Quantum flows neural network for variational solutions of the Schrödinger equation

Content

The computational technology of highly expressive parametric neural-network-functions has allowed machine learning to make a major foray into disciplines of natural sciences. The neural network functions may be effectively "fitted" to a loss function, given in the form of a variational principle or virial theorem, to provide solutions to quantum mechanical problems. Recently, a few deep neural network models for solving the electronic Schrödinger equation were developed [1-3], demonstrating both outstanding computing efficiency and accurate results.

Here, we present a new quantum-flow-neural-network approach for obtaining variational solutions of the Schrödinger equation. At the core of the method is an invertible neural network composed with the general basis of orthogonal functions [4], which provides a more stable framework for simultaneous optimization of the ground state and a lot of excited states. We apply our approach to calculations of the vibrational energy levels of polyatomic molecules as well as of electronic energies in a single-active-electron approximation. The results show a considerable improvement of variational convergence for the ground and the excited states.

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