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Recovery of polymer folding landscapes from univariate time series and its dimensionality reduction using machine learning JIANG WANG, Department of Physics, University of Illinois at Urbana-Champaign, ANDREW FERGUSON, Materials Science and Engineering, University of Illinois at Urbana-Champaign — The stable conformations and motions of polymers and macromolecules are governed by their underlying free energy surface. By integrating ideas from dynamical systems theory with nonlinear manifold learning, we have developed an approach to recover single-molecule free energy surfaces from univariate time series of a single system observable. Using the method of delays, we expand the time series into a high dimensional phase space in which, by Takens' Theorem, the dynamics are equivalent to those of the molecule in real space. We then apply nonlinear manifold learning algorithm (diffusion maps and nonliear PCA) to extract a low-dimensional representation of the free energy surface that is diffeomorphic (i.e., a smooth transformation) to that which would have been recovered from a complete knowledge of all system degrees of freedom. We have validated our approach in molecular dynamics simulations of a $C_{24}H_{50}$ n-alkane chain, demonstrating that the free energy surface extracted from the atomistic simulation trajectory is geometrically and topologically equivalent to that recovered from a knowledge of only the head-to-tail distance of the chain. Our approach lays the foundations to extract empirical single-molecule free energy surfaces directly from experimental data.

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