

DIFFUSION MAPS FOR SOLVING THE BACKWARD KOLMOGOROV PDES IN MODERATELY HIGH DIMENSIONS

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The diffusion map algorithm introduced by Coifman and Lafon in 2006 as a nonlinear dimensional reduction tool with proven theoretical guarantees has an important ability to approximate differential operators on point clouds. We show that by changing the kernel function inherent in diffusion maps and using renormalizations one can approximate the Backward Kolmogorov Operator for the stochastic differential equation governing the dynamics of biomolecules or atomic clusters described in collective variables: time-reversible dynamics with position-dependent and anisotropic diffusion. Moreover, the point cloud used as an input does not need to be sampled from the invariant density but can be generated by any standard enhanced sampling algorithm. Using the solution to the Backward Kolmogorov PDE on a point cloud with appropriate boundary conditions one can identify reaction channels and calculate the transition rate between metastable states of interest. An application to alanine dipeptide in four collective variables whose configurational space is the four-dimensional torus will be discussed.

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