Wavelet Scattering Regression of Quantum Chemical Energies

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Abstract

We introduce multiscale invariant dictionaries to learn quantum chemical energies of organic molecules, from training data bases. Molecular energies are invariant to isometric atomic displacements, and are Lipschitz continuous to molecular deformations. Similarly to density functional theory, the molecule represented by an electronic density function. A multiscale invariant dictionary is calculated with wavelet scattering invariants. It cascades a wavelet transforms which separate molecular scales and compute interactions across scales. Sparse scattering regressions give state of the art results over data bases of organic molecules, with errors in the range of density functional theory softwares.