Towards a large deviation theory for strongly correlated systems

Guiomar Ruiz\(^{a,b,*}\), Constantino Tsallis\(^{a,c}\)

\(^{a}\) Centro Brasileiro de Pesquisas Físicas and National Institute of Science and Technology for Complex Systems, Rua Xavier Sigaud 1399, Rio de Janeiro, RJ, Brazil
\(^{b}\) Departamento de Matemática Aplicada y Estadística, Universidad Politécnica de Madrid, Pza. Cardenal Cisneros s.n., 28040 Madrid, Spain
\(^{c}\) Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA

**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 \(e^{-Np}\), \(p\) related to the entropy. Large deviations for a strongly correlated model characterized by indices \((Q, y)\) are studied, the \((N \to \infty)\) limit yielding \(Q\)-Gaussians \((Q \to 1\) recovers a Gaussian). Its large deviations are governed by \(e_q^{-Np} \propto \alpha/\gamma\left(3-\gamma-1\right)\), \(q > 1\), \(n = (Q - 1)/\gamma(3 - Q) + 1\). This illustration opens the door towards a large-deviation foundation of nonextensive statistical mechanics.

\(\odot\) 2012 Elsevier B.V. All rights reserved.

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

\[
S_q = k_B \left\{ 1 - \sum_{i=1}^{W} q_i p_i^q \right\}, \quad \left( q \in \mathbb{R}; \sum_{i=1}^{W} p_i = 1 \right) \tag{1}
\]

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 \(S_q^{A+B}/k_B = S_q^A/k_B + S_q^B/k_B + (1-q) S_q^{A}(A+B)/k_B\). Moreover, if probabilities are all equal, we straightforwardly obtain \(S_q = k_B \ln W\), with \(\ln z \equiv z^{1-1} = z\ln z\). If we extremize (1) with a constraint on its width (in addition to normalization of the probabilities \(\{p_i\}\)), we obtain

\[
p_i = e_q^{-\varphi_i^q}, \quad \sum_{j=1}^{W} e_q^{-\varphi_i^q} = 1
\]

\(e_q^z\) being the inverse function of the \(q\)-logarithmic function, i.e., \(e_q^z \equiv [1 + (1 - q)z]^{1/(1-q)}\) (\(e_q^2 = e^q\); \(\varphi_i\) are the energy levels; \(\varphi_q\) 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.
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 \( \{p_i\} \ (i = 1, \ldots, W) \) is defined as

\[
I_1 = -\sum_{i=1}^{W} p_i \ln \frac{p_i^{(0)}}{p_i},
\]

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

\[
I_1 = \ln W - \sum_{i=1}^{W} p_i \ln \frac{1}{p_i} = \ln W - \frac{1}{k_B},
\]

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

\[
I_q = -\sum_{i=1}^{W} p_i \ln \frac{p_i^{(0)}}{p_i} = \sum_{i=1}^{W} p_i \left[ \frac{p_i / p_i^{(0)}}{q-1} - 1 \right],
\]

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

\[
I_q = W^{q-1} \left[ \ln_q 1 - S_q / k_B \right],
\]

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

\[
I_1 = \ln 2 + p_1 \ln p_1 + p_2 \ln p_2,
\]

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

\[
r_1(x) = \ln 2 + x \ln x + (1-x) \ln (1-x),
\]

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

\[
I_q(x) = \ln_q 1 - 2^{q-1} \left[ x^q + (1-x)^q \right],
\]

which recovers expression (8) for \( q \rightarrow 1 \).

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 \( n \ (n = 0, 1, \ldots, N) \) heads, that are given by

\[
P_{N,n} = \frac{N!}{n! (N-n)!}. \tag{10}
\]

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

\[
P(N; n/N < x) = \sum_{\left\lfloor \frac{n}{N} x \right\rfloor} P_{N,n}, \tag{11}
\]

and it is straightforward to obtain that, in the \( N \rightarrow \infty \) limit,

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

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 \( q \)-Gaussians, whereas in [31,32] the models are scale invariant and yield \( q \)-Gaussians.

The simple model that we have just reviewed yields, for \( N \rightarrow \infty \), 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.
(1 ≤ Q < 2), which exactly converge onto Q-Gaussians in the limit N → ∞. The p_{N,n} in (11) are now given by

\[ p_{N,n} = \frac{p_Q(y_{N,n})}{\sum_{n=0}^{N} p_Q(y_{N,n})}, \]

where the Q-Gaussian is given by

\[ p_Q(z) \propto [1 + (Q - 1)z^2]^{-1/(Q-1)} \]

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

\[ ΔN = (N + 1)γ (δ > 0; 0 < γ < 1). \]

The model is fully determined by (Q, γ, δ). The left column of Fig. 2 shows how the distributions P(y) = \[ \frac{N}{N^q} p_{N,n} \] 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.,

\[ P(N; n/N < x) \propto e^{-Nq(x)} (0 ≤ x ≤ 1/2), \]

where we have heuristically obtained that

\[ q = \frac{Q - 1}{γ(3 - Q)} + (0 < x < 1/2; ∀δ), \]

hence,

\[ \frac{Q}{Q - 1} = 2 \frac{Q - 1}{Q - 1} (0 < x ≤ 1/2; ∀δ). \]

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) ∝ 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 ≤ 1/2, noted q_{[0<x<1/2]} and given by Eqs. (17) or (18). For all (Q, γ, δ) we have that

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

The rate function satisfies, for 0 < x ≤ 1/2,

\[ r_q(x; Q; γ; δ) = r_q(x; Q; γ; δ)^{1/δ} (δ > 0), \]

where r_q(x; Q; γ; δ) depends on the model parameters (Q, γ), as illustrated in Fig. 3 [notice that Eq. (15) yields ΔN ∼ (Nδ)_{1/δ} \ for N >> 1]. In all cases, due the above mentioned boundary effect, r_q(0) < \lim_{x→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).
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 [3,34,35].

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 whole class of applications between the individual random variables of the sequence.

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.

Acknowledgements

We acknowledge useful conversations with R. Bissacot, T.C.P. Lobato, S.T.R. de Pinho, H. Touchette and M.E. Vares, as well as financial support by the DGU-MEC (Spanish Ministry of Education) through Project PHB2007-0095-PC.

References