ENHANCING SAMPLING IN MOLECULAR DYNAMICS: INTEGRATING AUTOENCODERS AND LINEAR DISCRIMINANT ANALYSIS FOR THE IDENTIFICATION OF COLLECTIVE VARIABLES

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In molecular dynamics, transitions between conformations are rare events, making sampling a significant challenge. Enhanced sampling methods, such as the extended Adapted Biasing Force (ABF), rely on collective variables (CVs) to capture the slow parts of these transitions. While intuitive selection of CVs can sometimes be effective, it often fails to observe critical transitions. This study explores a novel approach using autoencoders combined with Linear Discriminant Analysis (LDA) to identify optimal CVs. By examining multiple topologies, we aim to maximize the likelihood of obtaining effective CVs, thereby improving the efficiency and accuracy of enhanced sampling methods in molecular dynamics.