FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

NMR-Solver: automated structure elucidation via large-scale spectral matching and physics-guided fragment optimization

Speaker: Yongqi Jin (Peking University)

Time: 2026-05-07, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Advisor: Weinan E (Peking University)

Abstract: Nuclear Magnetic Resonance (NMR) spectroscopy is one of the most powerful and widely used tools for molecular structure elucidation in organic chemistry. However, the interpretation of NMR spectra to determine unknown molecular structures remains a labor-intensive and expertise-dependent process. Here, we present NMR-Solver, a practical and interpretable framework for the automated determination of small organic molecule structures from 1D NMR spectra. Our method introduces an automated framework for molecular structure elucidation, integrating large-scale spectral matching with physics-guided molecular optimization that exploits atomic-level structure spectrum relationships in NMR. Evaluated on literature data and real-world experiments, NMR-Solver shows strong generalization, robustness, and practical utility in real-life scenarios. By integrating computational NMR analysis, deep learning, and interpretable chemical reasoning into a unified system, it facilitates a scalable, automated, and chemically meaningful solution for inverse problems in molecular science.