



復旦大學
FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

Optimization of Neural Network Wavefunctions in Variational Monte Carlo

Speaker: Yuyang Wang (Chinese Academy of Sciences)

Time: 2026-09-17, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Advisor: Xin Liu (Chinese Academy of Sciences)

Abstract: Variational Monte Carlo (VMC) with neural network wavefunctions is a powerful approach to ground-state calculations, but its performance depends critically on wavefunction optimization. In this talk, we will introduce VMC and focus on geometry-aware optimization methods for neural network wavefunctions, in particular stochastic reconfiguration (SR) and its variants. Among them, SPRING, inspired by the randomized Kaczmarz method, has shown strong empirical performance but is sensitive to the choice of a momentum-like parameter μ . We analyze this sensitivity and reveal a qualitative difference between $\mu < 1$ and $\mu = 1$. For $0 \leq \mu < 1$, we establish first-order convergence under weak moment assumptions allowing heavy-tailed Monte Carlo noise; for $\mu = 1$, we construct counterexamples showing divergence through accumulation along kernel-related directions. Motivated by these results, we propose PRIME-SR, an adaptive SR method that adjusts the momentum parameter based on spectral information and subspace overlap. Numerical experiments show that PRIME-SR achieves performance comparable to well-tuned SPRING while substantially improving robustness in neural wavefunction optimization.