Using Neural Networks to Learn Kinetic Energy Functional and Many-body Energy

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Many researches have been done to construct accurate kinetic energy functionals so that linear-scaling orbital-free DFT can be implemented. Here, instead of deriving analytically, we trained convolutional neural network trained to reproduce the Kohn–Sham kinetic energy of hydrocarbons from an input electron density. The output of the network is used as a nonlocal correction to conventional local and semilocal kinetic functionals. We show that this approximation qualitatively reproduces Kohn–Sham potential energy surfaces when used with conventional exchange correlation functionals. The density which minimizes the total energy given by the functional is also examined. We also examine the features in the density learned by the neural network to anticipate the prospects of generalizing these models.

The many-body energies in the many-body expansion (MBE) are often obtained via ab initio calculation. The number of many-body terms will increase tremendously with the total number of monomers in the cluster, which makes it difficult to be applied to large clusters (hundreds of monomers). In our work, we trained neural networks to learn the many-body energies of methanol so that the total energy of a large cluster can be derived from the MBE formula. We shows that our accuracy is comparable with ab initio method and thousands of many body energies can be evaluated in just seconds on GPU, which makes it possible to apply the MBE to large clusters. We also find that the permutation and rotation invariance can be achieved by augmenting the trained database.