Newcastle University

Open Research Case Study

NUBO – an open-source AI framework for optimisation

[1]Mike Diessner, [2]Kevin Wilson, [3]Richard Whalley

[1] PhD Candidate in Computing.. [2]Reader in Applied Statistics. [3]Senior Lecturer in Engineering.

Introduction and research context

Whenever air flows over an aircraft, a thin layer of turbulence is generated close to its surface that is responsible for over half of its energy consumption. Taming this turbulence reduces energy consumption and leads to monetary, environmental, and public health benefits due to reduced fuel costs and emissions. For context, just a 3% reduction in the turbulent forces acting on a long-range aircraft would save £1.2M in fuel and prevent the release of 3,000 tonnes of carbon dioxide per year [1]. With around 23,600 aircraft around the world, this is a billion-pound problem.

The Fluid Dynamics Lab at Newcastle University aims to find a solution to this problem by developing sensors and actuators through experiments in the wind tunnel. These experiments are expensive and complex as turbulence is a highly non-linear and multi-variable phenomenon. Hence, finding optimal parameters requires an advanced optimisation algorithm.

I am a postgraduate researcher at the Cloud Computing for Big Data CDT and have been developing methods and tools to optimise expensive black-box functions, such as physical experiments or computer simulators, for the past two years. In that time, we published two articles in open-access journals [2, 3] and released an open-source AI framework called NUBO along with a dedicated website1 and a preprint of our latest paper [4] offering rigorous documentation, guidance, and case studies.

Open research practices

Expensive black-box problems are encountered across many disciplines motivating us to make our tools and methods accessible to as many researchers as possible. To that end, we have used several open research practices. Firstly, we released NUBO, **an open-source software package**, whose code is completely and freely available online at our GitHub repository2. It can be installed from the Python Package Index (PyPI) and focuses on transparency and accessibility via thorough documentation, references, and commented code. NUBO has been downloaded over 1,000 times within the first four weeks of its release. All dependencies are completely open-source and NUBO can be run online without any requirements, e.g. with Google Colab3.

Secondly, we published our investigation into the underlying algorithms in an **open-access journal** [2] with all data available from our GitHub repository4 to enable the verification of our results. Furthermore, we collaborated with Imperial College London to optimise an expensive computer simulator and published the results in another open-access journal [3].

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[1] https://nubopy.com

[2] https://github.com/mikediessner/investigating-BO

[3] https://colab.research.google.com/

[4] https://github.com/mikediessner/nubo

Thirdly, while our reference paper detailing all of NUBO's functionalities and capabilities is in review with an open-access journal, we made the paper available to the scientific community by publishing a **preprint** [4] on the open-access archive arXiv.

Finally, we published a **website**[5] offering thorough documentation of NUBO, including references and detailed explanations for all implemented algorithms and objects, a "getting started" guide aimed at non-experts, an ever-growing list of practical considerations, and many use cases.

Challenges, benefits, and lessons learned

Following open research principles generated additional costs in time and resources. For example, providing data and code with our publication required it to be formatted, commented, and uploaded to an openly available online repository. Furthermore, as more people can read and scrutinise our work, we spent more time double and triple-checking it (which is, of course, a good thing). In addition, publishing NUBO required deciding on a licence to use. This was completely new to us and we had to consult the University to decide.

Publishing NUBO as an open-source software package makes it accessible to the largest number of researchers and professionals. This allows them to optimise their problems and share their code with others, increasing scientific exchange and reproducibility. Making all contributions openly available minimises gate-keeping that often occurs when proprietary software is hidden behind a paywall. The licence also allows others to build upon NUBO to advance their projects in academia and industry. For ourselves, following open research practices increased the rigour and quality of our research, enabled future collaborations (e.g. the University of York approached us to optimise their experiments, with potential joint publications in the future), and made our research more trustworthy.

Conclusion

We have published an open-source software package along with two publications in scientific open-access journals with another one on the way (currently available as a preprint), and a website with rigorous documentation and guides. The increased time and resources we put into our work to follow open research principles paid off manyfold. Making NUBO freely available is not only beneficial for the wider academic community but has also opened new opportunities for us and our future research.

References

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[3] O'Connor J, Diessner M, Wilson K, Whalley RD, Wynn A, Laizet S (2023). "Optimisation and Analysis of Streamwise-Varying Wall-Normal Blowing in a Turbulent Boundary Layer." Flow, Turbulence and Combustion, pp. 1–29. doi:10.1007/s10494-023-00408-3.

[4] Diessner M, Wilson K, Whalley RD (2023). "NUBO: A Transparent Python Package for Bayesian Optimisation." arXiv preprint arXiv:2305.06709. doi:10.48550/arXiv.2305.06709.

[5] https://nubopy.com