Learning the dynamics of systems with memory : Generalized Langevin equations

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Generalized Langevin equations with non-linear forces and memory kernels are commonly used to describe the effective dynamics of coarse-grained variables in molecular dynamics. Such reduced dynamics play an essential role in the study of a broad class of processes, ranging from chemical reactions in solution to conformational changes in biomolecules or phase transitions in condensed matter systems. I will first discuss the derivation of the generalized Langevin equations, emphasizing the need for memory in the effective dynamics due to the lack of a proper separation of time scales[2]. Then, I will turn on the inference of such generalized Langevin equations from observed trajectories, using a maximum likelihood approach. This data-driven approach provides a reduced dynamical model for multidimensional collective variables, enabling the accurate sampling of their long-time dynamical properties at a computational cost drastically reduced with respect to all-atom numerical simulations. I will illustrate the potential of this method on several model systems, both in and out of equilibrium[1].

[1] H. Vroylandt, L. Goudenège, P. Monmarché, F. Pietrucci, B. Rotenberg. *Likelihood-based non-markovian models from molecular dynamics.* Proceedings of the National Academy of Sciences, **119(13)**, e2117586119, 2022. doi :10.1073/pnas.2117586119.

[2] H. Vroylandt, P. Monmarché. *Position-dependent memory kernel in generalized langevin equations : theory and numerical estimation*, 2022. doi :10.48550/arXiv.2201.02457.

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