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Learning Kinetically Consistent Coarse Grained Dynamics via Kernel-based Approximation of Koopman Generator

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Accurately detecting the coarse-grained coordinates is an essential task in the model discovery of complex systems, such as molecular dynamics. In many cases, such systems cannot be approximated properly with deterministic dynamics. An extension of Extended Dynamic Mode Decomposition (EDMD) has been introduced in [Klus et al., Physica D (2020)] to approximate the Koopman generator for the identification of stochastic dynamical systems. However, the selection of basis functions upon which the generator is approximated is a non-trivial task and needs to be done manually. By taking advantage of kernel methods introduced in [Klus, Entropy (2020)], we develop a kernel-based data-driven method to approximate the Koompan generator of a dynamical system. This method allows us to identify stochastic differential equations governing the coarse-grained model of a high-dimensional system. Dominant dynamics and metastabilities of the system in the reduced-order space, furthermore, can be obtained by the eigen-decomposition of the coarse-grained generator.
We numerically investigate the method using toy models and molecular dynamics problems and demonstrate that the results are thermodynamically and kinetically consistent with the full model.

Presenter: NATEGHI, Vahid