Detailed balance and entropy production in continuous-time Markov processes

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Round-table conference on statistical physics - March 10-11, 2022

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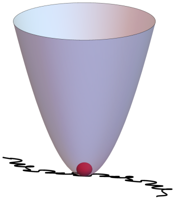
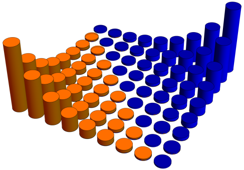
Motivation

- systems in contact with heat bath are dissipative
- change state of system $\rightarrow$ dissipate energy into heat bath
  - move Brownian particle through viscous environment
  - change occupation probability of lattice sites
- dissipation quantified by entropy production
- what is the minimum entropy production required for a given operation?
- what type of process realizes minimum entropy production?





1. Equilibrium, detailed balance and entropy production

Equilibrium and detailed balance

- classical statistical mechanics: systems in thermal equilibrium
- defining feature of equilibrium: detailed balance
  probability of transition $i \to j$: $P(i \to j) = P(j \to i)$ for any pair of states (i, j)
  - no currents in the system on average
  - one-to-one correspondence energy $\leftrightarrow$ probability

$$p^{\text{eq}}(i) = Z^{-1} e^{-\beta U(i)} \qquad \text{with} \qquad Z = \sum_i e^{-\beta U(i)}, \qquad \beta = \frac{1}{k_{\text{B}} T}$$

- detailed balance: probabilistic time-reversal symmetry

Entropy production out of equilibrium

- system out of equilibrium: no detailed balance, $P(i \to j) \neq P(j \to i)$ for some (i, j)
- trajectory of system: sequence of transitions $\Gamma = i_0 \to i_1 \to \ldots \to i_{N-1} \to i_N$
- time-reversed trajectory: $\Gamma^\dagger = i_N \to i_{N-1} \to \ldots \to i_1 \to i_0$

$$\Rightarrow \quad P(\Gamma) \neq P(\Gamma^\dagger) \qquad \text{for some } \Gamma$$

- use path probability $P(\Gamma)$ to define entropy production as Kullback-Leibler divergence

$$\Sigma = \sum_\Gamma P(\Gamma) \ln \left(\frac{P(\Gamma)}{P(\Gamma^\dagger)} \right) = D_{\mathsf{KL}}\left(P(\Gamma) \| P(\Gamma^\dagger)\right) \geq 0$$

- $\Sigma = 0$ only if $P(\Gamma) = P(\Gamma^\dagger)$ for all $\Gamma \to$ detailed balance

Continous-time Markov processes

- here: focus on Markov processes in continuous time
- transition probability independent of history $P(i \to j, t | k, s < t) = P(i \to j, t)$
- path probability factorizes

$$P(\Gamma) = P(i_N | i_{N-1}) P(i_{N-1} | i_{N-2}) \dots P(i_1 | i_0) P(i_0)$$

- entropy production: sum of individual transitions

$$\Sigma = \sum_{k=1}^{N} D_{\mathsf{KL}}\big(P(i_{k-1} \to i_k) \| P(i_{k-1} \to i_k)\big)$$

- two concrete types of dynamics: diffusion processes and jump processes

2. Diffusion processes: continuous state space

Diffusion processes

- diffusion process: continuous state-space $\boldsymbol{x} \in \mathbb{R}^d$
- dynamics described by overdamped Langevin equation

$$\dot{\boldsymbol{x}}(t) = \mu \boldsymbol{F}_t(\boldsymbol{x}(t)) + \sqrt{2\mu k_{\mathrm{B}} T}\boldsymbol{\xi}(t)$$

$\boldsymbol{F}_t(\boldsymbol{x})$ time-dependent force, μ mobility, T temperature

- $\boldsymbol{\xi}(t)$ Gaussian white noise: $\langle \boldsymbol{\xi}(t) \rangle = 0$, $\langle \xi_i(t) \xi_j(s) \rangle = \delta_{ij} \delta(t-s)$
- describes (interacting) Brownian particles in external force field

Fokker-Planck equation and entropy production

- equivalent description: Fokker-Planck equation for probability density $p_t(\boldsymbol{x})$

$$\partial_t p_t(\boldsymbol{x}) = -\boldsymbol{\nabla} \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})\big) \qquad \text{continuity equation}$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu\big(\boldsymbol{F}_t(\boldsymbol{x}) - k_{\mathrm{B}} T \boldsymbol{\nabla} \ln p_t(\boldsymbol{x})\big) \qquad \text{local mean velocity}$$

- short-time transition probability density Gaussian

$$p_{t+dt,t}(\boldsymbol{x}|\boldsymbol{y}) \simeq \left(\frac{1}{4\pi\mu k_{\mathrm{B}} T dt}\right)^{\frac{d}{2}} \exp\left[-\frac{1}{4\mu k_{\mathrm{B}} T dt}\Big\|\boldsymbol{x} - \big(\boldsymbol{y} + \mu \boldsymbol{F}_t(\boldsymbol{y}) dt\big)\Big\|^2\right]$$

- entropy production $\leftrightarrow$ local mean velocity

$$\Sigma = D_{\mathrm{KL}}\big(P(\Gamma)\|P^\dagger(\Gamma^\dagger)\big) = \frac{1}{\mu k_{\mathrm{B}} T} \int_0^\tau dt \int d\boldsymbol{x}\, \big\|\boldsymbol{\nu}_t(\boldsymbol{x})\big\|^2 p_t(\boldsymbol{x}) \geq 0$$

- $P^\dagger(\Gamma)$: path probability for time-reversed protocol $\boldsymbol{F}_t^\dagger(\boldsymbol{x}) = \boldsymbol{F}_{\tau-t}(\boldsymbol{x})$

Entropy production and thermodynamics

- equivalent expression for entropy production

$$\Sigma = \underbrace{\frac{1}{k_{\mathrm{B}}T}\left\langle \int_0^{\tau} dt\ \boldsymbol{F}_t(\boldsymbol{x}(t)) \circ \dot{\boldsymbol{x}}(t) \right\rangle}_{=-\frac{\Delta Q}{k_{\mathrm{B}}T}} + \Delta S \qquad\qquad S = -\int d\boldsymbol{x}\ \ln p_t(\boldsymbol{x}) p_t(\boldsymbol{x})$$

- second law of thermodynamics

$$\Delta S - \frac{\Delta Q}{k_{\mathrm{B}}T} = \Sigma \geq 0$$

- ΔS change in Gibbs-Shannon entropy of system
- ΔQ heat transfer from environment to system

Equilibrium and detailed balance

- in equilibrium: $\Sigma = 0 \Rightarrow \boldsymbol{\nu}_t(\boldsymbol{x}) = 0$ no flows
  - $\partial_t p_t(\boldsymbol{x}) = 0$: steady state $p^{\mathsf{st}}(\boldsymbol{x})$
  - $\boldsymbol{F}(\boldsymbol{x}) = k_{\mathsf{B}} T \boldsymbol{\nabla} \ln p^{\mathsf{st}}(\boldsymbol{x})$: conservative force $\boldsymbol{F}(\boldsymbol{x}) = -\boldsymbol{\nabla} U(\boldsymbol{x})$
- Boltzmann-Gibbs equilibrium density

$$p^{\mathsf{eq}}(\boldsymbol{x}) = Z^{-1} e^{-\frac{U(\boldsymbol{x})}{k_{\mathsf{B}} T}} \qquad \text{with} \qquad Z = \int d\boldsymbol{y}\, e^{-\frac{U(\boldsymbol{y})}{k_{\mathsf{B}} T}}$$

- equilibrium $\Leftrightarrow$ steady state in conservative force field
  - change of state $\partial_t p_t(\boldsymbol{x}) \neq 0 \Rightarrow \Sigma > 0$
  - nonconservative force $\boldsymbol{F}(\boldsymbol{x}) \neq -\boldsymbol{\nabla} U(\boldsymbol{x}) \Rightarrow \Sigma > 0$

Minimum entropy production

- minimum value of Σ for given change of state $p_0(\boldsymbol{x}) \to p_\tau(\boldsymbol{x})$?
  [Aurell, Mejia-Monasterio & Muratore-Ginanneschi, Phys. Rev. Lett. (2011)]

$$\inf_{\boldsymbol{\nu}_t, p_t} \left[\int_0^\tau dt \int d\boldsymbol{x} \left(\left\| \boldsymbol{\nu}_t(\boldsymbol{x}) \right\|^2 p_t(\boldsymbol{x}) - 2\psi_t(\boldsymbol{x}) \left[\partial_t p_t(\boldsymbol{x}) + \boldsymbol{\nabla} \cdot \left(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x}) \right) \right] \right) \right]$$

- minimum condition: gradient field $\boldsymbol{\nu}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla}\psi_t(\boldsymbol{x})$ with Hamilton-Jacobi equation

$$\partial_t \psi_t(\boldsymbol{x}) = \frac{1}{2} \left\| \boldsymbol{\nabla}\psi_t(\boldsymbol{x}) \right\|^2$$

- $\boldsymbol{\nu}_t^*(\boldsymbol{x}) = \mu(\boldsymbol{F}_t^*(\boldsymbol{x}) - T\boldsymbol{\nabla} \ln p_t^*(\boldsymbol{x})) \Rightarrow$ conservative force $\boldsymbol{F}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla} U_t^*(\boldsymbol{x})$

- optimal protocol: unique conservative force with constant entropy production rate

$$d_t \sigma_t^* = \frac{1}{\mu k_{\mathrm{B}} T} d_t \int d\boldsymbol{x} \left\| \boldsymbol{\nabla}\psi_t(\boldsymbol{x}) \right\|^2 p_t(\boldsymbol{x}) = 0$$

Relation to Wasserstein distance

- minimizing Σ dynamical problem: optimal process connecting initial and final state
- static problem: joint probability (coupling) $\Pi(\boldsymbol{x}, \boldsymbol{y})$ with marginals

$$\int d\boldsymbol{x}\ \Pi(\boldsymbol{x}, \boldsymbol{y}) = p_0(\boldsymbol{y}) \qquad \int d\boldsymbol{y}\ \Pi(\boldsymbol{x}, \boldsymbol{y}) = p_\tau(\boldsymbol{x})$$

- find optimal coupling $\Pi^*(\boldsymbol{x}, \boldsymbol{y})$ minimizing average distance

$$\mathcal{W}_2(p_\tau, p_0)^2 = \inf_{\Pi} \left(\int d\boldsymbol{x} \int d\boldsymbol{y}\ \|\boldsymbol{x} - \boldsymbol{y}\|^2 \Pi(\boldsymbol{x}, \boldsymbol{y}) \right)$$

- $\mathcal{W}_2(p_\tau, p_0)$ is called 2-Wasserstein distance: depends only on $p_0(\boldsymbol{x})$ and $p_\tau(\boldsymbol{x})$

Relation to Wasserstein distance

- central result of optimal transport theory: dynamic and static problem are equivalent [Benamou & Brenier, Numer. Math. (2000)]
- minimum entropy production $\triangleq$ Wasserstein distance [AD & Sakurai (2019)]

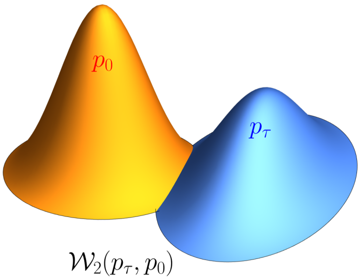
$$\Sigma^* = \frac{1}{\mu k_\mathrm{B} T \tau} \mathcal{W}_2(p_\tau, p_0)^2$$

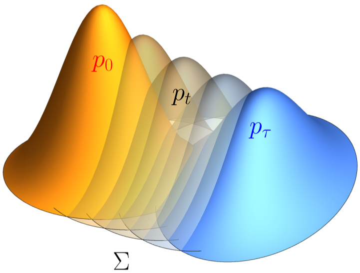
- recall $\Sigma^* = \tau \sigma^*$ with $\sigma^* = \text{const.}$

$$\sigma^* = \frac{1}{\mu k_\mathrm{B} T} u^2 \qquad \text{with} \qquad u = \frac{\mathcal{W}_2(p_\tau, p_0)}{\tau} \quad \text{“Wasserstein speed”}$$

- optimal process has constant speed with respect to Wasserstein distance
  Wasserstein speed $\rightarrow$ [Nakazato & Ito, Phys. Rev. Res. (2021)]

Relation to Wasserstein distance





Interim summary: diffusion processes

- optimal process is driven by conservative force
- optimal process has constant Wasserstein speed
- minimal entropy production $\hat{=}$ Wasserstein distance between initial and final state

$$\Sigma^* = \frac{1}{\mu k_{\mathrm{B}} T \tau} \mathcal{W}_2(p_\tau, p_0)^2$$

- minimal entropy production proportional to $1/\tau$ $\rightarrow$ fast process requires more dissipation

3. Jump processes: discrete state space

Jump processes

- discrete state space $i \in \{1, \ldots, N\}$
- transition from j to i: rate process with transition rates $W_t(i,j) \geq 0$
- occupation probability $p_t(i)$ follows Master equation

$$d_t p_t(i) = \sum_j \Big(W_t(i,j) p_t(j) - W_t(j,i) p_t(i) \Big)$$

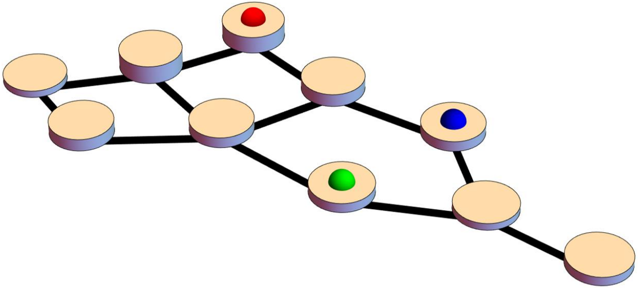
- short-time transition probability ($W_t(i,i) = 0$)

$$p_{t+dt,t}(i|j) \simeq \Big(1 - \sum_k W_t(k,j) dt \Big) \delta_{ij} + W_t(i,j) dt$$

- entropy production

$$\Sigma = \int_0^\tau dt \sum_{i,j} W_t(i,j) p_t(j) \ln \left(\frac{W_t(i,j) p_t(j)}{W_t(j,i) p_t(i)} \right) \geq 0$$

Jump processes



Thermodynamics

- equivalent expression for entropy production

$$\Sigma = \int_0^\tau dt \sum_{i,j} W_t(i,j) p_t(j) \ln \left(\frac{W_t(i,j)}{W_t(j,i)} \right) + \Delta S \qquad \text{with} \qquad S = -\sum_i \ln p_t(i) p_t(i)$$

- thermodynamic interpretation of transition rates

$$W_t(i,j) = \omega_t(i,j) \exp\left[-\frac{\beta}{2} A_t(i,j) \right]$$

$\omega_t(i,j) = \omega_t(j,i) \geq 0$ traffic, $\quad A_t(i,j) = -A_t(j,i)$ change in energy $\triangleq$ forces

- local detailed balance condition

$$\ln \left(\frac{W_t(i,j)}{W_t(j,i)} \right) = -\beta A_t(i,j) \quad \text{or} \quad W_t(i,j) = 0 \Leftrightarrow W_t(j,i) = 0$$

Equilibrium and detailed balance

- detailed balance $W_t(i,j)p_t(j) = W_t(j,i)p_t(j)$ for all (i,j)

$$\Rightarrow \quad d_t p_t(i) = 0 \qquad \text{and} \qquad \ln\left(\frac{W(i,j)}{W(j,i)}\right) = \ln p^{\text{st}}(i) - \ln p^{\text{st}}(j) = -\beta\big(U(i) - U(j)\big)$$

- equilibrium $p^{\text{eq}}(i) = Z^{-1}e^{-\beta U(i)} \Leftrightarrow$ steady state in an energy landscape
- time-dependent state $d_t p_t \neq 0$ or nonconservative driving $\Rightarrow \Sigma > 0$
- so far: completely analog to diffusion case

(Non-)Uniqueness of conservative forces

- diffusion case: one-to-one relation $U_t(\boldsymbol{x}) \leftrightarrow p_t(\boldsymbol{x})$
- jump case: one-to-one relation $U_t(i) \leftrightarrow p_t(i)$ only for fixed $\omega_t(i,j)$
- equilibrium state $p^{\mathrm{eq}}(i) = Z^{-1} e^{-\beta U(i)}$ independent of $\omega_t(i,j)$
- different combinations of $U_t(i)$ and $\omega_t(i,j)$ with same time evolution

Time evolution at vanishing entropy production

- minimum value of Σ for given change of state $p_0 \to p_\tau$?
- without any constraints: trivial answer $\Sigma = 0$!
  [Muratore-Ginanneschi, Mejia-Monasterio & Peliti, J. Stat. Phys. (2013)]
- define new transition rates ($\alpha \geq 1$) [AD, J. Phys. A (2022)]

$$W_t^\alpha(i,j) = \frac{1}{2p_t(j)}\Big(\alpha + \mathsf{sign}\big(J_t(i,j)\big)\Big)\Big|J_t(i,j)\Big|, \qquad J_t(i,j) = W_t(i,j)p_t(j) - W_t(j,i)p_t(i)$$

$$J_t^\alpha(i,j) = J_t(i,j) \quad \Rightarrow \quad d_t p_t(i) = \sum_j J_t^\alpha(i,j) \qquad \text{same time evolution}$$

- vanishing entropy production rate

$$\sigma_t^\alpha = \mathsf{atanh}\left(\frac{1}{\alpha}\right)\sum_{i,j}\Big|J_t(i,j)\Big| \xrightarrow[\alpha\to\infty]{} 0$$

Time evolution at vanishing entropy production

- rates $W_t^\alpha(i,j)$ correspond to fast transitions with small asymmetry
- overall transition rate measured by dynamical activity

$$\mathcal{A}_t = \sum_{i,j} W_t(i,j) p_t(j) \qquad \Rightarrow \qquad \mathcal{A}_t^\alpha = \frac{\alpha}{2} \sum_{i,j} \Big| J_t(i,j) \Big| \xrightarrow[\alpha \to \infty]{} \infty$$

- $\lim_{\alpha\to\infty} \sigma_t^\alpha \mathcal{A}_t^\alpha = \frac{1}{2}\Big(\sum_{i,j} |J_t(i,j)|\Big)^2$ tradeoff between dissipation and activity
- minimizing entropy "interesting" only with additional constraints

Fixed local traffic

- first possibility: fix local traffic $\omega_t(i,j)$ and p_t [Remlein & Seifert, Phys. Rev. E (2021)]

$$W_t(i,j) = \omega_t(i,j)\exp\left[-\frac{\beta}{2}A_t(i,j)\right]$$

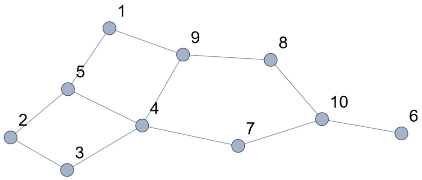
- conservative forces $A_t(i,j) = U_t(i) - U_t(j)$
- minimize σ_t with respect to $A_t(i,j) \Rightarrow A_t^*(i,j) \neq U_t(i) - U_t(j)$
- surprising result: entropy production rate minimized for nonconservative driving!
- connection between conservative forces and minimum entropy for jump processes?

Jump processes and graphs

- represent state space of jump process as graph
- states $i \in \{1, \ldots, N\} \to$ vertices

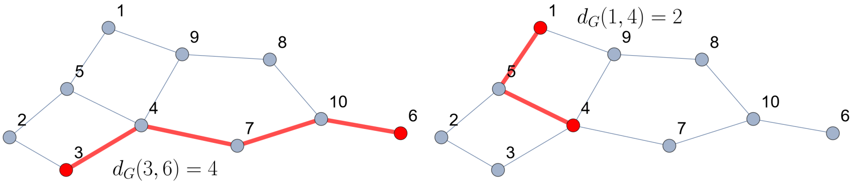
$$W_t(i,j) = k(i,j)\omega_t(i,j)\exp\left[-\frac{\beta}{2}A_t(i,j)\right] \qquad k(i,j) = k(j,i) = \begin{cases} 1 & i \leftrightarrow j \text{ allowed} \\ 0 & i \leftrightarrow j \text{ forbidden} \end{cases}$$

- $k(i,j)$ connectivity matrix of graph $\to$ edges



Wasserstein distance on graphs

- graph distance $d_G(i,j)$: length of shortest path between vertices i and j



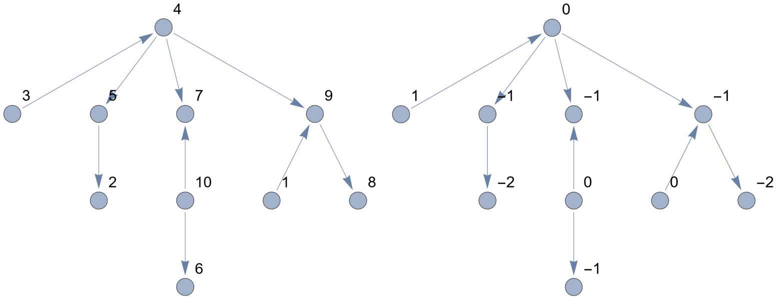
- Wasserstein distance between p_0 and p_τ

$$\mathcal{W}_G(p_\tau, p_0) = \inf_{\Pi} \left(\sum_{i,j} d_G(i,j)\Pi(i,j) \right) \quad \text{with}$$

$$\Pi(i,j) \geq 0, \qquad \sum_i \Pi(i,j) = p_0(j), \qquad \sum_j \Pi(i,j) = p_\tau(i)$$

Optimal coupling and energy landscape

- optimal coupling $\Pi^*(i,j)$ defines directed tree



- can always choose consistent “energy landscape” $\varepsilon(i)$ with $\Delta\varepsilon = \pm 1$
- mathematically: consequence of Kantorvich duality

Relation to jump processes

- computation of Wasserstein distance static problem
- what is the equivalent continuous-time dynamical problem?
- minimize average number of transitions $\mathcal{N} = \int_0^\tau dt\ \mathcal{A}_t$ at fixed connectivity $k(i,j)$ [AD, J. Phys. A (2022)]

$$\mathcal{W}_G(p_\tau, p_0) = \mathcal{N}^* = \inf_{W_t, p_t} \underbrace{\left(\int_0^\tau dt \sum_{i,j} W_t(i,j) p_t(j) \right)}_{=\mathcal{N}} \qquad \text{with}$$

$$d_t p_t(i) = \sum_j \big(W_t(i,j) p_t(j) - W_t(j,i) p_t(i) \big), \qquad W_t(i,j) = 0 \quad \text{if} \quad k(i,j) = 0$$

Optimal and symmetrized transition rates

- jump process minimizing $\mathcal{N}$ has transition rates

$$W_t^*(i,j) = \frac{\Pi^*(i,j)}{\tau p_t(j)} \qquad \text{with} \qquad p_t(i) = \left(1 - \frac{t}{\tau}\right) p_0(i) + \frac{t}{\tau} p_\tau(i)$$

- $\Pi^*(i,j) > 0 \Rightarrow \Pi^*(j,i) = 0$ one-directional transitions $\Rightarrow \Sigma = \infty$
- physically: minimizing $\mathcal{N}$ corresponds to $T \to 0$ limit $\Rightarrow \beta \Delta U \to \pm\infty$
- symmetrize transition rates ($\alpha \geq 1$)

$$W_t^\alpha(i,j) = \begin{cases} \frac{\alpha+1}{2} \frac{\Pi^*(i,j)}{\tau p_t(j)} & \text{if} \quad \Pi^*(i,j) > 0 \\ \frac{\alpha-1}{2} \frac{\Pi^*(j,i)}{\tau p_t(j)} & \text{if} \quad \Pi^*(j,i) > 0 \end{cases}$$

$$\Rightarrow \quad \Sigma^\alpha = 2\text{atanh}\left(\frac{1}{\alpha}\right) \mathcal{N}^*, \qquad \mathcal{N}^\alpha = \alpha \mathcal{N}^*$$

Minimum entropy production

- Σ^α is minimum entropy production for jump process with $\mathcal{N}^\alpha$ average transitions
- $\mathcal{N}^\alpha = \mathcal{N}$: relation between minimum entropy production and Wasserstein distance

$$\Sigma^* = 2\mathcal{N}^* \text{atanh}\left(\frac{\mathcal{N}^*}{\mathcal{N}}\right) = 2\mathcal{W}_G(p_\tau, p_0)\text{atanh}\left(\frac{\mathcal{W}_G(p_\tau, p_0)}{\mathcal{N}}\right) \qquad (\mathcal{N}, k(i,j)) \text{ fixed}$$

- large number of transitions $\mathcal{N} \gg \mathcal{W}_G(p_\tau, p_0)$

$$\Sigma^* \simeq \frac{2\mathcal{W}_G(p_\tau, p_0)^2}{\mathcal{N}} \qquad \text{diffusion case:} \quad \Sigma^* = \frac{\mathcal{W}_2(p_\tau, p_0)^2}{\mu k_\mathrm{B} T \tau}$$

- remark: [Van Vu & Hasegawa, Phys. Rev. Lett. (2021)]

$$\Sigma \geq \frac{\mathcal{W}_\mathrm{c}(p_\tau, p_0)^2}{\tau}$$

definition of $\mathcal{W}_\mathrm{c}$ depends on rates

Precision-dissipation tradeoff

- for arbitrary processes: lower bound $\Sigma \geq \Sigma^*$

$$\Sigma \geq 2\mathcal{W}_G(p_\tau, p_0)\text{atanh}\left(\frac{\mathcal{W}_G(p_\tau, p_0)}{\mathcal{N}}\right)$$

- $\mathcal{N}$ average number of transitions to transform p_0 into p_τ
  - large $\mathcal{N}$: many transitions in the "wrong" direction $\rightarrow$ low precision
  - small $\mathcal{N}$: almost all transitions in the "correct" direction $\rightarrow$ high precision

- precise operations require large dissipation

$$\Sigma \underset{\mathcal{N} \simeq \mathcal{W}_G}{\geq} \mathcal{W}_G(p_\tau, p_0) \ln\left(\frac{1}{1 - \frac{\mathcal{W}_G(p_\tau, p_0)}{\mathcal{N}}}\right)$$

- if $\mathcal{N} \simeq \tau\mathcal{A} \rightarrow$ tradeoff between dissipation and speed

Conservative forces and optimal process

- from properties of optimal coupling: energy landscape $\varepsilon(i)$ with $\Delta\varepsilon = \pm 1$

$$\beta U_t^*(i) = -\ln p_t(i) + 2\text{atanh}\left(\frac{\mathcal{W}_G(p_\tau, p_0)}{\mathcal{N}}\right)\varepsilon(i)$$

- optimal process with Σ^* driven by conservative forces
- constant speed with respect to Wasserstein distance

$$\mathcal{A}^* = \frac{\mathcal{W}_G(p_{t+dt}, p_t)}{dt} = \frac{\mathcal{W}_G(p_\tau, p_0)}{\tau}, \qquad \Sigma^* = \tau\sigma^* = \tau\mathcal{A}^*\text{atanh}\left(\frac{\mathcal{A}^*}{\mathcal{A}}\right)$$

- optimal process not unique: interpolation p_t arbitrary

Lower and upper bounds on Wasserstein distance

- computing Wasserstein distance: expensive combinatorial problem
- explicit expressions only in simple cases
  - one-dimensional chain $\mathcal{W}_G(p,q) = \sum_{i=1}^N \left| \sum_{j=1}^i (p(j) - q(j)) \right|$
  - complete graph $\mathcal{W}_G(p,q) = \frac{1}{2}\sum_{i=1}^N |p(i) - q(i)| = \delta(p,q)$ total variation distance
- complete graph has minimal distance between any two vertices $\Rightarrow \mathcal{W}_G(p,q) \geq \delta(p,q)$

$$\Sigma \geq 2\delta(p_\tau, p_0)\text{atanh}\left(\frac{\delta(p_\tau, p_0)}{\mathcal{N}}\right)$$

[Shiraishi, Funo & Saito, Phys. Rev. Lett. (2018)]

- maximal distance between any two vertices: diameter D_G of graph $\Rightarrow \mathcal{W}_G(p,q) \leq D_G$

Diffusion and jump processes

	diffusion, (μ, T)	jump process, ω_t	jump process, $\mathcal{A}_t$
force	conservative	nonconservative	conservative
$U_t \leftrightarrow p_t$	one-to-one	one-to-one	degenerate
minimum entropy	$\frac{\mathcal{W}_2(p_\tau, p_0)^2}{\mu k_B T \tau}$	$\frac{1}{2}\sigma_t^{\text{cons}} \leq \sigma_t^* \leq \sigma_t^{\text{cons}}$	$\mathcal{W}_G(p_\tau, p_0)\text{atanh}\left(\frac{\mathcal{W}_G(p_\tau, p_0)}{\mathcal{N}}\right)$
optimal process	constant speed	???	constant speed

- diffusion process: calculate $\mathcal{W}_2(p_\tau, p_0) \Leftrightarrow$ minimize Σ at fixed (μ, T)
- jump process: calculate $\mathcal{W}_G(p_\tau, p_0) \Leftrightarrow$ minimize Σ at fixed $\mathcal{N} \Leftrightarrow$ minimize $\mathcal{N}$

Thank you for your attention!

J. Phys. A **55**, 094001 (2022)

Minimum entropy production rate

- minimum value of Σ for given change of state $p_0(\boldsymbol{x}) \to p_\tau(\boldsymbol{x})$?
- first step: fix process $p_t(\boldsymbol{x})$, $t \in [0, \tau]$

$$\Sigma = \int_0^\tau dt\ \sigma_t \qquad \text{with} \qquad \sigma_t = \frac{1}{\mu k_\mathrm{B} T} \int d\boldsymbol{x}\ \left\|\boldsymbol{\nu}_t(\boldsymbol{x})\right\|^2 p_t(\boldsymbol{x})$$

$$\text{and} \qquad \partial_t p_t(\boldsymbol{x}) = -\boldsymbol{\nabla} \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})\big)\ (*)$$

- minimize entropy production rate σ_t with respect to $\boldsymbol{\nu}_t(\boldsymbol{x})$ under constraint $(*)$

$$\inf_{\boldsymbol{\nu}_t} \left[\int d\boldsymbol{x}\ \left\|\boldsymbol{\nu}_t(\boldsymbol{x})\right\|^2 p_t(\boldsymbol{x}) - 2 \int d\boldsymbol{x}\ \psi_t(\boldsymbol{x}) \Big(\partial_t p_t(\boldsymbol{x}) + \boldsymbol{\nabla} \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})\big) \Big) \right]$$

- $\psi_t(\boldsymbol{x})$ Lagrange multiplier $\to$ compute Euler-Lagrange equations

Minimum entropy production and conservative forces

- minimum condition: $\boldsymbol{\nu}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla}\psi_t(\boldsymbol{x})$ gradient field

$$\boldsymbol{\nu}_t^*(\boldsymbol{x}) = \mu\big(\boldsymbol{F}_t^*(\boldsymbol{x}) - T\boldsymbol{\nabla}\ln p_t(\boldsymbol{x})\big) \quad \Rightarrow \quad \boldsymbol{F}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla}U_t(\boldsymbol{x}) \quad \text{conservative force}$$

- minimum is unique: $\boldsymbol{\nabla}\cdot\big(p_t(\boldsymbol{x})\boldsymbol{\nabla}\psi_t(\boldsymbol{x})\big) = \boldsymbol{\nabla}\cdot\big(p_t(\boldsymbol{x})\boldsymbol{\nabla}\phi_t(\boldsymbol{x})\big) = \partial_t p_t(\boldsymbol{x})$
  $\Rightarrow \boldsymbol{\nabla}\psi_t(\boldsymbol{x}) = \boldsymbol{\nabla}\phi_t(\boldsymbol{x})$

- entropy production rate minimized by unique conservative force $\boldsymbol{F}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla}U_t(\boldsymbol{x})$
  [Maes & Netocny, J. Stat. Phys. (2014)]

Excess and housekeeping entropy

- system driven by a time-dependent nonconservative force $\boldsymbol{F}_t(\boldsymbol{x})$
- can find conservative force $\boldsymbol{F}_t^*(\boldsymbol{x}) = -\boldsymbol{\nabla} U_t(\boldsymbol{x})$ with same time evolution
- entropy production rate has two positive contributions

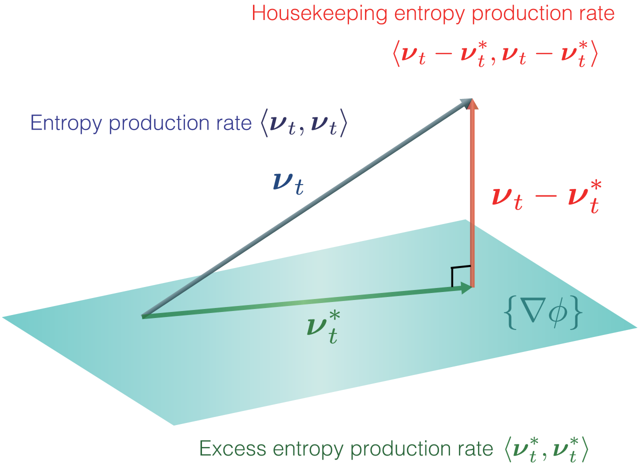
$$\sigma_t = \sigma_t^* + (\sigma_t - \sigma_t^*)$$

  - σ_t^* minimum entropy production for time evolution $p_t(\boldsymbol{x})$ ("excess entropy")
  - $\sigma_t - \sigma_t^*$ additional entropy production from nonconservative flows ("housekeeping entropy")

- corresponds to orthogonal terms in local mean velocity
  [AD, Sasa & Ito, Phys. Rev. Res. (2022)]

$$\int d\boldsymbol{x}\ \boldsymbol{\nu}_t^*(\boldsymbol{x}) \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) - \boldsymbol{\nu}_t^*(\boldsymbol{x})\big) p_t(\boldsymbol{x}) = \int d\boldsymbol{x}\ \psi_t(\boldsymbol{x}) \boldsymbol{\nabla} \cdot \Big(\big(\boldsymbol{\nu}_t(\boldsymbol{x}) - \boldsymbol{\nu}_t^*(\boldsymbol{x})\big) p_t(\boldsymbol{x})\Big) = 0$$

Excess and housekeeping entropy



[AD, Sasa & Ito, Phys. Rev. Res. (2022)]

Gaussian processes

- in general: no explicit solution for optimal protocol $U_t(\boldsymbol{x})$
- if initial and final state are Gaussian [AD, Sakurai, 2019]

$$U_t(\boldsymbol{x}) = -\frac{1}{\mu}\dot{\boldsymbol{m}}_t \cdot \boldsymbol{x} + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{m}_t) \cdot \boldsymbol{K}_t(\boldsymbol{x} - \boldsymbol{m}_t)$$

$$\boldsymbol{m}_t = \frac{t}{\tau}\boldsymbol{m}_\tau + \left(1 - \frac{t}{\tau}\right)\boldsymbol{m}_0$$

$$\boldsymbol{K}_t = k_{\mathrm{B}} T \boldsymbol{\Xi}_t^{-1} - \frac{1}{\mu}\int_0^\infty ds\ e^{-s\boldsymbol{\Xi}_t}\dot{\boldsymbol{\Xi}}_t e^{-s\boldsymbol{\Xi}_t}$$

$$\boldsymbol{\Xi}_t = \sqrt{\boldsymbol{\Xi}_0^{-1}}\left(\frac{t}{\tau}\sqrt{\sqrt{\boldsymbol{\Xi}_0}\boldsymbol{\Xi}_\tau\sqrt{\boldsymbol{\Xi}_0}} + \left(1 - \frac{t}{\tau}\right)\boldsymbol{\Xi}_0\right)^2\sqrt{\boldsymbol{\Xi}_0^{-1}}$$

- mean $\boldsymbol{m}_t$ and covariance matrix $\boldsymbol{\Xi}_t$ interpolate between initial and final value

Gaussian processes

- expressions simplify if initial and final covariance matrix commute $\mathbf{\Xi}_0 \mathbf{\Xi}_\tau = \mathbf{\Xi}_\tau \mathbf{\Xi}_0$

$$U_t(\boldsymbol{x}) = -\frac{1}{\mu} \dot{\boldsymbol{m}}_t \cdot \boldsymbol{x} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{m}_t) \cdot \boldsymbol{K}_t (\boldsymbol{x} - \boldsymbol{m}_t)$$

$$\boldsymbol{m}_t = \frac{t}{\tau} \boldsymbol{m}_\tau + \left(1 - \frac{t}{\tau}\right) \boldsymbol{m}_0$$

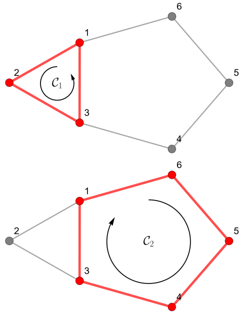
$$\boldsymbol{K}_t = k_\mathsf{B} T \mathbf{\Xi}_t^{-1} - \frac{1}{2\mu} \mathbf{\Xi}_t^{-1} \dot{\mathbf{\Xi}}_t$$

$$\mathbf{\Xi}_t = \left(\frac{t}{\tau} \sqrt{\mathbf{\Xi}_\tau} + \left(1 - \frac{t}{\tau}\right) \sqrt{\mathbf{\Xi}_0} \right)^2$$

Cycle affinities

- characterize nonconservative driving via cycle affinities
- state space $\triangleq$ connected graph
- decompose graph into cycles and calculate affinities

$$A(\mathcal{C}_1) = \ln\left(\frac{W(1,3)W(3,2)W(2,1)}{W(3,1)W(1,2)W(2,3)}\right)$$



- if $A(\mathcal{C}_1) = 0$ can find consistent energy landscape $E(1)$, $E(2)$, $E(3)$ along cycle

$$E(2) = E(1) + \beta^{-1} \ln\left(\frac{W(1,2)}{W(2,1)}\right)$$

- if $A(\mathcal{C}_1) \neq 0$ no consistent energy landscape $\rightarrow$ nonconservative driving

Cycle affinities

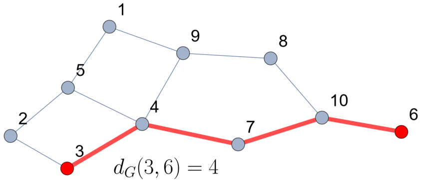
- conservative forces only if $A(\mathcal{C}) = 0$ for all $\mathcal{C}$ $\Leftrightarrow$ steady state satisfies detailed balance
- in steady state [Schnakenberg, Rev. Mod. Phys. (1976)]

$$\sigma^{\mathsf{st}} = \sum_{\mathcal{C}} J^{\mathsf{st}}(\mathcal{C}) A(\mathcal{C})$$

- minimum σ_t at fixed $\omega_t(i,j)$ leads to $A(\mathcal{C}) \neq 0$ [Remlein & Seifert, Phys. Rev. E (2021)]

Properties of optimal coupling

- optimal coupling $\Pi^*(i,j)$ not unique
  - shortest path not unique
  - $\Pi^*(6,3)$ moves probability from $3 \to 6$; same as $3 \to 4 \to 7 \to 10 \to 6$



- optimal coupling one-directional: $\Pi^*(i,j) > 0 \Rightarrow \Pi^*(j,i) = 0$
- edges with $\Pi^*(i,j) > 0$ can be chosen as tree

Minimum entropy production rate for given time evolution

- instead of p_0, p_τ and $\mathcal{N}$: specify time evolution p_t, $t \in [0, \tau]$ and activity $\mathcal{A}_t$

$$\sigma_t^* = 2\mathcal{A}_t^* \,\mathsf{atanh}\left(\frac{\mathcal{A}_t^*}{\mathcal{A}_t}\right) \quad \text{with}$$

$$\mathcal{A}_t^* = \frac{\mathcal{W}_G(p_{t+dt}, p_t)}{dt} \quad \text{Wasserstein speed} \triangleq \text{minimum activity}$$

- fixed p_t and $\mathcal{A}_t$: can further reduce entropy production even for conservative forces
- minimum entropy production process has constant Wasserstein speed $\mathcal{A}^* = \frac{\mathcal{W}_G(p_\tau, p_0)}{\tau}$

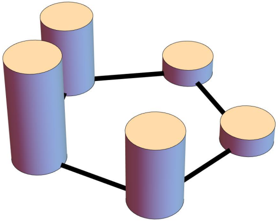
Example: pumping on a ring

- ring with N sites
- time-dependent energy landscape

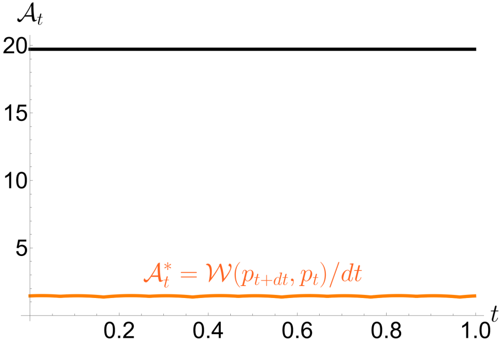
$$U_t(i) = \varepsilon_0\left(\frac{1}{2} - \frac{1}{2}\cos\left[2\pi\left(t + \frac{i-1}{N}\right)\right]\right)$$
$$W_t(i,j) = \omega_0 \exp\left[-\frac{\beta}{2}(U_t(i) - U_t(j))\right]$$

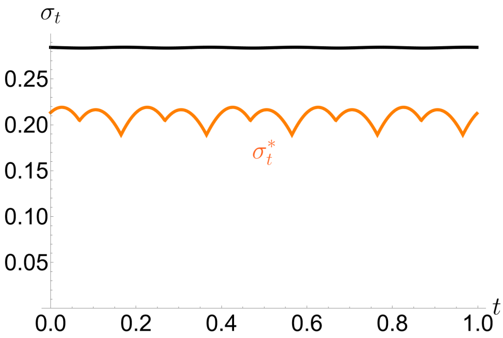
- potential minimum moves around ring $\to$ current
- fix p_t, $\mathcal{A}_t$ and minimize σ_t

Example: pumping on a ring

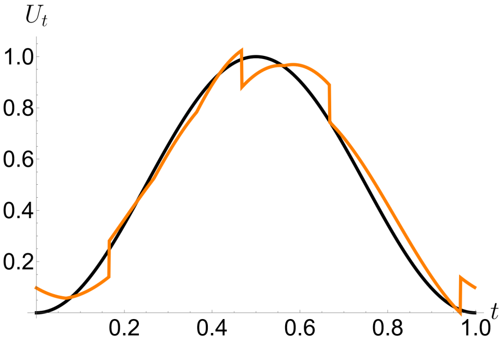


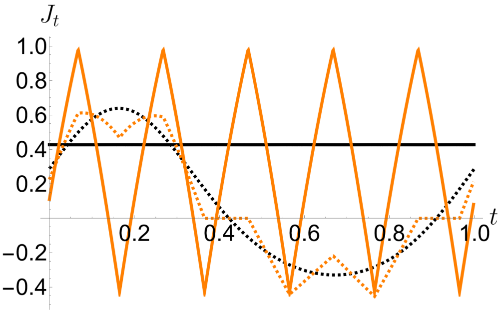
Fast transitions $\omega_0 = 10$



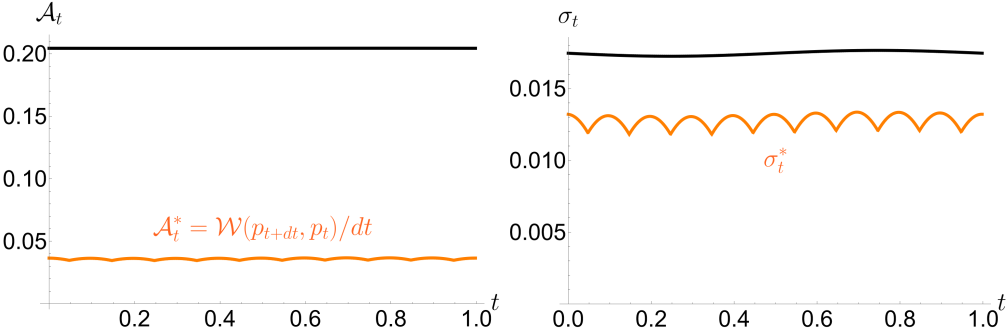


Fast transitions $\omega_0 = 10$

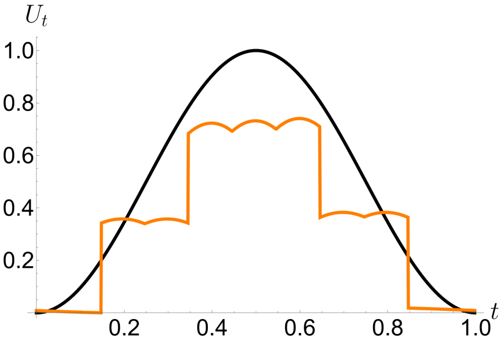


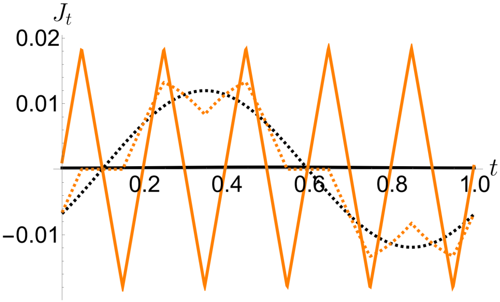


Slow transitions $\omega_0 = 0.1$



Slow transitions $\omega_0 = 0.1$





Conservative forces and detailed balance

- jump process, fixed $\omega_t(i,j)$: minimum entropy production rate for nonconservative force
- however: unique conservative force for given process p_t
- meaning of conservative force?
- conservative force minimizes

$$\eta_t = 2\sum_{i,j} W_t(i,j)p_t(j)\ln\left(\frac{W_t(i,j)p_t(j)}{W_t(j,i)p_t(i)}\right) - \left(\sqrt{W_t(i,j)p_t(j)} - \sqrt{W_t(j,i)p_t(i)}\right)^2$$

- similar properties to σ_t: $\eta_t \geq 0$ and $\eta_t = 0$ only in equilibrium

$$\sigma_t \leq \eta_t \leq 2\sigma_t$$

- η_t convex measure of detailed balance violation $\rightarrow$ "pseudo-entropy"?