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Generator-extended DMD method for control-affine SDEs

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Stochastic dynamics with metastability are a recurring theme in many scientific disciplines, for instance, in simulations of macro-molecules, in climate systems, and in applications of uncertainty quantification. Metastability describes the existence of long-lived macro-states in a dynamical system's state space, such that transitions between these macro-states are rare events. It is thus also closely related to control systems. There is a wide range of biased sampling algorithms, which seek to overcome the rare event nature of the dynamics using a time-dependent input.

In this study, we join the ideas of Koopman-based modeling and biased sampling. The key ingredient is the generator extended dynamic mode decomposition algorithm (gEDMD), a variant of EDMD to approximate the Koopman generator. For control-affine stochastic differential equations (SDEs), application of gEDMD reduces the Kolmogorov backward equation into an ODE that is bi-linear in expectation and input. This simplified structure can be utilized for designing controllers which are geared towards accelerated sampling of rare events.

In this talk, we will report on recent progress concerning the data-driven analysis of metastable systems using Koopman generators. First, we will introduce Koopman operators for (controlled) stochastic systems, the gEDMD method, and its application to optimal control problem. Second, we will present the numerical results showing that the gEDMD method for control-affine SDEs can be used to a) accurately predict the expectation of observable functions of interest for fixed control input; b) solve optimal control problems (OCPs) with integrated running cost and terminal cost; c) design OCPs which enforce accelerated transitions between metastable states.

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