APPROXIMATING COMMITTOR FUNCTIONS: OBJECTIVE FUNCTIONS AND TRAINING DATA SAMPLING

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The committor function is, for many applications, the best choice of collective variable to describe a transition from a metastable state to another one as it quantifies the probability that a configuration of a studied system undergoes a reaction.1,2 However, learning such a function is generally a challenging task due to the high dimensionality of the configuration space. In this work, after reviewing the existing methodologies to construct approximate committor functions, a new loss function based on the application of Ito's formula is proposed to learn the committor function with a neural network parametrization. After comparing the numerical results on the Müller–Brown potential with this new loss to those obtained with loss functions already proposed in the literature, the approach is coupled with the Adaptive Multilevel Splitting method to enhance the sampling of
the reactive trajectories.3,4 This methodology in which the committor function is iteratively learned only requires knowledge on the reactant and product states.

References

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