Entropy in continuous phase space

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Group seminar presentation

Entropy-producing processes of interest

- Discrete: Markov jump processes. Spontaneous transitions between discrete configurations $c \in \Omega$ with rates $w_{c \to c'}$
- Continuous, overdamped – "no momentum" following a DE of the form

$$\dot{q} = F(q) + \Gamma(q)\xi(t)$$

- Continuous, underdamped – full phase space required, e.g.

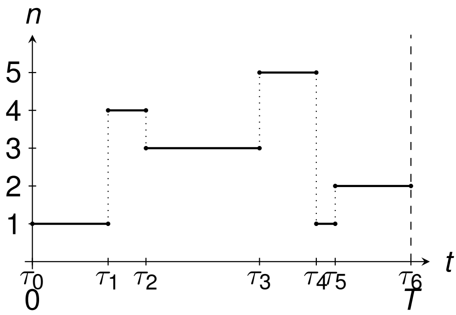
$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= F(q) - \gamma(p)p + \Gamma(p)\xi(t) \end{aligned}$$

Last time: Discrete systems

- Set of discrete microstates $c \in \Omega$
- Continuous time
- Transitions between the microstates at transition rates $w_{c \to c'}$

Stochastic trajectories

The evolution of a system looks like



$\rightarrow$ chain of states $\gamma : c_0 \rightarrow c_1 \rightarrow c_2 \rightarrow \ldots$ at times $t_0, t_1, t_2, \ldots$

Master equation

The dynamics of such a system are described by the Master equation:

$$\frac{\partial}{\partial t} P_c(t) = \sum_{c'} \left(P_{c'}(t) w_{c' \to c} - P_c(t) w_{c \to c'} \right)$$

Can be read as the sum of incoming and outgoing probability currents.

Entropy can be split up in two parts:

$$S_{\text{total}} = S_{\text{system}} + S_{\text{environment}}$$

System entropy along a stochastic trajectory γ:

$$S_{\text{system}}(t) = -\ln P_{c(t)}(t)$$

- Measure of how many different outcomes the system can have at time t - "how big is the pase space region that can be reached"
- Shannon entropy is the mean system entropy, i.e. the average over all configurations:

$$\langle S_{\text{System}}(t) \rangle = \sum_{c \in \Omega} -P_{c(t)}(t) \ln P_{c(t)}(t)$$

Entropy can be split up in two parts:

$$S_{\text{total}} = S_{\text{system}} + S_{\text{environment}}$$

Environmental entropy is easier to think about as a difference:

$$\Delta S_{\text{env}} = \ln w_{\rightarrow} - \ln w_{\leftarrow} = \ln \frac{w_{\rightarrow}}{w_{\leftarrow}}$$

- Measure of how much more likely a transition in one direction (*rate* $w_{\rightarrow}$) is compared to the reverse direction ($w_{\leftarrow}$).
- Each jump changes S_{env} discontinuously.

Continuous, overdamped systems

Space-continuous version of the master equation:

$$\dot{q} = F(q) + \Gamma(q)\xi(t)$$

with Force, Gaussian noise with $\langle \xi(t)\xi(t') \rangle \propto \delta(t - t')$, noise coefficient.

- How does environmental entropy translate to this system?
- What does “jump in the reverse direction” mean?

Continuous environmental entropy (overdamped)

Environmental entropy produced by this system along a trajectory γ starting at q_0:

$$\Delta S_{\text{env}} = \ln \frac{P[\gamma|q_0]}{P^\dagger[\gamma^\dagger|q_0^\dagger]} \cong \ln \frac{w_\rightarrow}{w_\leftarrow}$$

$\dagger$ stands for path and time reversal,

$$q^\dagger(t) = q(T-t) \qquad q_0^\dagger = q_T \qquad F^\dagger(x,t) = F(x, T-t)$$

Continuous, underdamped systems

Adding a friction term requires also considering momenta, making the full phase space necessary:

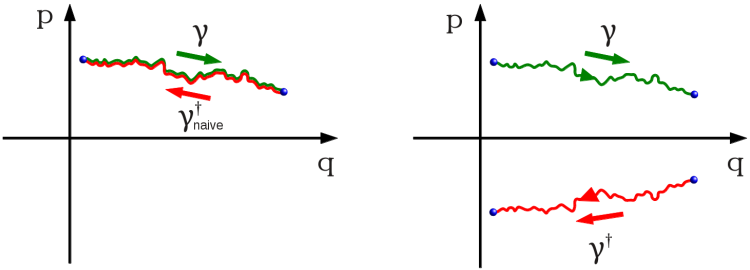
$$\dot{q} = p$$
$$\dot{p} = F(q) - \gamma(p)p + \Gamma(p)\xi(t)$$

The naive way of defining ΔS_{env} is just by carrying it over from the overdamped limit,

$$\Delta S_{\mathrm{env}} = \ln \frac{P[\gamma|q_0]}{P^\dagger[\gamma^\dagger|q_0^\dagger]}$$

However, this leads to momenta pointing in the other direction as velocities on the reverse path.

Spinney/Ford approach: reverse momenta



- Time reversal in the Hamiltonian formalism is equivalent to $p \to -p$
- Not all variables transform the same under $t \to -t$ – "odd and even variables" need to be distinguished:

$$\gamma = \{q(t), p(t)\} \longrightarrow \gamma^\dagger = \{\varepsilon q(T-t), \varepsilon p(T-t)\}$$

From the equations of motion to entropy

Rewrite the equations of motion to the corresponding Fokker-Planck equation

$$\dot{P}(x,t) = -\sum_i \partial_i \underbrace{\left(A_i(x,t)P(x,t) - \partial_i(D_i(x,t)P(x,t))\right)}_{J(x,t)}$$

where $x = (q, p)$

From this, the Green's function/short-time propagator $G_a(\boldsymbol{x}'|\boldsymbol{x}\ ; \mathrm{d}t)$ can be calculated, which ...

- solves the FP equation to lowest order in $\mathrm{d}t$
- is not unique, represented by the index a (similar to the Itō-Stratonovich dichotomy)
- Repeated application (convolution) yields the full propagagor

From equations of motion to entropy

After obtaining the (lengthy) expression for $G_a(\boldsymbol{x}'|\boldsymbol{x}\ ;\mathrm{d}t)$, the differential (short-term) entropy production is

$$\mathrm{d}S_{\mathrm{env}}(\boldsymbol{x}'|\boldsymbol{x};\ \mathrm{d}t) = \ln \frac{G_a(\boldsymbol{x}'|\boldsymbol{x};\ \mathrm{d}t)}{G_b(\boldsymbol{x}'^{\dagger}|\boldsymbol{x}^{\dagger};\ \mathrm{d}t)}$$

In the Spinney/Ford case (mirror momenta on the reverse path), this becomes

$$\mathrm{d}S_{\mathrm{env}}(q', p'|q, p;\ \mathrm{d}t) = \ln \frac{G_a(q', p'|q, p;\ \mathrm{d}t)}{G_b(q, -p|q', -p';\ \mathrm{d}t)}$$

Furthermore, Spinney/Ford show that $a = 1 - b$ is the right choice of parameters, which cancels them both out.

Spinney/Ford differential entropy production

Using this approach, we showed that the Spinney/Ford approach for the simplest case of constant $\gamma(p), \Gamma(p)$ yields

$$\mathrm{d}S_{\text{env}} = -\beta p \mathrm{d}p - \gamma \mathrm{d}t$$

This seems very implausible, as a resting particle ($p = 0$) produces negative entropy over time. This peculiar property of Spinney/Ford's approach motivated our research.

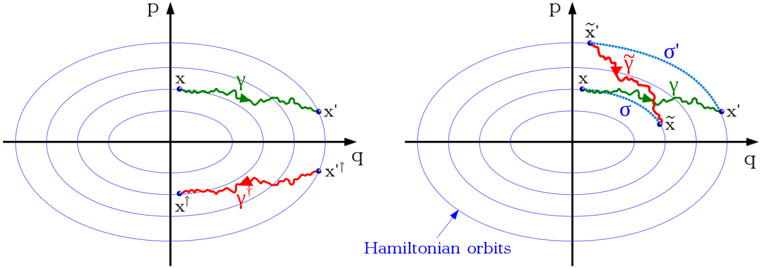
How to solve the problem?

- Deterministic systems should not produce entropy.
- Jumping to another state should produce environmental entropy.
- Entropy production should be local, and not require jumping to another region of phase space entirely.

Idea: What consitutes the “state” of a stochastic system? Could it be more than just a point in phase space?
Proposition: Identify the whole Hamiltonian trajectory as “the state” of a system. Switching trajectories produces entropy, staying on it doesn’t.

A new way of reversing paths

Can we redefine the path reversal to solve these issues?



- Forward trajectory stays the same as in Spinney/Ford
- Backward trajectory: Instead of reversing the path, consider how likely the reverse transition between orbits (instead of points) would have been

A new way of reversing paths

In formulas, this idea reads

$$\mathrm{d}S_{\mathrm{env}}(q', p' | q, p;\ \mathrm{d}t) = \ln \frac{G_a(q', p' | q, p;\ \mathrm{d}t)}{G_b(q + p\mathrm{d}t, p + f(q)\mathrm{d}t | q' - p'\mathrm{d}t, p' - f(q')\mathrm{d}t;\ \mathrm{d}t)}$$

Result for $\mathrm{d}S_{\mathrm{env}}$:

- Vanishes along the Hamiltonian flow (i.e. deterministic trajectories)
- $a = b = \frac{1}{2}$ turns out to be the right choice of parameters for the propagator ambiguity

Comparing the models

Differential entropy production $\mathrm{d}S_{\text{env}}$ is not observable, the expected (average) entropy production however is. What difference do the models make in the result?

$$\dot{S}_{\text{env}}(x) = \lim_{\mathrm{d}t \to 0} \frac{1}{\mathrm{d}t} \int_{\Omega} \mathrm{d}x' G_c(\boldsymbol{x}'|\boldsymbol{x};\ \mathrm{d}t)\mathrm{d}S_{\text{env}}(\boldsymbol{x}'|\boldsymbol{x};\ \mathrm{d}t)$$

$$\dot{S}_{\text{env}}(t) = \int_{\Omega} \mathrm{d}x' P(x,t)\dot{S}_{\text{env}}(x)$$

Results:

- The (third) ambiguity parameter c does not appear in the result in lowest order
- Both Spinney/Ford and the Flow model result in the same results, although the differential entropies are different

Example system

For a system obeying detailed balance (FP equation stationary):

$$\mathrm{d}S_{\text{env}} = \begin{cases} -\beta p(\mathrm{d}p + V'(q)\mathrm{d}t) - \frac{\beta}{2}\Gamma(p)^2\mathrm{d}t & \text{Spinney/Ford} \\ -\beta p(\mathrm{d}p + V'(q)\mathrm{d}t) & \text{Our model} \end{cases}$$

Because of the red term, only our result vanishes along the deterministic trajectory $\dot{p} = -V'(q)$. However,

$$\dot{S}_{\text{env}} = -\frac{1}{2}\Gamma(p)^2 + \frac{2}{3}\beta^2 p^2 \Gamma(p)^2 - \beta p \Gamma(p)\Gamma'(p)$$

is identical in both cases, as is the equilibrium entropy production,

$$\langle \dot{S}_{\text{env}} \rangle_{\text{DB}} = \int_\Omega \mathrm{d}p\mathrm{d}q \frac{e^{-\beta(\frac{p^2}{2} - V(q))}}{Z} \dot{S}_{\text{env}}(q,p) = 0$$

which is the desired result, as a system obeying detailed balance should not produce entropy in the environment.

Conclusion

- Spinney/Ford's differential entropy production shows odd behaviour in some cases
- Redefining the "backwards" path solves this issue, taking the non-stochastic Hamiltonian flow into accounthttps://news.ycombinator.com/item?id=5977495
- Both approaches yield the same physical quantity $\dot{S}_{\text{env}}$

Thanks for your attention!