Tensor Networks in Scientific Machine Learning

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Abstract: This project will address one of the biggest challenges in computational science: how to deal with extremely high-dimensional data. From high-dimensional partial differential equations to large-scale eigenvalue problems, the project aims to devise compressed representations for data and utilize them within exceedingly efficient downstream solvers. The methodology to be developed will offer more scalable alternatives to popular neural network representations of high-dimensional data and functions, with stronger mathematical guarantees and training based primarily on randomized numerical linear algebra rather than nonconvex optimization. The project's methodology will be drawn from the field of tensor networks, where high-order objects are encoded as contractions of several low-order objects. The first goal in the project will be to develop tensor network to tensor network solution operators for high-dimensional PDEs, through new tensor network structured neural networks. The other direction in the proposed work will be to explore, in collaboration with domain scientists, novel low-rank tensor ansatzes and algorithms for ground state energy calculations in quantum many-body systems. The project seeks to bring tensor networks into the mainstream of scientific machine learning.

The developed machinery will be applied to build novel tensor network to tensor network solution operators for PDEs, and to represent