Reconstruction of a density from its entropic moments

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Abstract. We describe a general reconstruction method of the density of a physical system from a finite number of entropic moments. These statistical quantities, which are integrals of the density to a power $\alpha \in \mathbb{R}$, may also represent some fundamental and/or experimentally accessible quantities of quantum-mechanical systems for specific values of α. We take advantage of the strategy recently used by us to solve the Hausdorff and Stieltjes entropic moment problems, where the main role is played by the inverse function of the density. In our method we first calculate such inverse function by use of an algorithm of minimization of the Fisher information measure of the density, and then we invert it. Two particular cases are discussed to illustrate the applicability of the method.

INTRODUCTION

The explicit determination of a density function from some known data about it is a basic inverse question posed in numerous scientific areas from statistics and analysis to physics. When these data are moments of a certain type (moments around the origin, central moments, factorial moments, absolute moments,...), the proof of the mere existence of the density is the aim of the moment problem of that type. Only for constructive proofs, what occurs very rarely, the moment problem technique is able to supply an explicit expression for the density. Methods to reconstruct the density from moments of almost any type abound in the literature [1- 10].

Recently we have posed and constructively solved the so-called entropic moment problem [11], which gives the necessary and sufficient conditions for the existence of a one-dimensional density provided the homogeneous density functionals called entropic moments (see below) are known. This problem, which has been shown for the Hausdorff case (i. e. for a density with a bounded set), is here extended to the Stieltjes case in Section 2. Therein, the generalization to D-dimensions is also pointed out. Finally, in Section 3 a practical method of reconstruction of the density from a finite number of entropic moments is discussed by closely following the lines of our paper [11].

The ordinary problem of moments [12, 13] asks when a given sequence of complex numbers may be represented as the moments around the origin of a non-negative measure, defined on the real line (Hamburger), on a half-line (Stieltjes), on a finite interval (Hausdorff) or on the unit circumference (the trigonometric moment problem). This is a classical topic in analysis which has illuminated an extraordinary number of scientific subjects from both standpoints, theoretical [12- 14] and applied [3, 7, 14, 15]. In particular, it has been used in many-body physics for the determination of rigorous re-

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lationships among physical quantities of many-particle systems within the framework of the density functional theory as well as in the design of algorithms for simulating fermionic systems [8, 15, 16].

The problem of entropic moments differs from the ordinary moment problem above mentioned in that it does not consider the moments-around-the-origin of a density function $\rho(x)$ on a set K, defined by

$$\mu_n = \int_K x^n \rho(x) dx \tag{1}$$

but the quantities

$$\omega_n = \int_K [\rho(x)]^n dx \tag{2}$$

which are called *frequency moments* of $\rho(x)$, $x \in K$, in probability and statistics [17-21]. It happens that estimators based on frequency moments are, at times, much better than the ordinary moment estimates for certain frequency curves [18, 19]. Moreover, the frequency moments are fairly efficient in the range where the ordinary moments are very inefficient [22]. This is so in some cases where the range K is unbounded and the density is poorly known [20].

It is interesting to remark that the frequency moments ω_n are location independent when $K = \mathbb{R}$ (Hamburger case); that is, two densities differing only in location have identical frequency moments. In these cases, the location parameter can be provided by the mode, the median or any other appropriate quantity [21].

We shall call the quantities ω_n as the *entropic moments* of the density function $\rho(x)$, because they are closely connected to the so-called Renyi and Tsallis entropies of $\rho(x)$ defined [23, 24] by

$$S_q^R := \frac{1}{1-q} \ln \int_K [\rho(x)]^q dx; \quad q > 0, \quad q \neq 1, \quad \int_K \rho(x) dx = 1 \tag{3}$$

and

$$S_q^T := \frac{1}{q-1} [1 - \int_K [\rho(x)]^q dx]; \quad q > 0, \quad q \neq 1, \quad \int_K \rho(x) dx = 1 \tag{4}$$

respectively. The entropic adjective allows us to identify more appropriately the moments ω_n from the other type of moments (moments around the origin, central moments, factorial moments, absolute moments, ...) of a frequency distribution.

In addition, the entropic moments ω_α for the three-dimensional case (see Sect. 2.3) have various physical meanings depending on the nature of the associated density function ρ (charge density, momentum density, ...). Indeed, they characterize some density functionals which describe certain physical quantities of fundamental and/or experimentally accessible character such as, up to a constant factor, the Thomas-Fermi kinetic energy ($\omega_{5/3}$), the Dirac exchange energy ($\omega_{4/3}$) and the electron average density (ω_2) of many-electron systems; see, e. g. Ref. [16].

THE HAUSDORFF AND STIELTJES ENTROPIC MOMENT PROBLEMS

The existence theorems associated to the Hausdorff and Stieltjes entropic moment problems and its generalization to D dimensions are given here. The constructive character of these theorems is emphasized for the Hausdorff problem.

The Hausdorff entropic moment problem.

Let $K = [0, a]$ with $a > 0$, and $\mathscr{M}(K)$ the set of real density functions $f(x)$ bounded on K and such that $f(0) = 1$ and $f(a) = 0$. We have obtained the following result for this set of functions.

Theorem 1 *The necessary and sufficient conditions which the given sequence of positive numbers $\omega_0, \omega_1, \ldots, \omega_n, \ldots$ must satisfy in order that a positive, decreasing and differentiable (a. e.) function $f(x), x \in K$, having these entropic moments (2) may exist, are given by*

$$\Sigma^k \frac{\omega_{m+1}}{m+1} \geq 0 \quad \textit{and} \quad \Sigma^k \omega_m \geq 0 \tag{5}$$

for $k, m = 0, 1, 2, \ldots$, and being

$$\Sigma^k \omega_m = \omega_m - \binom{k}{1} \omega_{m+1} + \cdots + (-1)^k \omega_{m+k}$$

Proof. Let us firstly prove the sufficiency condition. For convenience we adopt the notations

$$\mu_m \equiv \frac{\omega_{m+1}}{m+1}, \quad \nu_m \equiv \omega_m; \quad m = 0, 1, 2, \ldots$$

so that $\nu_m = m\mu_{m-1}$ for $m = 1, 2, \ldots$. If conditions (5) are fulfilled, the Hausdorff theorem for the ordinary moment problem on the interval $[0, 1]$ allows us to state [12] that

$$\exists! z(t) \geq 0 \text{ on } [0,1] \text{ such that } \int_0^1 t^m z(t) dt = \nu_m$$

and

$$\exists! g(t) \geq 0 \text{ on } [0,1] \text{ such that } \int_0^1 t^m g(t) dt = \mu_m$$

On the other hand, let us define

$$h(t) = \int_t^1 z(s) ds, \quad t \in [0, 1]$$

So, $h'(t) = -z(t)$. Moreover, starting from the definition of the moments of $h(t)$ and integrating by parts, it is observed that they exactly coincide with those of $g(t)$; then both functions are equal. Thus $g(t)$ is a decreasing function since $g'(t) = -z(t)$. We can define

$f(x)$ as its inverse with $x \in [g(1)=0, g(0)=a]$, which will be positive, decreasing and differentiable (a. e.). One should realize that in case that $g(t)$ is a constant $c > 0$ on some subintervals, this would provoke a jump discontinuity for $f(x)$ in $x = c$ and viceversa. Following the steps of Ref. [16], it is straightforward to obtain that

$$\int_0^a [f(x)]^m dx = v_m = \omega_m; \quad m = 0, 1, 2, \ldots$$

To prove necessity, we define the inverse of $f(x)$ as $h(t)$, $t \in [0,1]$, which is decreasing and differentiable (a. e.). A simple change of variable $t = f(x)$ allows us to find the following relationship between the entropic moments of $f(x)$ and the ordinary moments of $h(t)$:

$$\int_0^1 t^m h(t) dt = \frac{\omega_{m+1}}{m+1}, \quad m = 0, 1, 2, \ldots$$

Now we consider the function $z(t) = -h'(t)$, $t \in [0,1]$, and we realize that its ordinary moments are given by ω_m. Then, the direct application of the classical Hausdorff moment problem above mentioned leads us to the relations (5). □

The Stieltjes entropic moment problem

Let $K' = [0, \infty)$, and $M(K')$ the set of real density functions $f(x)$ bounded on K' and such that $f(0) = 1$. We can prove the following theorem in the same way as theorem 1, taking into account that now the auxiliary function $h(t)$ will be defined over $(0,1]$.

Theorem 2 *The necessary and sufficient conditions which the given sequence of positive numbers $\omega_1, \omega_2, \ldots, \omega_n, \ldots$ must satisfy in order that a positive, decreasing and differentiable (a. e.) function $f(x), x \in K'$, having these entropic moments 2 may exist, are given by*

$$\Sigma^k \frac{\omega_{m+1}}{m+1} \geq 0 \quad \text{and} \quad \Sigma^k \omega_m \geq 0 \tag{6}$$

for $k = 0, 1, 2, \ldots$ and $m = 1, 2, 3, \ldots$, and being

$$\Sigma^k \omega_m = \omega_m - \binom{k}{1} \omega_{m+1} + \cdots + (-1)^k \omega_{m+k}$$

Generalization to D dimensions

Let us now consider a spherically symmetric density function $\rho(r)$ on a D-dimensional sphere K of finite (Hausdorff) or infinite (Stieltjes) radius a. The corresponding frequency moments ω_n of the density $\rho(r)$ are now defined by

$$\omega_n = \Omega_D \int_0^a r^{D-1} [\rho(r)]^n dr$$

where $\Omega_D = 2\pi^{D/2}/\Gamma(D/2)$ is the D-dimensional solid angle and $r^{D-1} dr d\Omega_D$ the volume element. Then, the necessary and sufficient conditions of Theorems 1 and 2 are now given by

$$\Sigma^k \frac{D}{m+1} \omega_{\frac{m+1}{D}} \geq 0 \text{ and } \Sigma^k \omega_{\frac{m}{D}} \geq 0$$

The proof is carried out by following the same steps as in the previous theorems, although the function $f(r)$ is now given by

$$f(r) = [g^{-1}(r^D)]^D$$

instead of $f(r) = g^{-1}(r)$ (which corresponds to the particular case $D = 1$). Further details can be obtained from Ref. [16].

DENSITY RECONSTRUCTION

If the knowledge on a density $f(x)$ is restricted to a set of its entropic moments, rather than to the values of $f(x)$ over any subset or the whole set K, we can ask how we could reconstruct (if possible) the whole density from the knowledge of its entropic moments. In fact, associated to any moment problem there exists an inverse problem, namely that of the reconstruction of the corresponding density function. Moreover, in practical purposes we have at our disposal only a finite number of moments. The inverse Hausdorff (ordinary) moment problem given by equation (1), that is the determination of the density $\rho(x)$ from the moments around the origin $\{\mu_n\}_{n=0}^{\infty}$, was first proposed by Pafnuty Chebyshev [25]. It is a severely ill-conditioned problem because of the lack of a priori information and the large involved numerical instabilities [1- 6]. To avoid these instabilities, various regularization methods (Tikhonov, maximum-entropy methods, orthogonal-polynomials based methods,...) have been proposed; see [3] for a brief survey. The maximum-entropy method has been widely and efficiently used for scientific applications [3, 7- 9]. It consists in maximizing an entropic functional, and it allows us to find a density estimate which converges to the solution of the problem when the number of the involved moments increases.

Here we shall use a maximum entropy method to solve the inverse Hausdorff and Stieltjes entropic moment problems discussed in the previous section when the number of known entropic moments is finite. For illustration, let us restrict ourselves to the one-dimensional case. Based on the proof of Theorem 1 and 2, this method first computes the maximum-entropy estimate to the solution $z(t)$ of the inverse Hausdorff (Stieltjes) problem related to the sequence $\{\mu_n\}_{n=0}^{\infty}$ with $\mu_n \equiv \frac{\omega_{n+1}}{n+1}$. Then, the inverse of the estimated $z(t)$ is the desired approximated solution of our problem. Let us notice that, although we know that the asymptotic ($N \to \infty$) approach to $z(t)$ is inversible, the different N^{th} estimates to $z(t)$ may not have this property. In the case that there is not any inversible approach, our method is not applicable.

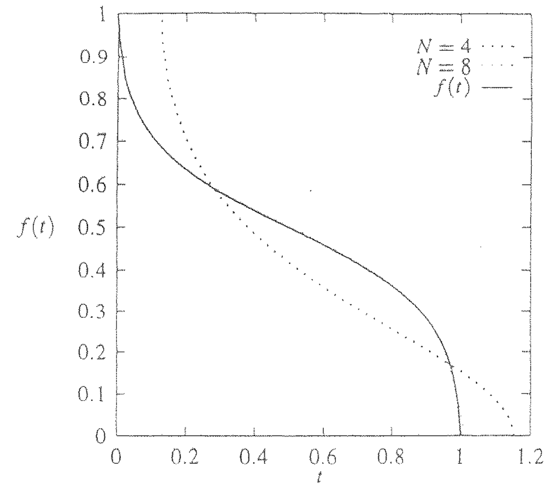

FIGURE 1. Density function $f(t) = \frac{1}{2} + \frac{1}{10} \ln\left(\frac{1}{At+B} - 1\right)$ and its estimates from the entropic moments ω_n, $n = 0, 1, \ldots, N$ with $N = 4$ and $N = 8$.

Although we may use any entropic functional to be maximized, we have chosen the Fisher information measure defined by

$$E_f \equiv \int_{[0,a]} \frac{[f'(x)]^2}{f(x)} dx$$

if $f(x) > 0$, and $E_f = 0$ if $f(x) \equiv 0$. Contrary to other entropic functionals (e. g., Boltzmann-Shannon information entropy, Burg entropy, positive L^2 entropy), this choice has the advantage of taking into account information from the derivative of the function, what is expected to have a strong smoothing effect on the estimate. In doing so we follow the operation lines of Borwein, Limber and Noll [10] to which we refer for further details.

To illustrate the method and the rate of convergence of the Fisher-information estimates for a function $f(t)$ on $[0,1]$ from its first $N+1$ entropic moments $\omega_n = \int_0^1 [f(t)]^n dt$, $n = 0, 1, \ldots N$, we have represented in Figure 1 the exact values and the Fisher estimates for the cases $N = 4$ and $N = 8$ of a specific function, namely

$$f(t) = \frac{1}{2} + \frac{1}{10} \ln\left(\frac{1}{At+B} - 1\right), \text{ with } A = \frac{1}{1+e^5} \text{ and } B = \frac{1}{1+e^{-5}} - \frac{1}{1+e^5}. \quad (7)$$

We visually notice in the figure the fast convergence of the method for this function as well as the good precision reached with nine entropic moments.

We show in Figure 2 the reconstruction of the function $f(t)$ given by Eq. (7) from the first $N+1$ moments around the origin $\mu_n = \int_0^1 f(t) t^n dt$ in the cases $N = 4$ and 8. The

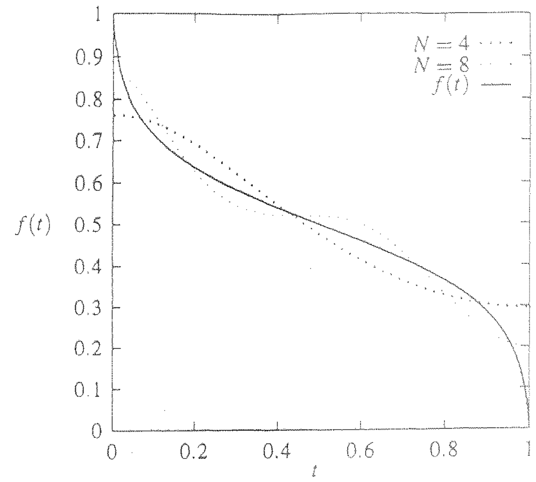

FIGURE 2. Density function $f(t) = \frac{1}{2} + \frac{1}{10} \ln\left(\frac{1}{At+B} - 1\right)$ and its estimates from the entropic moments μ_n, $n = 0, 1, \ldots, N$ with $N = 4$ and $N = 8$.

comparison of the two figures for each pair of corresponding cases, illustrates that there are functions that may be better estimated or reconstructed from the entropic moments (2) than from the ordinary moments (1). Needless to say that there exist other functions where the reciprocal situation occurs; consider, for example, the inverse of the function $f(t)$ given by Eq. (7)

Finally, in Figure 3 we show the exact value and the reconstruction from the entropic moments $\omega_i = \int_0^\infty [f(t)]^i dt$, $i = 1, \ldots, N$ of the density

$$f(t) = \ln\left(1 + \frac{1}{(1+t^2)}\right) / \ln 2. \quad (8)$$

We have represented the Fisher estimates for the cases $N = 5$ and $N = 11$. In this example it is not possible the reconstruction of the function $f(t)$ from any set of moments around the origin due to the fact that these moments $\mu_n = \int_0^\infty f(t) t^n dt$ does not exist for $n \geq 1$.

SUMMARY

We describe a practical procedure for the reconstruction of a density from a given finite number of entropic moments. These quantities, which are a special kind of homogeneous density functionals [26], have at times some specific physical meaning. This procedure has two steps. First it calculates the inverse function of the density by means of a minimization algorithm of the Fisher information measure, and then the desired density

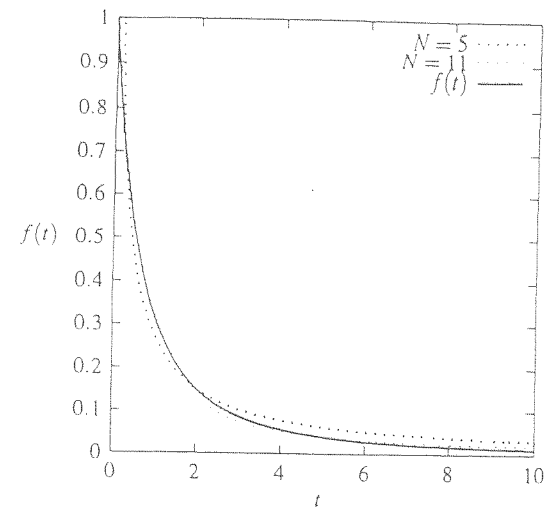

FIGURE 3. Density function $f(t) = \ln\left(1 + \frac{1}{(1+t^2)}\right) / \ln 2$. and its estimates from the entropic moments ω_n, $n = 1, \ldots, N$ with $N = 5$ and $N = 11$.

is numerically obtained by inversion. Two specific cases are used for illustration and to show the applicability for the procedure.

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