RELAXATION AND FLUCTUATION OF MACROVARIABLES

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Abstract

An extensive macrovariable X of a system of a large size Ω may have an extensive property of its probability distribution; namely the time-dependent probability function has the form

$$P(x,t) = C \exp \Omega\phi(x,t), \quad x = X/\Omega.$$

This ansatz has been proved by assuming a Markoffian process with transition probability satisfying a homogeneity condition. The function $\phi(x,t)$ can be identified with the action integral and the problem can be formulated by the Hamilton-Jacobi method, which is naturally related to a path-integral formalism. In normal cases, the distribution is Gaussian corresponding to a central limit theorem. Evolution of the mean value and the variance is determined by simple equations which contains the first and second moments of the basic transition probability.

Let X be an extensive macrovariable or a set of such variables in a large system with a size Ω, and x the corresponding density defined by

$$x = X/\Omega = \epsilon X, \qquad \epsilon = \Omega^{-1} \tag{1}$$

Examples are the numbers of molecules of certain species in a reaction vessel, the total spin in a magnetic (Ising spin) system, the population of certain class of people in a city and so on. The variable x is considered to make a stochastic process for which a time-dependent probability function $P(x,t)$ is defined. Some time ago, the author conjectured that this has an extensive property in the sense that it has the asymptotic form

$$P(x,t) = C \exp \Omega\phi(x,t) \tag{2}$$

for a large Ω[1]. This Ansatz was proved to be true under the assumption that the process $X(t)$ is Markoffian and its transition probability satisfies a certain condition of homogeneity to be given later. Recently, Suzuki has proved the Ansatz to hold under more general conditions[2). If the Ansatz (2) is valid, the deterministic path $x = y(t)$ will be determined by

$$\phi(x,t) = \max. \quad \text{for } x = y(t) \tag{3}$$

and the fluctuation

$$z = x - y(t)$$

is governed by the function ϕ. In normal cases, where ϕ is regular at $x = y$, the distribution is nearly Gaussian with the variance

$$\langle (x - y(t))^2 \rangle = -\varepsilon \phi''(y)^{-1} \equiv \varepsilon \sigma(t). \tag{4}$$

This corresponds to a central limit theorem for such a extensive macro-varialbe X.

Limiting ourselves to Markoffian cases, we assume that the process is described by the Chapman-Kolmogorov equation

$$\begin{aligned} P(X,t) = &-\int dr\ W(X\to X+r,t)\ P(X,t) \\ &+\int dr\ W(X-r \to X,t)\ P(X-r,t), \end{aligned} \tag{5}$$

where the transition probability W is assumed to be of the form

$$W(X\ X+r,\ t) = \Omega\ w(x,\ r,\ t); \tag{6}$$

in other words, the elementary jump of the state is essentially dependent on the density x and the magnitude of jump, the size Ω appearing only as the proportionality factor. This is a reasonable assumption realized in a great many cases of birth and death processes in physical and non-physical problems. Equation (5) can be written as

$$P(x,t) = -H(x,\ \varepsilon\frac{\partial}{\partial x},\ t)\ P(x,t) \tag{7}$$

with the operator H defined by

$$H(x,\ p,\ t) = \int dr\ (1 - e^{-rp})\ w(x,r,t) \tag{8}$$

or

$$H(x,\ p,\ t) = \sum_{n=1}^{\infty} \frac{(-)^{n-1}p^n}{n!}\ c_n(x,t) \tag{9}$$

where

$$c_n(x,t) = \int dr\ r^n\ w(x,r,t) \tag{10}$$

is the n-th moment of the transition probability.

We immediately notice that Eq. (7) is similar to a Schrödinger equation so that the asymptotic properties of the solution $P(x,t)$ for $\varepsilon \to 0$ may be treated in an analogous way. Referring to our paper[3] published about a year ago for the details, we summarize in the following some of the main points.

Propagation of the extensive property

The characteristic function $Q(\xi,t)$ is defined by

$$Q(\xi,\ t) = \int P(x,t)\ e^{ix\xi}\ dx\,. \tag{11}$$

It is shown that $Q(\xi,t)$ keeps the form

$$Q(\xi,\ t)\ \exp\ [\tfrac{1}{\varepsilon}\psi(i\varepsilon\xi,\ \varepsilon,\ t)] \tag{12}$$

if it is of this form at an initial time t_0.

By using the steepest descent evaluation, we have $P(x,t)$ in the form, Eq. (2). In particular, the extensivity holds for the initial condition $P(x,t_0) = \delta(x-x_0)$, so that the transition probability $P(x_0t_0|x,t)$ is extensive.

The proof assumes the convergence of cumulants of all orders and the analyticity of ψ. The propagation of extensivity may break down if these assumptions cease to be valid at some t.

Evolution equations

In normal cases, $P(x,t)$ is approximated by a Gaussian distrubution

$$P(x,\ t) \sim C\ \exp[\ -\frac{1}{2\varepsilon\sigma(t)}\ (x - y(t))^2]\,. \tag{13}$$

It is easily proved that $y(t)$ and $\sigma(t)$ obey the evolution equations,

$$\dot{y}(t) = c_1(y,\ t), \tag{14}$$

$$\dot{\sigma}(t) = 2\frac{\partial c_1}{\partial y}\sigma + c_2(y, t), \qquad (15)$$

which have been obtained by van Kampen from a different point of view.[4] These equations can easily be generalized to a many variable case;

$$\dot{y}_k(t) = c_{1k}(y,t), \qquad (16)$$

$$\dot{\sigma}_{jk}(t) = \sum_{\ell}(\sigma_{j\ell}\frac{\partial c_{1k}}{\partial y_\ell} + \frac{\partial c_{1j}}{\partial y_\ell}\sigma_{\ell k}) + c_{2jk}. \qquad (17)$$

These equations can be applied to a number of problems and lead to some important consequences. The standard Brownian motion corresponds to the assumption,

$$c_1(y) = -\gamma y, \qquad c_2 = \text{const.} \qquad (18)$$

The evolution equations then give immediately the well-known basic formulae for a Brownian motion. If $\gamma < 0$ in Eq. (18), $y = 0$ is unstable; the variance σ increases exponentially as y grows. An anomalous enhancement of fluctuation is seen to be a general phenomenon when a system departs from an unstable situation to reach a new stable equilibrium.

In a more than two variable case, there may arise a limit cycle for the motion $y(t)$. By a change of a parameter of the system, this may appear as a kind of phase transition.[5]

Hamilton-Jacobi formalism

Equation (7) gives

$$\frac{\partial}{\partial t}\phi = -H(x, \frac{\partial \phi}{\partial x}, t) \qquad (19)$$

to determine the function ϕ. The equations for the characteristics are then

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial x}, \qquad (20)$$

$$\frac{dJ}{dt} = -H + p\frac{\partial H}{\partial p} \equiv L, \qquad \frac{dq}{dt} = -\frac{\partial H}{\partial t}. \qquad (21)$$

To solve the Cauchy problem of Eq. (19) for a given initial function

$$\phi(x, t_0) = f(x),$$

we impose the initial condition

$$x(t_0) = \xi, \quad p(t_0) = f'(\xi), \quad J(t_0) = f(\xi)$$
$$q(t_0) = -H(\xi, f'(\xi), t_0) \qquad (22)$$

and find the solutions

$$x = x(t,\xi), \quad p = p(t,\xi), \quad J = J(t,\xi), \quad q = q(t,\xi).$$

This gives a parametric representation of $\phi(x,t)$ as

$$\phi(x,t) = J(t,\xi), \quad x = x(t,\xi). \tag{23}$$

This method is more general than using the evolution equations (14), (15); it can be used even when the variance σ does not exist.

Path-integral formulation

The asymptotic solution of Eq. (7) may also be represented by a path integral

$$P(x_0 t_0 | x\ t) = \int d\mathcal{B}(x(t)) \exp[\frac{1}{\varepsilon}\int_{t_0}^{t} ds\ L(x,\dot{x},s)], \tag{24}$$

where the Lagrangian L is that defined by Eq. (21).
The action integral

$$\phi = \int_{t_0}^{t} L(x(s),\ \dot{x}(s),\ s)\ ds \tag{25}$$

is maximized for the path which satisfies the Hamilton equation of motion, (20).

The Gaussian form (13) corresponds to the approximation

$$L(x,\ \dot{x},\ t) = -\frac{1}{2c_2(x,t)}\{\dot{x}(t) - c_1(x,t)\}^2. \tag{26}$$

If c_2 is a constant, the process is easily seen to be that described by the Langevin equation

$$\dot{x} = c_1(x,t) + R(t) \tag{27}$$

with a Gaussian white random noise

$$\langle R(t)\ R(t')\rangle = c_2\ \delta(t - t'). \tag{28}$$

The stochastic equation (27) is interpreted in Itô's sense, which is in accord with the Eq. (24) with the Lagrangian as given by (26).

Generalization to a field variable

So far we have confined ourselves to a single or a finite number of macrovariables. This is allowed for uniform systems. In non-uniform systems, we have to consider a field of macrovariables. The generalization of the asymptotic evaluation of fluctuations to such a case is not so direct. A scaling theory has been proposed by Mori in this connection.[6)]

Here we only remark that it is possible to extend our formalism to a field function $\psi(\vec{r},t)$ which follows the Langevin equation

$$\frac{\partial}{\partial t}\psi(\vec{r},t) = c_1(\psi,\vec{r},t) + R(\psi,\vec{r},t), \tag{29}$$

where R is a white noise. If R is characterized by its cumulants,

$$\begin{aligned} &\int \cdots\cdots \int \langle R(\psi,\vec{r}_1 t_1) \cdots\cdots R(\psi,\vec{r}_n t_n)\rangle_c d\vec{r}_1 dt_1 \cdots\cdots d\vec{r}_n dt_n \\ &\qquad r < r_j < r+\Delta r, \qquad t < t_j < t+\Delta t \\ &= c_n(\psi,\vec{r},t)\Delta\vec{r}\ \Delta t, \qquad\qquad n > 2\ , \end{aligned} \tag{30}$$

the characteristic function of $\partial\psi/\partial t$ is given by

$$\begin{aligned} &< \exp[-\int_{t_0}^{t_0+t} dt \int_\Omega dr\ \pi(\vec{r},t)\ \frac{\partial\psi}{\partial t}\ ]> \\ &= \exp\ [-\int_{t_0}^{t} dt \int_\Omega dr\ \mathcal{H}(\pi,\psi,\vec{r},t)\ ] \end{aligned} \tag{31}$$

with the "Hamiltonian"

$$\mathcal{H} = \sum_{n=1}^{\infty} \frac{(-)^{n-1}}{n!}\ \pi^n\ c_n(\psi,\vec{r},t). \tag{32}$$

If the volume Ω is large, an asymptotic evaluation can be made to obtain the distribution function of the field $\psi(\vec{r},t)$ in a path-integral form with the Lagrangian function

$$\mathcal{L}(\psi,\dot{\psi},\vec{r},t) = -\mathcal{H}(\pi,\psi,\vec{r},t) + \pi(\vec{r},t)\dot{\psi}\ . \tag{33}$$

This approach may be useful to treat non-uniform systems, but it has not been fully developed as yet.

Relaxation Spectra

Writing Eq. (7) as

$$\dot{P} = - \Gamma P \ , \tag{34}$$

we consider the eigenvalue problem

$$\Gamma\Psi_\alpha = \lambda_\alpha \Psi_\alpha . \tag{35}$$

We ask the asymptotic behavior of the eigenvalue spectrum for $\varepsilon \to 0$. It is seen that the eigenmodes are classified into two types. Normally, the first type of eigenmodes have eigenvalues independent of ε and corresponds to fluctuations around an equilibrium. The second type of eigenmodes have eigenvalues of the order of ε^{-1} and describe the decay of large deviations from equilibrium.

If the equilibrium is critical or marginal, the relaxation equation (14) becomes

$$\dot{y} = -\gamma y^k, \qquad k > 1 . \tag{36}$$

In such a case, there occurs an accumulation of eigenvalues at $\lambda = 0$, which corresponds to the phenomena of critical slowing down.

If Eq. (5) is a difference equation with the symmetry of detailed balance condition, the spectral density can be easily obtained with the use of the method of large perturbation introduced by Bethe many years ago. This treatment has also been described briefly in our previous paper.

References

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