Benchmarking Experiment Planning Algorithms for Autonomous Experimentation

Introduction

Some of the most urgent problems faced by the world today include energy crisis, global warming, pollution, waste management, and food security. All of these can be potentially solved by the discovery of novel materials. However, the commercialisation and wide-spread usage of a newly discovered material can take up to over a decade and half after the material is discovered. Such a large period of time grossly reduces both value and the effect that these materials can potentially have and, in some cases, may even render the material useless against the problem it was originally discovered to tackle.

The use of highly automated laboratories and artificial intelligence (AI) algorithms, in combination, holds the promise to greatly accelerate the development of new materials and their manufacturing processes. [1] These self-driving laboratories are being designed using concepts of computer science and AI. These laboratories will not only accelerate discovery and commercialisation of materials but also conserve valuable resources, that get used up in experimentation. Thus, the development of these laboratories for more efficient and accelerated discovery of materials is of great interest to chemists as well as computer scientists.

Research Question

Self-driving laboratories are being designed with the purpose of discovering and exploring autonomously using ML models and AI-guided robots. A recently developed python library, named OLYMPUS, provides easy access to ML algorithms for the development of such laboratory. [2]
OLYMPUS provides a wide variety of optimisation algorithms and also allows for integration of customized algorithms that can potentially be used for autonomous experiment planning. The use of appropriate algorithms for the problem at hand can lead to much greater experimental efficiencies as compared to traditional trial-and-error approaches. [3] This reduces the time and cost needed to discover a material or develop its manufacturing process, accelerating the discovery-to-commercialisation timeline in materials science.
However, the performance of different ML algorithms against various optimisation tasks in chemistry and materials science stand unclear, and as such it is difficult for the researcher to select the most suitable algorithm for the problem at hand. In this study, we will benchmark 20 optimisation algorithms against 10 characteristic problems in chemistry and materials science in order to answer the following questions:

1. Which algorithms require the least number of steps for optimisation?
2. Which algorithms are robust to output/measurement noise?
3. Which algorithms are robust to input noise, i.e., noise in the experimental conditions?

Research Methodology

OLYMPUS provides a set of 10 experimentally-derived data sets that correspond to optimisation problems within chemistry and material science (e.g., optimization of the yield of chemical reactions, calibration of analytical instruments, improvement of the photostability of solar cells). These datasets form the basis of Bayesian neural network models that can be used to simulate these experiments via OLYMPUS. These simulated experiments will be used for benchmarking the 20 algorithms present within the package.

The study will be conducted in three stages. Within each stage, 20 optimisation algorithms will be tested against the 10 OLYMPUS data sets. These algorithms are present within OLYMPUS as "Planners", via a standardized Python interface. We will repeat the simulated experiments 100 times to collect significant statistics. The performance of the algorithms will be measured by using standard performance metrics in optimization. One example a metric is the 'cumulative regret', which measures the rate at which the algorithms managed to improve upon the best solutions found. Another metric will measure how far from the true optimum the best solutions discovered by the algorithms are.

In the first stage, the simulations will be run without the introduction of artificial noise, emulating an ideal experimental scenario. The obtained results will be used to identify the algorithm that is capable of providing the best solutions in the least number of steps.

In the second stage, different levels of noise will be introduced into the (simulated) experimental measurements (e.g., the reaction yield). The results obtained from running these simulations will be used to evaluate the robustness of these algorithms against output noise.

Similar to the second stage, in the third stage, different levels of noise will be introduced into the data that corresponds to the inputs, i.e., the experimental conditions determining the outcome of the experiments (e.g., temperature and catalyst concentration). The results of these simulations will be used to evaluate the robustness of the ML algorithms against input noise.

Random noise will be introduced artificially, so to have full control over the amount of noise injected, which will allow us thorough statistical analysis. Due to the large number of simulations that have to be performed, the first three weeks will be devoted entirely to collecting statistical data and running simulations. The next 4 weeks will involve the statistical analysis of the collected data. The last week will involve the finalisation of benchmarking and the identification of recommendations for chemistry and materials science researchers intending to use ML algorithms to drive optimization in self-driving laboratories.

All of the stages can be completed in online mode and, even in an in-person setting, the approach will remain unchanged.

The training and planning prior to the research will include:

- Review of the planner classes and optimization algorithms present in OLYMPUS. This will allow me to familiarize with the theoretical aspects of optimization as well as the specific implementations.
- Review of the datasets present in OLYMPUS. This will allow me to understand the chemistry and materials science problems we are using as representative scientific tasks.
- Learning how to access the datasets, planners and emulators via the low-level interface of OLYMPUS. As I will need fine control of OLYMPUS, it is important for me to be familiar with the lower-level aspects of the code.
- Planning the amount of noise that will be introduced to each dataset for each set of simulations. This will allow us to use realistic levels of noise in our benchmarks.
- Selection of metrics to be used to benchmark the planners. I will review the optimization literature to identify possible metrics in addition to cumulative regret and distance from the optimum.

Additionally, before the start of the project I will learn how to access the computing resources of the Aspuru-Guzik group remotely. This will involve familiarisation with ssh, git, and the Unix shell.

Outcomes

The immediate and foremost outcome of this research will be increased knowledge and understanding of the robustness of optimisation algorithms towards specific research and data conditions. Based on the results of this research, I will prepare a set of guidelines for chemists and material scientists to help them make informed choices about the most suitable optimisation algorithms given their optimisation task and experimental conditions. This will guide a chemist's decisions as to which algorithm will be most efficient towards the optimization task that has to be solved, leading to faster, efficient and goal-oriented optimization. Ultimately, this work will impact the vision and development of autonomous laboratories, including their robotic structure, applications of optimisation algorithms and ML models.

Research Advisor

Alán Aspuru-Guzik is a professor of chemistry and computer science at the University of Toronto, the Canada 150 Research Chair in Theoretical Chemistry, a CIFAR AI chair, and a Fellow of the Vector Institute for AI. His work is at the interface of chemistry and computer science and he is a pioneer of AI-driven autonomous chemical laboratories. Prof. Aspuru-Guzik will supervise the research and will correspond every three weeks (including the beginning and end of the project) to discuss progress and findings. In addition, Dr. Matteo Aldeghi, a senior postdoc in the Aspuru-Guzik group, will be guiding the training and planning prior to the proposed start date. During the research period, Riley Hickman, a senior PhD student in the Aspuru-Guzik group, will be providing regular (weekly) supervision as well as day-to-day technical assistance.

References

1. Florian Häse et al. ‘Next-Generation Experimentation with Self-Driving Laboratories’ Accessed: January 10th, 2021 [Online] Available: https://www.sciencedirect.com/science/article/pii/S258959741930019X
2. Florian Häse, Matteo Aldeghi et al. ‘Olympus: a benchmarking framework for noisy optimization and experiment planning’ Accessed: January 10th, 2021 [Online] Available: https://iopscience.iop.org/article/10.1088/2632-2153/abedc8/meta
3. Stefan Langner et al. ‘Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems’ Accessed: January 10th, 2021 [Online] Available: https://onlinelibrary.wiley.com/doi/full/10.1002/adma.201907801