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Approximating Many-Electron Wave Functions using Neural Networks

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The use of neural networks for approximating fermionic wave functions has become popular over the past few years as their ability to provide impressively accurate descriptions of molecules, nuclei, and solids has become clear.

Most electronic structure methods rely on uncontrolled approximations, such as the choice of exchange-correlation functional in density functional theory or the form of the parameterized trial wavefunction in conventional quantum Monte Carlo simulations. Neural wave functions, on the other hand, are built from multilayer perceptrons, which are universal approximators. The network weights and biases that define a neural wave function may be optimized efficiently by combining variational Monte Carlo methods with automatic gradients calculated using back propagation. This approach produces results of consistent quality across highly diverse systems. In some cases, the variational optimization is capable of discovering quantum phase transitions unaided.

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