The energy dissipated tells us how far a system is from equilibrium

~~Irreversibility as divergence from equilibrium~~

David Andrieux I do research by myself, for fun

The entropy production is commonly used to gauge a system's distance from equilibrium, but this interpretation lacks formalization due to the absence of a natural equilibrium measure. This analysis shows that the entropy production of a Markov system measures its separation from specific equilibrium dynamics. These reference dynamics correspond to the closest reversible systems in the information-theoretic sense. This result yields new lower bounds for the entropy production and novel links between thermodynamics and information geometry.

TL;DR I formalize the intuitive notion that the energy lost when a system transports energy and matter depends on how far the system is from being at rest (i.e., at equilibrium)

I. IRREVERSIBILITY OF MARKOV CHAINS

What was already known

Let's consider a Markov chain characterized by a transition matrix $P = (P_{ij})$ on a finite state space of size N (our results directly extends to continuous time processes). The Markov chain is primitive, i.e., P^n has all positive entries for n larger than some n_0. The chain P then admits a unique stationary distribution π.

The entropy production of P takes the form [1–3]

$$\Delta_i S = \frac{1}{2} \sum_{ij} (\pi_i P_{ij} - \pi_j P_{ji}) \ln \frac{P_{ij}}{P_{ji}} . \tag{1}$$

Energy dissipated measures the difference between a process and its time-reversal

This expression only depends on P (and its stationary distribution π).

However, the entropy production (1) involves the reversed probabilities P_{ji}, which are proportional to the time-reversed dynamics $P^*_{ij} = (\pi_j/\pi_i) P_{ji}$. Intuitively, irreversibility thus arises from the difference between the dynamical randomness of the forward and the time-reversed processes [4]. This is formalized by writing the entropy production as

forward

Time direction

$$\Delta_i S = D_{KL}(P||P^*) ,$$

Energy lost

where

backward

$$D_{KL}(P||G) = \sum_{ij} \pi_i P_{ij} \ln \frac{P_{ij}}{G_{ij}} \geq 0$$

is the Kullback-Leibler divergence between P and G. Note that in this case $D_{KL}(P||P^*) = D_{KL}(P^*||P)$ even though D_{KL} is not symmetric in general.

II. IRREVERSIBILITY AS DIVERGENCE FROM EQUILIBRIUM

A different perspective

Examining the entropy production (1), no links to other dynamics beyond P^* are discernible. Yet, the entropy production can also be expressed as a divergence with respect to specific equilibrium systems $P^{(x)}$ associated with P:

NEW FORMULA!

$$\frac{1}{2} \Delta_i S = D_{sKL}\left(P||P^{(x)}\right) . \tag{2}$$

where $D_{sKL}(P||G) = D_{KL}(P||G) + D_{KL}(G||P)$ is the symmetrized KL divergence.

The relationship (2) holds for the two equilibrium dynamics

With the new formula:

$$P^{(e)} = s\left[(P \circ P^*)^{(1/2)}\right] \quad \text{and} \quad P^{(m)} = (P + P^*)/2 .$$

forward

Here $\circ$ denotes the Hadamard product, $P^{(1/2)}$ is the elementwise exponentiation, and the mapping s transforms a positive matrix K into a stochastic one as $s[K] = (1/\rho)\,\mathrm{diag}(\alpha)^{-1} K \,\mathrm{diag}(\alpha)$, where ρ is the largest eigenvalue of K and α its corresponding right eigenvector.

Energy lost

Equilibrium (nothing moves)

Eq. (2) is demonstrated in the appendix while its connection with information geometry and nonequilibrium thermodynamics is discussed in Section IV.

Works for special equilibrium states shown on next page

III. LOWER BOUNDS FOR THE ENTROPY PRODUCTION

Bonus content

Using that $D_{KL} \geq 0$, we directly obtain new bounds for the entropy production:

$$\Delta_i S \geq 2 \max\left[D_{KL}\left(P||P^{(e)}\right), D_{KL}\left(P^{(e)}||P\right)\right]$$

and

$$\Delta_i S \geq 2 \max\left[D_{KL}\left(P||P^{(m)}\right), D_{KL}\left(P^{(m)}||P\right)\right] .$$

Additional ways to estimate the energy lost - not critical but always nice to have

Additional bounds can be derived from these expressions. For example, $D(P^{(e)}||P) = -\ln\rho$ with ρ the largest eigenvalue of $P^{(1/2)} \circ P^{*(1/2)}$ (see the appendix for a demonstration). Then, using the standard bound for the Perron eigenvalue [5] leads to

$$\Delta_i S \geq -2 \ln\left[\max_i \sum_j \sqrt{P_{ij} P_{ji}}\right] \geq 0 .$$

This bound captures the symmetric part of the dynamics. Readers are invited to further explore related bounds.

Why this formula is INTERESTING

~~IV. DISCUSSION: INFORMATION GEOMETRY AND NONEQUILIBRIUM TRANSPORT~~

Expression (2) shows that irreversibility can be interpreted as arising from an 'information divergence' from equilibrium [6]. Indeed, $P^{(e)}$ and $P^{(m)}$ correspond to

Conceptual figure

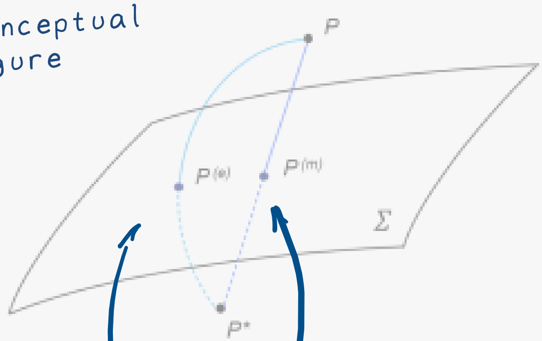

FIG. 1. **Geometry of the space of Markov chains.** The set of equilibrium dynamics is represented as a two-di[illegible] by the symmetrized KL-divergence [illegible] P and $P^{(e)}$ or $P^{(m)}$ [illegible] by integrating the Fisher information along the e-geodesic and the m-geodesic (solid lines). The dynamical equivalence class $[P]$ contains the e-geodesic (not shown) and provides additional structure and symmetries for nonequilibrium transport [9, 11, 12].

Among all possible equilibrium states, two play a special role. The core 'trick' of the paper was to identify these two states

the [illegible] equilibrium [illegible] in the information-theoretic sense [7–9]:

The new formula links different concepts from information theory and thermodynamics,

$$P^{(e)} = \arg\min_G D(G||P)\,, \quad P^{(m)} = \arg\min_G D(P||G)\,,$$

and they [illegible] to the e-geodesic and the m-geodesic, respectively (Fig. 1) [7, 8, 10]. In turn, the symmetrized KL-divergence is given by the integration of the Fisher information along the e-geodesic and the m-geodesic (Theorem 3.2 in [7]).

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In [illegible], recent advances in stochastics thermodynamics showed that transport properties display hidden structures and symmetries, including far from equilibrium [9, 11–13]. These structures take the form of dynamical equivalence classes, which, remarkably, contain $P^{(e)}$ and the e-geodesic [11, 13].

The finding (2) now expresses the entropy production as a divergence from equilibrium along both the e- and m-geodesic. Taken together, these results deepen the connections between thermodynamics and information geometry and suggest [illegible] structures for transport, especially far from equilibrium.

which is always neat, but also suggests hidden physical structures waiting to be discovered

Disclaimer. This paper is not intended for journal publication.

The END

APPENDIX: DEMONSTRATION OF EQ. (2)

To demonstrate the relationship (2), it will be useful to introduce the relative entropies

$$h(P|G) = -\sum_i \pi_i P_{ij} \ln G_{ij}$$

so that $D_{KL}(P||G) = h(P|G) - h(P|P)$.

Let's first demonstrate Eq. (2) when $P^{(x)} = P^{(e)}$. The symmetrized divergence reads

$$D_{sKL}(P||P^{(e)}) = D_{KL}(P^{(e)}||P) + D_{KL}(P||P^{(e)})\,.$$

The same log ratios $\ln P_{ij}/P^{(e)}_{ij}$ appear in both terms on the right hand side, and take the form

$$\ln \frac{P_{ij}}{P^{(e)}_{ij}} = \frac{1}{2}\ln\frac{P_{ij}}{P_{ji}} + \frac{1}{2}\ln\frac{\pi_i}{\pi_j} + \ln\frac{\alpha_i}{\alpha_j} + \ln\rho\,,$$

where we used that $P^{(e)}_{ij} = (1/\rho)\,(\alpha_j/\alpha_i)\sqrt{P_{ij}P_{ji}}$. Inserting this expression into $D_{KL}(P^{(e)}||P)$ we get that

$$\begin{aligned} D_{KL}(P^{(e)}||P) &= (1/2)[h(P^{(e)}|P) - h(P^{(e)}|P^*)] - \ln\rho \\ &= -\ln\rho\,. \end{aligned}$$

Here we used that the terms $\ln \pi_i/\pi_j$ and $\ln \alpha_i/\alpha_j$ vanish when averaged over a stochastic dynamics (see for example Lemma 4.3 (iii) in ref. [8]) to get the first equality. For the second equality, Lemma 4.3 (ii) from reference [8] shows that $h(P^{(e)}|P) - h(P^{(e)}|P^*) = 0$ since $P^{(e)}$ is reversible and the log ratios $\ln P_{ij}/P_{ji}$ are antisymmetric in (i,j).

In parallel we have

$$\begin{aligned} D_{KL}(P||P^{(e)}) &= (1/2)[h(P|P^*) - h(P|P)] + \ln\rho \\ &= (1/2)\Delta_i S + \ln\rho\,. \end{aligned}$$

Demonstration: Trying to keep it short but understandable

Here we also used that the terms $\ln \pi_i/\pi_j$ and $\ln \alpha_i/\alpha_j$ vanish when averaged over a stochastic dynamics. The last equality uses that $h(P|P^*) - h(P|P) = D_{KL}(P||P^*)$ is the entropy production (1). Summing the last two equations the terms $\pm\ln\rho$ cancel each other and we obtain Eq. (2). □

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Let's now demonstrate Eq. (2) when $P^{(x)} = P^{(m)}$. We have

$$\begin{aligned} D_{sKL}(P||P^{(m)}) &= (1/2)[h(P|P^*) - h(P|P)] \\ &\quad + (1/2)[h(P|P^{(m)}) - h(P^*|P^{(m)})] \\ &= (1/2)[h(P|P^*) - h(P|P)] \\ &= (1/2)\Delta_i S\,. \end{aligned}$$

The first equality is obtained by noting that π is also the stationary distribution of P^* and thus of $P^{(m)}$, and that $h(P^*|P) = h(P|P^*)$. The second equality comes from Lemma 4.3 (i) in reference [8]. Similar to the previous case with $P^{(e)}$, the last equality uses that $h(P|P^*) - h(P|P) = D_{KL}(P||P^*)$ is the entropy production (1). □

Note: The authors of Ref. [8] proved the Pythagorean identities $D(P||G) = D(P||P^{(m)}) + D(P^{(m)}||G)$ and $D(G||P) = D(G||P^{(e)}) + D(P^{(e)}||P)$ (Theorem 6.1). However, these identities require G to be reversible, and thus cannot be used to derive Eq. (2).

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Inspired by Claire Lamman, Phys. Today **77** (2024)

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