A note on $q$-Gaussians and non-Gaussians in statistical mechanics

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Abstract. The sum of $N$ sufficiently strongly correlated random variables will not in general be Gaussian distributed in the limit $N \to \infty$. We revisit examples of sums $x$ that have recently been put forward as instances of variables obeying a $q$-Gaussian law, that is, one of type $cst \times [1 - (1 - q)x^2]^{1/(1-q)}$. We show by explicit calculation that the probability distributions in the examples are actually analytically different from $q$-Gaussians, in spite of numerically resembling them very closely. Although $q$-Gaussians exhibit many interesting properties, the examples investigated do not support the idea that they play a special role as limit distributions of correlated sums.

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1. Introduction

The central limit theorem says that the sum of $N$ sufficiently weakly correlated random variables, when properly scaled with $N$ and in the limit $N \to \infty$, has a Gaussian probability distribution. In many places in physics, however, strongly correlated variables occur. Causes of strong correlations may be, for example, the presence of long-range interaction or memory effects. On the basis of a generalization of the statistical mechanical formalism \cite{1} it has been suggested that in certain strongly correlated systems such many-variable sums are distributed according to a $q$-Gaussian law. This law is a generalization of the ordinary Gaussian and arises, in particular, when one maximizes the generalized entropy which is at the basis of the theory. Pursuant to this idea $q$-Gaussians have been advanced to describe velocity distributions in a Hamiltonian mean-field model (HMF) of classical rotators \cite{2}, in turbulent Couette–Taylor flow \cite{3}, and in cellular aggregates \cite{4}; and were also proposed for the velocity distribution of galaxy clusters \cite{5} and the temperature fluctuations in the cosmic microwave background \cite{6}. In at least the case of the HMF, divergent interpretations of Monte Carlo results have led to vivid discussions in the literature (see e.g., \cite{7}–\cite{10}).

For a single variable $x$ the $q$-Gaussian probability distribution $G_q(x)$ is given by

$$G_q(x) = b^{1/2} C_q \left[ 1 - \frac{1 - q}{3 - q} b x^2 \right]^{1/(1-q)},$$  \hspace{1cm} (1.1)

where $C_q$ is a normalization constant and the scale factor $b$ controls the width. For $-\infty < q < 1$, which will be the range of $q$ values of interest to us, $G_q(x)$ is bell-shaped and...
has its support restricted to the interval \([-x_m, x_m]\), where \(x_m = (((1 - q)/(3 - q))b)^{-1/2}\). The denominator \(3 - q\) in (1.1) is there merely to guarantee that for \(q \to -\infty\) the support of the \(q\)-Gaussian remains finite. The special case \(G_{-\infty}\) is the block function equal to \((1/2)b^{1/2}\) on \([-b^{-1/2}, b^{-1/2}]\). For \(q \to 1\) expression (1.1) reduces to the ordinary Gaussian \(G_1(x) = (b/2\pi)^{1/2}\exp(-1/2bx^2)\).

Independently of their applicability in statistical mechanics, \(q\)-Gaussians have several interesting mathematical properties. For example, the multivariate \(q\)-Gaussian (for which \(x^2\) in (1.1) is replaced with a symmetric bilinear form \(\sum_{\mu\nu} x_\mu A_{\mu\nu} x_\nu\)) has marginal distributions that are \(q'\)-Gaussians with \(q' \neq q\) (see [11]).

We will be concerned specifically with the question of whether \(q\)-Gaussians can emerge as probability distributions of sums of correlated random variables. Attempts in the literature to demonstrate how such \(q\)-Gaussian distributions may arise, have consisted of constructing and numerically analysing simplified model systems. A successful model should not only explain the origin of the \(q\)-Gaussian, but also express the parameter \(q\) in terms of more common concepts such as interactions and correlations. These model studies leave for later investigation the question of whether the properties preassigned to the model may actually be realized in physical systems.

In this note we will examine two model systems taken from the recent literature [12,13]. Both feature sums that were put forward as candidates for being \(q\)-Gaussian distributed. We show by explicit calculation that in both examples the probability distributions are actually analytically different from \(q'\)-Gaussians, even though very closely resembling them numerically. Notwithstanding the interesting properties exhibited by \(q\)-Gaussians, the two examples studied therefore do not lend support to the idea that these functions play a role as limit distributions of correlated sums.

2. First example

2.1. A set of strongly correlated variables

Thistleton et al [12] consider what is probably the simplest imaginable instance of a strongly correlated system. It consists of \(N\) identically distributed variables \(u_1, u_2, \ldots, u_N\) such that the probability distribution \(P_1\) of each individual \(u_j\) is the block function

\[
P_1(u_j) = 1, \quad \left( -\frac{1}{2} \leq u_j \leq \frac{1}{2} \right),
\]

and \(P_1(u_j) = 0\) elsewhere. The \(u_j\) have, furthermore, strong mean-field type correlations, as expressed by their covariance matrix

\[
\langle u_j u_k \rangle = \begin{cases} 
\frac{1}{12} & (j = k), \\
r & (j \neq k),
\end{cases}
\]

where \(0 < r \leq 1\). The authors of [12] are then interested in finding the probability distribution \(P_N(U)\) of the scaled sum

\[
U = N^{-1} \sum_{j=1}^{N} u_j
\]

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and in obtaining its limit \( P(U) = \lim_{N \to \infty} P_N(U) \). It will turn out in this mean-field problem that in order for the limit \( N \to \infty \) to exist, the appropriate scaling is the one with \( N^{-1} \) given in (2.3) rather than the conventional one with \( N^{-1/2} \) applicable to independent variables. It is therefore clear that we cannot expect the limits \( r \to 0 \) and \( N \to \infty \) to commute.

Determining \( P_N(U) \) requires the knowledge of the full joint probability distribution \( P_N(u_1, u_2, \ldots, u_N) \) of the \( u_j \). This distribution is fixed implicitly by the way the \( u_j \) are constructed [12], namely, from a Gaussian distribution that one knows how to generate numerically. Let the \( N \) correlated Gaussian variables \( z_1, z_2, \ldots, z_N \) be distributed according to

\[
P_N^{\text{Gauss}}(z_1, z_2, \ldots, z_N) = \left[ (2\pi)^N \det M \right]^{-1/2} \exp \left( -\frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} z_j M^{-1}_{jk} z_k \right). \tag{2.4}\]

Then the \( z_j \) have the covariance matrix \( \langle z_j z_k \rangle = M_{jk} \), for which will take

\[
M_{jk} = \begin{cases} 1 & (j = k), \\ \rho & (j \neq k), \end{cases} \tag{2.5}\]

where \( \rho \in (0,1] \) is a parameter. It follows that the elements of the inverse matrix \( M^{-1} \) are

\[
M^{-1}_{jk} = \begin{cases} \alpha & (j = k), \\ -\beta & (j \neq k), \end{cases} \tag{2.6}\]

with

\[
\alpha = \frac{1 + (N - 2)\rho}{(1 - \rho)(1 + (N - 1)\rho)}, \quad \beta = \frac{\rho}{(1 - \rho)(1 + (N - 1)\rho)}. \tag{2.7}\]

The marginal distribution \( P_1^{\text{Gauss}}(z_j) \) of \( z_j \) derived from (2.4) is a Gaussian of unit variance. The variables \( u_j \) are now constructed [12] from the \( z_j \) according to

\[
u_j = \int_0^{z_j} dx \, P_1^{\text{Gauss}}(x) = \frac{1}{2} \text{erf} \left( \frac{z_j}{\sqrt{2}} \right), \quad (j = 1, \ldots, N). \tag{2.8}\]

Then \( u_j \) has the block distribution (2.1) and is correlated to the other \( u_k \) according to (2.2) with an \( r \) that may be determined as a function of \( \rho \).

On the basis of numerical evidence Thistleton et al [12] conjectured that the probability distribution \( P(U) \) of the scaled sum \( U \) of these variables was a \( q \)-Gaussian with an index \( q \) related to \( \rho \) according to

\[
q = \frac{1 - (5/3)\rho}{1 - \rho}. \tag{2.9}\]

This example is sufficiently simple to allow for an exact analytic treatment, which we will present now.
2.2. The limiting law $\mathcal{P}(U)$

In this subsection we replace the block function $P_1$ considered in (2.1) by an arbitrary symmetric function $P_1(u)$. Let there be $N$ correlated random variables $u_j$, $j = 1, 2, \ldots, N$ having an arbitrary symmetric marginal distribution $P_1(u_j)$ of unit variance and having correlations $(u_j u_k) = r$ for $j \neq k$. Variables $u_j$ having these properties may be obtained from the $z_j$ by

$$
\int_0^{z_j} dx P_1^{\text{Gauss}}(x) = \int_0^{u_j} dx P_1(x), \quad (j = 1, \ldots, N),
$$

(2.10)

which generalizes (2.8) and which we will abbreviate as

$$
u_j = h(z_j), \quad (j = 1, \ldots, N).
$$

(2.11)

The expression for the law $\mathcal{P}_N(U)$ follows directly from its definition,

$$
\mathcal{P}_N(U) = [(2\pi)^N \det M]^{-1/2} \int_{-\infty}^\infty dz_1 \ldots dz_N \delta \left(U - N^{-1} \sum_i h(z_i)\right)
$$

$$
\times \exp \left(-\frac{1}{2} \sum_{j,k} z_j M^{-1}_{jk} z_k \right).
$$

(2.12)

The quadratic form in the exponential in (2.12) simplifies according to

$$
\sum_{j,k} z_j M^{-1}_{jk} z_k = (\alpha + \beta) \sum_j z_j^2 - \beta \left(\sum_j z_j\right)^2.
$$

(2.13)

Upon substituting (2.13) in (2.12) and introducing integral representations for $\exp \left((1/2)\beta (\sum_j z_j)^2\right)$ and for the delta function, we find that the integrations on the $z_j$ factorize and we get

$$
\mathcal{P}_N(U) = [N(2\pi)^N \det M]^{-1/2} \int_{-\infty}^\infty \frac{d\nu}{\sqrt{2\pi}} e^{-\nu^2/2} \int_{-\infty}^\infty \frac{d\lambda}{2\pi} e^{-\lambda U}
$$

$$
\times \left(\int_{-\infty}^\infty dz e^{-(1/2)\alpha(\beta z^2 + \nu(N\beta)^{1/2} z + i\lambda N^{-1} h(z))} \right)^N.
$$

(2.14)

We use that $\alpha + \beta = 1/(1 - \rho)$ and shift from $z$ to a new variable of integration

$$
w = (1 - \rho)^{-1/2} (z - \nu(1 - \rho) (N\beta)^{1/2}).
$$

(2.15)

Completing the square in the exponential in (2.14) produces a factor $\exp \left((N\beta/2) \times (1 - \rho)\nu^2\right)$ which may be taken outside the integral and whose $N$th power combines with $\exp((-1/2)N\nu^2)$ to yield $\exp((-1/2)\gamma N\nu^2)$ where $\gamma = N(1 - \rho)/(1 + N(1 - \rho))$. The asymptotic $N$ dependence of this coefficient, namely $\gamma \simeq (1 - \rho)/\rho$, is the result of a cancellation of terms of order $N$. Using that $\det M = [1 + (N - 1)\rho]^{-1}$ and rearranging some of the prefactors we transform (2.14) into

$$
\mathcal{P}_N(U) = \left(\frac{1 - \rho}{2\pi[1 + (N - 1)\rho]}\right)^{1/2} \int_{-\infty}^\infty d\nu e^{-\gamma \nu^2} \int_{-\infty}^\infty d\lambda e^{-i\lambda U}
$$

$$
\times \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty dw e^{-(1/2)w^2 + i\lambda N^{-1} h(w + \nu\sqrt{1 - \rho})} \right)^N.
$$

(2.16)

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At this point we perform an asymptotic expansion in powers of $N^{-1}$ of the right-hand side of equation (2.16). This gives

$$\mathcal{P}(U) = \lim_{N \to \infty} \left( \frac{1 - \rho}{2\pi \rho} \right)^{1/2} \int_{-\infty}^{\infty} d\nu e^{-((1-\rho)/2\rho)\nu^2} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda U} \times \left( 1 + \frac{i\lambda}{N} \int_{-\infty}^{\infty} \frac{dw}{\sqrt{2\pi}} e^{-(1/2)w^2} h((w + \nu)\sqrt{1-\rho}) + O(N^{-2}) \right)^N.$$  

(2.17)

We now define

$$k(\nu) = U - \int_{-\infty}^{\infty} \frac{dw}{\sqrt{2\pi}} e^{-(1/2)w^2} h((w + \nu)\sqrt{1-\rho})$$  

(2.18)

and simplify (2.17) further to

$$\mathcal{P}(U) = \left( \frac{1 - \rho}{2\pi \rho} \right)^{1/2} \int_{-\infty}^{\infty} d\nu e^{-(1-\rho)/2\rho)\nu^2} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda k(\nu)}$$

$$= \left( \frac{1 - \rho}{2\pi \rho} \right)^{1/2} \int_{-\infty}^{\infty} d\nu e^{-(1-\rho)/2\rho)\nu^2} \delta(k(\nu)).$$  

(2.19)

Let $\nu_s(U)$ be the unique solution of

$$k(\nu_s) = 0,$$  

(2.20)

so that we may write $\delta(k(\nu)) = \delta(\nu - \nu_s)|k'(\nu_s)|^{-1}$. Then, in the general case under consideration here, our final result for the limit function $\mathcal{P}(U)$ follows from (2.19) as

$$\mathcal{P}(U) = \left( \frac{1 - \rho}{2\pi \rho} \right)^{1/2} |k'(\nu_s(U))|^{-1} \exp \left( -\frac{1 - \rho}{2\rho} [\nu_s(U)]^2 \right), \quad \left(-\frac{1}{2} \leq U \leq \frac{1}{2}\right),$$  

(2.21)

in which $k$ is defined by (2.18), $\nu_s$ by (2.20), and we have set $k' = dk/d\nu$.

2.3. Special case of a block function

The limit function $\mathcal{P}(U)$ given by equations (2.21), (2.18), and (2.20) can be found fully explicitly for the special case of the block function distribution (2.1) studied by Thistleton et al [12]. According to equations (2.8) and (2.11), we have in that case $h(z) = (1/2)\text{erf}(z/\sqrt{2})$, which when substituted in (2.18) yields

$$k'(\nu) = \pi^{-1/2} \kappa e^{-\kappa^2 \nu^2}, \quad \kappa \equiv \left( \frac{1 - \rho}{2(2 - \rho)} \right)^{1/2},$$

$$k(\nu) = U - \frac{1}{2} \text{erf}(\kappa \nu),$$

$$\nu_s = \kappa^{-1} \text{erf}^{-1}(2U),$$  

(2.22)

where $\text{erf}^{-1}$ denotes the inverse error function. After straightforward substitution of (2.22) in the general expression (2.21) we obtain

$$\mathcal{P}(U) = \left( \frac{2 - \rho}{\rho} \right)^{1/2} \exp \left( -\frac{2(1 - \rho)}{\rho} [\text{erf}^{-1}(2U)]^2 \right), \quad \left(-\frac{1}{2} \leq U \leq \frac{1}{2}\right).$$  

(2.23)

This is our end result for the distribution $\mathcal{P}(U)$ of the scaled sum $U$ in the special case studied by Thistleton et al [12]. It is not the $q$-Gaussian that the authors speculated it to be.

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2.4. Discussion of $\mathcal{P}(U)$

For $U \to \pm (1/2)$ we have that $\text{erf}^{-1}(2U) \to \pm \infty$ and therefore $\mathcal{P}(U) = 0$ outside the interval $[-1/2, 1/2]$. One may verify explicitly the normalization $\int_{-1/2}^{1/2} \mathcal{P}(U) \, dU = 1$. We consider now successively the limits $\rho \to 0$ and $\rho \to 1$. The inverse error function has the expansion [14]

$$\text{erf}^{-1}(2U) = \pi^{1/2}U + \frac{1}{3}(\pi^{1/2}U)^3 + \frac{7}{30}(\pi^{1/2}U)^5 + \frac{127}{360}(\pi^{1/2}U)^7 + \frac{4369}{22680}(\pi^{1/2}U)^9 + \cdots \tag{2.24}$$

For $\rho \ll 1$ it suffices to keep the first term in this expansion and substitution in (2.23) shows that in that limit $\mathcal{P}(U)$ approaches a Gaussian of variance $\rho/(4\pi)$. This Gaussian limit is nevertheless somewhat curious: whereas it is true that for $\rho \to 0$ the $N$ variables become independent, the usual Gaussian distribution associated with their sum would require a scaling with $N^{-1/2}$ instead of the present one with $N^{-1}$. Hence we have here the explicit demonstration of the non-commutativity of the limits $\rho \to 0$ and $N \to \infty$.

In the other limit, $\rho \to 1$, one sees directly that $\mathcal{P}(U)$ tends to unity on the interval $[-1/2, 1/2]$. This second limit is heuristically obvious since for $\rho = 1$ the random variables are fully correlated. For $0 < \rho < 1$ the function $\mathcal{P}(U)$ interpolates between a Gaussian and a block function. Since the $q$-Gaussian does the same for $1 > q > -\infty$, one may ask, for given $\rho$, whether there is a corresponding $q$ that gives the best fit. This will be done in the next subsection.

2.5. Best $q$-Gaussian fit to $\mathcal{P}(U)$

We try to find the best $q$-Gaussian fit to solution (2.23) by adjusting the values of $q$ and the width $b$ in (1.1). There is no unique way of defining a ‘best fit’. We will base ourselves on comparing the small-argument expansions of $\mathcal{P}(U)$ and $G_q(x)$. The one of $G_q(x)$ is immediate,

$$G_q(x) = b^{1/2}C_q \exp \left[ -\sum_{n=1}^{\infty} \frac{(1-q)^{n-1}}{n(3-q)^n} b^n x^{2n} \right]. \tag{2.25}$$

The expansion of $\mathcal{P}(U)$ is obtained by substituting (2.24) in (2.23) and going through the algebra. One finds

$$\mathcal{P}(U) = \left( \frac{2-\rho}{\rho} \right)^{1/2} \exp \left[ -\sum_{n=1}^{\infty} C_{2n} U^{2n} \right]$$

$$= \left( \frac{2-\rho}{\rho} \right)^{1/2} \exp \left[ -\frac{2(1-\rho)}{\rho} \sum_{n=1}^{\infty} c_{2n} \pi^n U^{2n} \right], \tag{2.26}$$

in which the coefficients $C_{2n}$ are defined by the $c_{2n}$ which in turn are given by

$$c_2 = 1, \quad c_4 = \frac{2}{3}, \quad c_6 = \frac{26}{25}, \quad c_8 = \frac{176}{315}, \quad c_{10} = \frac{8138}{11177}, \ldots \tag{2.27}$$

The $q$-Gaussian (2.25) contains two adjustable parameters, $q$ and $b$. For the best fit we will adopt the criterion that the coefficients of the quadratic and quartic terms in

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Figure 1. Solid line: the exact limit function $P(U)$ given by equation (2.23) for the case $\rho = 7/10$. Dotted line: the $q$-Gaussian approximation to this function for $q = -5/9$ (see text). The difference between the two curves is of the order of the thickness of the dotted line and just barely visible to the eye.

the expansions (2.25) and (2.26) coincide. This leads directly to the relation $C_4/C_2^2 = (1/2)(1-q)$. Working out the remaining algebra using (2.25), (2.26), and (2.27), we obtain

$$q = \frac{1 - (5/3)\rho}{1 - \rho}, \quad b = \frac{4\pi(1 - (2/3)\rho)}{\rho}.$$ (2.28)

The first one of these equations is precisely the result (2.9) conjectured by Thistleton et al [12] on the basis of their numerical simulations! As an example, we show in figure 1 the exact solution (2.23) for $\rho = 7/10$ (solid line) together with its $q$-Gaussian approximation (dotted line), which according to (2.28) has $q = -5/9$. The difference between the two is of the order of the thickness of the dotted line and just barely visible to the eye.

To get an analytic idea of the quality of the fit (2.28) we consider the ratio of the $q$-Gaussian approximation to the true solution. From (2.25) to (2.28) we deduce that

$$\frac{G_q(U)}{P(U)} = b^{1/2}C_q \left( \frac{\rho}{2 - \rho} \right)^{1/2} \exp \left[ -\frac{2(1 - \rho)}{\rho} \sum_{n=3}^{\infty} \epsilon_{2n} \pi^n U^{2n} \right],$$ (2.29)

where we set

$$\epsilon_{2n} = n^{-1} \left( \frac{4}{3} \right)^{n-1} - c_{2n}, \quad (n = 1, 2, \ldots).$$ (2.30)

By construction $\epsilon_2 = \epsilon_4 = 0$. It is remarkable that for the next few coefficients the terms in the difference (2.30) largely cancel. Evaluation gives, in particular,

$$\epsilon_6 = \frac{2}{135} = 0.01481, \quad \epsilon_8 = \frac{32}{945} = 0.03386, \quad \epsilon_{10} = \frac{822}{14175} = 0.05799.$$ (2.31)

The smallness of these coefficients explains analytically why the $q$-Gaussian fit (2.28) is so excellent.

Finally, we observe that with the criterion employed here the two functions $P$ and $G_q$ do not exactly coincide for $U = 0$. Using the explicit expression for $C_q$ we find for their

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ratio in the origin

\[
\frac{G_q(0)}{P(0)} = b^{1/2} C_q \left( \frac{\rho}{2 - \rho} \right)^{1/2} = \frac{3(2 - \rho)}{2(3 - 2\rho)} \frac{\Gamma(3/(2\rho) - 1/2)^2}{\Gamma(3/(2\rho) - 1)\Gamma(3/(2\rho))} = 1 - \frac{1}{144} \rho^2 + \cdots,
\]  

(2.32)

where the last line represents a small-\(\rho\) expansion. Again we see that the deviation from unity is very small. Hence our analysis confirms the high quality of the fit.

2.6. Remark on the general case (2.21)

The general case that we set out to consider in section 2.2 is specified by an arbitrary marginal one-variable distribution \(P_1(x)\). The corresponding limit distribution \(P(U)\) found in (2.21) is then obtained in terms of a function \(\nu_\ast(U)\) that follows from \(P_1(x)\) via relations (2.10), (2.11), (2.18), and (2.20). Although \(P(U)\) is not a \(q\)-Gaussian in the special case where \(P_1(x)\) is a block function, it is likely that an appropriate choice of \(P_1(x)\) will lead to a \(\nu_\ast(U)\) for which \(P(U)\) is a \(q\)-Gaussian. The conditions for this to happen constitute a rather complicated set of equations that we will not study here. The important point is that in the same way not only a \(q\)-Gaussian but any limit function \(P(U)\) out of a large class can be obtained; there is no indication that \(q\)-Gaussians play a special role.

3. Second example: the MTG sum

3.1. A special probability law

In an earlier attempt to construct a \(q\)-Gaussian distributed sum of variables, Moyano, Tsallis, and Gell-Mann (MTG) [13] proposed the expression

\[
R_N(n) = \sum_{i=N-n}^{N} (-1)^{i+n-N} \binom{n}{i} \left( \frac{p}{|i-(i-1)p\rho|^{1/\rho}} \right),
\]  

(3.1)

which depends on two parameters \(p\) and \(\rho\). The \(R_N(n)\) satisfy the normalization

\[
\sum_{n=0}^{N} \binom{N}{n} R_N(n) = 1
\]  

(3.2)

and \(\binom{N}{n} R_N(n)\) can be interpreted as the probability that the sum of \(N\) Boolean random variables, correlated in a special way (but remaining implicit), be exactly equal to \(n\). In this second example the starting point (3.1) is itself clearly motivated by the formalism of \(q\)-statistical mechanics: the last factor in the summand represents a so-called ‘\(q\)-product’ [13] with \(\rho\) in the role of \(1 - q\); in the singular limit \(\rho \to 0\) it reduces to \(p^{-i}\).

Moyano et al [13] were again interested in the large-\(N\) limit with \(n\) scaling as \(n = yN\), hence the limiting probability distribution

\[
\mathcal{R}(y) = \lim_{N \to \infty} N \binom{N}{yN} R_N(yN),
\]  

(3.3)

\footnote{In [13] our \(\rho\) introduced in section 3.1 is called \(1 - q\) and our \(q\) in section 3.4 is called \(q_\ast\).}

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where the first factor $N$ comes from the scaling between $n$ and $y$. They evaluated the sum (3.1) numerically for typical values of $p$ and $\rho$ and for $N$ up to 1000, taking extraordinary precautions to deal with the cancellations caused by the alternating signs. On the basis of their numerical results Moyano et al [13] conjecture that $R(y)$ is a double-branched $q$-Gaussian, the two branches joining in the centre and having the same $q$ but slightly different widths. After fitting they arrive at the relation

$$q = \frac{1 - 2\rho}{1 - \rho}. \quad (3.4)$$

The functional dependence of (3.4) on $\rho$ bears resemblance to that of $q$ in the first example, equation (2.9).

For simplicity we will restrict ourselves in what follows to the case $p = 1/2$, where some rewriting turns expression (3.1) into

$$R_N(n) = \frac{1}{2(1 - 2^{-\rho})} \sum_{j=0}^{n} (-1)^{n-j} \binom{n}{j} \frac{1}{[N - j + (2^\rho - 1)^{-1}]^{1/\rho}}. \quad (3.5)$$

Below we will show that it is possible, again, to evaluate this sum and find the limit function $R(y)$ analytically.

### 3.2. The limiting law $R(y)$

Upon employing in (3.5) the integral representation

$$\frac{1}{X^k} = \frac{1}{\Gamma(k)} \int_0^\infty d\alpha \alpha^{k-1} e^{-\alpha X} \quad (3.6)$$

with $X = N - j + (2^\rho - 1)^{-1}$ and $k = 1/\rho$ we find that the sum on $j$ represents the binomial expansion of $(e^{\alpha} - 1)^n$. We get

$$R_N(n) = \frac{1}{A_{\rho}} \int_0^\infty d\alpha \alpha^{(1-\rho)/\rho} e^{-(2^\rho - 1)^{-1}\alpha - N f(\alpha)} \quad (3.7)$$

with

$$A_{\rho} = 2\Gamma\left(\frac{1}{\rho}\right)(1 - 2^{-\rho})^{1/\rho},$$

$$f(\alpha) = \alpha - y \log(e^\alpha - 1). \quad (3.8)$$

The function $f(\alpha)$ has its maximum for $\alpha = \alpha^* \equiv \log(1 - y)$. In the large-$N$ limit the integral (3.7) is easily evaluated by the saddle point method with the result

$$R_N(n) = \left(\frac{2\pi}{N f''(\alpha^*)}\right)^{1/2} e^{-\alpha^* - N f(\alpha^*)} \left[1 + \cdots\right]$$

$$= \left(\frac{2\pi y(1 - y)}{N}\right)^{1/2} e^{N[y \log y + (1 - y) \log(1 - y)]} \left[1 + \cdots\right], \quad (3.9)$$

where the dots indicate terms that vanish as $N \to \infty$ and we recall that $y = n/N$. This should now be combined with the large-$N$ expression of the binomial coefficient,

$$\binom{N}{n} = [2\pi N y(1 - y)]^{-1/2} e^{-N[y \log y + (1 - y) \log(1 - y)]} \left[1 + \cdots\right], \quad (3.10)$$

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which results from straightforward application of Stirling’s formula. Combining (3.3) with (3.9) and (3.10) and setting

\[ a_\rho = \frac{2 - 2^\rho}{2^\rho - 1} \quad (3.11) \]

we obtain

\[ R(y) = A_\rho^{-1} (1 - y)^{a_\rho} \left[ - \log(1 - y) \right]^{(1-\rho)/\rho}, \quad (0 \leq y \leq 1). \quad (3.12) \]

This is our result for the distribution \( R(y) \) studied by Moyano et al [13] in their special case \( p = 1/2 \). Again, it is not the double-branched \( q \)-Gaussian that the authors [13] conjectured it to be (and which would have required it to be non-analytic at its centre).

3.3. Discussion of \( R(y) \)

The exponents \( a_\rho \) and \((1 - \rho)/\rho\) are both positive for \( 0 < \rho < 1 \), which is the interval of interest. Hence \( R(y) \) is bell-shaped and vanishes in \( y = 0 \) and 1. One may verify explicitly the normalization \( \int_0^1 R(y) \, dy = 1 \). As had to be expected, \( R(y) \) has no point of symmetry. It takes its maximum for \( y = y_\rho^* \) given by

\[ y_\rho^* = 1 - \exp \left( -\frac{1 - \rho}{\rho a_\rho} \right). \quad (3.13) \]

We consider again two limiting cases of interest. For \( \rho \to 0 \) one shows after some algebra that \( R(y) \) approaches a Gaussian centred at \( y = 1/2 \) and of variance \( \rho \log 2 \). For \( \rho \to 1 \) we have \( A_1 = 1 \) and \( a_1 = 0 \), whence it follows that \( R(y) \) is the block function \( R(y) = 1 \) on the interval \( 0 \leq y \leq 1 \). When \( \rho \to 1 \) the maximum \( y_1^* \) of the distribution has the non-trivial limit \( y_1^* \equiv \lim_{\rho \to 1} y_\rho^* = 1 - \exp \left( - (2 \log 2)^{-1} \right) = 0.5139 \ldots \), which is different from 1/2 in spite of \( R(y) \) being symmetric for \( \rho = 1 \). In summary, for \( 0 < \rho < 1 \), the sum \( R(y) \) varies between a Gaussian and a block function distribution, just as in the first example.

3.4. Best \( q \)-Gaussian fit to \( R(y) \)

We will again find the \( q \)-Gaussian that best fits the exact result (3.12). Upon expanding the latter around its maximum (3.13) one finds

\[ R(y) = \exp \left( - \sum_{j=2}^{\infty} D_j (y - y_\rho^*)^j \right), \quad (3.14) \]

which defines the coefficients \( D_j \). The best \( q \) will be determined as a function of \( \rho \) in the same way as above, that is, from the ratio of the coefficients of the quadratic and the quartic terms according to \((1/2)(1 - q) = D_4/D_2^2\). This procedure ‘averages’ over the asymmetry due to the cubic and higher order odd terms in (3.14) by simply neglecting them. After doing the algebra one finds (see footnote 2)

\[ q = 1 - \frac{11(1 - \rho)^2 - 12(1 - \rho)\rho a_\rho + 6\rho^2 a_\rho^2}{3(1 - \rho)\rho a_\rho^2}, \quad (3.15) \]
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Figure 2. Comparison of two relationships between $q$ and $\rho$. Solid line: equation (3.15) obtained analytically in this work. Dotted line: equation (3.4) conjectured by Moyano *et al* [13] on the basis of numerical work. The difference is hardly visible to the eye.

Figure 3. Solid line: the exact limit function $R(y)$ given by equation (3.12) for the case $\rho = 7/10$. Dotted line: the $q$-Gaussian approximation to this function for $q = -4/3$ (see text). We improved the fit visually by not centring the $q$-Gaussian at the exact maximum $y^*_\rho$ but shifting it very slightly to the left. The difference between the two curves is small but visible.

which has the small-$\rho$ expansion

$$q = 1 - \left[\frac{11}{3} (\log 2)^2 - 4 \log 2 + 2\right] \rho - \left[11 (\log 2)^3 - \frac{29}{3} (\log 2)^2 + 2\right] \rho^2 + \cdots$$

$$= 1 - 0.98907 \ldots \rho - 1.01889 \ldots \rho^2 + \cdots. \quad (3.16)$$

It appears from (3.15) that in this second example we do not reproduce the guess (3.4) based by MTG [13] on their numerical evaluation of $R(y)$. Nevertheless, the two relations between $q$ and $\rho$, equations (3.4) and (3.15), are in very close *numerical* agreement, as shown in figure 2. Concomitantly expansion (3.16), when compared to the expansion $q = 1 - \rho - \rho^2 + \cdots$ obtained from (3.4), shows a close numerical agreement between the coefficients.

In figure 3, finally, we show the limit function $R(y)$ for $\rho = 7/10$ together with its $q$-Gaussian approximation, which according to equation (3.4) has $q = -4/3$. No visible difference results if instead one were to take $q = -1.36074$ as would follow from (3.15).
Hence in this second example once more, things conspire such that it becomes extremely
difficult to distinguish the true curve from its $q$-Gaussian approximant.

4. Final remarks

Probability distributions shaped as $q$-Gaussians, if and when they occur, are interpreted
as a manifestation of a $q$-generalized statistical mechanics [1]. We have investigated
the emergence of $q$-Gaussians as probability distributions of \textit{sums of strongly correlated}
variables. The possible role of $q$-Gaussians in a wider context has remained outside the
scope of this work.

The literature examples discussed in this note illustrate the difficulty of identifying
$q$-Gaussians. Two cases where $q$-Gaussian distributions had been thought to occur, turn out
to correspond to analytically very different functions. The very close numerical agreement
does not detract from this distinction of principle. Although the first example does show
a way of fine-tuning correlations between random variables such that their sum becomes
$q$-Gaussian distributed, this method works for any one out of a large class of distributions
and does not hint at a special role for $q$-Gaussians. The probability laws constructed by
this kind of fine-tuning are \textit{limit distributions} in the plain sense that they appear when
the number $N$ of terms in the sum tends to infinity. They are not, however, or at least
have not been shown to be, \textit{attractors}, and this raises the question of why such finely
adjusted correlations would occur in physics. Efforts to let $q$-Gaussians play the role of
attractors within the framework of a $q$-generalized central limit theorem [15] have not yet
led to examples that we can subject to analysis.

The undeniably interesting properties of $q$-Gaussians make it worthwhile to investigate
the role they play in many-body systems in statistical mechanics. However, from
the examples studied in this work we draw the conclusion that, in the absence of
convincing theoretical arguments, one should exercise extreme caution when interpreting
non-Gaussian data in terms of $q$-Gaussians.

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References

[1] Tsallis C, 1988 \textit{J. Stat. Phys.} \textbf{52} 479
[2] Latora V, Rapisarda A and Tsallis C, 2001 \textit{Phys. Rev. E} \textbf{64} 056134
   Latora V, Rapisarda A and Tsallis C, 2002 \textit{Physica A} \textbf{305} 129
[3] Beck C, Lewis G S and Swinney H L, 2001 \textit{Phys. Rev. E} \textbf{63} 035303(R)
[4] Upadhyaya A, Rieu J-P, Glazier J A and Sawada Y, 2001 \textit{Physica A} \textbf{293} 549
[5] Lavagno A, Kaniadakis G, Rego-Monteiro M, Quarati P and Tsallis C, 1998 \textit{Astrophys. Lett. Commun.} \textbf{35} 449
[6] Bernui A, Tsallis C and Villela T, 2006 \textit{Phys. Lett. A} \textbf{356} 426
   Bernui A, Tsallis C and Villela T, 2007 \textit{Europhys. Lett.} \textbf{78} 19001
[7] Baldovin F and Orlandini E, 2006 \textit{Phys. Rev. Lett.} \textbf{96} 240602
   Baldovin F and Orlandini E, 2006 \textit{Phys. Rev. Lett.} \textbf{97} 100601
[8] Tsallis C, Rapisarda A, Pluchino A and Borges E P, 2007 \textit{Physica A} at press

\textit{J. Stat. Mech.} (2007) P06003

doi:10.1088/1742-5468/2007/06/P06003
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[9] Yamaguchi Y, Bouchet F and Dauxois T, 2007 J. Stat. Mech. P01020
[10] Bouchet F and Dauxois T, 2005 Phys. Rev. E 72 045103(R)
    Chavanis P-H and Sire C, 2005 Physica A 256 419
    Chavanis P-H, 2006 Eur. Phys. J. B 53 487
    Chavanis P-H, 2006 Physica A 365 102
[11] Umarov S and Tsallis C, 2007 Preprint cond-mat/0703553
[12] Thistleton W, Marsh J A, Nelson K and Tsallis C, 2006 unpublished
    Tsallis C, 2007 Workshop on the Dynamics of Complex Systems (Natal, Brazil, March 2007)
[13] Moyano L G, Tsallis C and Gell-Mann M, 2006 Europhys. Lett. 73 813
    See also Marsh J A, Fuentes M A, Moyano L G and Tsallis C, 2006 Physica A 372 183
    Tsallis C, 2006 Physica A 365 7
[14] http://functions.wolfram.com/GammaBetaErf/InverseErf/06/01/
[15] Umarov S, Tsallis C and Steinberg S, 2006 Preprint cond-mat/0603593v3