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The Reversibility and The Entropy Production of Markov Processes

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ABSTRACT. In this paper, we summarize some results of the criterion on the reversibility and irreversibility of stationary Markov processes, the background of which is the equilibrium and nonequilibrum in the statistical mechanics. These results include the circulation number, the general definition of the entropy production, Einstein formula, etc.

1. Introduction

Thermodynamic equilibrium (detailed balance) and nonequilibrium are well known and of interest among physicists [Ha], [Hi], [NP], [Sch]. The mathematical version of them is the symmetry (or reversibility) and nonsymmetry of stochastic processes defined as follows.

Consider a stochastic process $X = \{X_t : \quad t \in T\}$ (where $T = Z^+$ or R^+) with the state space $(E, \mathcal{B})$, given on the probability space $\{\Omega, \mathcal{F}, P\}$. Two measures $P^+[s,t]$ and $P^-[s,t]$ can be introduced on $\mathcal{F}_s^t$ as the distributions of $\{X_u : s \le u \le t\}$ and $\{X_{t-s+u} : s \le u \le t\}$, where

$$\mathcal{F}_s^t = \sigma(X_u : s \le u \le t)\,.$$

DEFINITION 1. *X is called reversible, if for any $t > s$,*

$$P^+[s,t] = P^-[s,t]. \tag{1}$$

when X is a homogeneous Markov process with transition probability $\{P(t, x, A)\}$ and initial distribution μ, then X is reversible iff X is stationary and

$$\int_A \mu(dx)\, P(t,x,B) = \int_B \mu(dx)\, P(t,x,A) \quad \forall A, B \in \mathcal{B} \text{ and } t \in T\,. \tag{2}$$

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If X is a discrete Markov chain with transition probability (p_{ij}) and initial distribution $\{\mu_i\}$, (2) is equivalent to

$$\mu_i p_{ij} = \mu_j p_{ji} \qquad \text{for any states } i \text{ and } j\ .$$

And when X is a diffusion process with transition probability density $p(t,x,y)$ and initial density $\mu(x)$, (2) is equivalent to

$$\mu(x)p(t,x,y) = \mu(y)p(t,y,x) \quad \forall t\,,x\,,y\,.$$

If X satisfies a Stratonovich SDE in R^n:

$$dX_t = \sigma(X_t) \circ dw_t + b(X_t)dt \tag{3}$$

with a unique invariant measure $\mu(x)dx$, then for the stationary diffusion starting from $\mu(x)dx$, (2) is equivalent to the condition that L is symmetric with respect to μ, i.e.,

$$\int Lf(x)g(x)\mu(x)dx = \int f(x)Lg(x)\mu(x)dx\,,$$

for any $f, g \in C_0^\infty$, where

$$L = \frac{1}{2}\sum_{i,j}\frac{\partial}{\partial x_i}a_{ij}(x)\frac{\partial}{\partial x_j} + \sum_i b_i(x)\frac{\partial}{\partial x_i}\,.$$

As we have seen above, equilibrium means that the distribution of the process does not change under time reversal. But this could not be true in many situations, especially for stochastic processes in live bodies, which are time sensitive. Therefore, it is important to understand what will happen when the system is in nonequilibrium and to understand the difference in path behavior between reversible processes and irreversible processes. Can we give a quantity that measures how far a nonequilibrium process is from reversibility? In this paper, we summarize some conclusions obtained in answering these question.

2. Circulations of Markov chains

Consider a countable state recurrent Markov chain with transition matrix $P = (p_{ij})$. Kolmogorov gave a criterion for the reversibility of a finite state Markov chain [K]:

THEOREM 1. *P is reversible with respect to its invariant measure μ iff for any state cycle: $i_1 \to i_2 \to \cdots \to i_s \to i_1$,*

$$p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_s i_1} = p_{i_s i_{s-1}} p_{i_{s-1} i_{s-2}} \cdots p_{i_1 i_s}\,.$$

It is natural to consider the path behavior along cycles of a reversible Markov chain. For a recurrent Markov chain, the path draws cycles one after another. Record each cycle once it forms, and delete it to avoid confusion and double-counting. Denote the number of times for each cycle R: $i_1 \to i_2 \to \cdots \to i_s \to i_1$ formed up to time T by $W_T(\omega, R)$. We have the following theorem about the path behavior along cycles of the Markov chain.

THEOREM 2 [QQ2].

$$\lim_{T\to\infty} \frac{1}{T} W_T(\omega, R) = J_R \quad a.s.$$

where

$$J_R = p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_s i_1} N(i_2|i_1) N(i_3|i_1, i_2) \cdots N(i_s|i_1, i_2, \ldots, i_{s-1})$$

and $N(i_k|i_1, i_2, \ldots, i_{s-1})$ $(k = 1, 2, \ldots, s)$ *are the taboo Green's functions of* P *starting from* i_k *back to* i_k *without touching* $i_1, i_2, \ldots, i_{k-1}$. *Moreover the product*

$$N(i_2|i_1) N(i_3|i_1, i_2) \cdots N(i_s|i_1, i_2, \ldots, i_{s-1}) \tag{4}$$

is independent of the order of $i_1, i_2, \ldots, i_s$, *and*

$$J_R = J_{R^-} (R^- : \ i_s \to i_{s-1} \to \cdots \to i_1 \to i_s)$$

whenever

$$p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_s i_1} = p_{i_2 i_1} p_{i_3 i_2} \cdots p_{i_1 i_s}. \tag{5}$$

COROLLARY 1. *A Markov chain* X *is reversible iff* $J_R = J_{R^-}$ *for every cycle* R.

Remark. For the finite state Markov chains, the product in (4) is the ratio

$$D(i_1, i_2, \ldots, i_{s-1}) / D(i_s),$$

where $D(i_s)$ and $D(i_1, i_2, \ldots, i_{s-1})$ are the determinants of the matrices formed by deleting the i_s-th row and column and i_1-th, i_2-th,..., i_{s-1}-th rows and columns form the matrix $(\delta_{ij} - p_{ij})$ respectively. This is the quantity expressed by tree terminologies in graph theory (see [Hi], [QQQ3]).

For a stationary diffusion on a circle with stationary density ρ:

$$dx_t = \sigma(x_t) \circ dW_t + b(x_t)\, dt,$$

where

$$\sigma(0) = \sigma(2\pi), \quad b(0) = b(2\pi).$$

Denote the number of winding times up to time T of X clockwise and counterclockwise by $W_T^+(\omega)$ and $W_T^-(\omega)$, respectively.

THEOREM 3. *For the diffusion* X *on the unit circle, the following two limits exist:*

$$J^+ = \lim_{T\to\infty} \frac{1}{T} W_T^+(\omega), \quad J^- = \lim_{T\to\infty} \frac{1}{T} W_T^-(\omega), \tag{6}$$

and

$$J^+ - J^- = -\frac{1}{2} a(x) \rho(x)' + b(x) \rho(x), \quad \frac{J^+}{J^-} = w(2\pi), \tag{7}$$

where

$$a(x) = \sigma(x)^2, \quad w(x) = \exp\left(\int_0^x \frac{b(x)}{a(x)}\,dx\right)$$

COROLLARY 2. *X is reversible iff $J^+ = J^-$.*

Remark. $J^+ - J^- = -\frac{1}{2}a(x)\rho(x)' + b(x)\rho(x) = v(x)\rho(x)$ where

$$v(x) = b(x) - \frac{1}{2}a(x)^{-1}\,\nabla \log\,\rho(x)$$

is nothing but Nelson's current velocity [N], and $J^+ - J^-$, introduced by Feller (see [F1] [F2]), is the flux used very often in physics for the probability flowing through point x. Also

$$\log \frac{J^+}{J^-} = \log w(2\pi)$$

is the so-called force in physics, corresponding to the chemical potential for a process in chemical reaction.

3. Entropy production

In physics, there are several quantities, called entropy productions, such as [Sch]

$$\text{ep} = \sum(\mu_i p_{ij} - \mu_j p_{ji}) \log \frac{\mu_i p_{ij}}{\mu_j p_{ji}} \tag{8}$$

for Markov chains and

$$\text{ep}d(x) = (\frac{1}{2}\nabla \log \rho(x) - A^{-1}b)^T\,A\,(\frac{1}{2}\nabla \log \rho(x) - A^{-1}b) \tag{9}$$

for diffusion processes, with A, b, ρ being its diffusion matrix, drift, and invariant density, respectively. It is claimed that systems far from equilibrium have positive entropy productions. The questions are: (1) What is the probabilistic meaning for those quantities? (2) Are these different formulas for entropy productions essentially the same thing? and (3) Is there a relationship between a system having positive entropy production and its being far from equilibrium?

The answers for these questions are given in Theorems 4 and 5.

DEFINITION 2. *The entropy production of a stochastic process $X = \{X_t : t \in T\}$ at time t is defined as*

$$\text{ep}(t) = \lim_{s \to t} \frac{1}{t-s} h(P^+[s,t], P^-[s,t]) \tag{10}$$

where $h(P^+[s,t], P^-[s,t])$ is the relative entropy.

$$h(P^+[s,t], P^-[s,t]) = \int \log \frac{dP^+[s,t]}{dP^-[s,t]}\,dP^+[s,t]\,,$$

if the limit (10) *exists.*

The following theorem tells that the entropy production defined above can be regarded as a criterion to characterize how far a process is from being reversible and that it coincides with the formulas in (8) and (9) given by physicists.

THEOREM 4. *For a Markov chain with transition matrix $P = (p_{ij})$ and distribution $\{\mu_i\}$ at time t,*

$$\mathrm{ep}(t) = \sum (\mu_i p_{ij} - \mu_j p_{ji}) \log \frac{\mu_i p_{ij}}{\mu_j p_{ji}}.$$

For a diffusion processes X given by (3) *in the introduction,*

$$\mathrm{ep}(t) = \int (\frac{1}{2}\nabla \log \rho(x) - A^{-1}b)^T A\, (\frac{1}{2}\nabla \log \rho(x) - A^{-1}b)\, \rho(x)\, dx\,.$$

THEOREM 5. *For the Markov chain as in Theorem* 4,

$$\mathrm{ep}(x) = \frac{1}{2}\sum_R (J_R - J_{R^-}) \log \frac{J_R}{J_{R^-}}$$

(*see* [QQ2]).

Theorem 5 says that reversibility of time is equivalent to the symmetry of the path behavior along cycles.

THEOREM 6. *The entropy production of the diffusion on the circle in Theorem* 5, *can be expressed as* [GQ1]*:*

$$\mathrm{ep} = (J^+ - J^-) \log \frac{J^+}{J^-}$$

and

$$J^+ - J^- = -a\rho' + b\rho\,,$$

$$\frac{J^+}{J^-} = \exp \int_0^{2\pi} \frac{b(x)}{a(x)}\, dx = w(2\pi)\,.$$

Remark. Theorem 6 shows that the entropy production of a diffusion on the unit circle is just the product of the 'flux' and 'force'.

4. The winding numbers of diffusions

For diffusions, it is not clear what is J_R as for Markov chains, so in its place we use the winding number.

Consider a stationary drifted Brownian motion in R^n with drift $b(x)$. Take any two of its components of X, say $X_t^{(k)}$ and $X_t^{(j)}$. Let

$$Z_t = (X_t^{(k)} - \alpha) + i(X_t^{(j)} - \beta) = e^{\gamma t + i\theta_t}\,,$$

and define θ_t as the winding angle around point (α, β) up to time t of the (k, j) component of X.

THEOREM 7. *Under some mild integrable conditions we have that* [GQX]

$$\lim_{t\to\infty} \frac{1}{t}\theta_t = c_1\varsigma + c_2$$

in law, where ς is a Cauchy random variable, c_1 and c_2 are two constants depending on the drift b. Furthermore, if X is reversible, then $c_2 = 0$ holds for $\forall(i,j)$ and (α, β), and the converse is also true.

5. Einstein formula

In this section, we state a formula of the stationary diffusion processes, which is an extension of the Einstein formula of the Ornstein-Uleneck process (see [E], [QGG], [QQ5]).

THEOREM 8 (EINSTEIN FORMULA). *Let X_t be a stationary diffusion process with bounded drift $b(x)$ and diffusion matrix $A(x)$ uniformly bounded from below and above. Then*

$$E \int_0^\infty b(X_t)^T b^*(X_t)\, dt = E\left(tr\, A(X_t)\right),$$

where $b^*(x)$ is the reverse drift:

$$b^*(x) = -b(x) + \frac{1}{2}A(x)\nabla \log \rho(x),$$

and $\rho(x)$ is the invariant density.

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