

Prediction of Density Matrix with Machine Learning

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ABSTRACT

The convergence of electronic structure calculations either Hartree-Fock (HF) or Kohn-sham density functional theory (KS-DFT) heavily depends on an initial guess for molecular orbitals (MO). In practice, these methods (HF or DFT) solve eigenvalue equations iteratively and aim to obtain the correct MO. For these approaches, typically this self-consistent algorithm (SCF) starts with an initial guess of the density matrix (DM) and then solves the eigenvalue equation iteratively until the solution reaches the desired convergence. The quality of an initial guess has a significant impact on the outcome of the SCF algorithm. If the quality is close to the converged density matrix, the SCF process will require a small number of iterations to converge, hence effectively the entire HF/DFT calculations can be accelerated. In this study, we established a machine learning (ML) predicted initial guess for DM, which can be an indomitable entity to speed up the SCF procedure compared to any other familiar guesses. The used theory framework is DFT. Furthermore, we applied this ML-based approach to generate the inter-atomic forces for AIMD (Ab-initio Molecular dynamics) simulations, to see whether this ML guess can allow us to bypass the SCF procedure [1].

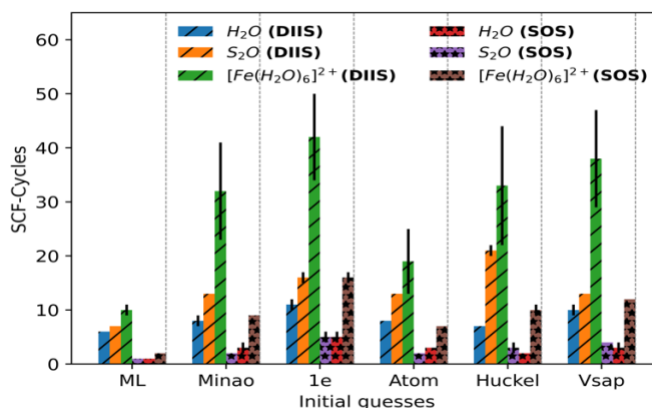


Figure 1 : This figure represents the average number of SCF steps were required to achieve the convergence for different initial guesses. X-axis reflects known guesses and Y is for the number of iterations.

References

- [1] Hazra S; Patil U; Sanvito S. Predicting The One-Particle Density Matrix With Machine Learning, arXiv: 2401.06533 (2024).