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KEYNOTE: A General Message Belief Propagation Framework for Quantum Computations

Monday, November 20, 2023 9:00 AM (1 hour)

The core computational tasks in quantum systems are the computation of expectations of operators, including reduced density matrices, and the computation of the ground state energy of a quantum system. Many tools have been developed in the literature to achieve this, including Density Functional Theory (DFT), Density Matrix Renormalization Group (DMRG) and other Tensor Network methods, Variational Monte Carlo (VMC) and so on. Recently, some methods based on Machine Learning have also been pioneered such as FermiNet and PauliNet and other Neural Variational methods. In this work we will build a bridge between the rich Machine Learning literature on Loopy Belief Propagation and its generalizations for posterior inference and the above mentioned quantum computational tasks. It was shown recently that LBP can be used to contract Tensor Networks and compute Reduced Density Matrices. Here we generalize this concept to a new class of generalized LBP methods, known as Region Graph BP and as a particular example we implemented TreeEP. We show that a very general framework exists that encompasses both classical LBP and quantum LBP, which can be used to compute expectations as well as ground state energies and states. We hope that this work will encourage cross fertilization between these two fields.

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