Model-based inference of protein dynamics based on MD data

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Abstract

Molecular Dynamics (MD) data is one major source of protein dynamics information, but it is still unclear how to use these data to elucidate the energy landscape of the protein structure space. We proposed a method to integrate thousands of MD trajectories to analyze the protein dynamics. We will use both geometric distance and dynamic distance to probe the grouping structure of conformations within the landscape. A parametric Bayesian approach is used to partition the structural space.