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Evolution based on chromosome affinity from a network perspective

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HIGHLIGHTS

- We examine the evolution of species from the affinity between individuals.
- We propose an evolutive algorithm that incorporates the some network properties.
- We also propose a method to characterize complex networks.
- Punctuated equilibria and stasis are related to the mutation and genetic crossover.
- The proposed model is appropriate to explain evolution of species in a network.

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ABSTRACT

Recent studies have focused on models to simulate the complex phenomenon of evolution of species. Several studies have been performed with theoretical models based on Darwin's theories to associate them with the actual evolution of species. However, none of the existing models include the affinity between individuals using network properties. In this paper, we present a new model based on the concept of affinity. The model is used to simulate the evolution of species in an ecosystem composed of individuals and their relationships. We propose an evolutive algorithm that incorporates the degree centrality and efficiency network properties to perform the crossover process and to obtain the network topology objective, respectively. Using a real network as a starting point, we simulate its evolution and compare its results with the results of 5788 computer-generated networks.

1. Brief introduction to models of evolution of species

After Charles Darwin published his major findings in 1859 [1], many theories have been proposed to explain the evolution of species. The data found in the specialized literature show that biological evolution occurs in intermittent bursts of activity separated by relatively long acquiescent periods rather than in a gradual manner [2,3]. The complex pattern of selection

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imposed on geographically structured populations by heterogeneous environments and coevolution can paradoxically remain in stasis at the species level for long periods of time. By contrast, some authors argue that genetic mechanisms cannot explain species-wide stasis [4–9]. The order–disorder conflict in the biological evolution route to equilibrium is an established concept of biological evolution that applies to this situation.

Several mathematical models have been used for biological research. For instance, there are simple models such as the Fibonacci sequence that describes population growth, or the game of life [10] that seeks convergence in cellular automata. Similarly, computational models have been proposed to simulate the evolution of species. We briefly discuss the three models used as a starting point to develop our model. Our model simulates the evolution of species, including the relationships between individuals (i.e., social and complex networks), and the processes of mutation, reproduction and crossover (i.e., processes based on Darwinian evolution).

- *Bak–Sneppen (BS) model*: the BS model [11] models biological evolution as a self-organized criticality system [11–13]. It was designed to preserve/capture the punctuated equilibria found in fossil records [8].
- *Penna model*: the Penna model is based on Darwinian evolution with mutations. It is a representation of the Darwinian conflict [14–18]. The Penna model uses binary variables to represent genes, where 0 represents ordinary genes and 1 represents harmful genes. Originally, the Penna model focused on problems of biological aging. Then, applications to several different evolutionary problems substantially increased the scope of the Penna model.
- Recently, some of us have proposed a simple model based on Darwin's theories of evolution [19]. In that model, a set of 32 alleles is used, formed by the numbers from 0 to 6, associated with each level of fitness, as chromosomes. The values range from the zero, which represents a totally unfit allele, to six, which represents complete fitness. We have observed that both stasis and punctuated equilibria were directly obtained from the mutation, selection of parents and genetic crossover.

In the literature, we can find several models on evolution of species. Models of evolutionary processes have been developed to study the evolution of species. Recently, a hydrophobicity scale based on self-organized criticality (SOC) was proposed by Moret and Zebende [20]. From this hydrophobicity scale some studies about evolution were proposed [21,9, 22–25]. As we also remark in this paper, the affinity criterion is used to promote the evolution of species.

This paper introduces a novel model based on the theory of networks [26–31]. Some of the properties of social and complex networks (e.g., centrality and efficiency indices) are used as criteria to perform the crossover process and to establish the network topology objective for the proposed evolutive algorithm.

With respect to the theory of networks, this study builds on three major areas: graph theory, social network analysis and the theory of complex networks. These areas have been used to investigate the behavior and structure of various complex systems represented by entities and their relationships, such as technological networks [32–34], biological networks [35,36], social networks [37–39], information networks [40–42], and semantic networks [43–47].

Ohtsuki et al. [48] have argued for a simple rule based on the benefit of altruistic acts, its costs and neighborhood to explain the evolution of cooperation in social networks.

The remainder of this paper is organized as follows. In Section 2, we present the description of the proposed model, including the concept of affinity used as a parameter for crossover, and the algorithm used to simulate the evolution of species. In Section 3, we extend the previous section and present the evolutionary algorithm based on affinity networks. In Section 4, we present the results obtained from the simulations. We present the concluding remarks of the paper in Section 5.

2. Description of the proposed model

Consider a system composed of entities (e.g., individuals, companies, computers, words, etc.) that establish relationships among themselves with a minimum degree of affinity. Each entity can have an arbitrary number of characteristics that will be used to determine whether two entities have affinity. The number of characteristics of an entity depends on the system.

Let us consider that an individual of a particular species has 14 key characteristics, each of which is coded as a binary number consisting of two bits. Therefore, 28 numbers are used to compose the chromosomes of the individuals of the affinity network. In summary, any ecosystem in the proposed model has any number of individuals and each individual has a chromosome with N_g characteristic genes; in this example, $N_g = 28$.

In the proposed affinity networks, the vertices are the individuals and the edges are the affinity relationships between the individuals. In the affinity networks, we do not include loops (i.e., an edge that connects a vertex to itself) or multiple edges connecting two vertices. The degree of affinity is defined as the percentage of similarity between a pair of individual chromosomes and is given by Eq. (1) as follows:

$$A_{ij} = \frac{1}{N_g} \sum_{i \neq j \in G,\, w=1}^{N_g} g_{iw} \equiv g_{jw} \tag{1}$$

where N_g is the number of chromosome genes, g_{kw} is the wth chromosome gene of an individual k, and operation $g_{iw} \equiv g_{jw}$ is given as follows:

$$g_{iw} \equiv g_{jw} = \begin{cases} 1, & g_{iw} = g_{jw} \quad \text{or} \\ 0, & \text{Otherwise.} \end{cases} \tag{2}$$

We propose a new model to simulate the evolution of species based not only on Darwinian evolution, using mutation, reproduction and crossover processes, but also on the similarity between individuals in an ecosystem. Using this context, to perform the simulations, we build the affinity networks at each generation. To do that, the proposed model uses two indices of network theory: degree centrality [49,37] and efficiency [50].

Mathematically, affinity networks can be represented and studied as graphs. A graph $G = (V, E)$ is a mathematical structure consisting of two sets V (finite and not empty) with elements called vertices (or nodes), and E (binary relation on V), with elements called edges [51]. The total number of vertices or cardinality of set V is $n = |V|$; and the total number of edges or cardinality of set E is $m = |E|$.

We use the Latora and Marchiori efficiencies model [50]. The global efficiency is defined as $E(G) = \frac{1}{n(n-1)} \sum_{i \neq j \in G} \frac{1}{d_{ij}}$, where d_{ij} is the geodesic distance, in terms of number of edges, between the vertices i and j. The local efficiency is defined as $E_{\text{loc}} = \frac{1}{n} \sum_{i \in G} E(G_i)$, where $E(G_i)$ is the efficiency of the local subgraph G_i (i.e. neighborhood of i) since $i \notin G_i$. During the simulations of the evolution of affinity networks, both efficiency indices were used to determine whether the network topology objective was obtained. For each "classical" network topology (i.e., random, small-world and scale-free), we propose three criteria as follows:

- *random networks*: the global efficiency and the local efficiency of the network must be similar to the global and local efficiency of an equivalent random network, i.e. $E_{\text{global}} \simeq E_{\text{globalRD}}$ and $E_{\text{local}} \simeq E_{\text{localRD}}$, for any value of undirected network's density, denoted by $\Delta = \frac{2m}{n(n-1)}$, i.e. the total number of existing edges divided by the maximum possible number of edges;
- *small-world networks*: the global efficiency of the network must be similar to the global efficiency of an equivalent random network, i.e., $E_{\text{global}} \simeq E_{\text{globalRD}}$, and the local efficiency of the network will be greater than the local efficiency of an equivalent random network, i.e. $E_{\text{local}} > E_{\text{localRD}}$, and $\Delta \leq 7\%$; and
- *scale-free networks*: the global efficiency of the network must be greater than the global efficiency of an equivalent random network, i.e., $E_{\text{global}} > E_{\text{globalRD}}$, while the local efficiency is much greater than the local efficiency of an equivalent random network, i.e., $E_{\text{local}} \gg E_{\text{localRD}}$, and $\Delta \leq 20\%$. If $\Delta > 20\%$, then $E_{\text{global}} \simeq E_{\text{globalRD}}$.

According to Latora and Marchiori [50], small-world networks achieve a local efficiency much greater than the local efficiency of an equivalent random network. Nevertheless, by using both Watts–Strogatz and Latora–Marchiori methods, this behavior is observed only when the network density is less than or equal to 7%. In the case of network densities greater than 7%, it is not possible to identify the topology between random and small-world networks. We have found that the global efficiency index can be accurately used to characterize scale-free networks because the network density is less than or equal to 20%. Fig. 1 shows the relationship between the average density and efficiencies (global in Fig. 1(a) and local in Fig. 1(b)) for the classical network topologies. We used 6000 computer-generated networks, i.e., 2000 random networks, 2000 small-world networks and 2000 scale-free networks, to create these results.

This approach, which more precisely identifies the objective topology of the affinity network, can be used as a method for characterizing the topological structure of a social and/or complex network.

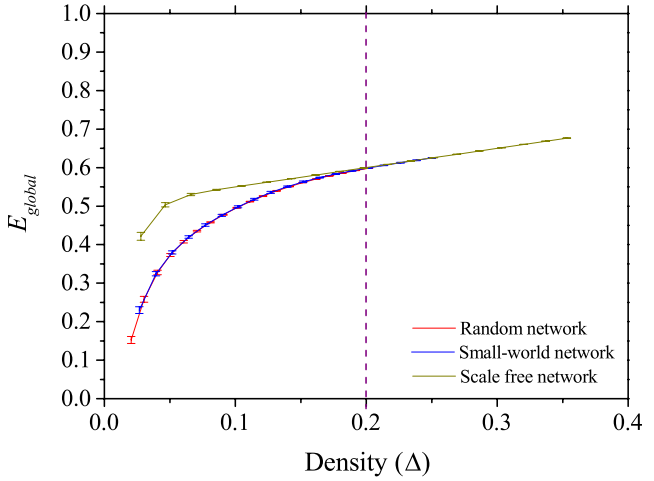
3. Evolutionary algorithm based on affinity networks

Using the ecosystem structure as a starting point, we developed an evolutionary algorithm based on Darwinian evolution theories and affinity networks. We noted that no models had yet been developed that included the affinity of chromosome pairs as a criterion for interaction (i.e., for reproduction and genetic crossover).

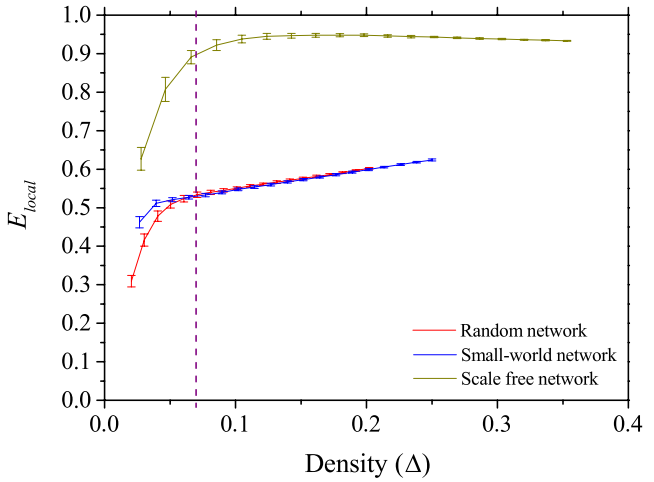
Four main characteristics define the proposed algorithm, as follows: (1) the affinity relationships are measured at each generation; (2) the fitness measurements of each individual are defined as the degree centrality (C_D) of the individual; (3) pairs of individuals with genetic similarity are selected for crossover; and (4) according to the probability of mutation, mutation may occur in the genes of each individual.

In terms of the algorithm, we summarize the model as follows:

1. *initialize the population*: a set of n individuals is randomly selected from a given population;
2. *Set number of generations*: set the maximum number of generations;
3. *set genetic compatibility*: set the value for the minimum affinity degree that will be used to identify the genetic compatibility. In other words, this parameter, A_f, is the minimum percentage of similarity between a pair of individual chromosomes;
4. *calculate the degree of affinity*: for each pair of individuals i and j, we compare the equivalent genes and count the number of genes that carry the same information; then we calculate the percentage of similarity between i and j according to Eq. (1);
5. *build the affinity network*: the affinity network is built at each generation using the status of the chromosomes (composed of N_g genes each) of the individuals. If two individuals i and j have a minimum degree of affinity between them ($A_{ij} \geq A_f$), they will be connected;
6. *calculate the individual fitness*: the fitness, $C_D(i)$, of each individual of the network at each generation is calculated to determinate the most fit individuals. These individuals are called the individual elite, $i_e \in I_E$;



(a) Global efficiency as a function of density shows that it is possible to characterize the network topology for $\Delta \leq 20\%$.



(b) Local efficiency as a function of density shows that it is possible to characterize the network topology for $\Delta \leq 7\%$.

Fig. 1. Global and local efficiencies for the classical network topologies as a function of density (Δ).

7. *select genes for crossover*: we randomly mark 50% of the genes of the population (N_g genes times n individuals) at each generation. This probability is denoted by P_c;
8. *perform the crossover process*: if a pair of individuals is connected, and one of them is an elite individual (i_e) and the other one is a non-elite individual, but at least one of its genes is marked from Step 7, a crossover process between them is performed, because the pair of individuals has at least a minimum degree of affinity (i.e., $A_{ij} \geq A_f$). Thus, only the marked genes of a non-elite individual will be replaced by equivalent genes of an $i_e \in I_E$ (Fig. 2(a)). The probability that two individuals i and j are chosen for crossover, P_{cross}, is therefore:

$$P_{\text{cross}} = \begin{cases} 1, & i \in I_E \text{ and } j \notin I_E \text{ and } j \text{ has at least one gene marked} \\ & \text{to be replaced by equivalent genes of } i \text{ and } A_{ij} \geq A_f \quad \text{or} \\ 0, & \text{Otherwise;} \end{cases} \tag{3}$$

9. *select genes for mutation*: we randomly mark 0.1% of the genes of all individuals at each generation. This probability is denoted by P_m;
10. *perform the mutation process*: a mutation is performed on each individual selected for mutation. If an individual has at least one gene marked in Step 9, its marked genes will be changed as follows: a gene coded as 1 is changed to 0 and a gene coded as 0 is changed to 1, i.e., we interchange 0s and 1s (Fig. 2(b)). The probability that an individual j is chosen for mutation, P_{mut}, is as follows:

$$P_{\text{mut}} = \begin{cases} 1, & j \text{ has at least one gene marked in Step 9} \quad \text{or} \\ 0, & \text{Otherwise;} \end{cases} \tag{4}$$

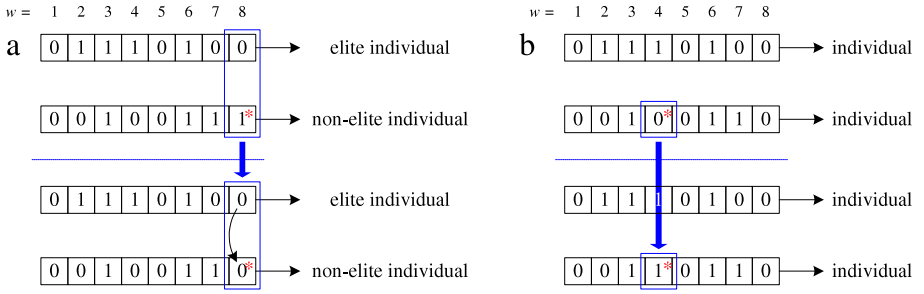


Fig. 2. Crossover and mutation processes: (a) for all conditions, the crossover process is performed considering that only the marked gene ($w = 8$) of the non-elite individual will be replaced by the equivalent gene of the elite individual; (b) for all conditions, the mutation process is performed considering that only the marked gene ($w = 4$) of the individuals will be replaced by its complement.

11. *calculate efficiencies*: calculate the global and local efficiencies to identify the network topology as discussed in Section 2;
12. Return to Step 4, unless the maximum number of generations has been reached, or unless the network topology objective is small-world (i.e., $E_{\text{global}} \simeq E_{\text{globalRD}}$ and $E_{\text{local}} > E_{\text{localRD}}$; for more details see Section 2).

4. Simulations and results

The simulations performed in this paper have included three important aspects: (i) an elite individual transmits its genetic characteristics; (ii) the measurement of the fitness consists of the individual degree centrality; and (iii) the measurement of the global and local efficiencies are used as parameters to determine the network topology and to verify if there has been evolution in the affinity networks.

We have simulated different scenarios considering a population of 93 individuals, whose chromosomes have 28 characteristic genes (for more details, see Section 2). In addition, we have used Eq. (1) to determine the degree of affinity (A_{ij}) between two individuals i and j.

To define not only the most appropriate value to represent the minimum genetic compatibility (A_f) between two individuals (Step 3 in the algorithm presented in Section 3) but also the percentage of the genes of all individuals who will be marked for mutation (Step 9 in the algorithm presented in Section 3), we performed approximately 163,000 simulations.

For the minimum genetic compatibility or minimum degree of affinity (A_f), we have used four values (i.e., 33,0%, 46,0%, 49,0% and 64,0%) obtained from the frequency distribution of affinities between all pairs of individuals that compose a randomly constructed ecosystem. Values less than 33% produced very dense networks in early generations, leading to the stagnation of evolution (i.e., continuous stasis and no punctuated equilibria). Values greater than 64% impact the evolutionary behavior in terms of the number of generations (i.e., many generations are needed to simulate the evolution). Thus we set the genetic compatibility at values from 49% (the average between 33% and 64%) to 46% (the most appropriate value for minimum degree of affinity).

For the percentage of the genes of all individuals who will be marked for mutation, P_m, we identified that the most appropriate value, for $N_g = 28$, is 0.1%. On the other hand, the percentage that does not present any stationary equilibria starts at 1.0%, as found by Moret et al. [19].

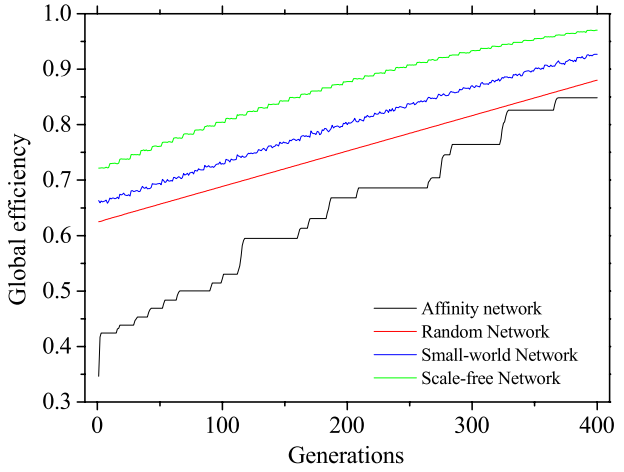
For the percentage of the genes of all individuals who will be marked for crossover, P_c, we found that, for $N_g = 28$, values greater than 50% result in a very fast evolution and values less than 50% result in a very slow evolution. For these reasons, we set $P_c = 50\%$.

Using values of $A_f = 46\%$ and $P_m = 0.1\%$, Fig. 3 shows that punctuated equilibria occur at different evolutionary times, similar to the evolution of a natural ecosystem [8]. In Fig. 3, both evolution curves of affinity networks for global and local efficiencies (Fig. 3(a) and (b), respectively) resemble the observed fossil record [2]. Using the minimum degree of affinity $A_f = 46\%$, we observed an evolution of the affinity network; recall that the local efficiency E_{local} of an affinity network is similar to E_{local} of an equivalent small-world network (Fig. 3(b)). In the affinity networks, a very small percentage of individuals is involved in the genetic improvement of the entire population.

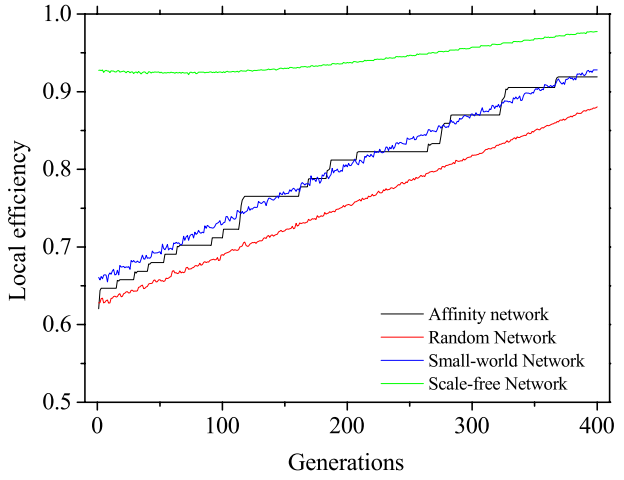
Although we have taken into account 500 generations in the simulations, after the 400th generation the small-world phenomenon disappears because the network density reaches very high values. Therefore, for Step 2 in the algorithm (see Section 3), we set the number of generations to 400.

In Table 1, we show the values of the basic network indices taken from the four networks at the 400th generation. The measured properties are: $n = |V|$ is the number of vertices; $m = |E|$ is the number of edges; Δ is the density; $\langle k \rangle$ is the average degree; C is the average clustering coefficient; L is the average minimal path length; E_{global} is the global efficiency; and E_{local} is the local efficiency.

The four networks at the 400th generation are dense ($\Delta > 75\%$) with small average degree $6.99 < \langle k \rangle < 8.65$. The results show that $L \to 1$, thus these networks tend to form a clique (i.e. a set of n vertices that are mutually connected). The networks also tend towards a high efficiency (i.e., E_{global} and E_{local} are greater than 80%). This behavior is due to the small size of the population (approximately 100) and low affinity between the individuals (0.30–0.46).



(a) Evolution of global efficiency.



(b) Evolution of local efficiency.

Fig. 3. Evolution of global and local efficiencies as function of number of generations for a mutation process equal to 0.1% of the population genes at each generation, and for a crossover process equal to 50% of the population genes at each generation. For these simulations we used 5788 networks.

Table 1
Basic network indices at the 400th generation.

Networks	n	$m = \|E\|$	Δ	$\langle k \rangle$	C	L	E_{global}	E_{local}
Scale free network	93	4023	0.94	8.65	0.95	1.05	0.97	0.97
Small-world network	93	3653	0.85	7.85	0.85	1.14	0.92	0.92
Random network	93	3253	0.76	6.99	0.76	1.23	0.88	0.88
Affinity network	93	3606	0.84	7.75	0.91	1.01	0.84	0.91

Thus, it is natural that the network converges to a clique. However, if we used high affinity values, as those observed in nature (0.999), the network would not converge to a clique, and the efficiency would not reach such a high value. Fig. 4 shows the evolution of a population of 100 individuals with a 32 bit chromosome length and 40% of their genes marked 1 at the generation 0. The results show the same shape as that in Fig. 3 for both evolutions of global and local efficiencies of the affinity network.

5. Discussion

This study concerns the evolution of species in a network-based ecosystem. We introduced a novel method to connect individuals using the degree of affinity between them. This model leads to consistent evolution processes. Mutation and crossover must take place throughout the evolution of a network-based ecosystem.

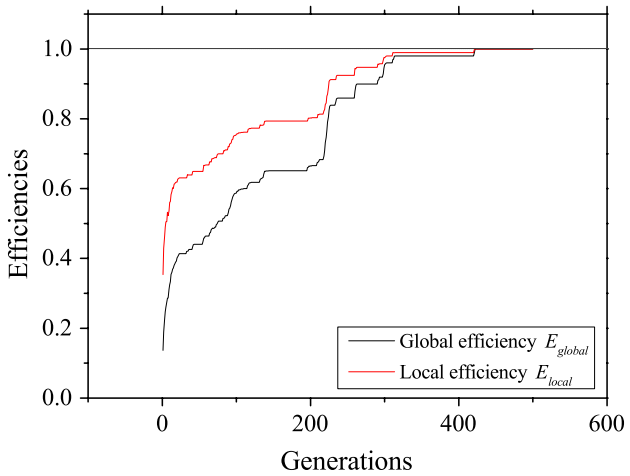


Fig. 4. Evolution of global and local efficiencies as a function of the number of generations for $A_f = 40\%$ affinity and 0.1% mutation. This figure is similar to the 'lineage through time' (LTT) plot, based on the temporal distribution of branch points in an experimental phylogenetic tree, shown in Fig. 2 of Ref. [8].

The results presented in Fig. 3 showed that punctuated equilibria and stasis throughout the generations in evolutions of both global and local efficiencies (Fig. 3(a) and (b), respectively) are consistent with those observed in fossil records [2]. This behavior is also found by Moret et al. [19].

The equilibria intervals are observed at different times of the evolution of species, revealing the natural tendency of the genetic engine to accumulate knowledge before the onset of a rapid change in individual characteristics, to best fit individuals to the their habitat.

The ecosystem is represented as an affinity network and the most fit individuals are those with $C_D(i) > \langle k \rangle$. We studied the evolution of the ecosystem by evaluating its global and local efficiencies with respect to its network topology. We can thus characterize the networks as small-world and scale-free networks at the 400th generation.

This approach, which more precisely identifies the objective topology of the affinity network, can be used as a method for characterizing the topological structure of social and/or complex networks.

Despite being a very simplified model of chromosomes, our approach reproduces the behavior of the evolution of biological systems (such as punctuated equilibria and stasis). The result obtained is similar to that obtained from fossil records.

Finally, the results of Fig. 1 can be used as a convergence criterion for this type of evolutionary algorithm. Thus, the proposed algorithm has a well-defined convergence criterion, which is not common in evolutionary algorithms.

As future work, we propose to study the connections of density (Δ) to real examples of evolution (e.g. phylogenetic trees of rhodopsin).

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