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Finding representative structures: pathway learning with Path Similarity Analysis-based subsampling CHENOU ZHANG, OLIVER BECKSTEIN, Arizona State Univ. — Many proteins function as macromolecular machines that switch between different conformational states. In order to understand the molecular mechanisms of such proteins, an important goal is to gain quantitative insights into the conformational transition. Molecular dynamics (MD) simulation have been used to sample such transition pathways but thermal noise from the stochastic nature of MD simulations may obscure the important stages in the transition. Hence finding a series of representative structures that are not affected by thermal fluctuations while retaining all important transition features can be a crucial prerequisite towards any further analysis. Here we demonstrate how to use Path Similarity Analysis (PSA) with the Hausdorff metric to find the most similar subset path with a given number of trajectory frames as the best representative subsampled trajectory. We discuss an iterative algorithm that minimizes the Hausdorff path distance under various additional constraints. We analyze the conformational transition pathway of the membrane transporter Mhp1. We show the convergence of our iterative subsampling algorithm and discuss its dependence on initial choices of frames and order parameter.

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