Converging the Infeasible: Machine Learning and Renormalization in Multiple scattering Simulations

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Abstract

Multiple scattering theory (MST) is a cornerstone for modeling spectroscopies such as photoemission, X-ray absorption, and electron diffraction. Despite its utility, MST simulations encounter significant computational bottlenecks, particularly in the low-energy regime (10–400 eV), where series expansions often diverge due to the spectral radius of the τ-matrix exceeding unity. While matrix inversion (MI) methods yield exact solutions, they are computationally prohibitive and constrained by storage limitations, especially for large systems.

To address these challenges, we propose integrating Bayesian optimization [1], a machine learning technique, with series expansion renormalization schemes [2] to enhance the convergence of MST series expansions. Renormalization, as introduced by Sébilleau and Natoli [3], mitigates divergence by reducing the spectral radius while maintaining accuracy. Bayesian optimization is employed to efficiently determine the optimal renormalization scheme and the corresponding parameter (e.g., ω), minimizing the number of trials required.

We tested this approach on a small cylindrical cluster of copper (001) consisting of 6 atoms at 10 eV kinetic energy, where the initial spectral radius was 1.01. After 60 iterations, Bayesian optimization identified the Π_1 renormalization scheme with ω=0.429+0.229i, reducing the spectral radius to 0.51. This improvement reduced the required scattering order to just 4. Furthermore, we demonstrated the transferability of optimized parameters by applying them to a larger cluster of 336 atoms. Despite the larger system's initial divergence (spectral radius = 1.13), the optimized parameters reduced the spectral radius to 0.87, enabling convergence and eliminating the need for re-optimization.

These results highlight significant reductions in computational time and memory requirements, making it feasible to simulate larger systems and complex phenomena in condensed matter physics. By coupling renormalization schemes with Bayesian optimization, this work offers a scalable and robust framework for modeling structural, electronic, and magnetic properties in materials science.

References

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