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Kinetically Consistent Coarse Graining using Kernel-based Extended Dynamic Mode Decomposition

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In this work, we show how kernel-based approximation to the Koopman generator –the kgEDMD algorithm – can be used to identify implied timescales and meta-stable sets in stochastic dynamical systems, and to learn a coarse-grained dynamics on reduced variables, which retains the essential kinetic properties of the full model. The centerpiece of this study is a learning method to identify an effective diffusion in coarse-grained space by leveraging the kgEMD model for the Koopman generator. By combining this method with force matching, a complete model for the effective dynamics can be inferred. Using a two-dimensional model system and molecular dynamics simulation data of alanine dipeptide and Chignolin, we demonstrate that the proposed method successfully and robustly recovers the essential theormodynamic and kinetic properties of the full model.

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