AutoOED: Automated Optimal Experiment Design Platform

Yunsheng Tian
Mina Konaković Luković
Timothy Erps
Michael Foshey
Wojciech Matusik

Computer Science & Artificial Intelligence Lab
Massachusetts Institute of Technology
Cambridge, MA 02139, USA

Abstract

We present AutoOED, an Optimal Experiment Design platform powered with automated machine learning to accelerate the discovery of optimal solutions. The platform solves multi-objective optimization problems in time- and data-efficient manner by automatically guiding the design of experiments to be evaluated. To automate the optimization process, we implement several multi-objective Bayesian optimization algorithms with state-of-the-art performance. AutoOED is open-source and written in Python. The codebase is modular, facilitating extensions and tailoring the code, serving as a testbed for machine learning researchers to easily develop and evaluate their own multi-objective Bayesian optimization algorithms. An intuitive graphical user interface (GUI) is provided to visualize and guide the experiments for users with little or no experience with coding, machine learning, or optimization. Furthermore, a distributed system is integrated to enable parallelized experimental evaluations by independent workers in remote locations. The platform is available at https://autooed.org.

Keywords: multi-objective optimization, Bayesian optimization, Pareto optimality, optimal experiment design, design of experiments

1. Introduction

Optimal Experiment Design (OED) problems in science and engineering often require satisfying several conflicting objectives simultaneously. These problems aim to solve a multi-objective optimization system and discover a set of optimal solutions, called Pareto optimal. Furthermore, the objectives are typically black-box functions whose evaluations are time-consuming and costly (e.g., evaluations can either measure real experiments or run expensive numerical simulations). Thus, the budget that determines the number of experiments can be heavily constrained. Hence, an efficient strategy for guiding the experimental design towards Pareto-optimal solutions is necessary. Recent advances in machine learning algorithms have facilitated optimization of various design problems, including chemical design (Griffiths and Hernández-Lobato, 2017), material design (Zhang et al., 2020), battery design (Attia et al., 2020), clinical drug trials (Yu et al., 2019), resource allocation (Wu et al., 2013), environmental monitoring (Marchant and Ramos, 2012), robotics (Martinez-Cantin et al., 2009). A machine learning concept that enables automatic guidance of the design process is Bayesian optimization (Shahriari et al., 2016). This concept is extensively...
studied in the machine learning and optimization community from a theoretical aspect and in the single-objective case. However, its potential applications in other fields with multi-objective problems are still not widely explored due to the lack of intuitive, easy to use, and open-source software. BoTorch (Balandat et al., 2020) is a recent library for Bayesian optimization, nevertheless, it lacks a GUI, does not support distributed usage, and is targeted for experts in coding. Auto-QChem (Shields et al., 2021) is a recent open-source software for experiment design in chemistry, but it does not optimize for multiple objectives and does not apply to fields other than chemistry.

AutoOED is an open-source platform for multi-objective optimization problems with a restricted budget of test samples. The platform automatically guides the design of experiments to be evaluated and quickly leads to the best performing designs. AutoOED is based on the concept of multi-objective Bayesian optimization (MOBO) and is entirely implemented in Python. The key features of this platform include:

- **Intuitive GUI**: An easy-to-use graphical user interface (GUI) is provided to directly visualize and guide the optimization progress and facilitate the operation for users with little or no experience with coding, optimization, or machine learning. The GUI is built using the Tkinter package with a model-view-controller (MVC) architecture.
- **Modular structure**: A highly modularized codebase and built-in visualization enable easy extensions and replacements of MOBO algorithm components. The platform can serve as a testbed for machine learning researchers to easily develop and evaluate their own MOBO algorithms.
- **Data-efficient experimentation**: As the platform aims to solve problems with expensive to evaluate or black-box objective functions, the number of experiments is limited to an order of several dozens. The platform employs an optimization strategy that rapidly advances the Pareto front with a small set of evaluated experiments.
- **Sequential and batch evaluations**: A standard feature supports evaluating a single experiment in each optimization iteration. To further reduce the optimization time, the platform parallelizes the evaluation process by enabling synchronous and asynchronous batch evaluations. Asynchronous batch evaluations are instrumental when multiple workers are running experiments, but their evaluations drastically vary in time.
- **Automation of experiment design**: The platform is designed for straightforward integration into an automatic experiment design optimization pipeline. The pipeline may include both physical experiments (see example at https://tinyurl.com/autooed-phys) and an expensive simulation setup (see example at https://tinyurl.com/autooed-sim).

**Distributed usage**: Besides the standard single-user version, to facilitate the platform’s use for a single design process by several users, we provide a distributed team version based on a centralized database. The database shares the optimization status to different roles in the experiment team (managers, scientists, technicians) and provides them with different tools for controlling and contributing to the experimental design process.

2. Platform Overview

To automate the optimization process and guide the experiments, AutoOED is based on the principles and algorithms of multi-objective Bayesian optimization (MOBO). MOBO is a data-driven approach that attempts to learn the black-box objective functions from
available data and find Pareto-optimal solutions in a data-efficient manner. AutoOED outputs the whole palette of designs on the Pareto front, enabling the user to choose the trade-off most suited for their application. In addition to the set of optimal solutions, our platform’s final product is the learned prediction models of the unknown objectives. The prediction provides the users with more insights into the potential outcomes of experiments. It helps them better understand the optimization problem to make informed decisions and guide the optimization process towards their preference.

As a full-stack software, the overall workflow of AutoOED from the front-end to the back-end is presented in Figure 1. Given an optimization problem, if the evaluation program is available, AutoOED can automatically guide the experimentation by alternating between optimization and evaluation. In this case, an optimization process starts first. The scheduler then orders evaluations in an asynchronous way, and the optimization restarts once the evaluations from the currently requested batch are all done. This process repeats until some stopping criterion is met and the evaluated results are automatically recorded in the database. Otherwise, if the evaluation program does not exist, users can still manually do the evaluations and enter results into the database.

![Figure 1: The overall workflow of the platform design.](image)

### 2.1 Modular Code Structure

Multi-objective Bayesian optimization typically consists of four core components: (i) an inexpensive surrogate model for the black-box objective functions; (ii) an acquisition function that defines sampling from the surrogate model and trade-off between exploration and exploitation of the design space; (iii) a multi-objective optimization solver to approximate the Pareto set and front; (iv) a selection strategy that proposes a single or a batch of experiments to evaluate next. These four components (see Figure 2) are implemented as core and independent building blocks of the AutoOEDs, making it highly modularized and easy to develop new algorithms and modules. A list of supported surrogate models, acquisition functions, solvers, and selection strategies can be found at the API reference section of our documentation.

![Figure 2: Algorithmic pipeline and core modules. The platform follows the multi-objective Bayesian optimization pipeline. A user can choose an approach for each module.](image)
2.2 Supported Algorithms and Features

We provide several popular and state-of-the-art multi-objective Bayesian optimization methods, including DGEMO (Luković et al., 2020), TSEMO (Bradford et al., 2018), USeMO (Belakaria and Deshwal, 2020), ParEGO (Knowles, 2006). To the best of our knowledge, DGEMO exhibits state-of-the-art performance for data-efficient, multi-objective problems with batch evaluations. Implemented algorithms also include NSGA-II (Deb et al., 2002) and MOEA/D (Zhang and Li, 2007), as they are some of the most widely used multi-objective evolutionary algorithms. Users can select an algorithm from this library that best fits the characteristics of their physical system or the optimization goals.

Additional features of the platform support: continuous, discrete, binary, categorical, and mixed design variables; linear and non-linear constraints handling in the design space; sequential and batch evaluations; synchronous and asynchronous batch evaluations. In the synchronous case, the algorithm starts a new iteration when all the requested evaluations from one batch are completed. The asynchronous batch evaluations are instrumental when evaluations drastically vary in time. To be more time-efficient, the asynchronous approach updates a model and requests a new evaluation as soon as one batch sample is completed. Our platform is especially beneficial for applications in areas such as finance, organization optimization, materials science, life sciences, chemistry, robotics, and the pharmaceutical industry, where the experiments are long (e.g., days or weeks) but can easily be carried out in parallel.

2.3 Graphical User Interface (GUI) and Distributed Usage

The GUI guides the user through a set of simple steps to configure the problem, such as the number of design and performance parameters, the parameter ranges and constraints, parallelization settings, and selection of the optimization algorithm. Other functional features include real-time display of design and performance space, exporting of the database and statistics, and support for linking custom evaluation scripts. We provide a manual GUI for entering the experiment data and example scripts that showcase how to interface the worker with simulation scripts (e.g., MATLAB structural analysis toolbox, see https://tinyurl.com/autooed-sim) or automated robotic platforms that perform experiments (see examples at https://tinyurl.com/autooed-phys).

For additional flexibility, a single experiment can be managed by several users from different computers. A distributed team version is based on a centralized database, providing secure data storage and retrieval. Users can be assigned different roles (scientist, technician, manager), and they will have different access and tools for controlling the experimental design process. This version helps the team collaborate more efficiently across the globe.

3. Concluding Remarks

AutoOED is released under the MIT license as a free and open-source platform that can be obtained at https://github.com/yunshengtian/AutoOED. This paper presents only a brief overview of the platform and its features. Comprehensive documentation and examples are available at https://autooed.readthedocs.io. The official webpage, as well as the past and ongoing projects using AutoOED, can be found at https://autooed.org.
Acknowledgments

We would like to acknowledge support and feedback for this project from Konica Minolta. M. K. Luković would like to acknowledge support from the Schmidt Science Fellowship.

References

Peter M Attia, Aditya Grover, Norman Jin, Kristen A Severson, Todor M Markov, Yang-Hung Liao, Michael H Chen, Bryan Cheong, Nicholas Perkins, Zi Yang, et al. Closed-loop optimization of fast-charging protocols for batteries with machine learning. *Nature*, 578 (7795):397–402, 2020.

Maximilian Balandat, Brian Karrer, Daniel R. Jiang, Samuel Daulton, Benjamin Letham, Andrew Gordon Wilson, and Eytan Bakshy. BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization. In *Advances in Neural Information Processing Systems 33*, 2020. URL http://arxiv.org/abs/1910.06403.

Syrine Belakaria and Aryan Deshwal. Uncertainty-aware search framework for multi-objective bayesian optimization. In *AAAI Conference on Artificial Intelligence (AAAI)*, 2020.

Eric Bradford, Artur M Schweidtmann, and Alexei Lapkin. Efficient multiobjective optimization employing gaussian processes, spectral sampling and a genetic algorithm. *Journal of global optimization*, 71(2):407–438, 2018.

Kalyanmoy Deb, Amrit Pratap, Sameer Agarwal, and TAMT Meyarivan. A fast and elitist multiobjective genetic algorithm: Nsga-ii. *IEEE transactions on evolutionary computation*, 6(2):182–197, 2002.

Ryan-Rhys Griffiths and José Miguel Hernández-Lobato. Constrained bayesian optimization for automatic chemical design. *arXiv preprint arXiv:1709.05501*, 2017.

Joshua Knowles. Parego: a hybrid algorithm with on-line landscape approximation for expensive multiobjective optimization problems. *IEEE Transactions on Evolutionary Computation*, 10(1):50–66, 2006.

Mina Konaković Luković, Yunsheng Tian, and Wojciech Matusik. Diversity-guided multiobjective bayesian optimization with batch evaluations. In *Advances in Neural Information Processing Systems 33, NeurIPS 2020, December 6-12, 2020, virtual*, 2020.

Roman Marchant and Fabio Ramos. Bayesian optimisation for intelligent environmental monitoring. pages 2242–2249, 10 2012. ISBN 978-1-4673-1737-5. doi: 10.1109/IROS.2012.6385653.

Ruben Martinez-Cantin, Nando Freitas, Eric Brochu, Jose Castellanos, and Arnaud Doucet. A bayesian exploration-exploitation approach for optimal online sensing and planning with a visually guided mobile robot. *Auton. Robots*, 27:93–103, 08 2009. doi: 10.1007/s10514-009-9130-2.
B. Shahriari, K. Swersky, Z. Wang, R. P. Adams, and N. de Freitas. Taking the human out of the loop: A review of bayesian optimization. *Proceedings of the IEEE*, 104(1):148–175, 2016.

Benjamin J Shields, Jason Stevens, Jun Li, Marvin Parasram, Farhan Damani, Jesus I Martinez Alvarado, Jacob M Janey, Ryan P Adams, and Abigail G Doyle. Bayesian reaction optimization as a tool for chemical synthesis. *Nature*, 590(7844):89–96, 2021.

J. Wu, W.Y. Zhang, S. Zhang, Y.N. Liu, and X.H. Meng. A matrix-based bayesian approach for manufacturing resource allocation planning in supply chain management. *International Journal of Production Research*, 51(5):1451–1463, 2013. doi: 10.1080/00207543.2012.693966. URL https://doi.org/10.1080/00207543.2012.693966.

Zhenning Yu, Viswanathan Ramakrishnan, and Caitlyn Meinzer. Simulation optimization for bayesian multi-arm multi-stage clinical trial with binary endpoints. *Journal of Biopharmaceutical Statistics*, 29:1–12, 02 2019. doi: 10.1080/10543406.2019.1577682.

Q. Zhang and H. Li. Moea/d: A multiobjective evolutionary algorithm based on decomposition. *IEEE Transactions on Evolutionary Computation*, 11(6):712–731, 2007.

Yichi Zhang, Daniel W Apley, and Wei Chen. Bayesian optimization for materials design with mixed quantitative and qualitative variables. *Scientific Reports*, 10(1):1–13, 2020.