

Machine Learning the External Potential

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ABSTRACT

Within the DFT framework, complete description of a molecular system is provided by the number of electrons and the exact external potential. In the absence of its exact functional form, a forest of approximations and parametrisations grew, each suited to specific chemistry but none universally reliable. In these, the densities and energies are obtained through numerical procedures until the self-consistency is achieved. Here, we present an alternative path toward the electron density *via* fitting the exact external potential to that expanded in a chosen molecular basis set. Using QM7b dataset, we train a machine learning model to predict the electron density matrix and, thus, the electronic energy from this basis-set-expanded external potential (Fig. 1). We discuss the implementation and performance of this approach for selected test sets.

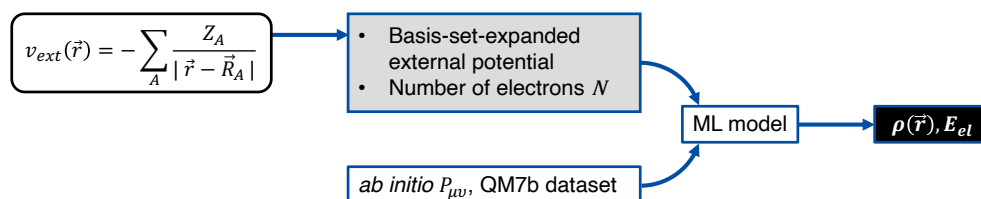


Figure 1. Predicting exact density from fitted external potential, expanded in a molecular basis set.