Introduction to Bayesian Optimization

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Bayesian Optimization Series

github.com/drewgjerstad/bayesian-optimization

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Introduction

Bayesian optimization refers to an optimization method that uses Bayesian inference to guide the optimizer make “better” decisions.

- This method achieves *unparalleled* sample efficiency.
- A statistical model is used to approximate the objective function.
- *Uncertainty* is inherent in optimization decisions, and uncertainty can be tackled via a Bayesian approach.

Motivation

Theoretical Motivation

- Black-box objective functions are functions that we can only interact with via its inputs and outputs meaning typical methods don't work.
- Expensive-to-evaluate objective functions are functions that require significant effort to obtain outputs but can be approximated and modeled using the Bayesian approach.
- Useful when objectives lack analytical evaluation.
- Useful when objectives have no efficient (if it exists) gradient.

Applications

The application potential of Bayesian optimization can be seen across several critical domains, especially those attempting to accelerate finding solutions to real-world scientific and engineering problems.

- Drug Discovery
- Molecule/Protein Discovery
- Materials Design
- AutoML (hyperparameter tuning)
- Engineering Decisions
- Many more...

Application: Drug Discovery

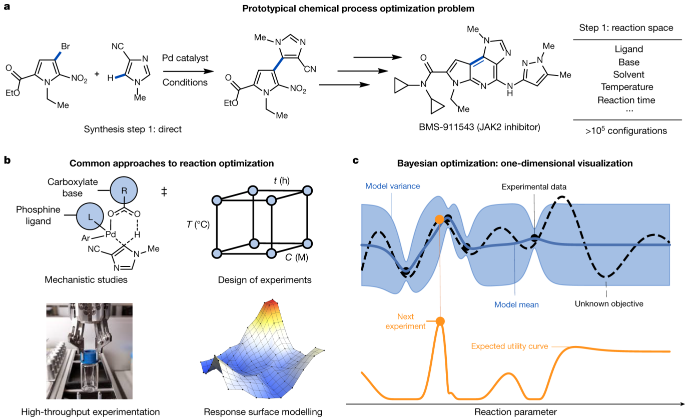

Figure 1: Overview of Drug Synthesis from *Bayesian optimization as a tool for chemical synthesis* by Shields et al. (2021)

Application: Molecule/Protein Discovery

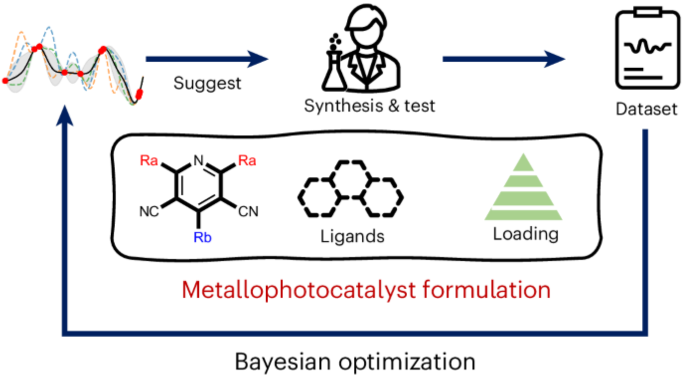

Figure 2: Closed Loop for Molecular Discovery from *Sequential closed-loop Bayesian optimization as a guide for organic molecular metallophotocatalyst formulation discovery* by Li et al. (2024)

Application: Materials Discovery

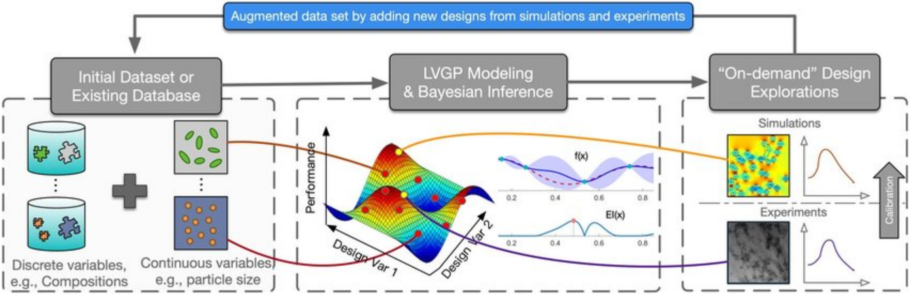

Figure 3: Material Design Framework from *Bayesian Optimization for Materials Design with Mixed Quantitative and Qualitative Variables* by Zhang et al. (2020)

Application: AutoML

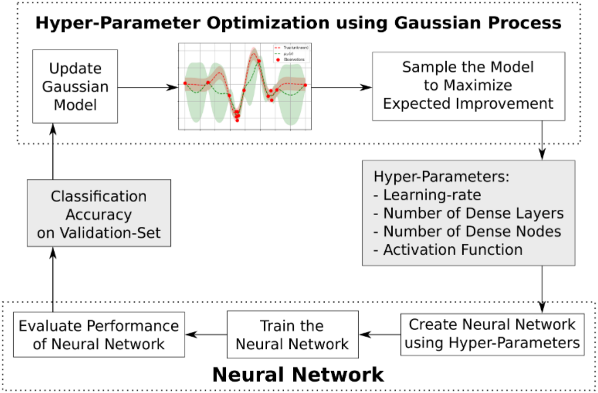

Figure 4: Framework for AutoML from *Achieve Bayesian optimization for tuning hyperparameters* by Edward Ortiz on *Medium* (2020)

Application: Engineering Decisions

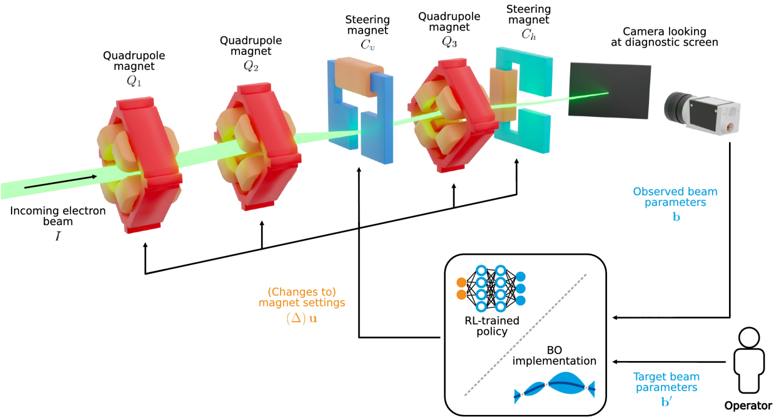

Figure 5: Framework for Particle Accelerator Tuning from *Reinforcement learning-trained optimisers and Bayesian optimisation for online particle accelerator tuning* by Kaiser et al. (2024)

Optimization Foundations

Optimization Foundations

Bayesian Foundations

Bayesian Foundations

The Bayesian Approach

The Bayesian Approach

Bayesian Optimization Workflow

Bayesian Optimization Workflow

Surrogate Models

Gaussian Processes

Acquisition Functions

Acquisition Function Optimizer

References

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