Reciprocity relations and generalized entropic quantifiers that lack trace-form

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Abstract

In this effort we show that the Legendre reciprocity relations, thermodynamics essential formal feature, are respected by any entropic functional, even if it is NOT of trace-form nature, as Shannons is. Further, with reference to the MaXent variational process, we encounter important cases, relevant to physical applications currently discussed in the research literature, in which the associated reciprocity relations exhibit anomalies. We show that these anomalies can be cured by carefully discriminating between apparently equivalent entropic forms.

KEYWORDS: Reciprocity relations, Maximum Entropy, Non trace form entropic functionals

1 Introduction

Renyi's entropy S_R is an important quantifier in variegated areas of scientific activity. We mentions as examples ecology, quantum information, the Heisenberg XY spin chain model, theoretical computer science, conformal field theory, quantum quenching, diffusion processes, etc. [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. and references therein. A typical Renyi-feature is the lack of trace form, since S_R is not of the form

$$S = \int dV f(\xi), \tag{1}$$

with dV the appropriate volume element, ξ a probability density (PD), and f an arbitrary smooth function of the PD. Instead, S_R is the logarithm of S above, for $f = [1/(q-1)]\xi^q$, q a real number.

In this work, we focus attention on thermodynamics' reciprocity relations and re-visit some issues concerning generalized entropies that, we believe, lack yet full adequate understanding. We focus attention on the canonical ensemble. Our aims are:

1. To establish whether general entropies that lack trace form, with Renyi's logarithm replaced by an arbitrary smooth functional G of f in (1), can be successfully described by Jaynes' MaxEnt variational treatment, so that reciprocity relations hold [12].
2. To analyze anomalies that sometimes arise with regards to the workings of MaxEnt's Lagrange multipliers [13].
3. To assess whether these anomalies can be eliminated.

2 Background: Legendre transform and reciprocity relations

For the Lagrange multipliers in the canonical ensemble we use this notation.

- λ_U is the energy U multiplier,
- λ_N is the normalization multiplier.

In statistical mechanics, these multipliers are always endowed with meaningful physical information [14].
Legendre's transform (LT) is an operation that converts a real function f_1 with real variable x into another f_2, of another variable y, keeping constant the information content of f_1. The derivative of f_1 becomes the argument of f_2.

$$f_2(y) = xy - f_1(x); \;\; y = f_1'(x) \Rightarrow \text{ reciprocity.} \tag{2}$$

LT' *reciprocity relations are thermodynamics' basic formal ingredient* [15]. For two functions S and μ_J one has

$$S(< A_1 >, \ldots, < A_M >) \; = \; \mu_J + \sum_{k=1}^{M} \; \mu_k \langle A_k \rangle, \tag{3}$$

with the A_i extensive variables and the μ_i *independent* intensive ones. Obviously, the Legendre transform main goal is that of changing the identity of our relevant independent variables. For μ_J we have

$$\mu_J(\mu_1, \ldots, \mu_M) = S - \sum_{k=1}^{M} \; \mu_k \, \langle A_k \rangle \, . \tag{4}$$

Note that for general entropic measures (other than Shannon-Gibbs') $\mu_J = \mu_J(\mu_1, \ldots, \mu_M)$ does not coincide with the normalization Lagrange multiplier. The three operative reciprocity relations become [15]

$$\frac{\partial \mu_J}{\partial \mu_k} = -\langle A_k \rangle \; ; \qquad \frac{\partial S}{\partial \langle A_k \rangle} \; = \; \mu_k \; ; \qquad \frac{\partial S}{\partial \mu_i} = \sum_k^M \mu_k \frac{\partial \langle A_k \rangle}{\partial \mu_i}, \tag{5}$$

the last one being the so-called Euler theorem. In Jaynes' philosophy [12] S is an information amount, to be maximized subject to *a priori known* values for the constraints $\langle A_k \rangle$.

3 General not-trace-form entropies and reciprocity

All trace form entropies can be successfully described by Jaynes' MaxEnt variational treatment, so that reciprocity relations hold, as demontrted in

[16]. Let us consider the general lack-of-trace-form instance (see (1 in the Introduction). One has, in the language of the Introduction,

$$S = G\left[\int dV f(\xi)\right], \tag{6}$$

with G an arbitrary smooth function. Then

$$S' = G' \int dV f'(\xi). \tag{7}$$

(Here S' denotes the functional derivative). Define $F = G'[f'(\xi)]$ and consider the inverse function of F, namely,

$$g = F^{-1}. \tag{8}$$

The MaxEnt variational problem ends up being

$$F - \lambda_N - \lambda_U U = 0, \tag{9}$$

so that the MaxEnt solution's PD ξ_{ME} is

$$\xi_{ME} = g(\lambda_N + \lambda_U U), \tag{10}$$

and the MaxEnt entropy reads

$$S_{ME} = G[\int dV f[g(\lambda_N + \lambda_U U)]]. \tag{11}$$

One also has

$$\frac{\partial \langle U \rangle}{\partial \lambda_U} = \int dV U g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{12}$$

and

$$0 = \frac{\partial}{\partial \lambda_U} \int dV \xi = \tag{13}$$

$$= \int dV g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U] = 0, \tag{14}$$

so that we arrive at the important relation [see (10)]

$$\frac{\partial S_{ME}}{\partial \lambda_U} = (QG')\frac{\partial}{\partial \lambda_U}\int dV f[g(\lambda_N + \lambda_U U)] = \tag{15}$$

$$= (QG')\int dV F'[g(\lambda_N + \lambda_U U)][g'(\lambda_N + \lambda_U U)][\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{16}$$

that using (14) gives

$$\frac{\partial S_{ME}}{\partial \lambda_U} = \lambda_U \int dV U g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{17}$$

which, according to (29) yields the Euler relation

$$\frac{\partial S_{ME}}{\partial \lambda_U} = \lambda_U \frac{\partial \langle U \rangle}{\partial \lambda_U}, \tag{18}$$

so that

$$\frac{\partial S}{\partial < U >} = \frac{\partial S}{\partial \lambda_U}\frac{\partial \lambda_U}{\partial < U >} = \lambda_U \frac{\partial < U >}{\partial \lambda_U}\frac{\partial \lambda_U}{\partial < U >} = \lambda_U, \tag{19}$$

the first reciprocity relation. Finally, introducing now the Jaynes parameter λ_J (the Legendre transform of S_{ME})

$$\lambda_J(\lambda_U) = S(< U >) - \lambda_U < U > (\lambda_U), \tag{20}$$

it is clear that

$$\frac{\partial \lambda_J}{\partial \lambda_U} = \frac{\partial S_{ME}}{\partial < U >}\frac{\partial < U >}{\partial \lambda_U} - \lambda_U \frac{\partial < U >}{\partial \lambda_U} - < U >= - < U >, \tag{21}$$

the second reciprocity relation. There exists a thermodynamics associated to the general entropic forms under study here, since Jaynes' MaxEnt approach successfully works.

4 Renyi's entropy S_R and reciprocity relations

We specialize the preceding discussion for S_R and ascertain, as should be expected, that it does work. This fact notwithstanding, if we try to explicitly write ξ_{ME}, as we will do in the following Section, problems arise. Because of such contradiction, it is worthwhile to repeat the preceding argument for S_R. One has

$$S = Q \ln [\int dV f(\xi)], \tag{22}$$

that becomes Renyi's one for $Q = (1-q)^{-1}$ and $f(\xi) = \xi^q$. One abbreviates also $h = \int dV f(\xi)$. Then

$$S' = (Q/h) \int dV f'(\xi). \tag{23}$$

Define $F = (Q/h)f'(\xi)$ and consider the inverse function of F, namely,

$$g = F^{-1};\;\; FF^{-1}(\nu) = \nu. \tag{24}$$

In this case

$$F = (Q/h)q\xi^{q-1};\;\; g(\xi) = [(h/Q)(\xi/q)]^{\frac{1}{q-1}};\;\; gF(\xi) = \xi, \tag{25}$$

The MaxEnt variational problem ends up being

$$F - \lambda_N - \lambda_U U = 0, \tag{26}$$

so that the MaxEnt solution ξ_{ME} is

$$\xi_{ME} = g(\lambda_N + \lambda_U U), \tag{27}$$

and the MaxEnt entropy reads

$$S_{ME} = Q \ln [\int dV f[g(\lambda_N + \lambda_U U)]]. \tag{28}$$

One also has

$$\frac{\partial \langle U \rangle}{\partial \lambda_U} = \int dV U g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{29}$$

and

$$0 = \frac{\partial}{\partial \lambda_U} \int dV \xi = \tag{30}$$

$$= \int dV g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U] = 0, \tag{31}$$

so that we arrive at the important relation [see (27)], after remembering that $F'g(\nu) = \nu$,

$$\frac{\partial S_{ME}}{\partial \lambda_U} = (Q/h)\frac{\partial}{\partial \lambda_U}\int dV f[g(\lambda_N + \lambda_U U)] = \tag{32}$$

$$= \int dV F'[g(\lambda_N + \lambda_U U)][g'(\lambda_N + \lambda_U U)][\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{33}$$

that using (31) gives

$$\frac{\partial S_{ME}}{\partial \lambda_U} = \lambda_U \int dV U g'(\lambda_N + \lambda_U U)[\frac{\partial \lambda_N}{\partial \lambda_U} + U], \tag{34}$$

which, according to (29) yields the Euler relation

$$\frac{\partial S_{ME}}{\partial \lambda_U} = \lambda_U \frac{\partial \langle U \rangle}{\partial \lambda_U}, \tag{35}$$

so that

$$\frac{\partial S}{\partial < U >} = \frac{\partial S}{\partial \lambda_U}\frac{\partial \lambda_U}{\partial < U >} = \lambda_U \frac{\partial < U >}{\partial \lambda_U}\frac{\partial \lambda_U}{\partial < U >} = \lambda_U, \tag{36}$$

the first reciprocity relation. Finally, introducing now the Jaynes parameter λ_J (the Legendre transform of S_{ME})

$$\lambda_J(\lambda_U) = S(< U >) - \lambda_U < U > (\lambda_U), \tag{37}$$

it is clear that

$$\frac{\partial \lambda_J}{\partial \lambda_U} = \frac{\partial S_{ME}}{\partial < U >}\frac{\partial < U >}{\partial \lambda_U} - \lambda_U \frac{\partial < U >}{\partial \lambda_U} - < U > = - < U >, \tag{38}$$

the second reciprocity relation.

5 MaxEnt-Renyi's peculiarities

This was detected in [13]. Let us return to

$$h = \int dV \xi^q, \tag{39}$$

$$F = (Q/h) f'(\xi); \tag{40}$$

$$F - \lambda_N - \lambda_U U = 0, \tag{41}$$

and set $f(\xi) = \xi^q$ (specify Renyi's case, with $Q = 1/(1-q)$). One has

$$\frac{q\xi^{q-1}}{(1-q)h} - \lambda_N - \lambda_U U = 0, \tag{42}$$

and now integrate (41) over ξdV. *The h in the denominator cancels the $\xi-$integral in the numerator!* Thus,

$$0 = \int dV \xi \{ \frac{(1-q)^{-1} q \xi^{q-1}}{h} - \lambda_N - \lambda_U U \} = \tag{43}$$

$$= \frac{q}{1-q} - \lambda_N - \lambda_U \langle U \rangle = 0, \tag{44}$$

leading to

$$\lambda_N = \frac{q}{(1-q)} - \lambda_U \langle U \rangle, \tag{45}$$

which *diverges* for $q == 1$. Also, one has

$$\frac{\partial \lambda_N}{\partial \lambda_U} = -\langle U \rangle - \lambda_U \frac{\partial \langle U \rangle}{\partial \lambda_U}, \tag{46}$$

which is an interesting Renyi relation, to be compared to the Legendre transform (see Sect.1)

$$\lambda_J = S - \lambda_U \langle U \rangle, \tag{47}$$

so that

$$\frac{\partial \lambda_J}{\partial \lambda_U} = -\langle U \rangle. \tag{48}$$

Summing up, we have a divergence at $q = 1$ in (45) that we should try to understand. In order to do so, we embark now on a detour.

6 Comparison with Tsallis' case

It is of interest to compare (45) above with its Tsallis' counterpart S_T. One has [17, 18, 19, 20]

$$S_T = \frac{1}{q-1}\int dV[\xi - \xi^q]. \tag{49}$$

Thus,

$$\int dV \xi \frac{\partial S_T}{\partial \xi} = \frac{1}{q-1}\int dV[\xi - q\xi^q], \tag{50}$$

leading to

$$dV\frac{1}{q-1}\int dV[\xi - q\xi^q] - \lambda_N - \lambda_U\langle U\rangle = 0. \tag{51}$$

Now, using ξ-normalization, this can be recast, using $\int dV\xi^q = 1+(1-q)S_T$,

$$qS_T - 1 - \lambda_N - \lambda_U\langle U\rangle = 0, \tag{52}$$

that should be compared to (**??**). Now, after adding and substracting S_T on the l.h.s.,

$$\lambda_J = S_T - \lambda_U\langle U\rangle = \lambda_N + 1 + (1-q)S_T. \tag{53}$$

In the limit $q \to 1$ this yields

$$\lambda_J = \lambda_N + 1, \tag{54}$$

the Boltzamnn-Gibbs classical result [12].

6.1 Tsallis' case alternative viewpoint

This alternative situation is also mentioned in [21]. Quite simply, S_T can cast in two identical fashions:

$$S_T = \frac{1}{q-1}\int dV[\xi - \xi^q] = \frac{1}{q-1} - \frac{1}{q-1}\int dV\xi^q, \tag{55}$$

which gives rise to two different variational problems. Using the second form one has

$$\int dV\xi \frac{\partial S_T}{\partial \xi} = \frac{q}{1-q} \int dV\xi^q, \tag{56}$$

and

$$\frac{q}{1-q} \int dV\xi^q - \lambda_N - \lambda_U \langle U \rangle = 0., \tag{57}$$

Using again $\int dV\xi^q = 1 + (1-q)S_T$, we are led to, after adding and substracting

$$\lambda_J = S_T - \lambda_U \langle U \rangle = \lambda_N - \frac{q}{1-q} + (1-q)S_T, \tag{58}$$

which in the limit $q \to 1$ results in a divergence!

What is happening here? The answer is that casting S_R as

$$S_T = \frac{1}{q-1} - \frac{1}{q-1} \int dV\xi^q, \tag{59}$$

assumes normalization from the very beginning, which *unduly restricts* the ξ-variational space. Additionally, we keep λ_N in the variation, which is an inconsistency. Thus, the accompanying divergence.

6.2 Surrogate Renyi entropy S_R^S

We just add zero to the Renyi definition in the fashion (b is a constant to be chosen later on)

$$S_R^S = \frac{bq}{1-q} \ln \left[\int dV\xi \right] + \frac{1}{1-q} \ln \left[\int dV\xi^q \right], \tag{60}$$

and thus

$$\int dV\xi \frac{\partial S_R^S}{\partial \xi} = \frac{q}{1-q}(b+1), \tag{61}$$

which vanishes if one chooses $b = -1$. Accordingly,

$$\lambda_N = -\lambda_U \langle U \rangle, \tag{62}$$

and the divergence has disappeared. We have discovered then that the original Renyi definition somehow assumes normalization from the beginning. In any case, λ_N does not tend to its Shannon counterpart as q tends to unity.

7 Conclusions

We have investigated here quite general entropies that lack trace form, a family of entropic functionals that includes as a distinguished member the celebrated Renyi entropy S_R. We studied for such family the validity of thermodynamics' reciprocity relations (RR) that would, in turn, legitimate an associated statistical mechanics, complying with the basic thermodynamics' tenets. We proved the RR exist for all possible entropies.

Our endeavors both illuminated and allowed us to understand the origin of the MaxEnt-Renyi peculiarities, discovered in [13], that seemingly impaired the associated RR for the particular entropic form S_R. Amongst these peculiarities, we single out a singularity in Eq. (45), connecting λ_N (normalization multiplier) with λ_U (energy multiplier) that emerges in the limit $q \to 1$. We found that the singularity can be removed if one replaces S_R by a surrogate quantifier S_R^S, essentialy equivalent to S_R but not identical to it. These two measures are given by different functionals of the probability density ξ, whose numerical values coincide if one explicitly takes into account the normalization of ξ.

A similar artifact is seen to apply to Tsallis entropy S_T when extremized with linear constraints. S_T can be cast in two different ways as a function of the probability density ξ, and for one of them a similar singularity emerges as well. In the alternative instance, instead, the $q \to 1$ limit makes Tsallis normalization multiplier to converge to the Shannon one.

We conclude that, if for some entropic form S_A the MaxEnt treatment displays a singularity, there should be an alternative way of writing S_A that overcomes the difficulty, as we have proved in Section 3 that RR are valid for any S_A.

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