

Mathematics Colloquium



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Learning to predict ground state properties of gapped Hamiltonians

Classical machine learning (ML) provides a potentially powerful approach to solving challenging quantum many-body problems in physics and chemistry. However, the advantages of ML over traditional methods have not been firmly established. In this work, we prove that classical ML algorithms can efficiently predict ground-state properties of gapped Hamiltonians after learning from other Hamiltonians in the same quantum phase of matter. By contrast, under a widely accepted conjecture, classical algorithms that do not learn from data cannot achieve the same guarantee.

Our proof technique combines mathematical signal processing with quantum manybody physics and also builds upon the recently developed framework of classical shadows. I will try to convey the main proof ingredients and also present numerical experiments that address the anti-ferromagnetic Heisenberg model and Rydberg atom systems.

This is joint work with Hsin-Yuan (Robert) Huang, Giacomo Torlai, Victor Albert and John Preskill, see [Huang et al., Provably efficient machine learning for quantum many-body problems, Science 2022]