LEARNING COLLECTIVE VARIABLES FOR ACCURATE TRANSITION RATE ESTIMATION

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We investigate the problem of learning collective variables (CVs) to minimize the error in transition rates in the reduced model. We propose a computational algorithm to learn collective variables based on the orthogonality relationship between the residence manifold and the level sets of the CVs (Legoll and Lelievre, 2010). The algorithm involves a feature mapping to account for symmetry groups, learning the residence manifold via diffusion maps (Coifman et al. 2008) and diffusion nets (Mishne et al. 2019), and learning CVs via autoencoders. We present three case studies: normal butane C4H10, Lennard-Jones-7 (LJ7) in 2D, and Lennard-Jones-8 (LJ8) in 3D. We successfully preserved the anti-gauche transition rate in the reduced model for butane with high accuracy. We used the committors of the reduced models in LJ7 and LJ8 as the reaction coordinate for the forward flux sampling. We also designed a stochastic control for sampling transition paths. The resulting transition rates and residence times agree with the brute-force estimates.

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