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Dynamics-driven evolution to structural heterogeneity in complex networks

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ABSTRACT

The mutual influence of dynamics and structure is a central issue in complex systems. In this paper we study by simulation slow evolution of network under the feedback of a local-majority-rule opinion process. If performance-enhancing local mutations have higher chances of getting integrated into its structure, the system can evolve into a highly heterogeneous small-world with a global hub (whose connectivity is proportional to the network size), strong local connection correlations and power-law-like degree distribution. Networks with better dynamical performance are achieved if structural evolution occurs much slower than the network dynamics. Structural heterogeneity of many biological and social dynamical systems may also be driven by various dynamics–structure coupling mechanisms.

1. Introduction

The underlying networks of many biological and social complex systems are distinguished from purely random graphs. These real-world networks often have the small-world property [1] and scale-free (power-law) vertex-degree profiles [2]; they have system-specific local structural motifs [3] and often are organized into communities [4,5] of different connection densities. In recent years models have been proposed to understand the structural properties of real-world complex systems [6,7]; among them the "rich-get-richer" mechanism of network growth by preferential attachment [2] gained great popularity. As the connection pattern affects considerably functions of a networked system, there may exist various feedback mechanisms which couple the system's dynamical performance (efficiency, sensitivity, robustness, ...) with the evolution of its structure. But the detailed interactions between dynamics and evolution are often unclear for real-world systems, and understanding complex networks from the angle of dynamics–structure interplay is still a challenging and largely unexplored research topic. Among the few theoretical works on dynamics-driven network evolutions from the physics and the computer science communities (see, e.g., Refs. [8–18] and review [19]), the main focus has been on network evolutionary games for which network dynamics and evolution occur on comparable timescales. A payoff function is defined for the system, and vertices change their local connections to optimize gains. In many complex systems, however, the dynamical performance of a network is a global property which cannot be predicted by only looking at the local structures. Most structural changes in such systems, on the other hand, take place locally and relatively randomly, without knowing their consequences to the system's dynamical performance. The timescales of network dynamics and network structural

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evolution can also be very different. Will dynamics–structure coupling mechanisms build highly nontrivial architectures out of random, blind, and local structural mutations?

In this work extensive simulations of dynamics-driven network evolution are performed on a simple model system, namely the local-majority-rule (LMR) opinion dynamics of complex networks. There are two main motivations for this study. First, earlier analytical and simulation studies [20–22] revealed that networks with heterogeneous structural organizations have remarkably better LMR dynamical performances than homogeneous networks. In complementary to these studies, we want to know, in this simple LMR dynamical system, to what extent the dynamical performance of a network can influence the evolution trajectory of the network's structure. Second, as LMR-like dynamical processes are frequently encountered in neural and gene-regulation networks and other biological or social systems, it is hoped that a detailed study of dynamics–structure coupling in the model LMR system will also shed light on the structural evolution and optimization in real-world complex systems.

In the simulation, a fitness value is assigned to a network to quantitatively measure its efficiency of LMR dynamical performance. A slow (in comparison with the LMR dynamics) mutation-selection process is performed on a population of networks, and networks of higher fitness values are more likely to remain in the population. The network population dynamics reaches a steady-state after passing through several transient stages. A steady-state network has high clustering coefficient [1] and strong local degree–degree correlations, and the fraction $P(k)$ of vertices in the network with degree k resembles a power-law distribution of $P(k) \propto k^{-\gamma}$ with $\gamma \approx 2$. Interestingly a global hub of degree proportional to network size N spontaneously emerges in the network. These results bring new insights on the optimized network organization for LMR dynamics. They are also consistent with the opinion that feedback mechanisms from dynamics to structure could be a dominant force driving complex networks into heterogeneous structures [19]. Hopefully this work will stimulate studies on the detailed interactions between dynamics and structure in more realistic complex systems.

2. Dynamics and evolution

The local-majority-rule dynamics runs on a network of N vertices and $M = cN/2$ undirected links, with c being the mean connectivity. The network's adjacency matrix $\mathbf{A}$ has entries $A_{ij} = 1$ if vertices i and j are connected by an edge or $A_{ij} = 0$ if otherwise. Each vertex i has an opinion (spin) $\sigma_i = \pm 1$ that can be influenced by its nearest-neighbors. At each time step t of the LMR dynamics, every vertex of the network updates its opinion synchronously according to $\sigma_i(t+1) = \text{sign}[h_i(t)]$, where $h_i(t) \equiv \sum_{j=1}^{N} A_{ij}\sigma_j(t)$ is the local field on vertex i (when $h_i(t) = 0$ we set $\sigma_i(t+1) = \sigma_i(t)$). Starting from an initial configuration $\vec{\sigma}(0) \equiv \{\sigma_1(0), \sigma_2(0), \ldots, \sigma_N(0)\}$, the LMR process will derive the system to a consensus state in which all the vertices share the same opinion. To measure a network's efficiency of performing the LMR process, we follow Refs. [20, 22] and choose the initial opinion patterns $\vec{\sigma}(0)$ to be *strongly disordered*, with $\sum_{i=1}^{N} \sigma_i(0) = \sum_{i=1}^{N} k_i\sigma_i(0) \equiv 0$ (k_i is the degree of vertex i); in other words a vertex (either randomly chosen or reached by following a randomly chosen edge) has probability one-half to be in the plus-opinion state. For networks containing $N \geq 1000$ vertices such strongly disordered patterns can be easily constructed: One first divide the vertices into two groups (G_+ and G_-) of equal size and assign spin $+1$ to vertices of group G_+ and spin -1 to vertices of group G_-; and as long as $\sum_{i=1}^{N} k_i\sigma_i \neq 0$, two vertices (one from G_+ and the other from G_-) are randomly chosen and their positions are exchanged if and only if this exchange does not cause an increase in the value of $|\sum_{i=1}^{N} k_i\sigma_i|$.

For a given network $\mathcal{G}$, we generate a total number $\Omega = 1000$ of strongly disordered initial opinion patterns $\vec{\sigma}^{\alpha}(0)$ and, for each of them we run the LMR dynamics for one time step to reach the corresponding pattern $\vec{\sigma}^{\alpha}(1)$. It has been shown in Ref. [20] that the characteristic relaxation time of the LMR dynamics is determined by the mean escaping velocity of the network's opinion pattern from the strongly disordered region. In the present work we calculate a fitness parameter f for network $\mathcal{G}$ according to

$$f(\mathcal{G}) = \frac{1}{\Omega} \sum_{\alpha=1}^{\Omega} \left| \frac{1}{N} \sum_{i=1}^{N} \sigma_i^{\alpha}(1) \right| . \tag{1}$$

For networks with the same size N and mean degree c, we have checked that those with higher fitness values have shorter mean LMR consensus times [23].

The fitness $f(\mathcal{G})$ as defined by Eq. (1) can also be evaluated using completely random configurations instead of random strongly disordered configurations as the initial conditions. When using random configurations as the initial conditions, we found that the main results of the present paper do not change, but the vertex–vertex correlation patterns of the network will be slightly affected (i.e., the R value defined by Eq. (2) will be more close to zero).

The network of a complex system is not fixed but changes with time. We focus on situations in which the typical timescale of network evolution is much longer than that of the dynamical process. In real-world systems, modifications of network structure often occur distributedly and locally. In accordance with this, in the simulation a simple local edge-rewiring scheme as demonstrated in Fig. 1 is employed (similar simulation results obtained with other local or global mutation schemes will be reported elsewhere [23]). For each vertex i of the network with probability (mutation rate) μ propose the following $(i, j) \to (i, k)$ edge redirection: randomly cut one of its edges (i, j) to vertex j and link this edge to vertex j's nearest-neighbors k. This proposal is rejected if (1) edge (i, k) already exists or (2) the degree of vertex j is less than a

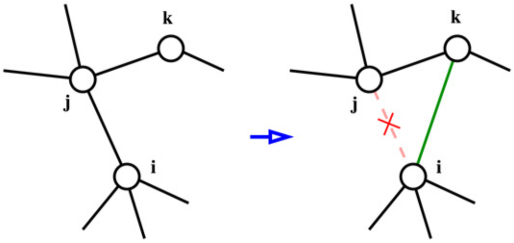

Fig. 1. Local edge redirection process. The edge rewiring $(i, j) \to (i, k)$ is accepted only if before the rewiring vertex i and k is not connected and that vertex j has vertex-degree higher than k_0.

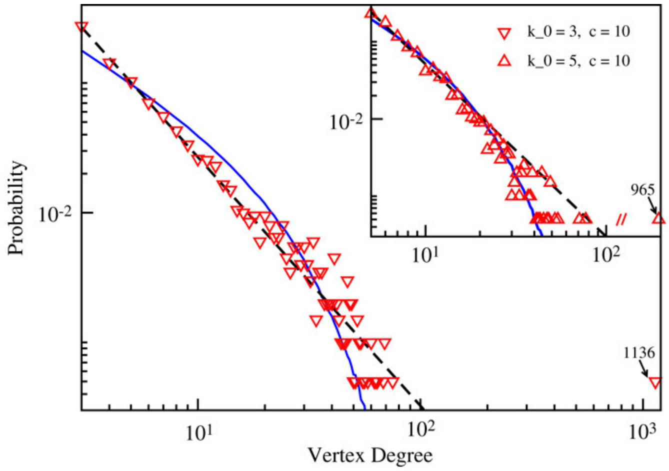

Fig. 2. (Color Online) The degree distribution for a steady-state network (under dynamics–structure coupling) of $N = 2000$ and $c = 10$, $k_0 = 3$ (down triangles) and $c = 10$, $k_0 = 5$ (up triangles). The dashed lines are the best power-law fit of the points with $\gamma = 1.92 \pm 0.02$ (main panel) and $\gamma = 2.24 \pm 0.04$ (inset). The solid lines are the corresponding degree distributions (as averaged over 200 samples) for steady–steady networks under only mutation but no selection. The mutation rate $\mu = 0.01$.

minimal value k_0 after cutting edge (i, j). We set $k_0 = 3$ or 5 in the simulation. The only motivation of setting a cutoff $k_0 > 1$ is to make sure that in the network there will not be an accumulation of dangling vertices of degree $k = 1$. The local edge rewiring process reserves the number of connected components of the network. If initially the network is connected, it will remain to be connected.

During each time step T of the evolution, the network is mutated by the above-mentioned random local scheme and the fitness difference δf between the new and the old network is estimated by Eq. (1). For the dynamics–structure coupling, a simple simulation rule could be to accept this mutation with probability unity if $\delta f \geq 0$ and with probability $\exp(\beta \delta f)$ if otherwise, with β controlling the strength of dynamics–structure coupling. When there is only mutation but no selection ($\beta = 0$), it has already been known that the steady-state network's vertex-degree profile decays exponentially for large degrees [24] (see also the solid lines of Fig. 2). Here we focus on the other limit of strong fitness selection ($\beta \gg 0$) and carry out the network evolution process through a population dynamics simulation of mutation and selection [15]: Starting with a set of $P = 25$ networks uniformly sampled from the ensemble of random networks of size N and mean connectivity c, at each round of the evolution each parent network generates $E = 3$ slightly mutated offsprings, resulting in an expanded population of $(E + 1)P$ networks; the fitness values of these networks are estimated and the P ones with the highest values survive and become parents for the next generation. The population dynamics runs for many steps until the system reaches a final steady-state. We have checked that the steady-states of the simulation are not affected with larger values of population parameters P and E [23].

3. Results

Fig. 2 shows the vertex-degree distribution of a network with size $N = 2000$ and mean degree c (=10) at evolution time $T = 2 \times 10^5$ under mutation rate $\mu = 0.01$. One remarkable feature is that the steady-state network has a global hub whose connectivity is proportional to N. This global hub samples the opinions of a finite population of the network (especially those of the low-degree vertices, see below) and serves as a global indicator of the system's state; its emergence is completely due to the dynamics–structure coupling. To some extent this global hub balances the influences of the minority high-degree vertices (see below) and those of the majority low-degree vertices. Such a global hub may correspond to news agencies and public medias in modern societies and to global transcription factors in biological cells.

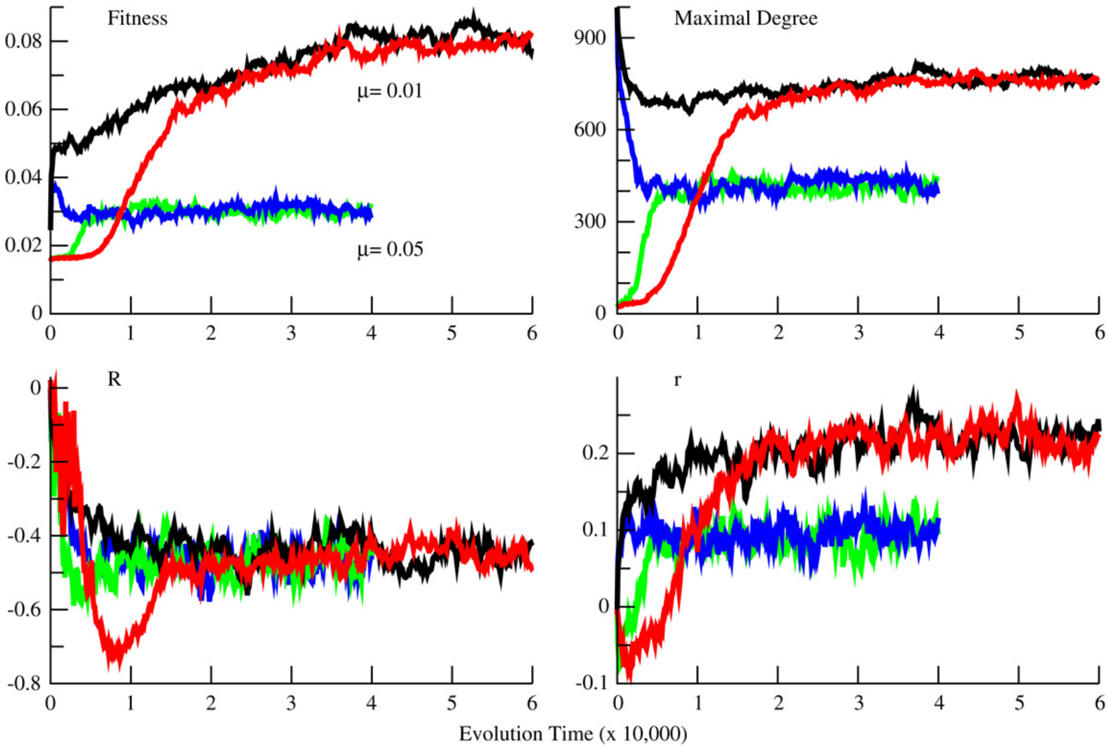

Fig. 3. (Color Online) The evolution of the mean fitness value, the mean maximal vertex-degree, the correlation index R (Eq. (2)), and the assortative-mixing index r (of the global hub-removed subnetwork) as a function of simulation steps. The network size is $N = 1000$, mean vertex-degree is $c = 10.0$, and minimal degree is $k_0 = 5$. The mutation rate is $\mu = 0.01$ (black and red curves, maximal evolution time to 6×10^4 steps) or $\mu = 0.05$ (blue and green curves, maximal evolution time to 4×10^4 steps). The population dynamics starts from an ensemble of random Poissonian networks (red and green curves, which initially are the two lower curves) or an ensemble of modified random Poissonian networks with a single vertex of degree $N - 1$ (black and blue curves, which initially are the two upper curves).

At mutation rate $\mu = 0.01$ the mean clustering coefficient [1] of the steady-state networks is about 0.0640 ± 0.0006 (for $N = 2000$ and $c = 10$), considerably larger than the mean value of 0.0048 ± 0.0008 for random Poissonian networks. The global hub is crucial for this small-world property: if it is removed, the remaining subnetwork has much reduced mean clustering coefficient 0.0089 ± 0.0002. There are strong degree–degree correlations in a steady-state network. First, the global hub prefers to interact with low-degree vertices. This preference can be measured by a parameter R defined by

$$R = \frac{k_{\mathrm{nn}}^{\mathrm{g}} - \langle k_{\mathrm{nn}}^{\mathrm{g}} \rangle_{\mathrm{rand}}}{\langle k_{\mathrm{nn}}^{\mathrm{g}} \rangle_{\mathrm{rand}} - k_0}, \tag{2}$$

where $k_{\mathrm{nn}}^{\mathrm{g}}$ is the mean degree of nearest-neighbors of the global hub and $\langle k_{\mathrm{nn}}^{\mathrm{g}} \rangle_{\mathrm{rand}}$ is the averaged value of this mean degree over an ensemble of randomly shuffled networks. The steady-state value is $R \approx -0.5$ for $N = 1000$, $c = 10$ and $\mu = 0.01$ (Fig. 3). By this preference the 'voices' of low-degree vertices have a larger chance to be heard by the whole system. Second, there are strong positive degree–degree correlations among vertices of a steady-state network (excluding the global hub). To measure the extent of these correlations, we calculate the assortative-mixing index r of the global hub-removed subnetwork following Ref. [25]. A steady-state assortative-mixing index of $r \approx 0.2$ for mutation rate $\mu = 0.01$ (Fig. 3) suggests that in the subnetwork high-degree vertices (except the global hub) are more likely than random to connect with other high-degree vertices.

The steady-state vertex-degree distributions for networks under dynamics–structure coupling deviate remarkably from those of the networks under only mutation (see Fig. 2). Besides the emergence of a global hub, the stead-state vertex-degree distribution resembles a power-law form of

$$P(k) = Ck^{-\gamma}, \quad k \geq k_0, \tag{3}$$

where C is a normalization constant. For the data-set of Fig. 2 with mean degree $c = 10$ and minimal degree $k_0 = 3$, the fitting reports a decay exponent of $\gamma \simeq 1.92$, while for the data-set with of $c = 10$ and $k_0 = 5$ the fitting gives $\gamma \simeq 2.24$. Scale-free networks with decay exponent $\gamma < 2.5$ have shown to be particularly efficient for LMR dynamics, and the mean relaxation time of the dynamics on such a network does not increase with network size N [20,22]. This work indicates that such heterogeneous optimal network structures might be reachable without employing any central planning and any intelligence. The system only needs to accumulate decentralized and local structural changes under the selection of dynamics–structure coupling. Networks with pronounced power-law degree distributions also emerged in other model systems with comparable dynamical and evolutionary timescales [16,17]. In real-world systems, it was noticed by Aldana [26] that a major fraction of scale-free complex networks has their decay exponent γ in the tiny range of $\gamma \in [2.0, 2.5]$.

The network evolution trajectory also shows interesting features. Starting from an ensemble of random Poissonian networks with size $N = 1000$ and mean degree $c = 10.0$, Fig. 3 shows that the evolution can be divided into four stages. In the first 'dormant' stage which lasts for about 5000 evolution steps for mutation rate $\mu = 0.01$, the degree distribution of the networks changes gradually into the form shown by the solid line in the inset of Fig. 2. The fitness values of the networks are small and increase only very slowly, the maximal vertex-degrees of the networks are also small, and the degree–degree correlations in the network are weak. This dormant stage is followed by a 'reforming' stage which lasts for about 10,000 steps for $\mu = 0.01$. A global hub emerges and its degree rapidly exceeds those of all the other vertices of the network, the subnetwork assortative index r also increases rapidly, and the degree distribution of the network becomes power-law-like at the end of this stage. This reforming stage has rapid increase in the mean fitness value; it follows by a long 'structural fine-tuning' stage (lasts for about 20,000 steps at $\mu = 0.01$) of slow increase in network fitness, maximal degree, and assortative mixing. Finally the network reaches the steady-state in which the network's fitness value saturates but its local structures are being modified continuously.

We have performed simulations with different initial conditions and confirmed that the steady-states are not affected [23]. For example, Fig. 3 demonstrates that the steady-state networks obtained from two different initial conditions share the same dynamical performances and the same structural properties. (If the network initially has a global hub of degree $N - 1$ but otherwise is completely random, during the evolution the degree of the global hub decreases but the fitness of the network increases (Fig. 3). This indicates that the existence of a global hub, heterogeneous degree profile, and strong local degree–degree correlations are all important for high dynamical performance.) On the other hand, the evolution process is greatly influenced by the network mutation rate μ. For the same network size N and mean connectivity c, the steady-state networks obtained with a lower network mutation rate μ have better dynamical performances (Fig. 3). As the network topology becomes heterogeneous, most local structural changes will tend to deteriorate the dynamical performance. When the mutation rate is relatively large, in one evolution step the probability for the combination of $L = N\mu$ local and distributed mutations to enhance the network's dynamical performance will decrease rapidly with L. The balance between structural entropy (randomness) and dynamical performance then makes the system cease to be further optimized. For the dynamics–structure interaction to work most efficiently, it is therefore desirable that the timescale of network evolution be much slower than the timescale of network dynamics.

4. Conclusion

In this paper, we have studied the evolution and optimization of complex networks from the perspective of dynamics–structure mutual influence. Through extensive simulation on a simple prototypical model process, the local-majority-rule dynamics, we showed that if there exist feedback mechanisms from a network's dynamical performance to its structure, the network can be driven into highly heterogeneous structures with a global hub, strong local correlations in its connection pattern, and power-law-like vertex-degree distributions. The steady-state networks reached by this dynamics-driven evolution will have better dynamical performance if network evolution occurs much slowly than the dynamical process on the network.

For the LMR dynamics specifically, this work confirmed and extended previous studies [20,22] by showing that scale-free networks with decay exponent $\gamma < 2.5$ indeed are optimal and can be reached without the need of any central planning. Besides the scale-free property and strong local structural correlations, a steady-state network also has a global hub which serves a global indicator of the system's state by sampling the opinions of a large fraction of the vertices of the system.

Real-world complex systems of course are much more complicated than the simple model systems studied in this paper. Different mechanisms may be contributing simultaneously to the evolution of a real-world complex network. The present paper suggested that the interplay between dynamics and structure can be an important driving force for the formation and stabilization of heterogeneous structures which are ubiquitous in biological and social systems [8,10,11,13,14,16–19]. A lot of efforts are needed to decipher the detailed dynamics–structure coupling mechanisms in many complex systems.

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