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Reciprocity relations and generalized, classic entropic quantifiers that lack trace-form

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HIGHLIGHTS

- Entropy functionals that lack trace form are investigated.
- We show that any such functional satisfies the Legendre reciprocity relations characteristic of thermodynamics.
- A given entropic form may display singularities in the relation between the associated MaXent Lagrange multipliers.
- We give examples and show how to remove them.

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ABSTRACT

In this effort we show that the Legendre reciprocity relations, thermodynamics' essential formal feature, are respected by general classic entropic functionals, even if they are NOT of trace-form nature, in contrast with Shannon's or Tsallis' cases. Further, with reference to the Maximum Entropy (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.

1. Introduction

The principle of maximum entropy (MaxEnt) is a powerful technique for estimating states of probabilistic models [1]. This principle states that the most suitable probability distribution compatible with the a priori known data is the one with largest entropy [1–3].

In a MaxEnt context, this paper studies quite general classic entropy functionals and their associated thermodynamics, with the idea of verifying whether the classical reciprocity relations remain valid in a general scenario involving functionals that lack trace form. The idea is also to re-visit some issues that lack yet full adequate understanding. We focus attention on the canonical ensemble.

As already mentioned, our main concern is to investigate the so-called non trace form entropies. Indeed, the Physics community has paid considerable attention to non-trace form entropic functionals in recent years [4–14]. These entropic measures have been applied to a variety of problems in the emerging field of complex systems theory. This kind of entropies have been found to be relevant in connection with diverse physical scenarios, ranging from processes described by nonlinear

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Fokker–Planck equations [11–13], to the thermodynamics of multifractal systems [14]. The importance of non trace form entropies has been highlighted by recent and remarkable contributions by Tempesta and collaborators concerning the property of composability of entropic measures [4–6]. An entropy is composable if its value for a composite system consisting of two statistically independent parts can be expressed in terms of the entropies of the constituent parts. In the case of trace form entropies the only composable ones are Boltzmann's and Tsallis'. However, in the realm of non trace form entropies, Tempesta has found a vast family of entropies of this nature, that are suitable for application in the natural sciences [6].

The foremost example of such an entropy is Renyi's one, advanced in 1961. It is the most general information measure that complies with additivity in joining independent systems or events [15–26]. If its logarithm is replaced by a continuous and monotonic function G, we obtain a rather general non trace-form entropy. We wish to ascertain whether it can be successfully described by Jaynes' MaxEnt variational treatment, so that reciprocity relations hold [1].

In addition, we wish to analyze anomalies that sometimes arise with regards to the workings of MaxEnt's Lagrange multipliers in the Renyi instance [27].

Our present analysis uncovers an interesting feature of the Jaynes' maximum entropy approach as applied to generalized entropies. Apparently equivalent entropic forms, that yield the same numerical value when evaluated on normalized probability densities ξ, lead to quite different MaxEnt results. Some of them exhibit singularities for particular values of the relevant entropic parameters, while others behave continuously in terms of these parameters. The paper is organized as follows:

- Section 2 presents background information.
- Section 3 is the core of the present effort. We show that, for any non trace form entropic functional, Legendre's reciprocity relations are respected. It was already known, since 1997, that this was true for trace form entropies. 20 years later we extend here the result to more general entropic forms (the non trace form ones).
- Section 4 specializes the general demonstration for the case of Renyi's functional.
- Section 5 discusses anomalies exhibited by Renyi's MaxEnt's Lagrange multipliers and makes comparisons with the Tsallis' instance.
- Section 6 is devoted to conclusions.

2. Background: Legendre transform and reciprocity relations

Here we briefly review the Legendre transform essentials, together with their associated Lagrange multipliers. These multipliers obey reciprocity relations that are extremely important in thermodynamics, so that any putative entropic functional must lead to a variational principle respecting them. The reciprocity relations constitute the basic link connecting thermodynamics with the probability density arising from the constrained optimization of an appropriate entropy measure. Indeed, the fundamental thermodynamics relations among entropy, energy, temperature, and other basic thermodynamics quantities can be identified with the aforementioned MaxEnt 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 [28].

Legendre's transform (LT) is an operation that converts a real function f_1 with real argument 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.

$$f_2(y) = xy - f_1(x); \quad y = f_1'(x) \Rightarrow \text{ reciprocity.} \tag{1}$$

Legendre Transform's *reciprocity relations are thermodynamics' basic formal ingredient* [29]. For two functions, an entropy S and its Legendre transform $\tilde{S}$, one has the relation given below [1], where $\langle A_i \rangle$ is the mean value of any function of phase space variables, that we may call a classical observable A_i, of which one is supposed to deal with M of them:

$$S(\langle A_1\rangle, \ldots, \langle A_M\rangle) = \tilde{S} + \sum_{k=1}^{M} \mu_k \langle A_k\rangle, \tag{2}$$

where μ_k is the Lagrange multiplier corresponding to the constraint $\langle A_k\rangle$. In standard thermodynamical scenarios the quantities $\langle A_i\rangle$ can be identified with extensive thermodynamic variables and the Lagrange multipliers μ_i with intensive ones. Obviously, the Legendre transform main goal is that of changing the identity of our relevant independent variables. For $\tilde{S}$ we have

$$\tilde{S}(\mu_1, \ldots, \mu_M) = S - \sum_{k=1}^{M} \mu_k \, \langle A_k\rangle \,. \tag{3}$$

Note that for general entropic measures (other than Shannon–Gibbs') $\tilde{S} = \tilde{S}(\mu_1, \ldots, \mu_M)$ does not coincide with the normalization Lagrange multiplier. The three operative reciprocity relations become [29]

$$\frac{\partial \tilde{S}}{\partial \mu_k} = -\langle A_k\rangle \,; \qquad \frac{\partial S}{\partial \langle A_k\rangle} = \mu_k \,; \qquad \frac{\partial S}{\partial \mu_i} = \sum_{k}^{M} \mu_k \frac{\partial \langle A_k\rangle}{\partial \mu_i}, \tag{4}$$