Parallel Thompson Sampling for Large-scale Accelerated Exploration of Chemical Space,

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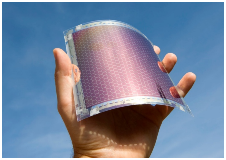
Joint work with James Requeima, Edward O. Pyzer-Knapp and Alan Aspuru-Guzik.

Drug and material design

Goal: find novel molecules that optimally fulfill various metrics.

About 10^8 compounds in databases, potential ones: $10^{20} - 10^{60}$.

Challenges:

- Evaluating molecular properties is slow and expensive.
- Chemical space is huge.

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  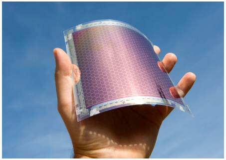

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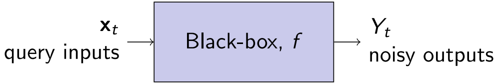
Bayesian optimization can accelerate the search.

Bayesian optimization aims to efficiently optimize **black-box** functions:

$$\mathbf{x}^\star = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

No gradients, observations may be **corrupted by noise**.



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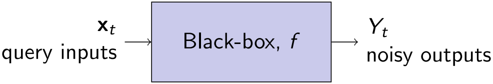

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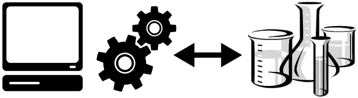
Main idea: replace expensive black-box queries with **cheaper computations** that will save additional queries in the long run.



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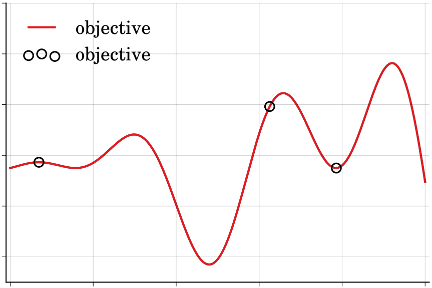

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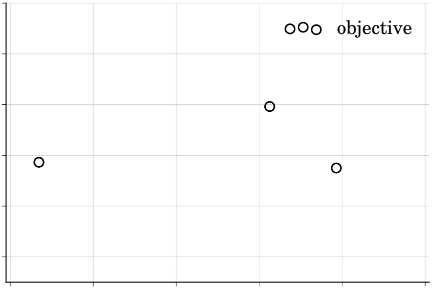

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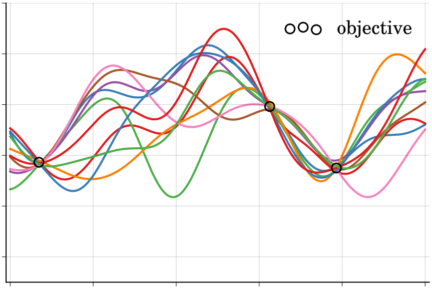

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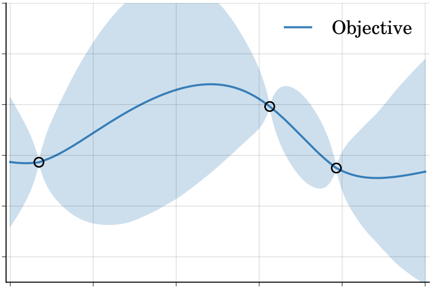

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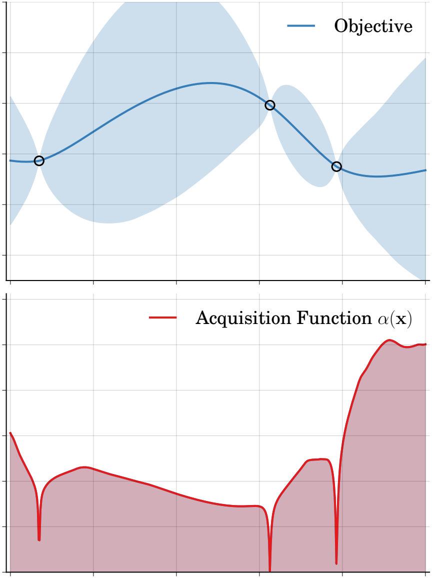

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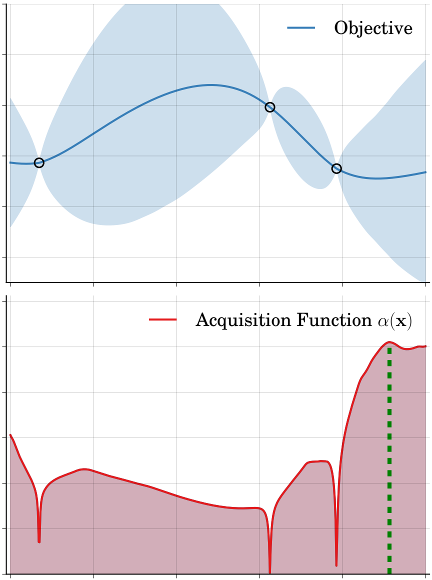

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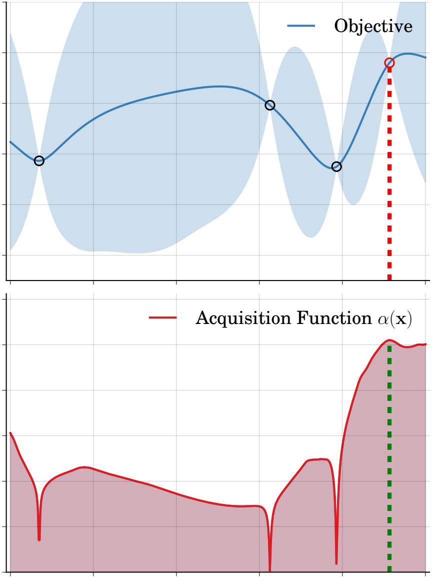

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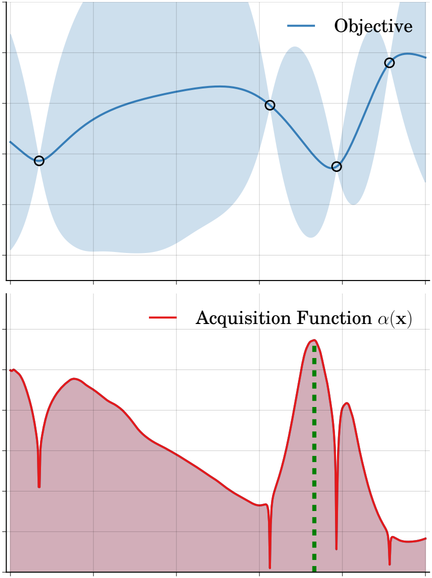

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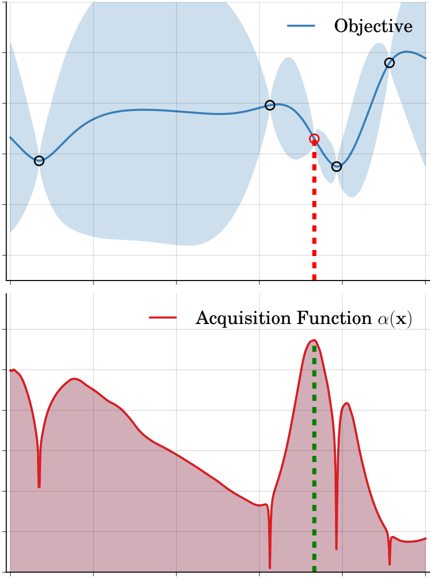

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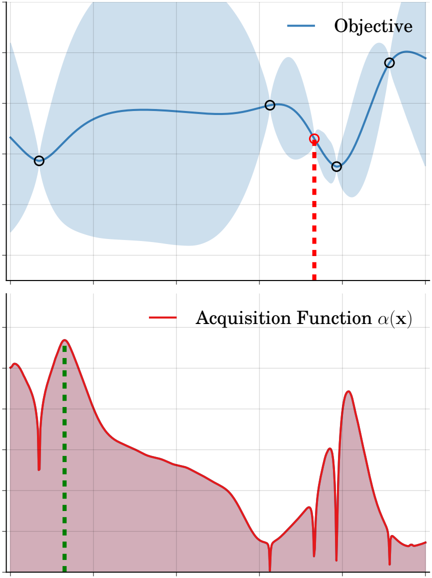

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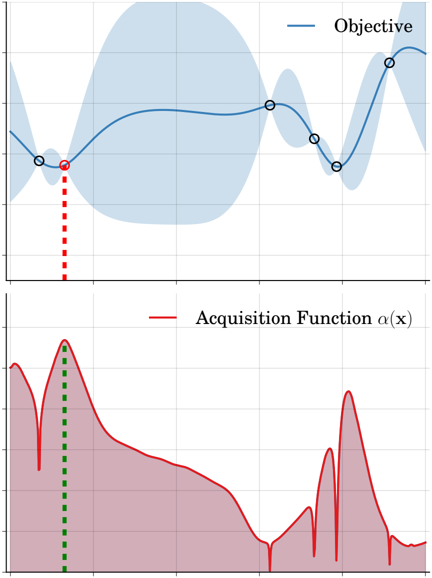

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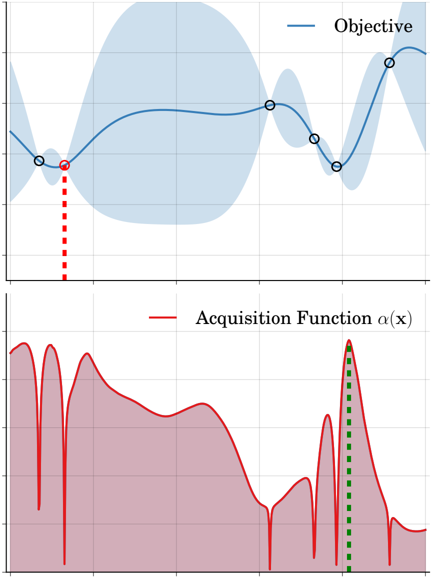

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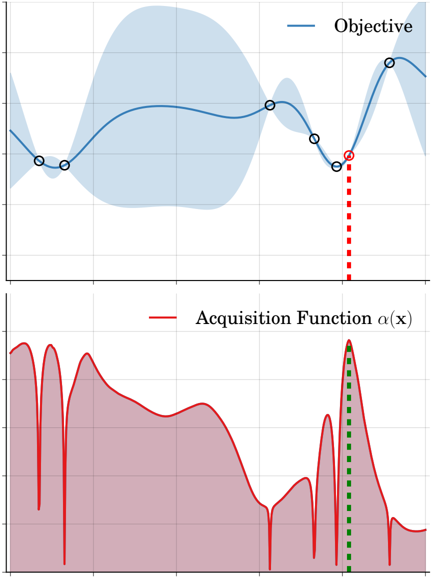

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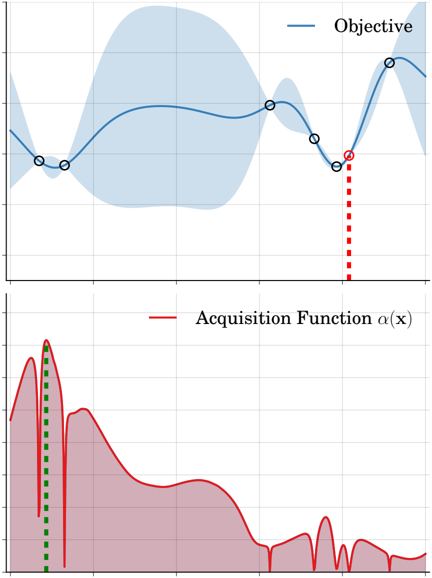

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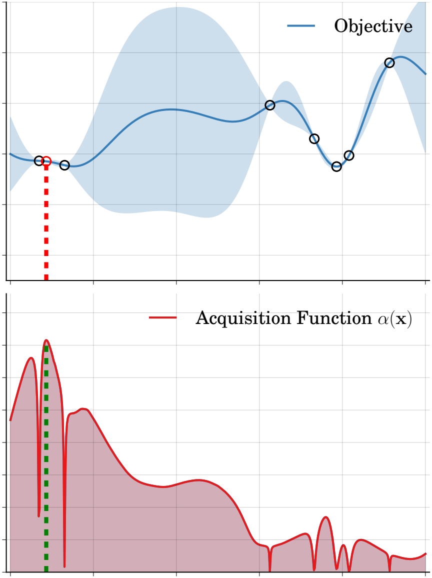

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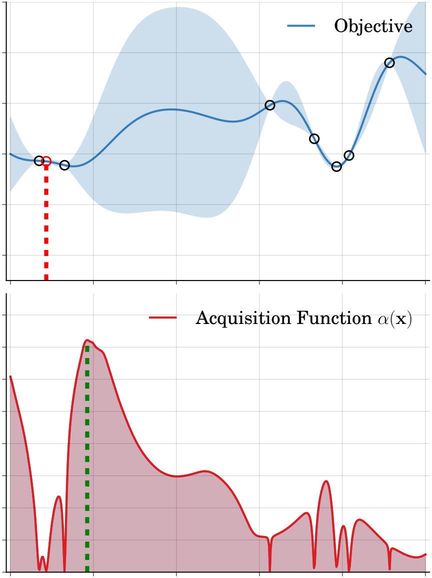

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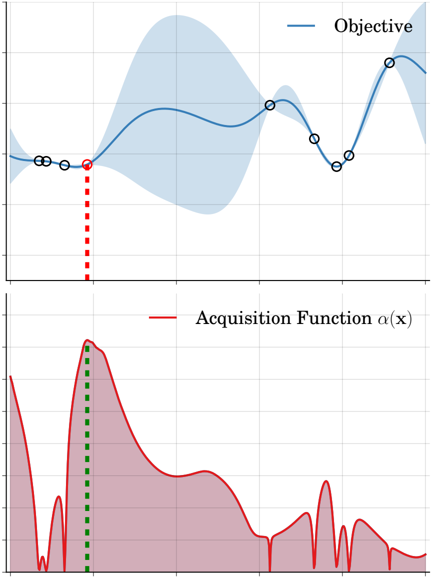

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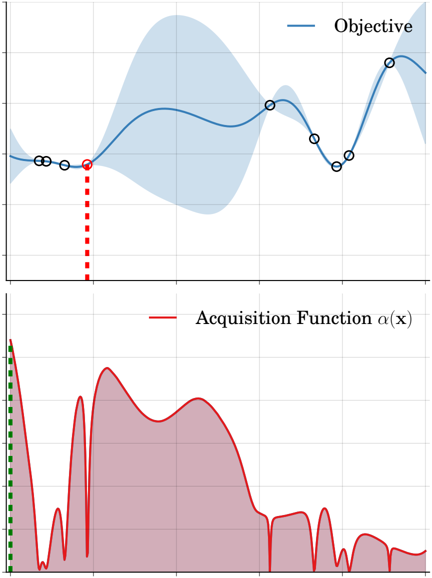

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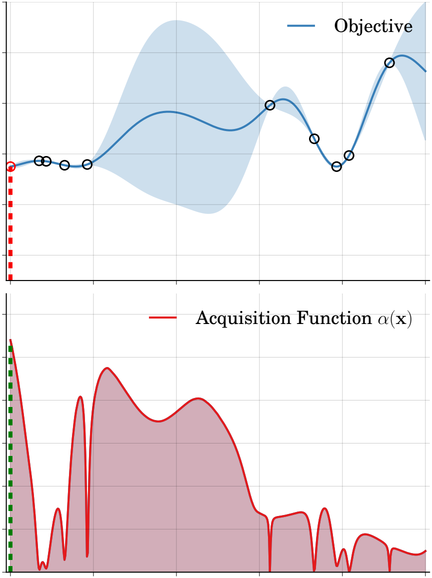

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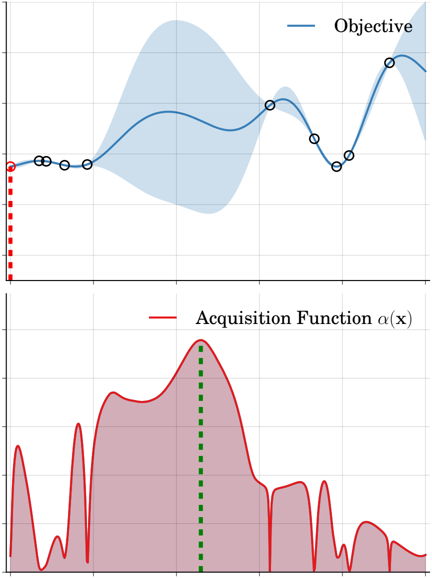

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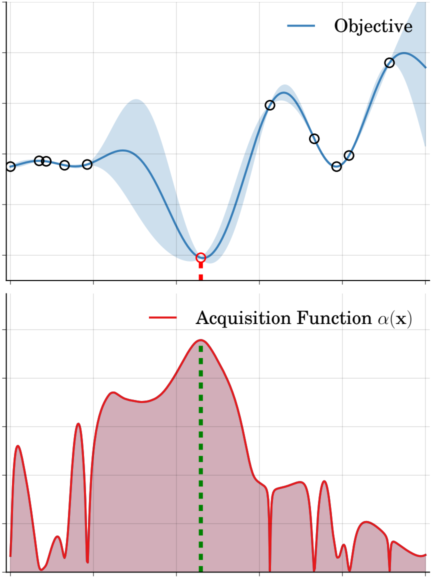

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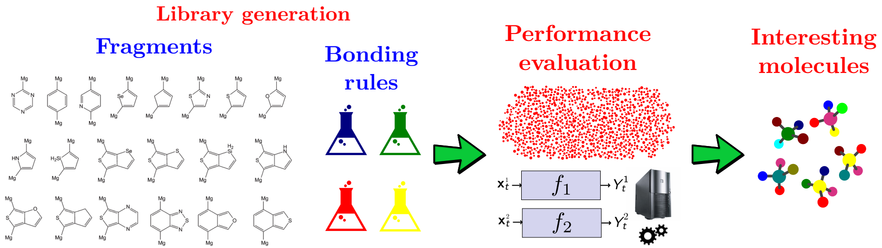

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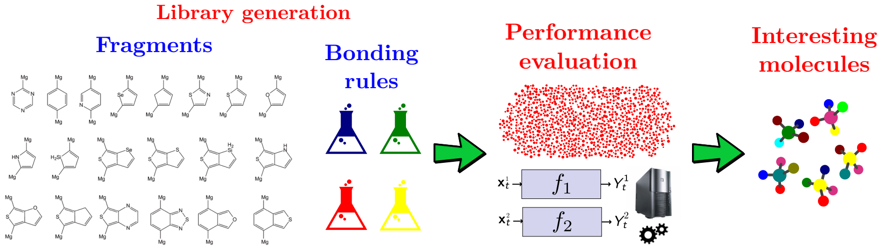

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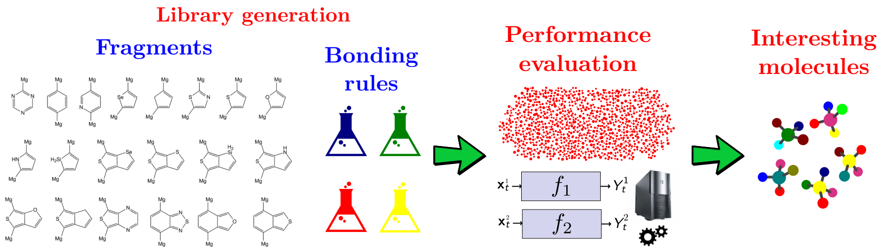

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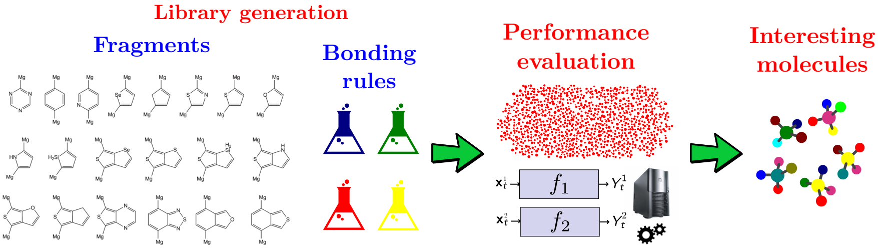

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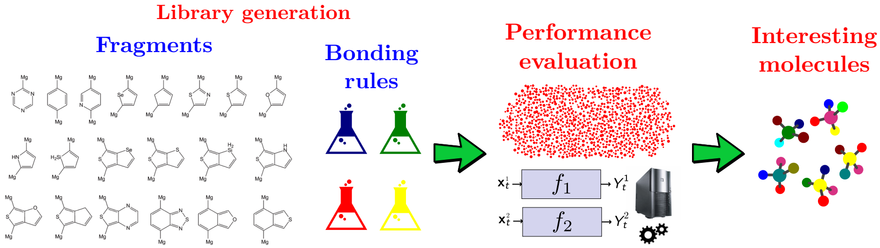

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3. How to collect data in **parallel** efficiently? e.g. with a **computer cluster**.

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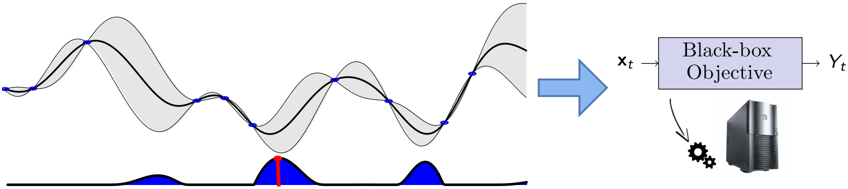

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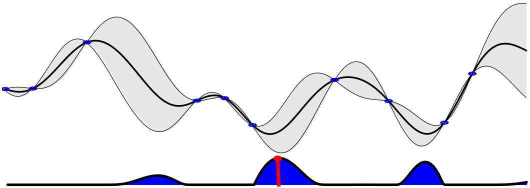

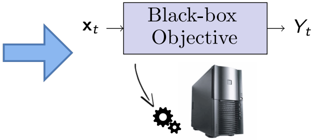

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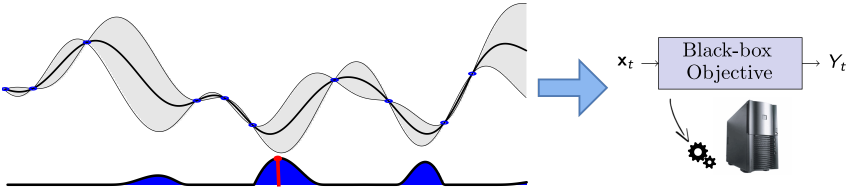

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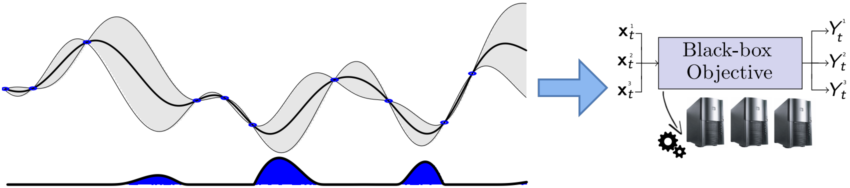

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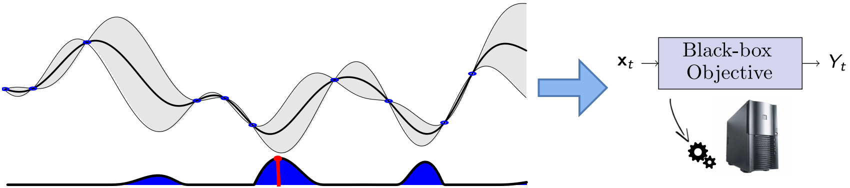

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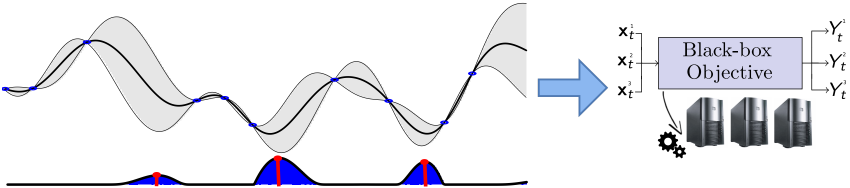

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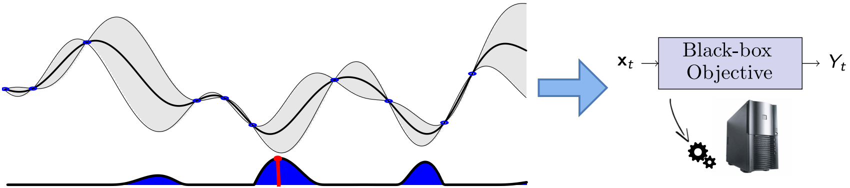

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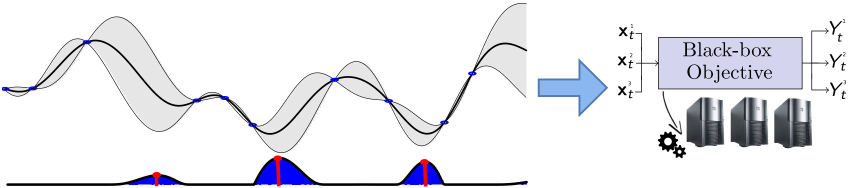

Parallel experiments should be highly informative but also diverse!

Traditional parallel BO

Parallel BO can be implemented by averaging the sequential acquisition function across data $\{\mathbf{y}_k\}_{k=1}^K$ **fantasized** at **pending** evaluation locations $\{\mathbf{x}_k\}_{k=1}^K$:

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Approximated by an **empirical average** across fantasies (samples) of $\{y_k\}_{k=1}^K$.

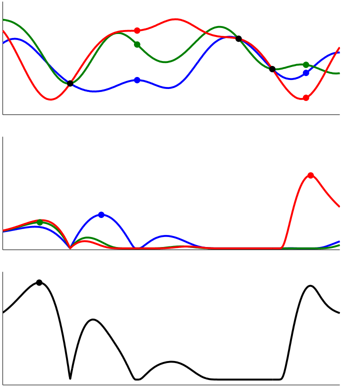
Traditional parallel BO

Figure source: Snoek et al. 2012.

Two pending evaluations, three fantasies.

Three **acquisition functions**, one per fantasy.

Average **acquisition function**.



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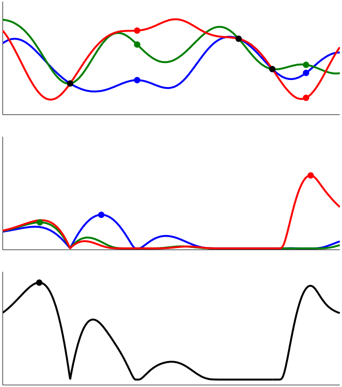

Challenges:

- Lack of scalability with **large batch sizes** and **large library sizes**.

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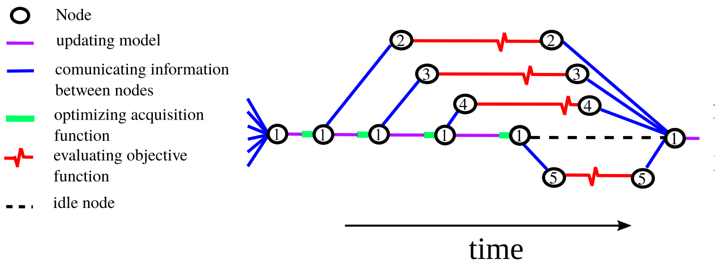

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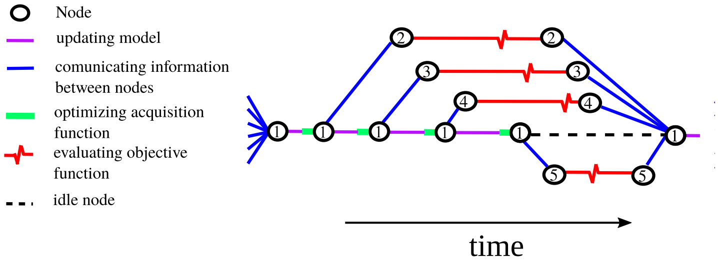

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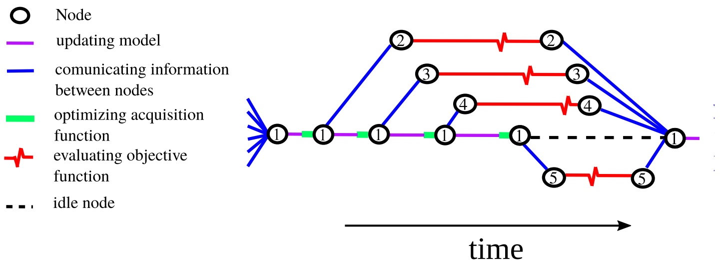

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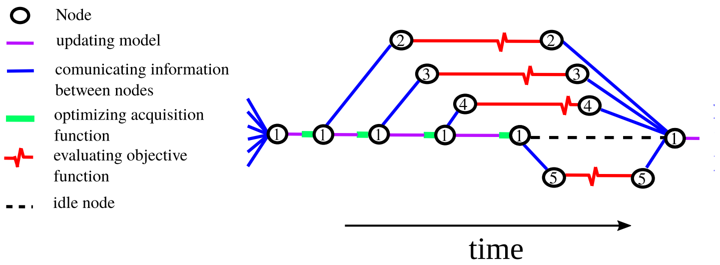

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Fails to exploit parallelism!

There is a need for methods that fully work in a **parallel and distributed manner**.

Thompson sampling (TS)

Sequential BO method that collects data by evaluating at $\mathbf{x} \sim p(\mathbf{x}_\star|\mathcal{D})$.

Implemented by drawing $f' \sim p(f|\mathcal{D})$ and then evaluating at $\mathbf{x} = \arg\min_{\mathbf{x}'} f'(\mathbf{x}')$.

The acquisition function is a **sample** from the posterior over functions!

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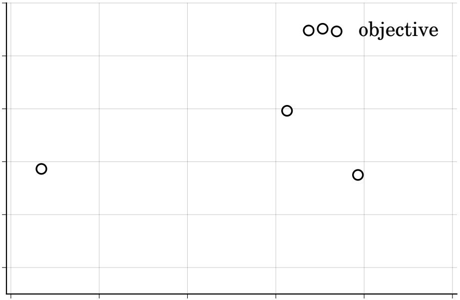

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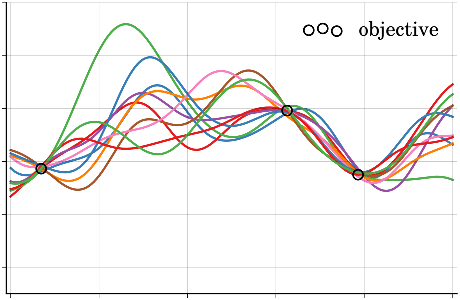

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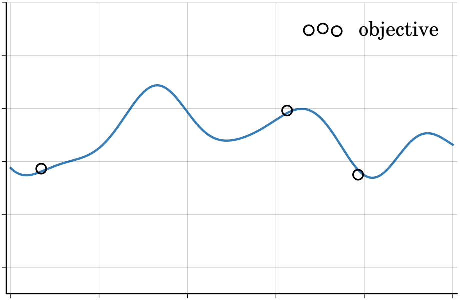

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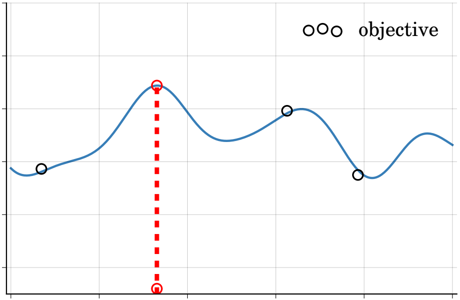

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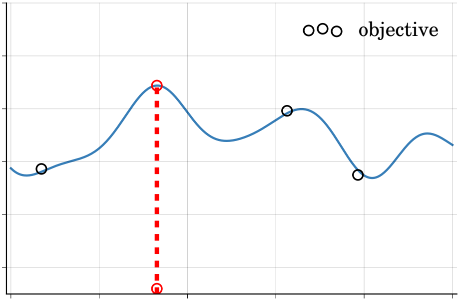

Exploitation: achieved because on average f' minimizes the prediction error.

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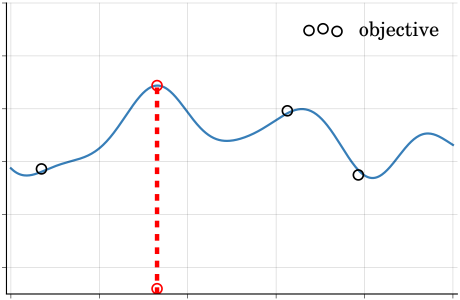

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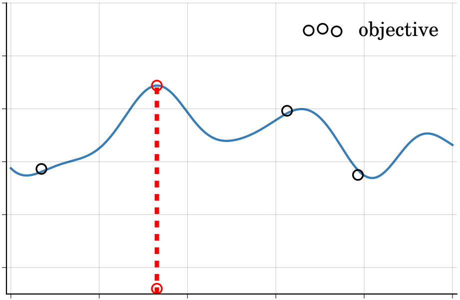

Very simple strategy that often works well in practice.

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TS as utility maximization and parallel TS

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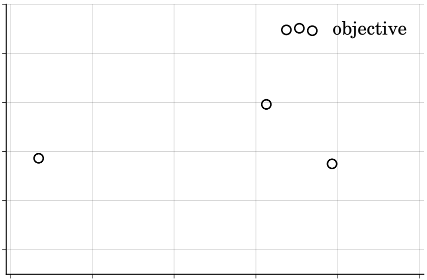
Our parallel TS is equivalent to running sequential TS multiple times!

Example



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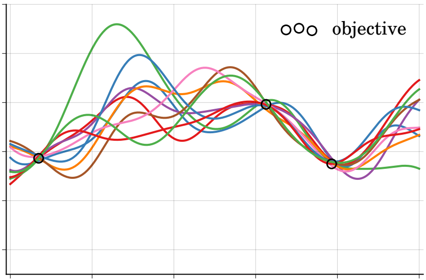

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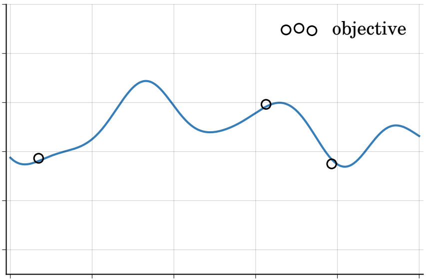

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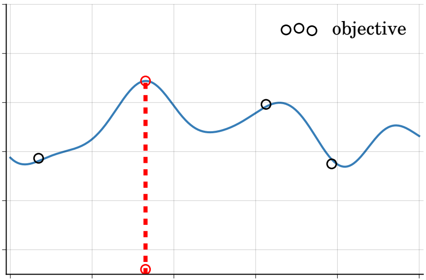

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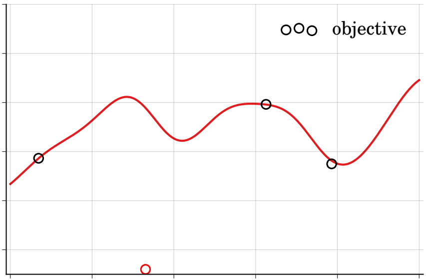

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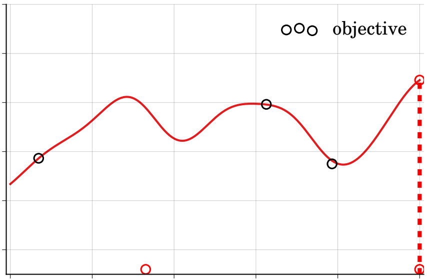

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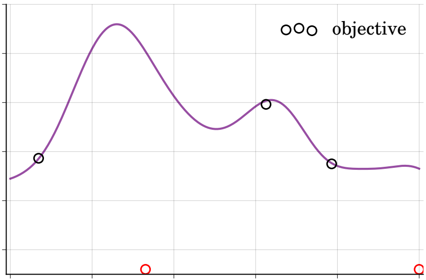

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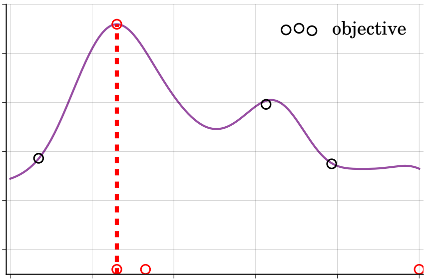

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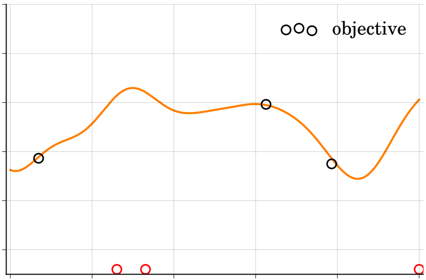

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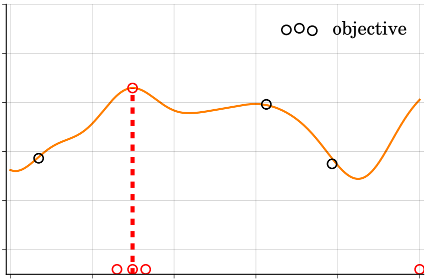

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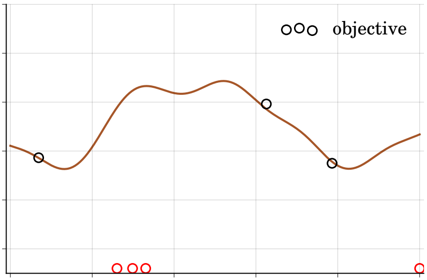

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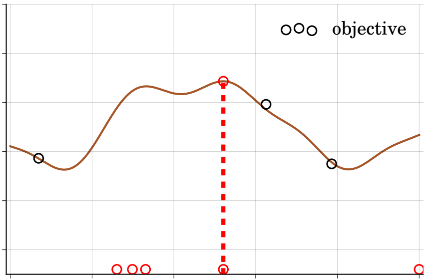

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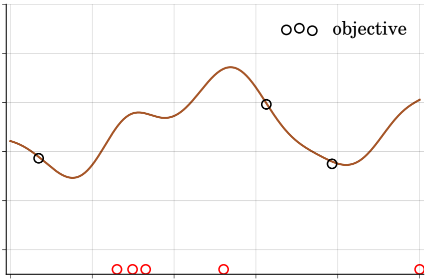

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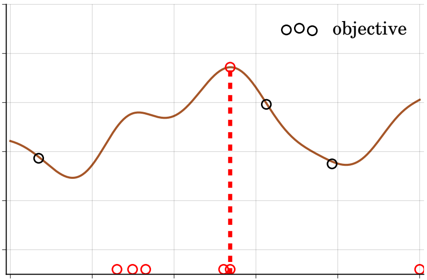

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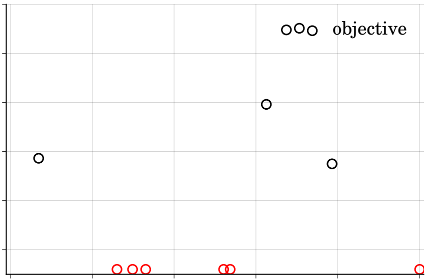

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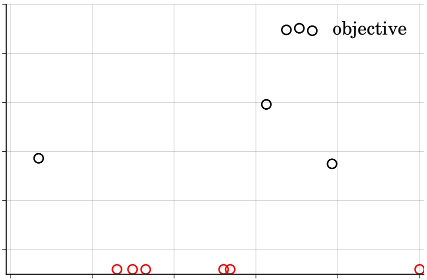
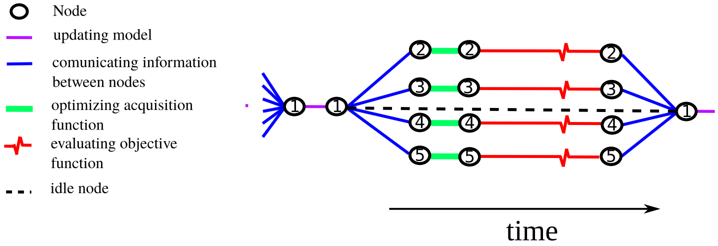


Each optimization problem can be done independently in a **different computer**.

Parallel Thompson sampling



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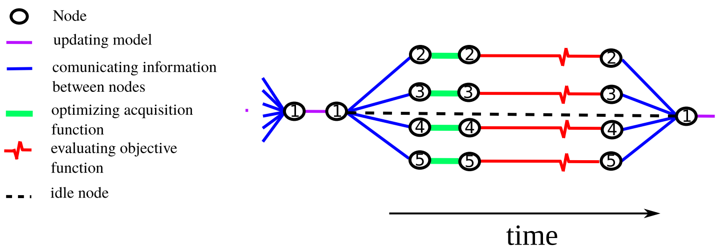


Works in a fully **parallel and distributed manner**.

Thompson sampling with Gaussian processes (GPs)

GPs are a **non-parametric models**, so sampling the model parameters $\boldsymbol{\theta}$ and optimizing $\mathbf{E}_{p(y|\mathbf{x},\boldsymbol{\theta})}[y]$ is not possible.

We approximate the objective function f as $f(\mathbf{x}) \approx \boldsymbol{\Phi}(\mathbf{x})\boldsymbol{\theta}$ with random features

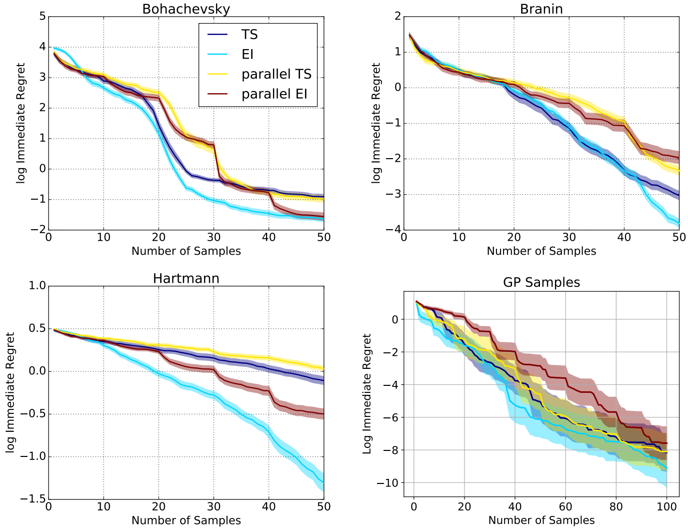
$$\boldsymbol{\Phi}(\mathbf{x}) = C\cos(\mathbf{W}^{\mathsf{T}}\mathbf{x} + \mathbf{b})\,, \tag{1}$$

where $\mathbf{W}, \mathbf{b} \sim p(\mathbf{W}, \mathbf{b})$, a distribution specified by the GP covariance function.

The prior for $\boldsymbol{\theta}$ is $\mathcal{N}(\mathbf{0}, \mathbf{I})$. The resulting **Bayesian linear regression model** is a parametric approximation to the original GP model.

Results with Gaussian process based models

Batch size: 10



Results with Bayesian neural networks

Data sets:

- CEP: Harvard Clean Energy Project data, 2.3M molecules.
- One-dose: percentage cell growth relative to control, 27,000 molecules.
- Malaria: drug concentration giving half max response, 19,000 molecules.

Batch sizes: 500 (CEP) and 200 (Malaria and One-dose).

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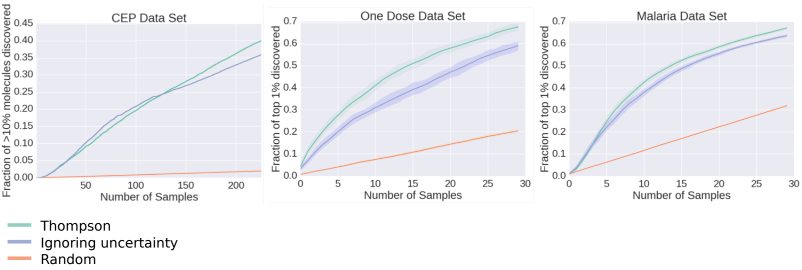
Batch sizes: 500 (CEP) and 200 (Malaria and One-dose).

Fraction of top 10% (CEP) or 1% (Malaria and One-dose) molecules found:



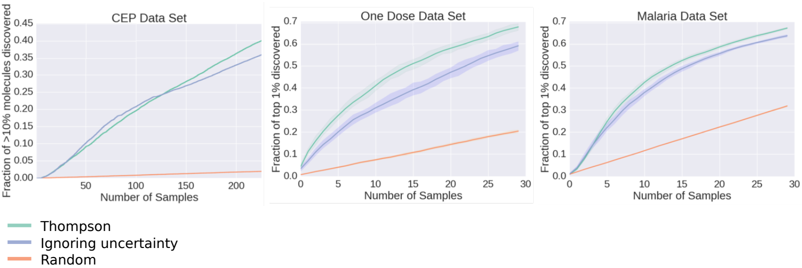
Results with Bayesian neural networks

Data sets:

- CEP: Harvard Clean Energy Project data, 2.3M molecules.
- One-dose: percentage cell growth relative to control, 27,000 molecules.
- Malaria: drug concentration giving half max response, 19,000 molecules.

Batch sizes: 500 (CEP) and 200 (Malaria and One-dose).

Fraction of top 10% (CEP) or 1% (Malaria and One-dose) molecules found:



BO gives 20× gains over random in CEP. Using uncertainty always helps.

Comparison with ϵ-greedy sampling

Table: Average rank and standard errors obtained by each method.

Method	**Rank**
$\epsilon = 0.01$	3.42±0.28
$\epsilon = 0.025$	3.02±0.25
$\epsilon = 0.05$	2.86±0.23
$\epsilon = 0.075$	3.20±0.26
Thompson	**2.51±0.20**

Take home message

Parallel Thompson sampling...

1. Batch BO method that runs in a **parallel and distributed manner**.
2. Can handle large batch sizes and large molecule libraries.
3. Comparable to non-scalable approaches in small problems with GPs.
4. Outperforms other alternative scalable approaches in large scale settings.

Thanks!