High-Dimensional Learning Rather Than Computing in Quantum Chemistry

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Physical functionals are usually computed as solutions of variational problems or from solutions of PDE, which may require huge computations for complex systems. Quantum chemistry calculations of large molecule energy is an example. Learning strategies do not simulate the physical system but estimate solutions by interpolating values provided by a training set of known examples. However, precise interpolations may require a number of examples which is exponential in the system dimension, and are thus untractable. This curse of dimensionality may be avoided by computing interpolations in smaller approximation spaces, which take advantage of physical invariants. We introduce deep multiscale learning architectures, which compute such invariant approximations, with iterated wavelet transforms. Numerical applications are shown for molecule energies in quantum chemistry, in relation with Density Functional Theory.