Using Machine Learning to Solve the Schrodinger Equation of Electronic Systems

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ABSTRACT

The most enthusiastic modeler claims to accurately predict chemical reaction thermodynamics, kinetics, and nonequilibrium dynamics. Unfortunately, current models, while more robust and predictive than in past years, are often either too approximate to provide a faithful representation of reality or too computationally expensive to yield answers within a reasonable time. The talk argues that it is imperative to develop new-generation electronic structure methods to aid experiments, as these face different yet similarly difficult circumstances. The talk introduces electronic structure models based on machine learning. It is argued that machine learning methods are best employed learning quantities rich in information, such as the electron density, density matrix, or even the wavefunction. These models are inherently more useful than those targeting single quantities such as energy, dipole, etc. Models for the one-electron density matrix of small to medium sized molecules are presented and the crucial role of imposing N-representability conditions is discussed. We also present methods to learn two-electron density matrices as a route for accounting for electronic correlation explicitly at low computational cost. The methods are available to the broader community as open-source Python implementations in the QMLearn software, http://qmlearn.rutgers.edu.