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Ab initio solution of the many-electron Schrödinger equation with deep neural networks

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Given access to accurate solutions of the many-electron Schrödinger equation, nearly all chemistry could be derived from first principles. Exact wave functions of interesting chemical systems are out of reach because they are NP-hard to compute in general, but approximations can be found using polynomially scaling algorithms. The key challenge for many of these algorithms is the choice of wave function approximation, or Ansatz, which must trade off between efficiency and accuracy. Neural networks have shown impressive power as accurate practical function approximators and promise as a compact wave-function Ansatz for spin systems, but problems in electronic structure require wave functions that obey Fermi-Dirac statistics. Here we introduce a novel deep learning architecture, the Fermionic neural network, as a powerful wave-function Ansatz for many-electron systems. The Fermionic neural network is able to achieve accuracy beyond other variational quantum Monte Carlo Ansatz on a variety of atoms and small molecules. Using no data other than atomic positions and charges, we predict the dissociation curves of the nitrogen molecule and hydrogen chain, two challenging strongly correlated systems, to significantly higher accuracy than the coupled cluster method, widely considered the most accurate scalable method for quantum chemistry at equilibrium geometry. This demonstrates that deep neural networks can improve the accuracy of variational quantum Monte Carlo to the point where it outperforms other ab initio quantum chemistry methods, opening the possibility of accurate direct optimization of wave functions for previously intractable many-electron systems.