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LLM and human-in-the-loop Bayesian optimization for chemical experiments

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Bayesian optimization has proven effective for optimizing expensive-to-evaluate functions in Chemical Engineering. However, valuable physical insights from domain experts are often overlooked. This article introduces a collaborative Bayesian optimization approach that integrates both human expertise and large language models (LLMs) into the data-driven decision-making process. By combining high-throughput Bayesian optimization with discrete decision theory, experts and LLMs collaboratively influence the selection of experiments via a human-LLM-in-the-loop discrete choice mechanism. We propose a multi-objective approach to generate a diverse set of high-utility and distinct solutions, from which the expert, supported by an LLM, selects the preferred solution for evaluation at each iteration. The LLM assists in interpreting complex model outputs, suggesting experimental strategies, and mitigating cognitive biases, thereby augmenting human decision-making while maintaining interpretability and accountability. Our methodology retains the advantages of Bayesian optimization while incorporating expert knowledge and AI-driven guidance. The approach is demonstrated across various case studies, including bioprocess optimization and reactor geometry design, showing that even with an uninformed practitioner, the algorithm recovers the regret of standard Bayesian optimization. By including continuous expert-LLM interaction, the proposed method enables faster convergence, improved decision-making, and enhanced accountability for Bayesian optimization in engineering systems.

Type of presentation

Invited Talk

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