

“Simulation-Based Inference for Parameter Identification in Complex Systems

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Training machine learning algorithms typically requires access to large datasets, yet in many scientific domains such datasets are scarce or difficult to obtain. One solution is to generate synthetic data through physics-based simulations, which can complement or substitute experimental measurements. A key challenge is how to construct such models, tune their baseline assumptions, and use them to generate large datasets that incorporate realistic noise and test–retest variability. Simulation-based inference (SBI) provides a framework for this process by combining simulated datasets with neural networks that learn mappings between parameters and observations. A critical step is validating the resulting inference networks. For spectral data, such as spectral data, conventional similarity measures like RMSE are often inadequate.

In this talk, I will introduce a workflow for developing a simulator, training SBI neural networks, tuning baseline models, and extending them to generate pathological outcomes representing large deviations from the baseline. I will then present a validation strategy that quantifies network performance using a system of complementary similarity measures and a majority-vote similarity index.

Thursday, September 25, 2025

4:00 - 5:20PM

MND1015

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