A Green-Kubo Formula for general Markov processes with continuous time parameter

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1 Background

1.1. What is Green-Kubo formula ?

1827 R. Brown

“ Pollen grains suspended in water perform a continual swarming motions. ”

1905, 1908, 1923, 1930, 1945 ... Einstein, Langevin, Smoluchowski,Wiener Ornstien, Uhlenbeck, Wang,

$x(t)$: the displacement of a Browmian particle of mass m is governed by Newton's second law

$$m\ddot{x} = -\frac{\dot{x}}{\mu} - \frac{\partial V}{\partial x} + f_{\text{Random}} \tag{1}$$

- $-\dfrac{\dot{x}}{\mu}$: Friction force due to viscosity of the fluid.

  $\mu = (6\pi\eta R)^{-1}$: mobility, $\quad \gamma = \dfrac{1}{m\mu}$: frictional factor
- $-\dfrac{\partial V}{\partial x}$: external potential V e.g. gravity
- f_{Random} : Random force of zero mean due to the impacts of fluid particles.

Hypothesis: $\gamma \gg 1$ **(Overdamped)**

The viscous term dominates the inertial one, so, ignore the acceleration. Then, Eq. (1)

$$m\ddot{x} = -\frac{\dot{x}}{\mu} - \frac{\partial V}{\partial x} + f_{\text{Random}}$$

reduces to Langevin Equation

$$\begin{aligned} \dot{x} &= -\mu\frac{\partial V}{\partial x} + \mu f_{\text{Random}} \\ &= -\mu\frac{\partial V}{\partial x} + \eta(t) \end{aligned} \quad (2)$$

Assume that η: zero mean and

$$\langle \eta(t), \eta(t')\rangle = D\delta(t-t') \quad (3)$$

D is related to "Diffusion of the Brownian particle"

If $V(x) = x^2$, (Particle connected to a Hookian spring), then, Eq. (2) is O-U equation

$$\dot{x} = -\mu x + \eta(t). \tag{4}$$

- Deterministic velocity: $v(x) = -\mu x$
- Stochastic velocity $\eta(t)$
- Mean position: $\langle x(t) \rangle \equiv E(x(t)) = x(0)e^{-\mu t} \to 0$ as $t \to \infty$
- Fluctuation around the mean position

$$\langle (x(t) - \langle x(t) \rangle)^2 \rangle \equiv Var(x(t)) \to \frac{D}{2\mu}, \text{ as } t \to \infty \tag{5}$$

In physics (canonical ensemble), once the Brownian particle reaches the equilibrium (stationary process) with the fluid at a temperature T, the probability of finding a Browian particle at position x is given

$$\mathcal{P}_{\text{equilibrium}}(x) = \frac{1}{\sqrt{2\pi k_B T}} \exp\left[-\frac{x^2}{2k_B T}\right]$$

k_B is Boltzmann constant.

Then, $\langle x^2 \rangle_{\text{equilibrium}} = k_B T$, by (5) $\langle x^2 \rangle_{\text{equilibrium}} = \frac{D}{2\mu}$

Now, obtaining the well-known Einstein relation

$$D = 2\mu k_B T \tag{6}$$

This equality connects the fluctuation of Noise (D) to the dissipation in the medium.

Equilibrium $\Rightarrow$ **Balance** between **Fluctuation** and **Dissipative**

Another derivation by Green (1952) and Kubo (1966)

at the equilibrium state

- The mean velocity of $x(t)$ at $(t, x(t))$ is

$$v(x(t)) \equiv -\mu x(t)$$

- The autocorrelation function of $v(x(t))$ is

$$R(t) \equiv E(v(x(0))v(x(t))) = \langle v(x(0))v(x(t))\rangle = \frac{\mu D^2}{2}e^{-\mu t} \qquad (7)$$

$\Phi(\omega)$ is Fourier transform of $R(t)$, it is the Power spectrum of $v(x(t))$. $\Phi(\omega)$ can be regraded as “energy” in the frequency ω.

- moreover, by direct computation

$$R(t) = \langle v(x(0))^2 \rangle D e^{-\mu t} \tag{8}$$

- So,

$$\frac{D^2}{2} = \int_0^\infty R(t)dt = \langle v(x(0))^2 \rangle D\mu \tag{9}$$

- In fact, $\langle v(x(0))^2 \rangle$ is kinetic energy, then $\langle v(x(0))^2 \rangle = k_B T$
- Therefore, obtain Einstein relation $D = 2\mu k_B T$ again.

The formula

$$\frac{D^2}{2} = \int_0^\infty \langle v(0)v(t)\rangle dt = \int_0^\infty R(t)dt \tag{10}$$

is called **Green-Kubo formula** (Green-Kubo relation). It is a special form of **Fluctuation-Dissipative Theorem**.

2 Main results

Stochastic processes and **deterministic or random dynamical systems** are considered as two of the most important mathematical approaches dealing with the problems in nonequilibrium statistical physics

- Qian, Guo, Guo, 1988, Green-Kubo formula holds for **reversible** diffusion processes
- Spohn, 1991, some linearized hydrodynamic system with fluctuation currents and hard core lattice gas in thermal equilibrium and
- Ruelle, 1999, smooth dynamical systems
- Qian, Qian, Zhang, 2003, ergodic **reversible, finite states** Markov Chains
- Jiang, Zhang, 2003, general **reversible** Markov processes by Spectral representation theory
- Chen, Chen and Qian, 2006, **irreversible** Markov Chains with **finite states** by Matrix analysis

Our main result: A Green-Kubo formula holds for general Markov processes under some mild conditions.

Problem: How to understand " Mean Velocity" and " Diffusion Coefficient" of a general Markov process X_t ??

The state space is not $\mathbf{R}^d$.

Solution:

We get information of Markov process X_t by observable

$$\varphi(X_t) = (\varphi_1, \varphi_2, \cdots, \varphi_m)(X_t)$$

Therefore, consider the " Mean Velocity" and " Diffusion Coefficient" of observable $\varphi(X_t)$.

Then, go back to Nelson 1966

Let $\mathcal{P}_t = \sigma\{X_s, s \le t\}$

Definition of Mean Forward Velocity of $\varphi(X_t)$

$$V\varphi(X_t) = \lim_{\Delta t \downarrow 0} E\Big[\frac{\varphi(X_{t+\Delta t}) - \varphi(X_t)}{\Delta t} \,|\, \mathcal{P}_t\Big] \tag{11}$$

Definition of Conditional Diffusion Coefficient of $\varphi(X_t)$

$$G\varphi(X_t) = \lim_{\Delta t \downarrow 0} \mathrm{E}\Big[\frac{(\varphi(X_{t+\Delta t}) - \varphi(X_t))^T(\varphi(X_{t+\Delta t}) - \varphi(X_t))}{\Delta t}|\mathcal{P}_t\Big], \tag{12}$$

X_t: stationary Markov process on a Polish space Ξ

μ: stationary probability distribution of X_t

P_t: transition semigroup of X_t on $L^2(\Xi, \mu)$, assume it is strongly continuous.

$\mathcal{A}$: generator of P_t.

$\mathcal{D}(\mathcal{A})$: the domain of the generator $\mathcal{A}$

Theorem: Green-Kubo formula: For the stationary Markov process $\{X_t\}_{t\geq 0}$, let

$$\mathcal{J} = \Big\{ f \in L^2(\Xi, \mu) : \lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0 \Big\}. \qquad (13)$$

Then for any $\varphi_i,\ \varphi_j \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J}$, and $\phi_i\phi_j \in \mathcal{D}(\mathcal{A})$

$$\langle G_{ij}\varphi(X_t)\rangle = \int_0^\infty \langle V\varphi_i(X_0)V\varphi_j(X_t)\rangle\, dt + \int_0^\infty \langle V\varphi_j(X_0)V\varphi_i(X_t)\rangle\, dt. \qquad (14)$$

or,

$$\big(\langle G\varphi(X_t)\rangle\big)_{i,j=1\ldots m} = \int_0^\infty \langle V\varphi(X_0)\otimes V\varphi(X_t)\rangle\, dt + \int_0^\infty \langle V\varphi(X_0)\otimes V\varphi(X_t)\rangle\, dt. \qquad (15)$$

Remark:

- If X_t is reservable, Green-Kubo formula is

$$\langle G_{ij}\varphi(X_t)\rangle = 2\int_0^\infty \langle V\varphi_i(X_0)V\varphi_j(X_t)\rangle\, d\,t \tag{16}$$

- The condition

$$\mathcal{J} = \left\{ f \in L^2(\Xi,\mu) : \lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0 \right\}$$

$$\varphi_i,\ \varphi_j \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J}$$

is sharp.

For example, $\dot{x} = 1$, $z(t) = e^{\mathrm{i}\,x(t)}$ can be regarded as a Markov process on $\mathbb{S}^1$. Lebesgue measure on $\mathbb{S}^1$ is its stationary distribution. This example was given by Deuschel at this May for us.

- $X = \{X_t\}_{t\geq 0}$ is a stationary diffusion on $\mathbb{R}^d$ with infinitesimal generator

$$\mathcal{A} = \frac{1}{2}\nabla\cdot\big(A(x)\nabla\big)+b(x)\cdot\nabla = \frac{1}{2}\sum_{i,j=1}^{d}\frac{\partial}{\partial x_i}a_{ij}(x)\frac{\partial}{\partial x_j}+\sum_{i=1}^{d}b_i(x)\frac{\partial}{\partial x_i}\,, \tag{17}$$

$$\varphi_i(x) = x_i, \varphi_j(x) = x_j$$

Assume: the stationary distribution of X_t have a positive smooth density $\rho(x)$, and all the condition in Theorem are satisfied. Thus,

$$V_i(x) \equiv V\varphi_i(x) = b_i(x) + \frac{1}{2}\sum_{k=1}^{d} \frac{\partial a_{ik}}{\partial x_k}(x), \tag{18}$$

$$V_j(x) \equiv V\varphi_j(x) = b_j(x) + \frac{1}{2}\sum_{k=1}^{d} \frac{\partial a_{jk}}{\partial x_k}(x), \tag{19}$$

$$G_{ij}\varphi(x) = a_{ij}(x) \tag{20}$$

Green-Kubo formula is

$$\int_{\mathbb{R}^d} a_{ij}(x)\rho(x)d\,x = \int_0^\infty \langle V_i(X_0)V_j(X_t)\rangle d\,t + \int_0^\infty \langle V_j(X_0)V_i(X_t)\rangle d\,t. \tag{21}$$

Sketch of Proof:

- Due to direct computation

$$\langle G_{ij}\varphi(X_t)\rangle = -\langle \mathcal{A}\varphi_i, \varphi_j\rangle_\mu - \langle \mathcal{A}\varphi_j, \varphi_i\rangle_\mu. \tag{22}$$

$$\int_0^\infty \langle V\varphi_i(X_0)V\varphi_j(X_t)\rangle\, d\,t = \int_0^\infty \langle P_t\mathcal{A}\varphi_j, \mathcal{A}\varphi_i\rangle_\mu\, d\,t \tag{23}$$

$$= \lim_{t\to\infty}\langle P_t\varphi_j, \mathcal{A}\varphi_i\rangle_\mu - \langle \varphi_j, \mathcal{A}\varphi_i\rangle_\mu. \tag{24}$$

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$$\lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0 \ \text{AND} \ \langle \mathcal{A}\varphi\rangle_\mu = 0$$

$$\Rightarrow$$

$$\lim_{t\to\infty}\langle P_t f, \mathcal{A}\varphi\rangle_\mu = 0$$

3 Examples

3.1. Stochastic evolution equations in Hilbert spaces

$$\begin{cases} d\,X_t = (AX_t + F(X_t))\,d\,t + B\,d\,W_t, \quad t \geq 0, \\ X_0 = x \in H, \end{cases} \tag{25}$$

Reamrk: Da Prato *et al*: Non symmetric dissipative stochastic systems.

Da Prato, G.,Debussche A. and Goldys, B., *Some properties of invariant measures of non symmetric dissipative stochastic systems.* Probab. Theory Relat. Fields 123 (2002), 355-380.

Theorem: 3.1 (Da Prato, G.,Debussche A. and Goldys, B.)
Under some conditions,...... $\omega + \kappa < 0$ and $C^{-1} \in L(H)$ and $F \in C_b^2(H;H)$, then we have for any $f \in L^2(H,\mu)$, μ is the invariant measure of X_t

$$\lim_{t\to\infty} \|P_t f - \langle f \rangle_\mu\|_{L^2(\mu)} = 0, \tag{26}$$

with exponential rate.

* That is to say, it is the same as $\mathcal{J} = L^2(H,\mu)$. There are many observables f enough to guarantee Green-Kubo formula holds for Eq. (25)

Proposition 3.2 (Da Prato 2004) Assume that $C \equiv BB^* = \mathbb{I}$ (identity operator) and $F \in C_b(H, H)$. Then

$$\mathcal{A} \text{ is symmetric if and only if } F = \frac{1}{2}\nabla \log \rho,$$

where $\rho = \frac{d\mu}{d\nu}$, the Radon-Nikodym derivative of μ with respect to ν, $\nu = N(0, Q_\infty)$.

Example :(Da Prato 2002) Stochastic Reaction-Diffusion Equation: $H = L^2(0,1)$,

$$\begin{cases} Af = \frac{\partial^2}{\partial\zeta^2}(af) + b\frac{\partial}{\partial\zeta}f + cf, \ f \in D(A) \\ D(A) = H^2(0,1) \cap H_0^1(0,1), \end{cases} \tag{27}$$

... ...

$$F(x) = \sum_{k=0}^{2m-1} a_k x^k, \ x \in \mathbb{R}, \ \ a_{2m-1} < 0$$

3.2. Critical interacting diffusion processes on $\mathbb{Z}^d$

Assume $d \geq 3$. Let $X_t = \{X_t(i),\ i \in \mathbb{Z}^d\}$

$$d\,X_t(i) = \sum_{j\in\mathbb{Z}^d} q_{ij} X_t(i)\,d\,t + \sqrt{a(X_t(i))}\,d\,B_t(i), \qquad i \in \mathbb{Z}^d, \tag{28}$$

(H1) $q_{ij} \geq 0,\ \ i \neq j$, and $Q = \{q_{ij}\}$ is of finite range.

(H2) $-q_{ii} = \sum_{j\neq i} q_{ij} = 1.$

(H3) $q_{ij} = q_{0(j-i)}$.

Shiga, T., *An interacting system in population genetics.* J. Math. Kyoto Univ. 20 (1980), 213-242.

Shiga, T., Shimizu, A., *Infinite dimensional stochastic differential equations and their applications.* J. Math. Kyoto Univ. 20 (1980), 395-416.

Deuschel, J. D., *Invariance principible and empirical mean large deviation of the critical Ornstein-Uhlenbeck process.* Ann. Probab. 17 (1989), 74-90.

- *The critical Ornstein-Uhlenbeck process*: $a(y) = 1$

  Proposition 3.3 (Chojnowska-Michalik, A., Goldys, B. 2002)

  The following conditions are equivalent.

  (i) The semigroup P_t is symmetric in $L^2(H, \mu)$.

  (ii) If $x \in \mathcal{D}(A^*)$ then $Cx \in \mathcal{D}(A)$ and

  $$ACx = CA^*x.$$

  (iii) $e^{tA}C = C(e^{tA})^*$ for all $t \geq 0$.

  Chojnowska-Michalik, A., Goldys, B., *Symmetric Ornstein-Uhlenbeck semigroups and their generators.* Probab. Theory Relat. Fields 124 (2002), 459-486.

This is to say, there are many critical Ornstein-Uhlenbeck processes on $\mathbb{Z}^d$ which are irreversible.

- *The continuous time stepping stone model:*

$$a(y) = y(1-y), \qquad y \in [0,1]$$

Feng, S., Schmuland, B., Vaillancourt, J., Zhou, X., *Reversibility of Interacting Fleming-Viot Processes with Mutation, Selection, and Recombination.* Arxiv preprint arXiv:0803.1492, 2008.

Their results imply this process is irreversible.

- *The measure-valued critical branching random walk*: $a(y) = y$

  We guess this process is irreversible, but we can not give a proof.

Deuschel (1989) show for all of the three above processes, for any $f \in L^2(\Xi, \mu)$, μ is the ergodic invariant measure.

$$\lim_{t\to\infty} \|P_t f - \langle f \rangle_\mu\|_{L^2(\mu)} = 0.$$

That is to say, it is the same as $\mathcal{J} = L^2(\Xi, \mu)$. There are many observables f enough to guarantee Green-Kubo formula holds for for all of the three above processes

4 Discussion

There are different understand for "Diffusion coefficient" and "Velocity" in statistical physics. So, different forms of Green-Kubo formulas are derived from different definitions.

Suppose that $(v_x(t), v_y(t))$ is the velocity. Let the instantaneous position be

$$x(t) = x(0) + \int_0^t v_x(s)d\,s \equiv x(0) + \delta x(t). \tag{29}$$

$y(t)$ is similar.

Definition: The asymptotic diffusion coefficient is defined by

$$\lim_{t\to\infty} \frac{d}{d\,t}\langle \delta x^2(t)\rangle.$$

- **Example 1** For the A-Langevin equations

$$\begin{bmatrix} d\,v_x(t) \\ d\,v_y(t) \end{bmatrix} = \begin{bmatrix} -r & \Omega \\ -\Omega & -r \end{bmatrix} \begin{bmatrix} v_x(t) \\ v_y(t) \end{bmatrix} d\,t + \sigma \begin{bmatrix} d\,B_1(t) \\ d\,B_2(t) \end{bmatrix}, \tag{30}$$

$r > 0, \Omega > 0$, Clearly, $(v_x(t), v_y(t))$ has an invariant distribution. It is shown by Balescu that

$$\lim_{t\to\infty} \frac{d}{d\,t}\langle \delta x^2(t)\rangle = 2\int_0^\infty \langle v_x(t)v_x(0)\rangle d\,t. \tag{31}$$

This is also named Green-Kubo formula.

Balescu, R., *Statistical Dynamics Matter out of Equilibrium.* London: Imperial College Press, 1997.

However, the process associated with a complete set of variables

$$\{\xi_t = (x(t), y(t), v_x(t), v_y(t))\}$$

is a Markov process. The mean forward velocity of $x(t)$ is exactly $v_x(t)$. But, the process $(\xi_t)_{t\geq 0}$ has no invariant distribution, which prevents our Green-Kubo formula from being used.

- **Example 2** Suppose $p(t)$ is the momentum. For the harmonic oscillator, the explicit equations of motions are

$$\begin{cases} d\,x = \frac{p}{m} d\,t \\ d\,p = (-m\omega_0^2 x - \gamma p) d\,t + \sqrt{2kTm\gamma}\, d\,B(t), \end{cases} \tag{32}$$

$(\xi_t = (x(t), p(t)))_{t \geqslant 0}$ is a Markov diffusion with invariant distribution

$$\rho(x,\, p) \;=\; \frac{\omega_0}{2\pi kT} \exp\{-\frac{m\omega_0^2 x^2}{2kT} - \frac{p^2}{2mkT}\}$$

Risken Risken, H., *The Fokker-Plank Equation.* 2nd Edition, Springer-Verlag, 1989.

Zwanzig, R., *Nonequilibrium Statistical Mechanics.* Oxford University Press, 2001.

Then

$$V(x(t)) = \frac{p(t)}{m}$$

Thus, we have that

$$\langle Gx(t) \rangle = \lim_{t\to\infty} \frac{d}{d\,t} \langle \delta x^2(t) \rangle = 2\int_0^\infty \langle \frac{p(t)}{m} \frac{p(0)}{m} \rangle \, d\,t. \qquad (33)$$

The asymptotic diffusion coefficient and the expectation of the conditional diffusion coefficient are identical now. This means these two different diffusion coefficients lead to the same Green-Kubo formula for this example.

Thank you!