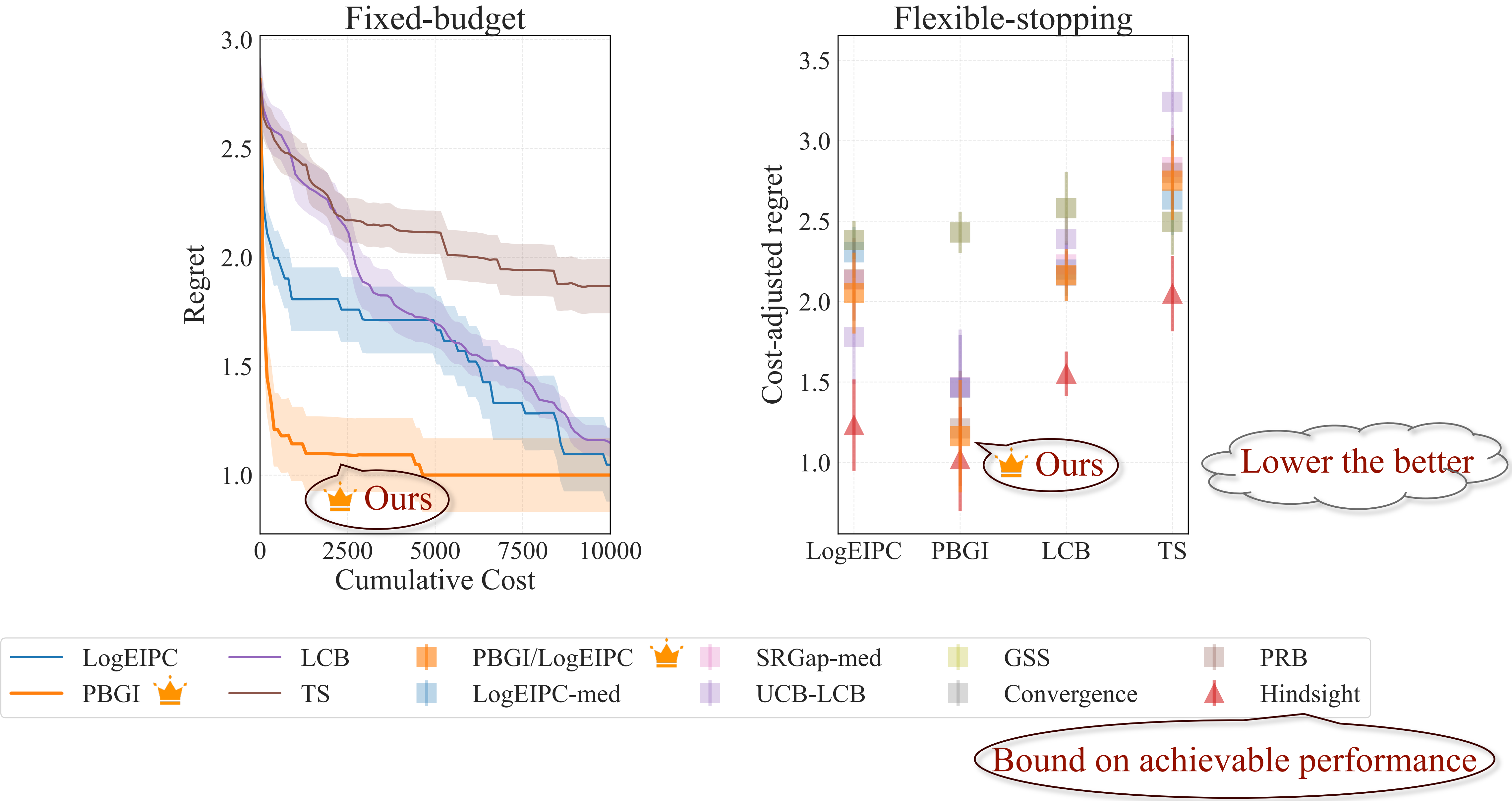
Gittins Index vs Baselines on AutoML Benchmark



New Design Principle: Gittins Index

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- Thompson sampling
- **Gittins Index**

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Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

$\mathbb{E}[R(\text{ours; PBGI})] \le R[\text{stopping immediately}]$

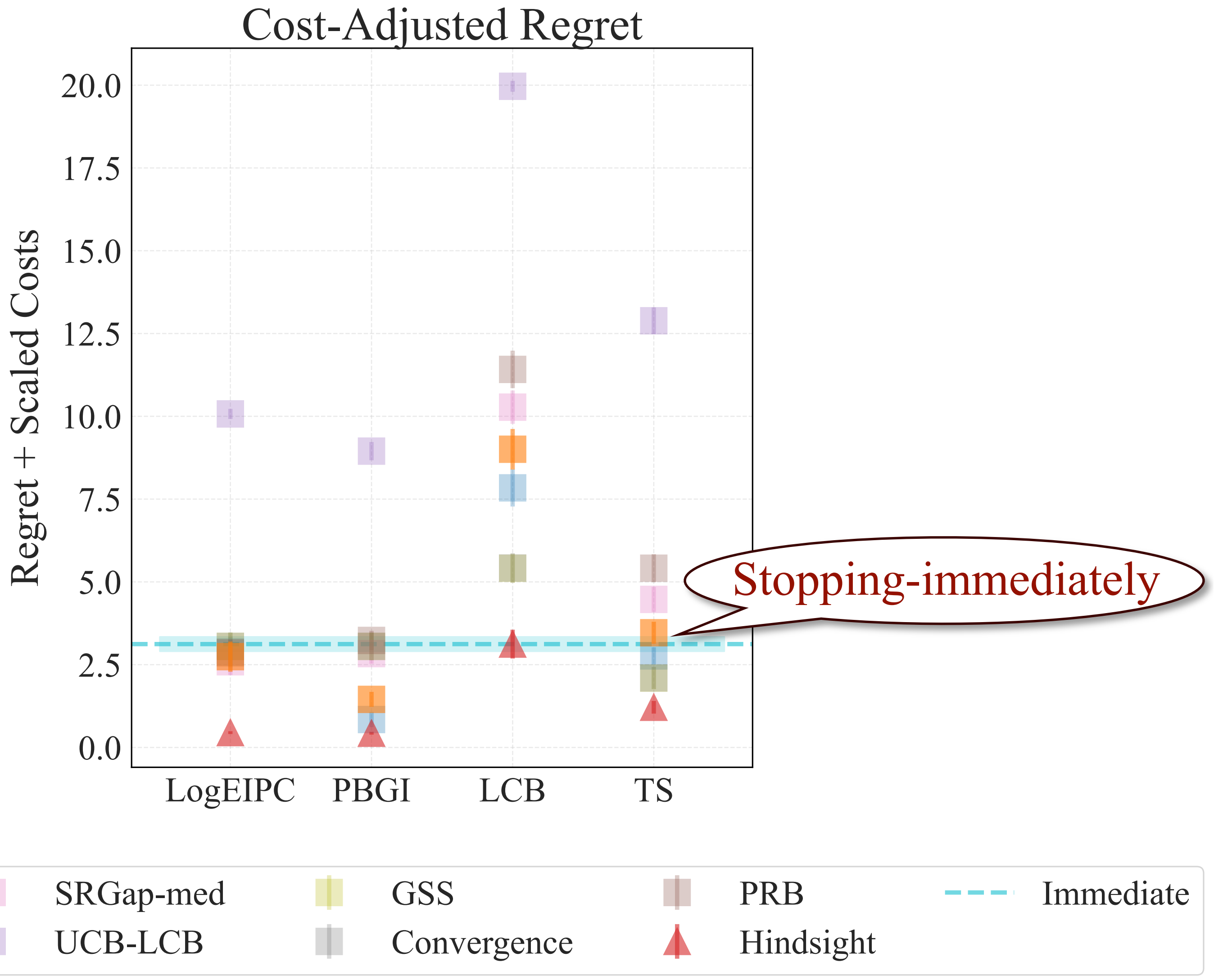
or LogEIPC

cost-adjusted regret

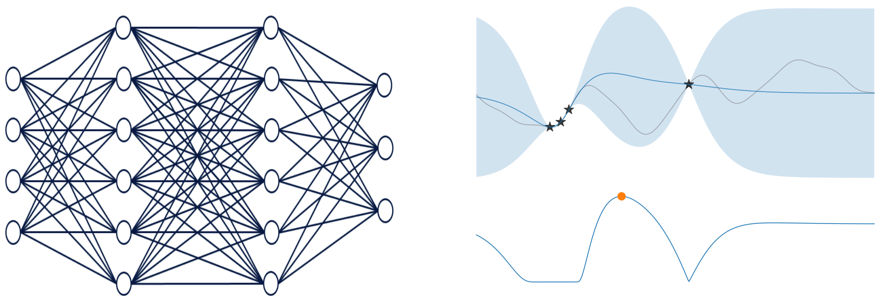
Implication:

- Matches the best achievable performance in the worst case (evaluations are all very costly).

- Avoids over-spending — a property many cost-unaware stopping rules lack.



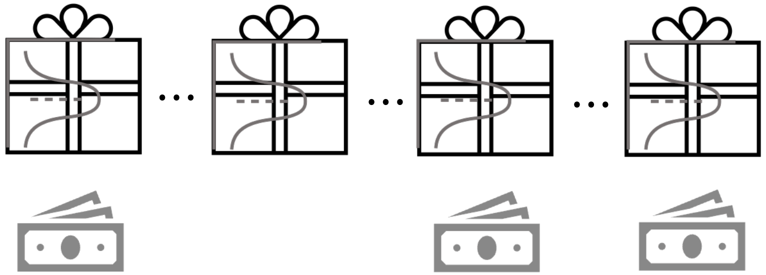
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

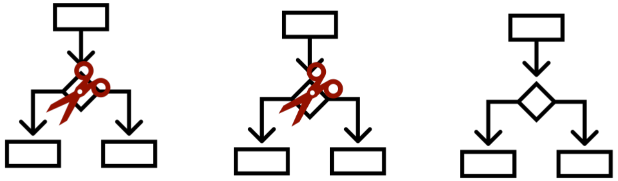
Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

Ongoing work



Sharper theoretical guarantees & black-box optimization w/ multi-stage feedback

"Cost-aware Stopping for Bayesian Optimization." Under review.

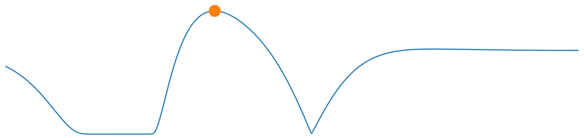
Recap: Bayesian Optimization

x →  → $f(x)$

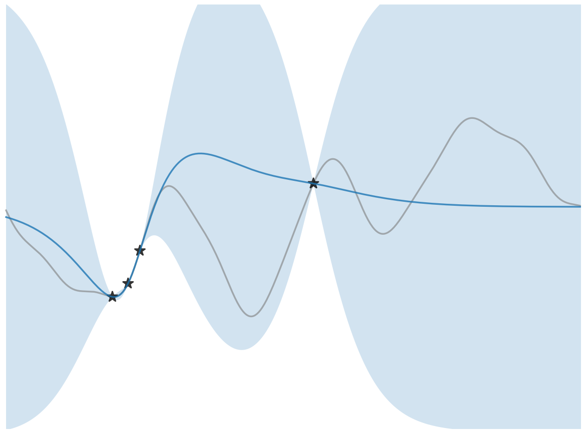
Black-box function

Select next input
(gradient-based optimization)

Update belief
(Bayes' rule)



Decision rule
(e.g., UCB, TS)



Probabilistic model
(e.g., Gaussian process)

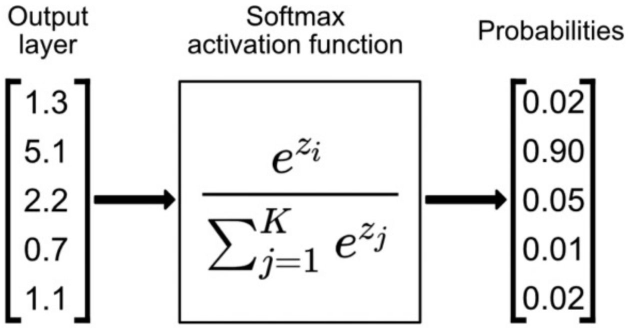
Ongoing: LLM-Driven Black-Box Optimization

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

Black-box function

Select next input
(LLM proposal)

Update belief
(feedback-augmented context)



$$\begin{bmatrix}1.3\\5.1\\2.2\\0.7\\1.1\end{bmatrix} \longrightarrow \boxed{\frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}} \longrightarrow \begin{bmatrix}0.02\\0.90\\0.05\\0.01\\0.02\end{bmatrix}$$

Decision rule
(e.g., Softmax sampling)

ChatGPT Gemini
deepseek Claude

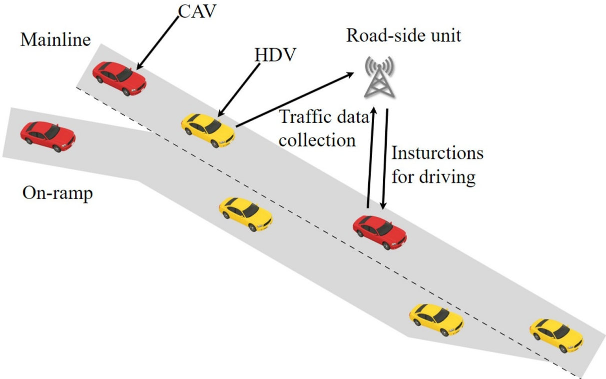
Probabilistic model
(large language model)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

x →



→ $f(x)$

(e.g., average speed)

Black-box function

(RL training & evaluation)

Update belief

(feedback-augmented context)

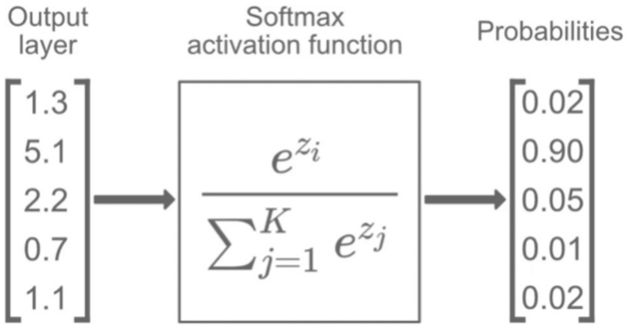
Probabilistic model

(large language model)

ChatGPT Gemini deepseek Claude

Decision rule

(e.g., Softmax sampling)



Select next input

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