Kauffman Boolean model in undirected scale-free networks

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We investigate analytically and numerically the critical line in undirected random Boolean networks with arbitrary degree distributions, including the scale-free topology of connections $P(k) \sim k^{-\gamma}$. We explain that the unattainability of the critical line in numerical simulations of classical random graphs is due to percolation phenomena. We suggest that recent findings of discrepancy between simulations and theory in directed random Boolean networks might have the same reason. We also show that in infinite scale-free networks the transition between frozen and chaotic phases occurs for $3 < \gamma < 3.5$. Since most critical phenomena in scale-free networks reveal their nontrivial character for $\gamma < 3$, the position of the critical line in the Kauffman model seems to be an important exception to the rule.

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Almost 40 years ago Kauffman proposed random Boolean networks (RBNs) for modeling gene regulatory networks [1]. Since then, in addition to its original purpose, the model and its modifications have been applied to many different phenomena like cell differentiation [2], immune response [3], evolution [4], opinion formation [5], neural networks [6], and even quantum gravity problems [7].

The original RBNs were represented by a set of N elements, $\Sigma_t = \{\sigma_1(t), \sigma_2(t), \ldots, \sigma_N(t)\}$, each element σ_i having two possible states: active (1) or inactive (0). The value of σ_i was controlled by k other elements of the network, i.e., $\sigma_i(t+1) = f_i(\sigma_{i_1}(t), \sigma_{i_2}(t), \ldots, \sigma_{i_k}(t))$, where k was a fixed parameter. The functions f_i were selected so that they returned values 1 and 0 with probabilities, respectively, equal to p and $1-p$. The parameters k and p determined the dynamics of the system (Kauffman network), and it has been shown that for a given probability p, there exists a critical number of inputs [13]

$$k_c = \frac{1}{2p(1-p)}, \tag{1}$$

below which all perturbations in the initial state of the system die out (*frozen phase*), and above which a small perturbation in the initial state of the system may propagate across the entire network (*chaotic phase*).

In fact, the behavior of the Kauffman model in the vicinity of the critical line $k_c(p)$ has become a major concern of scientists interested in gene regulatory networks. The main reason for this is the conjecture that living organisms operate in a region between order and complete randomness or chaos (the *edge of chaos*) where both complexity and rate of evolution are maximized [8–10]. Analogous behavior has been noted in Kauffman networks, which in the interesting region described by Eq. (1) show stability, homeostasis, and the ability to cope with minor modifications when mutated. The networks are stable as well as flexible in this region.

Recently, when data from real networks became available [11,12], a quantitative comparison of the edge of chaos in these data sets and RBN models brought the encouraging and promising message that even such a simple model may mimic characteristics of real systems quite well.

Since, however, real genetic networks exhibit a wide range of connectivities, the recent modifications of the standard RBN take into consideration a distribution of node degrees, $P(k)$. It has been shown that, if the random topology of the directed network is homogeneous (i.e., all elements of the network are statistically equivalent), then the network topology can be meaningfully characterized by the average in-degree $\langle k \rangle$, and the transition between frozen and chaotic phases occurs for [14]

$$\langle k \rangle_c = \frac{1}{2p(1-p)}. \tag{2}$$

On the other hand, if the network topology is characterized by a wide heterogeneity in the connectivity of elements, then it is useless to characterize the network by the average in-degree, and instead of $\langle k \rangle$ another parameter must be used. In the case of a power-law in-degree distribution $P(k) = [\zeta(\gamma) k^{\gamma}]^{-1}$, where $\zeta(\gamma)$ is the zeta function, the characteristic exponent γ is the relevant parameter. It has been shown that the critical line $\gamma_c(p)$ in the RBN model defined on scale-free networks is given by [15]

$$\frac{\zeta(\gamma_c - 1)}{\zeta(\gamma_c)} = \frac{1}{2p(1-p)}. \tag{3}$$

Since $2 < \gamma_c(p) < 2.5$, based on the result (3), it was claimed [16] that the abundance of scale-free networks with $2 < \gamma < 3$ in nature and society can be attributed to the presence of both phases, frozen and chaotic, only in such networks.

Recently, several authors [17,18] have provided a general formula for the edge of chaos in directed networks characterized by the joint degree distribution $P(k,q)$,

$$\frac{\langle kq \rangle}{\langle q \rangle} = \frac{1}{2p(1-p)}, \tag{4}$$

where k and q correspond to in- and out-degrees of the same node, respectively. The formula (4) shows that the position of the critical line depends on the correlations between k and q in such networks. It is also easy to show that the previous results (1)–(3) immediately follow from (4) if one assumes a lack of correlations $P(k,q)=P_{\rm in}(k)P_{\rm out}(q)$.

In this paper, we derive a general relation describing the position of the critical line in undirected RBNs with an arbitrary distribution of connections $P(k)$. Specific cases, including homogeneous as well as strongly heterogeneous (i.e., scale-free) random network topologies, are discussed. We also generalize our derivations to the case when the scale-free network topology is characterized not only by the exponent γ but also by the minimal node degree $k_{\min}=m$, which controls the density of connections. We show that for $\gamma \to \infty$ the parameter m corresponds to the original parameter k used in the standard Kauffman model defined on regular random graphs, in which the number of connections is the same for all elements.

In order to find the position of the critical line in RBN, one has to examine the sensitivity of its dynamics with regard to the initial conditions. In numerical studies such a sensitivity can be analyzed quite simply. One has to start with two initial states $\Sigma_0=\{\sigma_1(0),\sigma_2(0),\ldots,\sigma_N(0)\}$ and $\tilde{\Sigma}_0=\{\tilde{\sigma}_1(0),\tilde{\sigma}_2(0),\ldots,\tilde{\sigma}_N(0)\}$, which are identical except for a small number of elements, and observe how the differences between both configurations Σ_t and $\tilde{\Sigma}_t$ change in time. If a system is robust then the studied configurations lead to similar long-time behavior; otherwise differences develop in time. A suitable measure for the distance between the configurations is the overlap $x(t)$ defined as

$$x(t) = 1 - \frac{1}{N}\sum_{i=1}^{N} |\sigma_i(t) - \tilde{\sigma}_i(t)|. \tag{5}$$

Note that, in the limit $N\to\infty$, the overlap becomes the probability for two arbitrary but corresponding elements $\sigma_i(t)$ and $\tilde{\sigma}_i(t)$ to be equal. Moreover, the stationary long-time limit of the overlap $x=\lim_{t\to\infty} x(t)$ can be treated as the order parameter of the system. If $x=1$, then the system is insensitive to initial perturbations (frozen phase), while for $x<1$, the initial perturbations propagate across the entire network (chaotic phase).

In the following, we will partially reproduce the annealed computation (carried out by Derrida and Pomeau [13]), and generalize it to the case of undirected random graphs with arbitrary degree distribution. The case of directed networks has been studied by Aldana [15], and also by Lee and Rieger [17].

Thus, having in mind that $x(t)$ corresponds to the probability that a given element i possesses the same value in both configurations, $\sigma_i(t)=\tilde{\sigma}_i(t)$, two different situations have to be considered. If all the k_i inputs of $\sigma_i(t)$ are equal to the coresponding inputs of $\tilde{\sigma}_i(t)$, which occurs with probability $[x(t)]^{k_i}$, then one has $\sigma_i(t+1)=\tilde{\sigma}_i(t+1)$. On the other hand, if at least one of the k_i inputs of $\sigma_i(t)$ differs from its counterpart in $\tilde{\Sigma}_t$, which occurs with probability $1-[x(t)]^{k_i}$, then $\sigma_i(t+1)=\tilde{\sigma}_i(t+1)$ only if $f_i(\sigma_{i_1}(t),\ldots,\sigma_{i_{k_i}}(t)) = f_i(\tilde{\sigma}_{i_1}(t),\ldots,\tilde{\sigma}_{i_{k_i}}(t))$ regardless of the values of the inputs in each configuration. The probability of such an event is $p^2+(1-p)^2$. Taking all the above together, one finds that the probability $x(t+1)$ that $\sigma_i(t+1)=\tilde{\sigma}_i(t+1)$ averaged over all elements is given by

$$x(t+1) = \sum_{k=1}^{\infty} \left([x(t)]^k \times 1 + \{1-[x(t)]^k\}[p^2+(1-p)^2]\right)Q(k), \tag{6}$$

where $Q(k)$ represents the probability that an arbitrary link leads to the node of degree k. Of course, in regular random networks in which all nodes have the same connectivity the distribution $Q(k)=P(k)$ and Eq. (6) simplifies to the well-known equation considered in the seminal paper by Derrida and Pomeau [13]. In uncorrelated networks, $Q(k)$ corresponds to the degree distribution of the nearest neighbors,

$$Q(k) = \frac{k}{\langle k\rangle}P(k). \tag{7}$$

Equation (6) can be understood as a map $x(t+1)=M(x(t))$, where

$$M(x) \equiv 1 - 2p(1-p)\left(1 - \sum_{k=1}^{\infty} x^k Q(k)\right). \tag{8}$$

It can be shown that the change of stability of the fixed point of the map $x=M(x)$, which occurs when

$$\lim_{x\to 1^-} \frac{dM(x)}{dx} = 1, \tag{9}$$

determines the phase transition between the ordered and chaotic regimes (cf. [15].). Substituting (8) into (9), one gets the condition for the phase transition:

$$\frac{\langle k^2\rangle}{\langle k\rangle} = \frac{1}{2p(1-p)}. \tag{10}$$

In the following we will analyze Eq. (10) in classical random graphs and in scale-free networks where the second moment $\langle k^2\rangle$ becomes important (it diverges for $\gamma<3$).

Since in classical random graphs $\langle k^2\rangle=\langle k\rangle^2+\langle k\rangle$, Eq. (10) simplifies:

$$\langle k\rangle_c = \frac{1}{2p(1-p)} - 1. \tag{11}$$

Let us note that random undirected networks are formally equivalent to directed networks, in which every undirected link $i-j$ is replaced by two directed links: $i\leftarrow j$ and $i\to j$. The joint degree distribution characterizing such a directed network is given by $P(k,q)=P(k)\delta(k-q)$, where $P(k)$ corresponds to the node degree distribution in the original undirected network, and $\delta(k-q)$ is the Kronecker delta function. Now, substituting the obtained joined degree distribution into Eq. (4), one immediately gets our Eq. (11).

Comparing the formula (11) with (2), one can see that the critical curve in undirected networks has been shifted by 1 in comparison with the directed case. Figure 1 presents both equations as well as numerical simulations of undirected networks of three different sizes ($N=50$, 500, and 5000). While in the limit of large $\langle k\rangle$ the results, especially for large N, agree very well with Eq. (11) (see the inset), for $\langle k\rangle\to 1$ (i.e.,

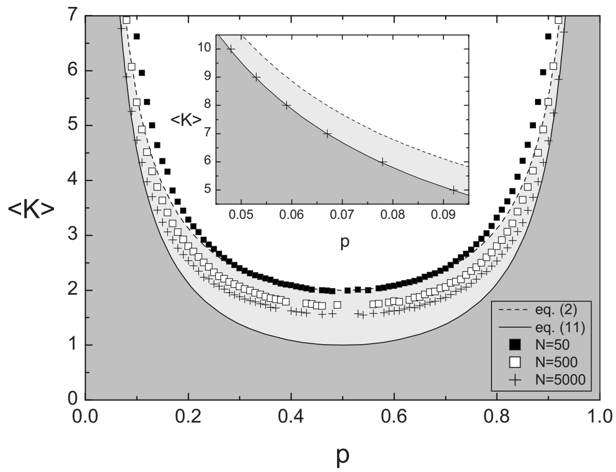

FIG. 1. Phase diagram of Kauffman model defined on classical random graphs. Frozen phase resulting from Eq. (11) is marked by the dark gray area. Light gray area shows the difference between directed and undirected networks.

$p\to 0.5$) they differ significantly. The discrepancy results from the fact that $\langle k\rangle=1$ corresponds to the percolation threshold in these networks. Because the size of the largest component near $\langle k\rangle=1$ is significantly smaller than the network size (the network is divided into several unconnected components), any perturbation cannot propagate across the entire system, and the frozen phase is more easily achieved. This means that it is impossible to verify Eq. (11) in this range. The closer we are to the percolation threshold, the smaller the networks (separated pieces of the whole network) we analyze. One can also show that if one introduces assortativity (i.e., positive degree-degree correlations) to the network the attainable critical connectivity can be significantly shifted toward $\langle k\rangle_c=1$. This happens because the percolation transition occurs for lower values of $\langle k\rangle$ in assortative networks [20,21]. Unfortunately, due to the correlations introduced, analytical treatment is much more difficult in this case.

Nevertheless, it seems to be possible to modify Eq. (11) by taking into consideration the size of the largest component in such networks. If this modification makes analytical results comparable with simulations, then it will have important implications for the directed case of the RBN. Recently, the critical (in the sense of attainability) value of the connectivity is such networks has been estimated as 1.87 by finite-size scaling methods [19] [which significantly deviates from the predictions of mean-field theory—cf. Eq. (2)]. Because the problem of percolation in directed networks is much more complicated (see [22,23]), the undirected case we study here (although less appropriate to model real networks) is the first step that has to be taken to understand the discrepancies observed in directed networks. We leave this issue for future work.

Now, let us analyze scale-free networks with the degree distribution given by a power law,

$$P(k)=[\zeta(\gamma,m)k^{\gamma}]^{-1}, \tag{12}$$

where $\zeta(\gamma,m)=\Sigma_{k=m}^{\infty}k^{-\gamma}$ is the generalized Riemann zeta function (normalization factor), and the parameter m represents the minimal node degree, i.e., it controls the density of connections in the considered networks. Now Eq. (10) takes the form

$$\frac{\zeta(\gamma-2,m)}{\zeta(\gamma-1,m)}=\frac{1}{2p(1-p)}. \tag{13}$$

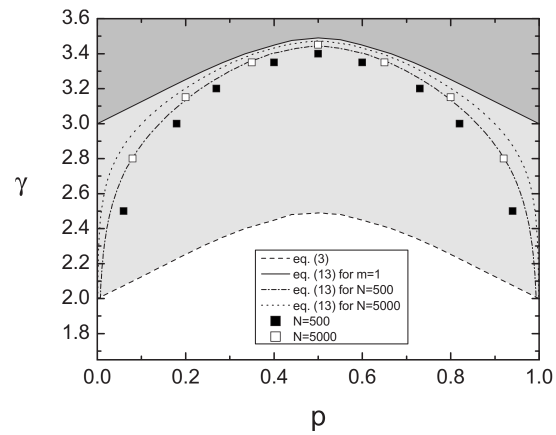

FIG. 2. Phase diagram of scale-free networks with $m=1$. Frozen phase resulting from Eq. (13) is marked by dark gray area. Light gray area shows the difference between directed and undirected networks. Points represent results of numerical simulations, while the two intermediate lines are solutions of Eq. (13) modified for finite networks (dot-dashed line for $N=500$, and dotted line for $N=5000$).

In Fig. 2 a comparison of the transcendental equations (13) (undirected network) for $m=1$ and (3) (directed network) is presented. Analytical curves taking into account the finite-size version of the distribution (12) (where the ζ functions have been replaced by finite sums), as well as results of the numerical simulations for $N=500$ and 5000 are also shown in the figure. One can see that, in the undirected case of infinite scale-free networks, the transition between the frozen and chaotic phases occurs for $3<\gamma<3.5$. This means that in the studied network the critical line has been shifted in comparison with the directed case by $\Delta\gamma=1$ toward larger values of the exponent γ.

The observation is interesting since most critical phenomena in scale-free networks reveal their nontrivial character for $\gamma<3$, making these networks interesting for researchers [24]. This happens because the second moment of the degree distribution is size dependent for $\gamma<3$ (it diverges for $N\to\infty$). For example, in the case of the percolation transition, this means that it is almost impossible to eliminate the giant connected component in such networks, i.e., they are ultraresilient against random damage or failure [25,26]. It also implies the lack of an epidemic threshold in such networks, i.e., the networks are prone to the spreading and the persistence of infections whatever the epidemic spreading rate is. Finally, in the Ising model defined on scale-free networks with $\gamma<3$, the critical temperature is size dependent. Taking all the above into consideration, the position of the critical line in the Kauffman model shows that scale-free networks with $\gamma>3$ may also exhibit interesting properties.

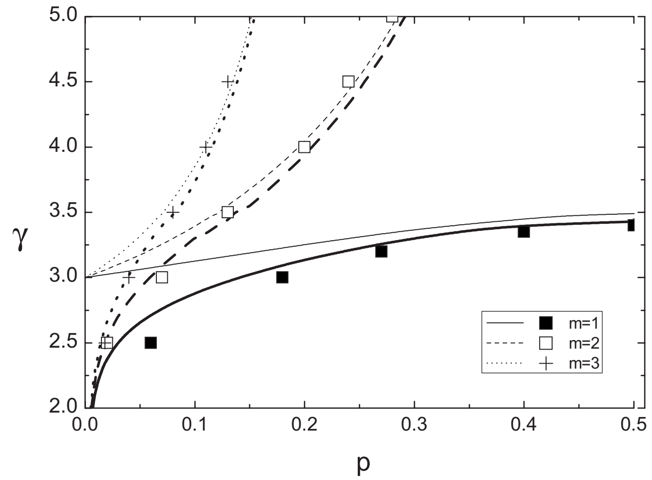

FIG. 3. Critical lines for scale-free RBNs with $m=1$ (solid lines and filled points), $m=2$ (dashed lines and open points), and $m=3$ (dotted lines and crosses). Thin lines are solutions of Eq. (13), while the thick lines are solutions of the same equation modified for networks of size $N=5000$. Points correspond to the results of numerical simulations.

In previous papers [15,16], it has been stated that the only natural parameter determining the network topology is the scale-free exponent γ. In this paper, we introduce the parameter m, which does not change the scale-free character of the node degree distribution, but allows us to control the density of connections. For $m=1$ we retrieve the original problem studied in [15,16]. In Figs. 3 and 4 we present the solutions of Eq. (13) for different values of the parameter m. As one can see, for $m>2$ the frozen phase is preserved only for sufficiently small and sufficiently large values of the parameter p. For a wide range of intermediate values of p, the frozen phase is unattainable.

It is worth noting that, in the limit $\gamma\to\infty$, the scale-free distribution (12) transforms into the Dirac delta function $\delta(k-m)$ [then $\langle k^2\rangle=\langle k\rangle^2$ and Eq. (10) simplifies to Eq. (1)]. This means that in this limit the scale-free RBN model transforms to the standard RBN model, where all elements have the same node degree. In Fig. 4 one can see that for $\gamma\to\infty$ and $m=2$ the width of the chaotic phase shrinks to zero. In

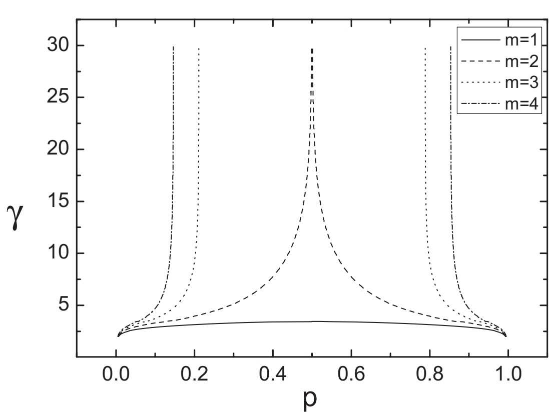

FIG. 4. Phase diagram of scale-free networks with different values of the parameter m.

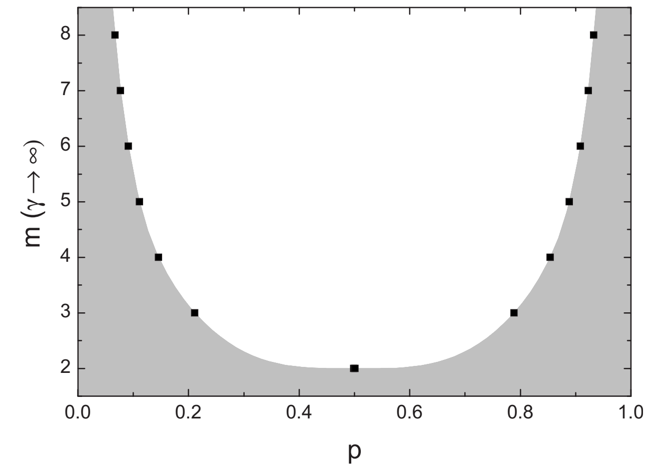

FIG. 5. Phase diagram of scale-free RBNs with $\gamma\to\infty$. The diagram coincides with the phase diagram of the standard RBN model. Points for a given m show the width of the chaotic phase taken from Fig. 4 for $\gamma=30$.

Fig. 5 we show this width for different values of the parameter m. In this figure one can easily recognize the phase diagram of the standard RBN model, in which for $p=0.5$ the critical value of the node degree is $m=k_c=2$.

In summary, we have investigated analytically and numerically the critical line in undirected random Boolean networks with arbitrary degree distribution, including homogeneous and scale-free topology of connections. Study of the undirected case of the RBN facilitates understanding of the impact of percolation phenomena on the unattainability of the critical line in numerical simulations of classical random graphs. We have shown also that in infinite scale-free networks the transition between the frozen and chaotic phases occurs for $3<\gamma<3.5$, i.e., the position of the critical line is shifted by $\Delta\gamma=1$ toward larger values of the exponent γ in comparison with the directed case. Since most critical phenomena in scale-free networks reveal their nontrivial character for $\gamma<3$, the position of the critical line in the Kauffman model seems to be an important exception to the rule.

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APPENDIX

In the following, we present an explanation of the method used in the numerical simulations.

To generate networks with the desired node degree distribution (scale-free in our case), we apply the method introduced by Bender and Canfield [27]. We assign for each node i a number k_i (taken from a specific degree sequence) of "stubs"—ends of edges emerging from the node. Then we choose pairs of these stubs uniformly at random and join them together to make complete edges. We do not allow loops (i.e., edges starting and ending at the same node) or multiple edges between the same pair of nodes.

In order to generate a power-law degree sequence we apply the procedure described in [28]. The procedure determines the minimal and maximal node degree, which allows us to control the density of the constructed network.

To determine the position of the critical line in the studied RBNs we calculate the Hamming distance H of two system configurations after a large number T_{end} of system updates. The two configurations differ at time $T=0$ in one randomly chosen bit. We set $T_{\mathrm{end}}=200$ and averaged calculations over 10 000 randomly generated networks (each network has a different topology of connections, different initial states, and different functions of nodes). We set p fixed and observe the dependence of $\langle H\rangle$ on $\langle k\rangle$ or on γ in Erdös-Renyi and scale-free networks, respectively. For the chaotic phase $\langle H(T_{\mathrm{end}})\rangle \gg \langle H(T=0)\rangle$, while for the frozen phase $\langle H(T_{\mathrm{end}})\rangle \to 0$. The phase transition occurs when $\langle H(T_{\mathrm{end}})\rangle = \langle H(T=0)\rangle$.

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