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LETTER TO THE EDITOR

Entropic sampling and natural selection in biological evolution

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Abstract. With a view to connecting random mutation on the molecular level to punctuated equilibrium behaviour on the phenotype level, we propose a new model for biological evolution, which incorporates random mutation and natural selection. In this scheme the system evolves continuously into new configurations, yielding non-stationary behaviour of the total fitness. Furthermore, both the waiting time distribution of species and the avalanche size distribution display power-law behaviours with exponents close to two, which are consistent with the fossil data. These features are rather robust, indicating the key role of entropy.

The idea of punctuated equilibrium, based on the new interpretation of the fossil record, holds that biological evolution proceeds not at a steady pace but in an intermittent manner [1]. Simple models attempting to describe such phenomena usually employ the extremal dynamics, which evolves the system by sequentially updating or mutating the species with the globally minimum value of fitness [2, 3]. This indeed drives the system into a self-organized critical state, characterized by power-law behaviour, and such extremal dynamics is regarded as an essential ingredient to achieve the self-organized criticality. In reality, however, there is no reason why mutation necessarily occurs in the species with the minimum fitness. On the contrary, on the molecular level most evolutionary changes and most of variability within a species are believed to be caused not by selection but by random drift of mutant genes which are selectively equivalent [4]. In contrast to such randomness on the molecular level, the fossil data exhibit critical behaviour on the phenotypic level: for example, it is known that the number M_t of genera with lifetime t displays the power-law behaviour $M_t \sim t^{-\alpha}$ with $\alpha \approx 2$ [5]. Here, the longer a genus exists in the ecosystem, the more sub-genera should be generated; it is thus expected that the number of sub-families is proportional to the length of the period of existence [6, 7]. Indeed recent analysis of fossil records has revealed such structure in the taxonomic system that the number M_n of taxa having n sub-taxa follows essentially the same power-law distribution $M_n \sim n^{-\alpha'}$ with $\alpha' \approx 1.84$ to 2.41 [8]. These imply that there does not exist a relevant time scale characterizing the length of the period during which a certain species dominates the population. Furthermore, it is known that a few mass extinction events as well as many background events (of smaller sizes) have occurred during the last 600 million years [9], which also exhibit power-law behaviour. Namely, the distribution of extinction events of size s is observed to follow $\tilde{M}(s) \sim s^{-\tau}$ with $1 \lesssim \tau \lesssim 2$ [10], again manifesting scale invariance.

This work attempts to provide a natural link between the behaviour on the molecular level and that on the phenotypic level. For this purpose, we propose a new model of evolution, which is more realistic than existing models, and show how the power-law behaviour emerges on the phenotype level. Our model incorporates the *random mutation* on the molecular level and introduces an additional step determining acceptance or rejection of a particular mutation. The latter mimics the *natural selection* process, connecting the molecular and phenotypic levels. Here the entropy of the ecosystem plays a key role: when information is transferred from the environment to the species via mutation, the information-theoretic entropy of the species drops. Although the subsequent (random) mutation may restore the previous level of the entropy by re-establishing disorder, the mutation is on the average oriented to lower the entropy during the process of evolution [6]. This corresponds to transferring information from the environment to the species in the viewpoint of information theory, where entropy stands for missing (negative) information. We consider various forms of the fitness function, and measure the waiting time distributions of the species having maximum fitness values as well as of a typical species. They all show power-law behaviour with exponents close to two. We also investigate the size distributions of ‘avalanches’, i.e. series of mutations triggered by single starting mutations, again to obtain power-law behaviour, which is consistent with the observed distribution of extinction events.

Consider an ecosystem consisting of N species, in interaction with the environment. The configuration of the ecosystem is described by $x \equiv \{x_i\}$, where x_i represents the configuration of the i th species. Usually, x_i is taken to be a number between zero and unity ($0 \leq x_i \leq 1$). We assume that the fitness of the i th species is modelled by a real function $f_i(x)$, which may in general depend upon the configuration of neighbouring species as well as its own configuration x_i . The total fitness $F(x)$ is then defined to be the sum of the fitness values of all species in the system:

$$F(x) = \sum_{i=1}^N f_i(x). \quad (1)$$

Accordingly, the phase space volume (or the number of accessible states) $\Omega(F)$ for a given value of the total fitness F reads

$$\Omega(F) = \prod_{j=1}^N \int_0^1 dx_j \delta \left[F - \sum_{i=1}^N f_i(x) \right] \quad (2)$$

the logarithm of which gives the entropy of the ecosystem.

In an ecosystem, mutation is an exception to the regularity of the process of DNA replication, which normally involves precise copying of the hereditary information encoded in nucleotide sequences. We thus choose randomly a single species in the system and mutate the chosen species only, since there is no obvious reason that mutations occur in the nearest neighbouring species simultaneously [11]. The natural selection via which the mutation is accepted or rejected is determined by the entropy in our scheme. We assume that the change in the total entropy $S_{\text{tot}} \equiv S + S_0$, where S and S_0 are the entropy of the ecosystem and that of the environment, respectively, is negligible during the information transfer from the environment to the ecosystem (i.e. the entropy flow from the ecosystem to the environment). Namely, the information transfer is assumed to be almost reversible. (Relaxation of the reversibility assumption will be discussed later.) The probability $P(x)$ of finding the system in configuration x in the stationary state is simply proportional to the number Ω_0 of accessible states for the environment:

$$P(x) \propto \Omega_0 = \exp[S_0] = C \exp[-S(F)] \quad (3)$$

where $C \equiv \exp[S_{\text{tot}}]$ is a constant and the entropy of the ecosystem, given by the logarithm of the number of accessible states for the system $S(F) = \ln \Omega(F)$, depends on the configuration through the total fitness $F \equiv F(x)$. The probability distribution given by equation (3) can be attained dynamically by imposing the detailed balance condition

$$\frac{W(x \rightarrow x')}{W(x' \rightarrow x)} = \exp[S(F) - S(F')] \quad (4)$$

where the transition probability $W(x \rightarrow x')$ describes the mutation from configuration x to configuration x' and $F' \equiv F(x')$ denotes the total fitness of the ecosystem in configuration x' . We thus compute the entropy change $\Delta S \equiv S(F') - S(F)$ during the process of mutation $x \rightarrow x'$, and accept the mutation when $\Delta S < 0$; for $\Delta S > 0$, the mutation is accepted with probability $\exp(-\Delta S)$. In consequence, the entropy of the ecosystem tends to decrease while that of the environment tends to increase, since the total entropy remains approximately constant (and cannot decrease in particular). Thus the entropy is directed to flow from the ecosystem to the environment.

Interestingly, the dynamics described by equation (4) precisely corresponds to the entropic sampling algorithm, which was successfully applied to the travelling salesman problem [12]. In this algorithm, the entropy of the ecosystem is estimated as follows: initially the entropy $S(F)$ is set equal to zero for all values of the total fitness F . We then obtain the histogram $H(F)$ of the total fitness for a short run, which gives a new estimation of $S(F)$:

$$S(F) = \begin{cases} S(F) & \text{for } H(F) = 0 \\ S(F) + \ln H(F) & \text{otherwise.} \end{cases} \quad (5)$$

This yields the entropy increasing as the run proceeds. Once the stationary state is reached, however, the increase due to more runs gives merely an additive constant (independent of F), which is obviously irrelevant. Note also that this sampling has characteristics of frequency-dependent selection [9] and yields a uniform distribution of the total fitness over the entire space, which appears natural in a real ecosystem. It assists the system to escape from a local maximum in the total fitness space and fall into a new local maximum, which corresponds to a metastable phenotype of the ecosystem. In this manner, the ecosystem is allowed to evolve into a new configuration by gathering information from the environment (i.e. by reducing its entropy). In particular, the additional step determining the acceptance/rejection of mutation naturally leads to correlations between the configuration before the mutation and that after it. For the simplest Bak-Sneppen (BS)-type fitness [2]

$$f_i = x_i \quad (6)$$

which allows the explicit evaluation of equation (2), the above algorithm indeed yields the entropy in perfect coincidence with that obtained from equation (2) (up to an irrelevant additive constant). This demonstrates the accuracy of the entropic sampling although other forms of the fitness function in general do not allow analytic calculation to be compared.

In most of the existing models, the total fitness remains constant once the stationary state is reached. This implies that the species in the present time and those in the past have the same average adaptive power to the environment, which does not appear to be true in reality [11]. In contrast, the new model, which takes into account the role of entropy, leads to non-stationary behaviour of the total fitness. In the entropic sampling algorithm, which is adopted in the new model, the mutation is encouraged to decrease the entropy of the ecosystem and to transfer information from the environment to the species. Here the entropy of the system increases if the system stays long in configurations with the same

value of F . Accordingly, the probability for the mutation making the system escape from a region of the same F is higher than that for the mutation having the system stay in that region, producing non-stationary behaviour. In this way the system evolves continuously into new configurations in the whole fitness landscape instead of staying at a single local maximum, which reflects the interactions with the changing environment.

To compare with the fossil data, which give the exponent α close to two in the power-law behaviours of M_t and M_n , we have chosen a species at random and measured the distribution of the interval between two consecutive mutations. The resulting (average) waiting time distribution $D(t)$ of the species, measured during the time 10^4 to 5×10^8 and averaged over five independent runs with different initial configurations, is shown in figure 1. It indeed exhibits a power-law behaviour [13], $D \sim t^{-\nu}$ for $t \geq 3$ with the exponent $\nu = 2.07 \pm 0.02$, which is consistent with the frequency distribution of taxa observed in the fossil data; this is significantly larger than the value 1.57 obtained in the conventional model with the extremal dynamics [14]. In reality the contributions of various species to the fossil record are not all equal and those species which have the maximum fitness values should dominate the record. This implies the relative importance of the species having the maximum fitness values in the comparison with the fossil data [6]. We have thus watched the species having maximum fitness and measured the waiting time distribution of such species during the same time interval, performing ten independent runs with different initial configurations. The resulting waiting time distribution of the species having maximum fitness again exhibits a power-law behaviour with the exponent $\nu = 2.11 \pm 0.04$. The overall features are similar to those of the average distribution shown in figure 1, but the power-law nature is more clear and accurate, yielding an almost perfect fit for $t \geq 3$. The almost identical behaviour apparently indicates the validity of the results regardless of the (unknown) relative importance in the contributions to the fossil data.

To check whether these features are sensitive to the specific choice of the fitness function, we have also considered other types of the fitness function, for example

$$f_i = \sum_j' (x_i - x_j - A_{ij})^2 \quad (7)$$

where the prime restricts the summation to nearest-neighbouring species of i on a square lattice and A_{ij} has been introduced to accommodate the possibility of ‘frustration’ in the interactions between species. Since the exact form of interactions between species is not available, A_{ij} are taken to be quenched random variables, taking the values between -5 and 5 . Unlike in equation (6), the fitness in (7) is determined not only by its own configuration but also by the configurations of neighbouring species, and can change due to the mutation in neighbouring species, which is presumably more realistic. The fitness given by equation (7) has been investigated in a system of 16^2 species arranged to form a square array with linear size $L = 16$. The same entropic sampling algorithm again yields the waiting time distribution of the species with maximum fitness values, which is fitted to the power-law behaviour with exponent $\nu = 2.08 \pm 0.07$, as shown in figure 2. The distribution has been measured during the time 10^4 to 2×10^7 , and five independent runs have been performed with different initial configurations and realizations of A_{ij} [13]. The average waiting time distribution of a typical species has also been obtained, revealing essentially the same power-law behaviour except for the exponent $\nu = 2.12 \pm 0.09$. We have also checked other distribution of A_{ij} , and found that the overall behaviour still does not change qualitatively. This apparently suggests that the general behaviour is rather insensitive to the specific form of the fitness function, giving support to the use of a simple model without knowing the precise dynamics of the evolution.

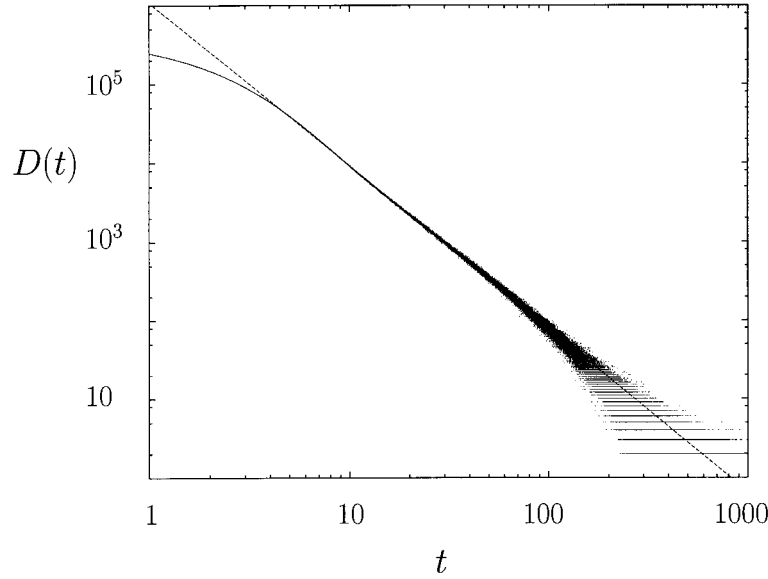


Figure 1. Average waiting time distribution of a typical species, measured during the time 10^4 to 5×10^8 , in the system of 100 species, with the BS-type fitness function. The time has been measured in units of the Monte Carlo steps per species. The dashed line corresponds to the least-squares fit of the data for $t \geq 8$, giving the slope -2.07 ± 0.02 .

When a mutation is accepted, the fitness of some species and consequently, the total fitness change. This in turn leads to a new value of the entropy, which determines the transition probability to other configurations, i.e. the mutation probability. Therefore, the acceptance/rejection of a mutation depends on that of the previous mutation, and the resulting correlations between the evolving configurations may be characterized by the distribution of ‘avalanches’, which stand for the series of (accepted) mutations triggered by single starting mutations. Since a mutation occurring on a species implies change of the species into another, avalanches correspond to extinctions of species, for which fossil data give a power-law behaviour in the size distribution, with the exponent τ between 1 and 2 [10]. To accommodate the large interval in the fossil analysis compared with the inverse of the mutation rate in nature, we have regarded the mutation accepted within Δ trials following a mutation as constituting an avalanche, and measured the distribution $\tilde{D}(s)$ of the avalanche events with size s for various values of the interval Δ . It is found that $\tilde{D}(s)$ indeed displays a power-law behaviour, $\tilde{D}(s) \sim s^{-\mu}$ with the exponent $\mu \approx 2$, unless Δ is too small. Figure 3 shows the behaviour of the avalanche size distribution for $\Delta = 10$, computed up to the time 10^6 in a system of 1000 species (with the BS-type fitness). The exponent is given by $\mu = 1.98 \pm 0.01$, which is consistent with the analysis of the fossil data. We have also considered larger values of the interval, up to $\Delta = 20$, and obtained almost the same power-law behaviour with μ hardly changing; we thus believe that such power-law behaviour is robust and persistent even for realistically large values of Δ .

We now consider the effects of irreversible information transfer in the natural selection process. In this case, the total entropy S_{tot} does not remain constant but increases during the information transfer, via which the ecosystem also increases its fitness F . It is thus plausible to assume that S_{tot} is an increasing function of F : $S_{\text{tot}}(F) \approx S_{\text{tot}}(F_0) + \beta(F - F_0)$, for some reference value F_0 , where $\beta \equiv \partial S_{\text{tot}} / \partial F|_{F=F_0} > 0$. This leads to the probability for the

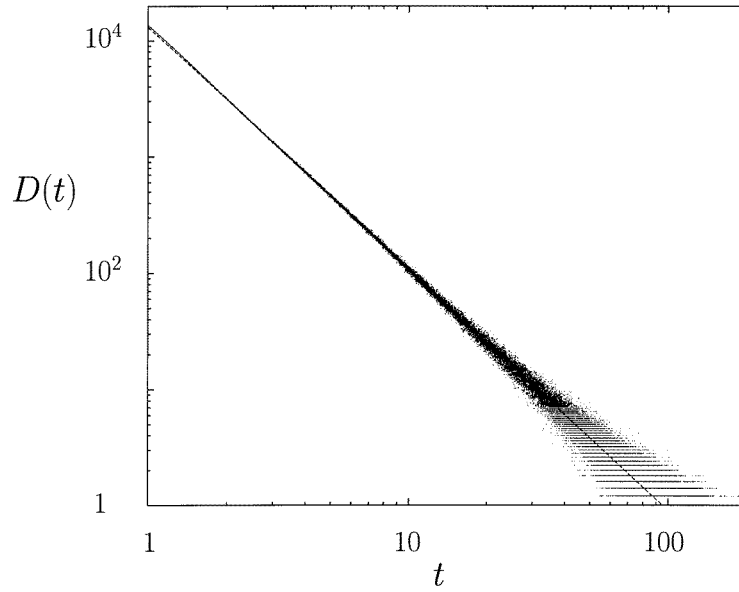


Figure 2. Waiting time distribution of the species having maximum fitness, measured during the time 10^4 to 2×10^7 , in the system of 16^2 species with the Gaussian fitness function. The dashed line represents the least-squares fit of the data for $t \geq 3$, with the slope -2.08 ± 0.07 .

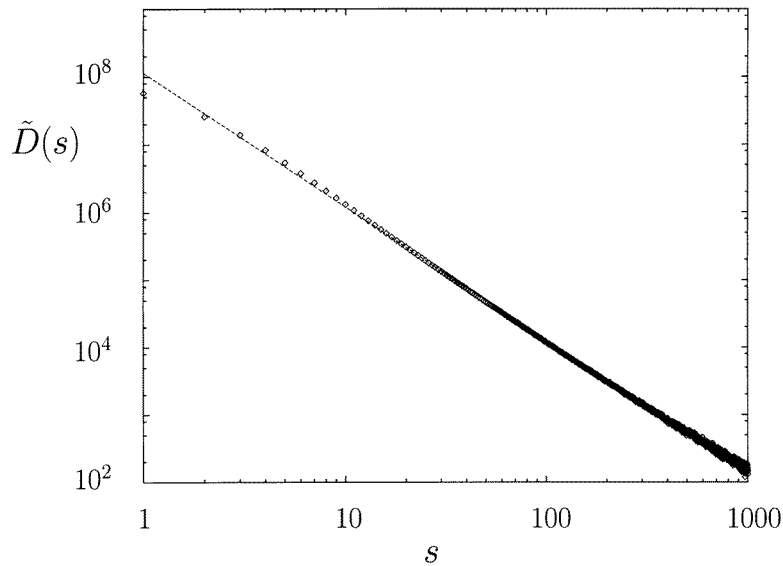


Figure 3. Avalanche size distribution measured with the interval $\Delta = 10$, in the system of 1000 species with the BS-type fitness function. The dashed line represents the least-squares fit of the data, with the slope -1.98 ± 0.01 .

ecosystem, $P(x) \propto \exp[\beta F - S(F)]$, which can be attained by the following algorithm. In determining acceptance or rejection of a mutation, we consider the change in the total fitness, ΔF , in addition to the entropy change ΔS , and select the new configuration according to the

probability $\min[1, e^{-\Delta S + \beta \Delta F}]$, where β measures the relative importance of the total fitness. This algorithm, where the available range of the total fitness is controlled by the term $e^{\beta \Delta F}$, yields qualitatively the same results: the system still displays the non-stationary behaviour of the total fitness and the power-law behaviour of the waiting time distribution with a similar value of the exponent. For example, for the fitness function given by equation (7), we obtain $\nu = 2.03 \pm 0.05$ unless β is too large. On the other hand, in the absence of the entropy term, the generalized algorithm reduces to the standard (Metropolis) importance sampling algorithm. This importance sampling, when used as an alternative to the entropic sampling in the natural selection process, fails to yield the power-law behaviour; instead it in general gives stretched exponential behaviour [15] which is rather close to the conventional exponential behaviour, in apparent disagreement with observation.

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