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Effective dynamics for discrete-in-time stochastic processes described by transfer operators

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Collective variables (CVs) play an important role in understanding the dynamics of high-dimensional metastable molecular dynamics. Given a set of CVs, effective dynamics of diffusion processes have been constructed using conditional expectations and their properties have been studied in previous works. In this talk, we extend the definition of effective dynamics to discrete-in-time Markov processes X_n. In particular, we show that the transition density of the effective dynamics solves a relative entropy minimization problem from certain family of densities to the transition density of X_n. We also show that many transfer operator-based data-driven numerical approaches essentially learn quantities of the effective dynamics. Finally, we discuss how our theoretical analysis can be converted into a numerical algorithm for identifying CVs. This is a joint work with Christof Schütte.

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