MATTHEW HIRN, Michigan State University

Learning many body physics via wavelet scattering transforms

Deep learning algorithms are making their mark in machine learning, obtaining state of the art results across computer vision, natural language processing, auditory signal processing and more. A wavelet scattering transform has the general architecture of a convolutional neural network, but leverages structure within data by encoding multiscale, stable invariants relevant to the task at hand. This approach is particularly relevant to data generated by physical systems, as such data must respect underlying physical laws. We illustrate this point through many body physics, in which scattering transforms can be loosely interpreted as the machine learning version of a fast multipole method (FMM). Unlike FMMs, which efficiently simulate the physical system, the scattering transform learns the underlying physical kernel from given states of the system. The resulting learning algorithm obtains state of the art numerical results for the regression of molecular energies in quantum chemistry, obtaining errors on the order of more costly quantum mechanical approaches.