Geometric analysis, Diffusion models, Reaction coordinates in Molecular Dynamics

Mary A. Rohrdanz[1], Wenwei Zheng[1], Mauro Maggioni[2], and Cecilia Clementi[1]

(1) Rice University, Department of Chemistry, Houston, Texas 77005, USA; (2) Duke University, Department of Mathematics, Durham, North Carolina 27708, USA

We view sets of configurations of a molecule along long trajectories as a set of points in high-dimensional state space, and analyze its local geometry to find a ***local intrinsic dimension*** and a ***local scale***, above the scale of noise but below the scale at which the set of trajectories curves, at which the set of configurations may be analyzed.

WIth these notions we construct ***locally scaled diffusion maps*** that yield *reaction coordinates* for the system, and associated low-dimensional nonlinear projections of the state space. The approach is highly robust, does not require the user to specify a fixed local scale, as in previous methods.

We demonstrate on several systems that the low-dimensional representation of the system and the reaction coordinates we find are able to accurately reproduce certain statistics of the dynamics, such as *reaction rates* between semi-stable configurations, and are able to capture some fine details of the energy landscape.

The methods proposed hold promise for larger and more complex molecules.