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Deep Wavelet Scattering for Quantum Energy Regression[1]

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Physical functionals are usually computed as solutions of variational problems or from solutions of partial differential equations, which may require huge computations for complex systems. Quantum chemistry calculations of ground state molecular energies is such an example. Indeed, if x is a quantum molecular state, then the ground state energy $E_0(x)$ is the minimum eigenvalue solution of the time independent Schrödinger Equation, which is computationally intensive for large systems. Machine learning algorithms do not simulate the physical system but estimate solutions by interpolating values provided by a training set of known examples $\{(x_i, E_0(x_i)\}_{i \leq n}$. However, precise interpolations may require a number of examples that is exponential in the system dimension, and are thus intractable. This curse of dimensionality may be circumvented by computing interpolations in smaller approximation spaces, which take advantage of physical invariants. Linear regressions of E_0 over a dictionary $\Phi = \{\phi_k\}_k$ compute an approximation $\widetilde{E}_0$ as: $\widetilde{E}_0(x) = \sum_k w_k \phi_k(x)$, where the weights $\{w_k\}_k$ are selected to minimize the error between E_0 and $\widetilde{E}_0$ on the training set. The key to such a regression approach then lies in the design of the dictionary Φ. It must be intricate enough to capture the essential variability of $E_0(x)$ over the molecular states x of interest, while simple enough so that evaluation of $\Phi(x)$ is significantly less intensive than a direct quantum mechanical computation (or approximation) of $E_0(x)$. In this talk we present a novel dictionary Φ for the regression of quantum mechanical energies based on the *scattering transform* of an intermediate, approximate electron density representation ρ_x of the state x. The scattering transform has the architecture of a deep convolutional network, composed of an alternating sequence of linear filters and nonlinear maps. Whereas in many deep learning tasks the linear filters are learned from the training data, here the physical properties of E_0 (invariance to isometric transformations of the state x, stable to deformations of x) are leveraged to design a collection of linear filters $\rho_x * \psi_\lambda$ for an appropriate wavelet ψ. These linear filters are composed with the nonlinear modulus operator, and the process is iterated upon so that at each layer stable, invariant features are extracted: $\phi_k(x) = \| ||\rho_x * \psi_{\lambda_1}| * \psi_{\lambda_2}| * \cdots * \psi_{\lambda_m} \|, \quad k = (\lambda_1, \ldots, \lambda_m), \ m = 1, 2, \ldots$ The scattering transform thus encodes not only interactions at multiple scales (in the first layer, $m = 1$), but also features that encode complex phenomena resulting from a cascade of interactions across scales (in subsequent layers, $m \geq 2$). Numerical experiments give state of the art accuracy over data bases of organic molecules, while theoretical results guarantee performance for the component of the ground state energy resulting from Coulombic interactions.

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