Three Dimensional Deep Learning and Many Body Physics

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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 many body problems, including those in quantum chemistry and materials science, are such examples. 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. Tractable algorithms compute interpolations in low dimensional approximation spaces, which leverage the underlying physical properties of the system.

In this talk we present a type of multiscale, multilayer convolutional network, called a wavelet scattering transform, for the regression of potential energies in many body physics. Through a cascade of multiscale wavelet filters and nonlinearities, this transform encodes the appropriate physical invariants and regularity properties of the physical system, and obtains regression errors on the order of quantum mechanical simulations, but at a fraction of the cost.