Abstract fluctuation theorem

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Abstract

We formulate an abstract fluctuation theorem which sheds light on mathematical relations between the fluctuation theorems of Bochkov-Kuzovlev, [B-K], and Jarzynski, [J], on one hand and those of Evans-Searles, [E-S], and Gallavotti-Cohen, [G-C], on the other.

1 Algebraic preliminaries

Let $\Phi : M \to M$ and $\Psi : M \to M$ be two dynamical systems in a broad sense. Later on we will specify them to be measurable maps, measure preserving or not, or diffeomorphisms. We start with a general framework, assuming only that Φ and Ψ are one-to-one maps of the phase space M.

Let $R : M \to M$ be an involution, i.e., $R^2 = R \circ R = Id$. We say that Φ is an *R-inverse* of Ψ if $R\Psi R\Phi = Id$, i.e., the following diagram commutes

$$\begin{array}{ccc} M & \xrightarrow{\Phi} & M \\ R\big\downarrow & & \big\downarrow R \\ M & \xrightarrow{\Psi^{-1}} & M \end{array}$$

Clearly if Φ is an R-inverse of Ψ, then Ψ is an R-inverse of Φ. If Φ is an R-inverse of itself then Φ is called *R-reversible*, or simply reversible.

Proposition 1 *Ψ is an R-inverse of Φ if and only for $S = R \circ \Phi$ and the involution $U : M \times M \to M \times M$, $U(x_1, x_2) = (Rx_2, Rx_1)$, the following diagram commutes*

$$\begin{array}{ccc} M & \xrightarrow{S} & M \\ \widetilde{\Phi}\big\downarrow & & \big\downarrow \widetilde{\Psi} \\ M \times M & \xrightarrow{U} & M \times M \end{array}$$

where $\widetilde{\Phi}(x) = (x, \Phi x)$ and $\widetilde{\Psi}(x) = (x, \Psi x)$.

Proof.

$$U\widetilde{\Phi}x = U\left(x, \Phi x\right) = (R\Phi x, Rx) = (Sx, \Psi R \Phi x) = \widetilde{\Psi} Sx. \qquad \square$$

We can immediately extend Proposition 1 to the space of trajectories of length $k+1, k \geq 1$. Let $M^{k+1} = M \times \cdots \times M, k \geq 1$ and $\widetilde{\Phi} : M \to M^{k+1}$ and $\widetilde{\Psi} : M \to M^{k+1}$ be defined as

$$\widetilde{\Phi}(x) = \left(x, \Phi x, \ldots, \Phi^k x\right), \quad \widetilde{\Psi}(x) = \left(x, \Psi x, \ldots, \Psi^k x\right). \tag{1}$$

We have then again that the involution $U = U_k : M^{k+1} \to M^{k+1}$,

$$U(x_0, \ldots, x_k) = (Rx_k, Rx_{k-1}, \ldots, Rx_0)$$

takes the trajectory of Φ starting at x into the trajectory of Ψ starting at Sx where $S = S_k = R \circ \Phi^k$. In other words we have again that $U_k \circ \widetilde{\Phi} = \widetilde{\Psi} \circ S_k$.

Let us now consider a set Z and a map $m : M \to Z$, which we think of as a measurement on the phase space M. In particular Z can be much "smaller" than M. We assume further that the involution R can be factored onto Z, i.e., there is an involution $r : Z \to Z$ such that $rm = mR$. We get then that the involution $T = T_k : Z^{k+1} \to Z^{k+1}$, $T\left(z_0, z_1, \ldots, z_k\right) = \left(rz_k, rz_{k-1}, \ldots, rz_0\right)$ takes the "time series" of Φ starting at x into the "time series" of Ψ starting at $S_k x$. More precisely we have the following

Proposition 2 *Let $m = m_k : M^{k+1} \to Z^{k+1}$ be the map*

$$m_k(x_0, x_1, \ldots, x_k) = (mx_0, mx_1, \ldots, mx_k).$$

We have the commuting diagram

$$\begin{array}{ccc} M & \xrightarrow{S_k} & M \\ \widetilde{\Phi}\big\downarrow & & \big\downarrow\widetilde{\Psi} \\ M^{k+1} & \xrightarrow{U_k} & M^{k+1} \\ m_k\big\downarrow & & \big\downarrow m_k \\ Z^{k+1} & \xrightarrow{T_k} & Z^{k+1} \end{array}$$

Proof. The commutativity of the upper part of the diagram is the generalized Proposition 1. We need only to establish the commutativity of the lower part. i.e., $m_k U_k = T_k m_k$.

$$\begin{aligned} m_k U_k(x_0, x_1, \ldots, x_k) &= m_k(Rx_k, \ldots, Rx_1, Rx_0) = (mRx_k, \ldots, mRx_1, mRx_0) \\ &= (rmx_k, rmx_{k-1}, \ldots, rmx_0) = T\left(mx_0, rmx_1, \ldots, mx_k\right) \end{aligned}$$

$\square$

In the special case of a reversible dynamical system, that is when $\Psi = \Phi$ we get that $S = S_k = R \circ \Phi^k, k \geq 1$ is an involution and although the dynamics itself cannot be factored in general to the space of measurements Z (or Z^k), the involution S has a natural factor T on Z^k, or more precisely on the space of time series (the space of measurements on finite trajectories of Φ, since this is exactly the range of $m_k \circ \widetilde{\Phi}$). Let us stress that the only requirement is that the involution R factors to Z.

Let us finally examine how this formalism works in the case of time dependent systems, i.e., let us consider two sequences of maps of M, $\Phi_1, \ldots, \Phi_k$ and $\Psi_1, \ldots, \Psi_k, k \geq 1$. We assume that each Ψ_i is an R-inverse of $\Phi_i, i = 1, \ldots, k$. Let us consider the time dependent dynamical systems $\Phi^j = \Phi_j \circ \cdots \circ \Phi_2 \circ \Phi_1$ and $\Psi^j = \Psi_{k-j+1} \circ \Psi_{k-j+2} \circ \ldots \Psi_k$, $j = 1, \ldots, k$.

Note the reversal of order in the definition of Ψ^i; it gives the impression of lacking physical meaning. However in some examples it can be interpreted as the arranged "time reversal of controls".

We can formulate an obvious time dependent generalization of Proposition 2. Namely if $\widetilde{\Phi}$ and $\widetilde{\Psi}$ is defined again by (1), with the modified meaning of $\Phi^j, \Psi^j, j = 1, \ldots, k$, then the commuting diagram of Proposition 2 holds.

2 Factors of measures

We keep all the assumptions of Section 1 with the addition that $M = (M, \mathcal{B}, \mu)$ is a measurable space, i.e., $\mathcal{B}$ is a σ-algebra of subsets of M and μ is a σ-finite measure. We assume that Φ, Ψ and R are measurable maps, that the involution R preserves the measure μ, and that $\Phi_* \mu = f\mu$, for some positive function f on M.

Proposition 3 *We have $\Psi_* \mu = g\mu$, where $g = (f \circ \Phi \circ R)^{-1}$. It follows that $g \circ \Psi = (f \circ R)^{-1}$.*

Proof. We have $\Phi_*^{-1} \mu = (f \circ \Phi)^{-1} \mu$ and $\Psi = R \circ \Phi^{-1} \circ R$. It follows that $\Psi_* \mu = (f \circ \Phi \circ R)^{-1} \mu$. $\square$

Clearly if $\Phi_*^k \mu = f^k \mu$ then $\Psi_*^k \mu = g^k \mu$, where $g^k = \left(f^k \circ \Phi^k \circ R\right)^{-1}$, for a fixed value of $k \geq 1$. (Note that k in f^k and g^k, is a superscript in these formulas and not a power.) Moreover this formula applies also to the case of time dependent systems described in Section 1. More precisely if $(\Phi_i)_* \mu = f_i \mu, i = 1, \ldots, k$, then $\Phi_*^k \mu = f^k \mu$ with

$$f^k = \prod_{i=1}^{k} f_i \circ \Phi_{i+1}^{-1} \circ \cdots \circ \Phi_k^{-1}$$

Let us consider the augmented maps

$$\widehat{\Phi} : M \to Z^{k+1} \times \mathbb{R}, \quad \widehat{\Psi} : M \to Z^{k+1} \times \mathbb{R},$$

defined by

$$\widehat{\Phi}x = \left(m_k \widetilde{\Phi}x, \ln f^k \circ \Phi^k \right) = \left(mx, m\Phi x, \ldots, m\Phi^k x, \ln \prod_{i=1}^{k} f_i(\Phi^i x) \right)$$

and the respective formula for $\widehat{\Psi}$. We also introduce the involution $\widehat{T} : Z^{k+1} \times \mathbb{R} \to Z^{k+1} \times \mathbb{R}$,

$$\widehat{T}(z_0, z_1, \ldots, z_k, a) = (rz_k, \ldots, rz_1, rz_0, -a).$$

We have the measure counterpart of Proposition 2.

Theorem 1 *The following diagram commutes*

$$\begin{array}{ccc} M & \xrightarrow{S_k} & M \\ \widehat{\Phi}\downarrow & & \downarrow\widehat{\Psi} \\ Z^{k+1} \times \mathbb{R} & \xrightarrow{\widehat{T}} & Z^{k+1} \times \mathbb{R} \end{array}$$

and

$$\widehat{T}_* \widehat{\Phi}_* \mu = e^{-a} \widehat{\Psi}_* \mu.$$

In the case of a probability measure μ, the measure $\widehat{\Phi}_*\mu$ represents the statistics of the time series of Φ augmented by the value of $\ln f^k \circ \Phi^k$. The measure $\widehat{\Psi}_*\mu$ has a similar meaning and the two probability distributions are related by the involutive symmetry $\widehat{T}$, namely the image of former under $\widehat{T}$ has the density e^{-a} with respect to the latter.

The last claim in Theorem 1 can be also formulated as

$$\widehat{T}_* \left(e^{-\frac{a}{2}} \widehat{\Phi}_* \mu \right) = e^{-\frac{a}{2}} \widehat{\Psi}_* \mu.$$

Hence in the case of R-reversible Φ, i.e., $\Psi = \Phi$ we get that the measure $e^{-\frac{a}{2}} \widehat{\Phi}_* \mu$ is invariant under the involution $\widehat{T}$.

Proof. In view of Proposition 2 to establish the commutativity of the diagram we need only to check that

$$g^k \circ \Psi^k \circ S_k = \left(f^k \circ \Phi^k \right)^{-1},$$

which follows immediately from Proposition 3.

Once the commutativity is established we get

$$\widehat{T}_*\widehat{\Phi}_*\mu = \widehat{\Psi}_*\left(R_*\Phi_*^k\mu\right) = \widehat{\Psi}_*\left(f^k \circ R\mu\right).$$

We conclude the proof by observing that by Proposition 3 the function $f^k \circ R$ equals to $\left(g^k \circ \Psi^k\right)^{-1}$, and hence it factors under $\widehat{\Psi}$ to the function on $Z^{k+1} \times \mathbb{R}$ equal to e^{-a}, where a is the last coordinate in $Z^{k+1} \times \mathbb{R}$. □

Let us assume further that Z comes with a reference measure ν invariant under the involution r. We introduce the measure λ on $Z^{k+1} \times \mathbb{R}$ equal to the product of ν^{k+1} on Z^{k+1} and the Lebesgue measure on $\mathbb{R}$. Clearly the measure λ is invariant under the action of the involution $\widehat{T}$. Under these assumptions we get immediately the following corollary of Theorem 1.

Theorem 2 *If the measures $\widehat{\Phi}_*\mu$ and $\widehat{\Psi}_*\mu$ are absolutely continuous with respect to the measure λ on $Z^{k+1} \times \mathbb{R}$ with densities equal to $p_+(z_0, z_1, \dots, z_k, a)$ and $p_-(z_0, z_1, \dots, z_k, a)$. then*

$$p_+(z_0, z_1, \dots, z_k, a) = e^a p_-(rz_k, \dots, rz_1, rz_0, -a).$$

3 Bochkov-Kuzovlev and Jarzynski scenarios

Theorem 1 provides a general scheme, special cases of which appeared earlier in different setups. For simplicity we will consider in this section only the case $k = 1$. We assume that the phase space M is a symplectic manifold with the symplectic form ω, and that the involution R is anti-symplectic, i.e., $R^*\omega = -\omega$. We consider a time dependent Hamiltonian $H(x, t)$ on M. We further assume that the Hamiltonian H is at every moment of time invariant under the involution R, i.e., $H(Rx, t) = H(x, t)$. Let us fix a time interval $[0, \tau]$ and let Φ be the "after time τ" symplectic map of M defined by the Hamiltonian dynamics of H. Let us consider the Hamiltonian $G(x, t) = H(x, \tau - t)$ and let Ψ be the "after time τ" symplectic map of M defined by the Hamiltonian dynamics of G. In the scenario of Jarzynski [J] the Hamiltonian G governs the process with the *" time reversed protocols"*.

Proposition 4 *Ψ is an R-inverse of Φ.*

Proof. By the definition of Ψ we get that Ψ^{-1} is the "after time τ" map of the Hamiltonian $-H(x, t)$. At the same time since the involution R is anti-symplectic the map $R\Phi R$ is also the "after time τ" map of the Hamiltonian $-H(x, t)$. □

In the the Bochkov-Kuzovlev scenario, [B-K], the Hamiltonian $H(x, t) = H_0(x) + H_1(x, t)$ with $H_1(x, t)$ representing a time dependent action on the system. Let χ be the Liouville measure on M and $\mu = \frac{1}{z}e^{-\beta H_0}\chi$ be the Gibbs probability measure, where z is the normalizing factor. We consider $Z = M$ with m the identity map, i.e., all variables are observed. We get that $\widehat{\Phi}x = (x, \Phi x, \beta H_0(\Phi x) - \beta H_0(x))$ and $\widehat{\Psi}x = (x, \Psi x, \beta H_0(\Psi x) - \beta H_0(x))$. Let us denote by P the probability defined by the Gibbs measure μ. Theorem 1 can be now reformulated as the following

Corollary 1 *For any subsets $A_0, A_1 \subset M$, and any real a and $\epsilon > 0$*

$$e^{\beta(a-\epsilon)} \leq \frac{P\left(x \in A_0, \Phi x \in A_1, |H_0(\Phi x) - H_0(x) - a| \leq \epsilon\right)}{P\left(x \in RA_1, \Psi x \in RA_0, |H_0(\Psi x) - H_0(x) + a| \leq \epsilon\right)} \leq e^{\beta(a+\epsilon)}.$$

In particular taking $A_0 = A_1 = M$ we obtain from Corollary 1 that

Corollary 2 *For any real a and $\epsilon > 0$*

$$e^{\beta(a-\epsilon)} \leq \frac{P\left(|H_0(\Phi x) - H_0(x) - a| \leq \epsilon\right)}{P\left(|H_0(\Psi x) - H_0(x) + a| \leq \epsilon\right)} \leq e^{\beta(a+\epsilon)}.$$

Corollary 3 *If $p_+ = p_+(a)$ and $p_- = p_-(a)$ are the densities with respect to the Lebesgue measure on $\mathbb{R}$ of the distributions of values of $H_0(\Phi x) - H_0(x)$ and $H_0(\Psi x) - H_0(x)$, respectively, then we have*

$$p_+(a) = e^{\beta a} p_-(-a).$$

In the Jarzynski scenario there is a Hamiltonian system on a symplectic manifold Z interacting with "heat baths", represented by another Hamiltonian system on a symplectic manifold Y. The joint Hamiltonian system lives on $M = Y \times Z$ and we take $m : M \to Z$ to be the projection on the second component. The Liouville measure χ on M is invariant under Φ, Ψ and R. However it is in general infinite. We introduce a probabilistic density $\rho = \rho(y)$ on Y, a *"prepared state of the heat baths"*. We apply Theorems 1 and 2 to the measure $\mu = \rho\chi$. We have

$$\Phi_*\mu = f\mu = \frac{\rho \circ \Phi^{-1}}{\rho}\mu.$$

In the Jarzynski scenario $\ln f \circ \Phi = \ln \rho - \ln \rho \circ \Phi$ quantifies the entropy production. The measure $\mu = \rho\chi$ on M is not probabilistic but it disintegrates into a family of probabilistic measures after fixing the Z component. Consequently the measure $\widehat{\Phi}_*\mu$ on $Z \times Z \times \mathbb{R}$ disintegrates into a family of probabilistic measures after fixing the first coordinate z_0. That gives us the "conditional" probabilities $P_+(\cdot|z_0)$. Similarly we obtain the family of "conditional" probabilities $P_-(\cdot|z_0)$ by considering the disintegration of the measure $\widehat{\Psi}_*\mu$. We obtain now Jarzynski detailed fluctuation theorem as a consequence of Theorem 2.

Corollary 4 *Denoting by* $p_+(z_1, a|z_0)$ *and* $p_-(z_1, a|z_0)$ *the densities of the probability measures* $P_+(\cdot|z_0)$ *and* $P_-(\cdot|z_0)$*, respectively, we have*

$$p_+(z_1, a|z_0) = e^a p_-(rz_0, -a|rz_1).$$

4 Evans-Searles and Gallavotti-Cohen scenarios

Let Φ be an R-reversible diffeomorphism of a Riemannian manifold M and μ a probabilistic volume element invariant under the involution R. Let $J(x) = |\det \mathcal{D}_x \Phi|$ be the Jacobian of the diffeomorphism Φ, and more generally $J_k(x) = \left|\det \mathcal{D}_x \Phi^k\right|$ be the Jacobian of Φ^k. We have $\Phi_* \mu = f\mu$ with $f(x) = \left(J(\Phi^{-1}x)\right)^{-1}$.

Hence the quantity $\ln \prod_{i=1}^k f(\Phi^i x) = -\ln J_k(x)$.

Taking $\Psi = \Phi$, $Z = M$ and $m = Id$, we get $\widehat{\Phi} = \left(x, \Phi x, \ldots, \Phi^k x, -\ln J_k(x)\right)$ and Theorem 1 gives us the Evans-Searles fluctuation theorem,[E-S].

Corollary 5 *For any subsets* $A_0, A_1, \ldots, A_k \subset M$*, any real* a*, and any positive* ϵ

$$e^{-a-\epsilon} \leq \frac{P\{x \in A_0, \ldots, \Phi^k(x) \in A_k, |\ln J_k(x) - a| \leq \epsilon\}}{P\{x \in RA_k, \ldots, \Phi^k(x) \in RA_0, |\ln J_k(x) + a| \leq \epsilon\}} \leq e^{-a+\epsilon},$$

where P *denotes the probability defined by the probabilistic volume element* μ.

In particular taking $A_0 = A_1 = \cdots = A_k = M$ in Corollary 5 we get

Corollary 6

$$e^{-a-\epsilon} \leq \frac{P\{|\ln J_k(x) - a| \leq \epsilon\}}{P\{|\ln J_k(x) + a| \leq \epsilon\}} \leq e^{-a+\epsilon}.$$

Corollary 7 *Let* $p_k = p_k(a)$ *denote the density with respect to the Lebesgue measure on* $\mathbb{R}$ *of the distribution of values of* $\ln J_k$*. We have*

$$p_k(a) = e^{-a} p_k(-a). \tag{2}$$

The property in Corollary 7 is stronger than the one in the Gallavotti-Cohen fluctuation theorem, [G-C], however it holds for the probability P defined by the reference Lebesgue measure μ on M, and not for the asymptotic state of the system.

We can get a little closer to the Gallavotti-Cohen formulation by observing that the distribution of values of

$$\sum_{i=-k}^{k} \ln J(\Phi^i x) = \ln J_{2k+1}(\Phi^{-k} x)$$

with respect to the probability measure $\Phi_*^k \mu$ coincides with the distribution of values of $\ln J_{2k+1}(x)$ with respect to the measure μ, and the density of this distribution being equal to $p_{2k+1}(a)$ has the symmetry (2). However it is not clear in general how to take the limit $k \to \infty$.

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