The Journal of Open Source Software

Odyssey

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DOI: 10.xxxxxx/draft

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Submitted: 06 February 2025
Published: unpublished

Summary

Bayesian optimisation (BO) is a popular approach for the optimisation of complex black-box functions and hyperparameters.(Frazier, 2018) Conceptually, BO involves fitting a surrogate model to observed data and then optimising an acquisition function that uses the surrogate to estimate the most beneficial points in the parameter space to sample for maximising or minimising the underlying objective function. By repeating the process of evaluating suggested points and updating the model, an optimal solution can be rapidly converged even in high-dimensional input spaces where alternatives such as grid sampling become prohibitively inefficient. Typically, a gaussian process is used as the surrogate model since it provides readily accessible uncertainties which are leveraged by the acquisition function in balancing the exploration of unobserved regions of the parameter space with the exploitation of known high-value regions.

In recent years, a notable application of BO has been in the chemical sciences where it has been applied for optimising the performance of materials and catalysts.(Shields et al., 2021; Wu et al., 2024) In particular, BO methods are typically the brains behind self-driving laboratories, which aim to accelerate materials discovery through a paradigm shift away from the slow trial-and-error approach that has traditionally been the basis of materials design and optimisation.(Tom et al., 2024)

Statement of need

Recent interest in BO has sparked the development of numerous software packages, each offering various acquisition functions, surrogate models, and Gaussian Process kernels, along with advanced methods like multi-fidelity and multi-objective optimization, and the handling of categorical, discrete, and numerical parameters. However, the lack of a standardized interface creates a significant barrier for using multiple BO packages seamlessly, which deters users from exploring and selecting the best method for the task.

Odyssey addresses this challenge as an open-source Python package designed to streamline the application of BO through providing a comprehensive framework that allows for the addition of new optimization algorithms, each with their unique underlying principles, while maintaining a consistent implementation approach. Popular BO methods for materials science are available out-of-the-box including BOTorch, BayBE, and SMAC3. Future work will develop a user-friendly GUI that can be used without any programming experience and further tutorials that guide users through setting up and running custom BO experiments.

References

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