A note on non-thermodynamical applications of non-extensive statistics

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Abstract

It is pointed out that the constraint to be imposed to the maximization of the entropy for processes outside the class of thermodynamical systems, is generally not well defined. In fact, any probability distribution can be derived from Jaynes’s principle with a suitable choice of the constraint. In the case of Tsallis’s non-extensive formalism, this implies that it is not possible to establish any connection between specific non-thermodynamical processes and non-extensive mechanisms and, in particular, to assign any unambiguous non-extensivity index $q$ to those processes.

Key words: Jaynes’s principle, Tsallis’s non-extensive thermostatistics, interdisciplinary applications

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Boltzmann-Gibbs thermostatistics bridges the microscopic description of physical systems that obey the laws of mechanics with the macroscopic picture drawn from the principles of thermodynamics. From a historical perspective, it reconciled the physics of thermal processes, fully congenial with our everyday-life experience, and the mechanicistic interpretation of the Universe as a huge ensemble of interacting particles—two views that, in the middle of the nineteenth century, were far from being perceived as compatible, both mathematically and philosophically [1].

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Physical systems whose microscopic degrees of freedom are governed by the equations of (classical or quantum) mechanics, and which have reached a state of macroscopic equilibrium, will hereafter be called *thermodynamical systems*. The Boltzmann-Gibbs formulation makes it possible to derive a theory for the collective equilibrium state variables of a thermodynamical system from its microscopic dynamics. At the same time, it gives origin to the mesoscopic (statistical) description level. An overwhelming corpus of experimental work validates the results of this procedure, both at mesoscopic and macroscopic levels. It is known, however, that Boltzmann-Gibbs thermostatistics fails to give a mathematically consistent description of certain physical systems – notably, those driven by gravitational and other long-range interactions – since the predicted values of some of their state variables diverge [2]. Though it is not clear whether such systems attain at all a state identifiable with macroscopic equilibrium [3], their thermodynamical properties would be characterized by non-extensive macroscopic variables.

In 1988, C. Tsallis proposed an extension of Boltzmann-Gibbs equilibrium thermostatistics based on a variational principle for a generalized form of the entropy [4],

$$S_q = -\sum_i p_i^q - \frac{1}{q-1},$$  \hspace{1cm} (1)

where $p_i$ is the probability that the thermodynamical system under study is found in its $i$-th quantum state and $q \in (-\infty, \infty)$. The fact that, for $q \neq 1$, the entropy $S_q$ is not additive with respect to the factorization of the probabilities, has led to the assumption that this formalism may provide consistent thermostatistical description of non-extensive systems. The parameter $q$ has been called non-extensivity index, since it measures the deviation from additivity of $S_q$.

In the canonical scenario, the generalized entropy (1) is maximized with respect to $p_i$, with the constraint of probability normalization,

$$\sum_i p_i = 1,$$  \hspace{1cm} (2)

and fixing the value of a generalized form of the mean energy [5],

$$\frac{\sum_i p_i^q \epsilon_i}{\sum_i p_i^q} = E_q,$$  \hspace{1cm} (3)

where $\epsilon_i$ is the energy of the $i$-th state. This canonical maximization procedure
yields the energy-dependent probability distribution

\[ p_i = Z^{-1}[1 + \beta(q - 1)\epsilon_i]^{-1/(q - 1)}, \]  

(4)

where \( Z \) is a normalization constant analogous to the partition function and \( \beta \) is an auxiliary parameter. The variational formulation of canonical Boltzmann-Gibbs thermostatistics is fully recovered in the limit \( q \to 1 \), where \( \beta \) reduces to the inverse temperature.

A remarkable property of Tsallis’s generalization is that it preserves the mathematical structure of standard thermostatistics for any value of \( q \) [6]. This noticeable feature justifies the rather unexpected form of the constraint (3), which replaces the usual definition of the mean energy \( E = \sum_i p_i \epsilon_i \). In a long series of publications [7], it has been shown that most of the theorems of equilibrium statistical mechanics, as well as many results concerning linear and nonlinear non-equilibrium properties, can be formally generalized in the frame of the extended formalism. Apart from this formal equivalence with Boltzmann-Gibbs thermostatistics, the relevance of the non-extensive formulation should be validated by the observation of actual thermodynamical systems with an energy distribution of the form (4). At the same time, the role of the quantity \( E_q \) as a macroscopic property of the system in question should be assessed, in comparison with the role of the mean energy \( E \) as a state variable of extensive systems. Until now, however, there is no conclusive evidence that non-extensive thermostatistics might correctly describe any thermodynamical system [8,9,10].

On the other hand, many real systems have been identified where the statistical distribution of their relevant variables—not of the energy, however—are well fitted with functions of the type of Eq. (4) [7]. To be specific, empirical distributions for quantities \( x \) defined over the semi-infinite range \((0, \infty)\) have been systematically fitted with the two-parameter function

\[ p(x) = N(1 + ax)^b, \]  

(5)

[cf. Eq. (4)] where \( N(a, b) \) is chosen in such a way that \( p(x) \) is normalized to unity. Through identification of \( p(x) \) with the distribution of Eq. (4), the fitting parameters \( a \) and \( b \) are used to assign an “inverse temperature” \( \beta \) and a non-extensivity index \( q \) to the empirical distribution under consideration. For quantities \( x \in (-\infty, \infty) \) the chosen function is, instead,

\[ p(x) = N(1 + ax^2)^b. \]  

(6)

This approach has been applied, for instance, to momentum distributions in elementary particle interactions [11], velocity distributions in diffusing bio-
logical systems [12], and volume and return distributions in financial processes [13]. In all the reported cases the result of the fitting seems to be quite good, a circumstance that has invariably led to the claim that the systems under study are governed by mechanisms characterized by non-extensivity. Frequently, moreover, connections have been established with presumably related concepts, such as self-similarity, scale invariance, non-ergodicity, meta- and quasi-equilibria, criticality, algorithmic complexity, et cætera [7,13,14].

Now, the fact that an empirical distribution is well fitted by a function derived from a variational principle analogous to that of canonical thermostatistics, does not necessarily mean that the nature of the underlying processes is the same as in a thermodynamical system, as described by equilibrium statistical mechanics, nor that the state of the system can be identified with canonical thermal equilibrium. The existence of a mechanical Hamiltonian formulation for processes such as, say, elementary interactions may be a matter of controversy, but a Hamiltonian-like realistic description of a biological population or the stock market should be out of question. However obvious, this remark raises a significant question associated with the maximization procedure that yields fitting functions such as those of Eqs. (5) and (6), and with Jaynes’s principle in general: Besides probability normalization, which is the “correct” constraint to be used in the canonical maximization of the entropy?

For extensive thermodynamical systems, numberless instances of experimental validation show that the mean energy $E$ is to be fixed. The formal equivalence of non-extensive thermostatistics with the Boltzmann-Gibbs formulation suggests in turn that constraint (3) may be necessary to deal with non-extensive thermodynamical systems (see, however, Ref. [9]). On the other hand, no rigorous justification can generally hold for any of the infinitely many constraints that can be imposed in the case of non-thermodynamical systems [15]. Assuming that the states of the system are well defined, any function $\phi(x)$ of the relevant variable $x$ may be used to introduce the average

$$
\Phi_q = \frac{\sum_i p_i^q \phi(x_i)}{\sum_i p_i^q},
$$

in full analogy with Eq. (3). Maximization of the entropy (1) under constraints (2) and (7) leads to

$$
p(x) = Z^{-1} [1 + \beta(q - 1)\phi(x)]^{-1/(q-1)}.
$$

This freedom in the choice of the variational constraint seems to have been systematically overlooked by those authors who applied non-extensive thermostatistics to the description of empirical data from non-thermodynamical systems. In fact, choosing fitting functions as in Eqs. (5) and (6) amounts to restricting $\phi(x)$ to $x$ and $x^2$, respectively.
Fig. 1. Distribution of (normalized) one-minute returns of 10 stocks of the New York Stock Exchange during 2001. The dotted line is a fitting with Eq. (6), which yields $q = 1.4$ [13]. The full line corresponds to a fitting with Eq. (8), taking $\phi(x) = |x|^{1.6}$. In this case, $q = 1.3$. The inset shows a close-up in linear scales.

An exception to this rule, which dramatically points out the necessity of considering more general constraints when studying non-thermodynamical systems, is given by the fittings of velocity-difference distributions in turbulent flows [16,17,18]. In this case, reasonable fittings with functions as in Eq. (8) are obtained only when $\phi(x)$ is allowed to take rather complicated forms, typically, $\phi(x) = x^{2\alpha}/2 - c \operatorname{sgn}(x)(|x|^\alpha - |x|^{3\alpha}/3)$ with $c \geq 0$ and $0 < \alpha < 1$. The circumstance that such form of $p(x)$ implies an unusual choice of the function being averaged in the variational constraint does not seem to have been discussed in the relevant literature, though.

The arbitrariness of the variational constraint for non-thermodynamical systems makes it possible to finely tune the fitting function by a suitable choice of $\phi(x)$. As an illustration, we show in Fig. 1 an empirical distribution of high-frequency stock returns in the New York Stock Exchange [19], along with two fittings. The dashed curve corresponds to the fitting function of Eq. (6), with $b = -2.5$ ($q = 1.4$) [13]. While the overall quality of the approximation is good, a systematic deviation from the empirical data is apparent for intermediate values of the distribution ($10^{-4} \lesssim p(x) \lesssim 10^{-2}$). This deviation is considerably reduced if, as shown by the full curve, the maximization of entropy is subject to constraint (7) with $\phi(x) = |x|^{1.6}$, which gives $q = 1.3$. As discussed above,
this constraint is as valid as any other, and has the advantage of yielding a
better fitting for the empirical data.

It immediately results from Eq. (8) that introducing the function

\[ \phi(x) = \frac{1}{q-1} [A p(x)^{1-q} + \phi_0] \]

(9)
in constraint (7) leads to a variational principle which exactly yields any given
distribution \( p(x) \). The constants \( A \) and \( \phi_0 \) fix the origin and units of measure
for the average \( \Phi_q \), while \( q \) establishes the connection between the shapes of
\( \phi(x) \) and \( p(x) \). Note that the index \( q \) can be chosen arbitrarily, and that a
different form of \( \phi(x) \) is obtained for each value of \( q \). For \( q \to 1 \), we get
\[ \phi(x) = A' \ln p(x) + \phi'_0. \]

The simple observation that any distribution can be derived from a variational
principle for the entropy if a suitable constraint is chosen, has far-reaching
consequences when interpreting the fitting of non-thermodynamical empirical
data in the frame of non-extensive statistics. In particular, it voids of meaning
any claim of connection between the fitted data and possible non-extensive
mechanisms underlying the system in question. A quantitative proof of this
assertion is provided by the fact that, for a given system, the non-extensivity
index \( q \) is not uniquely defined, and can in fact be given any value by an
appropriate choice of \( \phi(x) \). Any system, in fact, could be made “extensive” by
simply using the constraint that yields \( q = 1! \)

At this point, it could be argued that the kind of constraints arising from a
choice of \( \phi(x) \) as in Eq. (9) will generally be unconventional, typically involving
complicated functions of the relevant variables. We have seen that this is
in fact the case if the distributions of velocity-differences in turbulent flows
are forced to fit non-extensive thermostatistics. For other physical systems,
it has already been remarked that insisting to stick to a variational principle
may necessarily lead to consider “non-traditional” constraints [20]. For non-
physical systems, unfortunately, we can hardly discern between “traditional”
and “non-traditional” constraints. Without a rigorous argument to decide on
this point, no choice can possibly be dismissed on such basis.

In summary, we have pointed out that any probability distribution can be
derived from the entropic variational formalism that underlies Tsallis’s non-
extensive thermostatistics, if a suitable “state function” is chosen to define a
constraint for the maximization procedure. The same remark should hold for
any variational formalism based on Jaynes’s principle. While for macroscopic
Hamiltonian systems in thermodynamical equilibrium it is well established
that the mean energy is to be fixed, for non-thermodynamical systems it is gen-
erally not possible to argue for or against any choice. Therefore, any claim of
connection between non-thermodynamical processes and non-extensive mechanisms, based on the fitting of empirical probability distributions with the functions derived from Tsallis’s variational formalism, is essentially insubstantial. Such kind of fittings provide at most a phenomenological description of the systems in question, and bear little information on their true nature.

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