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Approximating Many-Electron Wave Functions using Neural Networks

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Exact wave functions of molecules and solid-state simulation cells containing more than a few electrons are out of reach because they are NP-hard to compute in general, but approximations can be found using polynomially scaling algorithms. A key challenge in many such approaches is the choice of an approximate parameterized wave function, which must trade accuracy for efficiency. Neural networks have shown impressive power as practical function approximators and promise as a way of representing wave functions for spin systems, but electronic wave functions have to obey Fermi-Dirac statistics. This talk describes a deep learning architecture, the Fermionic neural network, which is capable of approximating many-electron wave functions and greatly outperforms conventional approximations. Applications to a range of problems in molecular chemistry and solid-state physics will be discussed.

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