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On application of non–extensive statistical mechanics to studying ecological diversity

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Abstract. The concept of Tsallis entropy provides an extension of thermodynamics and statistical physics. In the ecology, Tsallis entropy is proposed to be a new class of diversity indices S_q which covers many common diversity indices found in ecological literature. As a new statistical model for the Whittaker plots describing species abundance distribution, the truncated exponential distribution is used to calculate the diversity and evenness indices. The obtained results in new model are graphically compared with those in previous publication in the same field of interests, and shows a good agreement. A further development of a thermodynamic theory of ecological systems that is consistent with entropic approach of statistical physics is motivated.

1. Introduction

In the history of science, the applications of thermodynamics and statistical physics, and their methods on research of complex systems, especially biological and ecological systems is not a new trend in interdisciplinary science [1–12]. The basic of these branches of physics brings new methodologies, new ideas and new understanding into ecological science [2, 3, 8–19]. One of the main interests in research of ecological systems is biological diversity, co–called biodiversity [20–30], which is used informally to refer to diversity at all levels of taxonomic organization, particularly the level of species. In order to make a quantitative knowledge of conceptual biodiversity [4, 31–37], many scientific ideas have been developed to provide possible approaches to an explicit definition of biodiversity. However, due to the complexity of the ecological systems, it is hardly to find a single and simple definition of biodiversity that would be accepted by all scientific communities who have different scientific backgrounds, even they still have ecological modelling and thermodynamics as a common platform.

In spite of scientifically conceptual controversy, some methods of measuring biological diversity are widely accepted to be used in ecological research such as Shannon–Wiener index (H) [38–40] and Simpson index (D) [31] which are derived from information and probability theories, respectively. The justification of Shannon–Wiener and Simpson indices in ecological investigation and their applicable conditions are temporally not the subject of this presentation, but some basic important discussion of the theme would found in literature. These indices, are acceptable for the communities because of its simplicity and ability to provide a single numerical value, a partial description of species richness (S) and species evenness (E) [32,41–48]for a given ecological system.

In their mathematical nature, Shannon–Wiener and Simpson indices are the functionals of some given distributions and have the mathematical expressions of different entropies – the most important physical quantity in thermodynamics and statistical physics which has been generalized and extended to provide its applicability not only in ecological research [31, 38, 39, 49, 50] , but also in many other fields of interests such as economics, sociology, etc. It has to notice that the entropy–like indices are not entropy in original meaning, they have their meaning in their certain context. The advantage of entropy formalism outside of physics is that the back connections to thermodynamic and statistical theories of collective behaviors in science of complexity supporting the evaluation of complex aspects that are not capable of measuring in complex systems.

In the framework of the mathematical similarity of biodiversity and entropy, a entropic approach is proposed to consider biological systems. As the very early attempt in the approach, a model for a rank abundance curve or Whittaker plot [51–54]which plays the role of a distribution function of a ecological system is the subject of consideration and the consistency of the model is evaluated in the context of the q–generalized entropy – Tsallis entropy (S_q) [55–58]. In general, the model in its mathematical form provides a possibility to analytically obtain all relevant indices needed to explore ecological characteristics of general ecological systems. The derivation of a thermodynamic theory for ecological systems will be left to the further investigation.

2. Diversity indices and entropy

To understand what a diversity index is, it could be referred to the simple definition in Wikipedia [59] as "A diversity index is a quantitative measure that reflects how many different types, such as species of animals or of plants, there are in a dataset, and at the same time take into account how evenly the basic entities such as individuals are distributed among those types. The value of a diversity index increases both when the number of types increases and when evenness increases. For a given number of types, the value of a diversity index is maximized when all types are equally abundant."

The Wikipedia's formulation of a diversity index supports for a large number of possibilities to develop a mathematical definition of diversity index based on so–called a rank abundance curve or Whittaker plot [52] within the satisfactory of the principle of maximization of desired quantity. In point of view of physicists, the most preferable quantity for the definition of a diversity index is the entropy [7, 15, 19, 53, 60–65], but mathematicians think of any functionals depending on probability that satisfy a set of the given conditions. Having different minds for a long time, the mathematicians and the physicists agree about some common mathematical definitions of diversity index as the same as the mathematical formulation of the entropy. In last decades, it is easy to find in any university textbook [11, 66] or internet the mathematical definition of well–known diversity indices and other relevant indices such as species richness and species evenness. To avoid conceptual misunderstanding, it would be worth to emphasize that entropies are reasonable indices of diversity, but this is no reason to claim that entropy is diversity. [67] In one hand, the similarity of diversity index and entropy provides the basic for thermodynamic and statistical physical theories of ecology, in other hand, the interpretation of physical equivalent quantities in those theories has to be realized with very careful and fruitful knowledge of ecological science.

2.1. True Diversity

In ecology, the numerical value of true diversity, or the effective number of types [10, 14, 23, 24, 33, 59, 68], is obtained by first taking the weighted generalized mean M_{q-1}

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$$M_{q-1} = \left(\sum_{i=1}^{C} p_i^q \right)^{q-1}, \tag{1}$$

of the proportional abundances of the types in the dataset, and then taking the reciprocal of M_{q-1} [32, 36, 37, 69, 70] as

$$\begin{aligned} {}^qD &= (M_{q-1})^{-1} \\ &= \left(\sum_{i=1}^{C} p_i^q \right)^{1/1-q}, \end{aligned} \tag{2}$$

where C is the total number of types in the dataset, and p_i is the proportional abundance of the ith type. In the expression (2), the parameter q is a positive number and often called as the order of the diversity.

From the equations (1) and (2), it is obvious to recognize that increasing the value of q increases the effective weight given to the most abundant species. This leads to obtaining a larger value of M_{q-1} and a smaller value of true diversity (${}^qD$) with increasing q. Furthermore, true diversity (2) approaches to the exponential of "the so–called Shannon entropy" in limit of $q = 1$

$$\lim_{q\to 0} {}^qD = \exp\left\{ - \sum_{i=1}^{C} p_i \ln p_i \right\}. \tag{3}$$

General form of true diversity would be the generating functional of many well–known diversity indices found in several literature of quantitative ecology [36].

2.2. Diversity Indices

Among the most common diversity indices, the Shannon–Wiener index (H) and Simpson index (D) are repeatedly recalled in this presentation because of their popularity not only in ecology, but also in physics, information theory, economics and so on. These indices have proved themselves as the powerful tool in interdisciplinary sciences reflecting the primary connection between physics and other sciences.

The Shannon–Wiener index, or the Shannon entropy,

$$\mathrm{H} = - \sum_{i=1}^{C} p_i \ln p_i, \tag{4}$$

was originally proposed by C. E. Shannon to quantify the information content in the information theory [38, 39] and has been a popular diversity index in the ecological literature. By bringing the information theory's meaning of Shannon entropy into ecology, the Shannon–Wiener index quantifies the uncertainty in predicting the species identity of an individual that is taken at random from the dataset.

As it was mentioned in the general expression of true diversity (3), Shannon–Wiener index is the logarithm of true diversity ${}^qD$ when q tends to 1

$$\mathrm{H} = \ln {}^1D. \tag{5}$$

The other common index being also very popular in ecology literature is the Simpson index, or the Gini–Simpson index

$$\begin{aligned} \mathrm{D} &= 1 - \sum_{i=1}^{C} p_i^2 \\ &= 1 - \left({}^2D\right)^{-1}. \end{aligned} \tag{6}$$

which was first introduced in 1949 by E. H. Simpson to measure the degree of concentration when individuals are classified into types. The same type of measure as this index can be also found in sociology, economics and management science which is known as the Blau index.

Two above common indices are obvious not the same, and have advantages and disadvantages in different scenarios of ecological calculations [14, 24, 27, 29, 33, 71]. For example, in experiences of ecologists, for a measure of dominance the Simpson index is quite good, and it is a poor indicator of richness, however the Shannon–Wiener index provides an immediate measure for both aspects of diversity [33, 35]. In mathematical impression, both Shannon–Wiener and Simpson indices are very similar to same definitions of entropy which is a very important quantity of thermodynamics and statistical physics where a new definition of entropy that extends statistical physics to new fields of interests is always the subject of consideration. It is surprised that the so–called Tsallis entropy [55–58]

$$S_q = \frac{1}{q-1}\left(1 - \sum_{i=1}^{C} p_i^q\right), \tag{7}$$

might be a good generalization of the Shannon–Wiener and Simpson indices because they are nothing but particular limiting cases of the Tsallis entropy with $q = 1$

$$\begin{aligned} \lim_{q\to 1} S_q &= S_1 \\ &= -\sum_{i=1}^{C} p_i \ln p_i \\ &= \mathrm{H}, \end{aligned} \tag{8}$$

and $q = 2$

$$\begin{aligned} \lim_{q\to 2} S_q &= S_2 \\ &= 1 - \sum_{i=1}^{C} p_i^2 \\ &= \mathrm{D}, \end{aligned} \tag{9}$$

respectively. In the expression (7) and its derivatives, C is the number of states, p_i is the probability of the i state, and q is a real parameter.

Within the methodology of analogical thinking [9], it is no doubt of applying the concept of Tsallis entropy to the concept of diversity to transform bulky and cumbersome calculations for each given diversity index into the single and unified platform with the help of Tsallis entropy [35]. This approach also offers an opportunity of taking into account the order of the diversity q in all possible calculating processes and revising this parameter in ordinary definition (2). It has to be noticed that the order of the diversity q in (2) and statistical generalization parameter q in (7) are generally not the same, but in only some particular cases both these parameters match each other. Further study of interchange between two interesting parameters is of long–term investigation in the future.

3. A rank abundance curve and exponential distribution

Before the diversity indices are calculated, the observable dataset must be processed and displayed as species abundance data. In practice, there are many different ways to visualize the species abundance distribution. Among them, the best known and most informative method is the rank (abundance) plot or dominance (diversity) curve termed Whittaker plots in celebration of their inventor [33, 52, 68, 72]. A typical visualization of species abundance data – rank abundance curve or Whittaker plot could be found in several textbooks and research on ecology [33, 52, 68, 72]. The more detailed information explaining why the Whittaker plot is the most preferable in study of diversity could be found in a number of university textbooks and references therein.

In theoretical view, it might be agreed that a simple numerical plot brings inside not so much useful contents and does not support a good generalization of the research. A number of statistical models was proposed to empirically fit a observed dataset with a given distribution function providing the possibility for comparing obtained results among different datasets. In the last eighty–year period, many statistical models have been proposed and developed to maximize the information extracted from large observed datasets in different ecological projects. Several arguments have been listed by investigators to prove or to support how and why one model is chosen, and to validate the results of the chosen model. The development makes calculations of diversity more complicated and controversial in all aspects [33, 68].

To avoid complexity caused by furnishing well–known statistical models, another statistical model based on the knowledge of Boltzmann – Gaussian transition [73], the well–known phenomenon in complexity science, is proposed. The distribution function of newly proposed model is simply an exponential function. Hence the number of different species in a dataset could not be infinite, the rank abundance curve of the given dataset has to be fitted by a truncated exponential distribution

$$\begin{aligned} D_C\left(x_i, \lambda\right) &= p_i \\ &= \begin{cases} \frac{\exp\left\{\frac{C}{\lambda}\right\}}{\lambda\left(\exp\left\{\frac{C}{\lambda}\right\}-1\right)} \exp\left\{-\frac{x_i}{\lambda}\right\} & \text{for } 0 \le x_i \le C \\ 0 & \text{otherwise,} \end{cases} \end{aligned} \tag{10}$$

where C is maximum value of species rank and λ is some rate parameter of the rank abundance curve under consideration. The model parameters C and λ are directly obtained from observed dataset.

The distribution function (10) allows to perform an analytical and exact calculation for Tsallis entropy. This property of the truncated exponential distribution can be made as one of all reasons why it is selected to be the distribution function of the statistical model under consideration. The resultant entropy reads

$$S_q = \frac{1}{q-1} \frac{1-\lambda\left(e^{\frac{Cq}{\lambda}}-1\right)\left(\lambda\left(e^{\frac{C}{\lambda}}-1\right)\right)^{-q}}{q}. \tag{11}$$

The Tsallis entropy S_q (11) is mathematical exact and supporting a construction of a formal thermodynamic and statistical theory for a class of assemblages which can be described by distribution function (10). The question on the accuracy of the newly proposed statistical model in comparison within a particular dataset should be the subject of ongoing consideration. Regardless of this question, the Tsallis entropy (11) will be used as root expression in calculating the diversity indices in below.

4. Results and discussions

As a primary attempt, in this section the proposed model is used to calculate some indices of diversity within the concept of the Tsallis entropy. Due to the lack of real data, the calculation of indices, in this work, is limited only with abstract and symbolic set of parameters C and λ, and the obtained results are justified with those of other works [24, 27, 33, 35, 71] by means of graphical comparison.

It is almost obvious to confirm that the Tsallis entropy as function of parameter q is one of the possible interpolations of the Shannon–Wiener and Simpson indices. Decreasing q elevates monotonically the graphics of entropy approaching the Shannon–Wiener and Simpson indices when $q = 1$ and $q = 2$, respectively. This reconfirms the initial assumption of similarity between the order of diversity and non–extensive parameter q and encourages the idea of using Tsallis entropy as a diversity index in ecological research.

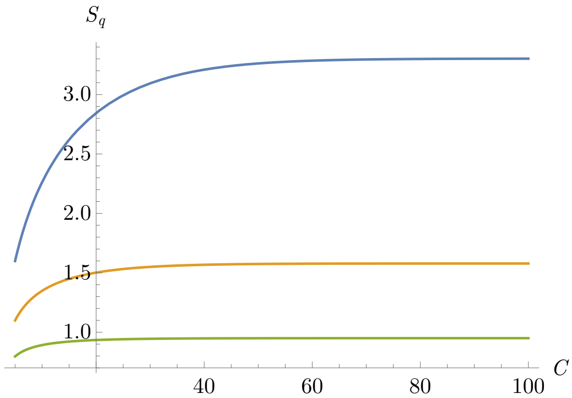

Figure 1. The Tsallis entropy (11) is the function of the total number of types in the dataset C with different values of non–extensive parameter q. The Shannon–Wiener index H and Simpson index D are the top and bottom lines corresponding to $q = 1$ and $q = 2$, respectively.

Treating the Tsallis entropy as a function of non–extensive parameter q with different fixed values of C shows the change of diversity index within variation of the total number of types in the dataset. There is no clear reason to unify parameter C and a hidden parameter of environment such as latitude, altitude or underground water . . . , however in some particular measurement, when several environmental factors are kept unchanged, the parameter C could be interpreted as one of those [33, 35].

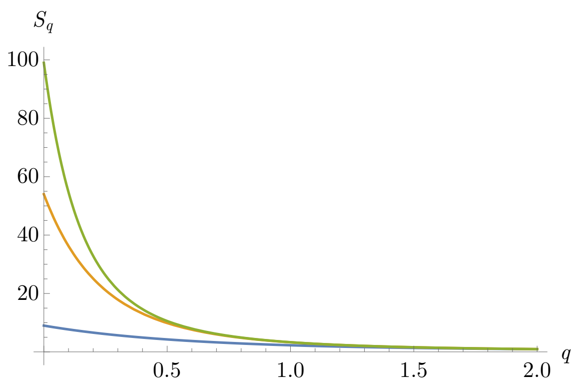

Figure 2. The Tsallis entropy (11) is the function of non–extensive parameter q with different values of the total number of types in the dataset C . Based on the abundance, the region with $q \leq 1$ emphasizes the richness whereas the region $q \geq 1$ emphasizes species dominance.

Another evaluation taking into account the role of the rate parameter λ supports an additional information to allow characterizing the global conditions as the single approximative one.

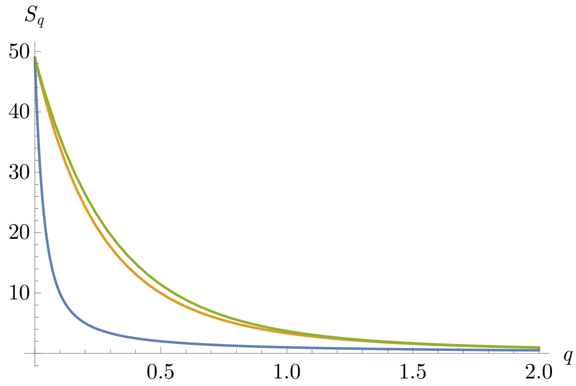

Figure 3. The Tsallis entropy (11) is the function of non–extensive parameter q with different values of the rate parameter λ.

Various mathematical behaviors of Tsallis entropy (11) are evaluated to show out the applicability of truncated exponential distribution and the new family of diversity indices in modelling the observed datasets and in searching the possible ecological meanings of each appearing parameter.

In one hand, the fitting parameters C and λ might contain an effective information of ecological systems, the non–extensive parameter q would be new well–defined order of diversity. The first relates strongly to the incompleteness of datasets hiding the uncertainty of the systems under consideration and observations, and the latter provides an alternative of reducing the influence of uncertainty in macroscopic results.

In consistence with that happens to the diversity indies, evenness indices are also considered as derivatives that have to be calculated for each dataset. In common sense, the evenness index reflects how close in numbers each species in a observed dataset is. Mathematically the evenness index is determined through a diversity index such as Shannon–Wiener index or Simpson index, a measure of biodiversity which quantifies how equal the community is numerically. In the context of Tsallis entropy, the evenness reads

$$E_q = \frac{S_q}{S_q^{max}} \ , \tag{12}$$

where S_q^{max} is the maximum value of S_q. It is not difficult to find out the analytical and exact expression of the evenness index in current situation as

$$S_q = \frac{1}{1-C^{1-q}} \frac{1-\lambda\left(e^{\frac{Cq}{\lambda}}-1\right)\left(\lambda\left(e^{\frac{C}{\lambda}}-1\right)\right)^{-q}}{q}. \tag{13}$$

Performing same manipulations as it was done with the diversity indies, allows to look mathematical behaviors of the evenness indices in more details. It is no doubt that the evenness index has a local minimum for each dataset. The existence of the local minimum in the current formalism is quite clear from the mathematical view, and actually agrees with the results found in [35].

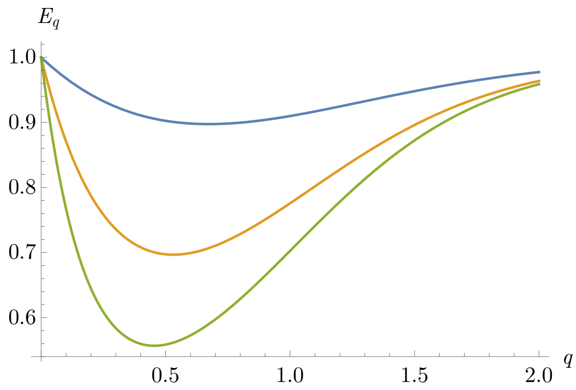

Figure 4. The evenness index (13) is the function of versus non–extensive parameter q with different values of the total number of types in the dataset C.

It is also clear that the values where the evenness indices E_q reach minimum increases for decreasing the total number of species C. The same impressions are in view of the rate parameter λ.

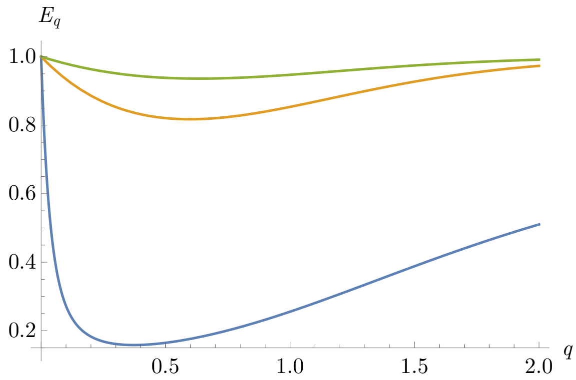

Figure 5. The evenness index (13) is the function of versus non–extensive parameter q with different values of of the rate parameter λ.

5. Conclusions

What has been done in this work is to propose a new statistical model based on truncated exponential distribution for the rank abundance curve of observed datasets. The model is simple and provides analytical calculations for diversity indices. Within the context of Tsallis entropy, which is an extension of statistical physics to other fields of interests in complexity, the diversity and evenness indices are exactly analytically obtained, and numerically evaluated to verify the applicability of the model in ecological science and to look for ecological meaning of parameters appeared in the model and in the Tsallis entropy.

Investigating mathematical behaviors of diversity and evenness indices shows that the non–extensive parameter q would be considered as the order of diversity while the total number of species and its rate parameter reflect an effective influence of environmental factors in statistics of ecology.

The model also motivates an idea to construct a consistent thermodynamic and statistical physical theory for ecological systems. This and many other open problems that could not be fully listed here, are waiting for further investigation.

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