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Fully-connected Neural Network for Orbital-free DFT: Exact Conditions and Non-local Information

Density Functional Theory (DFT) is one of the most successful methods for computing ground-state properties of molecules and materials. In its purest form ("orbital-free DFT"), it transforms a $3N$-dimensional interacting electron problem into one 3D integro-differential problem at the cost of approximating two functionals of the electron density $n(\mathbf{r})$, one of them being for the kinetic energy $T_s[n]$. Accurate approximations for this functional are currently missing, and in particular non-local contributions must be considered. Since ML approaches are good at handling non-locality and complex functional relationships, we started with a Fully-connected Neural Network (FNN) to model a semi-local expression for $T_s[n]$. FNN is simple but suitable for the purposes of maintaining the semi-local functional efficiency (linear scaling with the number of grid points) and achieve linear scaling for orbital-free DFT. We then further introduced exact physical conditions into the cost function and observed excellent agreement with exact kinetic energies in a 2-electron model system. Also, to include non-local information during the training for homonuclear diatomic molecules, we used additional information from the isolated atoms (such as their kinetic energy densities) and obtained energies that were comparable to those from the best semi-local analytical functionals (APBEK and rAPBEK) for a wide range of organic molecules.

Focus areas

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