Identifiable learning of dissipative dynamics

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1. Introduction

Complex dissipative systems appear across science and engineering, from polymers and active matter to learning algorithms. These systems operate far from equilibrium, where energy dissipation and time irreversibility govern their behavior but are difficult to quantify from data. In this work, we introduce a universal and identifiable neural framework [1] that learns dissipative stochastic dynamics directly from trajectories while ensuring interpretability, expressiveness, and uniqueness. Our method identifies a unique energy landscape, separates reversible from irreversible motion, and allows direct computation of the entropy production, providing a principled measure of irreversibility and deviations from equilibrium. This extends earlier ideas [2, 3, 4, 5]. Applications to polymer stretching in elongational flow and to stochastic gradient Langevin dynamics reveal new insights, including super-linear scaling of barrier heights and sub-linear scaling of entropy production rates with the strain rate, and the suppression of irreversibility with increasing batch size. Our methodology thus establishes a general, data-driven framework for discovering and interpreting non-equilibrium dynamics.

2. Universal and Identifiable Dissipative Dynamics

Universal and Identifiable Dissipative Dynamics (UIDD) is a neural framework for learning dissipative dynamics from discrete trajectory data. Its key innovation is a universal and identifiable dynamical formulation whose evolution is defined by the following Itô stochastic differential equation (SDE):

$$\begin{aligned}\dot{\mathbf{Z}}_t =& -[M(\mathbf{Z}_t) + W(\mathbf{Z}_t)]\nabla V(\mathbf{Z}_t) \\ &+ \nabla \cdot M(\mathbf{Z}_t) + \nabla \cdot W(\mathbf{Z}_t) + \sigma(\mathbf{Z}_t)\dot{\mathbf{B}}_t,\end{aligned} \tag{1}$$

where $V(\cdot)$ is a scalar potential, $M(\cdot)$ and $W(\cdot)$ are $D \times D$ matrix-valued functions. $M(z) = \sigma(z)\sigma^\top(z)/2$ is symmetric positive definite, while $W(z)$ is a banded antisymmetric matrix whose non-zero entries are confined to the first sub-diagonal and its corresponding counterparts.

In this model, the diffusion matrix $\sigma(\cdot)$ together with the white noise process $\dot{\mathbf{B}}_t$ models the thermal fluctuations. The symmetric matrix $M(\cdot)$ characterizes the energy dissipation of the system and is constructed in such a way that the model satisfies the fluctuation-dissipation relation, where we set $M = \sigma\sigma^\top/2$. The antisymmetric matrix $W(\cdot)$ models the time-irreversible phenomena, enabling the model to account for non-equilibrium effects. Notably, the proposed sub-diagonal form of W contains $D-1$ independent scalar functions, thereby guaranteeing that the number of scalar functions to be modeled in the drift coincides with the system dimension. As shown in the talk, these choices achieve simultaneously full expressive capacity and identifiability.

We employ a data-driven, machine-learning approach to reconstruct the stochastic dynamics in (1). The unknown functions W, V, and σ are each parameterized as trainable deep neural networks. Essential physical priors are encoded into the neural network, including the positive definiteness of $M = \sigma\sigma^\top/2$ and the integrability of $\rho = e^{-V}$, which ensures the existence of the invariant distribution. The model is trained on a dataset of multiple independent trajectories by maximizing the likelihood of the observed data. Once trained, identifiability allows for subsequent analysis of the dynamical properties of the system.

3. Numerical Results

We demonstrate the capabilities of UIDD by learning the dynamics of a 300-bead polymer chain stretching in elongational flow, a system with up to 900 degrees of freedom. Using coarse-grained representations learned from microscopic data, we show that UIDD reliably reconstructs consistent potential energy landscapes and reveals that the barrier height increases super-linearly with the strain rate. In addition, UIDD further quantifies both local and global EPR, uncovering a sub-linear scaling of EPR with strain rate and confirming that the system operates far from equilibrium. These findings were previously inaccessible due to non-identifiability. We further validate the non-equilibrium nature with single-molecule experimental data.

To further demonstrate its broad applicability, we also employ UIDD to investigate stochastic gradient Langevin dynamics, a widely used algorithm in Bayesian inference and non-convex optimization [**?**]. We quantify how mini-batching introduces state-dependent noise that breaks detailed balance and drives the system out of equilibrium. Our analysis reveals that the EPR decreases with the batch size before plateauing at larger batches, indicating a suppression of non-equilibrium behavior as stochasticity is reduced. In addition, we find that the sampling error follows a consistent trend, suggesting that the EPR can serve as a physically-grounded diagnostic for the sampling quality. Together, these applications illustrate the versatility of UIDD in uncovering and quantifying non-equilibrium behavior in complex stochastic processes across physically and algorithmically generated non-equilibrium systems.

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