Benchmarking and Optimization of UF3 Machine Learning Potential on Solids

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Ab initio calculations offer a promising theory-guided approach to materials discovery and design. Still, ab initio calculations are hindered by their computational cost, limiting the complexity of materials they can evaluate. Machine learning potentials (MLPs) have recently shown their utility in Molecular Dynamic simulations, reaching accuracies comparable to ab initio simulations at a fraction of the computational cost. This work which uses linear regression with a cubic B-spline basis to evaluate effective two- and three-body potentials — on elemental systems. We find that UF_3 has an accuracy comparable to that of benchmarks the recently published Ultra-Fast Potential (UF_3) —GAP, MTP, NNP(Behler Parrinello), and qSNAP MLPs while being two to three orders of magnitude faster. Apart from speed, another advantage of the UF_3 framework is its ability to visualize the learned two- and three-body potentials, helping identify possible "holes" in the learned potential. We perform extensive hyper- parameter (HP) optimization. For this, we separate HPs into inner and outer ones according to their computational cost. We then combine grid search on inner HPs with optimization algorithms from the Ray Tune library, leading to accurate and smooth potentials.