Continuous-time parametrization of neural quantum states for quantum dynamics

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Neural quantum states are a promising framework for simulating many-body quantum dynamics, as they can represent states with volume-law entanglement. As time evolves, the neural network parameters are typically optimized at discrete time steps to approximate the wave function at each point in time. Given the differentiability of the wave function stemming from the Schrödinger equation, here we impose a time-continuous and differentiable parameterization of the neural network by expressing its parameters as linear combinations of temporal basis functions with trainable, time-independent coefficients. We test this ansatz, referred to as the smooth neural quantum state (-NQS) with a loss function defined over an extended time interval, under a sudden quench of a non-integrable many-body quantum spin chain. We demonstrate accurate time evolution using simply a restricted Boltzmann machine as the instantaneous neural network architecture. Furthermore, we demonstrate that the parameterization is efficient in the number of parameters and the smooth neural quantum state allows us to initialize and evaluate the wave function at times not included in the training set, both within and beyond the training interval.

Tracking large chemical reaction networks and rare events by neural networks

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Stochastic reaction networks are widely used to model complex systems in various scientific fields, such as chemical kinetics, systems biology, and epidemiology, where randomness and discrete events play crucial roles. Solving the chemical master equation that governs these systems poses a significant computational challenge, especially in scenarios involving large state spaces and rare events. Previous work has demonstrated the potential of neural networks for approximating solutions to these equations, offering a flexible framework for modeling complex dynamics. We present a advancement in this approach by leveraging variational autoregressive neural networks, along with the implementation of more efficient optimizer to enhance training efficiency. These innovations improve the computational efficiency of our algorithm by at least tenfold, enabling us to track the dynamics of large stochastic reaction networks. Additionally, we incorporate enhanced sampling strategies to accurately track rare events, thereby expanding the range of problems that can be effectively addressed. The applications in challenging reaction networks, including the spatially extended reaction diffusion systems and the 16-species MAPK cascade network, demonstrate a reduction in computational cost while improving the accuracy of predictions over the previous neural-network method. The present approach thus enables more efficient modeling and simulation of stochastic reaction systems in general.