Networks between Professionals and Society: A Model for Protein Dependency

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We propose a network model with a fixed number of nodes and links with a dynamics which favors links between nodes differing in connectivity. Parameter regimes where the degree distributions follow power-laws, \( P(k) \sim k^{-\gamma} \), high clustering following \( C(N) \sim 1/N \) and small-world properties, with a network diameter following \( D(N) \sim A + B \log N \), are observed. Our model gives results comparable with real-world protein networks.

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I. INTRODUCTION

Over the last few years a large number of network models have been put forward, highly motivated by empirical studies of real-world networks.

The various models can be categorized belonging to one of three main classes of modeling paradigms. First, different variants of the random graph model of Erdős and Rényi are still used for comparison with many different models and empirical studies. The second group of network models are referred to as small-world models, first presented by Watts and Strogatz and are motivated by high clustering observed in many real-world networks. This group of network models aims to include both the idea of highly clustered networks and random graphs. Third, the construction of various scale-free models have been motivated by the discovering of power-law degree distributions in real-world networks, ranging from the World Wide Web to the network of Science collaboration and the web of human sexual contacts. This group of network models focuses on the dynamics of the network and aims to offer a universal theory of network evolution.

In the past few years, a wide range of concepts and measures for complex networks have been proposed and investigated. However, complex networks are most often described by three basic concepts.

The small-world concept describes the fact that there is a relative short path between any two nodes in most networks. The maximum of the shortest paths between any two nodes, referred to as the diameter, is often observed to grow logarithmically with the network size, \( N \). This property is not related to a particular organizing principle, and are observed in random graphs, small-world model networks and scale-free networks.

The clustering of a network is related to the formation of cliques of nodes being linked to each other. The clustering in most real networks is observed to be larger than the clustering in random graphs. Many proposed models of complex networks grasp this idea.

The third main characteristic for complex networks is the degree distribution. The degree distribution, \( P(k) \), gives the probability for a randomly selected node to be connected to \( k \) different other nodes. For a wide range of complex networks a power-law distribution \( P(k) \sim k^{-\gamma} \) has been observed. This deviates significantly from random graphs where links are placed randomly and from small-world models. In random graph models and in small-world models a large number of nodes have a degree close to the average degree of the network, \( \bar{k} \).

Over the last few years a wide range of protein networks have been studied. These networks are formed by direct physical interaction between pairs of proteins and proteins form the underlying structure for the propagation of various signals regulating the proteins. The motivation for the present study is the recent observation that protein networks guiding the biochemistry of living cells, the placement of links tends to occur between high and low connectivity nodes rather than between nodes of similar connectivity. The fact that one observe that the highly connected proteins are mostly connected to those with low connectivity, meaning that the highly connected nodes are well separated, is believed to increase the robustness of the networks. This observation is somewhat reminiscent of the networks that connect people with respect to their professional specialities. An example might be a network describing medical relations in terms of physician-patients relations. A physician (a highly connected node) has many patients (low connected node), but does not have a physician-patient relation to many other physicians. Patients do not have physician-patient relations with each other. The same argument goes for many networks describing relations based on a certain profession or some sort of specialization.

In the next section, we describe how we construct networks with the property that contrasting nodes are preferably attached through links by using a Monte Carlo technique. We then go on to show the results of our model simulations, focusing on the three main characteristics of complex networks, degree distributions, clustering and small-world properties. Finally we construct randomized versions of our networks and calculate the ratio between the degree distributions from the original
II. DESCRIPTION OF THE MODEL

Rather than attempting to construct a network that preferably connects highly contrasting nodes through reconstructing the process that may naturally have developed them, we take the Monte Carlo approach. Even though this is well-known and well understood technique, it is useful to remind the reader of its philosophy as we proceed. Given a probability distribution \( p(i, j) \) for having a link between nodes \( i \) and \( j \), the Monte Carlo method constructs a biased random walk through the set of different network configuration such that the relative frequency of encountering configurations with such a link present is proportional to \( p(i, j) \). This probability should not set any intrinsic scale for the network. The natural candidate for such a probability should then be a power law in the ratio \( k_i/k_j \). Hence, we propose the simplest form that accentuates the contrast between the connectivity of the two nodes \( i \) and \( j \) without bringing any intrinsic scales into the problem,

\[
p(i, j) = \left( \frac{\max(k_i, k_j)}{\min(k_i, k_j)} \right)^\beta.
\]

This may be rewritten in a more compact form as follows,

\[
p(i, j) = e^{-\beta H(i,j)},
\]

where

\[
H(i, j) = -\ln \left( \frac{k_i}{k_j} \right).
\]

The network we consider consists of \( N \) nodes with \( L \) undirected links between them. We term a given configuration of links between the nodes as \( \mathcal{G} \). The probability to find a given configuration \( \mathcal{G} \) is then

\[
\mathcal{P}(\mathcal{G}) = \prod_{\text{links}} p(i, j) = e^{-\beta H},
\]

where

\[
H = \sum_{\text{links}} -\ln \left( \frac{k_i}{k_j} \right).
\]

We see that formally, the probability for finding a given configuration \( \mathcal{G} \) follows the Boltzmann distribution with a Hamiltonian defined in Eq. 5. The parameter \( \beta \) has the formal appearance of an inverse temperature, but it should not be interpreted as anything more than the single remaining parameter in the probability when scale-freeness is implemented.

We implement the Monte Carlo procedure using the Metropolis algorithm \cite{14,15}, a well-known algorithm also previously used in different network models \cite{16}. In order to construct the random walk, we need the transitional probabilities \( \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') \) which have to obey detailed balance, \( \mathcal{P}(\mathcal{G}) \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') = \mathcal{P}(\mathcal{G}') \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') \). The Metropolis prescription consists in first defining a set of neighborhood configurations. These are in our case simply all configurations that can be reached from \( \mathcal{G} \) moving one link without placing two links between the same pair of nodes. The number of such neighboring states is \( \mathcal{L} = [N(N-1)/2]/(N(N-1)/2-L!)L! \). Next we define the partial transitional probability \( \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') = 1/\mathcal{L} \). If we now have that

\[
\mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') = \mathcal{P}(\mathcal{G}' \rightarrow \mathcal{G}) = \frac{1}{\mathcal{L}},
\]

the Metropolis construction of \( \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') \) from \( \mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') \) ensures that detailed balance is fulfilled. By construction, relation 6 is fulfilled. The transitional probability is now given by

\[
\mathcal{P}(\mathcal{G} \rightarrow \mathcal{G}') = \mathcal{P}(\mathcal{G}' \rightarrow \mathcal{G}) \min \left( 1, \frac{\mathcal{P}(\mathcal{G}')}{\mathcal{P}(\mathcal{G})} \right) = \frac{\min \left( 1, e^{-\beta \Delta H} \right)}{\mathcal{L}},
\]

where

\[
\Delta H = H(\mathcal{G}') - H(\mathcal{G}) .
\]

We emphasize at this point that it is essential that detailed balance to be fulfilled if the Monte Carlo algorithm is to produce configurations \( \mathcal{G} \) with probability proportional with the prescribed \( \mathcal{P}(\mathcal{G}) \) — and that this is fully ensured once Eq. 6 is fulfilled.

III. RESULTS

In figure 1 we show examples of networks with \( N = 50 \) nodes and average connectivity \( k = 4 \) for different values of the parameter \( \beta \) when the networks have reached equilibrium after \( \sim N^2 \) iterations. Our model allows so-called single nodes, i.e., nodes that are not connected to any other nodes. It is also possible to split the network in disjoint components. In figure 2 we show the probability, \( P(k) \), for a node being linked to \( k \) different other nodes for different values of the parameter \( \beta \). For small values of \( \beta \), the network behaves essentially as a random network. However, as \( \beta \) is increased, the importance of the contrast between the connectivity of each pair of nodes is increasingly accentuated. The effect of this is seen clearly in the diagrams for \( \beta \leq 0.8 \), where a power law appears. This is the regime where the model produces networks with the connectivity properties described in the Introduction. Furthermore, these networks are scale free, as power law in \( P(k) \) indicates.
There is a phase transition in the model associated with a $\beta = \beta_c$. In order to investigate this, we study moments of the nodal distribution $P_{N,\beta}(k)$, $\sum_k k^n P_{N,\beta}(k)$ ($n \geq 2$), for different network sizes $N$. As $N$ grows, $\sum_k k^n P_{N,\beta}(k)$ ($n \geq 2$) plotted as a function of $\beta$, converges towards a stepfunction with the step at critical $\beta_c$. By looking at the slope of the step and plot the slope intersection with the $\beta$-axis versus $1/N$ and finally extrapolating $1/N \to 0$, the numerical value of $\beta_c$ may be determined. The result of this analysis is shown in figure 3, and we find $\beta_c = 0.60$.

Figure 2 shows the cluster coefficient for different values of the parameter $\beta$ as a function of the network size, $N$. If we consider a single node $i$ with connectivity $k_i$, which means $k_i$ neighbors, we calculate the cluster coefficient $c_i$ as $c_i = m_i / M_{k_i}$, where $M_{k_i}$ is the highest possible number of links between $k_i$ ’s neighbors, $M_{k_i} = \frac{k_i(k_i - 1)}{2}$, while $m_i$ is the actual number of links between $k_i$’s neighbors. The mean cluster coefficient for a given temperature and a given network size, $C(\beta, N)$ is the average of all these $c_i$’s. For all values of $\beta$, we have a decreasing cluster coefficient as a function of the network size $N$, $C(\beta, N) \sim N^{-\omega}$ with $\omega$ close to 1 for all $\beta$. We observe that the largest clustering is found for intermediate values of $\beta$, close to $\beta_c$.

It is also possible to look at the average cluster coefficient for a node with connectivity $k_i$. These results are shown in figure 4 for different values of $\beta$. For high $\beta$, the model seems to show a power-law dependence for the clustering as a function of the degree, $k$, $c(k_i) \sim k^{-\gamma}$, with $\gamma$ close to 3. This means that nodes with low connectivity are typically better clustered than nodes with high connectivity. For $\beta = 0.0$, we have an exponent $\gamma = 0$ and this seems to be close to the situation for any $\beta$ below the critical value.

In many real-world networks one observes that there is a relative short path between any two nodes in the

FIG. 1: A network with $N = 50$ nodes with $\bar{k} = 4$ for different inverse temperature $\beta$ when the networks have reached equilibrium after $\sim N^2$ iterations.

FIG. 2: The probability $P(k)$ for a node to be linked to $k$ different other nodes for different $\beta$. These nodal distributions are averages for networks with $N = 2000$ nodes with $\bar{k} = 4$.

FIG. 3: Slope intersection with the $\beta$-axis for the stepfunction $\sum_k k^n P_{N,\beta}(k)$ ($n \geq 2$) as function of inverse network size, $1/N$. Extrapolation gives a critical $\beta_c = 0.60$. 

FIG. 4: The cluster coefficient for different values of $\beta$. These results are shown in figure 4 for different values of $\beta$. For high $\beta$, the model seems to show a power-law dependence for the clustering as a function of the degree, $k$, $c(k_i) \sim k^{-\gamma}$, with $\gamma$ close to 3. This means that nodes with low connectivity are typically better clustered than nodes with high connectivity. For $\beta = 0.0$, we have an exponent $\gamma = 0$ and this seems to be close to the situation for any $\beta$ below the critical value.
network. The maximum of the shortest paths between any two nodes in a network is most often referred to as the diameter of the network. In figure 6 we plot the mean diameter $D(N)$ as a function of the network size, $N$, for different $\beta$. $\blacklozenge: \beta = 0.0$, $\blacklozenge: \beta = 0.4$, $\blacklozenbox: \beta = 0.8$ and $\blacklozenbox: \beta = 1.2$.

A good illustration of connectivity correlations is to compare the network to a randomized network where the nodes have the same connectivity as in the original network but with randomized links. If $P(k_0, k_1)$ denotes the probability for a node with connectivity $k_0$ to be linked to a node with connectivity $k_1$ and $P_r(k_0, k_1)$ denotes the same probability in the randomized network, then the ratio $P(k_0, k_1)/P_r(k_0, k_1)$ is an interesting measure for the connectivity correlations which can extract some characteristics of the network. Figure 7 shows this ratio for two values of $\beta$, on either side of the critical $\beta_c$, $\beta = 0.4$ and $\beta = 0.8$. Because our network consists of undirected links, we have a symmetry around $k_0 = k_1$. We see regions in the $k_0 - k_1$-plane where connections between nodes with certain connectivities either are significantly enhanced or suppressed compared to randomized networks. The darker blue area around $k_0 = k_1$, reflects the tendency that it is less likely for two nodes with connectivities not differing much, to be connected. Along the $k_0$- or $k_1$-axis and close to these axis, we see an increased probability that nodes differing significantly in connectivity are connected. The same ratio for real-world protein networks show richer patterns [13], but it is possible to recognize some tendencies comparing it to our results. In areas around $k_0 = k_1$ we observe a reduced probability for two nodes with equal or close to equal connectivity to be connected, and we see an increased probability for nodes differing much in connectivity to be connected, observed close to the $k_0$- and $k_1$-axis [13].

IV. SUMMARY AND CONCLUSION

In this paper we have presented a network model with a static number of nodes and a static number of undirected links. Our model favors links between nodes differing in connectivity. We observe a series of characteristics observed in real-world networks. For small values of $\beta$, the network behaves essentially as a random network. As $\beta$ increases, the importance of the contrast between the connectivity of each pair of nodes increases,
and we observe scale free degree distributions indicated by power laws. We also observe a phase transition at $\beta = \beta_c = 0.60$. Our model gives networks with relative high clustering and a cluster coefficient decreasing with increasing network sizes as $C(N) \sim N^{-1}$. We observe the largest clustering for intermediate values of $\beta$ close to $\beta_c$. The small-world property in our network model is indicated by a diameter growing logarithmically with the network size, $D(N) \sim A + B \log N$. The diameter decreases for increasing values of $\beta$. Finally we constructed randomized versions of our networks in order to compare our results with real-world protein networks. Patterns in the connectivity correlation plot, $P(k_0, k_1)/P_r(k_0, k_1)$, for $\beta$-values on either side of the critical value for $\beta_c$, show similarities with patterns from real-world protein network. Connections between nodes with connectivities differing significantly are enhanced while connections between nodes with equal or almost equal connectivities are suppressed compared to randomized versions of the same networks.

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