The Lifting of Stochastic Processes and Entropy Production Rates

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Reference

Entropy Production and Its Potential Energy Representations:
Clausius' vs. Kelvin's views of the 2nd Law and irreversibility.
Yue Wang and Hong Qian, 2018.
https://arxiv.org/pdf/1805.09530.pdf

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Motivation

System with potential

- Consider a gradient force field $\boldsymbol{G}(\boldsymbol{x}) = \nabla g(\boldsymbol{x})$. Choose any curve C from P to Q.
- The work done along C is $\int_C \boldsymbol{G} \cdot \mathrm{d}\boldsymbol{s} = g(Q) - g(P)$, which is path independent.
- The reason is the existence of a potential function. Or equivalently, the work done along any closed path is 0.

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System with potential

- Consider an irreducible Markov chain with transition rate q_{ij}. The potential gain of a trajectory $i_1, \cdots, i_k$ is

$$\sum_{j=1}^{k-1} \log \frac{q_{i_{j+1} i_j}}{q_{i_j i_{j+1}}}.$$

- In general there is no global potential.

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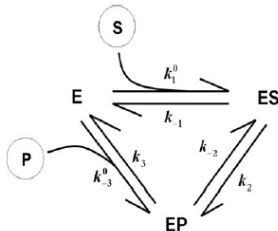
Open the cycle

- We can lift the above example to a line:

  $\cdots E \leftrightarrow ES \leftrightarrow EP \leftrightarrow E \leftrightarrow ES \leftrightarrow EP \leftrightarrow E \leftrightarrow ES \leftrightarrow EP \leftrightarrow \cdots$

- One can calculate the potential gain of a trajectory by its two ends alone. There exists a global potential.

- Goal: construct a new Markov chain with global potential. Different states have different potentials (calculated symbolically).

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Graph Theory

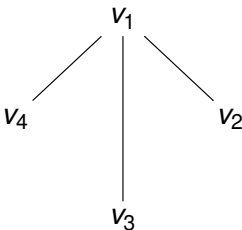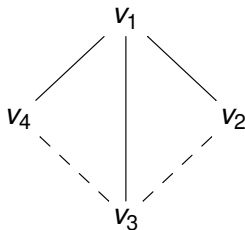- Consider an undirected connected graph with vertex set V and edge set E. Its first Betti number is $b(V, E) = |E| - |V| + 1$. This is the number of independent cycles.

- $b(V, E) \geq 0$. $b(V, E) = 0$ if and only if (V, E) is a tree. $b(V, E) = 1$ if and only if (V, E) has exactly one cycle.

- A subgraph of graph (V, E) is called a spanning tree if its vertex set is V, and it is a tree.

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Lemma

For graph (V, E), we can find $b(V, E)$ cycles $c_1, c_2, \cdots, c_{b(V,E)}$, such that each c_i contains an edge e_i^* which is not contained in any cycle c_j with $j \neq i$.

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- Now assign a direction for each edge in E. Consider the connection matrix ∂.

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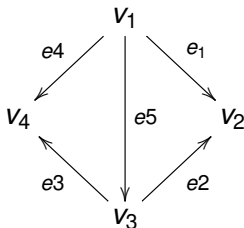
- $\partial = \begin{bmatrix} -1 & 0 & 0 & -1 & -1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}$

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Definition

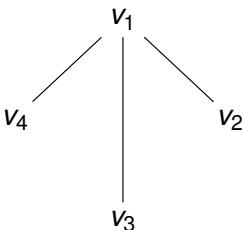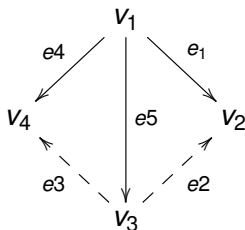An *algebraic cycle C* is an element in the null space of ∂.

The cycle v_1, v_2, v_3, v_4 (e_1, $-e_2$, e_3, $-e_4$) corresponds to an algebraic cycle, $(1, -1, 1, -1, 0)$.

Lemma

The $b(V, E)$ cycles in the previous lemma constitute a basis of the algebraic cycle space. When decomposing a cycle with this basis, the coefficients are the corresponding numbers of special edges.

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- Edge e_2 corresponds to $c_1 = (v_1, v_2, v_3)$ $(1, -1, 0, 0, -1)$.
  Edge e_3 corresponds to $c_2 = (v_1, v_3, v_4)$ $(0, 0, 1, -1, 1)$.

- $\{c_1, c_2\}$ is a basis, such that cycle $c_3 = (v_1, v_2, v_3, v_4)$
  $(1, -1, 1, -1, 0)$ can be expressed as $c_3 = c_1 + c_2$.

- Edges e_2 and e_3 appear once in c_3, that is why the
  coefficients are both 1.

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Potential of Markov chain

- For a Markov chain, the potential gain of a trajectory $i_1, \cdots, i_k$ is

$$\sum_{j=1}^{k-1} \log \frac{q_{i_{j+1} i_j}}{q_{i_j i_{j+1}}}.$$

- The potential gain only depends on the net number of each edge.

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Potential of Markov chain

- A function $f(i)$ is a **global potential** if the potential gain of a trajectory $i_1, \cdots, i_k$ is $f(i_k) - f(i_1)$.
- Global potential exists if and only if the potential gain of a closed trajectory is 0.
- A global potential is **proper** if different states have different potentials. (In the following, potential is always calculated symbolically.)

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Definition

Let X be a topological space. A covering space of X is a topological space C together with a continuous surjective map $p : C \to X$, such that for every $x \in X$, there exists an open neighborhood U of x, such that $p^{-1}(U)$ is a union of disjoint open sets in C, each of which is mapped homeomorphically onto U by p.

A path in X can be uniquely lifted to C with a given starting point. A path in C can be folded back to X.

Definition

A covering space is a universal covering space if it is simply connected.

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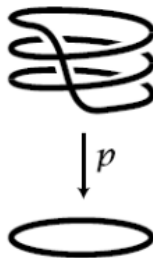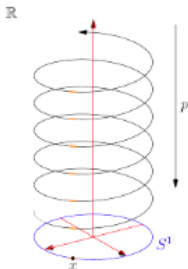
Examples of covering space.

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Algebraic Topology

- General space, such as connected graph or *n* dimensional torus, has universal covering space. If exists, universal covering space is unique.
- Universal covering space is a covering space of any covering space.
- For a finite graph, its covering space is still a graph. Each vertex in the covering space has an image vertex in the original graph, and they have the same neighbors.
- We say that the covering space is locally isomorphic to the original graph.

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Intuition

- For a finite irreducible Markov chain, the goal is to construct a new Markov chain with proper global potential.
- In the original Markov chain, cycles have non-zero potential gains, therefore we need to expand all cycles.
- A trivial idea: use the universal covering space of the original Markov chain. It is simply connected, therefore has no cycle. Global potential exists. The problem is that different states have the same potential.

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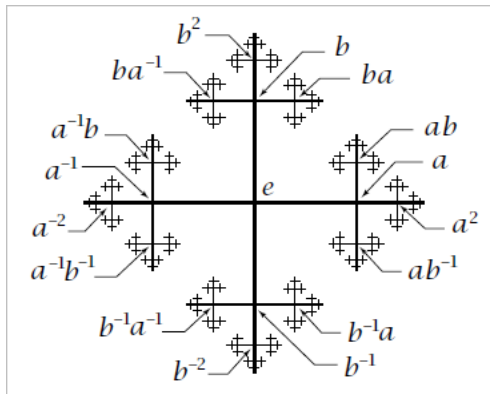
Universal covering space of wedge of two cycles. Corresponds to its fundamental group.

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Intuition

- Glue states with the same potential together, and the result is $\mathbb{Z}^2$, which is the abelianization of the fundamental group.
- $\mathbb{Z}^2$ is the fundamental group of $\mathbb{T}^2$. Implies the *n*-dimensional torus might be useful.

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Theorem (lifted version, Wang & Qian 2018)

For a finite Markov chain where $q_{ij} > 0 \Leftrightarrow q_{ji} > 0$, one can find another Markov chain with a proper global potential, and it is locally isomorphic with the original Markov chain. Such lifting is unique up to isomorphism.

Theorem (torus version, Wang & Qian 2018)

A Markov chain can be embedded into n-torus $\mathbb{T}^n$, such that a closed path has 0 potential gain if and only if it is homotopy trivial (can continuously shrink to a point).

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Method

- Let $n = b(V, E)$. Consider n-dimensional torus $\mathbb{T}^n$, which is a unit n-dimensional hypercube with opposite hypersurfaces glued together.
- Embed the spanning tree inside the torus. For each special edge, assign a different pair of hypersurfaces. Connect each special edge across the corresponding hypersurfaces.
- Lift $\mathbb{T}^n$ with the embedded graph to $\mathbb{R}^n$, its universal covering space.
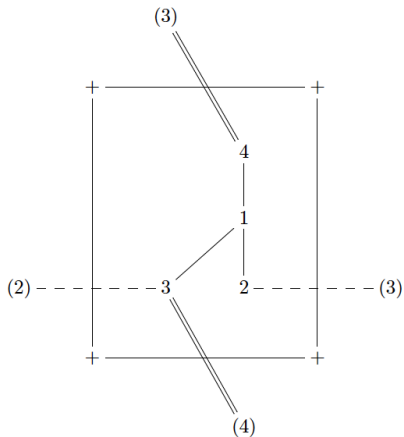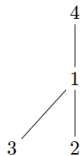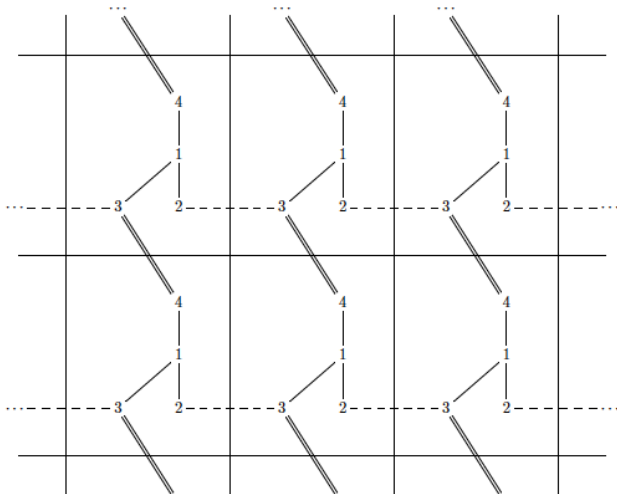
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For a finite Markov chain where $q_{ij} > 0 \Leftrightarrow q_{ji} > 0$, one can find another Markov chain with a proper global potential, and it is locally isomorphic with the original Markov chain. Such lifting is unique up to isomorphism.

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Proof: existence of global potential

- We have a natural coordinate structure $\mathbb{Z}^n$. Notice that the only way to change one coordinate, namely to cross one boundary, is to pass the corresponding special edge.

- For any closed path, the net number of each special edge is 0, since the coordinate change is 0.

- Fold the path back to the original Markov chain, then it is an algebraic cycle. An algebraic cycle is the linear combination of cycles in the basis, where the coefficients are the net numbers of special edges. Thus the net number of any edge is 0, and the potential gain is 0.

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Proof: properness of global potential

- If a path has 0 potential gain, then first the starting point and the ending point should be of the same state in the original Markov chain, otherwise the number of edges containing the starting point is odd.

- If the starting point and the ending point have the same state, but in different hypercubes, then at least one coordinate is different, thus the net number of the corresponding special edge is not 0. Therefore the potential gain is non-zero, a contradiction.

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Proof: uniqueness of lifting

- Consider the unique universal covering space. It is also the universal covering space of the lifted chain. States with the same potential are exactly the pre-image of a state in the lifted chain.
- Glue these states together, then the result is exactly the lifting chain. Therefore the lifting is independent with the choice of spanning tree.
- This finishes the proof of the lifted version.

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Theorem (torus version, Wang & Qian 2018)

A Markov chain can be embedded into n-torus $\mathbb{T}^n$, such that a closed path has 0 potential gain if and only if it is homotopy trivial (can continuously shrink to a point).

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Proof

- We have shown that in the lifted Markov chain, a path has 0 potential gain if and only if it is closed.
- In $\mathbb{T}^n$, a closed path is homotopy trivial, meaning that it could continuously shrink to a single point, if and only if its lifting in $\mathbb{R}^n$ is still closed. Remember that the fundamental group of $\mathbb{T}^n$ is $\mathbb{Z}^n$, and the universal covering space of $\mathbb{T}^n$ is $\mathbb{R}^n$.
- This finishes the proof of the torus version.

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Properties

- A path in the lifted Markov chain can be folded back to the original Markov chain (folded chain).
- The probability distributions satisfy $\bar{p}_i = \sum_\alpha p_{i_\alpha}$.
- For a closed path in the folded chain, the potential gain can be determined by the net numbers of special edges.
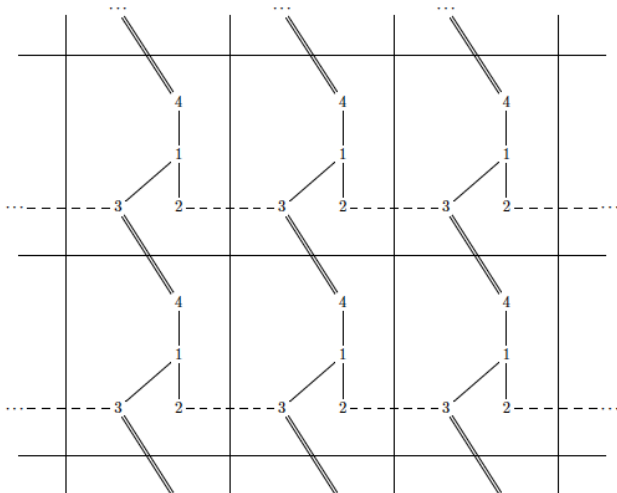
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Stationary distributions and measures

- The original irreducible Markov chain has a unique stationary distribution $\bar{\pi}_i$. Denote the probability distribution at time t as $\bar{p}_i(t)$. $\bar{p}_i(t) \to \bar{\pi}_i$.
- The periodic extension of $\bar{\pi}_i$, π_{i_α}, on the lifted chain, is a non-normalizable stationary measure.
- For the global potential φ_{i_α}, $\mu_{i_\alpha} = \exp(-\varphi_{i_\alpha})$ is a stationary measure with $\mu_{i_\alpha} q_{ij} = \mu_{j_\beta} q_{ji}$ (detailed balance).

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Stationary distributions and measures

- For the lifted chain, consider the relative entropy of $p_{i_\alpha}(t)$ with respect to any stationary measure θ_{i_α},

$$D_{KL}(p, \theta) = \sum_i \sum_\alpha p_{i_\alpha}(t) \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}}.$$

Lemma

$D_{KL}(p, \theta)$ *is monotonically decreasing.*

- The proof is equivalent transformation and $\log y \geq 1 - 1/y$. The equality holds if and only if $p_{i_\alpha}(t) = c\theta_{i_\alpha}$ for a constant c.

Yue Wang   Lifting and Entropy

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Stationary distributions and measures

Proposition

The lifted Markov chain has no stationary probability distribution.

Proof.

Assume there exists a stationary probability distribution η_{i_α}. Set $p(t) = \eta$, and $\theta = \pi$, then $D_{KL}(p(t), \pi)$ is a constant. This is true only if the equality holds in previous lemma, which means η and π only differ by a constant multiple. π is non-normalizable, so is η. $\qquad\square$

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Definition

For folded chain, the (instantaneous) entropy production rate $\bar{e}_p(t)$ is defined as

$$\bar{e}_p(t) = \frac{1}{\delta} \lim_{\delta \to 0} D_{KL}(\bar{P}_{[t,t+\delta]}, \bar{P}^-_{[t,t+\delta]}).$$

Here P is the probability distribution on the trajectory space. P^- is on the time inverse of the trajectory space.

•

$$\bar{e}_p(t) = \sum_{i \sim j} \left[\bar{p}_i(t)q_{ij} - \bar{p}_j(t)q_{ji} \right] \log \frac{\bar{p}_i(t)q_{ij}}{\bar{p}_j(t)q_{ji}}.$$

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Definition

For folded chain, free energy $\bar{F}(t)$ is defined as
$\bar{F}(t) = D_{KL}(\bar{p}(t), \bar{\pi})$.

- Its time derivative is

$$d\bar{F}(t)/dt = -\sum_{i \sim j} \left[\bar{p}_i(t)q_{ij} - \bar{p}_j(t)q_{ji} \right] \log \frac{\bar{p}_i(t)\pi_j}{\bar{p}_j(t)\pi_i}.$$

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Definition

For folded chain, housekeeping heat $\bar{Q}_{hk}(t)$ is defined as

$$\bar{Q}_{hk}(t) = \bar{e}_p(t) + \mathrm{d}\bar{F}(t)/\mathrm{d}t.$$

●

$$\bar{Q}_{hk}(t) = \sum_{i \sim j} \left[\bar{p}_i(t) q_{ij} - \bar{p}_j(t) q_{ji} \right] \log \frac{\pi_i q_{ij}}{\pi_j q_{ji}}.$$

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Definition

For lifted chain, the (instantaneous) entropy production rate $e_p(t)$ is defined as

$$e_p(t) = \frac{1}{\delta} \lim_{\delta \to 0} D_{\mathsf{KL}}(P_{[t,t+\delta]}, P^-_{[t,t+\delta]}).$$

Here P is the probability distribution on the trajectory space. P^- is on the time inverse of the trajectory space.

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$$e_p(t) = \sum_{i_\alpha \sim j_\beta} \left[p_{i_\alpha}(t) q_{ij} - p_{j_\beta}(t) q_{ji} \right] \log \frac{p_{i_\alpha}(t) q_{ij}}{p_{j_\beta}(t) q_{ji}}.$$

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Definition

For lifted chain, the free energy with respect to stationary measure θ, $F^{\theta}(t)$, is defined as $F^{\theta}(t) = D_{KL}(p, \theta)$.

- Its time derivative is

$$\mathrm{d}F^{\theta}(t)/\mathrm{d}t = - \sum_{i_{\alpha} \sim j_{\beta}} [p_{i_{\alpha}}(t)q_{ij} - p_{j_{\beta}}(t)q_{ji}] \log \frac{p_{i_{\alpha}}(t)\theta_{j_{\beta}}}{p_{j_{\beta}}(t)\theta_{i_{\alpha}}}.$$

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Definition

For lifted chain, the housekeeping heat with respect to stationary measure θ, $Q_{hk}^{\theta}(t)$, is defined as

$$Q_{hk}^{\theta}(t) = e_p(t) + \mathrm{d}F^{\theta}(t)/\mathrm{d}t.$$

-

$$Q_{hk}^{\theta}(t) = \sum_{i_\alpha \sim j_\beta} \left[p_{i_\alpha}(t)q_{ij} - p_{j_\beta}(t)q_{ji} \right] \log \frac{\theta_{i_\alpha}q_{ij}}{\theta_{j_\beta}q_{ji}}.$$

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Properties

- $e_p(t) \geq 0$.
- $\mathrm{d}F^\theta(t)/\mathrm{d}t \leq 0$.
- $Q_{hk}^\theta(t) \geq 0$. The proof relies on $\log y \geq 1 - 1/y$ and equivalent transformations.
- $e_p(t) = Q_{hk}^\theta(t) + [-\mathrm{d}F^\theta(t)/\mathrm{d}t]$, where all terms are non-negative.
- The same results are valid for folded chain.

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Folded chain

Since $\bar{p}(t)$ converges to $\bar{\pi}$, $\bar{F}(t)$ and $\mathrm{d}\bar{F}(t)/\mathrm{d}t$ converge to 0, $\bar{e}_p(t)$ and $\bar{Q}_{hk}(t)$ converge to the stationary entropy production rate

$$\bar{e}_p = \sum_{i \sim j} (\bar{\pi}_i q_{ij} - \bar{\pi}_j q_{ji}) \log \frac{\bar{\pi}_i q_{ij}}{\bar{\pi}_j q_{ji}}.$$

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Lifted chain

- For lifted chain, $p_{i_\alpha}(t) \to 0$. We cannot exchange summation and limit.
- Specifically, we consider the thermodynamic quantities with respect to the periodic stationary measure π and no-flux stationary measure μ.
- $Q_{hk}^\pi(t) \to \bar{e}_p$. $Q_{hk}^\mu(t) \equiv 0$.

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Main result

Theorem (Wang & Qian 2018)

Assume the initial distribution $p_{i_\alpha}(0)$ has finite covariance matrix. Then $e_p(t)$ converges to $\bar{e}_p$ in Cesàro's sense that $\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t)\mathrm{d}t = \bar{e}_p$.

- $\mathrm{d}F^\mu/\mathrm{d}t = -e_p \to -\bar{e}_p$ in Cesàro's sense, $\mathrm{d}F^\pi/\mathrm{d}t \to 0$ in Cesàro's sense.
- $e_p(t) = Q_{hk}^\theta(t) + [-\mathrm{d}F^\theta(t)/\mathrm{d}t]$, where all terms are non-negative. π and μ reach the maximum and minimum of Q_{hk}^θ, $\bar{e}_p$ and 0.

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Proof

- $\lim_{T\to\infty} \frac{1}{T} \int_0^T e_p(t)\mathrm{d}t = \bar{e}_p$ is equivalent with $F^\pi(T)/T \to 0$.

- $$F^\pi(t) = \sum_i \sum_\alpha p_{i_\alpha}(t) \log \frac{p_{i_\alpha}(t)}{\pi_i}$$

  $$= \sum_i \sum_\alpha p_{i_\alpha}(t) \log p_{i_\alpha}(t) - \sum_i \bar{p}_i(t) \log \bar{\pi}_i.$$

- The second term converges to a constant. The first term is $-h[p(t)]$, the Shannon entropy of $p(t)$.

- We only need to prove $h[p(T)]/T \to 0$.

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Proof

Lemma

For a continuous probability density function p on $\mathbb{R}^n$ with fixed covariance matrix Σ, its entropy $h[p]$ satisfies

$$h[p] \leq \frac{1}{2}\Big[n + \log\big(2^n \pi^n \det \Sigma\big)\Big].$$

The equality holds if and only if p is an n-dimensional normal distribution with covariance matrix Σ.

- We need a continuous distribution.
- We need to control the covariance matrix.

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A continuous space

- We embed the Markov chain into $\mathbb{R}^n$, and then substitute each single state with a hypercube. Construct a Markov process on these hypercubes. Transitions between states are now transitions between hypercubes (with the same rate), and the destinations are uniformly distributed in the hypercube.

- The distribution is continuous, and the entropy of this Markov process and the lifted Markov chain only differ by a constant.

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Control covariance

- We can choose G and Δt such that for any $0 \le \Delta t' \le \Delta t$, $i = 1, \cdots, n$,

$$\text{Var}\Big[\boldsymbol{X}_i(t + \Delta t') - \boldsymbol{X}_i(t) \Big] \le G \Delta t,$$

regardless of the value of $\boldsymbol{X}(t)$.

- Proof:

$$\text{Var}\Big[\boldsymbol{X}_i(t + \Delta t') - \boldsymbol{X}_i(t) \Big] \le \mathbb{E} N^2(t, t + \Delta t),$$

where $N(t, t + \Delta t)$ is the number of jumps in time interval $[t, t + \Delta t)$.

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- For a fixed $T > 0$, set $m = \lceil T/\Delta t \rceil$. Then

$$\text{Var}[\boldsymbol{X}_i(T)] = \text{Var}\{\boldsymbol{X}_i(0) + [\boldsymbol{X}_i(\Delta t) - \boldsymbol{X}_i(0)]$$

$$+ \cdots + [\boldsymbol{X}_i(T) - \boldsymbol{X}_i((m-1)\Delta t)]\}.$$

- $\text{Var}(\sum_{i=1}^n W_i) \leq n \sum_{i=1}^n \text{Var}(W_i)$.

-

$$|\text{Var}[\boldsymbol{X}(T)]_{jj}| \leq (m+1)(D + mG\Delta t),$$

where $D = \max_i \text{Var}[\boldsymbol{X}_i(0)]$.

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Control covariance

- $|\text{Cov}(Y, Z)| \leq \sqrt{\text{Var}[Y]\text{Var}[Z]}$. Thus

$$|\text{Cov}[\boldsymbol{X}(T)]_{ij}| \leq (m+1)(D + mG\Delta t).$$

- When T is large enough, $|\text{Cov}[\boldsymbol{X}(T)]_{ij}| \leq 2(T/\Delta t)^2 G\Delta t$.
- Thus $|\text{Cov}[\boldsymbol{X}(T)]_{ij}| \leq CT^2$, $\det\{\text{Cov}[\boldsymbol{X}(T)]\} \leq n!C^n T^{2n}$.

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Proof

Lemma

For a continuous probability density function p on $\mathbb{R}^n$ with fixed covariance matrix Σ, its entropy $h[p]$ satisfies

$$h[p] \leq \frac{1}{2}\Big[n + \log\big(2^n \pi^n \det \Sigma\big)\Big].$$

The equality holds if and only if p is an n-dimensional normal distribution with covariance matrix Σ.

- $\det\{\mathrm{Cov}[\boldsymbol{X}(T)]\} \leq n! C^n T^{2n}$, thus $0 \leq h[p(T)] \leq C' \log T$.
- $h[p(T)]/T \to 0$, thus $\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t)\mathrm{d}t = \bar{e}_p$.

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Conjectures

- We guess $\lim_{t\to\infty} e_p(t) = \bar{e}_p$, which requires $dh[p(t)]/dt \to 0$.
- We have shown that our lifting is the minimal lifting with global potential. We guess that it is also the maximal lifting with $e_p(t) \to \bar{e}_p$.

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Physical meaning

- For free energy with detailed balance stationary measure $\mu = \exp(-\varphi)$, $\mathrm{d}F^\mu/\mathrm{d}t = -e_p \to -\bar{e}_p$ in Cesàro's sense.

-
$$F^\mu(t) = \sum_{i_\alpha} p_{i_\alpha}(t) \log p_{i_\alpha}(t) + \sum_{i_\alpha} p_{i_\alpha}(t) \varphi_{i_\alpha}.$$

  The first term of rhs is controlled by $C' \log t$, and the second term is the mean potential energy.

- The entropy production of the folded Markov chain, which cannot be described by system status quantities directly, is reflected by the free energy/potential energy dissipation of the lifted Markov chain.

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Diffusion processes

- Consider a diffusion process $\bar{\boldsymbol{X}}(t)$ on n-dimensional torus $\mathbb{T}^n$:

$$\mathrm{d}\bar{\boldsymbol{X}}(t) = \bar{\boldsymbol{\Gamma}}(\bar{\boldsymbol{X}})\mathrm{d}\bar{\boldsymbol{B}}(t) + \bar{\boldsymbol{b}}(\bar{\boldsymbol{X}})\mathrm{d}t.$$

- Let $\boldsymbol{\Gamma}(\boldsymbol{x})$ and $\boldsymbol{b}(\boldsymbol{x})$ be the periodic extensions of $\bar{\boldsymbol{\Gamma}}(\bar{\boldsymbol{x}})$ and $\bar{\boldsymbol{b}}(\bar{\boldsymbol{x}})$, then we have a diffusion process $\boldsymbol{X}(t)$ on $\mathbb{R}^n$:

$$\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{\Gamma}(\boldsymbol{X})\mathrm{d}\boldsymbol{B}(t) + \boldsymbol{b}(\boldsymbol{X})\mathrm{d}t.$$

- The probability density function $f(\boldsymbol{x}, t)$ satisfies Kolmogorov forward equation:

$$\frac{\partial f(\boldsymbol{x}, t)}{\partial t} = -\nabla \cdot [\boldsymbol{b}(\boldsymbol{x})f(\boldsymbol{x}, t)] + \nabla \cdot \nabla \cdot \left[\boldsymbol{\Gamma}(\boldsymbol{x})\boldsymbol{\Gamma}^T(\boldsymbol{x})f(\boldsymbol{x}, t)/2 \right].$$

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- The probability density function satisfies

$$\bar{f}(\bar{\boldsymbol{x}}, t) = \sum_{i_1=-\infty}^{+\infty} \cdots \sum_{i_n=-\infty}^{+\infty} f(\bar{\boldsymbol{x}} + i_1 \boldsymbol{e}_1 + \cdots + i_n \boldsymbol{e}_n, t).$$

- A path on $\mathbb{T}^n$ can be lifted to $\mathbb{R}^n$, and a path on $\mathbb{R}^n$ can be folded back to $\mathbb{T}^n$.

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Diffusion processes

- In general there is no global potential.
- For Markov chain, there are finite cycles with non-zero potential gains. We expand (lift) all of them, so as to get a global potential.
- For diffusion process, there are infinite many cycles with non-zero potential gains. We only lift those main cycles ($\mathbb{T}^n = \prod_1^n \mathbb{S}^1$).

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Diffusion processes

- The lifted process has no stationary distribution.
- Thermodynamic quantities can be defined similarly.

Theorem (Wang & Qian 2018)

For any initial distribution $f(\boldsymbol{x}, 0)$ that has a finite covariance matrix, the entropy production rate of diffusion process $\boldsymbol{X}(t)$ on $\mathbb{R}^n$, $e_p(t)$, converges to $\bar{e}_p$ in Cesàro's sense that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t)\mathrm{d}t = \bar{e}_p.$$

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Thank you!