Non-unique way to generalize the Boltzmann-Gibbs distribution

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Abstract

Alternative definitions are given of basic concepts of generalized thermostatistics. In particular, generalizations of Shannon’s entropy, of the Boltzmann-Gibbs distribution, and of relative entropy are considered. Particular choices made in Tsallis’ nonextensive thermostatistics are questioned.

1 Introduction

Several choices have to be made when generalizing the Boltzmann-Gibbs distribution. In this note some of these choices are reviewed. Each time, two options are presented: an A-option, which is the choice made in Tsallis’ thermostatistics [1, 2, 3, 4], and a B-choice which corresponds with generalized thermostatistics as introduced by the author [5, 6]. Advantages and disadvantages of each of the options are discussed.

Starting point of the generalization is that the exponential function appearing in the Boltzmann-Gibbs distribution is replaced by some other increasing function. This idea goes back to the early days of Tsallis’ thermostatistics [7]. A generalization in this way is non-unique. As a consequence, historically made choices may now be questioned. If they appear to be suboptimal then the dilemma arises whether the standing formalism should be modified. The present paper tries to start this debate by clarifying possible choices and indicating their consequences.

In the next section deformed logarithmic and exponential functions are defined. Three sets of alternatives are presented in section 3. In the final section some preliminary conclusions are drawn.
2 Deformed logarithmic and exponential functions

The point of view adapted in the present paper is to replace the logarithmic
and exponential functions by arbitrary functions, which however share some
of the properties of the standard functions. In particular, following [5], a deformed
logarithmic function is denoted \( \ln_\kappa(x) \). It is defined for all positive \( x \), and is an
increasing and concave function. It is normalized so that \( \ln_\kappa(1) = 0 \). It could
be further normalized by requiring that

\[
\int_1^0 dx \ln_\kappa(x) = 1.
\]

However, some of the examples below do not satisfy this requirement. Therefore,
introduce the notation

\[
F_\kappa(x) = \int_1^x dy \ln_\kappa(y),
\]

and require only that \( F_\kappa(0) \) is a finite number.

The inverse of the deformed logarithmic function \( \ln_\kappa(x) \) is denoted \( \exp_\kappa(x) \).
Because the range of \( \ln_\kappa(x) \) can be less than the whole real line, let us convene that \( \exp_\kappa(x) = 0 \) when \( x \) is smaller than all values reached by \( \ln_\kappa(y) \) and \( \exp_\kappa(x) = +\infty \) when \( x \) is larger than all values reached by \( \ln_\kappa(y) \).

As an example, let us consider the definition of deformed logarithmic function as it is used in the context of Tsallis’ non-extensive thermostatistics. It is
denoted \( \ln_q(x) \), where \( q \) is a free parameter, which must lie between 0 and 2 in
order for \( \ln_q(x) \) to be a deformed logarithm according to the definition given
above. In what follows also an alternative definition will be needed. The latter
is denoted \( \ln_q^*(x) \). The two expressions are

\[
\ln_q(x) = \frac{1}{1-q}(x^{1-q} - 1) \\
\ln_q^*(x) = \frac{q}{q-1}(x^{q-1} - 1).
\]

A short calculation shows that

\[
F_q(0) = \int_1^0 dx \ln_q(x) = \frac{1}{2-q},
\]
\[
F_q^*(0) = \int_1^0 dx \ln_q^*(x) = 1.
\]

Hence, the deformed logarithm \( \ln_q(x) \) is not fully normalized. The inverse
functions are given by

\[
\exp_q(x) = [1 + (1-q)x]^{1/(1-q)},
\]
\[ \exp_q^* (x) = \left[ 1 + \frac{q-1}{q} x \right]^{1/(q-1)}_+, \quad (2) \]

where \([x]_+\) equals \(x\) when \(x\) is positive, and zero otherwise.

Another example of deformed logarithmic and exponential functions has been proposed by Kaniadakis [8, 9]. Yet another example is found in [6], where it is used to describe the equilibrium distribution of a single spin at the center of the Ising chain. In what follows, only the definitions (1, 2) will be used to illustrate the impact of alternatives in the context of Tsallis’ thermostatistics.

3 Three sets of alternatives

3.1 Entropy

Let us start with Shannon’s entropy functional, which for a discrete probability distribution can be written as

\[
I(p) = \sum_k p_k \ln \left( \frac{1}{p_k} \right) \\
= -\sum_k \int_0^{p_k} \text{d}x \left( 1 + \ln x \right). \quad (3)
\]

Given these expressions, the two obvious generalizations are

\[
I_A(p) = \sum_k p_k \ln_x \left( \frac{1}{p_k} \right) \\
I_B(p) = -\sum_k \int_0^{p_k} \text{d}x \left( F_x(0) + \ln_x x \right) \\
= -\sum_k \int_0^1 \text{d}x p_k (F_x(0) + \ln_x (xp_k)). \quad (4)
\]

Both definitions have all properties that one expects that an entropy functional should possess. An immediate advantage of \(I_B(p)\) over \(I_A(p)\) is that it is straightforward to calculate derivatives. E.g., the derivative w.r.t. temperature \(T\) is given by

\[
\frac{dI_B(p)}{dT} = -\sum_k (F_x(0) + \ln_x (p_k)) \frac{dp_k}{dT}. \quad (5)
\]

The latter property is very convenient when proving thermodynamic stability [6].

Let us now consider how the definitions (4) look like in the special cases that \(\ln_x(x)\) is taken equal to \(\ln_q(x)\), respectively \(\ln^*_q(x)\), as given by (1). One obtains

\[
I_A(p) = \sum_k p_k \ln_q \left( \frac{1}{p_k} \right)
\]

3
\[I_B(p) = - \sum_k \int_0^{p_k} dx (1 + \ln_q(x))\]
\[= \frac{1}{1-q} \left( \sum_k p_k^q - 1 \right).\]

Both definitions of entropy coincide. The resulting expression is Tsallis’ entropy [1]. It can also be written as (see formula (18) of [10])
\[I_A(p) = - \sum_k p_k^q \ln_q(p_k).\]

In the latter form generalization to arbitrary deformed logarithmic functions is not obvious.

For sake of completeness, the definitions of entropy are given now for the case of continuous distributions and for the quantum case. If \(\rho(\gamma)\) is a probability density over some phase space \(\Gamma\) then the expressions read
\[I_A(\rho) = \int_{\Gamma} d\gamma \rho(\gamma) \ln_n \left( \frac{1}{\rho(\gamma)} \right),\]
\[I_B(\rho) = - \int_{\Gamma} d\gamma \int_0^{\rho(\gamma)} dx \left( F_{\kappa}(0) + \ln_x x \right). \quad (6)\]

In the quantum case the entropy of a density matrix \(\rho\) is given by
\[I_A(\rho) = \text{Tr} \rho \ln_n \left( \frac{1}{\rho} \right),\]
\[I_B(\rho) = - \int_0^1 dx \text{Tr} \rho (F_{\kappa}(0) + \ln_x(x\rho)). \quad (7)\]

3.2 Canonical probability distributions
Given discrete energy levels \(H_k\), the Boltzmann-Gibbs distribution equals
\[p_k = \frac{1}{Z(T)} \exp(-H_k/T) = \exp(G(T) - H_k/T). \quad (8)\]

In this expression \(T > 0\) is the temperature. The normalization can be written either as a prefactor \(1/Z(T)\), or it can be included in the exponential as a term \(G(T)\). One clearly has \(Z(T) = \exp(-G(T))\). After generalization, the expressions become
\[p_k^A = \frac{1}{Z(T)} \exp_\kappa(-H_k/T),\]
\[p_k^B = \exp_\kappa(G(T) - H_k/T). \quad (9)\]
The expression for \( p^A_k \) has the advantage that an explicit expression for the normalization exists

\[
Z(T) = \sum_k \exp(-H_k/T).
\]

The definition of \( p^B_k \) has the advantage that it leads to an easy expression for \( \ln \kappa(p^B_k) \)

\[
\ln \kappa(p^B_k) = G(T) - H_k/T.
\]

The latter is very convenient when calculating the temperature derivative of the entropy. Indeed, one obtains immediately, using (5),

\[
\frac{dI_B(p^B)}{dT} = -\sum_k \left( 1 + \ln \kappa(p^B_k) \right) \frac{dp^B_k}{dT}
\]

\[
= -\sum_k \left( 1 + G(T) - H_k/T \right) \frac{dp^B_k}{dT}
\]

\[
= \frac{1}{T} \sum_k H_k \frac{dp^B_k}{dT}
\]

\[
= \frac{1}{T} \frac{dU}{dT},
\]

with the average energy \( U \) given by

\[
U = \sum_k p^B_k H_k.
\]

Relation (10) coincides with the thermodynamic definition of temperature as the inverse of the derivative of entropy with respect to average energy \( U \).

\[
\frac{1}{T} = \frac{dS}{dU}.
\]

This shows that \( p^B_k \) is the equilibrium probability distribution of the canonical ensemble with entropy functional \( I_B(p) \) and with average energy \( U \) defined in the usual way by (11). Moreover, the stability conditions, that \( S \) is a concave function of \( U \) and that \( U \) is an increasing function of \( T \), are satisfied. Generically, the corresponding \( A \)-quantities do not have such nice properties.

In the general case, it is very difficult to write an explicit formula expressing \( p^A_k \) in terms of \( p^B_k \). But this is feasible in the specific case that the deformed logarithm \( \ln_\kappa(x) \) is given by \( \ln_q(x) \), respectively \( \ln^*_q(x) \), as defined by (1). The expressions (9) become

\[
p^A_k = \frac{1}{Z(T)} \exp_q\left( -H_k/T \right)
\]

\[
= \frac{1}{Z(T)} \left[ 1 - (1-q)H_k/T \right]^{1/(1-q)}
\]
\[ p_k^B = \exp_q^* (G(T) - H_k/T) \]
\[ = \left[ 1 + \frac{q-1}{q} (G(T) - H_k/T) \right]^{1/(q-1)}. \]  
(13)

The first expression is the one introduced in [2]. The latter expression is found in [6]. The two expressions look similar but differ in a number of aspects. Let us try to match them. Replace \( q \) and \( T \) in the former expression by accented symbols \( q' \) and \( T' \). Then the two expressions coincide provided that
\[ q = 2 - q', \]
\[ G(T) = \frac{2-q}{1-q'} \left( Z(T')^{q'-1} - 1 \right), \]
\[ T = T' Z(T')^{1-q'}. \]

The latter expression makes clear that \( p_k^A \) and \( p_k^B \) have a completely different dependence on temperature \( T \). It is therefore obvious to check this temperature dependence in existing applications of the probability distribution \( p_k^A \). However, a first scan of the literature raises the conjecture that this temperature dependence has not at all been considered. There seems to be no evidence for temperature dependent probability distributions of the form (13), except of course in the \( q = 1 \)-case of the Boltzmann-Gibbs distribution.

It is straightforward to write down the extensions of (9) in case of continuous distributions, or in the quantum case.

### 3.3 Relative entropy

The relative entropy of a discrete probability distribution \( p \), given a discrete probability distribution \( r \), is defined by
\[ I(p||r) = \sum_k p_k \ln(p_k/r_k). \]  
(14)

It is only defined if \( r_k = 0 \) implies that also \( p_k = 0 \). Relative entropy is also called Kullback-Leibler distance. There are many ways to write (14), and hence, many alternative definitions of generalized relative entropy. Some possibilities are

\[ I_A(p||r) = -\sum_k p_k \ln_e \left( \frac{r_k}{p_k} \right), \]
\[ I_{B1}(p||r) = \sum_k \int_{r_k}^{p_k} dx \ln_e (x/r_k) \]
\[ = \sum_k \int_0^1 dx (p_k - r_k) \ln_e \left( 1 + \frac{p_k - r_k}{r_k} \right), \]
\[ I_{B2}(p||r) = \sum_k \int_{r_k}^{p_k} dx \left( \ln_e (x) - \ln_e (r_k) \right) \]
\[
\sum_{k} \int_{0}^{1} \, dx \, [p_k \ln_\kappa(xp_k) - r_k \ln_\kappa(xr_k) - (p_k - r_k) \ln_\kappa(r_k)].
\]

(15)

The main advantage of \(I_{B2}(p||r)\) over the other expressions is that, when \(r\) equals the equilibrium distribution \(p^B\), then one has (see [11])

\[
I_{B2}(p||p^B) = I_{B2}(p^B) - I_{B}(p) + \frac{1}{T} \sum_{k} (p_k - p_k^B) H_k.
\]

The quantity

\[
\sum_{k} p_k H_k - TI_{B}(p)
\]

is the free energy of the probability distribution \(p\) at temperature \(T\). The above result extends the standard result that non-equilibrium free energy is a convex function which reaches its minimum when \(p\) equals the equilibrium distribution (in casu \(p^B\)). This is called the variational principle (see [11]). The distance to the minimum, up to a factor \(T\), is the relative entropy. The other definitions of relative entropy do not have such a property.

Let us now compare the different definitions in case the deformed logarithms are given by [11]. One finds

\[
I_A(p||r) = - \sum_{k} p_k \ln_q(r_k/p_k)
\]

\[
= \frac{1}{q-1} \sum_{k} p_k^q \left( r_k^{1-q} - p_k^{1-q} \right),
\]

\[
I_{B1}(p||r) = \sum_{k} \int_{r_k}^{p_k} \, dx \, \ln_q^*(x/r_k)
\]

\[
= \frac{1}{q-1} \sum_{k} p_k^q \left( r_k^{1-q} - p_k^{1-q} \right),
\]

\[
I_{B2}(p||r) = \sum_{k} \int_{r_k}^{p_k} \, dx \, \left( \ln_q^*(x) - \ln_q^*(r_k) \right)
\]

\[
= \frac{1}{q-1} \sum_{k} \left( p_k^q - r_k^q - q r_k^{q-1} (p_k - r_k) \right).
\]

(16)

The first two expressions coincide, but clearly differ from the last one.

The formulas for relative entropy in case of continuous distributions are straightforward generalizations of the expressions (15). Quantization of relative entropy is not straightforward because two density matrices \(\rho\) and \(\sigma\) are involved. When these do not commute, then the order of operators is relevant. For \(I_A(p||r)\) and \(I_{B1}(p||r)\) there is no obvious quantum equivalent, while for \(I_{B2}(p||r)\) a possible quantum expression is

\[
I_{B2}(\rho||\sigma) = \int_{0}^{1} \, dx \, \text{Tr} \left[ \rho \ln_\kappa(x\rho) - \sigma \ln_\kappa(x\sigma) - (\rho - \sigma) \ln_\kappa(\sigma) \right].
\]

(17)
In the specific case that the deformed logarithms are of the form \( q = 1 \) then it is clear how to write quantum generalizations of all three definitions of relative entropy. From (16) follows

\[
I_A(\rho||\sigma) = I_B^1(\rho||\sigma) = \frac{1}{q-1} \left( \text{Tr} \rho^q \sigma^{1-q} - 1 \right) = \frac{1}{1-q} \text{Tr} \rho^q \left( \rho^{1-q} - \sigma^{1-q} \right),
\]

\[
I_B^2(\rho||\sigma) = \frac{1}{q-1} \text{Tr} \left[ \rho^q - \sigma^q - q \sigma^{q-1}(\rho - \sigma) \right].
\]

The former expression has been used in [12]. The latter expression is useful to prove a variational principle for the quantum case.

4 Discussion

The present paper studies generalized thermostatistics from the point of view that the exponential and logarithmic functions appearing in the Gibbs formalism are replaced by functions with similar properties. The obvious conclusion is that there is quite some freedom in choosing generalizations. Of course, there exist other points of view than the one presented here. In particular, this paper avoids the question of extensivity of macroscopic quantities like internal energy and entropy. The Gibbs formalism behaves nicely under decomposition of large systems into nearly independent subsystems. In non-extensive thermostatistics a more complex behavior is expected. The choices presented in this paper have not been evaluated from this point of view.

It is also necessary to reanalyze existing applications of Tsallis’ thermostatistics with the intention to test the different generalizations discussed in this paper. Apparently, such tests of the basic assumptions of generalized thermostatistics have been far from complete.

References

[1] C. Tsallis, *Possible Generalization of Boltzmann-Gibbs Statistics*, J. Stat. Phys. **52**, 479-487 (1988).

[2] E.M.F. Curado, C. Tsallis, *Generalized statistical mechanics: connection with thermodynamics*, J. Phys. A **24**, L69-72 (1991).

[3] C. Tsallis, R.S. Mendes, A.R. Plastino, *The role of constraints within generalized nonextensive statistics*, Physica A **261**, 543-554 (1998).

[4] S. Abe, A. Martinez, F. Pennini, A. Plastino, *Nonextensive thermodynamics relations*, Phys. Lett. A **281**(2-3), 126-130 (2001).

[5] J. Naudts, *Deformed exponentials and logarithms in generalized thermostatistics*, [arXiv:cond-mat/0203489](http://arxiv.org/abs/cond-mat/0203489), Physica A **316**, 1-12 (2002).

[6] J. Naudts, *Generalized thermostatistics and mean field theory*, [arXiv:cond-mat/0311444v3](http://arxiv.org/abs/cond-mat/0311444v3).
[7] C. Tsallis, *What are the numbers that experiments provide?* Quimica Nova 17, 468 (1994)

[8] G. Kaniadakis, *Nonlinear kinetics underlying generalized statistics,* Physica A296, 405-425 (2001).

[9] G. Kaniadakis, *Statistical mechanics in the context of special relativity,* Phys. Rev. E66, 056125 (2002).

[10] C. Tsallis, *Nonextensive statistics: theoretical, experimental and computational evidences and connections,* Braz. J. Phys. 29, 1-45 (1999).

[11] J. Naudts, *Continuity of $\kappa$-deformed entropies and relative entropies,* arXiv:math-ph/0208038v2.

[12] S. Abe, *Nonadditive generalization of the quantum Kullback-Leibler divergence for measuring the degree of purification,* quant-ph/0301136