Active Learning Scheme vs Conventional Optimization - developing a Python Framework

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Our project aims at efficiently solving the multi-objective optimization problem of getting a favorable chemical composition for permanent magnets which also yields the required physical properties.

In our case, the main effort required in this multi-objective optimization is the computation of a micro-magnetic simulation for each chemical composition. To reduce the computational effort we use a machine learning model as surrogate model to navigate through the design space to identify the most promising chemical compositions. This approach of combining machine learning and conventional optimization is called active learning scheme. Hence, we only need to simulate a few promising candidates along a Pareto-front which is updated in each iteration of the active learning scheme. The active learning scheme can save a lot of time and computational effort and prove very useful in recent research [1, 2, 3].

In order to solve the problem computationally and to build a basis for the optimization of other multi-objective optimization problems, we also develop an active learning scheme-Framework in Python. It allows building an active learning scheme with easily replaceable modules such as the machine learning model, the optimization algorithm or the initial data set. The software focuses on modularity, generalization and user-friendliness. This Python framework is built on top of the Pymoo library (version 0.6) [4], which provides a rich set of functionality for multi-objective optimization problem handling. The framework borrows and inherits many functions from Pymoo, and extends its capabilities by providing an interface to machine learning models to develop an active learning scheme.

Currently, the active learning scheme software in the proof-of-concept phase and so far we tested it on several test problems. We could verify that we can save up to 99 percent of computationally expensive simulations for convergence with a Design Space Tolerance of 5 percent.

Acknowledgements The financial support by the Austrian Federal Ministry of Labour and Economy, the National Foundation for Research, Technology and Development and the Christian Doppler Research Association is gratefully acknowledged.

References

[1] Alexander Kovacs et al: Physics-informed machine learning combining experiment and simulation for the design of neodymium-iron-boron permanent magnets with reduced critical-elements content. Frontiers in Materials, vol. 9 (2023).

[2] Hayate Yamano et al: Efficient optimization approach for designing power device structure using machine learning. Japanese Journal of Applied Physics, 62 SC1050 (2023).

[3] Auralee Edelen et al: Machine Learning for Orders of Magnitude Speedup in Multi-Objective Optimization of Particle Accelerator Systems. Phys. Rev. Accel. Beams 23, 044601 (2020).

[4] J. Blank and K. Deb, pymoo: Multi-Objective Optimization in Python, in IEEE Access, vol. 8, pp. 89497-89509, 2020,