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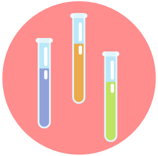
Near-linear Time Gaussian Process Optimization with Adaptive Batching and Resparsification

D. Calandriello* [1], **L. Carratino*** [2], A. Lazaric [3], M. Valko [1], L. Rosasco [2,4]

* equal contribution. [1] DeepMind, [2] MaLGa - UniGe, [3] Facebook, [4] MIT - IIT

Bayesian/Bandit Optimization

Set of candidates $\mathcal{A}$



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`for` $t = 1, \ldots, T$:

(1) Select candidate

(2) Receive noisy feedback

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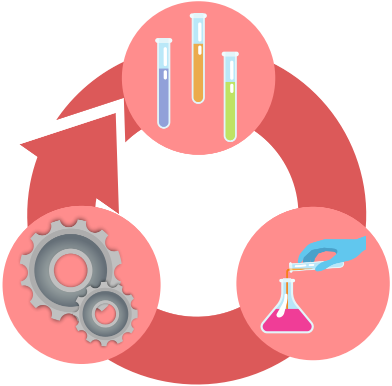

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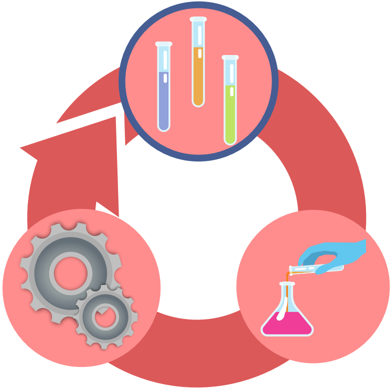

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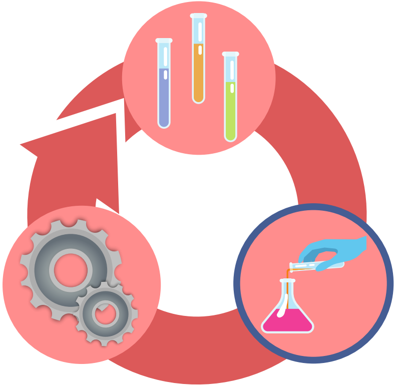

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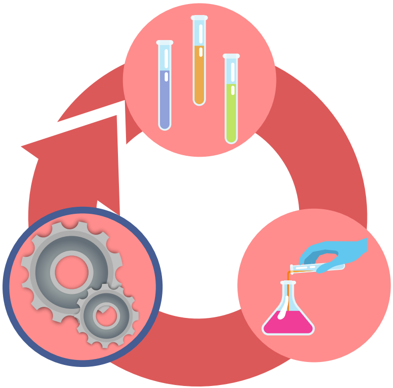

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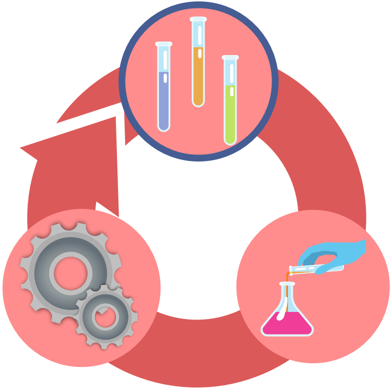

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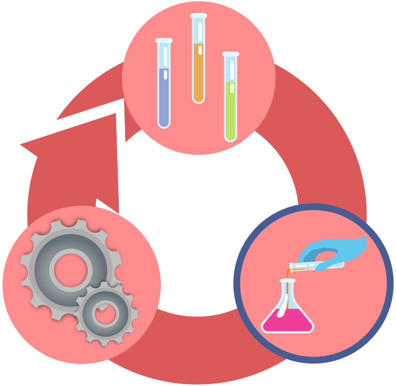

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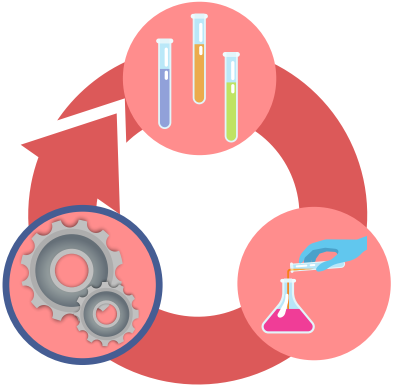

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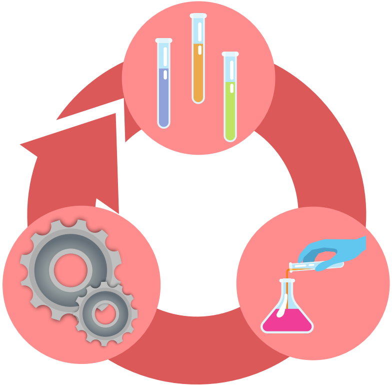

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Set of candidates $\mathcal{A} = \{x_1, \ldots, x_A\} \subset \mathbb{R}^d$,

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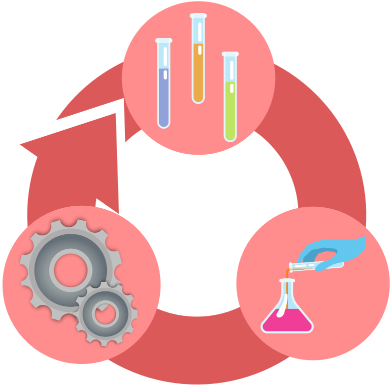

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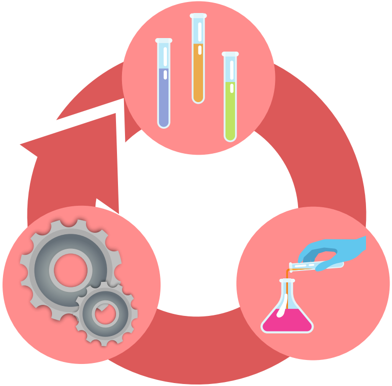

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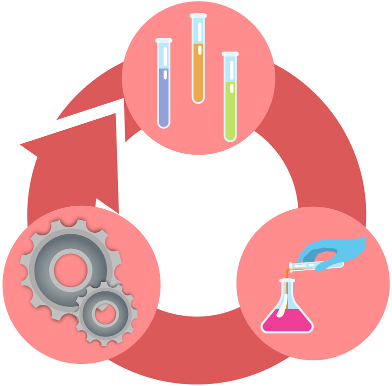

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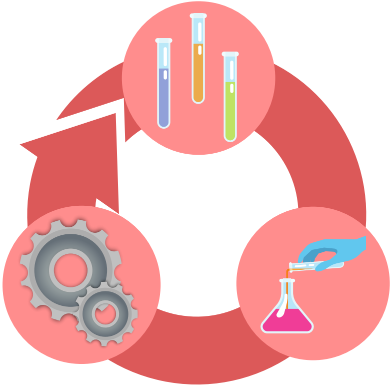

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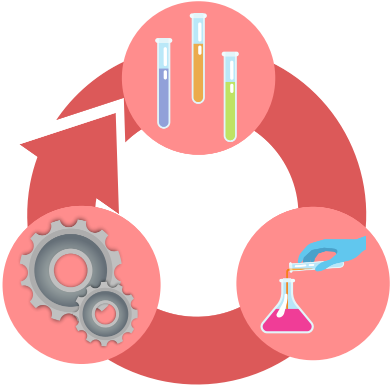

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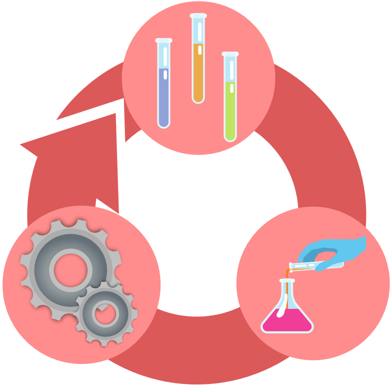

Performance measure: cumulative regret w.r.t. best x_*

$$R_T = \sum_{t=1}^{T} f(x_*) - f(x_t).$$

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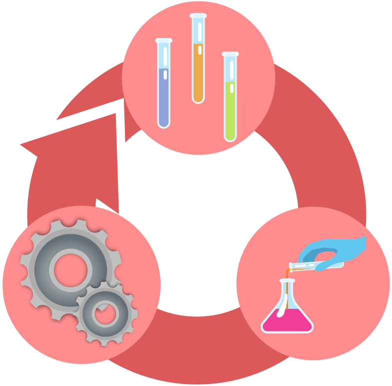

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💡 Use Gaussian process/kernelized Bandit to model f

Gaussian Process Optimization

🙂 Well studied: exploration vs exploitation $\rightarrow$ no-regret (low error)🙂

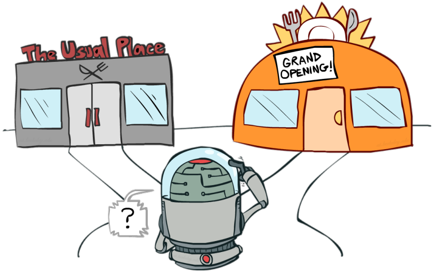

Image from Berkeley's CS 188

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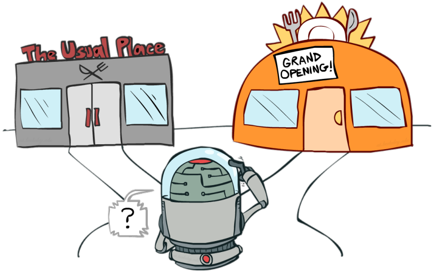

🤔 performance vs scalability ? 🤔

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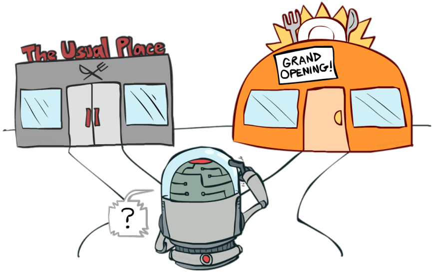

🤔 performance vs scalability ? 🤔

🙂 Batch BKB: no-regret and scalable 🙂

Why Scalable GP Optimization is Hard

Experimental
scalability

Computational
scalability

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Experimental scalability

sequential

vs

batch

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exact GP

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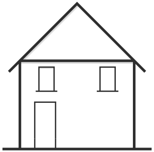
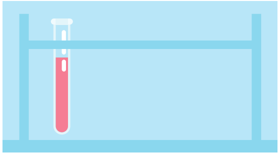


approximate GP

Why Scalable GP Optimization is Hard

Experimental scalability



sequential

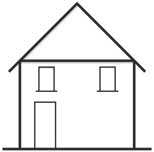
vs

batch

Computational scalability

exact GP

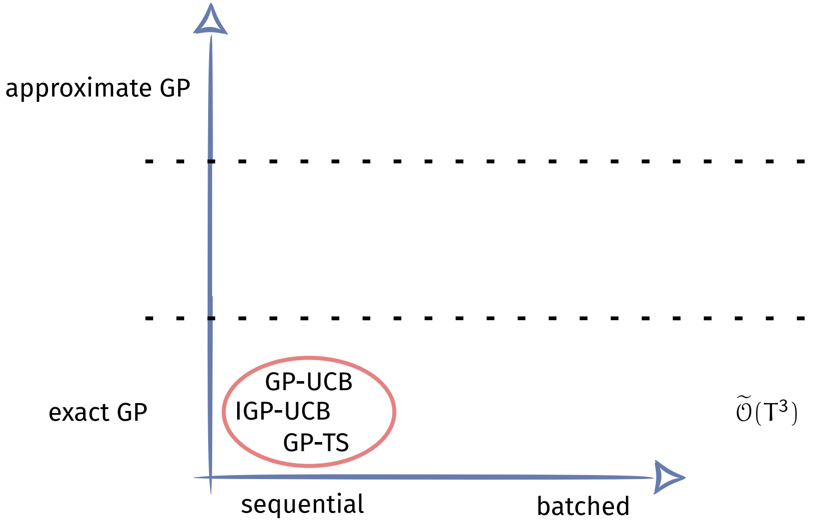
vs



approximate GP

🙁 Batching and approximations increase regret 🙁

Landscape of No-Regret GP Optimization



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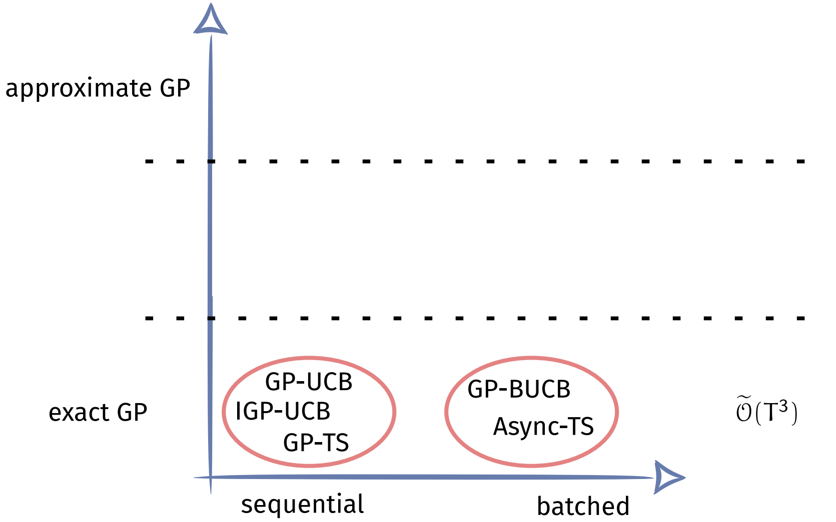

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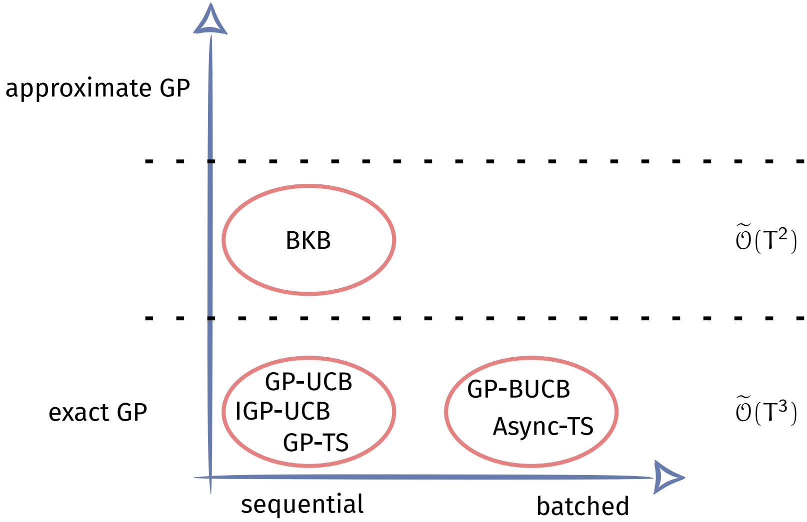

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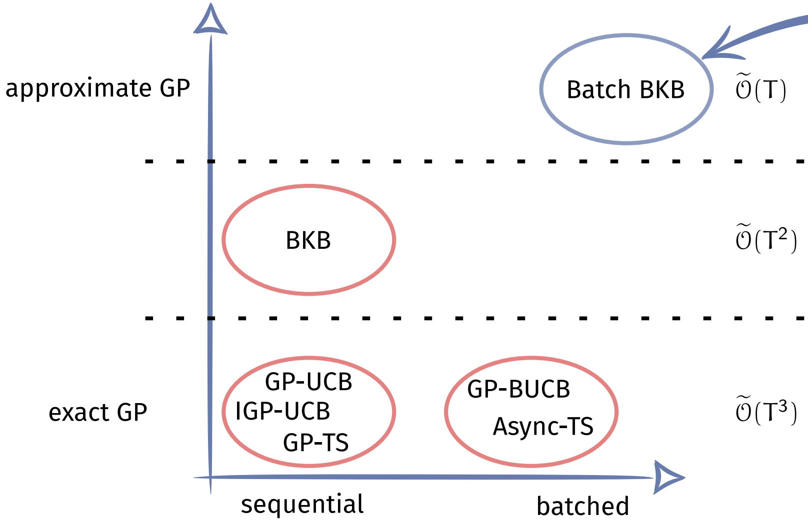

Our solution:
new adaptive schedule for
- batch-size
- approximation updates

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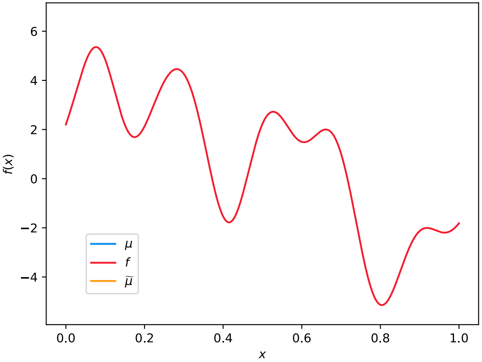
Choosing good candidates with GP-UCB



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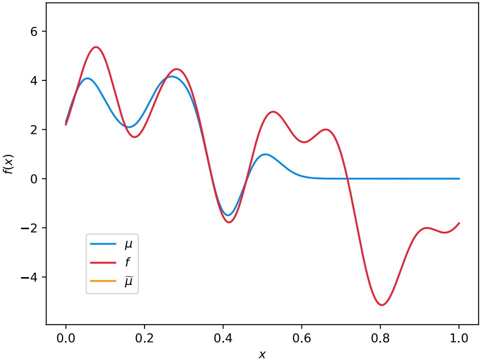
$$X_t = \{x_1, \dots, x_t\}, Y_t = \{y_1, \dots, y_t\}$$

Exact GP-UCB:

$$u_t(\cdot) = \mu(\cdot \mid X_t, Y_t)$$



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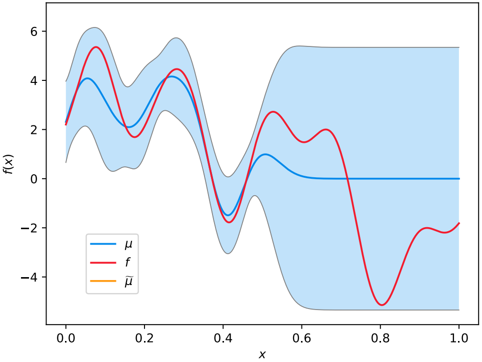

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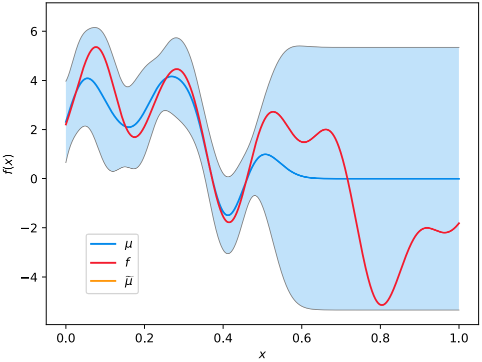
[Sri+10]: u_t valid UCB.



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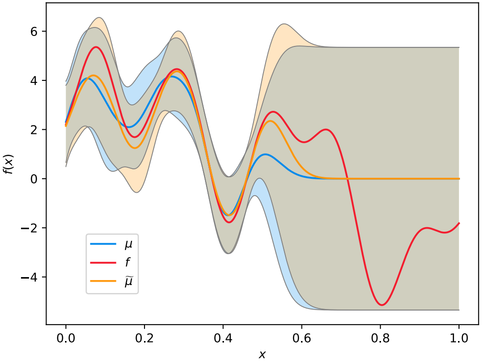

Sparse GP-UCB:

$$\widetilde{u}_t(\cdot) = \widetilde{\mu}(\cdot \mid X_t, Y_t, \mathcal{D}_t) + \widetilde{\beta}_t \widetilde{\sigma}(\cdot \mid X_t, \mathcal{D}_t)$$

with $\mathcal{D}_t \subset X_t$ inducing points

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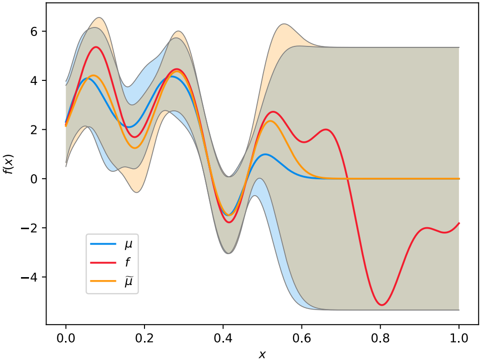
[Cal+19]: $\widetilde{u}_t$ valid UCB <u>if $\mathcal{D}_t$ updated at every t</u>.



Performance vs Scalability

Better performance: collect more feedback, update inducing points (resparsify)

$$\widetilde{u}_t(\,\cdot\,) = \widetilde{\mu}(\,\cdot\,|X_t, Y_t, \mathcal{D}_t) + \widetilde{\beta}_t \widetilde{\sigma}\ (\,\cdot\,|X_t, \mathcal{D}_t)$$

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Worse scalability: experimental cost, resparsification cost

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Worse scalability: <u>experimental cost</u>, <u>resparsification cost</u>

Improve scalability: <u>batching feedback (GP-BUCB)</u>, <u>batching resparsification ?</u>

Delayed Resparsification

New adaptive batching rule

$$\texttt{no-resparsify until} \sum_{i \in \text{Batch}} \widetilde{\sigma}(x_i) \geqslant 1$$

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“Not too big” Lemma: valid UCB

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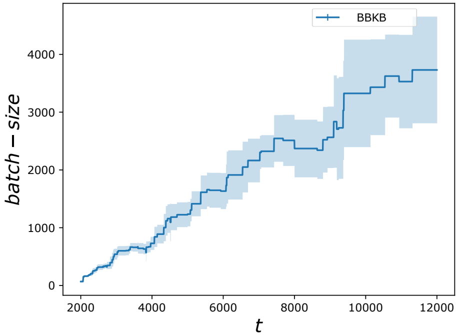
"Not too big" Lemma: valid UCB

"Not too small" Lemma: batch-size $= \Omega(t)$



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Batch-BKB

Theorem

*With high probability **Batch-BKB** achieves no-regret with time complexity $O(Td_{\mathit{eff}}^2)$, where $d_{\mathit{eff}} \ll T$ is the effective dimension / degrees of freedom of the GP.*

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Theorem

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Comparisons:

- 🙂 Same regret of GP-UCB/IGP-UCB and better scalability (form $O(T^3)$ to $O(Td_{eff}^2)$)
- 🙂 Larger batches than GP-BUCB
- 🙂 Better regret and better scalability than async-TS

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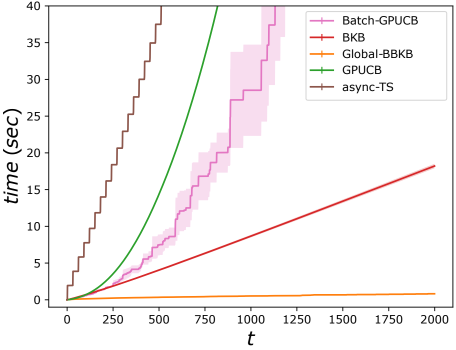
In practice: Scalability

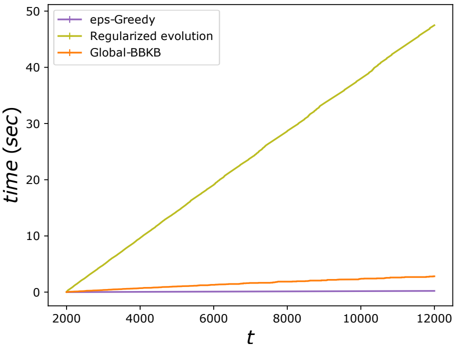
Cadata

$\mathcal{A} = 20640, d = 8, T = 2000$



NAS-bench-101

$\mathcal{A} = 12416, d = 19, T = 12000$



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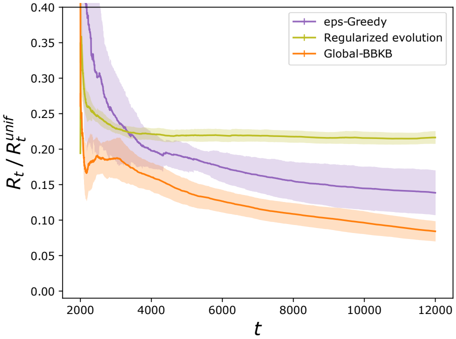
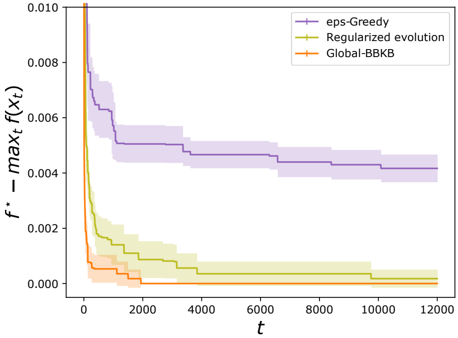
In practice: Performance

NAS-bench-101
Regret / Regret uniform



NAS-bench-101
Simple Regret



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Thank you