Long timescale behavior from trajectory data

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Abstract

The transition operator of a Markov process encodes all evolutionary statistics of the process. For example, the most slowly decorrelating functions of the process are encoded as certain eigenvectors of the transition operator. In cases of practical interest, however, the transition operator is not known in closed form. Instead our only access to the transition operator is through random trajectories of the Markov process. These observations have motivated a huge body of research focused on dynamical spectral estimation, which approximates eigenvectors of the transition operator and their corresponding eigenvalues using random trajectory data. Despite intense methodological development, the mathematical understanding of the error properties of dynamical spectral estimation remains incomplete. In this talk I will discuss our error analysis of a leading algorithm for dynamical spectral estimation, called the variational approach for conformation dynamics (VAC). We derive explicit mathematical relationships revealing the dependence of VAC error on key design parameters. In a second part of the talk I will describe algorithms that we are currently developing to compute predictions of long timescale phenomenon (i.e. rare events) using only relatively short trajectory data.

Speaker

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