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# Applied Math Ph.D. Seminar

## Generalization Error Estimate of a Machine Learning Method for Solving High Dimensional Schrödinger Eigenvalue Problems

**Speaker:** Hao Yu (Chinese Academy of Sciences)

**Time:** 2025-05-22, 16:10 to 17:00

**Location:** Rm 1801, Guanghua East Tower

**Advisor:** Pingbing Ming (Chinese Academy of Sciences)

**Abstract:** The high-dimensional Schrödinger eigenvalue problem plays a crucial role in various fields, such as computational chemistry, condensed matter physics and quantum computing. Though classical numerical methods have achieved great success in solving low-dimensional PDEs and eigenvalue problems, a major challenge persists: the curse of dimensionality. Recently, significant progress has been made in applying deep neural networks to solve PDEs and Schrödinger eigenvalue problems. In this talk, we introduce a machine learning method for computing eigenvalues and eigenfunctions of the Schrödinger operator with Dirichlet boundary conditions. The eigenvalues are deep in the spectrum. The cut-off function technique is employed to construct trial functions that precisely satisfy the Dirichlet boundary conditions. This approach outperforms the standard boundary penalty method, as demonstrated by the numerical tests. Under the assumption that the eigenfunctions belong to a spectral Barron space, we derive a dimension-free convergence rate of the generalization error bound of the method, and all constants in the error bounds grow at most polynomially. This assumption is verified by proving a new regularity result for the eigenfunctions when the potential lies in an appropriate spectral Barron space. Moreover, we prove a sharp accumulation rate of the generalization error and extend the generalization bound to the normalized penalty method, which is widely used in practice.