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Gaussian-Process Bayesian Optimization for the Design of a Precision Particle Physics Experiment

Monte-Carlo (MC) simulations are essential for designing particle physics experiments, as they enable us to evaluate and optimize key objectives—such as enhancing experimental sensitivity and performance. Since exhaustively sampling the full parameter space of experimental configurations is computationally prohibitive, sample-efficient methods to identify promising configurations are necessary. Bayesian optimization (BO) provides a principled framework for optimizing black-box functions by constructing a surrogate model and adaptively selecting promising parameter configurations. Many BO methods have theoretical convergence guarantees, typically relying on assumptions such as Lipschitz continuity or smoothness of the objective function. While these assumptions may not strictly hold in all cases, BO provides a sample-efficient and effective strategy for optimization.

In this study, we explore the use of BO with Gaussian processes [Chowdhury et al., 2019] in the design of an experiment searching for the electric dipole moment (EDM) of the muon at Paul Scherrer Institute [Adelmann et al., 2025]. We aim to optimize the injection of muons into the experiment to maximize the sensitivity to an EDM. To that end, we simulate our experiment using G4Beamline [Roberts & Kaplan, 2007], an MC framework for particle physics built on Geant4. We begin optimization with an initial set of parameter configurations, sampled using a quasi-random method to ensure broad coverage of the search space. We then use a Gaussian process as a surrogate model for the expensive simulation, and apply acquisition functions to choose new parameter combinations to simulate. By iteratively refining the surrogate model, we strategically sample parameter configurations that are likely to yield improvements for the sensitivity of the experiment.

Our study investigates the use of Bayesian optimization as an efficient method for parameter tuning in particle physics experiments. Using surrogate modeling and adaptive sampling, this approach offers a promising direction for optimizing complex experimental configurations.

References:

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