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Towards a large deviation theory for strongly correlated systems

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ABSTRACT

A large-deviation connection of statistical mechanics is provided by N independent binary variables, the $(N \to \infty)$ limit yielding Gaussian distributions. The probability of $n \neq N/2$ out of N throws is governed by e^{-Nr}, r related to the entropy. Large deviations for a strong correlated model characterized by indices (Q, γ) are studied, the $(N \to \infty)$ limit yielding Q-Gaussians ($Q \to 1$ recovers a Gaussian). Its large deviations are governed by $e_q^{-Nr_q}$ ($\propto 1/N^{1/(q-1)}$, $q > 1$), $q = (Q-1)/(\gamma[3-Q]) + 1$. This illustration opens the door towards a large-deviation foundation of nonextensive statistical mechanics.

1. Introduction

In his 1902 historical book *Elementary Principles in Statistical Mechanics* [1], Gibbs emphasizes that systems involving long-range interactions are intractable within the Boltzmann–Gibbs (BG) theory, due to the divergence of the partition function. Amazingly enough, this crucial remark is often overlooked in most textbooks.

To solve related complexities it was proposed in 1988 [2–5] a generalization of the BG theory, currently referred to as nonextensive statistical mechanics. It is based on the nonadditive entropy

$$S_q = k_B \frac{1 - \sum_{i=1}^{W} p_i^q}{q-1} \quad \left(q \in \mathcal{R}; \sum_{i=1}^{W} p_i = 1\right), \tag{1}$$

which recovers $S_{BG} = -k_B \sum_{i=1}^{W} p_i \ln p_i$ for $q \to 1$. If A and B are two probabilistically independent systems (i.e., $p_{ij}^{A+B} = p_i^A p_j^B$, $\forall (i,j)$), definition (1) implies the nonadditive relation $\frac{S_q(A+B)}{k_B} = \frac{S_q(A)}{k_B} + \frac{S_q(B)}{k_B} + (1-q)\frac{S_q(A)}{k_B}\frac{S_q(B)}{k_B}$. Moreover, if probabilities are all equal, we straightforwardly obtain $S_q = k_B \ln_q W$, with $\ln_q z \equiv \frac{z^{1-q}-1}{1-q}$ ($\ln_1 z = \ln z$). If we extremize (1) with a constraint on its width (in addition to normalization of the probabilities $\{p_i\}$), we obtain

$$p_i = \frac{e_q^{-\beta_q E_i}}{\sum_{j=1}^{W} e_q^{-\beta_q E_j}}, \tag{2}$$

e_q^z being the inverse function of the q-logarithmic function, i.e., $e_q^z \equiv [1 + (1-q)z]^{1/(1-q)}$ ($e_1^z = e^z$); $\{E_i\}$ are the energy levels; β_q is the effective inverse temperature.

Complexity frequently emerges in natural, artificial and social systems. It may be caused by various geometrical–dynamical ingredients, which include nonergodicity, long-term memory, multifractality, and other spatial–temporal long-range correlations between the elements of the system. During the last two decades, many such phenomena have been successfully approached in the frame of nonextensive statistical mechanics. Predictions, verifications and various applications have been performed in high-energy physics [6–11], spin-glasses [12], cold atoms in optical lattices [13], trapped ions [14], anomalous diffusion [15], dusty plasmas [16], solar physics [17,18], relativistic and nonrelativistic nonlinear quantum mechanics [19], among many others.

Large-deviation estimates are important in order to quantify the rates of convergence to equilibrium. They are therefore relevant for addressing the rigorous derivation concerning simplified models to describe complex systems. In fact it is known since several decades that the mathematical foundation of BG statistical mechanics crucially lies on the theory of large deviations (see [20,21] and references therein). To attain the same status for nonextensive statistical mechanics, it is necessary to q-generalize the large deviation theory itself. The purpose of the present effort precisely is to make a first step towards that goal through the study of a simple model.

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This Letter is organized as follows. In Section 2 we make some considerations about relative entropy associated with binary random variables, and a possible generalization for non-BG entropic random variables. In Section 3 we report some results of large deviation theory in a well-known model assuming independent probabilities and consequently a BG type relative entropy; we extend these results to a modified model that presents complexity due to strong correlations in Section 4. Finally, in Section 5 we summarize our results and conclusions.

2. Relative entropy

The *relative entropy* or *mutual information* for a random variable with discrete W events with probabilities $\{p_i\}$ $(i = 1, \dots, W)$ is defined as

$$I_1 = -\sum_{i=1}^{W} p_i \ln \frac{p_i^{(0)}}{p_i}, \tag{3}$$

where $p_i^{(0)}$ is a reference distribution [22]. By choosing $\{p_i^{(0)}\}$ as the uniform distribution (i.e., $p_i^{(0)} = 1/W$), we have

$$I_1 = \ln W - \sum_{i=1}^{W} p_i \ln \frac{1}{p_i} = \ln W - \frac{S_1}{k_B}. \tag{4}$$

Definition (3) and the nonadditive entropy S_q naturally lead to the generalization [24]

$$I_q = -\sum_{i=1}^{W} p_i \ln_q \frac{p_i^{(0)}}{p_i} = \sum_{i=1}^{W} p_i \frac{[(p_i/p_i^{(0)})^{q-1} - 1]}{q-1}, \tag{5}$$

where by once again choosing as $\{p_i^{(0)}\}$ the equiprobability distribution (i.e., $p_i^{(0)} = 1/W$), we have

$$I_q = W^{q-1}\left[\ln_q W - \frac{S_q}{k_B}\right]. \tag{6}$$

For $W = 2$ (e.g. tossing a coin to have *head* or *tail*), I_1 reads

$$I_1 = \ln 2 + p_1 \ln p_1 + p_2 \ln p_2 \tag{7}$$

and by identifying $(p_1, p_2) \to (x, 1-x)$, we establish [23]

$$r_1(x) = \ln 2 + x \ln x + (1-x)\ln(1-x), \tag{8}$$

as the inset of Fig. 1 shows. Generalized mutual information (5) now reads

$$I_q(x) = \frac{1}{1-q}\left[1 - 2^{q-1}\left[x^q + (1-x)^q\right]\right], \tag{9}$$

which recovers expression (8) for $q \to 1$.

In the following, we will apply these results to the problem of studying large deviations when tossing N times a fair coin or, equivalently, tossing one time N independent fair coins (BG entropic system) and when tossing N strongly correlated fair coins (non-BG entropic system).

3. Large deviations in *N* uncorrelated coins

Let us now exhibit some large deviation theory results on a standard example which consists in tossing N times a fair coin. This well-known model presents independent probabilities of obtaining n $(n = 0, 1, \dots, N)$ heads, that are given by

$$p_{N,n} = \binom{N}{n}\frac{1}{2^N}. \tag{10}$$

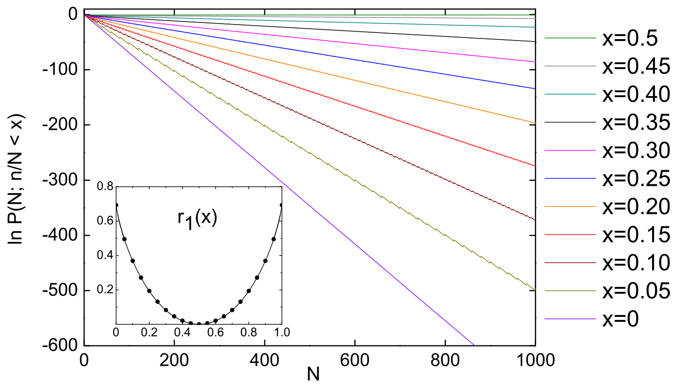

Fig. 1. Tossing N independent coins: the large-deviation probability $P(N; n/N < x)$ decays exponentially with N, and the slopes of the logarithms, $\ln P(N; n/N < x)$, provide the rate function numerical values $r_1(x)$, represented in the inset as dots. Continuous curve in the inset corresponds to Eq. (8).

The probability of having the ratio n/N smaller than x with $0 \leqslant x \leqslant 1/2$ (the case $1/2 \leqslant x \leqslant 1$ is totally symmetric) is given by

$$P(N; n/N < x) = \sum_{\{n \mid \frac{n}{N} < x\}} p_{N,n}, \tag{11}$$

and it is straightforward to obtain that, in the $N \to \infty$ limit,

$$P(N; n/N < x) \simeq e^{-N r_1(x)} \quad (0 \leqslant x \leqslant 1/2), \tag{12}$$

where the subindex 1 in the *rate function* $r_1(x)$ will soon become clear. In fact, this exponential decay with N, deeply related with the exponential decay with energy of the BG weight (namely, the $q = 1$ particular case of Eq. (2)), is verified in Fig. 1. In Section 2, it has been shown the analytical calculation of the rate function $r_1(x)$ for the present trivial model (8). The high-precision numerical calculation can be verified in Fig. 1.

4. Large deviation in *N* correlated coins

Let us now extend the above model to the case where the coins present strong correlations, so as to introduce complexity through a specific system and study the large-deviation behavior in a simple non-BG system. To deal with this problem, it is appropriate to refer to the recently proposed families of probabilistic models [31, 32] having q-Gaussians as limiting probability distribution. Let us incidentally mention that probabilistic scale invariance is not sufficient for obtaining q-Gaussians. Indeed, in [28] the model is scale invariant but the limit distribution is not q-Gaussian, whereas in [31,32] the models are scale invariant and yield q-Gaussians.

The simple model that we have just reviewed yields, for $N \to \infty$, a Gaussian distribution. This conforms to the Central Limit Theorem, valid for sums of many independent random variables whose variance is finite. This classical theorem has been q-generalized [27] (see also [28], as well as [29,30]) for a special class or correlations referred to as q-independence (1-independence recovers standard independence). The attractors in the probability space of q-independent models are q-Gaussians, which precisely extremize the (continuous form of the) entropy S_q when an appropriately generalized q-variance is maintained fixed. It is then this class of correlations that we are going to focus on here in order to illustrate how the classical large deviation theory can be generalized. We adopt the specific class of binary variable models introduced in [31]. These models consist in discretized forms of Q-Gaussians

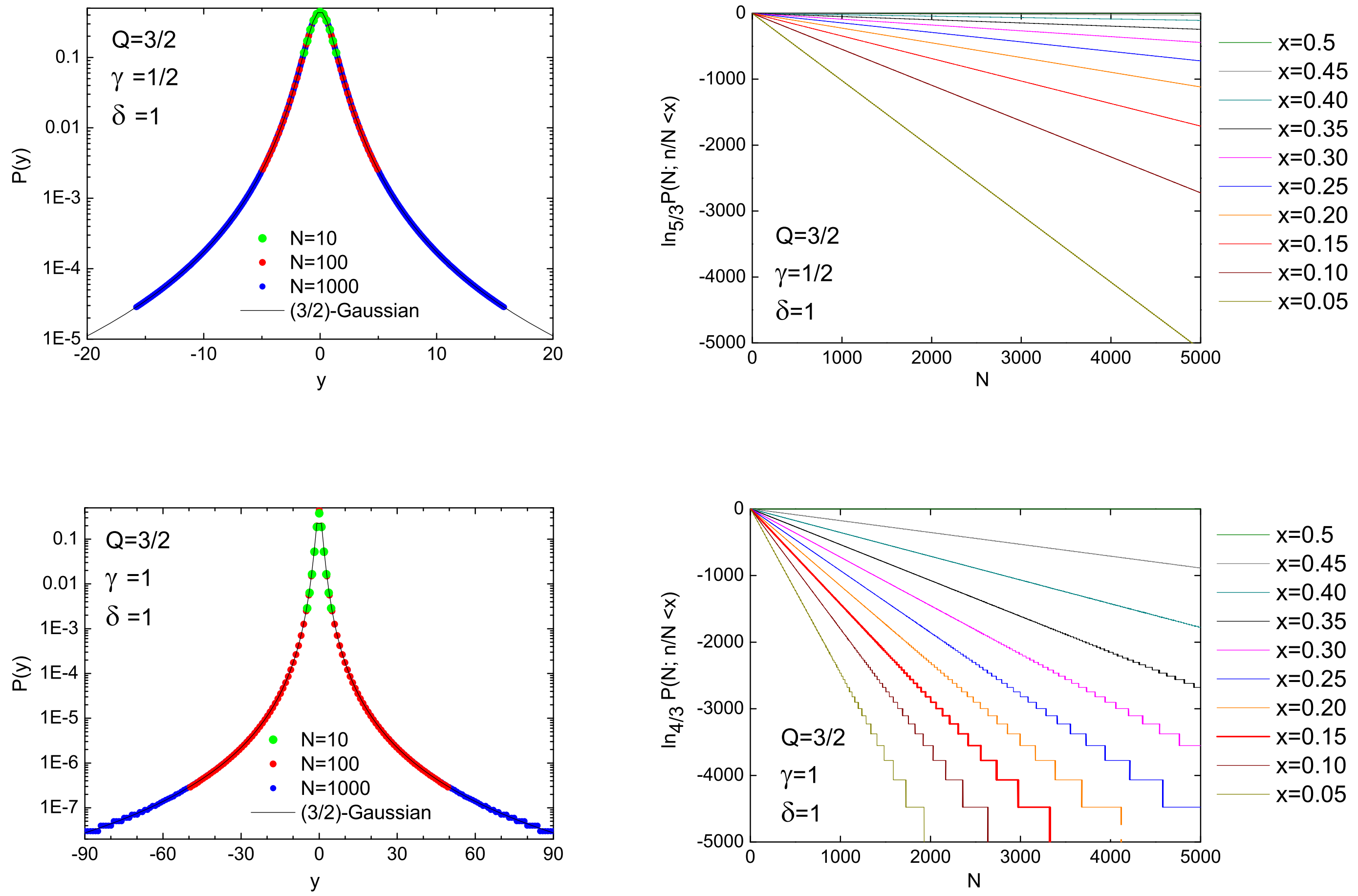

Fig. 2. Illustrative histograms of the discretized model (left column) and their corresponding distributions $P(N; n/N < x)$, in semi-q-log representation (right column). The cases $\gamma = 0$ and $\gamma = 1$ do not yield q-Gaussians with $Q > 1$ because the discretization never achieves the desired continuous limit (indeed, $\Delta_N = \delta$ and $\Delta_N/N \sim \delta$ respectively). The case $Q = 1$ yields a Gaussian with a specific discretization, which only in the $N \to \infty$ coincides with that of the independent-coin model.

($1 \leqslant Q < 2$),[1] which exactly converge onto Q-Gaussians in the limit $N \to \infty$. The $\{p_{N,n}\}$ in (11) are now given by

$$p_{N,n} = \frac{p_Q(y_{N,n})}{\sum_{n=0}^{N} p_Q(y_{N,n})}, \tag{13}$$

where the Q-Gaussian is given by

$$p_Q(z) \propto \left[1 + (Q-1)z^2\right]^{-1/(Q-1)} \tag{14}$$

and $y_{N,n}$ ($n = 0, 1, \ldots, N$) correspond to $(N+1)$ equally spaced points in the support of the discretized Q-Gaussian. More precisely, $y_{N,n} = \Delta_N(\frac{n}{N} - 1/2) \in [-\Delta_N/2, \Delta_N/2]$, where

$$\Delta_N = \delta(N+1)^{\gamma} \quad (\delta > 0; 0 < \gamma < 1). \tag{15}$$

The model is fully determined by (Q, γ, δ). The left column of Fig. 2 shows how the distributions $P(y) = \frac{N}{\Delta_N} p_{N,n}$ approach the corresponding Q-Gaussians while N increases.

We observe that, for each pair of values (Q, γ), $P(N; n/N < x)$ presents a q-logarithmic decay (see Fig. 2, right column), i.e.,

$$P(N; n/N < x) \simeq e_q^{-Nr_q(x)} \quad (0 \leqslant x \leqslant 1/2), \tag{16}$$

where we have heuristically obtained that

$$q = \frac{Q-1}{\gamma(3-Q)} + 1 \quad (0 < x \leqslant 1/2; \forall\delta), \tag{17}$$

hence,

$$\frac{1}{\gamma(q-1)} = \frac{2}{Q-1} - 1 \quad (0 < x \leqslant 1/2; \forall\delta). \tag{18}$$

We see that, for $Q = 1$ hence $q = 1$, Eq. (16) recovers Eq. (12). For $Q > 1$, we have $q > 1$, consequently $P(N; n/N < x) \propto 1/N^{1/(q-1)}$, i.e., *a power law instead of exponential*. We also verify that the value of q for $x = 0$, noted $q_{[x=0]}$, differs (possibly presumably due to a boundary effect) from the value corresponding to $0 < x \leqslant 1/2$, noted $q_{[0<x\leqslant 1/2]}$ and given by Eqs. (17) or (18). For all (Q, γ, δ) we have that

$$q_{[x=0]} = 2 - \frac{1}{q_{[0<x\leqslant 1/2]}}. \tag{19}$$

The rate function satisfies, for $0 < x \leqslant 1/2$,

$$r_q(x; Q; \gamma; \delta) = r_q(x; Q; \gamma; 1)\delta^{1/\gamma} \quad (\delta > 0), \tag{20}$$

where $r_q(x; Q; \gamma; 1)$ depends on the model parameters (Q, γ), as illustrated in Fig. 3 [notice that Eq. (15) yields $\Delta_N \sim (N\delta^{1/\gamma})^{\gamma}$ for $N \gg 1$]. In all cases, due the above mentioned boundary effect, $r_q(0) < \lim_{x\to 0} r_q(x)$. For comparison purposes we have also represented, in this same figure, $I_Q(x)$ as given by Eq. (9). We verify that, although it is of the same order of magnitude as $r_q(x)$, it does not coincide with the numerical results from Fig. 2 (neither coincide the corresponding $I_q(x)$'s, not shown in the figure). This cannot be considered as surprising since the present model includes, for $Q > 1$, nontrivial correlations between the N random variables, which have not been taken into account in the calculation of (9).

[1] Q-Gaussians are normalizable for $Q < 3$. But we limit the present illustrations to $Q \leqslant 2$ because, in the interval $2 < Q < 3$, a new regime appears to emerge (see Fig. 9 of [33]), which does not belong to the present scope.

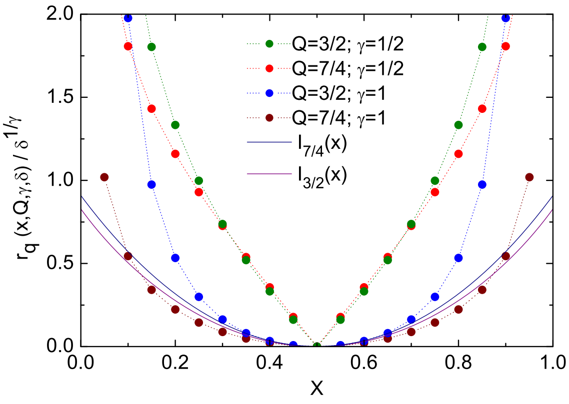

Fig. 3. Rate function $r_q(x)$ corresponding to typical values of (Q,γ). The continuous curves correspond to $I_Q(x)$ (Eq. (9) with $q \to Q$).

It is however remarkable that the exponent of the q-exponential (16) remains extensive (i.e., proportional to N) for all values of Q. Since the nature of this exponent is entropic, this results naturally reinforces the approach currently adopted in nonextensive thermostatistics, where, in the presence of strong correlations, one expects a value of the index q to exist such that S_q preserves the extensivity it has in the BG theory [3,34,5,35].

5. Conclusions

Sequences of correlated random variables different from the present ones, as well as their large deviation theory, are available in the literature [25]. In such sequences, the large deviation principle is still satisfied, as known mixing conditions on sequences of random variables [26] impose a limit on the strength of the correlations between the individual random variables of the sequence.

In the present study we address instead strongly correlated variables of a certain class. It appears to open the door to a q-generalization of virtually many, if not all, of the classical results of the theory of large deviations. In this sense, the present effort points a path which would be parallel to the q-generalization of the classical and Lévy–Gnedenko Central Limit Theorems [27]. Indeed, the present results do suggest the mathematical basis for the ubiquity of q-exponential energy distributions in nature, just as the q-generalized Central Limit Theorem suggests the ubiquity of q-Gaussians in nature.

It is quite remarkable that the argument of the q-logarithmic decay of large deviations remains extensive in our model. This result reinforces the fact that, according to nonextensive thermostatistics for a wide class of systems whose elements are strongly correlated, a value of the index q exists such that S_q preserves extensivity, in agreement with the well known thermodynamical requirement.

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