Benchmarking Optimization & Supervised Machine Learning Methods

Objectives

Understand potential of machine learning (ML) algorithms for calibrating computationally expensive energy density functionals using parallel computing resources given:

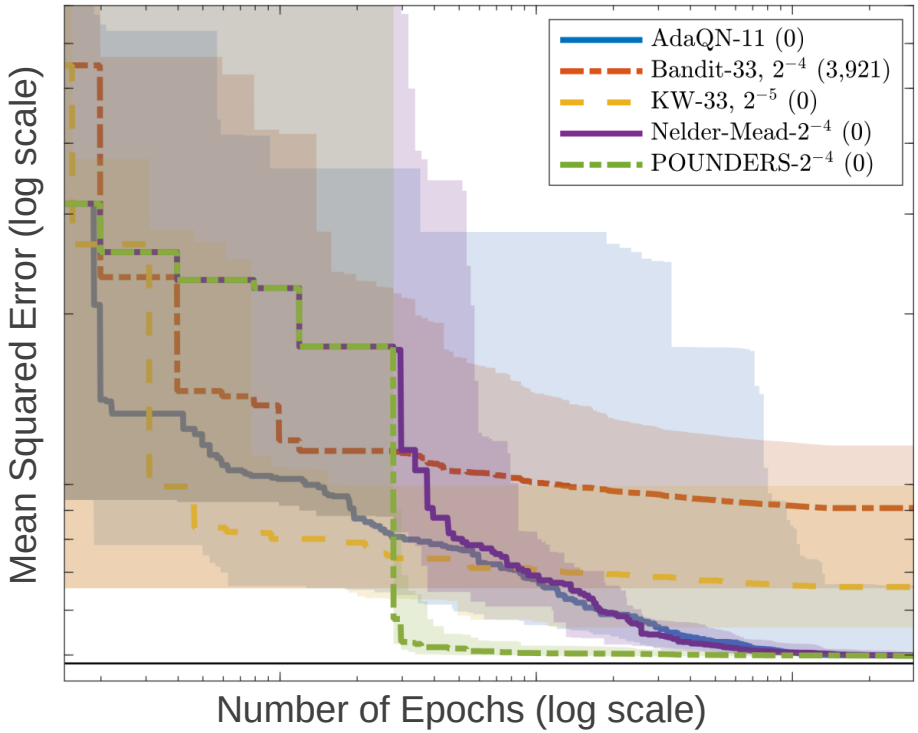
- Available training/experimental data (100s) much smaller than flagship ML uses (millions+)
- Derivatives are not available

Impact

- Reveals that targeted optimization methods typically outperform zeroth-order ML methods when little data are available for training computationally expensive nuclear physics models
- Provides actionable guidelines and directions for future research for leveraging parallel physics simulations in an energy-efficient manner
- Excellent results when applied to calibration of Fayans energy density functionals

Accomplishments

Publication: Bollapragada et al., *J. Phys. G:* **48** 024001 (2021)



Performance of best-tuned variants on an instance of calibrating the Fayans energy density functional. Solid lines indicate median performance; transparent bands indicate 25th-75th quantile performance. Best solutions are found in the allotted budget by POUNDERS; randomized methods achieve early reductions.