

Enhancing Sampling in Molecular Dynamics: Integrating Autoencoders and Linear Discriminant Analysis for Efficient Collective Variables

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In molecular dynamics, transitions between conformations are rare events, posing significant challenges for sampling. Enhanced sampling methods, such as the extended Adapted Biasing Force (eABF), utilize collective variables (CVs) to capture the slow components of these transitions. While intuitive selection of CVs can sometimes be effective, it often fails to capture critical transitions. Building on the work of my predecessor, this study explores a novel approach using autoencoders combined with Linear Discriminant Analysis (LDA) to identify optimal CVs. By validating our methods on semi-supervised datasets of a protein or an RNA, we aim to maximize the likelihood of obtaining effective CVs for various therapeutic targets, thereby improving the efficiency and accuracy of enhanced sampling methods in molecular dynamics.

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