Flexible construction of hierarchical scale-free networks with general exponent

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Extensive studies have been done to understand the principles behind architectures of real networks. Recently, evidences for hierarchical organization in many real networks have also been reported. Here, we present a new hierarchical model which reproduces the main experimental properties observed in real networks: scale-free of degree distribution $P(k) \sim k^{-\gamma}$ and power-law scaling of the clustering coefficient $C(k) \sim k^{-1}$. The major novelties of our model can be summarized as follows: (a) The model generates networks with scale-free distribution for the degree of nodes with general exponent $\gamma > 2$, and arbitrarily close to any specified value, being able to reproduce most of the observed hierarchical scale-free topologies. In contrast, previous models can not obtain values of $\gamma > 2.58$. (b) Our model has structural flexibility because (i) it can incorporate various types of basic building blocks (e.g., triangles, tetrahedrons and, in general, fully connected clusters of $n$ nodes) and (ii) it allows a large variety of configurations (i.e., the model can use more than $n - 1$ copies of basic blocks of $n$ nodes). The structural features of our proposed model might lead to a better understanding of architectures of biological and non-biological networks.

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Recently, the importance of hierarchical modularity in the context of biological networks \cite{12,13,14} and some non-biological networks \cite{12,13,14} has been pointed out and a number of theoretical models has been proposed. On the biological side, a major challenge is to understand the relationships among fundamental elements such as genes, proteins and chemical substrates in cells. It is believed that some groups of interlinked elements (i.e., functional modules) can carry out relevant tasks in a functional level \cite{12}. These functional modules can be integrated into larger groups, generating a hierarchical organization \cite{2}. Though experimental work is much more important, construction of adequate theoretical models is also important for better understanding of general principles behind architectures of biological networks.

Theoretical models for explaining real complex networks have evolved during the last years, from the classical random graph model \cite{7} and the small-world model \cite{8} to scale-free network models \cite{9,10,11}. The most important feature of scale-free networks is that the degree distribution $P(k)$ (frequency of the nodes that are connected to $k$ other nodes) decays as a power-law $P(k) \sim k^{-\gamma}$. In the earliest models of scale-free networks \cite{9,10}, probabilistic rules were employed to construct networks incrementally. After that, deterministic scale-free models introduced in \cite{12,13} were a step towards simulation of a modular topology. However, these models lack the power-law scaling of $C(k)$, because their nodes have clustering coefficient $C_i(k_i) = 0$. Recently, the modularity and hierarchical topology \cite{2,12,13} were introduced to explain all the observed properties in complex networks. These observed properties of real networks with $N$ nodes can be summarized as: scale-free of degree distribution $P(k) \sim k^{-\gamma}$, power-law scaling of the clustering coefficient $C(k) \sim k^{-1}$ and an independence of the network size $N$ and high value for the average of the clustering coefficient $C(N)$. The clustering coefficient for each node $i$ is defined as $C_i(k_i) = 2n_i/(k_i(k_i - 1))$, where $n_i$ denotes the number of edges connecting $k_i$ neighbors of node $i$, and $C(N)$ reads as $C(N) = \sum_i C_i(k_i)/N$. Finally, the function $C(k)$ is defined as the average clustering coefficient over nodes with the same degree $k$: $C(k) = \sum_{i:k_i=k} C_i(k_i)/N(k)$, where $N(k)$ is the number of nodes of degree $k$.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{(a) The RSMOB model \cite{2}. Initial cluster with four nodes, which are fully connected. After the first replication the network consists of 16 nodes ($4^2 = 16$). (b) The re-organized structure of (a) to show clearly the similarities and differences between the RSMOB model and our proposed model. (c) Our proposed hierarchical model up to $i = 2$. We note that only one copy (among four copies) exists with one edge connecting to the main hub. The number of such copies is not restricted. When the number grows, $\gamma$ also increases.}
\end{figure}

In \cite{2,3} Ravasz et al. (the RSMOB model in what follows) suggested a hierarchical model to incorporate all the mentioned observed properties in the same framework. The model starts with a fully connected module of four nodes (the number of nodes in the initial module can be different), and four identical copies are created, obtaining a network of $N = 16$ nodes in the first repli-
cation \((4^2 = 16\) nodes). This process can be repeated indefinitely. We illustrate the process in Fig. 1(a). It is mentioned in [2] that the model follows a power-law scaling for \(C(k) \sim k^{-\gamma}\) and holds a scale-free topology \(P(k) \sim k^{-\gamma}\), with \(\gamma = 1 + (\ln 4)/(\ln 3) \approx 2.26\). By modifying the number of nodes in the initial module, the value of \(\gamma\) changes. However, the value is constrained to \(2 < \gamma \leq 1 + (\ln 3)/(\ln 2) \approx 2.58\), which indicates a small range of possible applications.

In this article, we propose a new hierarchical model which integrates the observed properties of real networks in a single framework. The model can generate a scale-free topology with exponent \(\gamma > 2\), and arbitrarily close to any specified value. In addition, our model has structural flexibility because it can incorporate various types of basic building blocks (e.g., triangles, tetrahedrons), which might lead to better understanding of architectures of biological and non-biological networks.

Suppose that we have a network via \(n\) iterations. It is straightforward to see that the degree of the main hub is \(k = 2^i + 4\). Since one edge is appended to the \(j\)-th intermediate hub at the \((j+1)\)-th iteration, the degree \(k_j\) of the \(j\)-th intermediate hub will be \(k_j = (2^j + 4) + 1\), if \(2 \leq j < n\). We can see that the total number \(N_j\) of \(j\)-th intermediate hubs will satisfy \(N_j = 4^{(n-j)}\). From \(k_j = (2^j + 4) + 1\), we can write \(\ln k_j \approx j \ln 2\) and also from \(N_j = 4^{(n-j)}\), we have \(\ln N_j = (n-j) \ln 4 = c_j - j \ln 4\). From these expressions it is straightforward to write: \(\ln N_j = c_1 + \ln k_j^{-(\frac{n-j}{4})} = c_1 + \ln k_j^{-2}\). Hence, the number of hubs with degree \(k\) (i.e., distribution of hubs with degree \(k\)) in the proposed network follows the power-law \(N_j \propto k_j^{-2}\). However, we must notice that in a hierarchical network, the number of nodes with different degree \(k\) is scarce, therefore the probability distribution of node degree is properly defined as \(P(k) = (1/N_{tot})(N(k)/\Delta k)\), where \(N(k)\) is the number of nodes with degree \(k\), \(N_{tot}\) is the total number of nodes, and \(\Delta k\) means that nodes are binned into intervals according to degree \(k\). In addition, we note that for the hierarchical model, \(\Delta k\) changes linearly with \(k\) (i.e., \(\Delta k_{j+1} = k_{j+1} - k_j = 2^j \approx k_j\)). Hence, this linear dependence of \(\Delta k\) makes that the probability distribution follows in the proposed network the power-law \(P(k) \propto k^{-3}\). In general, that binning gives rise to \(\gamma = 1 + \gamma'\), where \(\gamma'\) means the exponent of the power-law distribution of hubs.

In order to explain an example of our model, we look at the structure depicted in Fig. 2(b). We see that there is a set of four triangles (fully connected cluster of three nodes) with upper nodes connected to the main hub. In Fig. 2(a) we notice that the initial cluster could have different structures and could be a fully linked initial cluster of 4, 5 nodes or even larger number of nodes. The initial cluster corresponds to the iteration of \(i = 1\). Fig. 2(b) shows the iteration of \(i = 2\) where four copies (the number of copies is selected according to the required \(\gamma\)) of the initial cluster are created and one node in each initial cluster is linked to the main hub. In addition, we note that only two out of the four triangles have all their vertices connected to the main hub. For brevity, we call a node in a copy corresponding to the main hub in the \(j\)-th iterations an \(j\)-th intermediate hub, and call a node which is not the main hub or an intermediate hub a non-hub node. In Fig. 2(c), we show the network with iteration of \(i = 3\). We make four replicas of the network in Fig. 2(b) and connect the second intermediate hubs in these copies to the main hub. The four non-hub nodes with the highest degree among the non-hub nodes in two copies are also connected to the main hub. In Fig. 2(d), we show the network with iteration of \(i = 4\) which is obtained by making four replicas of Fig. 2(c), following the same process explained above. This process can be iterated indefinitely. The degree distribution of this network is dominated by the intermediate hubs. There is a main hub at the top of the structure and new intermediate hubs appear at each iteration. In Fig. 2(c) we see four nodes as the second intermediate hubs.

FIG. 2: Topology and construction of our proposed model. (a) The model can start with arbitrary number of nodes which are fully connected. (b) Considering the initial cluster of three nodes, the two leftmost triangles have all their nodes connected to the main hub. This configuration is called the \((2+2)\) configuration. The degree of the main hub is calculated as \(k = 2^2 + 4\), where \(i\) is the number of iterations. (c) Four copies of (b) are made, and one node (the new main hub at this iteration) is added. Fig. 2(c) contains four nodes as the second intermediate hubs. Each of these hubs holds \(k\) edges, where \(k_j = (2^j + 4) + 1\) and \(j = 2\). (d) Following the same process, four copies of (c) are created. The process can be iterated indefinitely constructing a network with power-law \(P(k) \propto k^{-2}\). (e) Sketch of our model considering only the main hub with \(k\) links and the nodes in the bottom level (i.e., non-hub nodes) that are connected to the main hub. Since these non-hub nodes are connected by \(k'/2\) edges where \(k' = k - 4\), the clustering coefficient follows \(C(k) \approx 1/k\).
The construction can be generalized in the following way. We denote by \((l + m)\)-configuration one such that, at each (say the \(i\)-th) iteration, \(l + m\) copies of the network at the \((i - 1)\)-th iteration are created. With this configuration, we construct two types of connections between the copies and the main hub at the \(i\)-th iteration: connections between the \((i-1)\)-th intermediate hubs and the main hub, and connections between \(l^j\) non-hub nodes with the highest degree and the main hub.

We notice here that this configuration is flexible and can be modified. There are two important and modifiable factors: (i) the number of copies \((l + m)\) and the number of copies \((l)\) for which some of non-hub nodes are connected to the main hub, (ii) the basic building blocks (e.g., triangle, tetrahedron). The former determines the value \(\gamma\) and the latter affects the structure of network architecture.

Here we describe more about configuration of networks in our model. First we consider a configuration which is able to reproduce the observed value of \(\gamma = 3.25\) in language network, which has a hierarchical organization [4]. This network is generated connecting two words to each other if they appear as synonyms in the Merriam Webster dictionary [4]. We construct the network with the \((2 + 3)\) configuration \((k_j = (2^j + 5) + 1\) and \(N_j = 5^{n-j}\), and we obtain \(N_j \propto k_j^{-\frac{\ln(5^j)}{\ln 2}}\), where after binning we get \(\gamma = 3.3\). This value is in good agreement with the observed \(\gamma = 3.25\), which is not accessible with the RSMOB model. The reason is because the RSMOB model can only handle the case of \(m = 1\). Next we consider the general case. With \((l + m)\) configuration, we obtain \(k_j = \lfloor l + (l + m) \rfloor + 1\), \(N_j = (l + m)^{n-j}\), and \(N_j \propto k_j^{-\frac{\ln(l + m)}{\ln 2}}\), which indicates that by tuning the parameters \(l\) and \(m\) we have a network with exponent \(\gamma\), which is arbitrarily close to any required value above two.

From this construction of the hierarchical network we have several advantages if we compare with the RSMOB model [12]. First, \(\gamma\) can be arbitrarily close to any specified value above two, far from the restraints of the RSMOB model. Secondly, our procedure to generate the structure is more flexible and allows more variety of configurations. In Fig. 1(a) we show two iterations of the RSMOB model with 4 initial nodes, and in Fig. 1(c) we show the model up to \(i = 2\). Fig. 1(b) shows a re-organization of Fig. 1(a) to point out similarities and main differences between the RSMOB model and our proposed model. In the setup of Fig. 1, our model provides a dependence for the hubs as \(N_j \propto k_j^{-\frac{\ln(l + m)}{\ln 2}}\), and after binning we obtain \(\gamma = 1 + (\ln 4)/(\ln 3) \approx 2.26\), which is the same result provided by the RSMOB model. In addition, we are more flexible with our topology by increasing the number of copies. For example, with \((3 + 3)\) configuration, we obtain \(N_j \propto k_j^{-\frac{\ln(3^j)}{\ln 3}}\) and after binning we get the value of \(\gamma = 2 + (\ln 2)/(\ln 3) \approx 2.63\), which is not accessible with the RSMOB model [11].

Evidences for hierarchical organization in many real networks (biological and non-biological networks) have recently been reported. On the biological side, the metabolic network was analysed in [2, 16, 17] and the results showed that the value of exponent is \(\gamma = 2.2\), and the clustering coefficient \(C(k)\) scales as \(k^{-1}\). In [18] protein domain networks were analyzed using data from different domain databases and scale-free behaviors were reported with values of exponents: \(\gamma = 2.5\) (ProDom database), \(\gamma = 1.7\) (Pfam), and \(\gamma = 1.7\) (Prosite). A protein interaction network of \(S.\ ceriseus\) was studied in [19] and it was found that \(\gamma = 2.5\). In [20], the hierarchical signature of this network was revealed showing that \(C(k)\) scales as \(k^{-1}\). From non-biological networks, we can also find some examples which hold a scale-free topology integrated in the hierarchical organization [4]. Here, we only mention the type of network and the corresponding value of \(\gamma\): \(\gamma = 2.3\) for actor network [14], \(\gamma_{\text{out}} = 2.45\) and \(\gamma_{\text{in}} = 2.1\) (denoting the out and in-degree distribution respectively) for World Wide Web [14], \(\gamma = 2.1 \sim 2.2\) [21] for Internet at the AS level (interdomain level), and \(\gamma = 3.25\) for language network [4]. In all these cases the scaling of \(C(k)\) suggests the hierarchical organization [4]. For these examples with \(\gamma > 2\), our model is able to generate the scale-free topology with exponents arbitrarily close to the values shown above.

In Fig. 3 we show the degree distribution of our model with \((2 + 2)\) configuration, up to \(i = 8\). As we explained before, the tail of that distribution (hubs) should follow...
a power-law. Dashed-line indicates one which fits the degree of the hubs of our generated network. The meaning of this line is just distribution of nodes normalized to the total number of nodes. We see that the value of \( \gamma' \) is slightly different from the theoretical value of 2, but the difference comes from the approximation made from \( k_j = (2^j + 4) + 1 \) to \( \ln k_j \approx j \ln 2 \). If we plot the dots after subtracting 5 units in the axis of \( k \) and we fit them, we could find exactly \( \gamma' = 2 \), indicating that the difference between both results was coming from that approximation. However, we are interested in the probability distribution of node degree \( P(k) = (1/N_{tot})(N(k)/\Delta k) \). In Fig. 3 we show the probability distribution (triangles) after binning is applied for the hubs. In addition, we plot the probability distribution of the hubs after subtracting 5 units in the axis of \( k \) (squares). The continuous line is fitted to the squares and it shows a power-law probability distribution with exponent \( \gamma = 3 \).

It is worth noticing that we can also reproduce the distribution without explicit construction of the network. If we compute the values of \( 2^j + 5 \) (degree of hubs) versus the values of \( 4^{(n-j)} \) (the number of copies) for \( j = 1, \ldots, n \) and \( n = 20 \), we can obtain the power-law corresponding to \( \gamma' = 2 \) for the distribution of nodes and \( \gamma = 3 \) for the probability distribution after binning. It indicates that by generating a larger number of iterations in our model we are able to obtain exactly the predicted exponents.

In Fig. 4, we calculate \( C(k) \) for the \((2 + 2)\) and \((2 + 3)\) configurations in our model and we see the power-law scaling of \( C(k) \sim k^{-1} \), which is also a key feature of the hierarchical network. In Fig. 1(e) we show a sketch of our model considering only the main hub with \( k' = k - l - m \) edges to non-hub nodes. It is seen that there are \( k'/2 \) edges among the non-hub nodes. From this, it is straightforward to see that the clustering coefficient for non-hub nodes is: \( C(k) = (k'/2)/(k(k-1))/2 \approx 1/k \), showing the power-law scaling for the degree of clustering in our model. Concerning the average of the clustering coefficient \( C(N) \), its behavior in our model is independent of the network size \( N \) as a consequence of the power-law scaling of \( C(k) \), in agreement with the observed properties in metabolic networks.

It is interesting to note that our model holds a similarity with the model in [2, 4, 11], in particular with the preferential attachment feature. In that model, new nodes are being added in time step \( t \) and the probability that the new node is connected to an already present node \( i \) depends on the degree \( k_i \) of that node \( (k_i/\sum_j k_j) \). As we can see in Fig. 2, in each iteration we are adding a new node (main hub) plus copies of previous structures. The new hub is connected deterministically to the nodes in the non-hubs but only to those ones which have higher degree \( 2^j \). In that sense, a remanence of the preferential attachment concept is held in our model though the degree distribution for the non-hub nodes does not follow the power-law as in the RSMOB model.

In conclusion, we have presented here a new model to reproduce the main features of the hierarchical organization, which is one of the central challenges in the field of network science. Our model holds important properties as structural flexibility and its more general capability to generate values of \( \gamma > 2 \), being able to reproduce most of the observed scale-free topologies, even in networks with exponents above \( \gamma = 2.58 \), where the RSMOB model fails. Therefore, our model might be a useful tool to uncover the hierarchical features in biological and non-biological networks in a broader scope.

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It is worth noticing that although our proposed model is much more flexible than the RSMOB model, our model can not reproduce hierarchical networks with $\gamma < 2$. In our model, in order to control the value of $\gamma$, edges are connected from hubs to non-hub nodes. To reproduce hierarchical networks with $\gamma < 2$, too many edges from hubs to non-hub nodes would be required, which increases the complexity of the model. In addition, the fractalness of the network would be lost in this process.

Though non-hub nodes with the highest degree in $m$ copies are connected to the main hub, we can modify the construction such that required number of non-hub nodes are connected to the main hub. In order to maintain the power-law for $P(k)$ and $C(k)$, it is enough to connect the main hub (at the $i$-th iteration) with appropriate number of pairs of adjacent non-hub nodes. In such a case, exponent will be more flexible. However, fractalness of the network will be lost.