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Existence conditions and spreading properties of extreme entropy D-dimensional distributions

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Abstract

The extremization of the information-theoretic measures (Fisher information, Shannon entropy, Tsallis entropy), which complementary describe the spreading of the physical states of natural systems, gives rise to fundamental equations of motion and/or conservation laws. At times, the associated extreme entropy distributions are known for some given constraints, usually moments or radial expectation values. In this work, first we give the existence conditions of the maxent probability distributions in a D-dimensional scenario where two moments (not necessarily of consecutive order) are known. Then we find general relations which involve four elements (the extremized entropy, the other two information-theoretic measures and the variance of the extremum density) in scenarios with different dimensionalities and moment constraints.

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1. Introduction

The Fisher information [1,2] and the Shannon [3,4] and Tsallis [5,6] entropies are complementary information-theoretic measures of spreading of a probability distribution. The extremization methods of these information measures provide means to estimate the probability distributions of random variables from the knowledge of some given quantities related to these variables. They provide very useful constructive methods which objectively estimate the unknown distribution when only partial data are given. The least biased or minimally prejudiced estimate of the distribution consistent with the available data is that which extremizes the information-theoretic measure subject to the given data. The maximum entropy (maxent) method [7–9] associated to the Shannon entropy, which is the basis of

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the conventional or extensive statistical mechanics [10], is the most popular one; however, it does not always lead to an appropriate distribution function [11]. At present, the extremum Fisher information (exfinf) method is known [12] to provide the fundamental wave equations and/or the conservation laws of numerous natural systems at small and large scales. The maximization of the Tsallis entropy (maxtent) [6,13,14] has been recently encountered to be the basis of the modern non-extensive statistical mechanics [15]. The use of these information measures and their extremization is a subject of much current interest in density functional methods of multi-electronic systems [16–19].

Then, the knowledge of the existence conditions for these extremization problems and the spreading properties of the associated extremum information measures is a two-fold problem of great scientific relevance in natural sciences. Although the form of the extremum information distributions subject to some moment equality or inequality constraints is, at times, known (mostly for the maxent case), there are still numerous open questions about their existence conditions in spite of the efforts of many authors [10,18–36]. On the other hand, there has not been a systematical investigation into the spreading properties of these distributions. This situation is a serious lack not only from a conceptual standpoint but also because of its effects for a great deal of problems and phenomena in science, finances and engineering [18,25,26,37,38]. For a recent exhaustive review of the maxent problem until 2004 see Ref. [24].

Here we consider D-dimensional probability distributions because of numerous reasons; let us just mention that (i) numerous phenomena of physical systems in our three-dimensional world can be best explained via quantum-mechanical probability distributions with non-standard dimensionalities (e.g., quantum dots, quantum wells, quantum wires, ...) [39,40], (ii) it is commonly believed at present that the best way to explain the unification of all forces of physics is via the idea of higher dimensions [41], and (iii) they lead to important approximation techniques, based upon the ideas of D-scaling and perturbation expansions in $1/D$ [39,42,43]. In this paper we want to contribute to the solution of the problem mentioned above in the two following directions. First, we find the explicit necessary and sufficient condition for the existence of a D-dimensional extremum information distribution for a physical system with two given arbitrary radial expectation values. Second, we derive general relations among the extremized information-theoretic measures and the variance for scenarios with different dimensionalities and various given moment constraints.

The structure of the paper is the following. First, in Section 2, we fix the notation and definition of the information-theoretic measures involved in this D-dimensional work, and we describe briefly the general methodology used for corresponding extremization methods. Second, in Section 3, we obtain the existence condition of the maxent problem for a D-dimensional system with two arbitrary radial expectation values of not necessarily consecutive order, and some applications are given. Then, in Section 4, various information-theoretic properties of the extremizer density associated to the maxent, minfinf and maxtent problems (which measure its multi-dimensional spreading far beyond the familiar variance) are analytically and numerically discussed for a number of scenarios with different radial moment constraints. Finally, some conclusions and open problems are given.

2. Prolegomenon about information measures and their associated extremization methods

Here we describe the basic information-theoretic quantities (Fisher, Shannon, Renyi and Tsallis entropies) which, together with the variance, are mostly used to quantify the spreading of an absolutely continuous probability density $\rho(\vec{r})$ associated to the D-dimensional vector $\vec{r} = (x_1, x_2, \ldots, x_D)$, all over the space. Then we make some general comments about their corresponding extremum information methods. The variance of the density $\rho(\vec{r})$ is defined by

$$V_\rho = \int (r - \langle r\rangle)^2 \rho(\vec{r})\mathrm{d}^D r. \tag{1}$$

with $\langle r^m\rangle \equiv \int r^m \rho(\vec{r})\mathrm{d}^D r$.

The Shannon entropy S_ρ [3] and the Fisher information [1,2] I_ρ of the density are given by

$$S_\rho := -\int \rho(\vec{r}) \ln \rho(\vec{r})\mathrm{d}^D r \tag{2}$$

and

$$I_\rho := \int \rho(\vec{r}) \left(\frac{|\vec{\nabla}_D \rho(\vec{r})|}{\rho(\vec{r})}\right)^2 \mathrm{d}^D r, \tag{3}$$

respectively, where $\vec{\nabla}_D$ denotes the D-dimensional gradient operator. Finally, the Renyi [44] and Tsallis entropies [5, 6] are defined as

$$R_\alpha(\rho) = \frac{1}{1-\alpha} \ln\left(\int \left[\rho(\vec{r})\right]^\alpha \mathrm{d}^D r\right); \quad \alpha > 0, \alpha \neq 1 \tag{4}$$

and

$$T_\alpha(\rho) = \frac{1}{\alpha-1} \left\{1 - \int \left[\rho(\vec{r})\right]^\alpha \mathrm{d}^D r\right\}; \quad \alpha > 0, \alpha \neq 1 \tag{5}$$

respectively. It is well known that for $\alpha \to 1$, both entropies, R_α and T_α go to the Shannon value S_ρ. The extremum information method associated to a generic information-theoretic measure

$$Q \equiv \int \rho(\vec{r}) F[\rho(\vec{r})] \mathrm{d}^D r, \tag{6}$$

consists in the extremization of Q subject to the constraints of normalization to unity of the form

$$\int \rho(\vec{r}) \mathrm{d}^D r = 1 \tag{7}$$

and

$$\int \rho(\vec{r}) f_i(\vec{r}) \mathrm{d}^D r = a_i; \quad i = 1, 2, \ldots, n, \tag{8}$$

where $f_i(\vec{r})$ is a given function of $\vec{r}$ so that $f_0(\vec{r}) \equiv 1$. Using the method of Lagrange multipliers, one considers the functional

$$Q^* = Q + \sum_{i=0}^{n} \left[\lambda_i \int f_i(\vec{r}) \rho(\vec{r}) \mathrm{d}^D r - a_i\right], \tag{9}$$

where λ_i are the Lagrange multipliers, and sets its variation to zero so that

$$\delta Q^* = \int \left\{F\left[\rho(\vec{r})\right] + \sum_{i=0}^{n} \lambda_i f_i(\vec{r})\right\} \delta\rho(\vec{r}) \mathrm{d}^D r = 0. \tag{10}$$

This equation yields the density $\rho(\vec{r})$ which, with the multipliers λ_i determined from the $n+1$ equations given by (7) and (8), describes the extremum information probability density.

The maxent problem has a unique solution [22] which maximizes the Shannon entropy, whenever it exists, for the given set of moments $\{a\} = \{a_0 = 1, a_1, \ldots, a_n\}$. In contrast with this situation, the exfinf problems have multiple solutions. Then, the question is which solution to choose. It has been argued that the solution with no nodes (the ground-state solution) leading to the lowest Fisher information is the equilibrium one, so laying the foundations of the conventional or equilibrium thermodynamics based on the concept of Fisher information. The choice of linear superpositions of this ground state with excited state solutions leads us to non-equilibrium thermodynamics [45].

The maxent problem under different moment constraints in some scientific and engineering situations has been discussed in numerous places; see, e.g., Refs. [26,27,32,33,35,46,47]. For the analysis of the exfinf and maxtent problems we refer to Refs. [12,19,28,48,49] and [13,14,31], respectively. See Ref. [24] for detailed information. There are two kinds of exfinf problems in current use: the minimum Fisher information (minfinf) [12,28,48–50] and the extreme physical information (EPI) [12,51]. Nevertheless we do not distinguish between these two treatments for our present purposes. Let us only point out that the probability distribution which minimizes the Fisher information will be as non-informative as possible while still satisfying the constraints [50].

These four information-theoretic problems, although similar at first sight, are markedly different in their world views and applicability to physics [52,53]. Contrary to the EPI method, which does not depend upon arbitrary subjective choices, the maxent, minfinf and maxtent problems require the choice of arbitrary, subjectively defined inputs.

3. Existence conditions for the maxent problem

In this section we consider the reduced D-dimensional maxent problem, where one tries to approximate an absolutely continuous distribution $\rho(\vec{r})$ in $\Re^D$ from a finite number of radial expectation values

$$\langle r^m \rangle = \int r^m \rho(\vec{r}) \mathrm{d}^D r; \quad m = 0, 1, 2, \ldots, n, \tag{11}$$

where $\vec{r} = (r, \theta_1, \theta_2, \ldots, \theta_{D-1})$ describes the D-dimensional vector $\vec{r}$ in hyperspherical coordinates so that the hyperradius varies as $0 \leq r < \infty$, and the angles, $0 \leq \theta_j < \pi$ for $1 \leq j < D-2$ and $0 \leq \theta_{D-1} < 2\pi$. The volume element $\mathrm{d}^D r$ is

$$\mathrm{d}^D r = r^{D-1} \mathrm{d}r \mathrm{d}\Omega_D; \qquad \mathrm{d}\Omega_D = \left(\prod_{j=1}^{D-2} (\sin\theta_j)^{2\alpha_j} \mathrm{d}\theta_j \right) \mathrm{d}\theta_{D-1},$$

with $\alpha_j = \frac{D-j-1}{2}$. For the special case $D = 1$, remark that $r = x \in [0, \infty)$.

The application of the general considerations of the previous section to the Shannon entropy (2) provides that the maxent problem has a maximum entropy distribution whose density function is of the form

$$\rho^*(r) = \exp\left(-\sum_{i=0}^{n} \lambda_i r^i \right), \tag{12}$$

where the Lagrange multipliers λ_i, $i = 0, 1, \ldots, n$, are chosen to fulfill the conditions

$$\Omega_D \int_0^\infty r^m \exp\left(-\sum_{i=0}^{n} \lambda_i r^i \right) r^{D-1} \mathrm{d}r = \langle r^m \rangle; \quad m = 1, \ldots, n, \quad \text{and} \quad \langle r^0 \rangle = 1, \tag{13}$$

where Ω_D is the generalized solid angle

$$\Omega_D \equiv \int \mathrm{d}\Omega_D = \frac{2\pi^{D/2}}{\Gamma\left(\frac{D}{2}\right)},$$

so that $\Omega_1 = 2$, $\Omega_2 = 2\pi$ and $\Omega_3 = 4\pi$. For the case $n = 2$ (i.e. for given $\langle r \rangle$ and $\langle r^2 \rangle$) the determination of the associated Stieltjes problem [54] and the solvability of the integral relations (13) of the corresponding maxent problem [22,23,55] require that the involved radial expectation values satisfy the inequalities

$$\langle r \rangle^2 \leq \langle r^2 \rangle \leq \frac{D+1}{D} \langle r \rangle^2. \tag{14}$$

The lower bound to $\langle r^2 \rangle$ is a straightforward consequence of the non-negativity of the Hankel determinant

$$\begin{vmatrix} \langle r^0 \rangle & \langle r \rangle \\ \langle r \rangle & \langle r^2 \rangle \end{vmatrix} \geq 0$$

corresponding to the involved Stieltjes moment problem. Alternatively, the same result can be found by using the Hölder inequality. The upper bound to $\langle r^2 \rangle$ is obtained by means of the existence condition of the aforementioned maxent problem which, according to Einbu's theorem [22,24] or the Junk–Tagliani results [23,55], is given by

$$\mu_{D+1} \leq \frac{D+1}{D} \Omega_D \mu_D^2,$$

where the moments $\mu_{D+\alpha-1}$ are

$$\mu_{D+\alpha-1} = \frac{1}{\Omega_D} \langle r^\alpha \rangle; \quad \alpha > -D, \quad \text{and} \quad \mu_{D-1} = \Omega_D^{-1}. \tag{15}$$

In the application of the same procedure to the radial expectation values $\{\langle r^0\rangle = 1, \langle r^\alpha\rangle, \langle r^\beta\rangle\}$, i.e. to the moments $\{\mu_{D-1}, \mu_{D+\alpha-1}, \mu_{D+\beta-1}\}$, we have found the following inequalities:

$$\langle r^\alpha\rangle^{\frac{\beta}{\alpha}} \le \langle r^\beta\rangle \le f(D,\alpha,\beta)\langle r^\alpha\rangle^{\frac{\beta}{\alpha}}, \tag{16}$$

with $\beta > \alpha > 1 - D$ (if $\alpha < 0$, $\frac{\beta}{\alpha}$ must be integer), and the constant

$$f(D,\alpha,\beta) \equiv \left(\frac{\alpha}{D}\right)^{\frac{\beta}{\alpha}} \frac{\Gamma\left(\frac{\beta+D}{\alpha}\right)}{\Gamma\left(\frac{D}{\alpha}\right)}. \tag{17}$$

It is worth noticing that Eqs. (16) and (17) boil down to Eq. (14), and moreover when $D = 1$ the last expression contains the Dowson–Wragg condition [20] for the maxent problem associated to the univariate probability distributions when the first two moments are given.

The following desirable step forward is to find the existence conditions for the D-dimensional maxent distributions subject to the radial expectation values $\{\langle r^0\rangle = 1, \langle r^\alpha\rangle, \langle r^\beta\rangle, \langle r^\gamma\rangle; \gamma > \beta > \alpha\}$ or equivalently the moments $\{\mu_{D-1}, \mu_{D+\alpha-1}, \mu_{D+\beta-1}, \mu_{D+\gamma-1}; \gamma > \beta > \alpha > 0\}$. This would extend the celebrated Kociszewski [21] criteria for the existence of maximum entropy Stieltjes univariate ($D = 1$) distributions having prescribed the first three moments besides the normalization; that is, for given $\{\mu_0, \mu_1, \mu_2, \mu_3\}$. For completeness let us mention here that methodologies to obtain the desired existence inequalities for the four D-dimensional radial expectation values are possibly D-dimensional extensions of the Einbu theorems [22] or the Milano–Trento–Caracas maxent approach [29, 56,57] for the fractional lacunary Stieltjes moment problem.

4. Spreading properties of extremum information distributions

This section has three parts which correspond to the D-dimensional maxent, exfinf and maxtent problems. Each part begins with the determination of the distribution which extremizes the associated information-theoretic measure (namely, Shannon, Fisher or Tsallis, respectively) under some given constraints, and then the spread of the resulting extremum density is investigated by means of its information-theoretic measures other than that extremized, and its variance. The numerical analysis has been carried out for the charge density of the (D-dimensional) ground-state Hydrogen atom as distribution for computing the associated information measures as well as its radial expectation values as constraints.

4.1. The maxent problem

Following the method described in second section, the D-dimensional density which maximizes the Shannon entropy (2) with the known constraints $a_i = \langle f_i(\vec{r})\rangle$ is

$$\rho_S(\vec{r}) = \exp\left\{-\lambda_0 - \sum_{i=1}^{m} \lambda_i f_i(\vec{r})\right\}.$$

For this general problem, the existence conditions for $\rho_S(\vec{r})$ are yet unknown. Then we shall restrict ourselves to some simpler cases where such conditions do exist; namely, when the constraints are just one or two radial expectation values $\langle r^\alpha\rangle$ (moments $\mu_{D+\alpha-1}$) in addition to the normalization to unity.

Case 1: D-dimensional case with a given expectation value $\langle r^\alpha\rangle$. In this case the density which maximizes the Shannon entropy S_ρ is given by

$$\rho_S(\vec{r}) = \exp\{-\lambda_0 - \lambda_1 r^\alpha\}; \quad \alpha > 0, \tag{18}$$

where the Lagrange multipliers have, according to Eqs. (7) and (8), the form

$$\lambda_0 = \ln\left[\frac{2\pi^{\frac{D}{2}}\Gamma\left(\frac{D}{\alpha}\right)}{\alpha\Gamma\left(\frac{D}{2}\right)}\right] + \frac{D}{\alpha}\ln\left[\frac{\alpha}{D}\langle r^\alpha\rangle\right]$$

$$\lambda_1 = \frac{D}{\alpha\langle r^\alpha\rangle}.$$

Moreover, following (2) and (18), the corresponding value for the maximum entropy is

$$S_{\max} = A_0(\alpha, D) + \frac{D}{\alpha} \ln\left\langle r^\alpha \right\rangle, \tag{19}$$

with

$$A_0(\alpha, D) = \frac{D}{\alpha} + \ln\left[\frac{2\pi^{\frac{D}{2}}}{\alpha}\left(\frac{\alpha}{D}\right)^{\frac{D}{\alpha}} \frac{\Gamma\left(\frac{D}{\alpha}\right)}{\Gamma\left(\frac{D}{2}\right)}\right].$$

Also, according to Eqs. (1), (3), (5) and (7), we have found the values

$$V = A_1(\alpha, D)\left\langle r^\alpha \right\rangle^{\frac{2}{\alpha}}, \tag{20}$$

for the variance,

$$I = A_2(\alpha, D)\left\langle r^\alpha \right\rangle^{-\frac{2}{\alpha}}, \tag{21}$$

for the Fisher information, and

$$T_q = \frac{1}{q-1}\left\{1 - q^{-\frac{D}{\alpha}}\left[A_3(\alpha, D)\right]^{q-1}\left\langle r^\alpha \right\rangle^{\frac{D}{\alpha}(1-q)}\right\} \tag{22}$$

for the Tsallis entropy of the maximizer entropy (18), respectively. The coefficients A_i $(i = 1, 2, 3)$ are functions of parameters α and D as follows

$$A_1(\alpha, D) = \left(\frac{D}{\alpha}\right)^{-\frac{2}{\alpha}}\left\{\frac{\Gamma\left(\frac{D+2}{\alpha}\right)}{\Gamma\left(\frac{D}{\alpha}\right)} - \left(\frac{\Gamma\left(\frac{D+1}{\alpha}\right)}{\Gamma\left(\frac{D}{\alpha}\right)}\right)^2\right\} \tag{23}$$

$$A_2(\alpha, D) = \alpha^2\left(\frac{D}{\alpha}\right)^{\frac{2}{\alpha}} \frac{\Gamma\left(\frac{D-2}{\alpha} + 2\right)}{\Gamma\left(\frac{D}{\alpha}\right)} \tag{24}$$

$$A_3(\alpha, D) = \frac{\alpha}{2}\left(\frac{D}{\alpha}\right)^{\frac{D}{\alpha}} \frac{\Gamma\left(\frac{D}{2}\right)}{\pi^{\frac{D}{2}}\Gamma\left(\frac{D}{\alpha}\right)}, \tag{25}$$

which drastically simplify for specific values of α and D.

In Figs. 1 and 2 we have plotted the dependence of the four spreading measures (Shannon, variance, Fisher and Tsallis T_q with $q = 0.9$), calculated according to Eqs. (19)–(22) on the expectation order α and the dimensionality D of the system under consideration, respectively. From Fig. 1 we observe that, for the three-dimensional case, (i) the three global measures (Shannon, variance and Tsallis T_q) have an increasing behaviour with α, contrary to the decreasing monotonic behaviour of the local Fisher measure, (ii) the Tsallis entropy $T_{0.9}$ increases faster than the Shannon entropy, and both of them are systematically bigger than the Fisher information as α is increasing; the latter behaviour is not fulfilled by variance, and (iii) for a given expectation value, $T_{0.9} > S_{\max} > I$ always, $I > V$ for $\alpha < 24$ and $I < V$ for $\alpha > 24$.

From Fig. 2 we realize that, for fixed $\alpha = 2$, (i) the three global spreading measures increase, displaying a convex parabolic form in terms of the dimensionality D, (ii) the local Fisher measure has a decreasing convex form, and (iii) for a given dimensionality, it occurs that $T_{0.9} > S_{\max} > V$.

On the other hand, the algebraic manipulation of Eqs. (19)–(22) leads to the following mutual relations among the spreading measures under consideration. We find that

$$I = \frac{A_1(\alpha, D)A_2(\alpha, D)}{V}, \tag{26}$$

$$S_{\max} = F_1(\alpha, D) + \frac{D}{2}\ln V = F_2(\alpha, D) - \frac{D}{2}\ln I, \tag{27}$$

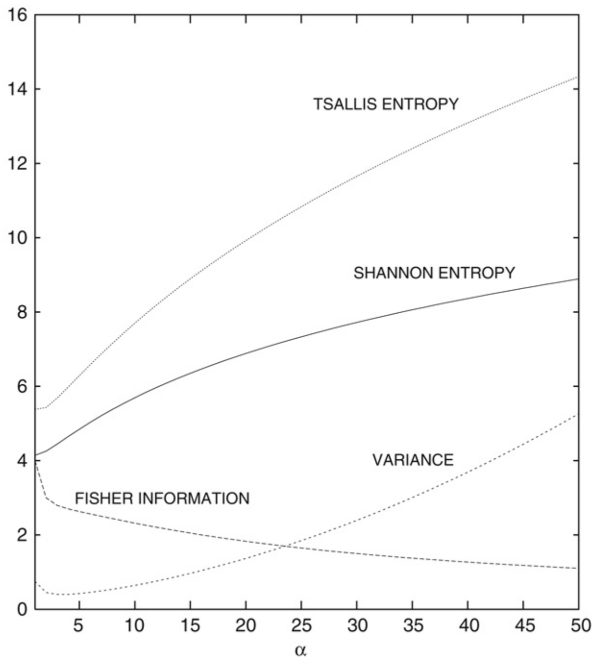

Fig. 1. Variance, Fisher information and Shannon and Tsallis (with $q = 0.9$) entropies for the maxent problem with the constraint $\langle r^\alpha \rangle$ as functions of the expectation order α in the three-dimensional case. Atomic units ($e = \hbar = m_e = 1$) are used.

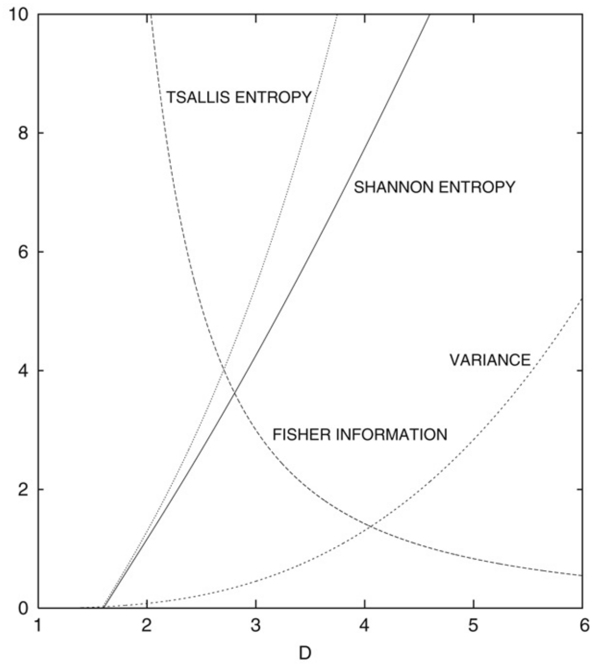

Fig. 2. Variance, Fisher information and Shannon and Tsallis (with $q = 0.9$) entropies for the maxent problem as functions of the dimension D constrained by the radial expectation value $\langle r^2 \rangle$. Atomic units ($e = \hbar = m_e = 1$) are used.

and

$$S_{\max} = F_3(\alpha, q, D) + \frac{1}{1-q} \ln\left[1 + (1-q)T_q\right], \tag{28}$$

where F_i $(i = 1, 2, 3)$ are simple relations of the coefficients A_i given by the expressions (23)–(25). The mutual relationships (26)–(28) among the four spreading measures drastically simplify when the dimensionality D and/or the other two involved parameters α and q are fixed.

Case 2: One-dimensional case with the given $\langle x\rangle$ and $\langle x^2\rangle$. In this case the maximizer density becomes

$$\rho_S(x) = \exp\left\{-\lambda_0 - \lambda_1 x - \lambda_2 x^2\right\}.$$

Here the existence conditions are known to be given by the inequalities (14) and (15). Moreover, operating similarly to the previous case we obtain that the maximum value of the Shannon entropy is a logarithmic function of the variance,

$$S_{\max} = \ln\sqrt{2\pi \mathrm{e}} + \frac{1}{2}\ln\left(\left\langle x^2\right\rangle - \langle x\rangle^2\right)$$

and the Fisher information I is exactly equal to the reciprocal of variance, so that

$$S_{\max} = \ln\sqrt{2\pi \mathrm{e}} - \frac{1}{2}\ln I.$$

Moreover, the Tsallis entropy of the maximizer density can be also explicitly expressed as

$$T_q = \frac{(2\pi)^{\frac{1-q}{2}}}{(1-q)\sqrt{q}}\left(\left\langle x^2\right\rangle - \langle x\rangle^2\right)^{\frac{1-q}{2}},$$

so that the following relation with the maximum Shannon entropy is fulfilled

$$S_{\max} = \frac{1}{2}(1-\ln 2\pi) + \frac{1}{1-q}\ln q + \frac{2}{1-q}\ln\left[1+(1-q)T_q\right].$$

4.2. The minfinf problem

In this case, the general method described in the second section shows that the D-dimensional density $\rho_F(\vec{r}) \equiv g(\vec{r})$ which minimizes the Fisher information (3) with the known constraints $a_i = \langle f_i(\vec{r})\rangle$ fulfills the differential equation

$$\left[\frac{\vec{\nabla}_D g(\vec{r})}{g(\vec{r})}\right]^2 + 2\vec{\nabla}_D\left[\frac{\vec{\nabla}_D g(\vec{r})}{g(\vec{r})}\right] + \lambda_0 + \sum_{k=1}^{m}\lambda_k f_k(\vec{r}) = 0, \tag{29}$$

where $\vec{\nabla}_D$ denotes the D-dimensional gradient operator. The case $D = 3$ has already been treated in detail [19]. For simplicity and transparency purposes we have restricted ourselves to a concrete yet fundamental three-dimensional case: the only constraint is $a_1 = \langle r^{-1}\rangle$, besides the normalization to unity. Then, the density $g(\vec{r})$ is given by [19]

$$g(r) = \pi^{-1}\left\langle r^{-1}\right\rangle^3 \exp\left(-2\left\langle r^{-1}\right\rangle r\right),$$

which corresponds to the minimal Fisher information

$$I_{\min} = 4\left\langle r^{-1}\right\rangle^2.$$

Moreover, this minimizer density $g(r)$ has the following values

$$V = \frac{3}{4\left\langle r^{-1}\right\rangle^2}$$

$$S = 3 + \ln\pi - 3\ln\left\langle r^{-1}\right\rangle$$

for the variance and the Shannon entropy, and

$$T_q = \frac{1}{q-1}\left[1 - \frac{\pi^{1-q}}{q^3}\left\langle r^{-1}\right\rangle^{3(q-1)}\right]; \quad q > 0, q \neq 1$$

for the Tsallis entropy. So that, they are mutually related by

$$I_{\min} = \frac{3}{V} = 4\pi^{\frac{2}{3}} e^2 \exp\left(-\frac{2}{3}S\right)$$

and

$$I_{\min} = 4\pi^{\frac{2}{3}} q^{\frac{2}{q-1}} \left[1 + (1-q)T_q\right]^{\frac{2}{3(q-1)}}, \quad q > 0, q \neq 1$$

so that for $q = 2$ one has that $T_2 = 1 - \frac{I_{\min}}{64\pi}$.

Similar analyses can be done for other concrete cases, such as $(a_0, a_1) = (1, \langle r^2\rangle)$ and $(a_0, a_1, a_2) = (1, \langle r^{-1}\rangle, \langle r^2\rangle), (1, \langle r^{-2}\rangle, \langle r^2\rangle)$, where the minimizer densities are known to exist [19]. We should point out, however, that for the general case mentioned above, neither the solution of Eq. (29) nor its existence conditions are known unless the constraints are specified. Unfortunately, this is even true for the particular cases where the constraints are one or various radial expectation values of generic order. The search of existence conditions for the minfinf problem just mentioned is an important yet open task, which lies beyond the scope of this work since it involves high-brow questions of partial differential equations of the type (29). On the other hand, it is worth to mention here the Frieden's [12,49,50] Lagrangian formalism for the minfinf problem and the Luo's application of the maxent and minfinf problems to a specific yet relevant system [53].

4.3. The maxtent problem

The maximizer density $\rho_T(\vec{r})$ of the three-dimensional maxtent problem given by Eqs. (5)–(10) with constraints $(a_0, a_1) = (1, \langle r^\alpha\rangle)$ depends on the value of q and α. There are three different cases:

- If $q > 1$ and $\alpha > 0$, the maximum entropy density only exists for a finite interval $r \in [0, a]$.
- If $0 < q < 1$ and $\alpha > \frac{3(1-q)}{q}$, the maximum entropy density exists for any value of r.
- If $q > 1$ and $-\frac{3(q-1)}{q} < \alpha < 0$, the maximum entropy density only exists for an unbounded interval $r \in [a, \infty)$.

For the first case, the extreme probability density is:

$$g_1(r) = C\left(\frac{1}{q}(a^\alpha - r^\alpha)\right)^{\frac{1}{q-1}}, \tag{30}$$

according to the general extremization method shown in the second section. C and a are functions of the Lagrange parameters; they have the following expressions

$$a = \left(\frac{3(q-1)+q\alpha}{3(q-1)}\langle r^\alpha\rangle\right)^{\frac{1}{\alpha}}$$

$$C = \frac{q^{\frac{1}{q-1}}\alpha}{4\pi B\left(\frac{3}{\alpha}, \frac{q}{q-1}\right)}\left(\frac{3(q-1)+q\alpha}{3(q-1)}\langle r^\alpha\rangle\right)^{-\frac{3}{\alpha}-\frac{1}{q-1}}$$

where $B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$ is the beta function.

This density has the following values

$$(T_q)_{\max} = \frac{1}{q-1}\left[1 - C_0(\alpha, q)\langle r^\alpha\rangle^{-\frac{3(q-1)}{\alpha}}\right] \tag{31}$$

for the maximal Tsallis entropy,

$$S = C_1(\alpha, q) + \frac{3(q-1)+\alpha-1}{\alpha(q-1)}\ln\langle r^\alpha\rangle, \tag{32}$$

$$V = C_2(\alpha, q)\langle r^\alpha\rangle^{\frac{2}{\alpha}}, \tag{33}$$

for the Shannon entropy and the variance, and

$$I = C_3(\alpha, q)\langle r^\alpha\rangle^{-\frac{2}{\alpha}}; \quad 1 < q < 2, \tag{34}$$

for the Fisher information. The coefficients $C_i(\alpha, q)$, $i = 0, 1, 2$ and 3, have the following expressions

$$C_0(\alpha, q) = \frac{q^q \alpha^{2q-1}(3(q-1))^{\frac{3(q-1)}{\alpha}}}{\left(4\pi B\left(\frac{3}{\alpha}, \frac{2q-1}{q-1}\right)\right)^{q-1}} (3(q-1)+q\alpha)^{-\frac{3(q-1)+q\alpha}{\alpha}} \tag{35}$$

$$C_1(\alpha, q) = \frac{1}{q-1}\left(\psi\left(\frac{q}{q-1}+\frac{3}{\alpha}\right)-\psi\left(\frac{q}{q-1}\right)\right) - \ln\left(\frac{\alpha}{4\pi B\left(\frac{3}{\alpha}, \frac{q}{q-1}\right)}\right) + \frac{3(q-1)+\alpha-1}{\alpha(q-1)}\ln\left(\frac{3(q-1)+\alpha q}{3(q-1)}\right) \tag{36}$$

$$C_2(\alpha, q) = \left(\frac{3(q-1)+q\alpha}{3(q-1)}\right)^{\frac{2}{\alpha}} \frac{\Gamma\left(\frac{q}{q-1}+\frac{3}{\alpha}\right)}{\Gamma\left(\frac{3}{\alpha}\right)}\left[\frac{\Gamma\left(\frac{5}{\alpha}\right)}{\Gamma\left(\frac{5}{\alpha}+\frac{q}{q-1}\right)} - \frac{\Gamma^2\left(\frac{4}{\alpha}\right)\Gamma\left(\frac{q}{q-1}+\frac{3}{\alpha}\right)}{\Gamma\left(\frac{3}{\alpha}\right)\Gamma^2\left(\frac{5}{\alpha}+\frac{q}{q-1}\right)}\right] \tag{37}$$

$$C_3(\alpha, q) = \frac{\alpha^2}{(q-1)^2}\left(\frac{3(q-1)+q\alpha}{3(q-1)}\right)^{-\frac{2}{\alpha}} \frac{B\left(\frac{1}{\alpha}+2, \frac{1}{q-1}-1\right)}{B\left(\frac{3}{\alpha}, \frac{q}{q-1}\right)} \tag{38}$$

where $\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$ is the digamma function.

Contrary to the previous extremization entropy problems where the extremizer density has an exponential form, now we have found the power law (30) as already pointed out [13–15,34,37,38]. To gain insight into this power-like maximizer density of the Tsallis entropy we have plotted in Figs. 3 and 4 the behaviour of the four spreading measures mentioned above with respect to the expectation order α and the non-extensivity parameter q, respectively. From Fig. 3 we notice that $I > (T_q)_{\max}$ (with $q = 1.7$) for any expectation value, having the maximum Tsallis entropy a widely extended convex shape. From Fig. 4, corresponding to $\alpha = 3$, we find that the Fisher information (i) monotonically increases as q increases, and (ii) $S > T_{q\max} > V$ for all values of the non-extensivity parameter. Besides, Fisher information crosses both Tsallis and Shannon measures at a critical q around 1.15 and 1.7 respectively.

Similar analyses can be done for the two remaining cases. Finally, for completeness, let us also mention the recent works of Brody, Buckley and Constantinou [38,58] where they maximize the Renyi entropy

$$R_\alpha(\rho) := \frac{1}{1-\alpha}\ln\int_0^\infty [\rho(x)]^\alpha\,dx$$

under the constraints $(a_0, a_1) = (1, \langle x^\alpha\rangle)$, $\alpha > 0$. They show that the solution of this one-dimensional maxrent problem has also the power-like form of the type (30), what should not be surprising since the Renyi and Tsallis entropies are mutually related by

$$R_\alpha(\rho) = \frac{1}{\alpha-1}\ln\left[1-(\alpha-1)T_\alpha(\rho)\right],$$

so that maximizing $R_\alpha(\rho)$ is tantamount to maximizing $T_\alpha(\rho)$. For extensive details about the vast literature on the maxtent problem, see Ref. [59].

5. Conclusions and open problems

A problem of extremum information asserts that one should choose as the least biased (minimally prejudiced or maximally unpresumptive) probability distribution that which extremizes the involved information-theoretic measure subject to some constraints known about the system. We have outlined the procedures for maximizing the Shannon and Tsallis entropies and a method for minimizing the Fisher information in scenarios with standard and non-standard dimensionalities under various constraints of moment or radial expectation type. These three information-theoretic

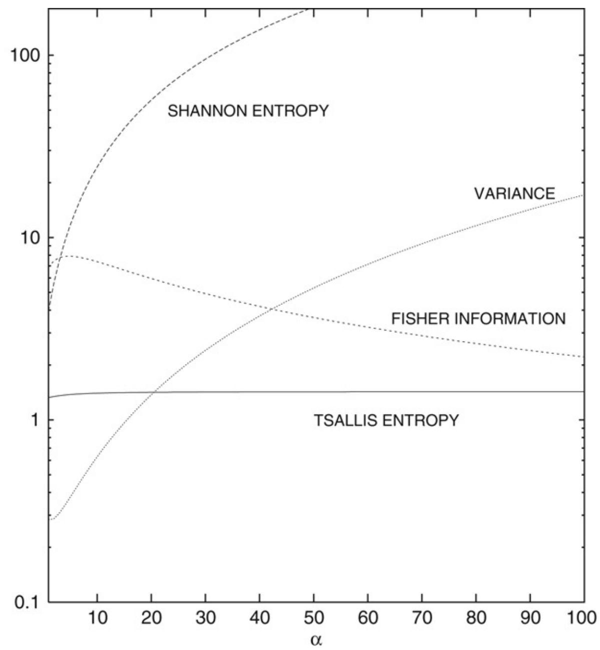

Fig. 3. Variance, Fisher information and Shannon and Tsallis (with $q = 1.7$) entropies in the three-dimensional maxtent problem with constraint $\langle r^{\alpha} \rangle$ as functions of the expectation order α in the three-dimensional case ($D = 3$). Atomic units ($e = \hbar = m_e = 1$) are used.

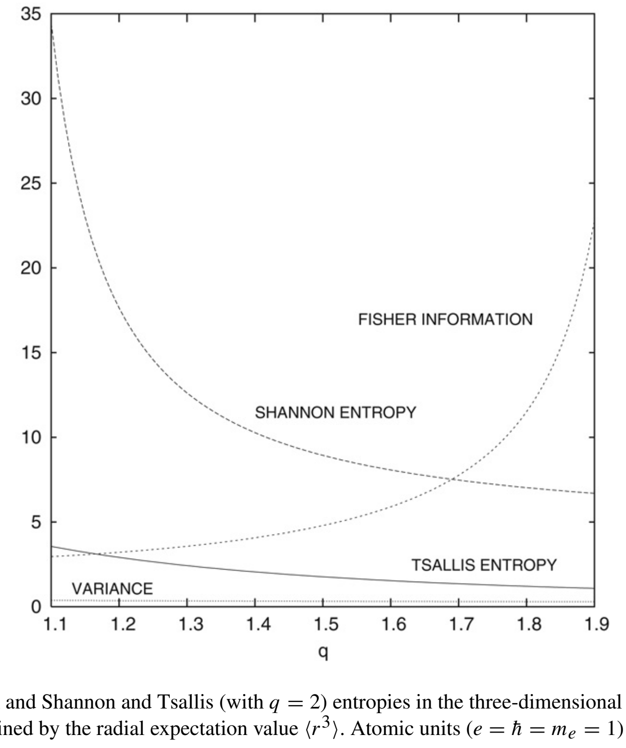

Fig. 4. Variance, Fisher information and Shannon and Tsallis (with $q = 2$) entropies in the three-dimensional maxtent problem as functions of the non-extensivity parameter q constrained by the radial expectation value $\langle r^3 \rangle$. Atomic units ($e = \hbar = m_e = 1$) are used.

measures are logarithmic (Shannon), power-like (Tsallis) and gradient (Fisher) functionals of the probability density; so, whilst the former two have a global character as the variance, the latter has a property of locality. It is worth noticing that the resulting Shannon maximizer density and Fisher minimizer density have an exponential form, in contrast to the Tsallis maximizer density which follows a power law.

We have investigated the spreading properties of the extremizer density associated to the three extremum information problems mentioned above (i.e., maxent, minfinf and maxtent). We have obtained the mutual functional relations and the explicit expressions of the variance, the extremized entropy and the other two information-theoretic measures of the extremizer density in terms of the moment constraints and the dimensionality of the system under consideration. Moreover, the D-dimensional maxent problem and maxtent problem with the constraints $(a_0, a_1) = (1, \langle r^\alpha \rangle)$ are numerically examined. It is found, in particular, that for the maximum entropy density the global measures increase with the expectation order α, while the Fisher information decreases. All the measures have a convex parabolic dependence on the dimensionality.

The existence condition for the D-dimensional maxent problem with the constraints $(a_0, a_1, a_2) = (1, \langle r^\alpha \rangle, \langle r^\beta \rangle)$ for $1 - D < \alpha < \beta$ and $\beta > 0$, is also obtained, extending to D dimensions and to arbitrary radial expectation values with non-necessarily consecutive orders the one-dimensional results of Dowson–Wragg for the two-first-moment constraints [20].

Finally let us point out some related open problems because of their intrinsic and technological relevance. First, to find the existence condition of the D-dimensional maxent problem (i) with the constraints $(1, \langle r^\alpha \rangle, \langle r^\beta \rangle, \langle r^\gamma \rangle)$, $\gamma > \beta > \alpha$ to generalize the one-dimensional Kociszewski's results [21] for the first three moments of lowest orders, (ii) with angular constraints, particularly of the type $\langle (\cos\theta)^\alpha \rangle$ and/or $\langle (\sin\theta)^\alpha \rangle$, and (ii) with mixed data such as $(\langle r^2 \rangle, \langle r^2 (\cos\theta)^2 \rangle)$. Second, to characterize the solutions and to obtain the existence conditions of the minfinf problem with the constraints $(1, \langle r^\alpha \rangle)$, where α is an arbitrary non-negative number. Third, to derive the existence conditions of the one-dimensional maxtent problem with the constraints $(1, \langle x^\alpha \rangle)$ and then to generalize it to D dimensions.

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