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The Onsager–Machlup theory for Markov processes with discrete time parameter: a characterisation of the detailed balance

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Abstract. The Onsager–Machlup (OM) function is introduced for a spatially uniform system evolving in accordance with a discrete time Markovian law. Circulation of probability flow is expressed in terms of the OM function. Equivalence is established between the two conditions: circulation $\equiv 0$ and the fulfilment of the detailed balance.

1. Introduction

There has been a renewed interest in Markovian models with discrete time parameter (Mayer-Kress and Haken 1981, Ito 1983). They are found to be good examples to study the influence of external random noises on the chaos of dynamical systems, one of the major subjects in recent non-equilibrium statistical mechanics (Nakamura 1978, Zippelius and Lücke 1981).

In contrast with the continuous time Markov models (Bach and Dürr 1978, Ito 1981), the role of the Onsager–Machlup (OM) function has hardly been studied for discrete time models. This paper aims at presenting a discrete time version of the characterisation of the detailed balance in terms of the OM function. Let us recall the characterisation for continuous time models (Ito 1981). Consider a master equation in R^n with a small parameter ε,

$$\partial p^\varepsilon(t, x)/\partial t = \varepsilon^{-1} \int \mathrm{d}r[w(x-\varepsilon r, r)p^\varepsilon(t, x-\varepsilon r) - w(x, r)p^\varepsilon(t, x)], \qquad (1)$$

which describes a spatially uniform system (van Kampen 1961, Kubo *et al* 1973). The OM function $L(\phi; \dot{\phi})$ is introduced by the Legendre transformation of H:

$$L(x; u) = (z, u) - H(x; z), \qquad u = \nabla_z H(x; z), \qquad (2)$$

where

$$H(x; z) = \int [\exp(z, r) - 1] w(x, r)\, \mathrm{d}r, \qquad (3)$$

and $(\cdot, \cdot)$ denotes the inner product. Net probability flow round a closed curve $\phi(t)$ $(0 \leq t \leq T)$ with $\phi(0) = \phi(T)$ has an asymptotic form $\exp(2I(\phi; \dot{\phi})/\varepsilon)$, where

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the circulation $I(\phi; \dot{\phi})$ round ϕ is given by

$$I(\phi; \dot{\phi}) = -\tfrac{1}{2}\int_0^T [L(\phi(t); \dot{\phi}(t)) - L(\phi(t); -\dot{\phi}(t))]\, dt. \tag{4}$$

Then the equivalence is found between the condition that $I(\phi; \dot{\phi}) = 0$ for any closed curve ϕ and the condition that the master equation (1) satisfies the detailed balance.

2. Onsager–Machlup function for discrete time systems

Let $(X^\varepsilon(t))_{0 \leq t < \infty}$ be a Markov process generated by the master equation (1). Let τ be the first jump time from $X^\varepsilon(0) = x$: $\tau = \inf\{t \geq 0;\ X^\varepsilon(t) \neq x\}$. Then $X^\varepsilon(\tau)$ is on a $\mathrm{d}r$-neighbourhood of $x + r$ with probability

$$p_\mathrm{d}^\varepsilon(x, r)\, \mathrm{d}r = \varepsilon^{-2} w(x, r/\varepsilon)\, \mathrm{d}r \Big/ \int \mathrm{d}r\, \varepsilon^{-2} w(x, r/\varepsilon) \tag{5}$$

(Doob 1953). This fact suggests that a discrete time version of X^ε, denoted by X_d^ε, has a one-step transition probability density p_d^ε given by (5). In the following, quantities corresponding to X_d^ε are indicated by associating a subscript d: H_d^ε, L_d^ε, I_d^ε etc, and the superscript ε is omitted if $\varepsilon = 1$: $H_\mathrm{d}^{\varepsilon=1} = H_\mathrm{d}$, $L_\mathrm{d}^{\varepsilon=1} = L_\mathrm{d}$ etc.

A simple calculation shows that the time derivative of a generating function of cumulants of X^ε

$$H^\varepsilon(x; z) = \lim_{\Delta t \downarrow 0} \Delta t^{-1} \log E[\exp(z, X^\varepsilon(\Delta t) - x) | X^\varepsilon(0) = x] \tag{6}$$

agrees with $H(x; z)$ given by (3) if we set $\varepsilon = 1$. Here $E[\cdot | X^\varepsilon(0) = x]$ represents the conditional expectation with a constraint $X^\varepsilon(0) = x$. H_d^ε, the corresponding quantity for X_d^ε, will be defined by (6) with $\Delta t = 1$ instead of taking the limit $\Delta t \downarrow 0$:

$$H_\mathrm{d}^\varepsilon(x; z) = \log E[\exp(z, X_\mathrm{d}^\varepsilon(1) - x) | X_\mathrm{d}^\varepsilon(0) = x] = \log\left(\int \mathrm{d}r\, \mathrm{e}^{(z,r)} w(x, r/\varepsilon)/(\varepsilon w(x))\right), \tag{7}$$

where

$$w(x) = \int \mathrm{d}r\, w(x, r). \tag{8}$$

The OM function L_d for X_d is obtained by the Legendre transformation of H_d.

Let us sketch how the OM function L_d is related to the probability flow. Solving (7) inversely, we have

$$\begin{aligned} w(x, r/\varepsilon)/\varepsilon w(x) &= \int \hat{\mathrm{d}}z\, \exp[H_\mathrm{d}^\varepsilon(x; \mathrm{i}z) - \mathrm{i}(z, r)] \\ &= \int \hat{\mathrm{d}}z\, \exp[H_\mathrm{d}(x; \mathrm{i}\varepsilon z) - \mathrm{i}(z, r)] \end{aligned} \tag{9}$$

with $\hat{\mathrm{d}}z = \mathrm{d}z/(2\pi)^n$, n being the dimension of the space variable. Take a smooth curve $\phi(t)$ $(0 \leq t \leq T)$, and set $x_j = \phi(\varepsilon j)$, $r_j = x_{j+1} - x_j$ $(j = 0, 1, \ldots, [T/\varepsilon] - 1 = N - 1)$. Here $[\cdot]$ is the Gauss symbol. From (5) we see that the probability density of making a transition $x_0 \to x_1 \to \ldots \to x_N$ is given by

$$\prod_{j=0}^{N-1} \frac{w(x_j, r_j/\varepsilon)}{\varepsilon w(x_j)} = \int \hat{\mathrm{d}}z_0 \ldots \hat{\mathrm{d}}z_{N-1} \exp\left(\varepsilon^{-1} \sum_{j=0}^{N-1} [H_{\mathrm{d}}(x_j; \mathrm{i}\varepsilon z_j)\varepsilon - \mathrm{i}(\varepsilon z_j, r_j/\varepsilon)\varepsilon]\right). \tag{10}$$

For sufficiently small ε, the augment

$$\varepsilon^{-1} \sum_{j=0}^{N-1} [H_{\mathrm{d}}(x_j; \mathrm{i}\varepsilon z_j)\varepsilon - \mathrm{i}(\varepsilon z_j, r_j/\varepsilon)\varepsilon]$$

will take the form of an integration

$$\varepsilon^{-1} \int_0^T \mathrm{d}t \, [H_{\mathrm{d}}(\phi(t); \mathrm{i}\varepsilon z(t)) - \mathrm{i}(\varepsilon z(t), \dot{\phi}(t))],$$

which is well approximated by

$$-\varepsilon^{-1} \int_0^T L_{\mathrm{d}}(\phi(t); \dot{\phi}(t)) \, \mathrm{d}t$$

if we take into account the most significant contribution from the extremal path. The above discussion shows that the probability flow round ϕ is of the order of $\exp(-\varepsilon^{-1} \int_0^T L_{\mathrm{d}}(\phi; \dot{\phi}) \mathrm{d}t)$, and that the net probability flow, defined by the ratio of the probability flow round ϕ to the one round $\hat{\phi}$ with $\hat{\phi}(t) = \phi(T-t)$, is given by $\exp(2I_{\mathrm{d}}(\phi; \dot{\phi})/\varepsilon)$. Here I_{d} is given by (4) with the replacement of L by L_{d}:

$$I_{\mathrm{d}}(\phi; \dot{\phi}) = -\tfrac{1}{2} \int_0^T [L_{\mathrm{d}}(\phi(t); \dot{\phi}(t)) - L_{\mathrm{d}}(\phi(t); -\dot{\phi}(t))] \, \mathrm{d}t. \tag{11}$$

In fact the above argument on the probability flow is justified in the following sense (Ventsel 1976). Consider a process $\tilde{X}^{\varepsilon}$ defined by

$$\tilde{X}^{\varepsilon}(t) = X_{\mathrm{d}}^{\varepsilon}([t/\varepsilon]), \tag{12}$$

so that one time step of $X_{\mathrm{d}}^{\varepsilon}$ corresponds to the interval ε in the actual time elapse. In (12), $[\cdot]$ is the Gauss symbol. Then for any $h > 0$, $\delta > 0$, there exists $\varepsilon_0 > 0$ such that, for $\varepsilon < \varepsilon_0$ the probability that $\tilde{X}^{\varepsilon}$ moves along ϕ, being inside the δ-tube around ϕ, satisfies an inequality

$$\exp[-\varepsilon^{-1}(S_{T,\mathrm{d}}(\phi) + h)] < P\left(\sup_{0 \le t \le T} |\tilde{X}^{\varepsilon}(t) - \phi(t)| < \delta\right) < \exp[-\varepsilon^{-1}(S_{T,\mathrm{d}}(\phi) - h)]$$

with $S_{T,\mathrm{d}}(\phi) = \int_0^T L_{\mathrm{d}}(\phi(t); \dot{\phi}(t)) \, \mathrm{d}t$.

3. A characterisation of the detailed balance

The detailed balance condition for $X_{\mathrm{d}}^{\varepsilon}$ is written as

$$q^{\varepsilon}(x - \varepsilon y) w(x - \varepsilon y, y)/\varepsilon w(x - \varepsilon y) = q^{\varepsilon}(x) w(x, -y)/\varepsilon w(x), \tag{13}$$

where $q^{\varepsilon}(x)$ is the stationary probability density. We suppose that $-\varepsilon \log q^{\varepsilon}(x)$ and its derivative $-\varepsilon \nabla \log q^{\varepsilon}(x)$ converge to a certain function $U(x)$ and its derivative

$\nabla U(x)$, respectively, in the limit of $\varepsilon \downarrow 0$. Then (13) is reduced to

$$\text{(P)} \qquad w(x, y) = w(x, -y) \exp[-(y, \nabla U(x))]. \tag{14}$$

We first show that the condition (P) implies

$$\text{(C)} \qquad I_{\rm d}(\phi; \dot{\phi}) = 0 \qquad \text{for any smooth closed curve } \phi. \tag{15}$$

By definition of the Legendre transformation

$$L_{\rm d}(\phi(t); \dot{\phi}(t)) = (z, \dot{\phi}(t)) - H_{\rm d}(\phi(t); z), \tag{16}$$

$$\dot{\phi}(t) = \nabla_z H_{\rm d}(\phi(t); z)$$
$$= \int y\, e^{(z,y)} w(\phi(t), y)\, dy \Big/ \int e^{(z,y)} w(\phi(t), y)\, dy. \tag{17}$$

Substituting $-y$ for y in the integrand of (17) and using (P), we have

$$-\dot{\phi}(t) = \int y\, e^{(\hat{z},y)} w(\phi(t), y)\, dy \Big/ \int e^{(\hat{z},y)} w(\phi(t), y)\, dy$$
$$= \nabla_{\hat{z}} H_{\rm d}(\phi(t); \hat{z}) \tag{18}$$

with

$$\hat{z} = -z + \nabla U(\phi(t)), \tag{19}$$

which asserts

$$L_{\rm d}(\phi(t); -\dot{\phi}(t)) = (\hat{z}, -\dot{\phi}(t)) - H_{\rm d}(\phi(t); \hat{z}). \tag{20}$$

Similarly

$$H_{\rm d}(\phi(t); z) = H_{\rm d}(\phi(t); \hat{z}). \tag{21}$$

Using the relations (16), (20), (21), we see

$$I_{\rm d}(\phi(t); \dot{\phi}(t)) = -\tfrac{1}{2} \int_0^T dt\, (z + \hat{z}, \dot{\phi}(t)) = -\tfrac{1}{2}[U(\phi(T)) - U(\phi(0))] = 0. \tag{22}$$

Conversely (C) implies (P) if $\lim_{y \to 0} w(x, y) \neq 0$ for any x. Take $\lambda > 0$ and substitute $\phi(\lambda t)$ for $\phi(t)$ in the relation $I_{\rm d}(\phi; \dot{\phi}) = 0$. Changing the variable $\lambda t \to t$, we obtain

$$\int_0^T [L_{\rm d}(\phi(t); -\lambda \dot{\phi}(t)) - L_{\rm d}(\phi(t); \lambda \dot{\phi}(t))]\, dt = 0.$$

Differentiating with respect to λ, and setting $\lambda = 1$, we have

$$\int_0^T (z + \hat{z}, \dot{\phi}(t))\, dt = 0 \tag{23}$$

with

$$z = \nabla_u L_{\rm d}(\phi(t); \dot{\phi}(t)), \tag{24}$$

$$\hat{z} = \nabla_u L_{\rm d}(\phi(t); -\dot{\phi}(t)). \tag{25}$$

Here ∇_u represents the derivation with respect to the second augment of $L_{\rm d}$. Since the relation (23) holds for any closed curve ϕ, there exists a potential function U such that

$$z+\hat{z}=U(\phi(t)). \tag{26}$$

By the one-to-one correspondence of the Legendre transformation, equations (24) and (25) are solved inversely as

$$\dot{\phi}(t)=\nabla_z H_{\mathrm{d}}(\phi(t);\, z) \tag{27}$$

$$-\dot{\phi}(t)=\nabla_{\hat{z}} H_{\mathrm{d}}(\phi(t);\, \hat{z}). \tag{28}$$

Rearranging the right-hand side of (28) with the use of (26), we have

$$\dot{\phi}(t)=\nabla_z \log\left(\int \mathrm{e}^{(z,y)} \exp[-(y, \nabla U(\phi(t)))] w(\phi(t), -y)\, \mathrm{d}y\right). \tag{29}$$

Eliminating $\dot{\phi}(t)$ from (27), (29), we obtain

$$\nabla_z \log\left(\int \mathrm{e}^{(z,y)} w(\phi(t), y)\, \mathrm{d}y\right)=\nabla_z \log\left(\int \mathrm{e}^{(z,y)} \exp[-(y, \nabla U(\phi(t)))] w(\phi(t), -y)\, \mathrm{d}y\right),$$

from which we get

$$\int \mathrm{e}^{(z,y)} \exp[-(y, \nabla U(\phi(t)))] w(\phi(t), -y)\, \mathrm{d}y = C \int \mathrm{e}^{(z,y)} w(\phi(t), y)\, \mathrm{d}y \tag{30}$$

with a constant C independent of z. Here we recall a fact proved by using the Weierstrass approximation theorem (Ito 1981). Given a continuous function f in R^n with a compact support, if $\int \mathrm{e}^{(z,y)} f(y)\, \mathrm{d}y=0$ for any z, then $f\equiv 0$. Taking this into account, we have from (30)

$$\exp[-(y, \nabla U(\phi(t))] w(\phi(t), -y) = Cw(\phi(t), y).$$

Take the limit $y\to 0$ and use the assumption $\lim_{y\to 0} w(x, y)\neq 0$, $\forall x\in R^n$. We then see that $C=1$, i.e. the condition (P) holds.

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