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A Time-Reversible Formulation of the H-Theorem

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An abstract theorem, which is an analogy of Boltzmann's H-theorm, is proved by the method of the ergodic theory. The theorem allows dynamical reversibility, i. e., in our formulation, it is not absolutely certain that entropy increases monotonically, but it is overwhelmingly unlikely that it decreases if the number of molecules is large enough. The theorem can be extended in two directions: the one is in continuous case and another of which is in the case of more general entropy. Finally, three instructive examples are shown satisfying the conditions of the theorems.

1 Introduction

The H-theorem by Boltzmann in statistical dynamics was abstractly reformulated by Yosida[5] (p. 392) and by others** who used Markov operators. As to the H-theorem, which asserts the increase of entropy for time, there have been some criticisms, e. g., the criticisms posed both by Loschmidt and by Zermelo-Poincarè. By the allowance of the existence of the fluctuations, we can answer these criticisms (for example, see Radushkevitch[4] Chap. 2 §6). The mathematical formulations, however, are not sufficient. Obviously, the method of Markov operators does not make models time-reversible, so such a formulation can not answer the criticisms.

In this paper, we propose one of the abstract models, which are time-reversible and to which the criticisms are irrelevant.

2 Preliminaries

Let $(A, \mathscr{A})$ be a measurable space, and $(A^N, \mathscr{A}^N)$ be a direct product measurable space of countablly infinite copies of $(A, \mathscr{A})$, where N is a set of all positive integers. Sometimes we denote $(A^N, \mathscr{A}^N)$ by $(X, \mathscr{X})$. For $x \in X$, x_i represents the i-th value of x, A_i represents the i-th space of A^N, and $\mathscr{A}_i$ is the σ-field of A_i, which is a copy of $\mathscr{A}$. Let S be the shift transformation on A^N, i. e., for $x \in X$, $(Sx)_i = x_{i+1}$. Clearly S is a measurable transformation on $(X, \mathscr{X})$. Similarly we introduce a measurable transformation S_n on $(A^n, \mathscr{A}^n)$, which is defined as: for $a \in A^n$, $(S_n\ a)_i = a_{i+1}$ if $i+1 \leq n$, and $(S_n\ a)_n = a_1$, i. e., S_n is a

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** It is also known that the similar inequality holds in quantum statistics (cf. von Neumann[3]) and also see Nakamura and Umegaki[2]).

cyclic rotation of a, where $A^n=\Pi_{i=1}^n A_i$ and $\mathscr{A}^n=\Pi_{i=1}^n \mathscr{A}_i$.

Let p_n be a probability measure on $(A^n, \mathscr{A}^n)$ and P be a probability measure on $(X. \mathscr{X})$. In such a situation we define:

DEFINITION 1. The probability measures p_n $(n=1, 2, \cdots\cdots)$ are *UI-convergent* (*convergent uniformly and inductively*) to the probability measure P if for all $\varepsilon>0$ there exists a number n_0, and for all n $(\geqq n_0)$ and all $B\in\mathscr{A}^n$

$$|p_n(B)-P(\tilde{B})|<\varepsilon,$$

where $\tilde{B}$ is an imbedding of B to X, i. e.,

$$\tilde{B}=\{x\in X:(x_1, x_2, \cdots\cdots, x_n)\in B\}.$$

Especially if p_n is a marginal distribution of P on $(A^n, \mathscr{A}^n)$, then p_n is UI-convergent to P trivially. The following lemma is obvious.

LEMMA 2.1 *p_n is UI-convergent to P if and only if*

$$\lim_{n\to\infty}||p_n-P||_n=0,$$

where $||\cdot||_n$ is a total variation of a measure on $(A^n, \mathscr{A}^n)$.

Let us assume that P is invariant under the transformation S and p_n's $(n=1, 2, \cdots)$ are invariant under S_n, i. e., for all $E\in\mathscr{X}$, $P(E)=P(S^{-1}E)$, and for all $F\in\mathscr{A}^n$, $p_n(F)=p_n(S_n^{-1}F)$.

For an element $a\in A^n$ and a set $B\in\mathscr{A}^n$, we put

$$r_n(B;a)=\frac{1}{n}\sum_{i=0}^{n-1}\chi_B(S_n{}^i\mathrm{a}), \tag{2.1}$$

where x_E is a characteristic function of a set E. Then, evidently $r_n(\cdot;a)$ is a probability measure on $\mathscr{A}^n$ for every $a\in A^n$, and $r_n(B;\cdot)$ is a measurable function on A^n for all $B\in\mathscr{A}^n$. For $x\in X$, the n-tuple $(x_1, x_2, \cdots, x_n)$ is regarded as a point of A^n, which we denote by $\pi_n(x)$. Clearly $r_n(\cdot;\pi_n(x))$ is a probability measure on $\mathscr{A}^n$ for all $x\in X$. Then we get:

LEMMA 2.2 *If P is ergodic with respect to S, then for every $B\in\mathscr{A}^m$ $(m\in N)$,*

$$r_n(\hat{B};\pi_n(x))\underset{\substack{n\to\infty\\(n\geqq m)}}{\longrightarrow}P(\tilde{B}) \qquad P\text{-a. e. } x,$$

where $\hat{B}$ is an imbedding of B $(\subseteq A^m)$ into A^n.

Proof. First, we see

$$r_n(\hat{B};\pi_n(x))=\frac{1}{n}\sum_{i=0}^{n-1}\chi_{\hat{B}}(S_n{}^i\pi_n(x))$$

$$=\frac{1}{n}\sum_{i=0}^{n-m}\chi_{\hat{B}}(S_n{}^i\pi_n(x))+\frac{1}{n}\sum_{i=n-m+1}^{n-1}\chi_{\hat{B}}(S_n{}^i\pi_n(x)). \tag{2.2}$$

Now we note that

$$\chi_{\hat{B}}(S_n{}^i\pi_n(x))=\chi_{\tilde{B}}(S^ix)$$

if $i\leqq n-m$, because $S_n{}^i\pi_n(x)\in\hat{B}$ is equivalent to $S_n{}^i(x_1,x_2,\cdots,x_n)\in\hat{B}$, and to $(x_{1+i}, x_{2+i}, \cdots x_{m+i})\in\hat{B}$ as $m+i\leqq n$, which is also equivalent to $S^ix\in\tilde{B}$. Hence (2.2) becomes

$$\frac{1}{n}\sum_{i=0}^{n-m}\chi_{\tilde{B}}(S^i x)+\frac{1}{n}\sum_{i=n-m+1}^{n-1}\chi_{\hat{B}}(S_n{}^i\pi(x))$$

$$=\frac{1}{n}\sum_{i=0}^{n-1}\chi_{\tilde{B}}(S^ix)+\frac{1}{n}\sum_{i=n-m+1}^{n-1}\{\chi_{\hat{B}}(S_n{}^i\pi_n(x))-\chi_{\tilde{B}}(S^ix)\}. \tag{2.3}$$

The first term of (2.3) is convergent to $P(\tilde{B})$ as P is an ergodic measure with respect to the transformation S, and the second term of (2.3) goes to 0. q.e.d.

As the almost everywhere convergence implies the convergence in probability, we get the following lemma.

LEMMA 2.3 *Under the same assumption as the previous lemma,* $r_n(\hat{B};\pi_n(x))$ *converges to* $P(\tilde{B})$ *in probability, i.e., for every* $\varepsilon>0$,

$$\lim_{n\to\infty}P\{x:|r_n(\hat{B};\pi_n(x))-P(\tilde{B})|\geqq\varepsilon\}=0. \tag{2.4}$$

3 A Time-Reversible H-theorem

Let φ_n be an invertible measure preserving transformation on A^n with respect to the measure p_n. Further, we assume the ergodicity of φ_n. Then by the ergodic theorem, for all $L^1(A^n, \mathscr{A}^n, p_n)$-function f, we see

$$\lim_{T\to\infty}\frac{1}{2T+1}\sum_{i=-T}^{T}f(\varphi_n{}^ia)=\int_{A^n}fdp_n \qquad p_n\text{-a.e. } a. \tag{3.1}$$

Let $F(t)$ be a logical proposition for the integer t, then we define:

DEFINITION 2. *A ratio of* $F(t)$ is a value of a limit

$$\lim_{T\to\infty}\frac{1}{2T+1}c\{t:-T\leqq t\leqq T, F(t)\text{ is true}\}$$

in case the limit exists, where $c(\cdot)$ is a counting measure on the set of all integers. Similarly *a ratio of a set* F_0 *of integers* is a ratio of a logical proposition "$t\in F_0$", if it exists. Sometimes we use above two notions indiscriminately.

By this terminology, we get the following lemma.

LEMMA 3.1 *Let m be an arbitrarily fixed positive integer, and p_n be UI-convergent to P. We assume that p_n is ergodic with respect to φ_n for all n. For every $\varepsilon>0$, every $\delta>0$ and every $B\in\mathscr{A}^m$, there exists a number n_0, and for all $n\geqq n_0$, the ratio of the inequality*

$$|r_n(\hat{B};\varphi_n{}^t a)-P(\tilde{B})|<\varepsilon \tag{3.2}$$

is greater than $1-\delta$, for almost everywhere $a\in A^n$ with respect to the measure p_n.

Proof. Let us denote

$$E_n=\{a:|r_n(\hat{B};a)-P(\tilde{B})|<\varepsilon\},$$

which belongs to $\mathscr{A}^n$. Then

$$\begin{aligned}\tilde{E}_n&=\{x:\pi_n(x)\in E_n\}\\&=\{x:|r_n(\hat{B};\pi_n(x))-P(\tilde{B})|<\varepsilon\},\end{aligned}$$

which belongs to $\mathscr{X}$. By Lemma 2.3,

$$\lim_{n\to\infty}P(\tilde{E}_n)=1. \tag{3.3}$$

As p_n is UI-convergent to P, we see

$$\lim_{n\to\infty}|p_n(E_n)-P(\tilde{E}_n)|=0. \tag{3.4}$$

From (3.3) and (3.4), there exists a number n_0 such that

$$p_n(E_n)>1-\delta \tag{3.5}$$

for all $n\geqq n_0$. Then

$$\begin{aligned}&\lim_{T\to\infty}\frac{1}{2T+1}c\{t:-T\leqq t\leqq T,\ |r_n(\hat{B};\varphi_n{}^t a)-P(\tilde{B})|<\varepsilon\}\\&=\lim_{T\to\infty}\frac{1}{2T+1}c\{t:-T\leqq t\leqq T,\ \varphi_n{}^t a\in E_n\}\\&=\lim_{T\to\infty}\frac{1}{2T+1}\sum_{t=-T}^{T}\chi_{E_n}(\varphi_n{}^t a)\\&=p_n(E_n)\end{aligned} \tag{3.6}$$

almost everywhere a by the ergodic theorem (3.1), and the last term is greater than $1-\delta$ by (3.5). q. e. d.

If $\mathscr{B}$ is a finite measurable partition of A^m (for some m), the entropy of $\mathscr{B}$ with respect to some probability measure $q(\cdot)$ is defined by

$$H(\mathscr{B};q) = -\sum_A q(A) \log q(A),$$

where the summation is taken over all atoms of $\mathscr{B}$ and 0 log 0 is assumed to be 0. Suppose that $\mathscr{B}$ has the atoms of equal measure with respect to P, i. e., if B is an atom of $\mathscr{B}$ and l is the number of atoms in $\mathscr{B}$ then $P(\widetilde{B})=1/l$. In this case the entropy of $\mathscr{B}$ with respect to P is equal to $\log l$, which is the maximum value of the entropy under assumption that the number of the atoms is l, and we put $H_0=\log l$. For all $a\in A^n$ and all integer t, $r_n(\cdot;\varphi_n{}^t a)$ is a probability measure, therefore we can construct the entropy of $\mathscr{B}$ with respect to such a measure. For this entropy we get the following theorem, under the same assumption as Lemma 3. 1.

THEOREM 3. 1 *For every* $\varepsilon>0$ *and* $\delta>0$ *there exists a number* n_0 *and for every* $n\geqq n_0$, *the ratio of the inequality*

$$H(\widehat{\mathscr{B}};r_n(\cdot;\varphi_n{}^t a)) \geqq H_0-\varepsilon \tag{3. 7}$$

is greater than $1-\delta$, *for almost everywhere* $a\in A^n$ *with respect to the measure* p_n.

Proof. As the function $-\sum_{i=1}^l x_i \log x_i$ is continuous on

$$\Delta^l=\{(x_1, \cdots, x_l)\in R^l : x_i\geqq 0 \;\; i=1, 2, \cdots, l, \; \sum_{i=1}^l x_i=1\},$$

there exists $\varepsilon'>0$ such that

$$-\sum_{i=1}^l x_i \log x_i \geqq H_0-\varepsilon \tag{3. 8}$$

if $|x_i-1/l|<\varepsilon'(i=1, 2, \cdots, l)$. For this ε', δ/l and an atom B, we apply Lemma 3. 1, then there exists a number $n_0'=n_0'(\varepsilon', \delta/l, B)$ and for all $n>n_0'$, the ratio of

$$|r_n(\widehat{B};\varphi_n{}^t a)-P(\widetilde{B})|<\varepsilon'$$

is greater than $1-\delta/l$ for a. e. a. Thus we put

$$n_0=\max\{n_0'(\varepsilon', \delta/l, B) : B \text{ is an atom of } \mathscr{B}\},$$

then for all $n>n_0$, the ratio of

$$[|r_n(\widehat{B};\varphi_n{}^t a)-P(\widetilde{B})|<\varepsilon' \text{ for all } B]$$

is greater than $1-\delta$ for a. e. a, because the "ratio" is an additive set function on the set of all integers, i. e., if ratios exist for sets F_1 and F_2 which are disjoint, then the ratio of $F_1 \cup F_2$ exists and equals to a sum of two ratios of F_1 and F_2.

Therefore, by (3. 8) the ratio of

$$H(\hat{\mathscr{B}}; r_n(\cdot; \varphi_n{}^t a)) \geqq H_0 - \varepsilon$$

is greater than $1-\delta$ almost everywhere a. q. e. d.

The above theorem is considered as a time-reversible analogy of the H-theorem in the statistical mechanics. That is, the theorem asserts that the macroscopic state remains in a neighborhood of the maximum entropy for arbitrarily long time, if the number of molecules is large enough. Subsequently, if the initial state happens to be at the small entropy, then the entropy increasing is probable in the next instant. The theorem takes a time-reversible form, in which the existance of fluctuations is allowed, even if the fluctuations are periodic. These circumstances are shown by some instructive examples in §5. Therefore the criticisms by Loschmidt and Zermelo-Poincaré are irrelevant to our time-reversible H-theorem.

4 Some Extensions

In the previous section, the time was discrete, thus let us consider the case of continuous time at first. For the parameter t in $\varphi_n{}^t$, we assume that the real value instead of integer is allowed and the following conditions are supplemented:

1. For all real value t, $\varphi_n{}^t$ is an invertible measure preserving transformation on $(A^n, \mathscr{A}^n, p_n)$,

2. for all t and s, $\varphi_n{}^t \varphi_n{}^s = \varphi_n{}^{t+s}$,

and

3. for all $\mathscr{A}^n$-measurable function f, $f(\varphi_n{}^t a)$ is a joint measurable function on $R^1 \times A^n$ as a function of a pair of variables (t, a).

The transformation which satisfies 1, 2 and 3 is called *a flow*. The flow is ergodic if for all t $\varphi_n{}^t E = E$ mod p_n implies $p_n(E)=0$ or 1. The following ergodic theorem for the flow is well known.

THEOREM (Ergodic Theorem for Flows) *If $\varphi_n{}^t$ is ergodic, then for any integrable function f,*

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(\varphi_n{}^t a) p_n(da) = \int f dp_n \quad \text{a. e.} \tag{4. 1}$$

The definition of the ratio given by Definition 2 is altered substituting the counting measure $c(\cdot)$ on the integers by a usual Lebesgue measure on the real axis. Moreover, replacing $\sum$ in the formula (3. 6) by $\int$, the proof of Lemma 3. 1 proceeds quite similarly, thus we conclude that Lemma 3. 1 holds even if time is continuous. Therefore Theorem 3.1 is also applicable to the continuous case.

Next, let us extend the concept of entropy. The amount

$$J(\mathscr{B};q,P)=\sum_A q(A)\log\frac{q(A)}{P(\tilde{A})} \tag{4.2}$$

is called the Kullback-Leibler entropy, where the summation is taken over all atoms of a finite partition $\mathscr{B}$. It is well known that this entropy is nonnegative and equal to zero if and only if $q(A)=P(\tilde{A})$ for all atom $\tilde{A}$. In case $P(\tilde{A})=1/l$, (4.2) becomes

$$\log l-\sum_A q(A)\log q(A)=H_0-H(\mathscr{B};q),$$

consequently the Kullback-Leibler entropy is a sort of difference between the maximum entropy and the usual entropy. Thus the notion of entropy increasing corresponds to decreasing of the Kullback-Leibler entropy. If we use the Kullback-Leibler entropy, we need not choose the partition of equi-atoms. Then Theorem 3.1 becomes the next theorem, the proof of which is similar.

THEOREM 4.1 *For any finite partition $\mathscr{B}$ of A^m and for any $\varepsilon>0$, $\delta>0$, there exists a number n_0, and for all $n>n_0$, the ratio of the inequality*

$$J(\hat{\mathscr{B}};r_n(\cdot;\varphi_n{}^t a),P)\leqq\varepsilon$$

is greater than $1-\delta$, almost everywhere a.

In case $\mathscr{B}$ posesses atoms of equi-measure, the above theorem reduces to Theorem 3.1.

5 Examples

At first, we raise a simple example: let A be $\{0, 1\}$, and P be a probability measure on A^N, which is coordinatewise-independent and $P([0]_j)=P([1]_j)=1/2$ for all $j\in N$ where $[i]_j=\{x\in X: x_j=i\}$. Obviously P is an ergodic measure with respect to the shift transformation S on A^N. For the transformation φ_n, we choose an operation which adds 1 to an element of A^n considered as a binary number, i.e., writing

$$a=(a_1, a_2, \cdots, a_n)\in A^n,$$

we put

$$\varphi_n a=(b_1, b_2, \cdots, b_n)$$

where b_i's are such that

$$b_n 2^{n-1}+b_{n-1}2^{n-2}+\cdots+b_1=a_n 2^{n-1}+a_{n-1}2^{n-2}+\cdots+a_1+1,$$

and particularly $(b_1,b_2,\cdots,b_n)=(0,0,\cdots,0)$ if $a=(1,1,\cdots,1)$. Then φ_n is an ergodic transformation on A^n with respect to the measure p_n which is a marginal distribution of P on $\mathscr{A}^n$. Let $\mathscr{B}$ be a partition of A^1, which posesses two atoms $\{0\}$ and $\{1\}$. Choosing 2 as a base of the logarithm and starting from $a=(0,0,\cdots,0)$, we get Fig. 1, which represents the variation of entropy with time, when $n=10$. Entropy decreases many times, however, it has a tendercy to increase in a long range time. The inverse operation of φ_n exists, as it is a minus-one-operation, thus we get the similar graph as Fig. 1 in the negative direction of time. Moreover we note that φ_n is a periodic transformation, hence it has the so-called Poincaré periode trivially.

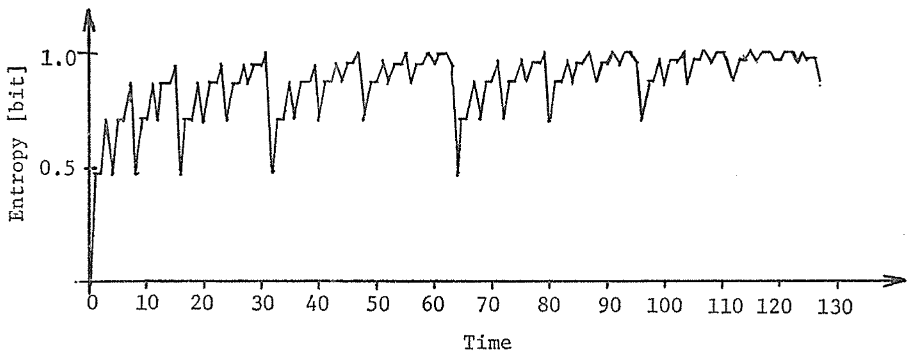

Fig. 1 The variation of entropy with time, advanced by binary addition.

We can make an example, in which p_n's differ from marginal distributions of P. Let $(X,\mathscr{X})$ be same as the first example, and

$$p_n(\{a\})=\begin{cases}0 & \text{if } a=(0,0,\cdots,0)\\ 1/(2^n-1) & \text{otherwise,}\end{cases}$$

where $a\in A^n$, then p_n converges uniformly and inductively to the probabity measure P defined in the first example. We choose φ_n as a linear transformation of a vector $a=(a_1,a_2,\cdots,a_n)$, which has a period 2^{n-1}, e.g.,

$$\varphi_n=\begin{bmatrix} 0 & 0 & \cdot & \cdot & \cdot & 0 & 1 \\ 1 & & & & & & b_1 \\ & 1 & 0 & & & & b_2 \\ & 0 & & & & & \vdots \\ & & & & & 1 & b_{n-1} \end{bmatrix},$$

where $(b_1, b_2, \cdots, b_{n-1})$ is a sequence of 0's and 1's such that

$$x^n + b_{n-1}x^{n-1} + \cdots + b_1 x + 1$$

is a primitive irreducible polynomial. Then we get the similar graph as Fig. 1.

The third example is one of the cases of continuous time. Let A be $[0, 2\pi)$, the half open interval of R^1, and let P be a countably infinite product of the normalized Lebesgue measure on $A=[0, 2\pi)$, and p_n is the marginal distribution of P. Put

$$\varphi_n{}^t a = (a_1 + \theta_1 t, a_2 + \theta_2 t, \cdots, a_n + \theta_n t), \tag{5.1}$$

where the coordinate-wise addition and multiplication are taken as modulo 2π, then it satisfies the conditions of the flow. If the equality

$$\sum_{i=1}^{n} m_i \theta_i = m \cdot 2\pi \tag{5.2}$$

does not hold for all integers $m_1, m_2, \cdots, m_n, m$. which are not zero simultaneously, then $\varphi_n{}^t$ is ergodic (See Kawada[1)]). For instance we choose

$$\theta_i = \pi \log_2 k_i \qquad i = 1, 2, \cdots, n, \tag{5.3}$$

where k_i is the $(i+1)$-th prime number, i. e., $k_1=3$, $k_2=5$, $k_3=7$, ……, then (5. 2) is equivalent to

$$k_1{}^{m_1} k_2{}^{m_2} \cdots k_n{}^{m_n} = 2^{2m} \tag{5.4}$$

which is impossible, i. e., choosing as (5. 3), $\varphi_n{}^t$ becomes ergodic. Choosing $\mathscr{B}$ as a partition of $[0, 2\pi)$ to the octants, we get Fig. 2 in case $n=24$. We can observe the fluctuations in the tendency of entropy increasing.

If our abstract H-theorem is applicable directly to the model of the perfect

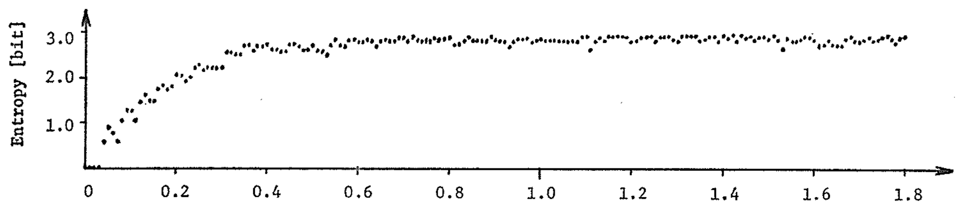

Fig. 2 The variation of entropy with time, advanced continuously by an irrational rotation.

elastic collision of the molecules, then the primitive H-theorem by Boltzmann can be rewritten into the time-reversible form. However, we meet the two difficult problems to do so, one of which is whether the model is ergodic or not, and the other of which is whether or not the invariant measure of the model of finite molecules converges to some shift-ergodic measure, when molecules increase. The second problem is related to a sort of law of large numbers, the consistency of which seems quite doubtful in many actual physical systems because it is probable that the system becomes more complicated and changes itself qualitatively when the number of molecules increases.

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