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BAYESIAN OPTIMIZATION FOR RECURRING, SIMULATION-BASED DECISION MAKING IN PRODUCTION AND LOGISTICS

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ABSTRACT

The thesis proposes a framework to accelerate Bayesian Optimization (BO) for recurrent simulation-based decision-making in production and logistics. BO is recognized for its sample efficiency but is often hindered by computational intensity, making it less suitable for scenarios requiring short-term decisions. The proposed framework TMPBO seeks to integrate transfer learning, meta-learning, and parallel computation to reduce optimization times and enhance convergence rates to make BO practical for operational decisions. The research will focus on leveraging historical optimization data and modern computing capabilities to improve BO's efficiency, making it viable for high-dimensional, multi-objective problems. The framework will be evaluated through a multi-stage process. The thesis aims to demonstrate that the TMPBO framework can offer significant advantages over classic BO and evolutionary algorithms in optimizing recurrent decision-making tasks.

1 INTRODUCTION

In modern production and logistics, efficient decision-making is crucial for maintaining operational excellence. Bayesian Optimization is a promising approach to optimize noisy and costly black-box functions by building a surrogate model, typically a Gaussian Process, to approximate the function. This surrogate is then used by the acquisition function (e.g. Expected Improvement) to determine the next sampling point (Frazier 2018). While this method is sample-efficient, it is also computationally intensive compared to methods like Evolutionary Algorithms, leading to longer optimization times (Lan et al. 2022). These longer times can render Bayesian Optimization impractical for short-term decision-making, where rapid responses are often necessary to adapt to dynamic conditions and avoid costly delays. In such scenarios, the ability to quickly identify optimal or near-optimal solutions is essential to ensure smooth and uninterrupted operations, making the balance between accuracy and speed a critical consideration.

In many simulation-based decision-making scenarios, decisions are recurrent, meaning similar decisions are made periodically based on similar data, as seen in Material Requirements Planning (MRP) or production planning (Savolainen et al. 2022). This recurrence offers an opportunity: by leveraging historical optimization data, referred to as source data or source models, we can accelerate the optimization process for current problems, known as target data or target models (Feurer et al. 2018). To achieve this acceleration, we apply concepts from transfer learning and meta learning, which are well-established in machine learning. These techniques, combined with parallel computation - whether of entire algorithms or through GPU computing can significantly enhance the efficiency of Bayesian Optimization. This approach makes it suitable for addressing recurrent short-term problems, transforming simulation combined with Bayesian Optimization into a viable tool for short-term decision-making in production and logistics.

2 TMPBO FRAMEWORK

Our aim is to develop a framework to accelerate the optimization process of Bayesian Optimization for recurrent simulation-based decision-making. We hypothesize that integrating transfer learning, meta-learning, and parallelization will significantly reduce computational time and improve convergence rates, while maintaining satisfactory optimization results. To validate this, we conduct evaluations over three stages with increasing complexity, resulting in the optimization of high-dimensional, multi-objective problems with continuous and discrete parameters, typical in production and logistics. The evaluation use case is a stochastic MRP simulation, though the framework is designed to be transferable to other parametrization problems.

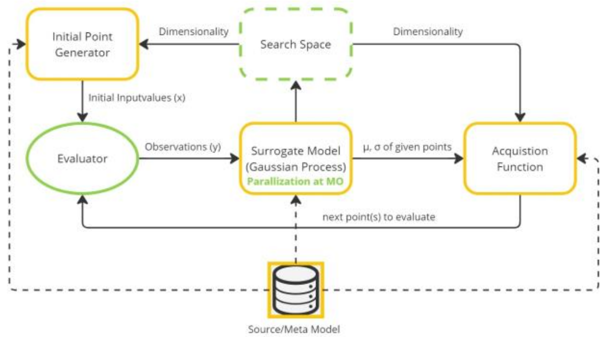

Figure 1: Overview of the Bayesian Optimization Framework with its key components. The color coding indicates the approaches used in TMPBO to address each component: yellow represents transfer and meta-learning, while green indicates parallelization. The search space is depicted with a dotted line to signify its implicit nature, as it is dependent on the modeling of the surrogate model. The arrows illustrate the flow of information.

Figure 1 illustrates the Bayesian Optimization Framework. The components highlighted in green will be optimized through parallelization of whole algorithms, leveraging modern computing capabilities. The yellow components will utilize techniques from transfer learning or meta-learning to incorporate historical data, enhancing initial model performance and reducing cold-start inefficiencies. We implement the framework in BoTorch, which is based on PyTorch, to take advantage of CUDA for efficient parallel computations (Balandat et al. 2020). This choice enables scalable processing capabilities crucial for handling high-dimensional optimization tasks. In the first step, we will conduct a comprehensive literature review to identify promising approaches for each component. Where necessary, we will modify the approaches to fit the framework's needs. We benchmark and select these approaches separately based on performance and compatibility with other BO components.

The selected approaches will be integrated into the TMPBO framework (Transfer learning, Meta-learning, and Parallelization for Bayesian Optimization), which will undergo evaluation over multiple stages. The framework will be benchmarked against classic Bayesian Optimization and state-of-the-art evolutionary algorithms.

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