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Maximization of Tsallis entropy in the combinatorial formulation

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Maximization of Tsallis entropy in the combinatorial formulation

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Abstract. This paper presents the mathematical reformulation for maximization of Tsallis entropy S_q in the combinatorial sense. More concretely, we generalize the original derivation of Maxwell-Boltzmann distribution law to Tsallis statistics by means of the corresponding generalized multinomial coefficient. Our results reveal that maximization of S_{2-q} under the usual expectation or S_q under q-average using the escort expectation are naturally derived from the combinatorial formulations for Tsallis statistics with respective combinatorial dualities, that is, one for additive duality and the other for multiplicative duality.

1. Introduction

Since the introduction of Tsallis entropy[1] in 1988 for a generalization of Boltzmann-Gibbs statistics (BG statistics), the maximum entropy principle has been the main approach along the Jaynes' original idea[2]. Jaynes developed Shannon's monumental achievement as pioneer of information theory in 1948 for the new method nowadays called maximum entropy principle (MEP) in mathematical physics. Originally, Jaynes applied the maximization of Shannon entropy under a constant expectation to the mathematical reformulation of Boltzmann-Gibbs statistics. On the other hand, the standard and well accepted introduction for Boltzmann-Gibbs statistics has been to count the number of accessible microstates[3]. From the traditional point of view in statistical physics, the counterpart for the number of accessible microstates in Tsallis statistics has been missing. For this purpose, the q-multinomial coefficient was introduced from the mathematics of the q-exponential and it was shown to have a natural generalization of the one-to-one correspondence between the usual multinomial coefficient and Shannon entropy[4]. This relation also reveals the additive duality ($q \leftrightarrow 2-q$) in Tsallis statistics. After that, the q-multinomial coefficient was generalized to cover the four typical mathematical structures: the additive duality ($q \leftrightarrow 2-q$), the multiplicative duality ($q \leftrightarrow 1/q$), the q-triplet and the multifractal-triplet[5]. Based on these mathematical results, the maximization of Tsallis entropy is reformulated in the combinatorial sense.

This paper consists of 4 sections including this introduction. In order to clarify the essential idea, an important and simple example of Jaynes' MEP for Boltzmann-Gibbs statistics is first given in the section 2. In the following section 3, the MEP for Tsallis statistics is reformulated using the above combinatorial formula. The section 4 concludes the paper.

2. A simple example of Jaynes' MEP for BG statistics

The present example was originally used by Boltzmann and later simplified in [6]. In order to clarify the mathematical formulations for MEP in Tsallis statistics from the combinatorial point of view, this example is generalized in the next section.

Suppose that n dice are thrown on the table and the total number of spots showing is nU_1. What proportion of the dice are showing face $i, i = 1, \cdots, 6$?

Let n_i be the number of the spots showing face i when n dice are thrown. Then there are $\begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix}$ such ways. This is a macrostate labeled by $(n_1, \cdots, n_6)$ corresponding to $\begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix}$ microstates. Each microstate has a probability $\frac{1}{6^n}$ which directly comes from the principle of equiprobability. To find the most probable macrostate, we wish to maximize $\begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix}$ under the constraint observed on the total number of spots, $\sum_{i=1}^{6} in_i = nU_1$. This maximization problem is formulated as

$$\text{maximize} : \begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix} \tag{1}$$

$$\text{constraint} : \sum_{i=1}^{6} in_i = nU_1 \tag{2}$$

Using the Stirling's formula, the number of microstates $\begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix}$ is approximated to Shannon entropy in the following sense.

$$\ln \begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix} \simeq nS_1 \left(\frac{n_1}{n}, \cdots \frac{n_6}{n} \right) \tag{3}$$

Thus, the logarithm ln is a monotone increasing function and we define $p_i := \frac{n_i}{n}$, so that the above maximization problem is equivalent to the following form.

$$\text{maximize} : S_1 \left(p_1, \cdots p_6 \right) \tag{4}$$

$$\text{constraint} : \sum_{i=1}^{6} ip_i = U_1 \tag{5}$$

The above equivalence was originally given by G.Wallis in 1962 [7] after the original paper of Jaynes [2]. This maximization problem is well known to be solved through the Lagrange multiplier method:

$$L := S_1 \left(p_1, \cdots p_6 \right) - \alpha \left(\sum_{i=1}^{6} p_i - 1 \right) - \beta_1 \left(\sum_{i=1}^{6} ip_i - U_1 \right) \tag{6}$$

and its solution is given by

$$p_i^* = \frac{\exp\left(-\beta_1 i\right)}{Z} \quad (i = 1, \cdots, 6) \tag{7}$$

where β_1 is chosen so that $\sum_{i=1}^{6} ip_i^* = U_1$. Thus, the most probable macrostate is $(np_1^*, \cdots, np_6^*)$ where $n_i^* = np_i^*$ dice show face i. In statistical physics, β_1 is the inverse temperature, i.e.,

$$\frac{\partial S_1}{\partial U_1} = \beta_1. \tag{8}$$

In the next section, the above equivalence between two maximization problems is generalized to Tsallis statistics in accordance with the same procedure as above.

3. Reformulation of Jaynes' MEP for Tsallis statistics in the combinatorial sense

3.1. Preliminaries

The mathematical structure in Tsallis statistics was recently found to be originated from the very fundamental nonlinear differential equation [8][9](See the appendix):

$$\frac{dy}{dx} = y^q. \tag{9}$$

The solution to the above equation is given by the so-called q-exponential:

$$y = \exp_q(x) := [1 + (1-q)x]^{\frac{1}{1-q}} \tag{10}$$

defined for $x \in \mathbb{R}$ satisfying $1 + (1-q)x > 0$. In the course of the above derivation, the inverse to the q-exponential is appeared.

$$\ln_q x := \frac{x^{1-q} - 1}{1-q} \tag{11}$$

which is called q-logarithm defined for $x > 0$.

Then the q-product $\otimes_q$ is introduced as a natural generalization of the exponential law in the following way:

$$\ln_q(x \otimes_q y) = \ln_q x + \ln_q y, \tag{12}$$

$$\exp_q(x + y) = \exp_q(x) \otimes_q \exp_q(y). \tag{13}$$

Thus, the q-product is concretely determined [10][11].

Definition 1 *(q-product) For any $x, y > 0$ satisfying $x^{1-q} + y^{1-q} - 1 > 0$,*

$$x \otimes_q y := \left[x^{1-q} + y^{1-q} - 1\right]^{\frac{1}{1-q}} \tag{14}$$

is the q-product.

By means of the q-product (14), the q-factorial is naturally defined in the following form.

Definition 2 *(q-factorial) For a natural number $n \in \mathbb{N}$ and $q > 0$, the q-factorial $n!_q$ is defined by*

$$n!_q := 1 \otimes_q \cdots \otimes_q n. \tag{15}$$

Thus, we concretely compute the q-Stirling's formula [4].

Proposition 3 *(q-Stirling's formula) Let $n!_q$ be the q-factorial defined by (15). The rough q-Stirling's formula $\ln_q(n!_q)$ is computed as follows:*

$$\ln_q(n!_q) = \begin{cases} \dfrac{n \ln_q n - n}{2-q} + O(\ln_q n) & \text{if} \quad q \neq 2, \\ n - \ln n + O(1) & \text{if} \quad q = 2. \end{cases} \tag{16}$$

The above rough q-Stirling's formula is obtained by the approximation:

$$\ln_q(n!_q) = \sum_{k=1}^{n} \ln_q k \simeq \int_1^n \ln_q x dx. \tag{17}$$

The rigorous derivation of the q-Stirling's formula is given in [4].

In order to define the q-multinomial coefficient, the q-ratio $\oslash_q$, the inverse operation to the q-product $\otimes_q$, is also needed and similarly defined from the requirements:

$$\ln_q (x \oslash_q y) = \ln_q x - \ln_q y, \tag{18}$$

$$\exp_q (x - y) = \exp_q (x) \oslash_q \exp_q (y). \tag{19}$$

Then, we define the q-ratio $\oslash_q$[10][11].

Definition 4 *(q-ratio) For any $x, y > 0$ satisfying $x^{1-q} - y^{1-q} + 1 > 0$,*

$$x \oslash_q y := \left[x^{1-q} - y^{1-q} + 1\right]^{\frac{1}{1-q}} \tag{20}$$

is the q-ratio.

We apply these formulations, q-product and q-ratio, to the definition of the q-multinomial coefficient [4].

Definition 5 *(q-multinomial coefficient) For $n = \sum_{i=1}^{k} n_i$ and $n_i \in \mathbb{N}\ (i = 1, \cdots, k)$, the q-multinomial coefficient is defined by*

$$\left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array}\right]_q := (n!_q) \oslash_q \left[(n_1!_q) \otimes_q \cdots \otimes_q (n_k!_q)\right]. \tag{21}$$

Based on these formulations, Tsallis entropy is derived as a natural generalization of the usual correspondence (3) [4].

Theorem 6 *When $n \in \mathbb{N}$ is sufficiently large, the q-logarithm of the q-multinomial coefficient coincides with Tsallis entropy (23) in the following correspondence:*

$$\ln_q \left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array}\right]_q \simeq \begin{cases} \dfrac{n^{2-q}}{2-q} \cdot S_{2-q}\left(\dfrac{n_1}{n}, \cdots, \dfrac{n_k}{n}\right) & \text{if} \quad q > 0,\ q \neq 2 \\ -S_1(n) + \sum\limits_{i=1}^{k} S_1(n_i) & \text{if} \quad q = 2 \end{cases} \tag{22}$$

where S_q is Tsallis entropy:

$$S_q(p_1, \ldots, p_k) = \frac{1 - \sum\limits_{i=1}^{k} p_i^q}{q-1} \tag{23}$$

and $S_1(n) := S_1\left(\frac{1}{n}, \cdots \frac{1}{n}\right) = \ln n$.

See [4] for the details and its proofs.

Therefore, Tsallis entropy is found to be the information measure uniquely determined by the nonlinear differential equation (9) [9]. Moreover, the parameter q in Tsallis statistics coincides with the parameter q in the generalized dimension D_q for multifractal systems in the following sense [12]:

$$\exp\left(S_q^{\text{Rényi}}(p_i)\right) = \exp_q\left(S_q^{\text{Tsallis}}(p_i)\right) = \exp_{1/q}\left(S_{1/q}^{\text{Tsallis}}(P_j)\right) \simeq \varepsilon^{-D_q} \tag{24}$$

where $S_q^{\text{Rényi}}$ is the Rényi entropy:

$$S_q^{\text{Rényi}} := \frac{\ln \sum\limits_{i=1}^{k} p_i^q}{1-q}, \tag{25}$$

P_j is the so-called escort distribution defined by

$$P_j := \frac{p_j^q}{\sum_{i=1}^{k} p_i^q} \quad (j = 1, \cdots, k), \tag{26}$$

and D_q is the generalized dimension:

$$D_q := \lim_{\varepsilon \to 0} \frac{1}{q-1} \frac{\ln \sum_{i=1}^{k} p_i^q}{\ln \varepsilon}. \tag{27}$$

In the following subsections, the maximization problem in Tsallis statistics is reformulated in the combinatorial sense in accordance with the section 2.

3.2. *Maximization of S_{2-q} under the normal expectation*

In Tsallis statistics, the maximization of (1) under the constraint (2) is generalized in the following form:

$$\text{maximize} : \begin{bmatrix} & n & \\ n_1 & \cdots & n_6 \end{bmatrix}_q \tag{28}$$

$$\text{constraint} : \sum_{i=1}^{6} i n_i = n U_1 \tag{29}$$

The q-logarithm $\ln_q$ is also a monotone increasing function and we define $p_i := \frac{n_i}{n}$, so that the above maximization problem is equivalent to the following form.

$$\text{maximize} : S_{2-q}\left(p_1, \cdots p_6\right) \tag{30}$$

$$\text{constraint} : \sum_{i=1}^{6} i p_i = U_1 \tag{31}$$

Here we used the one-to-one correspondence (22). The maximization of S_{2-q} under the normal expectation (31) has been considered in some papers [13][14]. The thermodynamic relation is obtained as

$$\frac{\partial S_{2-q}}{\partial U_1} = \beta_1. \tag{32}$$

See [14] for the details.

Note that this β_1 is the same as β_1 in (8). This case is due to the additive duality $q \leftrightarrow 2-q$ in Tsallis statistics. The multiplicative duality $q \leftrightarrow 1/q$ is also well known in Tsallis statistics, which maximization problem is reformulated in the similar combinatorial sense from the slight generalization of the correspondence (22).

3.3. *Maximization of S_q under the q-average (q-normalized expectation)*

In order to find the multiplicative duality $q \leftrightarrow 1/q$ in the relation between a generalized multinomial coefficient and Tsallis entropy, some generalizations of the mathematical formulas in the subsection 3.1 are introduced in [5].

Definition 7 *((μ,ν)-factorial) For a natural number $n \in \mathbb{N}$ and $\mu,\nu \in \mathbb{R}$, the (μ,ν)-factorial $n!_{(\mu,\nu)}$ is defined by*

$$n!_{(\mu,\nu)} := 1^{\nu} \otimes_{\mu} 2^{\nu} \otimes_{\mu} \cdots \otimes_{\mu} n^{\nu}. \tag{33}$$

where $\nu \neq 0$.

Definition 8 *((μ,ν)-multinomial coefficient) For $n = \sum_{i=1}^{k} n_i$ and $n_i \in \mathbb{N}$ $(i = 1, \cdots, k)$, the (μ,ν)-multinomial coefficient is defined by*

$$\left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array} \right]_{(\mu,\nu)} := \left(n!_{(\mu,\nu)}\right) \oslash_{\mu} \left[\left(n_1!_{(\mu,\nu)}\right) \otimes_{\mu} \cdots \otimes_{\mu} \left(n_k!_{(\mu,\nu)}\right) \right]. \tag{34}$$

where $n!_{(\mu,\nu)}$ is the (μ,ν)-factorial defined in (33).

Proposition 9 *((μ,ν)-Stirling's formula) Let $n!_{(\mu,\nu)}$ be the (μ,ν)-factorial defined by (33). The (μ,ν)-Stirling's formula $\ln_{\mu}\left(n!_{(\mu,\nu)}\right)$ is computed as follows:*

$$\ln_{\mu}\left(n!_{(\mu,\nu)}\right) = \begin{cases} \dfrac{n \ln_{\mu} n^{\nu} - \nu n}{\nu(1-\mu)+1} + O(\ln_{\mu} n) & \text{if} \quad \nu(1-\mu)+1 \neq 0, \\ \nu(n - \ln n) + O(1) & \text{if} \quad \nu(1-\mu)+1 = 0. \end{cases} \tag{35}$$

This formula is computed by the approximation:

$$\ln_{\mu}\left(n!_{(\mu,\nu)}\right) = \sum_{k=1}^{n} \ln_{\mu} k^{\nu} \simeq \int_{1}^{n} \ln_{\mu} x^{\nu} dx. \tag{36}$$

Based on these results, we obtain the one-to-one correspondence between the (μ,ν)-multinomial coefficient and Tsallis entropy as follows.

Theorem 10 *When n is sufficiently large, the μ-logarithm of the (μ,ν)-multinomial coefficient coincides with Tsallis entropy (23) as follows:*

$$\frac{1}{\nu} \ln_{\mu} \left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array} \right]_{(\mu,\nu)} \simeq \begin{cases} \dfrac{n^q}{q} \cdot S_q\left(\dfrac{n_1}{n}, \cdots, \dfrac{n_k}{n}\right) & \text{if} \quad q \neq 0 \\ -S_1(n) + \sum\limits_{i=1}^{k} S_1(n_i) & \text{if} \quad q = 0 \end{cases} \tag{37}$$

where $\nu \neq 0$,

$$\nu(1-\mu)+1 = q, \tag{38}$$

S_q is Tsallis entropy (23) and $S_1(n) := S_1\left(\frac{1}{n}, \cdots \frac{1}{n}\right) = \ln n$.

See [5] for the details and its proofs.

The multiplicative duality $q \leftrightarrow 1/q$ in (37) is recovered when $\nu = q$. Then, μ is determined as $\mu = \frac{1}{q}$ from (38), so that we obtain

$$\ln_{\frac{1}{q}} \left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array} \right]_{\left(\frac{1}{q},q\right)} \simeq n^q \cdot S_q\left(\frac{n_1}{n}, \cdots, \frac{n_k}{n}\right) \tag{39}$$

which reveals the multiplicative duality "$q \leftrightarrow \frac{1}{q}$".

In order to give the combinatorial formula of the maximization of S_q under the constraint the q-average (q-normalized expectation) in [15], the generalized multinomial coefficient on the left side of (39) is rewritten by means of the "form" of the q-multinomial coefficient (21).

$$\left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_k \end{array}\right]_{\left(\frac{1}{q},q\right)} = \left[\begin{array}{ccc} & n^q & \\ n_1^q & \cdots & n_k^q \end{array}\right]_{\frac{1}{q}} \tag{40}$$

Note that $\left[\begin{array}{ccc} & n^q & \\ n_1^q & \cdots & n_k^q \end{array}\right]_{\frac{1}{q}}$ does not satisfy the definition of (21) because $\sum_{i=1}^k n_i^q \neq n^q$,i.e., $\sum_{i=1}^k \left(\frac{n_i}{n}\right)^q \neq 1$[1]. Instead of this inconsistency involved in the formula (40), we apply the distribution determined from $\left(n_1^q, \cdots, n_k^q\right)$ to the constraint. Summarizing the maximization problem in combinatorial form, we have

$$\text{maximize} : \left[\begin{array}{ccc} & n & \\ n_1 & \cdots & n_6 \end{array}\right]_{\left(\frac{1}{q},q\right)} \left(= \left[\begin{array}{ccc} & n^q & \\ n_1^q & \cdots & n_6^q \end{array}\right]_{\frac{1}{q}} \right) \tag{41}$$

$$\text{constraint} : \sum_{i=1}^6 i \frac{n_i^q}{\sum_{j=1}^6 n_j^q} = U_q \tag{42}$$

where this U_q is slightly different from U_1 because the q-dependent expectation (q-average) is employed in the above maximization problem. Remark that the q-average (q-normalized expectation) does not depend on the summation $\sum_{i=1}^k n_i = n$. Using (37), the above maximization problem is equivalent to the following form.

$$\text{maximize} : S_q\left(p_1, \cdots, p_6\right) \tag{43}$$

$$\text{constraint} : \sum_{i=1}^6 i \frac{p_i^q}{\sum_{j=1}^6 p_j^q} = U_q \tag{44}$$

The thermodynamic relation has been already obtained as

$$\frac{\partial S_q}{\partial U_q} = \beta_q \left(\sum_{j=1}^6 p_j^q \right) = \beta \tag{45}$$

where $\beta_q := \frac{q}{q+(1+\alpha)(1-q)}\beta$, α and β are the Lagrange multipliers. β_q is the generalized inverse temperature which coincide with $1/kT_q$ (T_q: the physical temperature [17]). See [18] for the details. In addition, Obviously, $\frac{\partial S_q}{\partial U_q} = \beta$ is a natural generalization of (8).

4. Conclusion

This paper presents the two combinatorial formalisms for the well-known maximum entropy problems in Tsallis statistics. One is the use of the usual expectation and the other is the q-average. More general combinatorial formalism for Tsallis entropy can be obtained if one uses the one-to-one correspondence (37). But the combinatorial meanings in the generalized multinomial coefficient are still missing, which is remained as a future work.

[1] This case naturally leads us to the maximization of S_q under the constraint $\sum_{i=1}^k i p_i^q = U$, which has been proposed in [16] and used for several years. Since the paper [15] in 1998, this constraint has never been applied for MEP in Tsallis statistics, because some requirements as expectation are missing. (e.g., $\sum_{i=1}^k p_i^q \neq 1$.)

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Appendix

	Boltzmann-Gibbs statistics	Tsallis statistics
fundamental equation	$\frac{dy}{dx} = y$	$\frac{dy}{dx} = y^q$
fundamental function	exponential function	q-exponential function
information measure	Shannon entropy	Tsallis entropy
multiplication	$\times$ (product)(independence)	$\otimes_q$ (q-product)
q	$q = 1$	$q \neq 1$ (q in the generalized dimension D_q)
fundamental operator	differential operator $\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h)-f(x)}{h}$	Jackson's q-differential operator $\frac{d_q f}{d_q x} = \frac{f(qx)-f(x)}{(q-1)x}$
divergence	Kullback-Leibler divergence	α-divergence $q = \frac{1-\alpha}{2} \quad (\alpha \neq \pm 1)$

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