Universal Fluctuation-Response Relations of Nonequilibrium Dynamics

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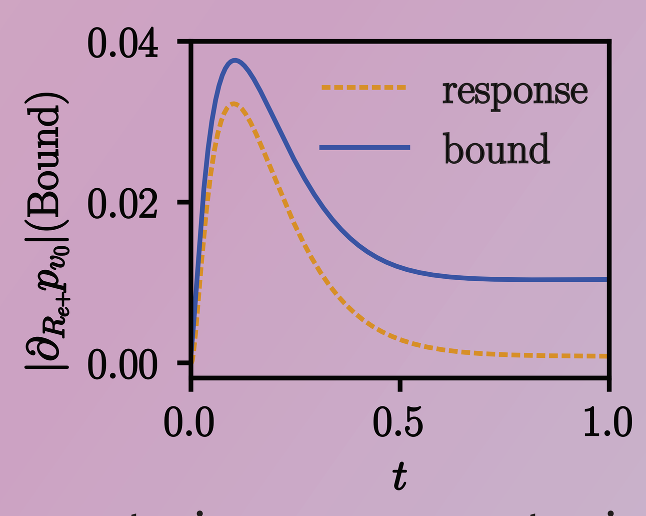
Abstract

Markov dynamics can effectively describe a wide range of thermodynamic and biological processes. Understanding how such systems respond to changes in environmental variables or external inputs is crucial for predicting and controlling their behaviors. We presents universal thermodynamic bounds on the responsiveness of any Markov system toward environmental changes. The systems of interest can be arbitrarily far from stationary state. The central element of this work is the introduction of information geometry on the manifold of probability distributions of stochastic trajectories. This work lays the foundation for understanding biological processes, engineering artificial systems, and exploring the fundamental principles governing complex systems far from equilibrium.

Sensitivity Relation

$$|\partial_{R_{e\pm}}\langle Q\rangle| \le \sqrt{\mathrm{Var}[Q]}\cdot\frac{\sqrt{\mathcal{A}_{e\pm}}}{R_{e\pm}}$$

System's sensitivity on observable Q to transition rate change is upper bounded by its variance and the dynamical activity $\mathcal{A}_{e\pm}$ (total number of transitions during the process).

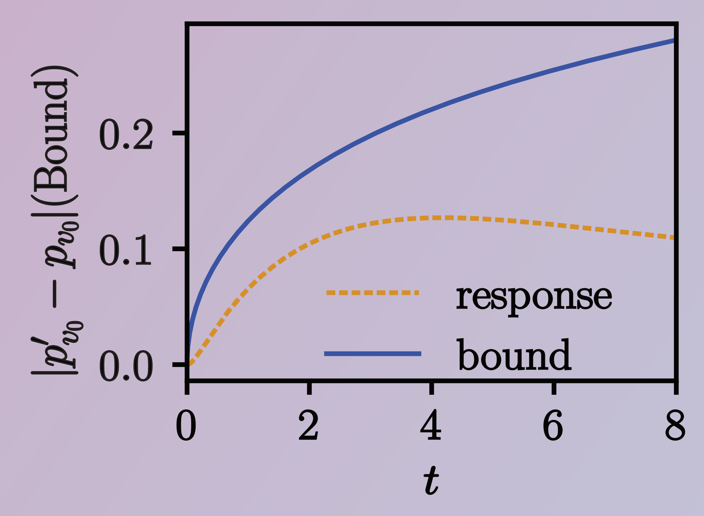


capturing non-monotonic transitiant response

Finite Response Relation

$$|\langle Q\rangle' - \langle Q\rangle| \le 2\max_{X_\tau}|Q|\cdot\sin(G_{e\pm})$$

where $G_{e\pm} = \left|\sqrt{R'_{e\pm}\tau} - \sqrt{R_{e\pm}\tau}\right|$

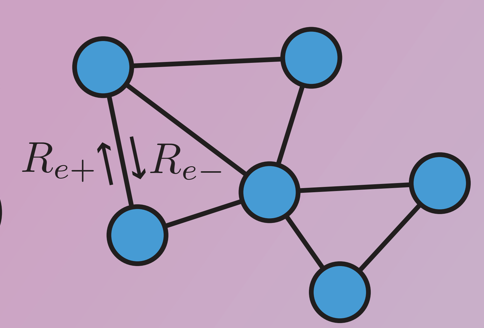


System's response on observable Q to finite rate change is upper bounded by quantities related to the dynamical activity.

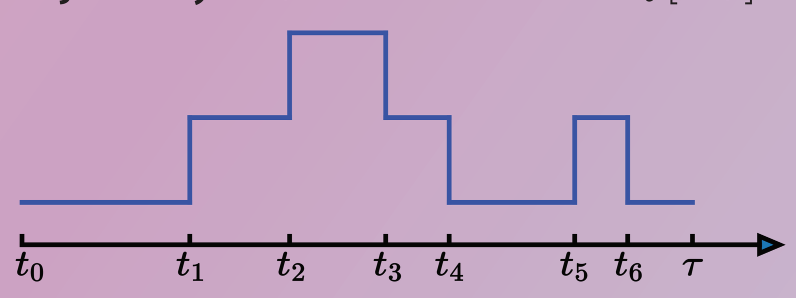
System and Setup

Markov dynamics

$$\frac{\partial \boldsymbol{p}(t)}{\partial t} = R\cdot \boldsymbol{p}(t)$$



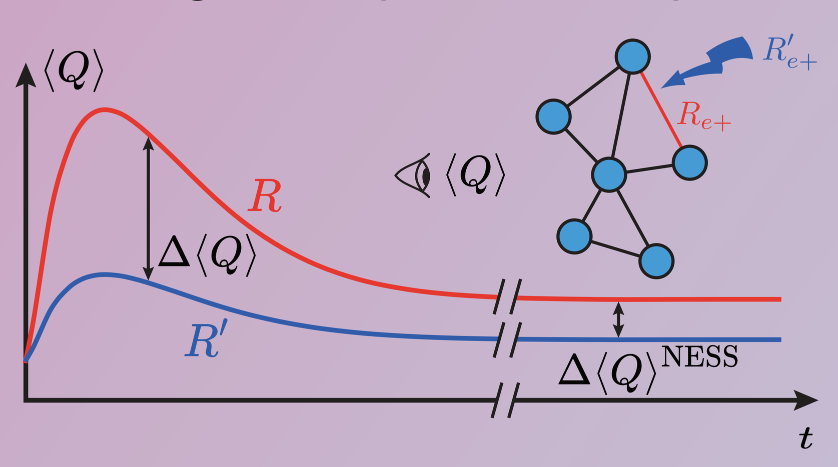
Trajectory X_τ & Observable $Q[X_\tau]$:



$X_\tau = ((x_0,t_0),(x_1,t_1),\cdots,(x_n,t_n))$

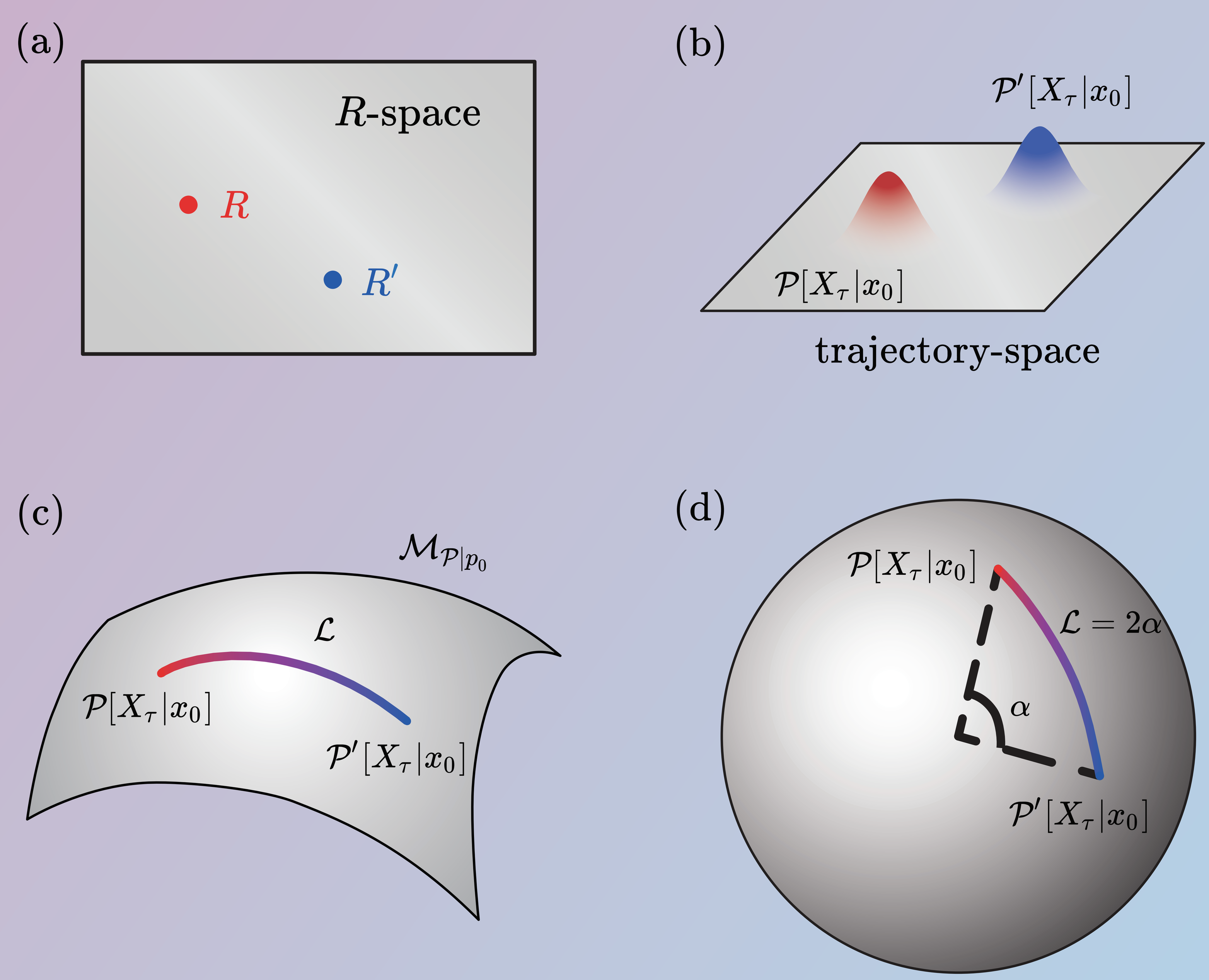
$Q = Q[X_\tau]$

Modeling non-equilibrium response



response: $\Delta\langle Q\rangle = |\langle Q\rangle' - \langle Q\rangle|$

Geometric Sturcture of Trajectory Probabilities



Relations between four spaces to capture Markov Processes. (a) The space of all possible probability rate matrices. (b) Distributions of stochastic trajectories in the trajectory space. (c) The manifold of trajectory probabilities equipped with Fisher information metric. (d) Isometric embedding from trajectory manifold to a hypersphere of radius 2 in Euclidean space.

Reference:

A. Pagare*, Z. Zhang*, J. Zheng*, Z. Lu. *J. Chem. Phys.* 160, 171101 (2024)

J. Zheng*, Z. Lu†. arXiv: 2403.10952

arXiv paper