Quantifying higher-order entropy production in organized nonequilibrium states

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Abstract

The entropy production rate reflects the dissipation of free energy in a nonequilibrium state, and it is necessary for many biological functions. Nevertheless, trivial systems can display large entropy production, and it is yet an open challenge to characterize the out-of-equilibrium states of living systems and their operational meaning. We present a way to decompose the entropy production rate of a system, capturing how much of it is generated from higher-order interactions between its components. Our method combines recent information-geometric decompositions of the entropy production rate with a hierarchical decomposition of forces into k-body stochastic interactions.

Introduction Living systems maintain themselves in organized nonequilibrium states by continually harvesting and dissipating free energy from their environment. The rate of free energy dissipation is often termed the ‘entropy production rate’ (EPR), as it quantifies how fast the entropy of a system and its environment grows (for example, it can quantify the rate at which a biological motor burns ATP into heat, increasing the entropy of the environment). For molecular systems, the EPR can be expressed in a remarkable information-theoretic way as the Kullback-Leibler (KL) divergence between forward and backward fluxes, Eq. (2) below. For coarse-grained systems, this expression can still be meaningfully interpreted as the temporal irreversibility of a stochastic process, reflecting a definite arrow of time.

The EPR has various operational consequences, in terms of precision of fluctuating observables and speed of dynamical evolution (Horowitz and Gingrich, 2020). More generally, positive EPR is necessary to display rich dynamical behavior like reproduction, homeostasis, and information processing. Recently, EPR has been suggested as a useful indicator for distinguishing organized states in macroscopic systems, such as brains involved in different tasks or states of consciousness (Lynn et al., 2021; de la Fuente et al., 2023).

Nevertheless, the EPR presents limitations as an indicator of organized nonequilibrium steady states in many-body systems. In principle, steady-state EPR can be arbitrarily large even in simple systems, such as well-mixed chemical solutions or electrical resistors. In these cases, the EPR reflects the additive contribution of many independent components (molecules, heating elements, etc.). This is different from EPR in systems with interactions and large-scale organization, such as active matter (Ro et al., 2022), nonequilibrium spin glasses (Aguilera et al., 2022), and biological systems. In such cases, we expect EPR to also arise from higher-order effects generated by interaction in the driving forces, as well as entropic forces that reflect emergent higher-order correlations in steady-state.

Here we investigate how to capture the contribution to EPR corresponding to interactions between components, not only pairwise but also of higher orders. We investigate this question in using a standard model of a nonequilibrium spin model, the kinetic Ising model, which displays a rich phenomenology under asymmetric couplings (Aguilera et al., 2022). Our goal is to investigate the relationship between higher order EPR and the organization of the nonequilibrium states of the spin glass. Understanding of this higher-order EPR could lead to an understanding of the operational meaning of this decomposition in terms of bounds on statistical fluctuations, and to understand how these contributions can be measured in real-world experiments.

Method We consider a discrete-state system described by a probability distribution $p(\mathbf{x}, t)$ over states $\mathbf{x} = \{x_1, \ldots, x_N\}$ at time t and a stochastic process with transition rates $R(\mathbf{y}|\mathbf{x})$. The system evolves according to a master equation

$$\dot{p}(\mathbf{y}, t) = \sum_{\mathbf{x}:\mathbf{x}\neq\mathbf{y}} \left(R(\mathbf{y}|\mathbf{x})p(\mathbf{x}, t) - R(\mathbf{x}|\mathbf{y})p(\mathbf{y}, t)\right). \quad (1)$$

The change of system’s Shannon entropy $S = -\sum_{\mathbf{x}} p(\mathbf{x}, t) \log p(\mathbf{x}, t)$ is $\dot{S} = -\sum_{\mathbf{x}} \dot{p}(\mathbf{x}, t) \log p(\mathbf{x}, t)$. Thermodynamics can be introduced when the condition of ‘local detailed balance’ (LDB) holds, meaning that the entropy increase of the environment (e.g., due to heat flow) can be written as $\sum_{\mathbf{x}\neq\mathbf{y}} R(\mathbf{y}|\mathbf{x})p(\mathbf{x}, t) \log \frac{R(\mathbf{y}|\mathbf{x})}{R(\mathbf{x}|\mathbf{y})}$ (Van den Broeck and Esposito, 2015). The combination of system and environment entropy increase is called the entropy

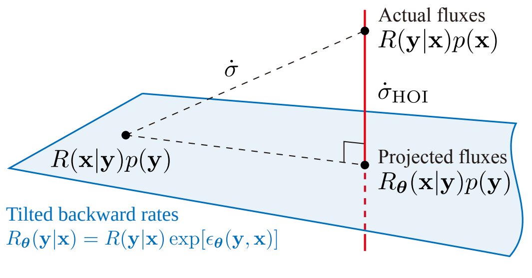

Figure 1: Illustration of the EPR decomposition in Eq. 3.

production rate (EPR), written as

$$\begin{aligned}\dot{\sigma} =& \sum_{\mathbf{x}\neq\mathbf{y}} R(\mathbf{y}|\mathbf{x})p(\mathbf{x},t) \log \frac{R(\mathbf{y}|\mathbf{x})p(\mathbf{x},t)}{R(\mathbf{x}|\mathbf{y})p(\mathbf{y},t)} \\ =& D(R(\mathbf{y}|\mathbf{x})p(\mathbf{x},t) \,\|\, R(\mathbf{x}|\mathbf{y})p(\mathbf{y},t)), \end{aligned} \tag{2}$$

where $D(p(\mathbf{x})\|p(\mathbf{x})) = \sum_{\mathbf{x}}(p(\mathbf{x}) \ln \frac{p(\mathbf{x})}{q(\mathbf{x})} - p(\mathbf{x}) + q(\mathbf{x}))$ is the generalized KL divergence. EPR is nonnegative in consistency with the Second Law, and it strictly positive for nonequilibrium irreversible processes. EPR is a measure of breaking of time irreversibility, even in the absence of LDB.

We decompose EPR by extending a recent framework that integrates nonequilibrium thermodynamics and information geometry (Kolchinsky et al., 2022). We combine this framework with a hierarchical decomposition of many-body interactions into a sequence of k-body terms (independent, pairwise, triplets, etc., Amari, 2001). Our approach provides a decomposition of EPR that is more general (Horowitz and Gingrich, 2020; Lynn et al., 2022) and interpretable (Ito et al., 2020) than previous approaches, because it does not require special dynamics, and because it has simple operational meaning in terms of uncertainty relations and fluctuations.

To apply this framework, we define a manifold of backward stochastic processes under a tilted rate matrix $R_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{y}) = R(\mathbf{x}|\mathbf{y}) \exp\left[\epsilon_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{y})\right]$, where $\epsilon_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{y})$ is a function parametrized by $\boldsymbol{\theta}$. Each such manifold will represent forces represented by k-body interactions. We then find the parameters in terms of the projection $\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} D\left(R(\mathbf{y}|\mathbf{x})p(\mathbf{x},t) \,||\, R_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{y})p(\mathbf{y},t)\right)$, resulting in a Pythagorean relation (Amari, 2001)

$$\begin{aligned}\dot{\sigma} =& \underbrace{D\left(R_{\boldsymbol{\theta}^*}(\mathbf{x}|\mathbf{y})p(\mathbf{y},t) \,\|\, R(\mathbf{x}|\mathbf{y})p(\mathbf{y},t)\right)}_{\text{lower-order EPR}} \\ &+ \underbrace{D\left(R(\mathbf{y}|\mathbf{x})p(\mathbf{x},t) \,\|\, R_{\boldsymbol{\theta}^*}(\mathbf{x}|\mathbf{y})p(\mathbf{y},t)\right)}_{\text{higher-order EPR, } \dot{\sigma}_{\text{HOI}}} \end{aligned} \tag{3}$$

Results We study the EPR decomposition in a nonequilibrium spin model of two homogeneous populations $a \in \{1,2\}$ of $N = 100$ spins $x_{a,i} = \pm 1$ with asymmetric population couplings $\mathbf{J} = \left[\begin{smallmatrix} 1 & 1 \\ -1 & 1 \end{smallmatrix}\right]$ (see Fig. 2). Spins are updated following a simoid rate applied asynchronously, i.e.

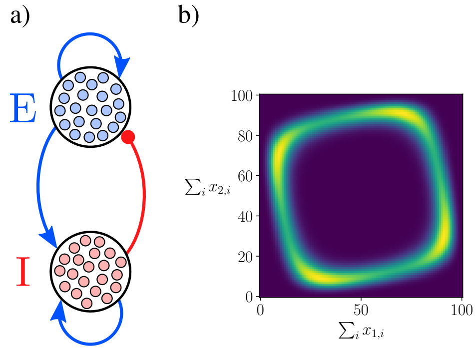

Figure 2: a) Excitatory-inhibitory spin model. b) NESS probability distribution for aggregated variables $\sum_i s_i^a$ for $\beta = 2$.

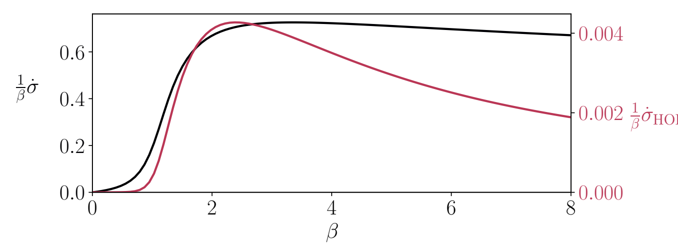

Figure 3: EPR and higher-order EPR of the two oscillatory population in Fig. 2 for different values ofβ. Higher-order ERP is close to zero for the disordered phase ($\beta < 1$) and peaks around $\beta = 2$ where the system displays stochastic self-sustained oscillations. As the behaviour of the system becomes more deterministic for larger β, high-order ERP decreases, while ERP remains high.

assuming $\mathbf{y} = \mathbf{x}^{[i,a]}$ ($^{[i,a]}$ being a spin-flip operator applied to $x_{a,i}$),

$$R(\mathbf{y}|\mathbf{x}) = \frac{1}{1 + \exp\left[-2\beta y_{a,i} \sum_{b,j} J_{ab} x_{b,j}\right]}, \tag{4}$$

otherwise $R(\mathbf{y}|\mathbf{x}) = 0$. The system resembles simple models of excitatory and inhibitory neuron populations. In steady state, if β is sufficiently high ($\beta > 1$ in the large size limit), the system undergoes an Andronov-Hopf bifurcation bifurcation from a disordered state to self-sustained stochastic oscillations. For larger values of β oscillations become more deterministic.

We measure the decomposition of the EPR that cannot be reduced to pairwise interactions, using $\epsilon_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{y}) = \exp[\,\theta_{i,a,\emptyset} + \theta_{i,a,0} x_{i,a} + \sum_{j,b} \theta_{ij,b} x_{i,a} y_{j,b}\,]$ (assuming $\mathbf{y} = \mathbf{x}^{[i,a]}$). Fig. 3 shows that, while EPR grows as oscillations emerge, a small fraction of ERP higher-order terms peak around $\beta = 2$, where oscillations emerge, but the system maintains some level of stochasticity.

References

Aguilera, M., Igarashi, M., and Shimazaki, H. (2022). Nonequilibrium thermodynamics of the asymmetric sherrington-kirkpatrick model. *arXiv preprint arXiv:2205.09886*.

Amari, S.-I. (2001). Information geometry on hierarchy of probability distributions. *IEEE transactions on information theory*, 47(5):1701–1711.

de la Fuente, L. A., Zamberlan, F., Bocaccio, H., Kringelbach, M., Deco, G., Perl, Y. S., Pallavicini, C., and Tagliazucchi, E. (2023). Temporal irreversibility of neural dynamics as a signature of consciousness. *Cerebral Cortex*, 33(5):1856–1865.

Horowitz, J. M. and Gingrich, T. R. (2020). Thermodynamic uncertainty relations constrain non-equilibrium fluctuations. *Nature Physics*, 16(1):15–20.

Ito, S., Oizumi, M., and Amari, S.-i. (2020). Unified framework for the entropy production and the stochastic interaction based on information geometry. *Physical Review Research*, 2(3):033048.

Kolchinsky, A., Dechant, A., Yoshimura, K., and Ito, S. (2022). Information geometry of excess and housekeeping entropy production. *arXiv preprint arXiv:2206.14599*.

Lynn, C. W., Cornblath, E. J., Papadopoulos, L., Bertolero, M. A., and Bassett, D. S. (2021). Broken detailed balance and entropy production in the human brain. *Proceedings of the National Academy of Sciences*, 118(47):e2109889118.

Lynn, C. W., Holmes, C. M., Bialek, W., and Schwab, D. J. (2022). Decomposing the local arrow of time in interacting systems. *Physical review letters*, 129(11):118101.

Ro, S., Guo, B., Shih, A., Phan, T. V., Austin, R. H., Levine, D., Chaikin, P. M., and Martiniani, S. (2022). Model-free measurement of local entropy production and extractable work in active matter. *Physical Review Letters*, 129(22):220601.

Van den Broeck, C. and Esposito, M. (2015). Ensemble and trajectory thermodynamics: A brief introduction. *Physica A: Statistical Mechanics and its Applications*, 418:6–16.