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Accelerating Quantum Chemistry Calculations: Machine Learning for Efficient Evaluation of Electron-Repulsion Integrals

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Abstract : A crucial objective in quantum chemistry is the computation of the energy levels of chemical systems. This task requires electron-repulsion integrals as inputs, and the steep computational cost of evaluating these integrals poses a major numerical challenge in efficient implementation of quantum chemical software. This work presents a moment-based machine-learning approach for the efficient evaluation of electron-repulsion integrals. These integrals were approximated using linear combinations of a small number of moments. Machine learning algorithms were applied to estimate the coefficients in the linear combination. A random forest approach was used to identify promising features using a recursive feature elimination approach, which performed best for learning the sign of each coefficient but not the magnitude. A neural network with two hidden layers were then used to learn the coefficient magnitudes along with an iterative feature masking approach to perform input vector compression, identifying a small subset of orbitals whose coefficients are sufficient for the quantum state energy computation. Finally, a small ensemble of neural networks (with a median rule for decision fusion) was shown to improve results when compared to a single network.

Keywords : quantum energy calculations, atomic orbitals, electron-repulsion integrals, ensemble machine learning, random forests, neural networks, feature extraction
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