

SCD Colloquium

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Dynamical simulation via quantum machine learning with
provable generalization

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Dynamical simulations of quantum systems, processing data from quantum experiments, and quantum machine learning (QML) are three applications where quantum algorithms are expected to outperform classical methods. Moreover, such applications have the potential to transform our understanding of many-body quantum systems. While much attention has been paid to these fields independently, less attention has been paid to the potential of combining them. Here we discuss the possibility of using QML methods to develop algorithms for experimentally probing and simulating quantum systems. A central strategy, common to both goals, is to develop QML algorithms for learning circuit representations of quantum processes.

For such algorithms to have any chance of being successfully implemented on non-trivial problems any time soon, it's critical that their training data requirements are manageable. In this talk, we present a bound that ensures this. Namely, we establish out-of-distribution generalization for learning an unknown unitary using a quantum neural network and for a broad class of training and testing distributions. In particular, we show that one can learn the action of a unitary on entangled states using only product state training data. Since product states can be prepared using only single-qubit gates, this advances the near-term prospects of QML for learning quantum processes and further opens up new methods for the classical and quantum compilation of quantum circuits.

Based on these insights, we propose a QML-based algorithm for simulating quantum dynamics on near-term quantum hardware and rigorously prove its resource efficiency in terms of qubit and training data requirements. We also demonstrate the viability of this algorithm through numerical experiments, both in classical simulations and quantum hardware. Finally, we embed this algorithm in a broader framework for using QML methods for quantum dynamical simulation on NISQ devices.

The talk will focus on references: [arXiv:2204.10268](https://arxiv.org/abs/2204.10268) and [arXiv:2204.10269](https://arxiv.org/abs/2204.10269).