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Estimation of Tsallis' q-index in Non-extensive Systems

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Abstract. In this work we derive a microscopic estimation formula for the parameters in the q-exponential distribution, appearing in Tsallis statistics. This avoids the need for fitting a (cumulative) probability distribution to obtain q.

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INTRODUCTION

The $q-$exponential family of probability distributions is a common statistical model that generalizes the canonical (Boltzmann-Gibbs) distribution of statistical mechanics, appearing frequently in non-equilibrium or non-extensive systems, chaotic systems and fractals, among other phenomena. It is defined as

$$P(\vec{x}|\beta,q) = \frac{1}{Z}\exp(-\beta H(\vec{x});q), \tag{1}$$

where the notation $\exp(y;q)$ represents the $q-$exponential function,

$$\exp(y;q) = \Theta(1+(1-q)y)\,[1+(1-q)y]^{\frac{1}{1-q}}, \tag{2}$$

which reduces to the usual exponential function $\exp(y)$ in the limit $q \to 1$. Here H is some relevant "descriptor" function (usually the Hamiltonian, in Physics applications) and Z is a normalization constant (a partition function). These $q-$exponential distributions can be derived, in an analogous way as Jaynes' method of maximum entropy [1], from maximization of a generalized, non-extensive entropy [2],

$$S_q = k_B\frac{1}{q-1}\left(1-\int d\vec{x}P(\vec{x}|R)^q\right), \tag{3}$$

known as Tsallis entropy, subject to appropriate constraints fixing the expected energy. In the limit $q \to 1$, S_q reduces to the usual Shannon-Gibbs entropy

$$S = -k_B\int d\vec{x}P(\vec{x}|R)\ln P(\vec{x}|R) \tag{4}$$

and Eq. 1 recovers the Boltzmann-Gibbs distribution,

$$P(\vec{x}|R) = \frac{1}{Z}\exp(-\beta H(\vec{x})). \tag{5}$$

There is no constructive method to obtain q from a given set of observed states $\vec{x}$ (or measurements of H), and the usual route is to accumulate an histogram to approximate P (or the cumulative distribution function associated with P) and use nonlinear least-squares methods to fit q. Recently, a maximum likelihood method has been proposed [3].

In this work we present a simple estimation formula for the q index in a q-exponential distribution, with potential applications in numerical simulations of non-extensive systems.

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DERIVATION

We will only consider the case $q \leq 1$, as this ensures the correct normalization of P. In fact, without this condition the theory has been shown to be internally inconsistent [4].

We can always express Eq. 1 as a canonical distribution

$$P(\vec{x}|\beta,q) \propto \exp(-\tilde{H}(\vec{x};\beta,q)), \tag{6}$$

with a new fictitious Hamiltonian $\tilde{H}(\vec{x};\beta,q)$, defined as

$$\tilde{H}(\vec{x};\beta,q) = -\ln\Theta(1-(1-q)\beta H(\vec{x})) - \frac{1}{1-q}\ln(1-(1-q)\beta H(\vec{x})). \tag{7}$$

Now we can use the recently proposed *conjugate variables theorem* (CVT) [5], which is a convenient relationship between averages for a canonical distribution, generalizing the equipartition theorem and hypervirial theorems. For the canonical distribution of Eq. 5, CVT implies

$$\Big\langle \nabla\cdot\vec{v} \Big\rangle = \beta \Big\langle \vec{v}\cdot\nabla H(\vec{x}) \Big\rangle. \tag{8}$$

Due to the way we defined the new Hamiltonian $\tilde{H}$ (Eq. 6) the corresponding fictitious Lagrange multiplier has a value of 1, and CVT holds as

$$\Big\langle \nabla\cdot\vec{v} \Big\rangle = \Big\langle \vec{v}\cdot\nabla \tilde{H}(\vec{x};\beta,q) \Big\rangle. \tag{9}$$

Substituting the definition of $\tilde{H}$ to put it in terms of the original Hamiltonian we obtain

$$\Big\langle \nabla\cdot\vec{v} \Big\rangle = \beta(1-q)\Big\langle \frac{\delta(1-(1-q)\beta H)\vec{v}\cdot\nabla H}{\Theta(1-(1-q)\beta H)} \Big\rangle + \beta\Big\langle \frac{\vec{v}\cdot\nabla H}{1-(1-q)\beta H} \Big\rangle, \tag{10}$$

and we note the first term of the right-hand side vanishes for $q \leq 1$, as the probability in Eq. 1 is zero on the hypersurface imposed by the delta function. We finally arrive at

$$\Big\langle \nabla\cdot\vec{v} \Big\rangle = \beta\Big\langle \frac{\vec{v}\cdot\nabla H}{1-(1-q)\beta H} \Big\rangle, \tag{11}$$

from which a system of equations can be obtained for q and β by replacing different choices of the (arbitrary) $\vec{v}$ vector field (the only requirement being that every choice of $\vec{v}$ is differentiable). We can improve readability by using the substitution

$$\vec{v} = (1-(1-q)\beta H)\vec{\omega}, \tag{12}$$

leading to the more familiar form

$$\Big\langle \nabla\cdot\vec{\omega} \Big\rangle = \beta\left[\Big\langle \vec{\omega}\cdot\nabla H \Big\rangle + (1-q)\Big\langle \nabla\cdot(H\vec{\omega}) \Big\rangle\right]. \tag{13}$$

In this form, the first term is the usual (canonical) CVT, and the extra "non-extensive" term vanishes in the limit $q \to 1$. Using $\vec{\omega} = g(\vec{x})\vec{\chi}/(\vec{\chi}\cdot\nabla H)$, we get

$$\Big\langle \hat{\beta} g \Big\rangle + \Big\langle \frac{\vec{\chi}\cdot\nabla g}{\vec{\chi}\cdot\nabla H} \Big\rangle = \beta\left[\Big\langle g \Big\rangle + (1-q)\left(\Big\langle \hat{\beta} H g \Big\rangle + \Big\langle \frac{\vec{\chi}\cdot\nabla(gH)}{\vec{\chi}\cdot\nabla H} \Big\rangle\right)\right], \tag{14}$$

where

$$\hat{\beta} = \nabla\cdot\left(\frac{\vec{\chi}}{\vec{\chi}\cdot H}\right) \tag{15}$$

is the most general estimator for the inverse temperature [6, 7]. Two particular cases easily yield the desired system of equations. For simplicity we choose $g = 1$ and $g = H$, which gives

$$\langle \hat{\beta} \rangle = \beta\left[1 + (1-q)\left(1 + \Big\langle \hat{\beta} H \Big\rangle\right)\right] \tag{16}$$

$$\left\langle \hat{\beta} H \right\rangle + 1 = \beta \left[\langle H \rangle + (1-q) \left(\left\langle \hat{\beta} H^2 \right\rangle + 2 \langle H \rangle \right) \right]. \tag{17}$$

Combining Eqs. 16 and 17 we finally arrive at an expression for $1-q$ (which is of course not unique) depending only on microscopical averages, namely

$$1-q = \frac{\langle \hat{\beta} \rangle \langle H \rangle - \langle \hat{\beta} H \rangle - 1}{\left(1 + \langle \hat{\beta} H \rangle\right)^2 - \langle \hat{\beta} \rangle \left(2 \langle H \rangle + \langle \hat{\beta} H^2 \rangle\right)}. \tag{18}$$

This expression, along with Eq. 13 constitutes our main result. Once q is computed using this formula, then β can be computed using either Eq. 16 or 17.

For a non-extensive Hamiltonian with kinetic degrees of freedom,

$$H(\vec{x}, \vec{p}) = K(\vec{p}) + \Phi(\vec{x}) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \Phi(\vec{x}) \tag{19}$$

(where K is the kinetic energy) such as the HMF (Hamiltonian mean field) model [8], we already have a widely used estimator for the inverse temperature, the kinetic estimator $\hat{\beta}_K$ defined as

$$\hat{\beta}_K = \frac{3N}{2K} = \frac{1}{k_B T_K} \tag{20}$$

which is nothing but the typical formula used in molecular dynamics simulations,

$$\frac{3}{2} N k_B T_K = \sum_{i=1}^{N} \frac{p_i^2}{2m_i}. \tag{21}$$

Note that for the Boltzmann-Gibbs case,

$$\left\langle \delta \hat{\beta} \delta H \right\rangle = \left\langle \hat{\beta} H \right\rangle - \left\langle \hat{\beta} \right\rangle \left\langle H \right\rangle = -1 \tag{22}$$

and then from Eq. 18 we recover the fact that $1-q=0$.

APPLICATIONS

The q-Gaussian Distribution

The non-extensive analog of the ubiquitous Gaussian distribution is the so-called q-Gaussian distribution. It has the form

$$P(x|q, \mu, \sigma) = \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2; q\right) \tag{23}$$

which is a particular case of Eq. 1 with

$$H(x) = \frac{(x-\mu)^2}{2} \tag{24}$$

$$\beta = 1/\sigma^2. \tag{25}$$

Using the one-dimensional version of Eq. 13,

$$\left\langle \omega'(x) \right\rangle = \beta \left[(2-q) \langle \omega H' \rangle + (1-q) \langle \omega' H \rangle \right]. \tag{26}$$

and providing two different choices of $\omega(x)$ we can construct a system of equations for β and q. First we use $\omega(x) = (x-\mu)/2$, obtaining

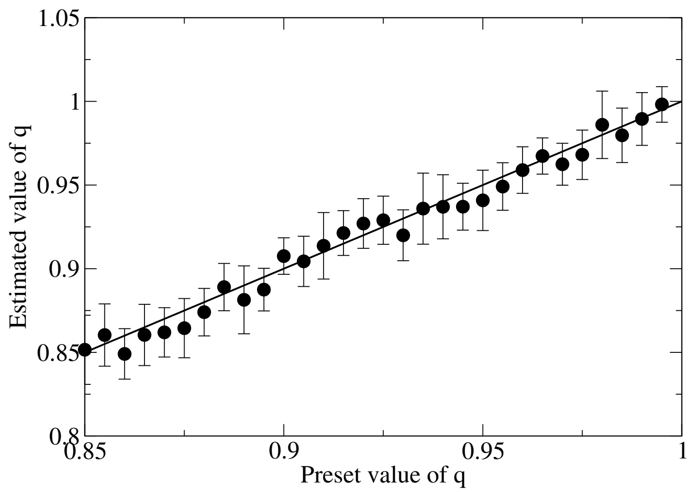

FIGURE 1. Preset and estimated values of q for μ =20, σ =5 and q between 0.85 and 1. The straight solid line represents the perfect estimation. Filled circles are the averages over 10 different realizations of the numerical experiment for each simulated value of q, with a dispersion indicated by the error bars.

$$\beta \langle H \rangle (2+3(1-q)) = 1. \tag{27}$$

Then, for $\omega(x) = \frac{(x-\mu)^3}{4}$, we get

$$\beta \langle H^2 \rangle \left(1+\frac{5}{2}(1-q)\right) = \frac{3}{2}\langle H \rangle. \tag{28}$$

Combining Eqs. 27 and 28 we finally obtain

$$1-q = \frac{1}{3}\left(\frac{4\langle H^2 \rangle}{5\langle H^2 \rangle - 9\langle H \rangle^2} - 2\right). \tag{29}$$

Figure 1 shows the numerical evaluation of Eq. 29 using data sampled from different q-Gaussian distributions (with μ =20, σ =5 and q ranging from 0.85 to 1) by means of a Metropolis-Hastings [9] procedure. The burning time was 5×10^5 steps and the samples for averaging were taken every 100 steps for a total of 1×10^4 samples.

CONCLUDING REMARKS

We have derived microscopic expressions for the q index appearing in q-exponential (Tsallis) distributions with $q \leq 1$, both in the case of an arbitrary Hamiltonian (here the estimation formula involves estimators $\hat{\beta}$ for the inverse temperature) and for the case of a q-Gaussian distribution. Numerical experiments on the q-Gaussian case demonstrate the accuracy of the formula.

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