Stochastic Thermodynamic Interpretation of Information Geometry

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(Received 6 January 2018; published 18 July 2018)

In recent years, the unified theory of information and thermodynamics has been intensively discussed in the context of stochastic thermodynamics. The unified theory reveals that information theory would be useful to understand nonstationary dynamics of systems far from equilibrium. In this Letter, we have found a new link between stochastic thermodynamics and information theory well-known as information geometry. By applying this link, an information geometric inequality can be interpreted as a thermodynamic uncertainty relationship between speed and thermodynamic cost. We have numerically applied an information geometric inequality to a thermodynamic model of a biochemical enzyme reaction.

DOI: 10.1103/PhysRevLett.121.030605

The crucial relationship between thermodynamics and information theory has been well studied in the last decades [1]. Historically, thermodynamic-informational links had been discussed in the context of the second law of thermodynamics and the paradox of Maxwell's demon [2]. Recently, several studies have newly revealed thermodynamic interpretations of informational quantities such as the Kullback-Leibler divergence [3], mutual information [4–6], the transfer entropy and information flow [7–19]. The above interpretations of informational quantities are based on the theory of stochastic thermodynamics [20,21], which mainly focus on the entropy production in stochastic dynamics of small systems far from equilibrium.

The information thermodynamic relationship has been attractive not only in terms of Maxwell's demon, but also in terms of geometry [22–28]. Indeed, differential geometric interpretations of thermodynamics have been discussed especially in a near-equilibrium system [22,29–34]. Moreover, the technique of differential geometry in information theory, well-known as information geometry [35], has received remarkable attention in the fields of neuroscience, signal processing, quantum mechanics, and machine learning [36–38]. In spite of the deep link between information and thermodynamics, the direct connection between thermodynamics and information geometry has been elusive, especially for nonstationary and nonequilibrium dynamics. For example, G. E. Crooks discovered a link between thermodynamics and information geometry [22,32] based on the Gibbs ensemble, and then his discussion is only valid for a near-equilibrium system.

In this Letter, we discover a fundamental link between information geometry and thermodynamics based on stochastic thermodynamics for the master equation. We mainly report two inequalities, derived thanks to information geometry, and we interpret them within the theory of stochastic thermodynamics. The first inequality connects the environmental entropy change rate to the mean change of the local thermodynamic force rate. The second inequality can be interpreted as a kind of thermodynamic uncertainty relationship, or thermodynamic trade-off relationship [39–51], between the speed of a transition from one state to another and the thermodynamic cost related to the entropy change of thermal baths in a near-equilibrium system. We numerically illustrate these two inequalities on a model of a biochemical enzyme reaction.

Stochastic thermodynamics.—To clarify a link between stochastic thermodynamics and information geometry, we start with the formalism of stochastic thermodynamics for the master equation [20,21], which is also known as the Schnakenberg network theory [52,53].

Here, we consider a $(n+1)$-states system. We assume that transitions between states are induced by n_{bath}-multiple thermal baths. The master equation for the probability p_x $(\geq 0, \sum_{x=0}^{n} p_x = 1)$ to find the state at $x = \{0, 1, \ldots, n\}$ is given by

$$\frac{d}{dt} p_x = \sum_{\nu=1}^{n_{\mathrm{bath}}} \sum_{x'=0}^{n} W^{(\nu)}_{x' \to x} p_{x'}, \tag{1}$$

where $W^{(\nu)}_{x' \to x}$ is the transition rate from x' to x induced by νth thermal bath. We assume a nonzero value of the transition rate $W^{(\nu)}_{x' \to x} > 0$ for any $x \neq x'$. We also assume the condition

$$\sum_{x=0}^{n} W^{(\nu)}_{x' \to x} = 0, \tag{2}$$

or, equivalently, $W^{(\nu)}_{x' \to x'} = -\sum_{x \neq x'} W^{(\nu)}_{x' \to x} < 0$, which leads to the conservation of probability $d(\sum_{x=0}^{n} p_x)/dt = 0$. Equation (2) indicates that the master equation is then given by the thermodynamic flux from the state x' to x [52],

$$J^{(\nu)}_{x' \to x} := W^{(\nu)}_{x' \to x} p_{x'} - W^{(\nu)}_{x \to x'} p_x, \tag{3}$$

