How Constraints Affect Evolution of Entropy – Strengthened Second Laws

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with

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STOCHASTIC THERMODYNAMICS

- All 20th century statistical physics concerns systems either at thermal equilibrium or close to it, with very few non-static degrees of freedom

- Quick, raise your hand if you "are close to thermal equilibrium"

- Almost *no* system outside the lab is governed by 20th century stat. phys.

!!!!!

- **Salvation**! 21st century has seen a major revolution in statistical physics, allowing us to describe systems arbitrarily far from thermal equilibrium:

Stochastic Thermodynamics

STOCHASTIC THERMODYNAMICS

MAJOR STRENGTHENINGS OF SECOND LAW WHENEVER (SEEMINGLY) INNOCUOUS CONSTRAINTS HOLD

- ***Speed limit theorems****:*
  - Strictly positive lower bound on dissipation of any non-static process

- ***Thermodynamic uncertainty relations****:*
  - Strictly positive lower bound on dissipation of any process that gives high statistical precision in value of integrated current

- ***Integral fluctuation theorems****:*
  - Strictly positive lower bound on dissipation of any process that has randomness in how much dissipation it produces

- ***Many more:***
  - Kinetic uncertainty relation, thermodynamic correlation inequality, etc.

STOCHASTIC THERMODYNAMICS

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Here I describe two more

These strengthened second laws apply to any process that is either

- modular (all digital devices and biological systems)
- periodic (all digital devices)

DEPENDENCE OF {lots of things} ON INITIAL DISTRIBUTION

Arbitrary physical process $\underline{P}(x_1 \mid x_0)$ taking $p_0 \rightarrow p_1$

Arbitrary "cost function" $C(p_0) = F(p_0) - [S(\underline{P}p_0) - S(p_0)]$ where F(.) is linear

- $F(p_0)$ = Heat flow into system; $C(p_0)$ is **dissipated work**
- $F(p_0) = \int_0^1 dt \sum_x \left(\frac{\partial p_t(x)}{\partial t} \ln p_t^{st}(x) \right)$; $C(p_0)$ is **nonadiabatic EP**

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Define q_0 as minimizer of cost function:

$$C(p_0) \ = \ C(q_0) + [C(p_0) - C(q_0)]$$

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Define q_0 as minimizer of cost function:

$$C(p_0) \;=\; \boldsymbol{C(q_0)} + [C(p_0) - C(q_0)]$$

$C(q_0)$ is called ***residual cost***

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Define q_0 as minimizer of cost function:

$$C(p_0) = C(q_0) + \left[\boldsymbol{C(p_0) - C(q_0)}\right]$$

$C(q_0)$ is called residual cost

$$C(p_0) - C(q_0) = D(p_0 \,||\, q_0) - D(\underline{P}p_0 \,||\underline{P}q_0) \geq 0$$

where D(. || .) is relative entropy (KL divergence)

$D(p_0 \,||\, q_0) - D(\underline{P}p_0 \,||\underline{P}q_0)$ is called ***mismatch cost***

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$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

Wolpert, D., Kolchinsky, A., *New J. Phys.* (2020)
Riechers, P., Gu, M., *Phys. Rev. E* (2021)
Ouldridge, T., Wolpert, D., *New J. Phys. (2023)*
Manzano, G., Kardes, G., Roldan, E., Wolpert D., *Phys. Rev. X* (2024)

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Any nontrivial physical process that results in zero thermodynamic cost for one initial distribution ***will be costly*** for any other initial distribution

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Holds for *Langevin dynamics*, (open) *quantum thermodynamics*, *non-Markovian dynamics*, *nonconservative forces*, *unidirectional transitions*.

Also holds at *trajectory level*.

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q_0 is minimizer of cost function:

$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

Often can solve for q_0 in closed form.
Example: It is stationary state of dynamics for $C(p_0)$ = nonadiabatic EP
Example: It is equilibrium distribution for $C(p_0)$ = EP

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$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

This formula is exact, not a bound

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$F(p_0) = \Sigma_x \, p(x) \, f(x)$ for some function f(x)

$$
\begin{aligned}
C(p_0) &= C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)] \\
&\geq D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)
\end{aligned}
$$

Given q_0, this lower bound is *completely* independent of details of the physical process.

Just like second law is.

In particular, none of the restrictions in the SLT, TUR, KUR etc.

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$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$
$$\geq D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)$$

Only effect of changing f(.) or $\underline{P}$(.) on the mismatch cost is to change q_0

LOWER BOUNDS ON MISMATCH COST

Arbitrary physical process $\underline{P}(x_1 \mid x_0)$ taking $p_0 \rightarrow p_1$

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$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

Example:

- Suppose your process *unavoidably generates a lot of heat;*
  - Then residual entropy production is large.
  - Then f(x) is large for all x, on scale of ln|X| (maximum entropy)

- Often when this happens $max_x f(x) - min_x f(x)$ is also large
  - Means $q_0(x)$ is very close to edge of simplex
  - Means **mismatch cost is large for all p_0 not too close to q_0**

Worst case mismatch cost: $max_x f(x) - min_x f(x) - \ln|X|$

LOWER BOUNDS ON RESIDUAL COST

Continuous-time Markov process taking $\underline{P}(x_1 \mid x_0)$ taking $p_0 \rightarrow p_1$

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$$C(p_0) = C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

"**Thermodynamic Speed limit theorem (SLT)**" bounds $C(q_0)$:

$$C(q_0) \geq \frac{L(p_0, p_1)^2}{2\, A_{tot}}$$

where

$L(p, p') = |p, p'|$ is L_1 distance
A_{tot} = average number system state changes during the process if start with distribution q_0

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"**Thermodynamic Speed limit theorem (SLT)**" bounds $C(q_0)$:

$$C(q_0) \geq 2W(q_0, Pq_0)\tanh^{-1} \frac{W(q_0, Pq_0)}{A_{tot}}$$

where

$W(p, p') = |p, p'|$ is Wasserstein distance through the network of possible state transitions

- Lots of other SLTs

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"**Thermodynamic Uncertainty Relation (TUR)**" bounds $C(q_0)$:

$$C(q_0) \geq \frac{2kB[E(J)]^2}{Var(J)}$$

where

$J = \Sigma_{x,x'} \, d(x, x')$ for all state changes x to x′ during the process if start with distribution q_0

and

$d(a, b)$ is an arbitrary "deviation function" obeying $d(a, b) = -d(b, a)$

- Lots of strengthened (but more complicated) TURs

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$$C(p_0) \;=\; C(q_0) + [D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)]$$

In contrast to thermodynamic uncertainty relations,
speed limit theorems, etc.,
mismatch cost bound is often large in macroscopic processes

MISMATCH COST IN PERIODIC PROCESSES

A physical process over a space X that repeats (e.g., a periodic process)

So over N iterations, the sum-total mismatch cost (lower bound on cost) is:

$$\sigma(N\lambda) \geq \inf_{q \in \Delta_X} \sum_{t=0}^{N-1} \left[D(P^t p_0 \,||\, q) - D(P^{t+1} p_0 \,||\, Pq) \right]$$

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KEY POINT: Since the process repeats, q is the same in each repetition.
However, $P^t p_0$ will differ over repetitions.

Therefore

At most one mismatch cost in the sum can equal 0 in general

- *Independent of the physical details of the underlying process*
(just like second law of thermodynamics)

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KEY POINT: Since the process is periodic, q is the same in each period.
However, $P^t p_0$ will differ over periods.

Therefore

At most one mismatch cost in the sum can equal 0 in general

A **strictly positive** lower bound on cost for ***any*** periodic process

Ex: Positive lower bound on entropy production (EP) for any digital device

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- Kolchinsky, A., DHW *Phys. Rev. E* (2021)
- Riechers, P., Gu, M., *Phys. Rev. E* (2021)
- Ouldridge, T., DHW *New J. Phys. (2023)*
- Manzano, G., Kardes, G., Roldan, E., DHW *Phys. Rev. X* (2024)
- DHW (14 co-authors), PNAS in press (2024)
- Yadav, A., Caravelli F., and DHW, arXiv:2411.16088 (2024)

Some papers soon to be submitted on strengthened second law that apply in

- Any (Shannon) communication channel
- Any Matlab program