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Maximum-entropy principle: ecological organization and evolution

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Abstract In the present paper, we have first studied the role of the maximum-entropy principle to explain the concept of organization of a physical system in the decreasing law of entropy with the increase of external constraints imposed on the system. We have then considered an open ecosystem (living) and determined a quantitative measure of ecological organization from the consideration of the thermodynamics of irreversible processes. Finally, we have tried to explain the evolution of the ecosystem in the light of Prigogine's principle of "order through fluctuation."

Keywords Maximum-entropy principle · Open system · Constraints · Ecological organization · Evolution

1 Introduction

In recent years, great efforts have gone into explaining the structure and function of complex ecosystems from the point of view of non-equilibrium thermodynamics [1–7]. Ecosystems may be considered as open systems exchanging energy, nutrients, and biomass with the environment. Ecosystem development shows an irreversible and non-repeatable history, a tendency expressed through the concept of entropy in the second law of thermodynamics. Besides the balance equations of momentum, energy and mass of all components of an ecosystem, the concept of entropy is inevitable in the understanding of ecosystems. Entropy and entropy production play a vital role in the understanding of the stability and evolution of complex ecosystems [2–5]. Another important aspect of entropy is the characterization of the organization of a system that plays a significant role in the evolution of a biological system. Organized systems are functionally complex and carry functional information [8, 9].

In the present paper, we have approached the problem of organization from the decreasing law of entropy with increasing of external constraints imposed on the system.

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The decreasing law of entropy is a characteristic of an organized system. The extent of organization at any stage is quantified by the loss of entropy (or gain of information). The paper consists of two parts. In the first part, we have tried to make an entropic analysis of organization. The methodology is based on Jaynes's maximum entropy principle and its extension for a generalized form of external constraints imposed on the system. An information-theoretic approach to the study of organization and self-organization of a system on the basis of the maximum-entropy principle is first due to Jumarie [10, 11]. Jumarie's approach is mathematical and is without application. A general theory of organization in physical and biological systems based on maximum entropy principle was also developed by Majernik [12, 13]. In this article, we present a more physical approach with biological application. In the second part, we have considered an open ecosystem (living) and determined a quantitative measure of ecological organization on the basis of non-equilibrium thermodynamics. This measure plays a significant role in the study of stability and evolution of the ecosystem [4, 6]. The evolution or self-organization of an ecosystem that corresponds to the decreasing law of entropy has been explained in the light of Prigogine's principle of "order through fluctuation" [14–17].

2 Open system: constraints and variation of entropy

We consider a system immersed in an environment. Let $P = (p_1, p_2, .., p_n)$ be the probability distribution of microstates of the system satisfying the normalization condition

$$f_0 : \sum_{i=1}^{n} p_i = 1. \tag{2.1}$$

The Boltzmann–Shannon entropy of the system with probability distribution $P = (p_1, p_2, .., p_n)$ of the microstates is given by [1, 18, 19]

$$H(P) = -k \sum_{i=1}^{n} p_i \ln p_i, \tag{2.2}$$

where $k(> 0)$ is the Boltzmann constant used to measure the entropy in thermodynamic units.

Let us first consider a system isolated from the environment by an adiabatic wall. Let S_0 be the entropy (thermodynamic) of the system in statistical equilibrium, and let it be equal to the maximum of the Boltzmann–Shannon entropy (2.2) subject to the normalization condition (or constraint f_0) (2.1)

$$S_0 = \text{Max}_{\{f_0\}} H(P) = \text{Max} \{H(P|f_0)\}, \tag{2.3}$$

where $H(P|f_0)$ is the conditional entropy of P subject to the known constraint f_0.

Let an external constraint (or environmental influence or disturbance) f_1 be imposed on the system in statistical equilibrium. The system then becomes open and changes take place within the system. The external constraint f_1 may, for example, be the replacement of the adiabatic wall by a diathermal wall, thus turning the isolated system into a closed one.

The constraint f_1 can then be represented mathematically by the fixed value of the average energy:

$$f_1 : \sum_{i=1}^{n} p_i E_i = \overline{E} \text{ (fixed)},$$

where E_i is the energy of the ith state. After some time, the system comes to the state of statistical equilibrium with the environment. Let S_1 (say) be the thermodynamic entropy of the system in the new statistical equilibrium, and it is obtained by maximizing the Boltzmann–Shannon entropy (2.2) subject to the constraints $\{f_0, f_1\}$, so that

$$S_1 = \text{Max}_{\{f_0, f_1\}} H(P) = \text{Max}\,\{H(P|f_0, f_1)\} \tag{2.4}$$

after proper thermodynamic identification of Lagrange's undetermined parameters. From [18],

$$\{H(P|f_0)\} > \{H(P|f_0, f_1)\}\,, \tag{2.5}$$

and we have then the inequality

$$S_0 > S_1 \tag{2.6}$$

implying a decrease of the entropy with the imposition of a new external constraint f_1 on the system. The inequality (2.6) is, however, not always true. For example, if the constraint f_1 consists of the withdrawal of a partition between two bodies forming an isolated system, it would result in the increase of entropy [15]. We can avert such a situation by the concept of an entropy-bath (or entrostat) environment whose entropy does not change significantly as a result of its interaction with (or influence on) the system [20]. This is analogous to the concept of a heat bath in statistical mechanics [21]. Let us make the concept of external constraint more clear. The constraint $\{f_i\}$ may not necessarily be confined to the linear constraints of the type of fixed values of average energy and particles of a physicochemical system or limitation of resources for an ecological system. The external constraints may be of different types determined by boundary conditions. Then, extending the set of constraints $\{f_i\}$ and generalizing the maximum-entropy principle for generalized forms of constraints, we have the result [10, 11]:

If S_i is the entropy (thermodynamic) of the system subject to the constraints $\{f_0, f_1, ..., f_i\}$ imposed on the system, we have then the inequality

$$S_i > S_{i+1}, \quad (i = 0, 1, 2...) \tag{2.7}$$

leading to the decreasing sequence of entropies of stationary states of the system

$$S_0 > S_1 > S_2 > .... > S_i > ...... \tag{2.8}$$

The different entropies $\{S_\alpha\}$ correspond to the different degrees of openness of the system. The different degrees of openness of the system correspond to the different values (or strengths) of the external constraints or entrostat influence on the system. We can identify the different degrees of openness by the parameter α, and each value of α corresponds to a certain stationary state of entropy S_α. The limiting value of the sequence (2.8) occupies the extreme position: (a) $\alpha = 0$, which is the stationary state of the completely isolated state (openness is zero) of the system and (b) $\alpha = \alpha_{\max}$, which corresponds to the maximum (or total) openness of the system with $S_{\alpha_{\max}} = 0$. The criteria of entropy change under the influence of external constraints can then be stated briefly as follows [20]:

1. To reduce the entropy S_i to S_{i+1}, it is necessary to increase the openness of the system from $\alpha = i$ to $\alpha = i + 1$ (i.e., to increase entrostat influence). To increase entropy in the system from $\alpha = i + 1$ to $\alpha = i$, it is necessary to reduce the openness from $\alpha = i + 1$ to $\alpha = i$ (i.e., to reduce the entrostat influence).
2. If the entropy of a non-stationary state $S > S_\alpha$, then the process of entropy reduction prevails; if $S < S_\alpha$, the process of entropy increase prevails; if $S = S_\alpha$, the actions of reducing and increasing entropy will compensate each other and the system will become stationary. As emphasized by Prigogine, we thus see that, in a system out of equilibrium, the entropy may either increase or decrease depending on the strength of the external constraints [15].

Let us now consider the quantity

$$\delta S = S_\alpha - S \tag{2.9}$$

as the change of entropy in transition from an initial non-stationary state to a stationary state of openness α. It can be divided into two parts:

$$\delta S = S_\alpha - S = (S_0 - S) + (S_\alpha - S_0). \tag{2.10}$$

The first part $(S_0 - S)$ is always positive and the second part $(S_\alpha - S_0)$ is negative in view of the decreasing sequence of entropies (2.8). If $|(S_\alpha - S_0)| > (S_0 - S)$, then $S_\alpha < S$, implying the process of entropy reduction or the process of organization prevailing in the system. On the contrary, if $|(S_\alpha - S_0)| < (S_0 - S)$, then $S < S_\alpha$, implying the process of entropy increase or the process of disorganization prevailing in the system. The second part $(S_\alpha - S_0)$ thus plays a significant role in the characterization of entropy variation. It, depending on the strength of the external constraints or environmental influences imposed on the system, is like the negentropy (or free-energy) flow from the environment to the system. It regulates the organization or disorganization of the system. In the next section, we shall show that the process of entropy reduction or organization $(S > S_\alpha)$ prevails in an open ecosystem immersed in an environment. We shall also study the evolution of the open ecosystem from the increasing law of organization in line with Prigogine's principle of "order through fluctuation" consistent with the above characterization of entropy variation.

3 Ecosystem: measure of organization and criteria of evolution

In order to describe an ecosystem properly, we must specify two basic points: (1) we must specify the interaction between the components of the system and (2) we must specify the interaction between the system and the external world. Mathematically, the second law influences the evolution equations through the boundary conditions or the systematic constraints intervening explicitly within the rate equations describing the system. The ecosystem communicates with the external world through a separating surface $\sum$. In general, conditions prevailing in the external world are not identical with those inside the ecosystem. In particular, the number of individuals of species i per unit area or volume inside and outside are different. Similarly, energy per unit area or volume is different. These differences are felt by the system as constraints including a flow of matter and energy within $\sum$. The ecosystem is, thus, an open, non-equilibrium system [16]. A non-equilibrium system as emphasized by Rosen [9] is an organized system. Our problem is now to find out the measure of the extent of organization of the ecosystem.

We consider an ecosystem A, immersed in an environment A_0. The environment A_0 is very large compared to the ecosystem and completely regulates the behavior of the ecosystem. As before, we assume the environment to be an entrostat or entropy bath. Let $N_i(i = 1, 2, ..., n)$ be the concentration of the ith substance (or species) and $N_i^0(i = 1, 2, ..., n)$ be that for the stationary equilibrium state of the ecosystem with the environment. Let $\mu_i(i = 1, 2, .., n)$ be the chemical potential of the ith species or substance and $\mu_{i0}(i = 1, 2, .., n)$ be that for the equilibrium state of the ecosystem with the environment. We assume the ecosystem to be isothermic with the environment. We consider an ideal gas (or solution) model of the ecosystem [1]. The ecosystem dynamics can be considered as a movement in the potential field with chemical potential [1, 4]

$$\mu_i = \mu_{i0} + RT \ln \frac{N_i}{N_i^0}, \tag{3.1}$$

where T is the common temperature of the ecosystem and the environment and R is the gas constant. The affinity (thermodynamic force) for the reaction (or transition) of the concentrations $N = (N_1, N_2, .., N_n)$ to the stationary equilibrium state $N^0 = (N_1^0, N_2^0, ..., N_n^0)$ is given by [4, 7]

$$X_i = \mu_i - \mu_{i0} = RT \ln \frac{N_i}{N_i^0}, \tag{3.2}$$

and the corresponding rate (or thermodynamic flux) is given by

$$J_i = \frac{dN_i}{dt}. \tag{3.3}$$

Then, according to the thermodynamics of irreversible processes, the rate of change of entropy is given by [15]

$$\frac{dS}{dt} = \sum_{i=1}^{n} J_i X_i = RT \sum_{i=1}^{n} \frac{dN_i}{dt} \ln \frac{N_i}{N_i^0}. \tag{3.4}$$

So the change of entropy of the open ecosystem in transition from some non-stationary state (current state) to the stationary state of thermodynamic equilibrium with the environment is given by

$$\begin{aligned} S^0 - S &= RT \sum_{i=1}^{n} \int_{N_i}^{N_i^0} \ln \frac{N_i}{N_i^0} \frac{dN_i}{dt} dt \\ &= -RT \sum_{i=1}^{n} \left[N_i \ln \frac{N_i}{N_i^0} - \left(N_i - N_i^0 \right) \right], \end{aligned} \tag{3.5}$$

which is a negative quantity, so that

$$S^0 < S. \tag{3.6}$$

We thus see a decrease of entropy of the ecosystem as result of free-energy consumption by the system from the environment. In the terminology of Section 2, the decrease of entropy is a result of external constraints (or entrostat influence or boundary conditions).

The ecosystem, as we have said, is an open, non-equilibrium system [16]. Our problem is to find out the measure of the extent of organization of the ecosystem. The organization results from the external constraints or boundary conditions imposed on the system. We can define the extent of organization of a non-equilibrium state by the loss of entropy

$$O = S - S^0 = RT \sum_{i=1}^{n} \left[N_i \ln \frac{N_i}{N_i^0} - \left(N_i - N_i^0 \right) \right]. \tag{3.7}$$

The system is self-organizing if [10, 11]

$$\frac{dO}{dt} > 0$$

or

$$\frac{d}{dt} \sum_{i=1}^{n} \left[N_i \ln \frac{N_i}{N_i^0} - \left(N_i - N_i^0 \right) \right] > 0, \tag{3.8}$$

where we have omitted the positive factor RT.

Let us now try to explain the concept of self-organization or evolution from the point of view of Prigogine's principle of "order through fluctuation" [14]. For this, we investigate the behavior of a stationary state $(N_1^0, N_2^0, ..., N_n^0)$ subject to external constraints (or environmental influences or disturbances). As a result of the disturbance, the stationary state $(N_1^0, N_2^0, ..., N_n^0)$ is displaced to a neighboring non-stationary state $(N_1, N_2, ..., N_n)$ such that

$$N_i = N_i^0 + \delta N_i, \quad (i = 1, 2, ..., n), \tag{3.9}$$

where $\delta N_i (i = 1, 2, ..., n)$ are the deviation or perturbation from the stationary values $(N_1^0, N_2^0, ..., N_n^0)$. These perturbations δN_i are a certain type of fluctuation (stochastic elements) as Prigogine emphasized to build a generalized thermodynamics, which includes a macroscopic theory of fluctuation.

Assuming $\delta N_i (i = 1, 2, ..., n)$ are very small, and neglecting higher powers of δN_i, we have

$$O \simeq RT \sum_{i=1}^{n} \frac{(\delta N_i)^2}{N_i^0}. \tag{3.10}$$

The expression (3.10) is positive definite and can be considered as a Liapunov function [4]. The criteria of stability of the stationary state $(N_1^0, N_2^0, ..., N_n^0)$ are then given by

$$\frac{d}{dt} \left[\sum_{i=1}^{n} \frac{(\delta N_i)^2}{N_i^0} \right] < 0. \tag{3.11}$$

If the stationary state $(N_1^0, N_2^0, ..., N_n^0)$ is stable, the system will remain within the domain of attraction of the stationary state, and there can be no evolution of the system. If the external constraints are strong enough to drive the system sufficiently from the stationary state $(N_1^0, N_2^0, ..., N_n^0)$, it will give rise to an ordered state. In that state, we must have the criteria of instability of the stationary state, leading to the inequality

$$\frac{d}{dt} \left[\sum_{i=1}^{n} \frac{(\delta N_i)^2}{N_i^0} \right] \geq 0, \tag{3.12}$$

whence the system will evolve out of the domain of attraction of the stationary state. We have to wait until the system settles down to a new stationary state. New external constraints imposed on the system may result in another instability, and so on. We shall have, then, a succession of instabilities arising from the external constraints (environmental influences) resulting in the increase of the ecological organization. The evolution of the ecosystem is thus associated with an irreversible increase in organization resulting in the transition of the system from an ordered state to a more ordered state. This is in line with Prigogine's principle of "order through fluctuation" [14–17].

4 Conclusion

The aim of this paper is to make an entropic analysis of organization in both physical and ecological systems. Some characteristic features of the methods and principles adopted and the results obtained are as follows:

1. The paper is based on the methods and principles of non-equilibrium thermodynamics and statistical mechanics. The maximum-entropy principle of statistical mechanics plays a significant role in the characterization of the decreasing law of entropy for an organized system. Thermodynamics of irreversible processes plays a dominant role in the characterization of ecological organization and evolution.
2. The entropy of the system decreases if a new external constraint is imposed on the system. This decreasing law of entropy with the increase of constraints is a characteristic property of an organized system. So a system would be organizing if there is a creation of constraints that cause the entropy to decrease. It would be self-organizing whenever there is self-creation of constraints. The origin of the constraints lies in some physical bounds on the environment of the system, such as the limitations of resources—food, nutrients, etc. [10]. In the special case of a multi-level hierarchical system, the lower level is subject to the constraints by the upper level, and one may assume that it is the upper-level sub-system itself that creates these constraints [10, 22].
3. The extent of organization of a non-equilibrium system at any state has been measured by the entropy loss $(S - S^0)$ or by the gain of information from the equilibrium stage to the present stage. This leads to the identification of organization with information [8, 23].
4. Openness of a system is the characteristic requirement for an organized system. The different entropies S_α correspond to the different degrees of openness and, hence, to the different extents of organization.
5. The openness of a system and the decreasing law of entropy have been explained through the concept of an entropy bath or entrostat, which is a new approach to the study of self-organization in physical, biological, and social systems [21]. The reverse of the inequalities (2.8) can be averted with the help of entropy bath.
6. In the context of ecology, the chemical potential μ_k appearing in (3.2) is known as the biological potential of the kth species [5]. Its expression, given by (3.2), represents the distance of the system from thermodynamic equilibrium. It acts as a thermodynamic force driving the system from the equilibrium state [1, 2].
7. In the derivation of the expression of the extent of ecological organization, we have assumed an ideal gas solution or mixture model of the ecosystem. The ecosystem can be treated as an ideal solution within a certain approximation. The main difference

from the common physicochemical solutions is the wide distance of the ecosystem from the thermodynamic equilibrium expressed by the inequality $\mu \gg kT$ [1].

8. Evolution has been discussed as a thermodynamic feature of the ecosystem. In biology or sociology, the idea of evolution is associated with an irreversible increase of organization, giving rise to the creation of more and more complex structures [14]. This is opposite to the thermodynamic evolution of isolated systems, which is directed to a continuous disorganization, which is the evolution to the most probable state, or maximum disorder. Nowadays, biologists realize that the second law applies to a system as a whole living system plus the environment, and this is perfectly compatible with entropy lowering in the organisms. This is the technique we have employed in our discussion of Section 2. In Section 2, we have represented the effect of environmental influences or external constraints by $\{f_i\}$ and their extension for the application of the maximum-entropy principle.
9. The increasing law of ecological organization (2.8) has been explained in the light of Prigogine's principle of "order through fluctuation" [14–17]. The deviations $\delta N_i (i = 1, 2, ..., n)$ are certain types of fluctuations as emphasized by Prigogine [14–17], resulting from the external constraints imposed by the environment on the ecosystem. In the evolution process, the different levels of organization result from the succession of instabilities arising from the successive impositions of external constraints or influences of the environment on the system.
10. In conclusion, the paper is an attempt to relate ecological and physical systems in order to provide a common platform for the description of both theoretical physics and biology [24, 25].

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