THE ENTROPY PRODUCTION AND IRREVERSIBILITY OF MARKOV PROCESSES

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In nonequilibrium statistical physics, the entropy production and the irreversibility (nondetailed balance) play very important roles. For the simple case of the Markov chains, it is shown that a stationary Markov chain is reversible iff its entropy production vanishes[1,2], and entropy production characterizes how far from reversibility it is. In the present note, we give a general probabilistic definition of the entropy production for a stochastic process and also its explicit formulas in some important concrete cases, i.e. Markov chains and the diffusions. Indeed, these formulas perfectly meet the expression of the entropy production defined by some physicists and chemists in terms of "flux" and "force" of chemical reaction[3-5].

Consider a stochastic process $\{X_t, P; t \in \mathscr{T}\}$ (where $\mathscr{T}$ is the real number set R_1, the interger set Z, or an interval of R_1). Set

$$\mathscr{F}_s^t = \sigma(\{X_r; s \leqslant r \leqslant t, r \in \mathscr{T}\}),$$

(the σ-field generated by $\{X_r; s \leqslant r \leqslant t, r \in \mathscr{T}\}$. Obviously, the two measures $P^+_{[s,t]}$, and $P^-_{[s,t]}$, can be introduced from $\{X_r; s \leqslant r \leqslant t, r \in \mathscr{T}\}$ and $\{X_{t-r}; 0 \leqslant r \leqslant t-s, r \in \mathscr{T}\}$ on $\mathscr{F}_s^t$ respectively. Let

$$\widetilde{P}_{[s,t]}(A) = \frac{1}{2}(P^+_{[s,t]}(A) + P^-_{[s,t]}(A)) \tag{1}$$

(for $\forall A \in \mathscr{F}_s^t$). It is easy to see that $\widetilde{P}_{[s,t]}$ is also a probability measure on $\mathscr{F}_s^t$ and that $P^+_{[s,t]}$ and $P^-_{[s,t]}$ are absolutely continuous with respect to $\widetilde{P}_{[s,t]}$. Then we have

$$\begin{aligned} P^+_{[s,t]}(A) &= \int_A \frac{dP^+_{[s,t]}}{d\widetilde{P}} d\widetilde{P}_{[s,t]}, \\ P^-_{[s,t]}(A) &= \int_A \frac{dP^-_{[s,t]}}{d\widetilde{P}} d\widetilde{P}_{[s,t]}, \end{aligned} \tag{2}$$

where $\frac{dP^+_{[s,t]}}{d\widetilde{P}}$ and $\frac{dP^-_{[s,t]}}{d\widetilde{P}}$ are respectively the Radon-Nikodyn derivatives of $P^+_{[s,t]}$ and $P^-_{[s,t]}$ with respect to $\widetilde{P}_{[s,t]}$. Then, by (1) and (2)

$$\frac{1}{2}\left(\frac{dP^+_{[s,t]}}{d\widetilde{P}} + \frac{dP^-_{[s,t]}}{d\widetilde{P}}\right) = 1 \quad (\text{a.e. } d\widetilde{P}).$$

Since $\frac{dP^+_{[s,t]}}{d\widetilde{P}}(\omega)$ and $\frac{dP^-_{[s,t]}}{d\widetilde{P}}(\omega)$ cannot vanish at the same time (a.e. $d\widetilde{P}$),

$$\frac{dP^+_{[s,t]}}{dP^-_{[s,t]}} \triangleq \frac{dP^+_{[s,t]}}{d\tilde{P}} \Big/ \frac{dP^-_{[s,t]}}{d\tilde{P}} \quad (\text{a.e. } d\tilde{P})$$

can be well defined.

Definition 1 (*Reversibility*). A stochastic process $\{X_t, P; t \in \mathscr{T}\}$ is reversible if for $\forall\, s, t \in \mathscr{T}$, $P^+_{[s,t]} = P^-_{[s,t]}$.

Definition 2 (*Instantaneous Entropy Production and Its Density*). If $\mathscr{T}$ is discrete, the instantaneous entropy production and its density are defined as

$$e_p(t) = E^P\left(\log \frac{dP^+_{[t,t+1]}}{dP^-}(\omega)\right), \tag{3_1}$$

$$e_p(t, x) = E^P\left(\log \frac{dP^+_{[t,t+1]}}{dP^-}(\omega) \,|\, X_t = x\right), \tag{3_2}$$

respectively. If $\mathscr{T}$ is continuous, we define the entropy production and its density as

$$e_p(t) = \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left[E^P\left(\log \frac{dP^+_{[t,t+\Delta t]}}{dP^-}(\omega)\right)\right], \tag{4_1}$$

and

$$e_p(t, x) = \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left[E^P\left(\log \frac{dP^+_{[t,t+\Delta t]}}{dP^-}(\omega) \,|\, X_t = x\right)\right], \tag{4_2}$$

respectively, if the limit exists.

It is easy to see that

$$e_p(t) = \lim_{\Delta t \downarrow 0} \frac{1}{2\Delta t}\left[E^{P^+}\left(\log \frac{dP^+_{[t,t+\Delta t]}}{dP^-}(\omega)\right) - E^{P^-}\left(\log \frac{dP^-_{[t,t+\Delta t]}}{dP^+}(\omega)\right)\right]$$

and

$$(e_p't) \geqslant 0, \qquad e_p(t, x) \geqslant 0.$$

Surely, $\{X_t, t \in \mathscr{T}\}$ is reversible iff $e_p(t) = 0$, and $e_p(t)$ characterizes how far from reversibility the process is. For a Markov chain with density matrix $\boldsymbol{Q} = (q_{i,j})$, and the distribution $\phi_i(t) \triangleq P(X_t = i)$, we have

$$e_p(t) = \frac{1}{2}\sum_{i,j} \log \frac{\phi_i(t) q_{i,j}}{\phi_j(t) q_{j,i}} (\phi_i(t) q_{i,j} - \phi_j(t) q_{j,i}) \geqslant 0,$$

$$e_p(t, x) = \sum_j \log \frac{\phi_i(t) q_{i,j}}{\phi_j(t) q_{j,i}} q_{i,j}.$$

For a diffusion process $\{X_t, t \in R_1^+\}$, we can prove that

$$e_p(t) = \int \left[\frac{1}{2}(\nabla \log \phi(t, x) - 2\boldsymbol{A}^{-1}\boldsymbol{b}(x))^T \boldsymbol{A} (\nabla \log \phi(t, x) - 2\boldsymbol{A}^{-1}\boldsymbol{b}) - \frac{\partial \log \phi(t, x)}{\partial t}\right] \phi(t, x) dx,$$

$$e_p(t, x) = \frac{1}{2}(\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b})^T \boldsymbol{A} (\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b}) - \frac{\partial \log \phi(t, x)}{\partial t},$$

where $\boldsymbol{A}, \boldsymbol{b}, \phi$ are the diffusion coefficient matrix, the drift vector and the probability density of X_t respectively. We prove the above result by using Girsanov's formula in the second case.

For a stationary diffusion, the above equations can be reduced to

$$e_p(t) = \frac{1}{2}\int (\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b})^T \boldsymbol{A}(\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b})\phi(x)dx,$$

and

$$e_p(t, x) = \frac{1}{2}(\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b})^T \boldsymbol{A}(\nabla \log \phi - 2\boldsymbol{A}^{-1}\boldsymbol{b}).$$

Therefore a stationary diffusion is reversible iff

$$\nabla \log \phi = 2\boldsymbol{A}^{-1}\boldsymbol{b}.$$

Hence reversibility implies that

$$\int_l \boldsymbol{A}^{-1}\boldsymbol{b}dx = 0$$

holds for any smooth closed curve l in state space. This is nothing but the condition for a diffusion to be symmetric[6,7]. The details of the proof will appear elsewhere.

References

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