

Maximum Entropy Models for Quantum Systems

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Abstract: We show that for a finite von Neumann algebra, the states that maximise Segal's entropy with a given energy level are Gibbs states. This is a counterpart of the classical result for the algebra of all bounded linear operators on a Hilbert space and von Neumann entropy.

Keywords: entropy; von Neumann algebra; Gibbs states

1. Introduction

Let $\mathbb{B}(\mathcal{H})$ be the algebra of all bounded linear operators on a Hilbert space \mathcal{H} , and let tr be the canonical trace on $\mathbb{B}(\mathcal{H})$. For a state ρ on $\mathbb{B}(\mathcal{H})$ represented by a density matrix D , its von Neumann entropy is defined by

$$S(\rho) = -\text{tr } D \log D.$$

Now, let H be the Hamiltonian of a physical system whose (bounded) observables are represented by $\mathbb{B}(\mathcal{H})$. The expected value of the energy in the state ρ is given by

$$\rho(H) = \text{tr } DH.$$

Let E , belonging to the spectrum of H , be a fixed energy level. We are interested in the states for which the expected value of the energy equals E ; i.e., in the states ρ such that $\rho(H) = E$. The classical result says that the maximal value of the entropy for such states is attained for a so-called *Gibbs state*; that is, a state with the density matrix $\frac{e^{\beta H}}{\text{tr } e^{\beta H}}$ for some $\beta \in \mathbb{R}$. In this note, we aim to show a similar result in the situation where $\mathbb{B}(\mathcal{H})$ is replaced by a finite von Neumann algebra, and the von Neumann entropy is replaced by Segal's entropy.

2. Preliminaries and Notation

Let \mathcal{M} be a finite von Neumann algebra with a normal finite faithful trace τ , identity $\mathbb{1}$, and predual \mathcal{M}_* . As usual, we assume that τ is normalised (i.e., $\tau(\mathbb{1}) = 1$), so τ is itself a normal faithful state. By \mathcal{M}^+ , we shall denote the set of positive operators in \mathcal{M} , and by \mathfrak{S} , the set of normal states of \mathcal{M} (i.e., $\mathfrak{S} = \{0 \leq \rho \in \mathcal{M}_* : \rho(\mathbb{1}) = 1\}$). For $x \in \mathcal{M}$, the spectrum of x will be denoted by $\text{sp } x$.

The trace τ can be extended to the space $L^1(\mathcal{M}, \tau)$ consisting of densely defined closed operators affiliated with \mathcal{M} such that for each $z \in L^1(\mathcal{M}, \tau)$, $\tau(z)$ is finite; in particular, $\mathcal{M} \subset L^1(\mathcal{M}, \tau)$.

Let \mathcal{N} be a von Neumann subalgebra of \mathcal{M} . There exists a normal faithful conditional expectation $\mathbb{E}: \mathcal{M} \rightarrow \mathcal{N}$ such that $\tau \circ \mathbb{E} = \tau$. This expectation can be extended to a map from $L^1(\mathcal{M}, \tau)$ onto $L^1(\mathcal{N}, \tau|_{\mathcal{N}})$, denoted by the same symbol, which retains the basic properties of the original conditional expectation; in particular,

$$\tau(\mathbb{E}z) = \tau(z), \quad z \in L^1(\mathcal{M}, \tau),$$

and

$$\mathbb{E}(zx) = z\mathbb{E}x, \quad x \in \mathcal{M}, z \in L^1(\mathcal{N}, \tau|\mathcal{N}).$$

For each $0 \leq \rho \in \mathcal{M}_*$, there is a selfadjoint positive operator $h_\rho \in L^1(\mathcal{M}, \tau)$ such that

$$\rho(x) = \tau(xh_\rho) = \tau(h_\rho x), \quad x \in \mathcal{M}.$$

By analogy with the case $\mathbb{B}(\mathcal{H})$, the h_ρ as above will be called the *density matrix* of ρ . The Segal entropy of ρ —denoted by $S(\rho)$ —is defined as

$$S(\rho) = -\tau(h_\rho \log h_\rho),$$

where h_ρ is the density matrix of ρ ; i.e., for the spectral representation of h_ρ

$$h_\rho = \int_0^\infty \lambda e(d\lambda),$$

we have

$$S(\rho) = -\int_0^\infty \lambda \log \lambda \tau(e(d\lambda)).$$

Let us note that Segal's entropy is well-defined (though it may be minus infinity) and nonpositive for the states, since, on account of the inequality

$$-\lambda \log \lambda \leq 1 - \lambda,$$

we have

$$\begin{aligned} S(\rho) &= -\int_0^\infty \lambda \log \lambda \tau(e(d\lambda)) \leq \int_0^\infty (1 - \lambda) \tau(e(d\lambda)) \\ &= \tau\left(\int_0^\infty e(d\lambda)\right) - \tau\left(\int_0^\infty \lambda e(d\lambda)\right) = \tau(\mathbb{1} - h_\rho) = 1 - \rho(\mathbb{1}), \end{aligned}$$

and the right-hand side of the inequality above is always finite, and equals zero for ρ being a state.

The Segal entropy in connection with quantum measurement theory was employed in [1], where it was shown that a weakly repeatable measurement is a maximal state entropy one, and that under some natural conditions, the converse is true, even in a slightly stronger form; i.e., a maximal state entropy measurement satisfying these conditions is repeatable (The reader should be warned that the definition of Segal's entropy adopted in [1] differs from ours by a minus sign, so the conclusions there are about minimal entropy instead of maximal). So far, Segal's entropy has not found many other applications in physics or information theory, and we hope that this paper may arouse some interest among physicists or information theorists for this notion.

Some further properties of Segal's entropy were investigated in [2–8].

3. Maximum Segal's Entropy States

The function introduced below plays a crucial role in our further considerations.

Lemma 1. *Let h be a selfadjoint element in \mathcal{M} which is not a multiple of the identity, and let f be defined as*

$$f(t) = \frac{\tau(he^{th})}{\tau(e^{th})}, \quad t \in \mathbb{R}.$$

The function f is strictly increasing.

Proof. We have

$$f'(t) = \frac{\tau(h^2 e^{th}) \tau(e^{th}) - [\tau(h e^{th})]^2}{[\tau(e^{th})]^2}.$$

Define on \mathcal{M} a scalar product $\langle \cdot | \cdot \rangle$ by the formula

$$\langle x | y \rangle = \tau(x^* y), \quad x, y \in \mathcal{M}.$$

For $x = h e^{th/2}$ and $y = e^{th/2}$, we obtain by the Schwarz inequality

$$[\tau(h e^{th})]^2 = |\langle x | y \rangle|^2 \leq \langle x^* | x \rangle \langle y^* | y \rangle = \tau(h^2 e^{th}) \tau(e^{th}).$$

Hence, $f'(t) \geq 0$ for all $t \in \mathbb{R}$ with the equality if and only if $h e^{th/2} = \lambda e^{th/2}$ for some λ which contradicts the assumption. Thus, $f'(t) > 0$ for all $t \in \mathbb{R}$, and we arrive at the conclusion of the lemma. \square

In what follows, we fix an arbitrary Hamiltonian h (i.e., h is a selfadjoint element of \mathcal{M}) and put

$$\lambda_m = \min\{\lambda : \lambda \in \text{sp } h\}, \quad \lambda_M = \max\{\lambda : \lambda \in \text{sp } h\}.$$

For each $t \in \mathbb{R}$, we define the Gibbs states ρ_t as the states with density matrices $h_t = \frac{e^{th}}{\tau(e^{th})}$. Let us begin with the following simple observation.

Lemma 2. *The following inclusion holds*

$$\{\rho(h) : \rho \in \mathfrak{S}\} \subset [\lambda_m, \lambda_M].$$

Moreover, if for some Gibbs state ρ_β we have $\rho_\beta(h) = \lambda_m$ or $\rho_\beta(h) = \lambda_M$, then, respectively, $h = \lambda_m \mathbb{1}$ or $h = \lambda_M \mathbb{1}$.

Proof. We have

$$\lambda_m \mathbb{1} \leq h \leq \lambda_M \mathbb{1},$$

consequently, for each $\rho \in \mathfrak{S}$ we get—applying ρ to the elements of the inequality above—

$$\lambda_m \leq \rho(h) \leq \lambda_M,$$

which shows the inclusion.

Furthermore, assume for example that for some $\beta \in \mathbb{R}$, we have $\rho_\beta(h) = \lambda_M$. Then,

$$0 = \rho_\beta(\lambda_M \mathbb{1} - h) = \tau(h_\beta(\lambda_M \mathbb{1} - h)) = \tau(h_\beta^{1/2}(\lambda_M \mathbb{1} - h)h_\beta^{1/2}),$$

and since

$$h_\beta^{1/2}(\lambda_M \mathbb{1} - h)h_\beta^{1/2} \geq 0,$$

and τ is faithful, we obtain

$$h_\beta^{1/2}(\lambda_M \mathbb{1} - h)h_\beta^{1/2} = 0,$$

which yields $h = \lambda_M \mathbb{1}$. In the same way, we show that $h = \lambda_m \mathbb{1}$ if $\rho_\beta(h) = \lambda_m$. \square

The result above shows that for the Gibbs states we cannot have $\rho_t(h) = \lambda_m$ or $\rho_t(h) = \lambda_M$ unless h is a multiple of the identity. However, the values between λ_m and λ_M can be attained as shown in the following proposition.

Proposition 1. Let $E \in (\lambda_m, \lambda_M)$. Then, there is a unique $\beta \in \mathbb{R}$ such that for the Gibbs state ρ_β , we have $\rho_\beta(h) = E$.

Proof. Let f be the function as in Lemma 1; in particular, we have

$$f(t) = \rho_t(h).$$

Take an arbitrary $\alpha \in (\lambda_m, \lambda_M)$, and observe that

$$f(t) = \frac{\tau(he^{th})}{\tau(e^{th})} = \frac{\tau(he^{t(h-\alpha\mathbb{1})})}{\tau(e^{t(h-\alpha\mathbb{1})})}, \quad t \in \mathbb{R}.$$

Let

$$h = \int_{\lambda_m}^{\lambda_M} \lambda e(d\lambda)$$

be the spectral representation of h . We have

$$\begin{aligned} f(t) &= \frac{\int_{[\lambda_m, \alpha]} \lambda e^{t(\lambda-\alpha)} \tau(e(d\lambda)) + \int_{[\alpha, \lambda_M]} \lambda e^{t(\lambda-\alpha)} \tau(e(d\lambda))}{\int_{[\lambda_m, \alpha]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) + \int_{[\alpha, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda))} \\ &\geq \frac{\int_{[\lambda_m, \alpha]} \lambda e^{t(\lambda-\alpha)} \tau(e(d\lambda)) + \alpha \int_{[\alpha, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda))}{\int_{[\lambda_m, \alpha]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) + \int_{[\alpha, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda))}. \end{aligned} \quad (1)$$

Since $\lambda - \alpha < 0$ for $\lambda \in [\lambda_m, \alpha)$, we obtain for such λ

$$\lim_{t \rightarrow \infty} e^{t(\lambda-\alpha)} = 0,$$

and the Lebesgue Dominated Convergence Theorem yields

$$\lim_{t \rightarrow \infty} \int_{[\lambda_m, \alpha]} \lambda e^{t(\lambda-\alpha)} \tau(e(d\lambda)) = \lim_{t \rightarrow \infty} \int_{[\lambda_m, \alpha]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) = 0.$$

To estimate the remaining integral, take an arbitrary fixed $\gamma \in (\alpha, \lambda_M)$ to obtain

$$\begin{aligned} \int_{[\alpha, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) &\geq \int_{[\gamma, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) \\ &\geq \int_{[\gamma, \lambda_M]} e^{t(\gamma-\alpha)} \tau(e(d\lambda)) = e^{t(\gamma-\alpha)} \tau(e([\gamma, \lambda_M])). \end{aligned}$$

Since $e([\gamma, \lambda_M]) \neq 0$ and $\gamma - \alpha > 0$, we get

$$\lim_{t \rightarrow \infty} e^{t(\gamma-\alpha)} \tau(e([\gamma, \lambda_M])) = +\infty,$$

consequently,

$$\lim_{t \rightarrow \infty} \int_{[\alpha, \lambda_M]} e^{t(\lambda-\alpha)} \tau(e(d\lambda)) = +\infty.$$

The estimates obtained yield (after passing to the limit in Formula (1)),

$$\lim_{t \rightarrow \infty} f(t) \geq \alpha,$$

and since α was arbitrary in (λ_m, λ_M) , it follows that

$$\lim_{t \rightarrow \infty} f(t) \geq \lambda_M.$$

On the other hand, since $f(t) = \rho_t(h)$, Lemma 2 yields the inequality $\lambda_m \leq f(t) \leq \lambda_M$; hence,

$$\lim_{t \rightarrow \infty} f(t) = \lambda_M.$$

An analogous reasoning leads first to the inequality

$$\lim_{t \rightarrow -\infty} f(t) \leq \lambda_m,$$

and hence

$$\lim_{t \rightarrow -\infty} f(t) = \lambda_m.$$

Now, since f is continuous and increasing, the Darboux property yields that for each $E \in (\lambda_m, \lambda_M)$ there is a unique $\beta \in \mathbb{R}$ such that

$$E = f(\beta) = \rho_\beta(h). \quad \square$$

Now we are in a position to prove the main result of the paper.

Theorem 1. *Let h be a Hamiltonian in \mathcal{M} , and let $E \in (\lambda_m, \lambda_M)$ be arbitrary, where λ_m and λ_M are as before. Then, there exists a unique $\beta \in \mathbb{R}$ such that*

$$\sup\{S(\rho) : \rho \in \mathfrak{S}, \rho(h) = E\} = S(\rho_\beta);$$

that is, the maximal value of Segal's entropy for the states in which the energy level is fixed is attained for a Gibbs state. Moreover, this Gibbs state is the only one for which the maximal value of entropy is attained.

Proof. Let $\beta \in \mathbb{R}$ be such that for the Gibbs state ρ_β

$$\rho_\beta(h) = E;$$

according to Proposition 1, the β as above exists and is unique. For h_β being the density matrix of ρ_β , we have

$$\log h_\beta = \beta h - \log \tau(e^{\beta h}) \mathbb{1}.$$

Let $\rho \in \mathfrak{S}$, with the density matrix h_ρ , be such that $\rho(h) = E$. We have

$$\begin{aligned} \tau(h_\rho \log h_\beta) &= \tau(h_\rho (\beta h - \log \tau(e^{\beta h}) \mathbb{1})) \\ &= \beta \tau(h_\rho h) - \tau(\log \tau(e^{\beta h}) h_\rho) \\ &= \beta \rho(h) - \log \tau(e^{\beta h}) \tau(h_\rho) = \beta E - \log \tau(e^{\beta h}). \end{aligned}$$

On the other hand,

$$\begin{aligned} S(\rho_\beta) &= -\tau(h_\beta \log h_\beta) = -\tau(h_\beta (\beta h - \log \tau(e^{\beta h}) \mathbb{1})) \\ &= -\beta \tau(h_\beta h) + \log \tau(e^{\beta h}) \tau(h_\beta) \\ &= -\beta \rho_\beta(h) + \log \tau(e^{\beta h}) = -\beta E + \log \tau(e^{\beta h}), \end{aligned}$$

and thus

$$S(\rho_\beta) = -\tau(h_\rho \log h_\beta). \quad (2)$$

Now the basic inequality

$$\tau(a(\log a - \log b)) \geq 0 \quad (3)$$

obtained in ([7], Theorem 1) for density matrices a and b of states ρ_a and ρ_b , respectively, with finite entropy, yields that for all ρ with finite entropy, we have

$$S(\rho) = -\tau(h_\rho \log h_\rho) \leq -\tau(h_\rho \log h_\beta) = S(\rho_\beta),$$

and since ρ was arbitrary, the claim follows.

Now assume that for some state ρ with density matrix h_ρ such that $\rho(h) = E$, we have

$$S(\rho) = S(\rho_\beta).$$

On account of Equality (2), this yields

$$\tau(h_\rho \log h_\rho) = \tau(h_\rho \log h_\beta). \quad (4)$$

Let \mathcal{A} be the von Neumann algebra generated by h_ρ (more precisely, \mathcal{A} is the (abelian) algebra generated by the spectral projections of h_ρ), and let \mathbb{E} be a faithful normal conditional expectation from \mathcal{M} onto \mathcal{A} such that $\tau \circ \mathbb{E} = \tau$. The operator $h_\rho \log h_\beta$ —as a product of an operator from $L^1(\mathcal{M}, \tau)$ and an operator from \mathcal{M} —is in $L^1(\mathcal{M}, \tau)$, so we may apply conditional expectation \mathbb{E} to it, obtaining

$$\tau(h_\rho \log h_\rho) = \tau(\mathbb{E}(h_\rho \log h_\beta)) = \tau(h_\rho \mathbb{E}(\log h_\beta)). \quad (5)$$

The function $(0, +\infty) \ni t \mapsto \log t$ is operator concave; hence, from Jensen's inequality, we obtain (keeping in mind that h_β is bounded)

$$\mathbb{E}(\log h_\beta) \leq \log \mathbb{E}h_\beta,$$

consequently,

$$h_\rho^{1/2} \mathbb{E}(\log h_\beta) h_\rho^{1/2} \leq h_\rho^{1/2} (\log \mathbb{E}h_\beta) h_\rho^{1/2},$$

which yields the inequality

$$\begin{aligned} \tau(h_\rho \mathbb{E}(\log h_\beta)) &= \tau(h_\rho^{1/2} \mathbb{E}(\log h_\beta) h_\rho^{1/2}) \\ &\leq \tau(h_\rho^{1/2} (\log \mathbb{E}h_\beta) h_\rho^{1/2}) = \tau(h_\rho \log \mathbb{E}h_\beta). \end{aligned} \quad (6)$$

Relations (5) and (6) now yield

$$\tau(h_\rho \log h_\rho) \leq \tau(h_\rho \log \mathbb{E}h_\beta);$$

i.e.,

$$\tau(h_\rho (\log h_\rho - \log \mathbb{E}h_\beta)) \leq 0.$$

Since $\mathbb{E}h_\beta$ is a density matrix, we get (by virtue of Inequality 3),

$$\tau(h_\rho (\log h_\rho - \log \mathbb{E}h_\beta)) = 0.$$

Now $\mathbb{E}h_\beta$ (and consequently, $\log \mathbb{E}h_\beta$) are in \mathcal{A} , so $\log \mathbb{E}h_\beta$ commutes with h_ρ , and from the equality above we infer—taking into account ([7], Theorem 2)—that

$$h_\rho = \mathbb{E}h_\beta,$$

in particular, h_ρ is bounded.

Now let \mathcal{B} be the (abelian) von Neumann algebra generated by the Hamiltonian h (in particular, we have $h_\beta \in \mathcal{B}$ and $\log h_\beta \in \mathcal{B}$), and let \mathbb{F} be a normal faithful conditional expectation from \mathcal{M} onto \mathcal{B}

such that $\tau \circ \mathbb{F} = \tau$. The function $[0, +\infty) \ni t \mapsto t \log t$ is operator convex, so from Jensen's inequality we obtain

$$\mathbb{F}h_\rho(\log \mathbb{F}h_\rho) \leq \mathbb{F}(h_\rho \log h_\rho).$$

By virtue of Inequality (3) and the fact that $\mathbb{F}h_\rho$ is a density matrix, from Equality (4) we get

$$\begin{aligned} \tau(\mathbb{F}h_\rho(\log h_\beta)) &= \tau(\mathbb{F}(h_\rho \log h_\beta)) = \tau(h_\rho \log h_\beta) = \tau(h_\rho \log h_\rho) \\ &= \tau(\mathbb{F}(h_\rho \log h_\rho)) \geq \tau(\mathbb{F}h_\rho(\log \mathbb{F}h_\rho)) \geq \tau(\mathbb{F}h_\rho(\log h_\beta)). \end{aligned}$$

Thus, we have

$$\tau(\mathbb{F}h_\rho(\log h_\beta)) = \tau(\mathbb{F}h_\rho(\log \mathbb{F}h_\rho)) = \tau(\mathbb{F}(h_\rho \log h_\rho)). \quad (7)$$

Since

$$\mathbb{F}(h_\rho \log h_\rho) - \mathbb{F}h_\rho(\log \mathbb{F}h_\rho) \geq 0,$$

and

$$\tau(\mathbb{F}(h_\rho \log h_\rho) - \mathbb{F}h_\rho(\log \mathbb{F}h_\rho)) = 0,$$

the faithfulness of τ yields

$$\mathbb{F}(h_\rho \log h_\rho) = \mathbb{F}h_\rho(\log \mathbb{F}h_\rho).$$

From ([3], Appendix B.5), it follows that

$$h_\rho = \mathbb{F}h_\rho;$$

i.e., Equality (7) becomes

$$\tau(h_\rho \log h_\beta) = \tau(h_\rho \log h_\rho),$$

or

$$\tau(h_\rho(\log h_\rho - \log h_\beta)) = 0. \quad (8)$$

Now, since $h_\rho = \mathbb{F}h_\rho \in \mathcal{B}$, it follows that h_ρ and h_β commute, and from Equality (8) we obtain—referring once more to ([7], Theorem 2)—that

$$h_\rho = h_\beta,$$

which ends the proof. \square

Remark 1. It should be noted that the equality

$$\tau(h_\rho(\log h_\rho - \log h_\beta)) = 0 \quad (9)$$

means that

$$S(\rho, \rho_\beta) = 0,$$

where $S(\rho, \rho_\beta)$ is the relative entropy of the states ρ, ρ_β . This relative entropy is defined in ([4], Chapter 5) by means of the relative modular operator, but it can be shown that for finite von Neumann algebras with a normal faithful finite trace τ , we have

$$S(\rho, \rho_\beta) = \tau(h_\rho(\log h_\rho - \log h_\beta)).$$

Now, referring to ([4], Corollary 5.6) gives the equality

$$\rho = \rho_\beta.$$

In our approach, we have chosen a simpler and more straightforward way without reference to any advanced theory of von Neumann algebras; in particular, to a rather sophisticated definition of the relative entropy based on the notion of the relative modular operator.

4. Conclusions

We have shown that for an arbitrary finite von Neumann algebra \mathcal{M} with a normal finite trace τ , a state that maximises Segal's entropy with a given energy level is a unique Gibbs state, i.e., a state ρ_β defined for $\beta \in \mathbb{R}$ by the formula

$$\rho_\beta(x) = \tau\left(x \frac{e^{\beta h}}{\tau(e^{\beta h})}\right), \quad x \in \mathcal{M},$$

with some fixed selfadjoint $h \in \mathcal{M}$. This result is analogous to the classical one concerning von Neumann's entropy defined by means of the canonical trace on the full algebra $\mathbb{B}(\mathcal{H})$. Since the definition of Segal's entropy applied to the full algebra and the canonical trace leads to von Neumann's entropy, it would be interesting to obtain such a result for Segal's entropy in the case of semifinite von Neumann algebras. Another interesting question would be extending Segal's definition to the states with their density matrices not necessarily in the algebra, and proving the maximisation condition in this case. However, in both the cases a serious difficulty arises, namely, an appropriate definition of Gibbs state is not clear due to the fact that the operator $e^{\beta h}$ need not be of trace class. Overcoming these difficulties seems to be an interesting challenge.

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