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 partial differential equations, which may require huge computations for complex systems. Quantum chemistry calculations of molecular ground state energies is such an example. Machine learning algorithms 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 that is exponential in the system dimension, and are thus intractable. 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 in a similar vein to deep neural networks, which compute such invariant approximations via iterated wavelet transforms. Theoretical results relating these architectures to the Coulomb potential from classical physics will motivate numerical applications for molecular energies in quantum chemistry, in relation with Density Functional Theory.

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