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MaxEnt, second variation, and generalized statistics

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HIGHLIGHTS

- We revisit the idea of second variation of the entropic functional.
- We apply it to q-statistics.
- We show that only for heavy-tail distributions the existence of a maximum of the entropy is guaranteed.

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ABSTRACT

There are two kinds of Tsallis-probability distributions: heavy tail ones and compact support distributions. We show here, by appeal to functional analysis' tools, that for lower bound Hamiltonians, the second variation's analysis of the entropic functional guarantees that the heavy tail q-distribution constitutes a maximum of Tsallis' entropy. On the other hand, in the compact support instance, a case by case analysis is necessary in order to tackle the issue.

1. Introduction

During more than 25 years, an important topic in statistical mechanics theory revolved around the notion of generalized q-statistics, pioneered by Tsallis [1]. It has been amply demonstrated that, in many occasions, the celebrated Boltzmann–Gibbs logarithmic entropy does not yield a correct description of the system under scrutiny [2]. Other entropic forms, called q-entropies, produce a much better performance [2]. One may cite a large number of such instances. For example, non-ergodic systems exhibiting a complex dynamics [2].

The non-extensive statistical mechanics of Tsallis has been employed to fruitfully discuss phenomena in variegated fields. One may mention, for instance, high-energy physics [3,4], spin-glasses [5], cold atoms in optical lattices [6], trapped ions [7], anomalous diffusion [8,9], dusty plasmas [10], low-dimensional dissipative and conservative maps in dynamical systems [11–13], turbulent flows [14], Levy flights [15], the QCD-based Nambu, Jona, Lasinio model of a many-body field theory [16], etc. Notions related to q-statistical mechanics have been found useful not only in physics but also in chemistry, biology, mathematics, economics, and informatics [17–19].

In this work we revisit the subject by appeal, in a classical MaxEnt phase–space framework, to the second variation of functionals. We find that such analysis guarantees a maximum of the Tsallis entropy only in the case of the heavy tail distributions. Our present treatment makes it advisable, on a more general MaxEnt framework, to always look at the second functional variation. We begin our discussion by remembering the concept of second variation.

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2. Second variation of a functional

The essential concept that we need here is that of *increment h of a functional*. Note that the general theory of Variational Calculus has been developed in a Banach Space (BS) [20]. Particularly important BS instantiations are, of course, Hilbert's space and classical phase–space.

The MaxEnt approach in Banach space requires a first variation that should vanish and a second one that ascertains the nature of the pertinent extremum. This second variation is not usually encountered in MaxEnt practice, since one believes that the entropy possesses a global maximum. This second functional variation is the protagonist of the present endeavor. The approach is described in detail, for instance in the canonical book by Shilov [20] (for local minima). It is simply explained.

One needs to evaluate the increment h of a functional F at the point y of the Banach space one is dealing with. One has

$$F(y+h) - F(y) = \delta^1 F(y,h) + \frac{1}{2}\delta^2 F(y,h^2) + \varepsilon(h) \tag{2.1}$$

where

$$\lim_{h\to 0} \frac{\|\varepsilon(h)\|}{\|h\|^2} = 0. \tag{2.2}$$

By definition, $\delta^1 F(y,h)$ is the first variation of F (if it is linear in h). $\delta^2 F(y,h)$ is F's second variation, quadratic in h. If y is an extremum of F then

$$\delta^1 F(y,h) = 0 \tag{2.3}$$

and it is a local minimum if

$$\delta^2 F(y,h) \geq C\|h\|^2 \quad C > 0, \tag{2.4}$$

or a local maximum if

$$\delta^2 F(y,h) \leq C\|h\|^2 \quad C < 0 \tag{2.5}$$

where C is a constant and $\|h\|$ stands for the norm of h. Accordingly, if the functional F has an extremum at the element y (of the Banach space) then Eq. (2.3) is fulfilled, and if there exists such a constant $C > 0$ (respectively: <0) that Eq. (2.4) (respectively: Eq. (2.5)) is true, then the functional F attains at y a minimum (respectively: a maximum).

In phase–space, the object of our present concerns,

$$\|h\|^2 = \int_M h^2 \, \mathrm{d}\mu \tag{2.6}$$

where M is the region of phase–space one is interested in and μ the associated measure-volume for the concomitant space. We start our consideration with reference to the orthodox instance.

3. Motivation

The following considerations should motivate the reader to seriously consider the importance of elementary notions of functional analysis in q-statistics.

3.1. q-Exponentials as linear functionals or distributions

A generalized function (or *distribution*) is a *continuous functional* defined on a space of test-functions [21]. A typical such test space is the so-called $\mathcal{K}$ space of Schwartz, of infinitely differentiable functions with compact support.

One can prove [21] that x_+^α, defined by

$$\begin{aligned} x_+^\alpha &= x^\alpha, \quad \text{for } x > 0, \\ x_+^\alpha &= 0, \quad \text{for } x \leq 0 \end{aligned} \tag{3.1}$$

is a distribution possessing single poles at integers $\alpha = -k$ with residues (at the pole)

$$R = \frac{(-1)^k}{(k-1)!}\delta^{(k-1)}(x), \tag{3.2}$$

with $k = 1, 2, \ldots, n, \ldots$ [21].

A function is a particular instance of a distribution, called *regular* distribution. A singular distribution is that which cannot represented as a function. For example, Dirac's delta is such a singular distribution. Tsallis' q-exponentials e_q, defined as

$$e_q(x) = [1 + (q-1)x]_+^{\frac{1}{1-q}}, \tag{3.3}$$

become clearly a distribution defined via

$$e_q(x) = [1 + (q-1)x]_+^{\frac{1}{1-q}} = [1 + (q-1)x]^{\frac{1}{1-q}} \quad \text{if } 1 + (q-1)x > 0$$
$$e_q(x) = 0 \quad \text{otherwise}. \tag{3.4}$$

Computations involving e_q should fruitfully appeal to distribution theory.

3.2. An instructive example for second variations [20]

Generally, the minimal condition

$$\delta^2 F(y, h) \geq C\|h\|^2, \tag{3.5}$$

with $C > 0$ cannot be naively replaced by the weaker restriction

$$\delta^2 F(y, h) \geq 0. \tag{3.6}$$

Consider, for instance, minimizing the functional

$$F(y) = \int_0^1 y^2(x)[x - y(x)] \, dx. \tag{3.7}$$

It is easily seen that

$$y(x) \equiv 0, \tag{3.8}$$

gives a functional extremum for $F(y)$, that is, for y given by (3.8) one has

$$\delta^1 F(y, h) = 0. \tag{3.9}$$

The second variation

$$\delta^2 F(y, h) = \int_0^1 x h^2(x) \, dx, \tag{3.10}$$

is >0 for any function $h(x) \neq 0$. Thus, one may naively assume that (3.8) yields a minimum for $F(y)$.

To disprove such an assertion it is enough, given $\epsilon > 0$, to consider as $y(x)$ any non-negative function that is positive at $x = 0$, does not exceed $\epsilon - x$ for $x < \epsilon$, and vanishes for $x \geq \epsilon$. For example, let $y(x) = \epsilon - x$ for $x < \epsilon$ and $y(x) = 0$ for $x \geq 0$. Then,

$$F(y) = \int_0^\epsilon (\epsilon - x)^2 (2x - \epsilon) \, dx = -\frac{\epsilon^4}{6}! \tag{3.11}$$

For a $y(x) \equiv 0$, $F = 0$, but the functional does not possess a minimum there.

Similar considerations regarding local maxima apply if one considers the restriction

$$\delta^2 F(y, h) \leq C\|h\|^2, \tag{3.12}$$

with $C < 0$, that cannot be replaced by the weaker condition

$$\delta^2 F(y, h) \leq 0. \tag{3.13}$$

Choose, for instance, the functional

$$F(y) = \int_0^1 y^2(x)[y(x) - x] \, dx, \tag{3.14}$$

and repeat the above analysis.

4. Applying second variation

4.1. Boltzmann–Gibbs' statistics

In the general case the prior information consists of N mean values corresponding to the observables $\langle R_i \rangle$, $i = 1, \ldots, N$: However, the points we are about to make here emerge already at the simplest level of just one observable, the Hamiltonian H (canonical ensemble). We limit ourselves to this instance in this work. Additionally, we assume that H is lower bounded. The MaxEnt variational functional becomes

$$F_S(P) = -\int_M P \ln(P) \, d\mu + \alpha \left(\int_M PH \, d\mu - \langle U \rangle \right) + \gamma \left(\int_M P \, d\mu - 1 \right), \tag{4.1}$$

with P the probability density MaxEnt is designed to encounter. H is the Hamiltonian whose mean value is called $\langle U\rangle$. Finally, α and γ will represent Lagrange multipliers. We consider now F_S's increment.

$$F_S(P+h)-F_S(P) = -\int_M (P+h)\ln(P+h)\,\mathrm{d}\mu + \alpha\left[\int_M (P+h)H\,\mathrm{d}\mu - \langle U\rangle\right] + \gamma\left(\int_M (P+h)\,\mathrm{d}\mu - 1\right) + \int_M P\ln(P)\,\mathrm{d}\mu - \alpha\left(\int_M PH\,\mathrm{d}\mu - \langle U\rangle\right) - \gamma\left(\int_M P\,\mathrm{d}\mu - 1\right). \tag{4.2}$$

We can also write

$$F_S(P+h)-F_S(P) = \int_M \left[(-1-\ln(P)+\alpha H+\gamma)\,h - \frac{h^2}{2P}\right]\mathrm{d}\mu + O(h^3). \tag{4.3}$$

From (4.3) we find the first variation with its associated Euler–Lagrange equation plus the second variation as well. One has

$$-1-\ln(P)+\alpha H+\gamma = 0 \tag{4.4}$$

$$-\int_M \frac{h^2}{P}\,\mathrm{d}\mu \le C\|h\|^2. \tag{4.5}$$

From (4.4) one gathers that

$$P = \frac{\mathrm{e}^{-\beta H}}{Z}$$
$$Z = \int_M \mathrm{e}^{-\beta H}\,\mathrm{d}\mu, \tag{4.6}$$

with Z the system's partition function and β proportional to the inverse temperature. Eq. (4.5) yields

$$-\int_M \frac{h^2}{P}\,\mathrm{d}\mu = -Z\int_M h^2\mathrm{e}^{\beta H}\,\mathrm{d}\mu \le -Z\int_M h^2\,\mathrm{d}\mu = -Z\|h\|^2. \tag{4.7}$$

Notice that we can pass from the second to the third integral because $\mathrm{e}^{\beta H}$ is always greater than unity. *This is a trivial point here, but not so when we consider Tsallis' statistics below*. Looking at (4.7) we see that one can choose $C=-Z$. Remark that these are *classical* considerations. Problems with (4.6) at $T=0$ are thus not surprising, on account of Thermodynamics' third law. As a bonus, we discover here that the bound-constant C is the partition function itself.

4.2. Tsallis' statistics

Here there is no single way of computing mean values for the theory [2]. Several options are available, that are today considered equivalent for all practical purposes [2,22], because there is a "dictionary" that univocally relates two given probability densities $P_1 - P_2$, obtained using two different mean-values' choices [22]. We consider in this work the three more important such choices and restrict ourselves to quadratic Hamiltonians. We insist in stating that the q-exponential is defined as ($x=\beta H\ge 0$)

$$\begin{aligned} e_q(-x) &= [1-(1-q)x]^{1/(1-q)}, \quad \text{if } (1-q)x\le 1; \\ &= 0 \quad \text{otherwise (Tsallis' cutoff)}, \end{aligned} \tag{4.8}$$

that tends to the ordinary exponential as $q\to 1$. One speaks of long tailed distributions for $[1-(1-q)x]\ge 0$ for all $x>0$ and compact-support ones whenever the Tsallis cutoff becomes operative for some x-values.

4.3. Orthodox linear choice

One evaluates mean values in the customary fashion, linear in P, i.e., $\langle R\rangle = \int_M RP\,\mathrm{d}\mu$. The concomitant Tsallis functional is

$$F_S(P) = -\int_M P^q\ln_q(P)\,\mathrm{d}\mu + \alpha\left(\int_M PH\,\mathrm{d}\mu - \langle U\rangle\right) + \gamma\left(\int_M P\,\mathrm{d}\mu - 1\right). \tag{4.9}$$

For the increment we have

$$F_S(P+h)-F_S(P) = -\int_M (P+h)^q\ln_q(P+h)\,\mathrm{d}\mu + \alpha\left[\int_M (P+h)H\,\mathrm{d}\mu - \langle U\rangle\right] + \gamma\left[\int_M (P+h)\,\mathrm{d}\mu - 1\right] + \int_M P^q\ln_q(P)\,\mathrm{d}\mu - \alpha\left(\int_M PH\,\mathrm{d}\mu - \langle U\rangle\right) - \gamma\left(\int_M P\,\mathrm{d}\mu - 1\right). \tag{4.10}$$

Eq. (4.10) can be recast as (see Appendix B)

$$F_S(P+h)-F_S(P)=\int_M\left[\left(\frac{q}{1-q}\right)P^{q-1}+\alpha H+\gamma\right]h\,\mathrm{d}\mu-\int_M qP^{q-2}\frac{h^2}{2}\,\mathrm{d}\mu+O(h^3). \tag{4.11}$$

Eq. (4.11) leads to the following equations:

$$\left(\frac{q}{1-q}\right)P^{q-1}+\alpha H+\gamma=0, \tag{4.12}$$

$$-\int_M qP^{q-2}h^2\,\mathrm{d}\mu\le C\|h\|^2. \tag{4.13}$$

Eq. (4.12) is the Euler–Lagrange one while (4.13) gives bounds originating from the second variation. Thus, (4.12) entails (using the procedure given in Ref. [23])

$$\alpha=\beta qZ^{1-q} \tag{4.14}$$

$$\gamma=\frac{q}{q-1}Z^{1-q} \tag{4.15}$$

$$P=\frac{[1+\beta(1-q)H]^{\frac{1}{q-1}}}{Z}=e_{2-q}(-\beta H)/Z, \tag{4.16}$$

$$Z=\int_M[1+\beta(1-q)H]^{\frac{1}{q-1}}\,\mathrm{d}\mu. \tag{4.17}$$

For Eq. (4.13) we have,

$$W=-\int_M qP^{q-2}h^2\,\mathrm{d}\mu=-\int_M qZ^{2-q}[1+\beta(1-q)H]^{\frac{q-2}{q-1}}h^2\,\mathrm{d}\mu. \tag{4.18}$$

In order to obtain a bound, we need to find a constant C (independent, in particular, of H). Thus, one needs to make sure that the bracket

$$[1+\beta(1-q)H]\ge 0. \tag{4.19}$$

This entails

$$0<q\le 1. \tag{4.20}$$

In such a case, the integral without the bracket is smaller than or equal to the integral with the bracket and we have

$$W\le -qZ^{2-q}\|h^2\|=-C\|h^2\|. \tag{4.21}$$

The present arguments, based on (4.19), *guarantee* an entropic maximum only for long-tail (or heavy-tail) Tsallis distributions. For compact support distributions, the present arguments are inconclusive. The maximum may or may not exist. One should further investigate things on a case-by-case fashion. For instance, if $q>1$, the bracket $[1+\beta(1-q)H]$ might remain positive for low enough β. We will discuss this possibility in a different section below.

4.4. Curado–Tsallis mean values

A second alternative way of obtaining mean values has been advanced in Ref. [24], where the authors define

$$\langle U\rangle=\int_M P^qH\,\mathrm{d}\mu, \tag{4.22}$$

so that the MaxEnt Lagrangian F_S becomes

$$F_S(P)=-\int_M P^q\ln_q(P)\,\mathrm{d}\mu+\alpha\left(\int_M P^qH\,\mathrm{d}\mu-\langle U\rangle\right)+\gamma\left(\int_M P\,\mathrm{d}\mu-1\right), \tag{4.23}$$

and for the functional increment one writes (see Appendix B)

$$\begin{aligned}F_S(P+h)-F_S(P)=&-\int_M(P+h)^q\ln_q(P+h)\,\mathrm{d}\mu+\alpha\left[\int_M(P+h)^qH\,\mathrm{d}\mu-\langle U\rangle\right]\\&+\gamma\left[\int_M(P+h)\,\mathrm{d}\mu-1\right]+\int_M P^q\ln_q(P)\,\mathrm{d}\mu-\alpha\left(\int_M P^qH\,\mathrm{d}\mu-\langle U\rangle\right)\\&-\gamma\left(\int_M P\,\mathrm{d}\mu-1\right).\end{aligned} \tag{4.24}$$

Expansion in order of up to h^2 is now demanded for (A) $(P+h)^q$, (B) $\ln_q(P+h)$, and the product (A) (B). Keeping only terms of order h and h^2, one deduces from (4.24) that the linear term in h yields

$$-\frac{q}{q-1}[1-\alpha(q-1)H]P^{q-1}+\gamma=0, \tag{4.25}$$

while the h^2-term generates

$$-\int_M q[1-\alpha(q-1)H]P^{q-2}h^2\,\mathrm{d}\mu\le C\|h\|^2. \tag{4.26}$$

Using (4.25) produces here (with the procedure of Ref. [23]):

$$\alpha=-\beta \tag{4.27}$$

$$\gamma=-\frac{q}{q-1}Z^{1-q} \tag{4.28}$$

$$P=\frac{[1-\beta(1-q)H]^{\frac{1}{1-q}}}{Z}=e_q(-\beta H)/Z, \tag{4.29}$$

$$Z=\int_M[1-\beta(1-q)H]^{\frac{1}{1-q}}\,\mathrm{d}\mu \tag{4.30}$$

while (4.26) leads to

$$\begin{aligned}W&=-\int_M q[1-\alpha(q-1)H]P^{q-2}h^2\,\mathrm{d}\mu\\&=-\int_M qZ^{2-q}[1+(q-1)\beta H]^{\frac{q-2}{1-q}+1}h^2\\&=-Z^{2-q}q\int_M[1+\beta(q-1)H]^{\frac{1}{q-1}}h^2\,\mathrm{d}\mu.\end{aligned} \tag{4.31}$$

Again, in order to obtain a constant bound we need the bracket in the last line above to be positive. This entails, again, heavy-tail distributions, here implying

$$q\ge 1. \tag{4.32}$$

Thus,

$$C=qZ^{2-q}. \tag{4.33}$$

The obvious demand $q>0$ is satisfied given (4.32). As in the preceding subsection, the present arguments *guarantee* an entropic maximum only for long-tail Tsallis distributions. For compact support ones, these arguments are inconclusive. The maximum may or may not exist. One should further investigate things on a case-by-case fashion. For instance, if $q<1$, the bracket $[1+\beta(q-1)H]$ might remain positive for low enough β. We will discuss this possibility in a future section below.

4.5. Tsallis–Mendes–Plastino (TMP) mean values

Following Ref. [23] we tackle the relationships

$$\langle U\rangle=\frac{\int_M P^qH\,\mathrm{d}\mu}{\int_M P^q\,\mathrm{d}\mu}. \tag{4.34}$$

Our Lagrangian reads now

$$F_S(P)=-\int_M P^q\ln_q(P)\,\mathrm{d}\mu+\alpha\left(\int_M P^qH\,\mathrm{d}\mu-\int_M P^q\,\mathrm{d}\mu\langle U\rangle\right)+\gamma\left(\int_M P\,\mathrm{d}\mu-1\right). \tag{4.35}$$

Thus (see Appendix B),

$$\begin{aligned}F_S(P+h)-F_S(P)&=-\int_M(P+h)^q\ln_q(P+h)\,\mathrm{d}\mu+\alpha\left[\int_M(P+h)^qH\,\mathrm{d}\mu-\int_M(P+h)^q\,\mathrm{d}\mu\langle U\rangle\right]\\&\quad+\gamma\left[\int_M(P+h)\,\mathrm{d}\mu-1\right]+\int_M P^q\ln_q(P)\,\mathrm{d}\mu-\alpha\left(\int_M P^qH\,\mathrm{d}\mu-\int_M P^q\,\mathrm{d}\mu\langle U\rangle\right)\\&\quad-\gamma\left(\int_M P\,\mathrm{d}\mu-1\right).\end{aligned} \tag{4.36}$$

This simplifies to

$$F_S(P+h)-F_S(P) = \int_M \left\{\left[-\frac{1}{q-1}+\alpha(H-\langle U\rangle)\right]qP^{q-1}+\gamma\right\} h\,\mathrm{d}\mu \\ -\frac{1}{2}\int_M [1-\alpha(q-1)(H-\langle U\rangle)]qP^{q-2}h^2\,\mathrm{d}\mu + O(h^3). \tag{4.37}$$

Now we gather that

$$\left[-\frac{1}{q-1}+\alpha(H-\langle U\rangle)\right]qP^{q-1}+\gamma = 0 \tag{4.38}$$

$$-\frac{1}{2}\int_M [1-\alpha(q-1)(H-\langle U\rangle)]qP^{q-2}h^2\,\mathrm{d}\mu \le C\|h\|^2. \tag{4.39}$$

From (4.38) one finds, with the usual procedure (see Ref. [23]):

$$\alpha = -\frac{\beta}{1-\beta(1-q)\langle U\rangle}, \tag{4.40}$$

$$\gamma = \frac{qZ^{1-q}-[1-\beta(1-q)\langle U\rangle]}{(q-1)[1-\beta(1-q)\langle U\rangle]}, \tag{4.41}$$

$$P = \frac{[1-\beta(1-q)H]^{\frac{1}{1-q}}}{Z}, \tag{4.42}$$

$$Z = \int_M [1-\beta(1-q)H]^{\frac{1}{1-q}}\,\mathrm{d}\mu. \tag{4.43}$$

A bit of algebra produces, from the above relations,

$$W = -\int_M [1-\alpha(q-1)(H-\langle U\rangle)]qP^{q-2}h^2\,\mathrm{d}\mu \\ = q\int_M -kT\frac{1-(1-q)H}{kT+(q-1)\langle U\rangle}P^{q-2}h^2\,\mathrm{d}\mu, \tag{4.44}$$

and setting $P^{q-2} = Z^{2-q}e_q(-\beta H)^{q-2}$,

$$W = -qZ^{2-q}\int_M \frac{[1+(q-1)\beta H]^{1/(q-1)}}{1+\beta(q-1)\langle U\rangle}h^2\mathrm{d}\mu. \tag{4.45}$$

One sees that, as in the two preceding instances, the bracket $[1+(q-1)\beta H]$ must be positive (long-tails!) so as to find a constant bound. This entails

$$q \ge 1, \tag{4.46}$$

and one has

$$W \le -qZ^{2-q}\int_M \frac{1}{1+\beta(q-1)\langle U\rangle}\|h\|^2 \le C\|h\|^2, \tag{4.47}$$

that is

$$C = q\frac{1}{1+\beta(q-1)\langle U\rangle}Z^{2-q}, \tag{4.48}$$

and we obtain the required bound for the entropy to become maximal. Moreover, from (4.47), we get, once again, the here redundant condition $q > 0$. As in the preceding two subsections, here our arguments *guarantee* an entropic maximum only for long-tail Tsallis distributions. For compact support distributions, the present arguments remain inconclusive. The maximum may or may not exist. One should further investigate things on a case-by-case fashion. The comment made below Eq. (4.33) is also pertinent here.

5. Example: the Harmonic Oscillator (HO)

Consider the simple Hamiltonian (in phase space) $H = P^2 + Q^2$. We will reconfirm the second variation functional restrictions encountered above in the concomitant three q-statistics cases.

5.1. Linear constraint $\langle U\rangle$

We start by remembering (4.11), that required $q \leq 1$. One has

$$-\int_M qP^{q-2}h^2\,\mathrm{d}\mu = -\int_M qZ^{2-q}[1+\beta(1-q)(P^2+Q^2)]_+^{\frac{q-2}{q-1}}h^2\,\mathrm{d}\mu$$
$$\leq -\int_M qZ^{2-q}[1+\beta(1-q)(P^2+Q^2)]_+^{\frac{1}{1-q}}h^2\,\mathrm{d}\mu \leq -qZ^{2-q}\int_M h^2\,\mathrm{d}\mu = -qZ^{2-q}\|h\|^2, \tag{5.1}$$

since

$$[1+\beta(1-q)(P^2+Q^2)]_+^{\frac{1}{1-q}} \geq 1. \tag{5.2}$$

We reobtain the restriction on heavy-tail Tsallis distributions.

5.2. Curado–Tsallis nonlinear constraints

We recall (4.35) and (4.36). We had here the restriction $q \geq 1$ and deal now with

$$-\int_M q[1-\alpha(q-1)(P^2+Q^2)]P^{q-2}h^2\,\mathrm{d}\mu = -\int_M Z^{2-q}q[1+\beta(q-1)(P^2+Q^2)]_+^{\frac{1}{q-1}}h^2\,\mathrm{d}\mu$$
$$\leq -\int_M qZ^{2-q}h^2\,\mathrm{d}\mu = -qZ^{2-q}\|h\|^2. \tag{5.3}$$

Since $q \geq 1$ we have $[1+\beta(q-1)(P^2+Q^2)]_+^{\frac{1}{q-1}} \geq 1$. Heavy tails once again!

5.3. TMP constraints

Here we must go back to (4.46). The operative restriction is $q \geq 1$. Accordingly,

$$-\int_M [1-\alpha(q-1)(P^2+Q^2-\langle U\rangle)]qP^{q-2}h^2\,\mathrm{d}\mu = -\frac{qZ^{2-q}}{1+\beta(q-1)\langle U\rangle}\int_M [1+\beta(q-1)(P^2+Q^2)]_+^{\frac{1}{q-1}}h^2\mathrm{d}\mu$$
$$\leq -\frac{qZ^{2-q}}{1+\beta(q-1)\langle U\rangle}\|h\|^2 \leq C\|h\|^2. \tag{5.4}$$

We need again to appeal to heavy tail distributions.

6. The compact support instance

We now consider the case of compact support probabilistic distributions in the formulation of Curado–Tsallis (similar arguments can be made for the other two possibilities). In such a case we need to satisfy, for a maximum, the relation

$$-Z^{2-q}q\int_M [1+\beta(q-1)H]^{\frac{1}{q-1}}h^2\,\mathrm{d}\mu \leq C\|h\|^2. \tag{6.1}$$

A maximum is not guaranteed if $0 < q < 1$. Consider now in more detail such a q-interval. H must be bounded by above in all phase space. By choosing β sufficiently small, the bracket above does take a minimum positive value Δ and then we have

$$-Z^{2-q}q\Delta^{\frac{1}{1-q}}\|h\|^2 \leq C\|h\|^2. \tag{6.2}$$

Thus, selecting

$$-Z^{2-q}q\Delta^{\frac{1}{1-q}} = C \tag{6.3}$$

we conclude that entropy does exhibit a maximum. Another way of viewing this argument is to consider that H has a maximum value R. Consider $q < 1$. More specifically, $q = 0.5$. Then our critical bracket reads

$$[1-0.5\beta R] > 0, \tag{6.4}$$

entailing, for $\beta = 1/kT$,

$$T > \frac{R}{2k}, \tag{6.5}$$

i.e., a *minimum* temperature in order to guarantee the desired maximal condition that concerns us here. One might wish to speculate that, for lower temperatures, since no entropic maximum is possible, equilibrium might not be reached.

6.1. Bounded Hamiltonian

Let us, for instance, H be given by

$$H = (P^2 + Q^2)\mathcal{H}(P_0^2 + Q_0^2 - P^2 + Q^2) \tag{6.6}$$

where $\mathcal{H}$ is Heaviside's step function. We need $[1 + \beta(q-1)H]$ to be positive.

Selecting $q = \frac{1}{2}$ and $\beta = 1/kT$ small enough we have:

$$0 \leq P^2 + Q^2 \leq P_0^2 + Q_0^2 < \frac{2}{\beta}, \tag{6.7}$$

and thus

$$T > (P_0^2 + Q_0^2)/2k, \tag{6.8}$$

so we wee that the higher the energy, the higher the temperature's lower bound. Finally,

$$\Delta = 1 - \frac{\beta}{2}(P_0^2 + Q_0^2). \tag{6.9}$$

7. Conclusions

Our second variation bounds are given, for the three Tsallis' cases, by the C-bounds (4.21), (4.33), and (4.48), respectively. Note that, since Z vanishes at $T = 0$, we cannot guarantee there a finite bound C, as required by the second variation protocol.

The three bounds yield exactly the same conclusion: entropic maxima are guaranteed only for long tail Tsallis distributions. For compact support distributions (CSD), the present arguments are inconclusive. The maximum may or may not exist. One should further investigate things on a case-by-case fashion, as we have done, for particular instances, in Section 6.

We saw there that, in the case of CSDs, a maximum entropy is attained only if the temperature is high enough. The bounded Hamiltonian example of Section 6 seems to suggest that the higher the mean energy, the higher the T-lower bound for reaching maximal entropies corresponding to equilibrium states.

Summing up, the three Tsallis treatments, that were proved to yield identical predictions for mean values in Ref. [22], still give the same results concerning the requirements for entropic maxima.

It is almost trivial to show that, for lower bounded Hamiltonians, a quantum n-levels treatment yields identical conclusions (see Appendix A).

Our present treatment makes it advisable, on a more general MaxEnt standpoint, to always look at the second functional variation.

Appendix A

We consider a quantum system with n discrete levels of positive energies ϵ_i, probabilities p_i, and increments h_i. The probability-vector P and increment-vector h belong to l^2. Consider, for instance, the orthodox linear choice for mean values, i.e., one evaluates mean values in the customary fashion, linear in the probabilities. The concomitant functional is

$$F_S(P) = -\sum_{i=1}^{n} p_i^q \ln_q(p_i) + \alpha\left(\sum_{i=1}^{n} p_i\epsilon_i - \langle U\rangle\right) + \gamma\left(\sum_{i=1}^{n} p_i\right). \tag{A.1}$$

For the increment we have

$$\begin{aligned} F_S(P+h) - F_S(P) &= -\sum_{i=1}^{n}(p_i+h_i)^q \ln_q(p_i+h_i) + \alpha\left[\sum_{i=1}^{n}(p_i+h_i)\epsilon_i - \langle U\rangle\right] \\ &\quad + \gamma\left[\sum_{i=1}^{n}(p_i+h_i) - 1\right] + \sum_{i=1}^{n} p_i^q \ln_q(p_i) - \alpha\left(\sum_{i=1}^{n} p_i\epsilon_i - \langle U\rangle\right) - \gamma\left(\sum_{i=1}^{n} p_i - 1\right). \end{aligned} \tag{A.2}$$

Eq. (A.2) can be recast as

$$F_S(P+h) - F_S(P) = \sum_{i=1}^{n}\left[\left(\frac{q}{1-q}\right)p_i^{q-1} + \alpha\epsilon_i + \gamma\right]h_i - \sum_{i=1}^{n} q p_i^{q-2}\frac{h_i^2}{2} + O(h^3). \tag{A.3}$$

Eq. (A.3) leads to the following equations:

$$\left(\frac{q}{1-q}\right)p_i^{q-1} + \alpha\epsilon_i + \gamma = 0, \tag{A.4}$$

$$-\sum_{i=1}^{n} q p_i^{q-2} h_i^2 \leq C\|h\|^2. \tag{A.5}$$

Eq. (A.4) is the Euler–Lagrange one while (A.5) gives bounds originating from the second variation. Thus, (A.4) entails

$$\alpha = \beta q Z^{1-q} \tag{A.6}$$

$$\gamma = \frac{q}{q-1} Z^{1-q} \tag{A.7}$$

$$p_i = \frac{[1+\beta(1-q)\epsilon_i]^{\frac{1}{q-1}}}{Z} \tag{A.8}$$

$$Z = \sum_{i=1}^{n} [1+\beta(1-q)\epsilon_i]^{\frac{1}{q-1}}. \tag{A.9}$$

For the bound given by (A.5) we have

$$W = -\sum_{i=1}^{n} q p_i^{q-2} h_i^2 = -\sum_{i=1}^{n} q Z^{2-q} [1+\beta(1-q)\epsilon_i]^{\frac{q-2}{q-1}} h_i^2. \tag{A.10}$$

To obtain a constant bound, independent of the ϵ_i, we must demand $[1+\beta(1-q)\epsilon_i] \geq 0$ (long tail distribution!). Accordingly,

$$W = -\sum_{i=1} q Z^{2-q} [1+\beta(1-q)\epsilon_i]^{\frac{1}{1-q}} h_i^2 \leq -q Z^{2-q} \sum_{i=1}^{n} h_i^2 = -q Z^{2-q} \|h\|^2. \tag{A.11}$$

From (A.11) we see that $C = -qZ^{2-q}$ and $q > 0$. As $q \leq 1$ we have finally for q the bounds $0 < q \leq 1$.

Appendix B

Consider a functional of P called $F_S(P)$, given by

$$F_S(P) = -\int_M P^q \ln_q(P)\, \mathrm{d}\mu = \frac{1}{q-1} + \int_M \frac{P^q}{1-q}\, \mathrm{d}\mu. \tag{B.1}$$

Thus, we can write

$$F_S(P+h) = -\int_M (P+h)^q \ln_q(P+h)\, \mathrm{d}\mu = \frac{1}{q-1} + \int_M \frac{(P+h)^q}{1-q}\, \mathrm{d}\mu. \tag{B.2}$$

Accordingly,

$$F_S(P+h) = \frac{1}{q-1} + \int_M \frac{P^q + qP^{(q-1)}h + \frac{q(q-1)}{2} P^{q-2} h^2}{1-q}\, \mathrm{d}\mu + O(h^3). \tag{B.3}$$

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