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D. Sulz

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Time Integration in Quantum Dynamics using Tree Tensor Networks

This talk studies the numerical solution of high-dimensional tensor differential equations. The prohibitive computational cost and memory requirements of numerically simulating such equations are often referred to as the curse of dimensionality. Such prohibitively large differential equations arise in many fields of application such as plasma physics, machine learning, radiation transport, or quantum physics. Dynamical low-rank approximation offers a promising approach to overcome the curse by representing the high-dimensional tensors in a low-rank format and solving a projected differential equation on a low-rank manifold. The low-rank manifold considered in this talk is the manifold of tree tensor networks. The time integration of tree tensor networks requires the update of each low-rank factor. Several numerical schemes to compute this time integration are proposed in this thesis. All of these methods fall into the class of Basis Update and Galerkin (BUG) integrators, where all basis matrices are evolved through a small matrix differential equation and all core tensors by a Galerkin step. We present a rigorous error analysis of all integration schemes, demonstrating robustness with respect to small singular values. This is important since small singular values can lead to numerical instabilities as they correspond to high curvatures in the corresponding low-rank manifold. Remarkable properties like rank-adaptivity, parallelism, norm and energy preservation, and the diminishing of energy in gradient systems are discussed. Further, the representation of the right-hand side of a differential equation in tree tensor network format is discussed for a class of long-range interacting Hamiltonians. Efficient constructions of these tree tensor network operators are provided, and bounds on the maximal tree rank for an exact and approximated representation of the operator are discussed. Numerical experiments for problems from quantum physics verify theoretical results and investigate the applicability of dynamical low-rank approximation to many-body quantum systems in detail.