

Geometric Methods for the Approximation of High-dimensional Dynamical Systems

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We discuss a geometry-based statistical learning framework for performing model reduction and modeling of stochastic high-dimensional dynamical systems. We consider two complementary settings. In the first one, we are given long trajectories of a system, e.g. from molecular dynamics, and we discuss new techniques for estimating, in a robust fashion, an effective number of degrees of freedom of the system, which may vary in the state space of then system, and a local scale where the dynamics is well-approximated by a reduced dynamics with a small number of degrees of freedom. We then use these ideas to produce an approximation to the generator of the system and obtain, via eigenfunctions of an empirical Fokker-Planck question, reaction coordinates for the system that capture the large time behavior of the dynamics. We present various examples from molecular dynamics illustrating these ideas. In the second setting we only have access to a (large number of expensive) simulators that can return short simulations of high-dimensional stochastic system, and introduce a novel statistical learning framework for learning automatically a family of local approximations to the system, that can be (automatically) pieced together to form a fast global reduced model for the system, called ATLAS. ATLAS is guaranteed to be accurate (in the sense of producing stochastic paths whose distribution is close to that of paths generated by the original system) not only at small time scales, but also at large time scales, under suitable assumptions on the dynamics. We discuss applications to homogenization of rough diffusions in low and high dimensions, as well as relatively simple systems with separations of time scales, and deterministic chaotic systems in high-dimensions, that are well-approximated by stochastic differential equations.