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Testing Machine Learning Methods on Density Functional Theory and Simple Toy Model[1] KEVIN VU, JOHN SNYDER, KIERON BURKE, University of California, Irvine — Kohn-Sham density functional theory (KS-DFT) is a ubiquitous electronic structure method characterized by its relatively high accuracy and low computational cost. However, deficiencies in KS-DFT hamper its efficacy and thus present ongoing avenues of research. The application of machine learning (ML) to KS-DFT is a novel approach which can potentially circumvent many of the drawbacks inherent in KS-DFT. To explore ML's efficacy, we tested it on a simple toy function to see how well our model performed. We examined the dependence of the ML model on the different parameters of the problem and noted how the error of the model responded to changes in each. We also tested the method on the density functional of the standard 1D particle in a box system in order to observe how effective it was in yielding the correct energies. The results showed that ML consistently provided an accurate approximation to the exact functions, demonstrating great promise for the viability of our method. Future efforts will focus on refining the method and continuing to clarify the relationships between the parameters and the ML error.

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Kevin Vu
University of California, Irvine

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