NONLINEAR MODEL REDUCTION FOR SLOW-FAST STOCHASTIC SYSTEMS NEAR UNKNOWN INVARIANT MANIFOLDS

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We are interested in model reduction for certain classes of high-dimensional stochastic dynamical systems. Model reduction consists in estimating a low-dimensional stochastic dynamical system that approximates, in a suitable sense (e.g. at certain spatial or temporal time-scale), the original system, or at least some observables of the original system. Typically such reduced models may be faster to simulate (e.g. because of their lower dimensionality) and may offer important insights on the dynamical behavior of the original system.
Motivated by examples and applications, including molecular dynamics, we consider a special, well-studied class of stochastic dynamical systems that exhibit two important properties. The first one is that the dynamics can be split into two timescales, a slow and a fast timescale, and the second one is that the slow dynamics takes place on, or near to, a low-dimensional manifold M, while the fast dynamics can be thought of as consisting of fast oscillations off that manifold.
Given only access to a black-box simulator from which short bursts of simulations can be obtained, and a (possibly small) set of reasonable initial conditions, we design an algorithm that outputs an estimate of the manifold M, a process representing the effective stochastic dynamics on M, which has averaged out the fast modes, and a simulator of such process. The fast modes are not assumed to be small, nor orthogonal to M.
This simulator is efficient in that it exploits the low dimension of the manifold M, and takes time steps of size dependent only the regularity of the effective process, and therefore typically much larger than that of the original simulator, which had to resolve the fast modes in high dimensions. Furthermore, the algorithm and the estimation can be performed on-the-fly, leading to efficient exploration of the effective state space, without losing consistency with the underlying dynamics. This construction enables fast and efficient simulation of paths of the effective dynamics, together with estimation of crucial features and observables of such dynamics, including the stationary distribution, identification of metastable states, and residence times and transition rates between them.

This is joint work with X.-F. Ye and S. Yang.