Qualms concerning Tsallis’ Use of the Maximum Entropy Formalism

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Abstract

Tsallis’ ‘statistical thermodynamic’ formulation of the nonadditive entropy of degree-\(\alpha\) is neither correct nor self-consistent.

It is well known that the maximum entropy formalism \(\[1\]\), the minimum discrimination information \(\[2\]\), and Gauss’ principle \(\[3, 4\]\) all lead to the same results when a certain condition on the prior probability distribution is imposed \(\[5\]\). All these methods lead to the same form of the posterior probability distribution; namely, the exponential family of distributions.

Tsallis and collaborators \(\[6\]\) have tried to adapt the maximum entropy formalism that uses the Shannon entropy to one that uses a nonadditive entropy of degree-\(\alpha\). In order to come out with analytic expressions for the probabilities that maximize the nonadditive entropy they found it necessary to use ‘escort probabilities’ \(\[7\]\) of the same power as the nonadditive entropy.

If the procedure they use is correct then it follows that Gauss’ principle should give the same optimum probabilities. Yet, we will find that the Tsallis result requires that the prior probability distribution be given by the same unphysical condition as the maximum entropy formalism and, what is worse, the potential of the error law be required to vanish. The potential of the error law is what information theory refers to as the error \(\[8\]\); that is, the difference between the inaccuracy and the entropy. Unless the ‘true’ probability distribution, \(P = (p(x_1), p(x_2), \ldots, p(x_m))\) coincides with the estimated probability distribution, \(Q = (q(x_1), q(x_2), \ldots, q(x_m))\), the error does not vanish. Moreover, we shall show that two procedures of averaging, one using the escort probabilities explicitly, do not give the same result, and the relation between the potential of the error law and the nonadditive entropy requires the latter to vanish when the former vanishes.

Let \(X\) be a random variable whose values \(x_1, x_2, \ldots, x_m\) are obtained at \(m\) independent trials. Prior to the observations the distribution is \(Q\), and after the observations the unknown probability distribution is \(P\). The observer has
at his disposal the statistic
\[ \hat{a} = \frac{1}{m} \sum_{i=1}^{m} x_i \]
to help him formulate a guess as to the form of \( Q \). Gauss’ principle assumes that the probability distribution \( P \) depends on a parameter \( a \)
\[ a = E(X) = \sum_{i=1}^{m} x_i p(x_i), \quad (1) \]
such that the arithmetic mean, \( \hat{a} \), is the maximum likelihood estimate of \( a \). Furthermore, \( P \) will depend upon the parameter \( a \) in such a way that there is a value \( a^0 \) for which \( p(x_i; a^0) = q(x_i) \), the prior distribution.

The maximum likelihood estimate,
\[ \frac{\partial}{\partial a} \log L(a) = 0, \]
will lead to the exponential family of distributions when the log-likelihood function
\[ \log L(a) = \sum_{i=1}^{m} \log p(x_i; a). \]
The likelihood equation
\[ \frac{\partial}{\partial a} \psi(x_i; a) = 0, \]
where \( \psi(x_i; a) = \log p(x_i; a) \), is the same as requiring
\[ \sum_{i=1}^{m} (x_i - a) = 0, \]
and any deviations in one will immediately lead to deviations in the other. Hence, they must be proportional to one another. Choosing the coefficient of proportionality, as the second derivative of some appropriate scalar function, \( V \), gives
\[ \frac{\partial}{\partial a} \psi(x_i; a) = V''(a)(x_i - a), \quad (2) \]
where the prime stands for differentiation with respect to the argument. The scalar potential, \( V(a) \), must be independent of the \( x_i \) because the left-hand side is only a function of \( x_i \) and a similar equation for \( x_j \) would lead to a contradiction. We assume that the potential is such that \( V(a^0) = 0 \). Consequently, (2) can be rewritten as
\[ \frac{\partial}{\partial a} \psi(x_i; a) = \frac{\partial}{\partial a} \{V'(a)(x_i - a) + V(a)\}. \]

Integrating from \( a_0 \) to \( a \) gives
\[ \psi(x_i; a) = \psi(x_i; a^0) + \lambda(a)(x_i - a) + V(a), \]
where $\lambda(a) = V'(a)$. In the usual case that the log-likelihood function is logarithmic, we get an exponential family of distributions

$$\log p(x_i; a) = \log q(x_i) + \lambda(a)(x_i - a) + V(a)$$

(3)

Averaging both sides with respect to the probability distribution $P$ gives

$$\sum_{i=1}^{m} \{ p(x_i; a) \log p(x_i; a) - p(x_i; a) \log q(x_i) \} = V(a)$$

In information theory, the first term is the negative of the Shannon entropy, the second term is the inaccuracy, and the right hand side is the error [8]. On the strength of Shannon’s inequality,

$$\sum_{i=1}^{m} p(x_i; a) \log \left( \frac{p(x_i; a)}{q(x_i)} \right) = V(a) \geq 0$$

(4)

the inaccuracy cannot be smaller than the Shannon entropy. Shannon’s inequality follows very simply from the arithmetic-geometric mean inequality,

$$\prod_{i=1}^{m} x_i^{p(x_i; a)} \leq \sum_{i=1}^{m} x_i p(x_i; a)$$

with $x_i = q(x_i)/p(x_i; a)$.

When $Q$ is the uniform distribution, i.e., $q(x_i) = 1/m \forall i$, Shannon’s inequality, (4), becomes

$$S_0(1/m) - S_1(P) = V(a)$$

which we have referred to as the entropy reduction caused by the application of a constraint that produces a finite value of $a$ [9]. $S_0(1/m) = \log m$ is the maximum entropy, and it is known as the Hartley entropy in information theory. Classically, the entropy is defined to within a constant; only entropy differences are measurable.

However, all that we have said so far does not apply to equilibrium thermodynamics [4]. If we average [4] with respect to the $Q$ distribution, instead of the $P$ distribution, and use Shannon’s inequality, $\sum_{i=1}^{m} q(x_i) \log [q(x_i)/p(x_i; a)] \geq 0$, we immediately run into a problem because $V(a)$ must now be necessarily negative. In statistical mechanics, $q(x_i)$ represents the surface of constant energy of a hypersphere of high dimensionality [10]. Because of its high dimensionality, the volume of the hypersphere lies very close to its surface so that $q(x_i)$ can be thought of as the volume of phase space occupied by the system. Averages are performed with respect to this non-normalizable prior probability distribution [10]. In order to keep the error $V(a)$, which will soon be identified as the thermodynamic entropy, positive, it is necessary to introduce a sign change in (3).

This sign change can be rationalized in the following way. The exponential factor, $e^{\lambda(a)x_i}$, will not overpower the rapidly increasing factor of the density of
states, \( q(x_i) \). However, the density of states cannot increase faster than a certain power of the radius, \( x_i \), of the phase space volume, which is proportional to \( x_i^m \) in a hypersphere of \( m \)-dimensions. What is needed is an even more rapidly decreasing exponential factor \( \exp(-\lambda x_i) \).

According to the Boltzmann-Planck interpretation, \( q(x_i) \) is not a normalized probability, but, rather, a ‘thermodynamic’ probability, being proportional to the volume of phase space occupied by the system. The (random) entropy \( S(x_i) \) is defined as the logarithm of the thermodynamic probability

\[
S(x_i) = \log q(x_i)
\]

The phase average is given by

\[
E[X] = \frac{\sum_{i=1}^{m} x_i q(x_i)}{\sum_{i=1}^{m} q(x_i)}.
\]

The thermodynamic entropy is the phase space average of \( \log [q(x_i)/p(x_i; a)] \) \( \text{viz.} \)

\[
S(a) = \frac{\sum_{i=1}^{m} q(x_i) \log[q(x_i)/p(x_i; a)]}{\sum_{i=1}^{m} q(x_i)}
\]

and its Legendre transform

\[
S(a) - \lambda(a) a = \log Z(\lambda),
\]

defines the logarithm of the generating function, \( Z(\lambda) \). The inaccuracy now appears as the difference between the thermodynamic entropy and the average of the random entropies

\[
- \sum_{i=1}^{m} q(x_i) \log p(x; a) = S(a) - \frac{\sum_{i=1}^{m} q(x_i) S(x_i)}{\sum_{i=1}^{m} q(x_i)} \geq 0. \quad (5)
\]

The inequality follows from the facts that \( S \) increases in the wide sense and is concave. The expectation \( a \) can be taken either with respect to \( P \) or \( Q \). The two averages must necessarily coincide for otherwise there would not be a single general thermodynamics, but rather a “microcanonical thermodynamics” and a separate “canonical thermodynamics” \( \text{[11]} \). Taken with respect to \( Q \), \( \text{[5]} \) is Jensen’s inequality for a concave function, where the \( Q \) has positive components but are otherwise arbitrary. Taken with respect to the normalized \( P \), \( \text{[6]} \) is the Jensen-Petrović inequality \( \text{[12]} \), where \( \sum_{i=1}^{m} p_i(x_j) \geq x_j \) for each \( j = 1, \ldots, m \). The average of \( m \) variables is likely to be considerably greater than any of its components. Then, if \( S \) is increasing,

\[
S \left( \sum_{i=1}^{m} x_i p(x_i) \right) \geq S(x_j)
\]

for \( j = 1, \ldots, m \). Multiplying by \( q(x_j) \) and summing gives back \( \text{[5]} \). This does not mean that \( S(x_i)/x_i \) should not decrease: A sufficient condition for \( S(\sum_{i=1}^{m} x_i) \leq \sum_{i=1}^{m} S(x_i) \) is that \( S(x_i)/x_i \) should decrease.
That $S(x_i)$ is an increasing function and $S(x_i)/x_i$ decreases, i.e., it is anti-star shaped, are the criteria for inequality attenuation [13]. Fluctuations give rise to inaccuracy [6], and, in their absence a function of the average is equal to an average of the function.

Therefore, if the exponential probability distribution, (3), is to coincide with Gauss’ error law, written in terms of the concavity of the entropy, 

$$\log p(x; a) = S(x_i) - S'(a)(x_i - a) - S(a) = \frac{1}{2}S''(\tilde{a})(x_i - a)^2$$

(6)

where $\tilde{a}$ lies between $x_i$ and $a$, then sign changes are needed. When this is done (3) becomes

$$\log p(x; a) = \log q(x_i) - \lambda(a)(x_i - a) - V(a).$$

(7)

A comparison of (6) and (7) shows that the entropy, $S(a)$, is the potential, $V(a)$, that determines the error law [4]. The concavity of the entropy ensures that the exponent will be negative and hence $p(x; a)$ will be less than unity. The parameter, $\lambda(a)$, is still the derivative of the scalar potential, $V(a)$, but since this potential now coincides with the thermodynamic entropy, $S(a)$, the Lagrange multiplier $\lambda(a)$ is now identified as the internal variable in the entropy representation.

Information theoretic entropies, and the entropy reduction of the thermodynamics of extremes [9], are not amenable to the previous thermodynamic interpretation, where the entropy is defined as the logarithm of the volume of phase space occupied by the system. Since all the volume lies very near of the surface in a thermodynamic system of high dimensionality, the volume of phase space will coincide with the surface area, which is referred to as the structure function [10].

Rather, we consider the $P$ and $Q$ as two sets of complete probability distributions. For a given probability distribution, $Q$, we seek the set of probability $P$ which most closely resemble $Q$. This is the minimum discrimination statistic of Kullback [2].

In order to derive the nonadditive entropies of degree-$\alpha$, the logarithm is replaced by the well-known elementary limit

$$\log p(x; a) \rightarrow \frac{p^{\alpha-1}(x; a) - 1}{\alpha - 1} = \psi(x_i; a),$$

and a similar relation for $\log q(x_i)$ in the exponential law we get

$$\frac{p^{\alpha-1}(x; a) - q^{\alpha-1}(x_i)}{\alpha - 1} = \lambda(a)(x_i - a) + V(a).$$

(8)

\footnote{In what turned out to be a futile attempt to justify Tsallis’ formalism, Plastino and Plastino [14] considered a structure function for the energy of the form $E_i^{m-1}$. Assuming a bounded phase space—for no given reason—whose total energy is $E_0$, they identified the Tsallis exponent as $\alpha = (m-2)/(m-1)$, and, at the same time, defined the inverse temperature as $\beta = (m-1)/E_0$. What they failed to realize is that in order to define a temperature $m$ must be much greater than 1 so that $\alpha \equiv 1$. More precisely $m$ must be large enough to validate the use of Stirling’s formula [4]. If the conditions under which they claim Tsallis’ statistical mechanics applies, then it cannot be applied to thermodynamic systems for such systems would be far to small to be capable of defining intensive quantities like temperature and pressure.}
Multiplying (8) by $p(x_i; a)$, and summing give

$$I_\alpha(Q) - S_\alpha(P) = \frac{\sum_{i=1}^{m} p(x_i; a) \left( p^{\alpha-1}(x_i; a) - q^{\alpha-1}(x_i) \right)}{\alpha - 1} = V(a) \geq 0$$

where

$$I_\alpha(Q) := \frac{1 - \sum_{i=1}^{m} p(x_i; a)q^{\alpha-1}(x_i)}{\alpha - 1}$$

has been referred to as the inaccuracy [22], and

$$S_\alpha(P) = \frac{1 - \sum_{i=1}^{m} p^\alpha(x_i)}{\alpha - 1}$$

(9)

has been referred to as the Tsallis entropy [16] in the physical literature, but has been well known in information theory since the late 1960’s [17, 18, 19, 20, 21, 22, 23]. We will henceforth suppress the dependence of the probability distribution $P$ on the average $a$, because Tsallis’ statistical thermodynamics make no pretext at statistical inference. The inaccuracy is a convex function of $Q$, for a given $P$, provided $\alpha \leq 2$. The inaccuracy is defined as the sum of the entropy of degree-$\alpha$, (9), and the error, $V(a)$. The inaccuracy has the property that

$$\lim_{q \to 1} I_\alpha(Q) = S_\alpha(1/m).$$

The negative of the error is what we have called the entropy reduction, $\Delta S$ [9].

Now the inequality in (8) follows from H¨older’s inequality. Consider the case when all the $P$ are rational; then they can be expressed in the form $p(x_i) = x_i / \sum_{i=1}^{m} x_i$, and $Q$ is the uniform distribution, $q(x_i) = 1/m \forall i$. Expression (8) then becomes

$$\left( \frac{\sum_{i=1}^{m} x_i^\alpha}{\left( \sum_{i=1}^{m} x_i \right)^\alpha} - m^{1-\alpha} \right) = V(a)$$

because of H¨older’s inequalities [24]

$$m^{-1}\sum_{i=1}^{m} x_i > \left( \sum_{i=1}^{m} x_i^\alpha \right)^{1/\alpha} m^{-1/\alpha} \quad \text{for} \quad \alpha > 1.$$

Now, Tsallis and collaborators [6] find that the maximization procedure of the nonadditive entropy [9] with respect to the constraint

$$a_\alpha = E_\alpha(X) = \frac{\sum_{i=1}^{m} x_i p^\alpha(x_i)}{\sum_{i=1}^{m} p^\alpha(x_i)}$$

(10)

using the escort probabilities [7], yields the stationary condition [6]

$$p(x_i) = \frac{[1 - (1 - \alpha) \lambda_\alpha (x_i - a_\alpha)]^{1/(1-\alpha)}}{Z_\alpha(\lambda_\alpha)}$$

(11)
where
\[ \lambda_\alpha = \lambda \sum_{i=1}^{m} p^\alpha(x_i) \] (12)
and \( \lambda \) is the Lagrange multiplier for a constraint \( \text{(10)} \). The normalization condition of the \( p(x_i) \) gives the partition function as
\[ Z_\alpha(\lambda_\alpha) = \sum_{i=1}^{m} [1 - (1 - \alpha)\lambda_\alpha(x_i - a_\alpha)]^{1/(1-\alpha)}. \] (13)

At best, (11) can be considered as an implicit relation for the probabilities since (12) contains the probabilities explicitly through (12).

In order to reduce Gauss’ principle (8) to something that even vaguely looks like the ‘optimal’ probabilities (11) that maximize the Tsallis entropy \( \text{(9)} \), it is necessary to:

1. assume that \( P \) is an incomplete distribution,
2. set \( q(x_i) = 1 \) \( \forall i \), and
3. set \( V(a) = 0 \).

We then obtain
\[ \frac{p(x_i)}{\sum_{i=1}^{m} p(x_i)} = \frac{[1 + (\alpha - 1)\lambda_\alpha(x_i - a_\alpha)]^{1/(\alpha-1)}}{Z_\alpha(\lambda_\alpha)}, \]
where the partition function is given by (13), and we used the escort probabilities \( \text{(10)} \) to define the parameter \( a \), rather than the weighted average \( \text{(11)} \).

Rather, if we take (7), and introduce the approximation
\[ \frac{p^{1-\alpha}(x_i) - 1}{1 - \alpha} \rightarrow \log p(x_i), \]
and a similar expression for \( q(x_i) \) we get
\[ \frac{p^{1-\alpha}(x_i) - q^{1-\alpha}(x_i)}{1 - \alpha} = -\lambda_\alpha(x_i - a_\alpha) - V(a_\alpha). \] (14)

Setting \( q(x_i) = 1 \) and \( V(a_\alpha) = 0 \), and requiring the probability distribution \( P \) to be normalized result in (11), or, equivalently,
\[ p^{1-\alpha}(x_i) = \frac{1 - (1 - \alpha)\lambda_\alpha(x_i - a_\alpha)}{Z_\alpha^{1-\alpha}(\lambda_\alpha)}. \]

Multiplying both sides by \( p^\alpha(x_i) \) and summing give \( Z_\alpha^{1-\alpha}(\lambda_\alpha) = \sum_{i=1}^{m} p^\alpha(x_i) \).
provided $\lambda_\alpha$ is given by the escort average, [10]. Rather, if raise both sides of [10] to the power $\alpha$, sum, and rearrange, we get

$$Z_\alpha(\lambda_\alpha) = \sum_{i=1}^{m} p^\alpha(x_i) = \sum_{i=1}^{m} [1 - (1 - \alpha) \lambda_\alpha (x_i - a_\alpha)]^{\alpha/(1-\alpha)} \neq Z_\alpha(\lambda_\alpha).$$

The only difference between the two forms of averaging is that in the first case use has been made of the escort probability average, [10]. Since the two results do not coincide, we conclude that there is something amiss with the escort probability average, [10].

Moreover, if we take the $\alpha \to 1$ limit in (14) we obtain

$$Z_1(\lambda_1) = \sum_{i=1}^{m} e^{-\lambda_1(x_i - a)},$$

which is not the correct expression for the partition function even in the unphysical case of a density of states equal to unity.

Finally, multiplying both sides of (14) by $p^\alpha(x_i)$, and summing, result in

$$1 - \sum_{i=1}^{m} q(x_i) [p(x_i)/q(x_i)]^\alpha = -\sum_{i=1}^{m} p^\alpha(x_i) V(a_\alpha).$$

If we now set $q(x_i) \equiv 1 \forall i$, we come out with

$$S_\alpha(P) = \sum_{i=1}^{m} p^\alpha(x_i) V(a_\alpha). \quad (15)$$

This shows the correspondence between Shannon entropy and the potential $V(a)$ in the $\alpha \to 1$ limit, that was alluded to above in the thermodynamic formulation which takes into account a non-normalized prior probability distribution. However, we have set the prior probability distribution equal to unity, as in the maximum entropy method, and, furthermore, in order to derive the probability distribution [11] from Gauss’ law we had to assume that $V$ is identically zero. Relation (15) would, consequently, require the vanishing of the nonadditive entropy, (9).

Based on the foregoing results, we can only conclude that Tsallis’ ‘statistical thermodynamic’ formulation of the nonadditive entropy of degree-\alpha is neither correct nor self-consistent.

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