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# A VARIATIONAL CHARACTERIZATION OF FINITE MARKOV CHAINS

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**Summary.** We prove a one-dimensional version of a theorem of O. E. Lanford and D. Ruelle [4] in equilibrium statistical mechanics which characterizes Gibbs states as those states which minimize the free energy. It is shown that a stationary Markov process is the most random (has the large stentropy) among all strictly stationary processes with the same energy. This energy is based on a potential $U$ which determines the transition matrix $M$ of the Markov chain with minimal free energy.

Let $\mathscr{T}$ be the class of *translation invariant states* (strictly stationary processes) defined as follows. The statement $\mu \in \mathscr{T}$ will mean that $(\Omega, \mathscr{F}, \mu)$ is a probability space, with $\Omega = \{1, 2, \cdots, n\}^{\mathbb{Z}}$, $\mathscr{F}$ is the $\sigma$-field generated by the cylinder sets of $\Omega$, and $\mu$ is a countably additive probability measure on $(\Omega, \mathscr{F})$ which is invariant under the shift $T$ which is defined by $(T\omega)_k = \omega_{k+1}$, $k \in \mathbb{Z}$. If $I_N$ is the cylinder $\{1, 2, \cdots, n\}^{[1,2,\cdots,N]}$, then the cylinder set probabilities will be denoted

$$\mu_N(i) = \mu\{\omega : \omega_1 = i_1, \cdots, \omega_N = i_N\},\ i = (i_1, i_2, \cdots, i_N) \in I_N,\ N \geqq 1\ .$$

For each $\mu \in \mathscr{T}$ and each $N \geqq 1$ we define the entropy (randomness in $[1, N]$) by

$$S_N(\mu) = -\sum_{i \in I_N} \mu_N(i) \log \mu_N(i)\ ,$$

with convention $0 \log 0 = 0$. Clearly $0 \leqq S_N(\mu) \leqq N \log N$, and it is known (the proof goes just as in 7.2.3. of [5] in the case $n = 2$) that the *specific entropy*

$$(1) \qquad s(\mu) = \lim_{N\to\infty} N^{-1} S_N(\mu)\ , \qquad \mu \in \mathscr{T}$$

exists and is an *affine*, *upper semi-continuous* function on $\mathscr{T}$ (in the vague topology of $\mathscr{T}$ as a subset of the continuous positive linear functionals on $C(\Omega)$).

Now we introduce a nearest neighbor pair *potential* $U(i, j)$, $1 \leqq i, j \leqq n$, to be thought of as an energy of interaction between $\omega_k$ and $\omega_{k+1}$ when $\omega_k = i$, and $\omega_{k+1} = j$. Then the average energy in an interval $[1, N]$ is

$$E_N(\mu) = \sum_{i \in I_N} \mu_N(i) \sum_{k=1}^{N-1} U(i_k, i_{k+1})\ .$$

Clearly the limit

$$(2) \qquad e_U(\mu) = \lim_{N\to\infty} N^{-1} E_N(\mu) = \sum_{r=1}^{n} \sum_{s=1}^{n} \mu_2(r, s) U(r, s)$$

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exists. It is called the *specific energy* of $\mu$ with respect to $U$, and is a *continuous affine* function on $\mathscr{T}$. As in statistical mechanics ([5] Chapter 7) we now define the free energy in the interval $[1, N]$ as $F_N(\mu) = E_N(\mu) - S_N(\mu)$, and the *specific free energy* as

$$f_U(\mu) = e_U(\mu) - s(\mu), \qquad \mu \in \mathscr{T}. \tag{3}$$

It will be crucial that $f_U(\mu)$ is a *lower semi-continuous affine* function on $\mathscr{T}$.

Consider now the class $\mathscr{M} \subset \mathscr{T}$ of positive stationary Markov processes (briefly *Markov states*) defined as follows. An element $\mu$ of $\mathscr{T}$ is in $\mathscr{M}$ if there exists a strictly positive $n \times n$ *stochastic matrix* $M = \{M(i, j)\}$, such that

$$\mu_N(i) = \varphi(i_1)M(i_1, i_2)M(i_2, i_3) \cdots M(i_{N-1}, i_N), \qquad i \in I_N, N \geqq 1, \tag{4}$$

where $\varphi$ is the unique invariant probability measure for $M$ (that is $\varphi(k) > 0$ for $1 \leqq k \leqq n$, $\varphi(1) + \cdots + \varphi(n) = 1$, $\varphi M = \varphi$).

Given a potential $U$ we define the positive matrix $Q = Q_U$ by the Boltzmann formula

$$Q(i, j) = e^{-U(i,j)}, \qquad 1 \leqq i, j \leqq n. \tag{5}$$

Let $\lambda = \lambda(U)$ be the largest (positive) eigenvalue of $Q$. Let $l$ and $r$ denote the left and right eigenvectors of $Q$ corresponding to $\lambda$, normalized so that $l(i) > 0$, $r(i) > 0$ for $1 \leqq i \leqq n$ and $l \cdot r = \sum l(i)r(i) = 1$. Define $M$ as the positive stochastic matrix

$$M(i, j) = \frac{1}{\lambda(U)} \frac{Q(i, j)r(j)}{r(i)}, \qquad 1 \leqq i, j \leqq n. \tag{6}$$

Note that $M$ has the invariant probability vector $\varphi(\varphi M = \varphi)$ given by

$$\varphi(i) = l(i)r(i), \qquad 1 \leqq i \leqq n. \tag{7}$$

Finally, let $\nu = \nu^{(M)}$ denote the *Markov state* defined by the transition matrix $M$ and its invariant vector $\varphi$ in accordance with (4), (5), (6) and (7). Now we can formulate the variational characterization of $\nu$. It asserts that $\nu$ is the most random of all states $\mu \in \mathscr{T}$ which have the same specific energy as $\nu$ (i.e., such that $e_U(\mu) = e_U(\nu)$). An analogous, more general, result can be stated and proved for the class of all stationary Markov processes (not necessarily with strictly positive $M$) if one permits the potential $U$ to assume the value $+\infty$.

THEOREM. *Let $U$ be given. Then*

$$f_U(\mu) \geqq -\log \lambda(U) \qquad \textit{for all } \mu \in \mathscr{T} \tag{8}$$

*with equality if and only if $\mu$ is the Markov state $\nu = \nu^{(M)}$ defined above in terms of $U$. Conversely, given $\nu \in \mathscr{M}$, one must choose a potential of the form*

$$U(i, j) = -\log \lambda - \log M(i, j) + h(i) - h(j), \qquad 1 \leqq i, j \leqq n, \tag{9}$$

*where h is an arbitrary function, if one wants $\nu$ to minimize the free energy $f_U$, and to give it the minimum value $-\log \lambda$.*

The converse of the theorem is a direct consequence of its first part, and of the definitions (2), (5), and (6). The main first part will be proved in three stages. Stage I will show that (8) holds with equality when $\mu = \nu^{(M)}$. In Stage II we assume that $\mu \neq \nu^{(M)}$ but that $\mu$ is ergodic, and show that $f_U(\mu) > -\log \lambda(U)$. Finally in Stage III we prove strict inequality in (8) for an arbitrary $\mu \in \mathscr{T}$ such that $\mu \neq \nu^{(M)}$. Throughout the proof we shall write $\nu^{(M)} = \nu$.

*Stage* I. With $M$ and $\varphi$ defined by (5), (6), (7),

$$\begin{aligned}\sum_{k=1}^{N-1} U(i_k, i_{k+1}) &= -\log \prod_{k=1}^{N-1} Q(i_k, i_{k+1}) \\ &= -(N-1)\log \lambda(U) - \log \prod_{k=1}^{N-1} M(i_k, i_{k+1}) \\ &\qquad -\log r(i_1) + \log r(i_N) \\ &= -(N-1)\log \lambda(U) - \log \nu_N(i) + \log \varphi(i_1) - \log r(i_1) \\ &\qquad + \log r(i_N)\,, \qquad\qquad i \in I_N\,.\end{aligned}$$

Hence, averaging with respect to $\mu$,

$$E_N(\mu) = -N \log \lambda(U) - \sum_{i \in I_N} \mu_N(i) \log \nu_N(i) + c\,,$$

where $c$ is a constant (depending on $U$ and $\mu$, but not on $N$). Thus

$$\text{(10)}\qquad \begin{aligned}\frac{1}{N} F_N(\mu) &= \frac{E_N(\mu) - S_N(\mu)}{N} \\ &= -\log \lambda(U) + \frac{1}{N} \sum_{i \in I_N} \mu_N(i) \log \frac{\mu_N(i)}{\nu_N(i)} + \frac{c}{N}\,.\end{aligned}$$

The sum in (10) is nonnegative in view of the elementary inequality $x \log x \geqq x - 1$ for $x \geqq 0$. Therefore

$$N^{-1} F_N(\mu) \geqq -\log \lambda(U) + c/N$$

with equality when $\mu = \nu$. Hence, letting $N \to \infty$,

$$\text{(11)}\qquad f_U(\mu) = \lim_{N \to \infty} N^{-1} F_N(\mu) \geqq -\log \lambda(U)\,, \qquad \mu \in \mathscr{T}\,,$$

with equality when $\mu = \nu$.

*Stage* II. Observe that

$$\text{(12)}\qquad s(\mu) \leqq N^{-1} S_N(\mu)\,, \qquad N \geqq 1\,,$$

in view of the well-known subadditivity property (cf. [5] 7.2.10)

$$S_{N_1+N_2}(\mu) \leqq S_{N_1}(\mu) + S_{N_2}(\mu)\,, \qquad N_1 \geqq 1,\ N_2 \geqq 1,\ \mu \in \mathscr{T}.$$

Also note that

$$\text{(13)}\qquad E_N(\mu) = (N-1) e_U(\mu)\,, \qquad N \geqq 2,\ \mu \in \mathscr{T}.$$

It follows from (12) and (13) that for each $N \geqq 2$

$$f_U(\mu) \geqq N^{-1}F_N(\mu) + N^{-1}e_U(\mu) ,$$

and in view of (10) there is a constant $c'$ (independent of $N$) such that

$$(14) \qquad f_U(\mu) \geqq -\log \lambda(U) + \frac{1}{N}\left[c' + \sum_{i \in I_N} \mu_N(i) \log \frac{\mu_N(i)}{\nu_N(i)}\right], \qquad N \geqq 2 .$$

Let $\mathscr{E}$ denote the subset of $\mathscr{T}$ consisting of *ergodic states* (states $\mu$ such that $A = \mathscr{F}$ and $A = TA$ implies $\mu(A) = 0$ or 1). We shall prove that

$$(15) \qquad f_U(\mu) > -\log \lambda(U) \qquad \text{for } \mu \in \mathscr{E},\ \mu \neq \nu .$$

This will be done by showing that the sum in (14) tends to $+\infty$ as $N \to \infty$, when $\mu \in \mathscr{E}$, $\mu \neq \nu$. First note that the Markov state $\nu$ is in $\mathscr{E}$, since the shift $T$ is mixing for $\nu$, by the ergodic theorem for Markov chains. Next observe that $\mu$ and $\nu$ are mutually singular if $\mu \in \mathscr{E}$ and $\mu \neq \nu$. This follows from Birkhoff's ergodic theorem by choosing a cylinder set $A \in \mathscr{T}$ such that $\mu(A) \neq \nu(A)$, setting

$$f_N(\omega) = N^{-1} \sum_{k=1}^{N} 1_A(T^k\omega) , \qquad \omega \in \Omega$$

and noting that the set on which $f_N \to \mu(A)$ has $\mu$-measure one, and $\nu$-measure zero. Following Doob ([2] page 343–348) we now define the stochastic process of *likelihood ratios*

$$(16) \qquad \begin{aligned} x_N(\omega) &= \nu_N[i(\omega)]/\mu_N[i(\omega)] && \text{if } \mu_N[i(\omega)] \neq 0 \\ &= 0 && \text{otherwise,} \end{aligned}$$

for $N \geqq 1$, on the probability space $(\Omega, \mathscr{F}, \mu)$. As shown by Doob this process is a *martingale* with respect to the increasing family of $\sigma$-fields $\mathscr{F}_N$ generated by $\{i_1(\omega), i_2(\omega), \cdots, i_N(\omega)\}$. As shown by Doob, the martingale $x_N$ converges (a.e. $\mu$) to the Radon-Nikodym derivative of $\nu$ with respect to $\mu$—hence to zero since $\mu$ and $\nu$ are mutually singular. Now let $y_N(\omega) = -\log x_N(\omega)$. If $E$ denotes expectation with respect to $\mu$ measure, we have

$$(17) \qquad E[y_N] = \sum_{i \in I_N} \mu_N(i) \log \frac{\mu_N(i)}{\nu_N(i)} ,$$

and (15) will be proved if $Ey_N \to +\infty$ as $N \to \infty$. Since $y_N \to +\infty$ (a.e. $\mu$) it suffices to show that the negative part of $y_N$ has uniformly bounded expectation. This follows from

$$E[y_N^-] = E[(\log x_N)^+] \leqq E[(x_N - 1)^+] \leqq E[x_N] = 1 , \qquad N \geqq 1 .$$

*Stage* III. Let $\mathscr{K} = \mathscr{K}_U$ be that subset of $\mathscr{T}$ on which $f_U$ assumes its minimum value. We have seen in Stage I that $\nu \in \mathscr{K}$. Since $f_U$ is a lower semi-continuous function it follows that $\mathscr{K}$ is closed, and since $\mathscr{T}$ is compact, so is $\mathscr{K}$. Since $f_U$ is affine we know that $\mathscr{K}$ is convex. We want to show that $\mathscr{K}$ consists of the single point $\nu$. By the Krein-Milman theorem ([1] page 95) this will be so if and only if *$\mathscr{K}$ has only one extreme point*. From the definition of $\mathscr{K}$ it is immediate that every extreme point of $\mathscr{K}$ is also an extreme point of $\mathscr{T}$. But if $\mu$ is an extreme point of $\mathscr{T}$, then it is in $\mathscr{E}$. (If $\mu$ were not in $\mathscr{E}$ we could choose $A \in \mathscr{F}$, with $0 < \mu(A) < 1$, $TA = A$, and express $\mu$ as a convex combination of the measures $\mu_1$, $\mu_2$, both in $\mathscr{T}$, defined by $\mu_1(B) = [\mu(A)]^{-1}\mu(A \cap B)$, $\mu_2(B) = [\mu(A^c)]^{-1}\mu(A^c \cap B)$, $B \in \mathscr{F}$.) Thus the problem is reduced to showing that $\mathscr{K}$ contains no ergodic states other than $\nu$, and this was the result of Stage II. Therefore the proof is complete.

REMARK. We wish to thank H. Kesten for suggesting the use of martingale theory in Stage II of the proof. This approach is much simpler than the proof of Lanford and Ruelle [4] which depends on the study of how $\mathscr{K}$ behaves as $U$ varies in a suitable Banach space of interactions. Another indirect proof was given by R. Holley [3] depending on the time evolution of a Markov process with state space $\mathscr{T}$. In principle the present method seems adaptable to the case of Gibbs states on $\Omega = \{0, 1\}^{Z^d}$ with $d \geqq 2$, since the process analogous to $\{x_N\}$ in (16) (with $N$ replaced by a sequence of expanding cubes) continues to form a martingale. However, the estimates leading to (15) seem to break down since there are boundary terms present which must be shown to be small compared to the expectation in (17).

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