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Reconstructing Protein Folding Trajectories from Low-Dimensional Experimental Time Series

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66-110

Abstract: Data-driven modeling and machine learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. In the first part of this talk, I will describe an approach integrating ideas from dynamical systems theory and nonlinear manifold learning to reconstruct multidimensional protein folding funnels from the time evolution of single experimentally measurable observables. In the second part of this talk, I will describe our use of deep learning to estimate slow collective variables from molecular simulation trajectories and the use of these coordinates to train highly efficient latent space molecular simulators. By combining these two ideas it is possible to reconstruct all-atom molecular configurations from one-dimensional time series in experimentally measurable observables.