Machine-learning for quantum dissipative dynamics

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Accurate simulations of quantum dynamics in complex condensed-phase systems are our gateway to understanding many physical, chemical, and biological processes. Exact numerical simulations often require computational resources that scale exponentially with the number of simulated time steps and the size of the system. Approximate perturbative or quantum-classical methods are often only reliable at short simulation times, rendering such methods inapplicable to study long-time quantum phenomena. I will present several methods for simulating long-time dynamics of dissipative quantum systems, including physics-based and machine-learning-based approaches. Specifically, I will show how many different types of machine learning models including artificial neural networks and kernel ridge regression models can efficiently and accurately simulate complex quantum dynamics across different regimes. Best models considerably reduce the required computational time for long-time simulations with no compromise in accuracy providing new routes for simulating quantum dynamics for arbitrarily long times, starting with computationally feasible short-time dynamical information.