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Extract the thermodynamic and kinetic information from protein simulations using dimensionality reduction

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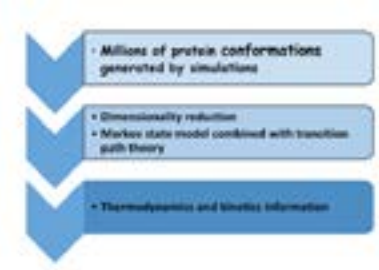
In the study of protein thermodynamics and kinetics, it is of paramount importance to characterize protein free energy landscapes. Dimensionality reduction is a valuable tool to complete the task. We have evaluated several methods of dimensionality reduction, including linear and nonlinear methods, such as principal component analysis, Isomap, locally linear embedding, and diffusion maps. A series of criteria was used to assess different aspects of the embedding qualities. Our results have shown that there is no clear winner in all aspects of the evaluation and each dimensionality-reduction method has its limitations in a certain aspect. The linear method, principal component analysis, is not worse than the nonlinear ones in some respects for our peptide system. We have also developed a mathematical formulation to demonstrate that an explicit Euclidean-based representation of protein conformation space and the local distance metric associated to it improve the quality of dimensionality reduction. For a certain sense, clustering protein conformations into macro-clusters to build a Markov state model is also an approach of dimensionality. We have tested inherent structure and geometric structure for state space discretization and demonstrated that the macro-cluster based on inherent structure give a meaningful state space discretization in terms of conformational features and kinetics.



Biography

Shuanghong Huo received her PhD in Computational Chemistry from Boston University. She did her Postdoctoral training at UC-San Francisco. She is a Professor of Chemistry and Biochemistry at Clark University, Worcester, USA. Her research interest is in protein folding, misfolding, and aggregation. Recently, her group is developing dimensionality reduction methods and graph representations of protein free energy landscapes.

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