THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS
STUDENT SEMINAR

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Efficient Long-range Convolutions for Point Clouds in Deep Learning

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Jones Laboratory, Room 303

ABSTRACT

The efficient treatment of long-range interactions for point clouds is a challenging problem in many scientific machine learning applications. To extract global information, one usually needs a large window size, a large number of layers, and/or a large number of channels. This can often significantly increase the computational cost. In this work, we present a novel neural network layer that directly incorporates long-range information for a point cloud. This layer leverages the convolutional theorem coupled with the non-uniform Fourier transform. The resulting global all-to-all convolution operation can be performed in nearly-linear time asymptotically with respect to the number of input points. This layer is a particularly powerful tool when combined with local convolution as together they offer efficient and seamless treatment of both short- and long-range interactions. We showcase this framework by introducing a neural network architecture that combines LRC-layers with short-range convolutional layers to accurately learn the energy and force associated with a N-body potential. We also exploit the induced two-level decomposition and propose an efficient strategy to train the combined architecture with a reduced number of samples.