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Discover committor-consistent path by neural networks

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A significant challenge faced by atomistic simulations is the difficulty, and often impossibility, to sample the transitions between metastable states of the free-energy landscape associated to slow molecular processes. Importance-sampling schemes represent an appealing option to accelerate the underlying dynamics by smoothing out the relevant free-energy barriers, but require the definition of a suitable reaction-coordinate (RC) models expressed in terms of compact low-dimensional sets of collective variables (CVs). While most computational studies of slow molecular processes have traditionally relied on educated guesses based on human intuition to reduce the dimensionality of the problem at hand, a variety of machine-learning (ML) algorithms have recently emerged as powerful alternatives to discover a meaningful CV capable of capturing the dynamics of the slowest degrees of freedom. Considering a simple paradigmatic situation in which the long-time dynamics is dominated by the transition between two known metastable states, we compare two variational data-driven ML methods based on Siamese neural networks aimed at discovering a meaningful RC model—the slowest decorrelating CV of the molecular process, and the committor probability to first reach one of the two metastable states. One method is the state-free reversible variational approach for Markov processes networks (VAMPnets), or SRVs—the other, inspired by the transition path theory framework, is the variational committor-based neural networks, or VCNs. The relationship and the ability of these methodologies to discover the relevant descriptors of the slow molecular process of interest is illustrated with a series of simple model systems. We also show that both strategies are amenable to importance-sampling schemes through an appropriate reweighting algorithm that approximates the kinetic properties of the transition.

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