

Dynamic pattern evolution on scale-free networks

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A general class of dynamic models on scale-free networks is studied by analytical methods and computer simulations. Each network consists of N vertices and is characterized by its degree distribution, $P(k)$, which represents the probability that a randomly chosen vertex is connected to k nearest neighbors. Each vertex can attain two internal states described by binary variables or Ising-like spins that evolve in time according to local majority rules. Scale-free networks, for which the degree distribution has a power law tail $P(k) \sim k^{-\gamma}$, are shown to exhibit qualitatively different dynamic behavior for $\gamma < 5/2$ and $\gamma > 5/2$, shedding light on the empirical observation that many real-world networks are scale-free with $2 < \gamma < 5/2$. For $2 < \gamma < 5/2$, strongly disordered patterns decay within a finite decay time even in the limit of infinite networks. For $\gamma > 5/2$, on the other hand, this decay time diverges as $\ln(N)$ with the network size N . An analogous distinction is found for a variety of more complex models including Hopfield models for associative memory networks. In the latter case, the storage capacity is found, within mean field theory, to be independent of N in the limit of large N for $\gamma > 5/2$ but to grow as N^α with $\alpha = (5 - 2\gamma)/(\gamma - 1)$ for $2 < \gamma < 5/2$.

random network | Boolean dynamics | cellular automata | associative memory

The biosphere contains many complex networks built up from rather different elements such as molecules, cells, organisms, or machines. Despite their diversity, these networks exhibit some universal features and generic properties, a topic of much recent interest (1–6). One important result of this recent activity is a classification scheme for the structure of networks in terms of their topology and connectivity (5, 6). The basic elements of each network can be represented by nodes or vertices and their interrelations by edges between these vertices. By definition, the degree, k , of a given vertex is equal to the number of edges connected to it. In this way, each network is characterized by its graph, a well defined mathematical object (7). Four large subsets of network graphs have been characterized in terms of their connectivity properties: regular ordered and random networks, which have been studied for a long time, as well as small-world (1) and scale-free (4) networks. The latter types of networks are characterized by a degree distribution, $P(k)$, that decays as $P(k) \sim 1/k^\gamma$ with decay exponent γ .

Many biological, social, and technological networks are found to be scale-free (5, 6). To explain this abundance, several mechanisms have been proposed, some of which are related to the growth of networks with preferential attachment rules (5, 8). The impact of network architecture on network integrity or resilience has also been investigated (6, 9–11). Upon random removal of a finite fraction of vertices, a scale-free network with decay exponent $2 < \gamma < 3$ will always keep a giant component. In contrast, if a tiny fraction of the most highly connected vertices is selectively removed, such a network will also break up into many small components. Applying this insight to the case of disease spreading on networks, one realizes that infective diseases have a high probability to affect the whole network (12) unless one immunizes the most highly connected vertices (13).

Random removal of vertices is equivalent to the process of site percolation on the initial network (9, 10). Likewise, disease spreading is intimately related, in the long time limit, to bond

percolation (6, 10). In general, the elements of real networks are dynamic and exhibit various properties that change with time. A more detailed description of the network dynamics is then obtained in terms of dynamical variables associated with each vertex of the network. We will consider processes on networks that evolve fast compared with any changes in the network topology, which is therefore taken to be time-independent. Two examples for such dynamical processes are provided by the regulation of genetic networks that exhibit a changing pattern of active and inactive genes (see, e.g., ref. 14) or by neural networks that can be characterized by firing and nonfiring neurons (see, e.g., ref. 15).

To identify universal features and generic properties, it is often convenient to use discrete dynamical variables and to allow each vertex to attain several distinct states. The network is then characterized, at each moment in time, by a certain pattern of these internal vertex states, and the time evolution of these patterns represents the global dynamics of the whole network.

The study of discrete dynamical processes on ordered and random networks has a long history. Ordered networks have been studied in the context of neural computation (16, 17), cellular automata or Boolean dynamics (18, 19), and dynamic Ising models (20). Random networks with random Boolean dynamics were introduced in the context of gene expression and studied as prototypes of random cellular automata (21–23). Discrete dynamic processes on small-world networks were discussed in ref. 2, whereas analogous processes on scale-free networks have only been addressed rather recently (24–26).

Random networks as originally studied in mathematics (5–7) are characterized by a Poissonian degree distribution as given by $P(k) = \langle k \rangle^k e^{-\langle k \rangle} / k!$, where $\langle k \rangle = \sum k P(k)$ denotes the mean value of the vertex degree k . In contrast, scale-free networks are characterized by $P(k) \sim k^{-\gamma}$ with decay exponent γ for an intermediate range of k -values that can be defined as follows. To avoid disconnected subgraphs, it is useful to introduce a certain minimal degree $k_0 > 0$. Furthermore, a large but finite network containing N vertices is also characterized by a certain maximal degree k_N . These two “cutoffs” can be incorporated in a particularly simple way via the explicit form (9)

$$P(k) = (1/\mathcal{A})k^{-\gamma} \quad \text{for } k_0 \leq k \leq k_N \\ = 0 \quad \text{otherwise} \quad [1]$$

with the normalization factor $\mathcal{A} \equiv \sum P(k)$ and $k_N = k_0 N^{1/(\gamma-1)}$ (see *Degree Distribution and Maximal Vertex Degree* in Supporting Text, which is published as supporting information on the PNAS web site).

Many scale-free networks are characterized by decay exponents γ that fall into the narrow range $2 < \gamma \leq 5/2$ as observed in ref. 24. Indeed, table 2 of ref. 5 contains a list of ten scale-free networks with $2 < \gamma < 5/2$, one with $\gamma = 2.5$, and only three with $2.5 < \gamma < 3$. The lower boundary value $\gamma = 2$ is easy to understand since it ensures that the mean vertex degree $\langle k \rangle = \sum k P(k)$ remains finite in the limit of large N . The upper boundary

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with $0 \leq Q(t) \leq 1$. Note that the ordering probability Q differs, in general, from the overall probability to find any vertex in the spin-up state. The latter probability is given by $\langle q \rangle \equiv \sum_k P(k)q_k$. Special patterns for which $\langle q \rangle = Q$ are provided by k -independent probabilities $q_k = q$. In particular, for the all-spin-down pattern with $q_k = 0$ for all k and for the all-spin-up pattern with $q_k = 1$ for all k , one has $Q = \langle q \rangle = 0$ and $Q = \langle q \rangle = 1$, respectively.

If we know the ordering probability Q at a certain time t , we can calculate the probabilities q_k at the next time step. Indeed, it follows from the majority rule dynamics as defined by Eq. 2 that

$$q_k(t+1) = \sum'_m \left(1 - \frac{1}{2} \delta_{m,k/2}\right) B_{k,m} Q^m(t) (1-Q(t))^{k-m}, \quad [4]$$

where the prime at the summation symbol indicates that this sum runs over all integer m with $k/2 \leq m \leq k$, δ is the Kronecker symbol, and $B_{k,m} \equiv k!/[m!(k-m)!]$ are the binomial coefficients. Finally, summation of the left-hand side of Eq. 4 leads to the evolution equation

$$Q(t+1) = \Psi(Q(t)) \quad [5]$$

for the ordering probability Q with the evolution function

$$\Psi(Q) \equiv \sum_k \sum'_m \left(1 - \frac{1}{2} \delta_{m,k/2}\right) k P(k) B_{k,m} Q^m (1-Q)^{k-m} / \langle k \rangle \quad [6]$$

for random graphs with no vertex degree correlations as considered here.

The evolution equation (5) has two stable fixed points at $Q = 0$ and $Q = 1$, and an unstable one at $Q = 1/2$. The fixed points with $Q = 0$ and $Q = 1$ correspond to the all-spin-down and all-spin-up patterns, respectively. The unstable fixed point with $Q = 1/2$ represents the phase boundary between these two ordered patterns; the corresponding boundary patterns are characterized by probabilities $\hat{q}_k$, which satisfy

$$\hat{Q} \equiv \sum_k k P(k) \hat{q}_k / \langle k \rangle = 1/2 \quad \text{or} \quad N \langle k \rangle \hat{Q} = M, \quad [7]$$

where M is the total number of edges. A subset of these boundary patterns is provided by those patterns for which the probabilities $\hat{q}_k = 1/2$ for all vertex degrees k . Therefore, the order parameter of these systems is taken to be

$$y \equiv Q - \hat{Q} = Q - 1/2, \quad [8]$$

which vanishes for all boundary patterns.

In the next section, we will compare the mean field trajectories obtained from the evolution equation (5) with the pattern evolution obtained from computer simulations. In the latter case, one starts from a certain initial pattern and applies the majority rule dynamics as given by Eq. 2 to each vertex of the network. Since we want to be able to use the same initial pattern for both mean field theory and computer simulations, we will define the enlarged set of *strongly disordered patterns* that consists (i) of the boundary patterns characterized by Eq. 7 and (ii) of additional patterns characterized by probabilities $\tilde{q}_k$ that lead to $Q = \tilde{Q} = 1/2 \pm 1/2M$ and, thus, to the order parameter

$$\tilde{y} \equiv \sum_k k P(k) \tilde{q}_k / \langle k \rangle - 1/2 = \pm 1/2M = \pm 1/\langle k \rangle N, \quad [9]$$

which vanishes in the limit of large network size N . A pattern with probabilities $\tilde{q}_k$ can be obtained from a boundary pattern by simultaneously flipping two spins with opposite orientations on a k and $(k+1)$ vertex.

The evolution equation for the order parameter $y = Q - 1/2$ can be directly obtained from the corresponding equation (7) for Q and is given by $y(t+1) = \Psi(1/2 + y(t)) - 1/2$. In the vicinity of the unstable fixed point with $Q = 1/2$ and $\Psi(1/2) = 1/2$, the latter equation can be linearized and becomes

$$y(t+1) \approx \Psi'(1/2)y(t) \quad \text{with} \quad \Psi'(1/2) \equiv d\Psi/dQ|_{Q=1/2} \quad [10]$$

for small $y(t)$. Iterating this equation n times from an initial time t_0 up to a final time t_1 , one obtains the time difference

$$\Delta t_{01} \equiv t_1 - t_0 \approx \frac{\ln|y(t_1)| - \ln|y(t_0)|}{\ln \Psi'(1/2)} \quad [11]$$

in the limit of small $y(t_0)$.

It follows from the explicit expression (Eq. 6) for the evolution function $\Psi(Q)$ that the derivative $\Psi'(1/2)$ at the unstable fixed point with $Q = 1/2$ diverges for a scale-free network with decay exponent $\gamma \leq 5/2$ in the limit of large network size N . More precisely, one obtains the asymptotic behavior

$$\begin{aligned} \Psi'(1/2) &\approx c_\gamma k_0^{1/2} && \text{for } \gamma > 5/2 \\ &\approx c_\gamma k_0^{1/2} \ln(N) && \text{for } \gamma = 5/2 \\ &\approx c_\gamma k_0^{1/2} N^{\alpha/2} && \text{for } 2 < \gamma < 5/2 \end{aligned} \quad [12]$$

in the limit of large N with $\alpha = (5 - 2\gamma)/(\gamma - 1)$, where c_γ is a dimensionless γ -dependent coefficient (see *Derivation of Eq. 12* in *Supporting Text*).

Results and Discussion

Decay of Strongly Disordered Patterns. Now, consider an initial state of the network at time $t = t_0$ that corresponds to a strongly disordered pattern with order parameter $y(t_0) = \tilde{y} = \pm 1/2M \sim 1/N$ as in Eq. 9. For $t > t_0$, such an initial pattern evolves according to the majority rule dynamics that leads to an increase in the absolute value of the order parameter y and, thus, to the growth of order. We will characterize this decay of the strongly disordered patterns by the decay time t_d , which is the time it takes to reach a pattern with an order parameter y_* that satisfies $|y_*| \geq 1/4$. In addition, we have also estimated the probability to reach the completely ordered patterns when one initially starts from strongly disordered ones.

Within mean field theory, the decay time t_d follows from Eq. 11 and is given by $t_d \approx \ln(\langle k \rangle N) / \ln(\Psi'(1/2))$ for large $\langle k \rangle$ or large N . This expression behaves as

$$\begin{aligned} t_d &\sim \ln(N) && \text{for } \gamma > 5/2 \\ &\sim \ln(N) / \ln \ln(N) && \text{for } \gamma = 5/2 \\ &\sim 2(\gamma - 1)/(5 - 2\gamma) && \text{for } 2 < \gamma < 5/2 \end{aligned} \quad [13]$$

in the limit of large network size N . Thus, for scale-free networks with decay exponent $2 < \gamma < 5/2$, strongly disordered patterns always decay after a *finite* number of iteration steps even in the limit of large N . In contrast, for networks with $\gamma > 5/2$, the decay time diverges as $\ln(N)$. The latter behavior for $\gamma > 5/2$ also applies to Poissonian networks and is, thus, consistent with recent results for opinion spreading on social networks (28).

We have confirmed these mean field predictions by computer simulations. To avoid both disconnected and tree-like network graphs, the simulations were performed for networks with a relatively large mean vertex degree $\langle k \rangle$ and minimal vertex degree $k_0 > 1$. In Fig. 1, we display the time evolution of the absolute value of the order parameter, $|y| = |Q - 1/2|$, as

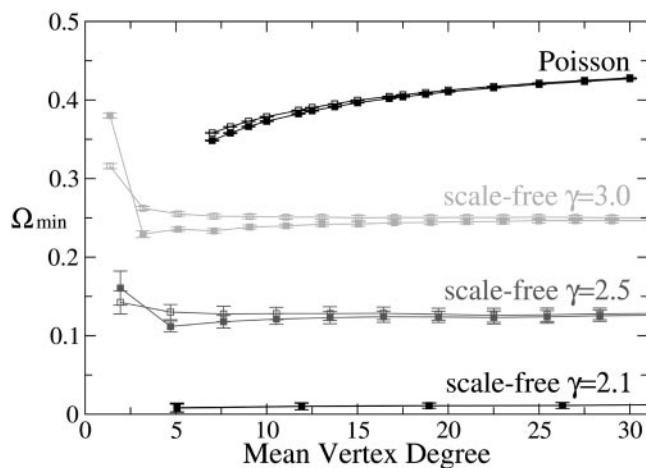


Fig. 4. Minimal fraction $\Omega_{\min}$ of spins that one has to flip to induce a transition from the all-spin-down to the all-spin-up pattern. All networks have $N = 10^5$ vertices but differ in their degree distribution, which was Poissonian or scale-free with $\gamma = 3.0$, $\gamma = 2.5$, and $\gamma = 2.1$. The open squares were obtained from the analytical expression (Eq. 14); the filled squares were obtained through exact enumerations where each data point represents an average over 100 network realizations.

is smaller than 0.6×10^{-2} for $2^{10} \leq n \leq 2^{18}$ (see Fig. 7, which is published as supporting information on the PNAS web site).

To see how the time evolution of the order parameter depends on the mean vertex degree $\langle k \rangle$, the same set of simulations was also performed for three networks with $\langle k \rangle = 10$ and $k_0 \geq 2$. The corresponding decay time distributions are found to be rather similar to those displayed in Fig. 2 (see Fig. 8, which is published as supporting information on the PNAS web site). The main difference is that the approach to the completely ordered patterns is slowed down (see Figs. 9 and 10, which are published as supporting information on the PNAS web site). Additional simulations for mean vertex degree $\langle k \rangle = 7$ and $\langle k \rangle = 5$ show that the time to reach the completely ordered patterns further increases with decreasing $\langle k \rangle$. These simulation results are consistent with those obtained for random Poissonian networks (31) but are rather different from the behavior found for tree-like networks (29) and for d -dimensional hypercubic lattices with $d \geq 3$ (30).

As emphasized in refs. 30 and 31, spin patterns, which evolve according to local majority dynamics, can be trapped in metastable states corresponding to several spin-up and spin-down domains. In addition, the domain boundaries may not be completely frozen but may contain “blinkers,” i.e., single spins that continue to flip after each time step. It is not difficult to see that domain boundaries and blinkers are likely to occur for spin patterns on tree-like graphs (33), leading to the glassy dynamics found for Cayley trees (29). Somewhat surprisingly, multidomain patterns with blinkers are also typical for d -dimensional hypercubic lattices with $d \geq 3$ as shown in ref. 30. In contrast, our simulations give strong evidence that, for scale-free networks with $k_0 > 1$, disordered patterns typically evolve toward the two completely ordered patterns provided the networks are connected and the mean vertex degree $\langle k \rangle$ is sufficiently large. The case $k_0 = 1$ is special since the graphs tend to be tree-like, and their dynamics is presumably characterized by blinkers as well.

Selective Spin Flips. Now, let us look at a different aspect of the response behavior. We start from the all-spin-down pattern and ask how many spins we have to flip to reach another pattern that evolves toward the all-spin-up pattern under the local majority dynamics.

If we flipped the spins on a randomly chosen set of vertices, we would have to flip, in general, of the order of $N/2$ spins. However, we can induce such a global transition in a much more efficient way if we flip primarily those spins that are located on the highly connected vertices. This is illustrated in Fig. 4, which displays the *minimal fraction* of spins, $\Omega_{\min}$, which one has to flip to transform the all-spin-down pattern into the all-spin-up pattern. An analytical estimate for this minimal fraction can be obtained from the explicit relation for the boundary patterns as given by Eq. 7 if one considers such patterns with $\hat{q}_k = 0$ for $k_0 < k < k_*$ and $\hat{q}_k = 1$ for $k_* < k < k_N$, where the intermediate k -value k_* is determined by the requirement that the spin pattern represents a boundary pattern with ordering probability $Q = \hat{Q} = 1/2$ (see *Derivation of Eq. 14 in Supporting Text*). For large vertex number N , this leads to the asymptotic estimate

$$\Omega_{\min} \approx [(1 + N^{-(\gamma-2)/(\gamma-1)})/2]^{(\gamma-1)/(\gamma-2)} \approx 2^{-(\gamma-1)/(\gamma-2)}. \quad [14]$$

This minimal fraction does *not* depend on the mean vertex degree $\langle k \rangle$ and vanishes very rapidly as $\sim \exp(-|const|/(\gamma-2))$, i.e., as an essential singularity in $\gamma-2$. Both properties are fully confirmed by the numerical results (see Fig. 4). For $\gamma = 3$, for example, the asymptotic estimate (Eq. 14) leads to $\Omega_{\min} \approx 1/4$ in perfect agreement with the numerical results shown in Fig. 4. This sensitivity of ordered spin patterns to selective spin flips has been independently observed in ref. 25.

Thus, a scale-free network with a decay exponent γ that is close to $\gamma = 2$ has the additional property that one needs to selectively flip only a very small fraction of the spins to induce a transition from one ordered pattern to the other. This property provides a very efficient way for the system to adapt its state in response to varying external conditions. Note, however, that in contrast to the behavior of the response time, the dependence of the minimal fraction $\Omega_{\min}$ on the decay exponent γ does not exhibit a sharp borderline at $\gamma = 5/2$.

Dynamic Behavior of More Complex Models. The main features of the pattern evolution described above are quite generic and remain valid for various extensions and generalizations of the majority rule dynamics. One particularly interesting generalization is obtained if we extend our mean field theory to Hopfield models (17, 27) that address the maximal storage capacity $S_{\max}$ of associative memory networks. This capacity, which represents the largest possible number of patterns that can be stored in the network, is found to behave as

$$\begin{aligned} S_{\max} &\sim k_0 N^\alpha && \text{for } 2 < \gamma < 5/2 \text{ and} \\ &\sim k_0 \ln^2(N) && \text{for } \gamma = 5/2 \end{aligned} \quad [15]$$

with $\alpha = (5-2\gamma)/(\gamma-1)$ in the limit of large network size N (see *Hopfield Models on Scale-Free Networks in Supporting Text*). In contrast, for $\gamma > 5/2$, the maximal storage capacity $S_{\max}$ does *not* grow with the network size N for large N . It has been recently argued that some functional networks in the human brain are indeed scale-free with $\gamma \approx 2.1$ (32, 34). Thus, for these latter networks, our mean field theory predicts that the storage capacity grows as N^α with $\alpha \approx 0.73$, which is almost as fast as in the original Hopfield model on complete graphs that have the constant vertex degree $k = N-1$ and are characterized by $\alpha = 1$.

We have also extended our analysis of the majority rule dynamics to a variety of other models including Potts models on nondirected networks as well as to Ising models on directed networks (see *Extension to Directed Scale-Free Networks in Supporting Text*). For all of these generalizations, we find that $\gamma = 5/2$ represents a borderline case for the dynamic pattern evolution.

