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Computational applications of nonextensive statistical mechanics[☆]

Constantino Tsallis [*]

Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, Brazil
Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA

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ABSTRACT

Computational applications of the nonextensive entropy S_q and nonextensive statistical mechanics, a current generalization of the Boltzmann–Gibbs (BG) theory, are briefly reviewed. The corresponding bibliography is provided as well.

1. Introduction

Entropy is an ubiquitous concept [1]. Indeed, it emerges in both conservative and dissipative systems, in physical as well as nonphysical contexts. This comes from the fact that it is a functional of probability distributions, and can therefore be used with profit in a considerable variety of manners, for natural, artificial and even social systems. The concept of entropy naturally emerges in statistical mechanics, one of the most important theoretical approaches in contemporary physics. Specifically, Boltzmann–Gibbs (BG) statistical mechanics is essentially based on a specific connection between the Clausius thermodynamic entropy S and the set of probabilities $\{p_i\}$ $(i = 1, 2, \ldots, W)$ of the microscopic configurations of the system. This connection is provided by the Boltzmann–Gibbs (or Boltzmann–Gibbs–von Neumann–Shannon) entropy S_{BG} defined (for the discrete case) through

$$S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i, \tag{1}$$

where k is a positive constant, the most usual choices being either the Boltzmann constant k_B, or just unity ($k = 1$).

This entropic functional and its associated statistical mechanics address a large amount of interesting systems, and have been successfully used along over 130 years. However, very many complex systems escape to its domain of applicability. As an attempt to improve the situation, a generalization of Eq. (1) was proposed in 1988 [2]. See Table 1, where the *q-logarithm* is defined as

$$\ln_q x \equiv \frac{x^{1-q} - 1}{1-q} \quad (x > 0;\ q \in \mathcal{R};\ \ln_1 x = \ln x), \tag{2}$$

the inverse function, the *q-exponential*, being

$$e_q^x \equiv [1 + (1-q)x]_+^{\frac{1}{1-q}} \quad (q \in \mathcal{R};\ e_1^x = e^x), \tag{3}$$

with $[z]_+ = z$ if $z \geq 0$, and zero otherwise. We verify that $\ln_q e_q^x = e_q^{\ln_q x} = x$, $\forall x$.

☆ Invited paper.

* Corresponding address: Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, Brazil. Tel.: +55 21 2141 7190; fax: +55 21 2141 7515.

E-mail address: tsallis@cbpf.br.

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Table 1
The *nonadditive* entropy S_q ($q \neq 1$), and its particular, *additive*, limiting case $S_{BG} = S_1$

Entropy	Equal probabilities ($p_i = 1/W, \forall i$)	Arbitrary probabilities ($\sum_{i=1}^{W} p_i = 1$)
$q = 1$	$S_{BG} = k \ln W$	$S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i = k \sum_{i=1}^{W} p_i \ln \frac{1}{p_i}$
$\forall q$	$S_q = k \ln_q W$	$S_q = k \frac{1-\sum_{i=1}^{W} p_i^q}{q-1} = k \sum_{i=1}^{W} p_i \ln_q \frac{1}{p_i}$

If we consider a system composed by two probabilistically *independent* subsystems A and B, i.e., $p_{ij}^{A+B} = p_i^A p_j^B \ \forall (ij)$, we straightforwardly verify that

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q)\frac{S_q(A)}{k}\frac{S_q(B)}{k}. \tag{4}$$

Therefore, S_{BG} is *additive* [3], and S_q ($q \neq 1$) is *nonadditive*. The entropy S_q leads to a natural generalization of BG statistical mechanics, currently referred to as *nonextensive statistical mechanics*, [2,4,5]. The nonextensive theory focuses on nonequilibrium stationary (or quasi-stationary) states in the same way the BG theory focuses on thermal equilibrium states. Recent reviews of the theory and its various applications (see, for instance, [6] for a recent review of astrophysical applications, whose lines the present review partially follows) can be found in [7–9], and a regularly updated bibliography is available at [10].

2. Extensivity of the nonadditive entropy S_q

From its very definition, additivity depends *only* on the functional form of the entropy. Extensivity *also* depends on the system. Indeed, the entropy $S(N)$ of a given system composed by N (independent or correlated) elements is said *extensive* if $\lim_{N\to\infty} S(N)/N$ is finite, i.e., if $S(N)$ scales like N for large N, *hence matching the classic thermodynamic behavior*. Consequently, for systems whose elements are independent or weakly correlated, S_{BG} is extensive, whereas S_q is nonextensive for $q \neq 1$. There are, in constrast, systems whose elements are strongly correlated, having as a consequence that S_q is extensive only for a special value of q, noted q_{ent}, with $q_{ent} \neq 1$. In other words, S_q is nonextensive for any value of $q \neq q_{ent}$. In particular, for such anomalous systems, S_{BG} is nonextensive, hence inadequate for thermodynamical purposes at the limit $N \to \infty$ (*thermodynamic limit*). There are finally systems that are even more complex, and for which there is no value of q such that $S_q(N)$ is extensive. Such strongly anomalous systems remain outside the realm of nonextensive statistical mechanical concepts, and are not addressed here.

Abstract probabilistic models with either $q_{ent} = 1$ or $q_{ent} \neq 1$ are exhibited in [11]. Physical realizations are exhibited in [12] for strongly entangled systems. For example, the block entropy of magnetic chains in the presence of a transverse magnetic field at its critical value and at $T = 0$, belonging to the universality class characterized by the *central charge* c [13], yield [12]

$$q_{ent} = \frac{\sqrt{9+c^2}-3}{c} \quad (c > 0). \tag{5}$$

Therefore, for the one-dimensional Ising model with short-range interactions (hence $c = 1/2$), we have $q_{ent} = \sqrt{37} - 6 \simeq 0.08$, and for the one-dimensional isotropic XY model with short-range interactions (hence $c = 1$), we have $q_{ent} = \sqrt{10} - 3 \simeq 0.16$. At the $c \to \infty$ limit, we recover the BG value $q_{ent} = 1$ ($q_{ent} = 1/2$ for $c = 4$; see [14] for $c = 26$).

3. Entropy production per unit time

Let us illustrate on one-dimensional unimodal nonlinear dynamical systems $x_{t+1} = f(x_t)$ some interesting concepts, namely that of *sensitivity to the initial conditions* and that of *entropy production per unit time*. A system is said *strongly chaotic* (or just *chaotic*) if its Lyapunov exponent λ_1 is positive, and *weakly chaotic* if it vanishes. The *sensitivity to the initial conditions* ξ is defined as

$$\xi(t) \equiv \lim_{\Delta x(0)\to 0} \frac{\Delta x(t)}{\Delta x(0)}. \tag{6}$$

If $\lambda_1 > 0$, we typically have

$$\xi(t) = e^{\lambda_1 t}. \tag{7}$$

The *entropy production per unit time* K_1 in such a system is defined as

$$K_1 \equiv \lim_{t\to\infty} \lim_{W\to\infty} \lim_{M\to\infty} \frac{S_{BG}(t)}{t}, \tag{8}$$