Spectral Estimation of the Koopman operator for Stochastic Reaction Networks

Ankit Gupta
Department of Biosystems Science and Engineering, ETH Zürich ankit.gupta@bsse.ethz.ch

Coauthor(s): Prof. Mustafa Khammash

Special session: Recent Advances in Monte Carlo Methods for Forward and Inverse Problems for Stochastic Reaction Networks, Parts I and II

Intracellular reaction networks are characterized by stochastic dynamics, often modeled as continuous-time Markov chains (CTMCs). However, computational analysis and inference of these stochastic models face significant challenges due to the curse of dimensionality, resulting in an excessively large state-space. The aim of this talk is to address some of these challenges by proposing a novel approach centered around estimating the Koopman operator associated with CTMCs. Leveraging the compact nature of this operator, we develop a Monte Carlo method for its efficient estimation, requiring only a limited number of simulated trajectories. Operating in the frequency domain, our method provides a computable error bound for the estimate. Through illustrative examples, we demonstrate how the estimated Koopman operator facilitates parameter inference from experimental data and enables efficient analysis of various properties of the stochastic model, including parameter sensitivities and the frequency content of its trajectories.