

Pathway Model and Nonextensive Statistical Mechanics

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Abstract The established technique of eliminating upper or lower parameters in a general hypergeometric series is profitably exploited to create pathways among confluent hypergeometric functions, binomial functions, Bessel functions, and exponential series. One such pathway, from the mathematical statistics point of view, results in distributions which naturally emerge within nonextensive statistical mechanics and Beck-Cohen superstatistics, as pursued in generalizations of Boltzmann-Gibbs statistics.

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1 Introduction

The celebrated Boltzmann-Gibbs (BG) statistical mechanics, in its classical version, typically holds for many-body systems whose microscopic nonlinear dynamics is *ergodic*, either in the entire Γ phase space, or in at least one of its subspaces determined by relevant symmetry considerations. For example, for classical ferromagnets (say the infinite-spin Heisenberg ferromagnet in three dimensions) exhibiting a second order phase transition, ergodicity applies to the entire Γ phase space for temperatures above the critical one, and only to one of the subspaces generated by the corresponding breakdown of symmetry for temperatures below the critical one. Analogous requirements must be satisfied for quantum systems, where the role of the Γ phase space is played by the appropriate Hilbert or Fock spaces. A fundamental question arises for the plethora of physical systems which violate ergodicity in the sense just mentioned: *Is it possible to have for them a statistical mechanical theory similar to the usual one, and also connected to thermodynamics?*

It was suggested in 1988 (1) that this is indeed possible based on a simple hypothesis, namely the generalization of the BG entropy, given (say in its continuous version) by

$$S_{BG} = \int dx \cdot p(x) \ln p(x) \quad (1)$$

The generalization that was then proposed is given by

$$S_q = k \frac{1 - \int dx [p(x)]^q}{q-1} \quad (q \in \mathfrak{R}; S_1 = S_{BG}) \quad (2)$$

Before proceeding, let us mention here that entropic forms generalizing the Boltzmann-Gibbs-Shannon-von Neumann one has in

fact a long history in information theory, cybernetics and related areas (2, 3). Indeed, along the years, the same or similar or related forms have been introduced again and again as possible mathematical functionals. For example, the Renyi form (defined here below) has been useful as a characterization of multifractal geometry. It appears, however, to be inadequate for thermodynamics since it is not concave for an important range of its parameter q , namely for $q > 1$, where many physical systems exist. Although independently postulated, the entropic functional S_q turns out to be mathematically very close to those of Havrda-Charvat, Daroczy, Lindhard-Nielsen, and Mathai-Rathie. In physics, this type of functional was used (1, 4, 5) to propose the generalization of the celebrated Boltzmann-Gibbs theory, including the Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein distributions, as well as their connections to thermodynamics.

The extremization of S_q under appropriate constraints (nonvanishing first moment, or nonvanishing second moment if the first moment is zero) yields the q -exponential form ($p(x) \propto e_q^{-\beta_1 x}$, or $p(x) \propto e_q^{-\beta_2 x^2}$ respectively), where $e_q^z \equiv [1 + (1-q)z]_+^{1/(1-q)}$, being $[u]_+ = u$ if $u > 0$, and zero otherwise; $e_1^z = e^z$. These functions belong to a complex net of related and more general functions, whose systematic discussion constitutes the aim of the present paper.

The above q -exponential functions emerge in a considerable amount of natural, artificial and social systems. For example (i) The velocity distribution of (cells of) *Hydra viridissima* follows a $q=3/2$ PDF (6); (ii) The velocity distribution of (cells of) *Dictyostelium discoideum* follows a $q=5/3$ PDF in the vegetative state

and a $q=2$ PDF in the starved state (7); (iii) The velocity distribution in defect turbulence (8); (iv) The velocity distribution of cold atoms in a dissipative optical lattice (9); (v) The velocity distribution during silo drainage (10, 11); (vi) The velocity distribution in a driven-dissipative 2D dusty plasma, with $q=1.08\pm 0.01$ and $q=1.05\pm 0.01$ at temperatures of 30000°K and 61000°K respectively (12); (vii) The spatial (Monte Carlo) distributions of a trapped $^{136}\text{Ba}^+$ ion cooled by various classical buffer gases at 300 K (13); (viii) The distributions of price returns and stock volumes at the stock exchange, as well as the volatility smile (14, 15, 16, 17); (ix) The distributions of returns of magnetic field fluctuations in the solar wind plasma as observed in data from Voyager 1 (18) and from Voyager 2 (19); (x) The distributions of returns in the Ehrenfest's dog-flea model (20, 21); (xi) The distributions of returns in the coherent noise model (22); (xii) The distributions of returns of the avalanche sizes in the self-organized critical Olami-Feder-Christensen model, as well as in real earthquakes (23); (xiii) The distributions of angles in the HMF model (24); (xiv) The distribution of stellar rotational velocities in the Pleiades (25); (xv) The relaxation in various paradigmatic spin-glass substances through neutron spin echo experiments (26); (xvi) Various properties directly related with the time dependence of the width of the ozone layer around the Earth (27); (xvii) The distribution of transverse momenta in high energy collisions of electron-positron, proton-proton, and heavy nuclei (e.g., Pb-Pb and Au-Au) (28, 29, 30, 31, 32, 33, 34), the flux of solar neutrinos (35), and the energy distribution of cosmic rays (36); (xviii) Various properties for conservative and dissipative nonlinear dynamical systems (37, 38, 39, 40, 41, 42, 43, 44, 45); (xix) The degree distribution of (asymptotically) scale-free networks (46, 47), and others.

The length of this list illustrates the relevance of a deeper understanding of the connections of the q -exponential functions with other functions (derivable or not from various entropic forms) within a variety of pathways, some of which also emerge in applications. This leads us to the next Section.

2 Hypergeometric Series

Consider a confluent hypergeometric series

$${}_1F_1(a; b; x) = \sum_{r=0}^{\infty} \frac{(a)_r}{(b)_r} \frac{x^r}{r!} \quad (3)$$

$$(c)_r = c(c+1)\dots(c+r-1), \quad (c)_0 = 1, c \neq 0$$

If we want to remove the denominator parameter, then a well known technique in the area of special functions is to replace x by bx and then take the limit when $b \rightarrow \infty$. Due to the fact that

$$\lim_{b \rightarrow \infty} \frac{b^r}{(b)_r} = \lim_{b \rightarrow \infty} \frac{b^r}{b(b+1)\dots(b+r-1)} \quad (4)$$

we have

$$\lim_{b \rightarrow \infty} {}_1F_1(a; b; bx) = {}_1F_0(a; ; x) = (1-x)^{-a}, \quad |x| < 1 \quad (5)$$

Hence a pathway between the binomial function $(1-x)^{-a}$ and the ${}_1F_1$ series is given by the limit of $\frac{b^r}{(b)_r}$

when $b \rightarrow \infty$. Going the other way one can build up a bridge between ${}_1F_0$ and ${}_1F_1$ by introducing $\frac{b^r}{(b)_r}$ into a

${}_1F_0$ series. That is,

$$\sum_{r=0}^{\infty} (a)_r \frac{x^r}{r!} \approx \sum_{r=0}^{\infty} \frac{(a)_r}{(b)_r} \frac{(bx)^r}{r!} = {}_1F_1(a; b; bx) \quad \text{for large } b \quad (6)$$

Similarly one can go back and forth from a Bessel function ${}_0F_1$ to a ${}_1F_0$ or to a ${}_0F_0$ which is the exponential series. Let us look at going from a binomial series to an exponential series.

$$(1-x)^a = \sum_{r=0}^{\infty} (a)_r \frac{x^r}{r!} \Rightarrow \lim_{a \rightarrow \infty} \frac{(a)_r}{r!} \left(\frac{x}{a}\right)^r = \sum_{r=0}^{\infty} \frac{x^r}{r!} = e^x \quad (7)$$

In other words,

$$e^{-cx} = \lim_{a \rightarrow \infty} \sum_{r=0}^{\infty} \frac{(-a)_r}{r!} \left(\frac{cx}{a}\right)^r = \lim_{a \rightarrow \infty} \left(1 - \frac{cx}{a}\right)^a = \lim_{a \rightarrow 1} [1 - c(1-\alpha)x]^{1/(1-\alpha)} \quad (8)$$

Thus a pathway between the exponential function $e^{-cx}, c > 0$ and the binomial function $[1 - c(1-\alpha)x]^{1/(1-\alpha)}$ can be created with the help of the pathway parameter α . When α is very close to 1, the binomial and exponential functions are very close to each other and they will be farther apart when α is away from 1. Observe that $e^{-cx}, c > 0, 0 < x < \infty$ and $[1 - c(1-\alpha)x]^{1/(1-\alpha)},$

$0 < x < \frac{1}{c(1-\alpha)}, c > 0, \alpha < 1$ or $[1 + c(\alpha-1)x]^{-1/(\alpha-1)}, c > 0, \alpha > 1, x > 0$ are integrable functions and hence one can create statistical densities out of them. Thus a pathway connecting the three types of densities

$$f_1(x) = \lambda_1 x^\gamma e^{-cx}, \quad c > 0, x > 0$$

$$f_2(x) = \lambda_2 x^\gamma [1 - c(1-\alpha)x]^{1/(1-\alpha)}$$

$$c > 0, \alpha < 1, 0 < x < \frac{1}{c(1-\alpha)} \quad (9)$$

$$f_3(x) = \lambda_3 x^\gamma [1 + c(\alpha-1)x]^{-1/(\alpha-1)}$$

$$c > 0, \alpha > 1, 0 < x$$

where $\lambda_1, \lambda_2, \lambda_3$ are the appropriate normalizing constants, can be created with the help of the pathway parameter α . Observe that in f_1, f_2 and f_3 one can replace x by $|x|, -\infty < x < \infty$ or x by $|x|^\delta, \delta > 0$ and still all the three forms can create densities. Note that f_1 stays in the exponential/gamma type densities, f_2 stays as a type-1 beta form and f_3 a type-2 beta form. By exploiting these observations, Mathai has introduced (48) the pathway model connecting exponential type and binomial type functions.

Another rich area is the class of Bessel functions. As indicated above, a Bessel function can be written in terms of a hypergeometric function ${}_0F_1(;b;x)$ and one can remove the denominator parameter b by replacing x by bx and then using the limit $b \rightarrow \infty$. In other words,

$$\lim_{b \rightarrow \infty} {}_0F_1(;b;-bx) = {}_0F_0(;;-x) = e^{-x} = \lim_{\alpha \rightarrow 0} {}_0F_1\left(\frac{1}{1-\alpha}; -\frac{x}{1-\alpha}\right) \tag{10}$$

Thus α can provide a pathway between Bessel functions and exponential functions. If the exponential form gives the stable situation, then the parameter α will provide a pathway between stable and chaotic situations. So far this area is not explored. In this connection one can obtain an interesting result by using the integral representation of a Gauss hypergeometric function ${}_2F_1$, namely,

$${}_2F_1(a,b;c;-z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 x^{a-1} (1-x)^{c-a-1} (1+zx)^{-b} dx \tag{11}$$

$\Re(a) > 0; \Re(c-a) > 0; |z| < 1$

Hence,

$${}_1F_1(a;c;-z) = \lim_{b \rightarrow \infty} {}_2F_1(a,b;c;-\frac{zx}{b}) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 x^{a-1} (1-x)^{c-a-1} (1+\frac{zx}{b})^{-b} dx = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 x^{a-1} (1-x)^{c-a-1} e^{-zx} dx \tag{12}$$

$|x| < 1, |z| < 1$

Thus a pathway between ${}_1F_1$ and ${}_2F_1$ is given by (12). Many such results can be obtained by using this technique of eliminating one or more numerator or denominator parameters from a general hypergeometric series ${}_qF_q$.

Thus for a real scalar random variable x , the pathway density can be written in the following form:

$$f_4(x) = \lambda_4 |x|^\gamma [1 - a(1-\alpha)|x|]^{1-\alpha} \tag{13}$$

$a > 0, 1 > a(1-\alpha)|x|, \alpha < 1$

A more general form of the pathway density is the following:

$$f_5(x) = \lambda_5 |x|^\gamma [1 - a(1-\alpha)|x|^\delta]^{1-\alpha} \tag{14}$$

where $\alpha > 0$ and $(\eta, \delta, \gamma, \alpha)$ are such that $f_5(x)$ is normalizable. A large number of commonly used statistical densities can be seen to be particular cases of (14), details may be seen in (48, 49, 50). From the point of view of mathematical statistics, nonextensive statistics (1, 4, 5, 52, 53, 54) with constant density of states is a particular case of (14) for $\gamma = 0, x > 0$. The case $\gamma \neq 0$ can be seen as the particular case when the density of states is given by a power law (which is quite frequent in many physical systems). One of the

forms of the Beck-Cohen superstatistics (55, 56) is a special case of (14) for $\gamma = 0, \alpha > 1, x > 0$.

3 Density from Optimization of Entropy

In situations when an appropriate density is selected, one guiding principle is the maximization of entropy. Entropy or a measure of uncertainty in a scheme or "information" in a scheme is traditionally measured by Shannon entropy. Consider a discrete distribution $P' = (p_1, \dots, p_k)$, $p_i > 0, i = 1, \dots, k$ $p_1 + \dots + p_k = 1$ This may also be looked upon as the sample space or the sure event S is partitioned into mutually exclusive and totally exhaustive A_1, \dots, A_k events $A_1 \cup \dots \cup A_k = S, A_i \cap A_j = \emptyset$ for all i and $j, i \neq j$ with the probability of the event A_i , denoted by $p_i = \Pr(A_i); i = 1, \dots, k$. If any p_i is allowed to take the value zero also, then $p_i \geq 0; i = 1, \dots, k$.

Shannon entropy on this scheme is $S(P)$, where

$$S(P) = -\sum_{i=1}^k p_i \ln p_i \tag{15}$$

When a $p_i = 0$ $p_i \ln p_i$ is to be interpreted as zero. Several characterization theorems on $S(P)$ or axiomatic definitions may be seen from (3). There are several extensions or generalizations of the measure $S_k(P)$. Classical generalizations in information theory are the Havrda-Charvát measure $H_{k,\alpha}^{\alpha}(P)$, and the Rényi measure $R_{k,\alpha}(P)$, where

$$H_\alpha(P) = \frac{\sum_{i=1}^k P_i^\alpha - 1}{2^{1-\alpha} - 1}; R_\alpha(P) = \frac{\sum_{i=1}^k P_i^\alpha}{1-\alpha}; \alpha \neq 1, \alpha > 0 \tag{16}$$

These are generalizations in the sense that when $\alpha \rightarrow 1$, $H_\alpha(P) \rightarrow S(P)$ and $R_\alpha(P) \rightarrow S(P)$. Out of these, $S(P)$ and $R_\alpha(P)$ are additive and $H_\alpha(P)$ is nonadditive. The additivity property is defined as follows: Consider a bivariate discrete distribution in the sense $p_{ij} > 0, i = 1, \dots, m; j = 1, \dots, n$ such that $\sum_{i=1}^m \sum_{j=1}^n p_{ij} = 1$. What happens if there is the product probability property (PPP), which in statistical literature is known as statistical independence. What happens is that $p_{ij} = p_i q_j, p_1 + \dots + p_m = 1; q_1 + \dots + q_n = 1$ or there is the product probability property. When PPP holds, if the entropy in the joint distribution $(P; Q) = (p_{ij}); i = 1, \dots, m; j = 1, \dots, n$ is the sum of the entropies on P and Q then we say that there is additivity. It is easily seen that there is additivity in $S(P)$ and $R_\alpha(P)$, that is,

$$R_\alpha(P, Q) = R_\alpha(P) + R_\alpha(Q) \text{ and } S(P, Q) = S(P) + S(Q) \tag{17}$$

This additivity holds due to the logarithmic nature of the function in $S_k(P)$ and $R_\alpha(P)$ and the logarithm of a product of positive quantities being the sum of the logarithms. It is explained in (49) that logarithmic function enters into an entropy measure due to the recursivity axiom which leads into a logarithmic function necessarily.

In the following we will concentrate on the q -type of generalization of entropy measures, and review, for completeness, how the extremization of generalized entropies yields the probability density which correspond to stationary states. It was postulated (1) the entropy

$$S_\alpha(P) = \sum_{i=1}^k \frac{p_i^{\alpha-1}}{1-\alpha}; \quad \alpha \neq 1, \alpha > 0 \quad (18)$$

To avoid confusion, let us mention that, in most of the literature of nonextensive statistical mechanics, the index α is noted q , and the entropy S_α is noted S_q . The Shannon form is obtained as the $q \equiv \alpha \rightarrow 1$ limit.

The normalizing factor in Havrda-Charvát entropy $H_\alpha(P)$, namely $(2^{1-\alpha} - 1)$, is replaced by $(1-\alpha)$. In the continuous case, the nonadditive entropy upon which nonextensive statistical mechanics is built is then,

$$S_\alpha(f) = \frac{\int_x [f(x)]^\alpha dx - 1}{1-\alpha}; \quad \alpha \neq 1, \alpha > 0 \quad (19)$$

Over all functions f , what is that particular f which will optimize the nonadditive entropy in (19)? If calculus of variation principle is used, then the Euler equation for optimizing the entropy S_α under the restrictions

$$\int_x f(x) dx = 1 \quad \text{and} \quad \int_x x f(x) dx = E(x) = \text{fixed} \quad (20)$$

$$f(x) \geq 0, \forall x$$

will yield the equation,

$$\frac{\partial}{\partial x} [f^\alpha - \lambda_1 f - \lambda_2 x f] = 0 \Rightarrow \Rightarrow f = (\lambda + \lambda_2 x)^{\frac{1}{\alpha-1}} = \lambda [1 + (\alpha-1)x]^{\frac{1}{\alpha-1}} \quad (21)$$

by taking $\frac{\lambda_2}{\lambda_1} = \alpha - 1$ and $\frac{\lambda_1}{\lambda_1} = \lambda$, where λ_1 and λ_2 are

Lagrangian multipliers. The quantity λ can act as the normalizing constant. The condition $E(x) = \text{fixed}$, where E denotes the expected value, can be interpreted as the principle of conservation of the quantity x . When $\alpha \rightarrow 1$, $f = \lambda e^{-x}$ which is an exponential function. The derivation in (21) does not yield nonextensive statistics in its most convenient form. But (21) gives an exponential function when $\alpha \rightarrow 1$ and this exponential function is directly related to what is known in the literature as the q -exponential function. In order to circumvent some difficulties, it was replaced ((1, 5)) the second condition that $E(x)$ is fixed by fixing the expected value in the escort distribution. The escort density is given by

$$g(x) = \frac{f^\alpha(x)}{\int_x f^\alpha(x) dx} \quad (22)$$

and then nonextensive statistics has the form

$$f = \lambda [1 - (1-\alpha)x]^{\frac{1}{1-\alpha}} \quad (23)$$

This form can produce densities for $\alpha < 1$, $\alpha > 1$ and $\alpha \rightarrow 1$ and further, this form satisfies the power-law differential equation

$$\boxed{x f'(x) = -f(x)} \quad (24)$$

One can introduce a general measure of entropy, which in the discrete and continuous cases are denoted by $M_\alpha(P)$ and $M_\alpha(f)$ respectively, where

$$M_\alpha(P) = \frac{\sum_{i=1}^k p_i^{2-\alpha} - 1}{\alpha - 1}; \quad M_\alpha(f) = \frac{\int_x [f(x)]^{2-\alpha} dx - 1}{\alpha - 1} \quad (25)$$

$$\alpha \neq 1, \alpha < 2$$

A characterization of $M_\alpha(P)$ is given in (49) (see also (49, 50, 51)). If $M_\alpha(f)$ is optimized under the conditions that $E(x) = \text{fixed}$ and that $f(x)$ is a density, then the Euler equation becomes

$$\frac{\partial}{\partial x} [f^{2-\alpha} - \lambda_1 f + \lambda_2 x f] = 0 \Rightarrow \Rightarrow f = \lambda [1 - a(1-\alpha)x]^{-\frac{1}{1-\alpha}} \quad (26)$$

where $a > 0$; $1 - a(1-\alpha)x > 0$ and $\frac{\lambda_2}{\lambda_1}$ is taken as

$a(1-\alpha)$ with $a > 0$ and $\left(\frac{\lambda_1}{2-\alpha}\right)^{\frac{1}{1-\alpha}}$ is taken as λ . Observe

that (26) readily gives densities for $\alpha < 1, \alpha > 1$ and $\alpha \rightarrow 1$. Further, the entropy itself can be expressed as

$$M_\alpha(P) = \frac{E(p^{1-\alpha}) - 1}{\alpha - 1}; \quad M_\alpha(f) = \frac{E[f^{1-\alpha}(x)] - 1}{\alpha - 1} \quad (27)$$

where $(1-\alpha)$ can be interpreted as the strength of information in f and this expected value is also associated with Kerridge's "inaccuracy" measure. As a simple mathematical remark, let us mention that if the entropy in (25) is optimized in an *ad hoc* manner, namely that for all $f(x)$ such that $f(x) \geq 0$ for all,

$x > 0, \int_x f(x) dx < \infty, \int_x [x^{\gamma(1-\alpha)}] f(x) dx = \text{fixed}$ and

$\int_x [x^{\gamma(1-\alpha)+\delta}] f(x) dx = \text{fixed}$ then we end up with the density

$$f(x) = \lambda x^\gamma [1 - a(1-\alpha)x^\delta]^{-\frac{1}{1-\alpha}}; \quad a > 0, -\infty < \alpha < \infty \quad (28)$$

and λ is the normalizing constant. Through trivial changes in the notation, this expression recovers that of (14).

As already mentioned, for $\gamma = 0, \delta = 1$ in (28) one has a particular case of nonextensive statistics. For $a > 0, \alpha > 1$ in (28) one has a particular case of the superstatistics of Beck and Cohen (55, 56). For $\alpha < 1$, (28) gives a generalized type-1 beta form for $0 < x^\delta < 1/a(1-\alpha)$, and for $\alpha > 1$, (28) gives a generalized type-2 beta form. Superstatistics can produce only the type-2 beta form and not the type-1 beta form.

4 Final Remarks

We utilize the established technique of eliminating upper or lower parameters in a general hypergeometric series to create pathways among confluent hypergeometric functions, binomial functions, Bessel functions, and exponential series. Mathai's pathway, from the mathematical statistics point of view, results in distributions which also emerge within nonextensive statistics and Beck-Cohen superstatistics, pursued as generalizations of Boltzmann-Gibbs statistics. It was shown that this pathway model can also be

derived by optimizing a generalized entropic measure. Through Mathai's pathway approach, exponential and binomial type functions are connected through the pathway model parameter. The same pathway model also leads to a link between Bessel functions and exponential functions. The pathway model covers statistical densities emanating in nonextensive statistics and Beck-Cohen superstatistics as special cases of (28). Related results are obtained by optimizing a general measure of entropy in (26) (see also (1, 5, 51)). An open problem is identified that would allow to entropically derive a general density of the form (28) within physically meaningful circumstances. Summarizing, relations between Mathai's pathway model and nonextensive statistics and Beck-Cohen superstatistics were exhibited.

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