

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, evidence for hierarchical organization in many real networks has also been reported. Here, we present a hierarchical model that reproduces the main experimental properties observed in real networks: scale-free of degree distribution $P(k)$ [frequency of the nodes that are connected to k other nodes decays as a power law $P(k) \sim k^{-\gamma}$] and power-law scaling of the clustering coefficient $C(k) \sim k^{-1}$. The major points 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 cannot 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 nonbiological networks.

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I. INTRODUCTION

Recently, the importance of hierarchical modularity in the context of biological networks [1–3] and some nonbiological networks [4–6] 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 [1]. These functional modules can be integrated into larger groups, generating a hierarchical organization [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 [30] have evolved during recent years, from the classical random graph model [7] and the small-world model [8] to scale-free network models [9–12]. 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 [9–11], probabilistic rules were employed to construct networks incrementally. After that, deterministic scale-free models introduced in [13,14] were a step toward 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 [2–4] 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 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 (*local clustering*) 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 .

In [2,4] Ravasz, Somera, Mongru, Oltvai, and Barabási suggested a hierarchical model (the RSMOB model in what follows) 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 replication ($4^2 = 16$ 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 $C(k) \sim k^{-1}$ and holds a scale-free topology $P(k) \sim k^{-\gamma}$, with $\gamma = 1$

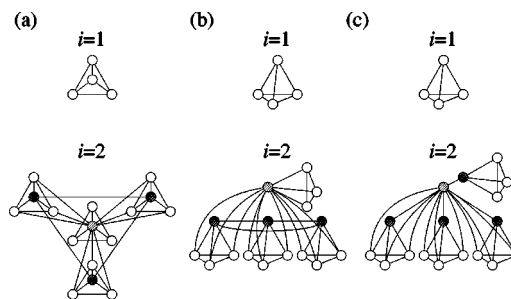


FIG. 1. (a) The RSMOB model [2]. Initial cluster with four nodes, which are fully connected. After the first replication the network consists of 16 nodes ($4^2 = 16$). (b) The reorganized structure of (a) to show clearly the similarities and differences between the RSMOB model and our proposed model. (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, γ also increases.

$+(\ln 4)/(\ln 3) \approx 2.26$. By modifying the number of nodes in the initial module, the value of γ 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. Figure 1(b) shows a reorganization of Fig. 1(a) to point out the main structural differences between the RSMOB model and our proposed model shown in Fig. 1(c).

In this article, we propose a 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.

II. THE MODEL

A. Architecture of the model: Examples

In order to explain some examples 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 clusters 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 four, five, or even larger number of nodes. The initial cluster corresponds to the iteration of $i=1$. Figure 2(b) shows the iteration of $i=2$ where four copies (the number of copies is selected according to the required γ) 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. This configuration is called the (2+2) configuration. In general, we will see that we can generate a network with $(l+m)$ configuration. For brevity, we call a node in a copy corresponding to the main hub in the j th iteration a *j*th intermediate hub, and call a node that is not the main hub or an intermediate hub a *nonhub 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 nonhub nodes with the highest degree among the nonhub 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.

Suppose that we have a network via n iterations. It is straightforward to see that the degree of the main hub is $k = 2^n + 4$. 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

$$k_j = (2^j + 4) + 1, \tag{1}$$

if $2 \leq j < n$. We can also see that the total number N_j of j th intermediate hubs will satisfy

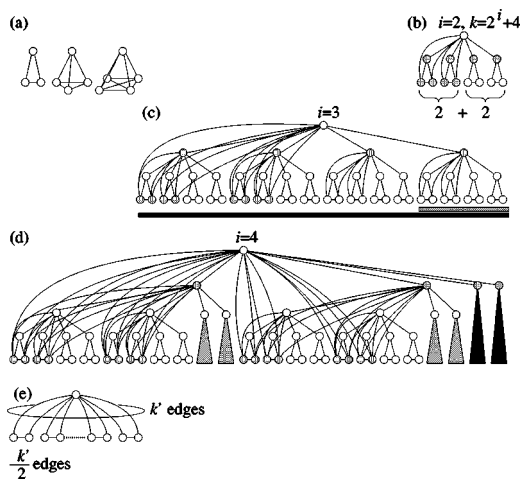


FIG. 2. Topology and construction of our proposed model. (a) The model can start with an arbitrary number of nodes which are fully connected. (b) Considering the initial cluster of three nodes, the two leftmost triangles have all their nodes connected to the main hub. This configuration is called the (2+2) configuration. The degree of the main hub is calculated as $k = 2^i + 4$, 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. (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., nonhub nodes) that are connected to the main hub. Since these nonhub nodes are connected by $k'/2$ edges where $k' = k - 4$, the clustering coefficient follows $C(k) \approx 1/k$.

$$N_j = 4^{(n-j)}. \tag{2}$$

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 $\ln N_j = (n-j) \ln 4 = c_1 - j \ln 4$. From these expressions it is straightforward to write

$$\ln N_j = c_1 + \ln k_j^{-(\ln 4/\ln 2)} = c_1 + \ln k_j^{-2}. \tag{3}$$

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 Δk means that nodes are binned into intervals according to degree k [2]. In addition, we note that for the hierarchical model, Δk 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 Δk makes the probability distribution to follow in the proposed network the power law

$$P(k) \propto k^{-3}. \tag{4}$$

In general, that binning gives rise to $\gamma = 1 + \gamma'$, where γ' means the exponent of the power-law distribution of hubs [2]. Finally, we can describe more about configuration of networks in our model by showing another example. First we

consider a configuration that is able to reproduce the observed value of $\gamma=3.25$ in a language network, which has a hierarchical organization [4]. This network is generated by 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 $N_j \propto k_j^{-(\ln 5/\ln 2)}$, 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 that the RSMOB model can only handle the case of $m=1$.

B. General case

The construction can be generalized in the following way. We denote by the $(l+m)$ 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^i nonhub nodes with the highest degree and the main hub. With the $(l+m)$ configuration, the degree of the main hub is $k=[l^i+(l+m)]$ and since one edge is connected to the j th intermediate hub at the $(j+1)$ th iteration, the degree of the k_j of the j th intermediate hub will be

$$k_j=[l^j+(l+m)+1]. \quad (5)$$

The total number N_j of j th intermediate hubs will read as

$$N_j=(l+m)^{n-j}. \quad (6)$$

From these expressions we can obtain the power-law distribution of hubs

$$N_j \propto k^{-\gamma'}, \quad (7)$$

where

$$\gamma' = \frac{\ln(l+m)}{\ln l}. \quad (8)$$

After binning, we find that the probability distribution in the proposed network follows the power law

$$P(k) \propto k^{-\gamma}, \quad (9)$$

where $\gamma=1+\gamma'$.

Equation (8) indicates that by tuning the parameters l and m we have a network with exponent γ , which is arbitrarily close to any required value above 2.

We remark that although Eqs. (8) and (9) give us the value of the exponent γ of the power-law probability distribution, this value can differ slightly from the value obtained by numerical calculation if the network is not very large. The reason is that to obtain Eq. (8), we approximated $k_j=(l^j+l+m)+1$ as $\ln k_j \approx j \ln l$. This is the reason that in the probability distribution obtained by numerical calculations, we will remove $(l+m+1)$ units from the x axis for the main hub and intermediate hubs in order to verify the mathematical derivation [see Fig. 3(b)]. However, as we will see later, the

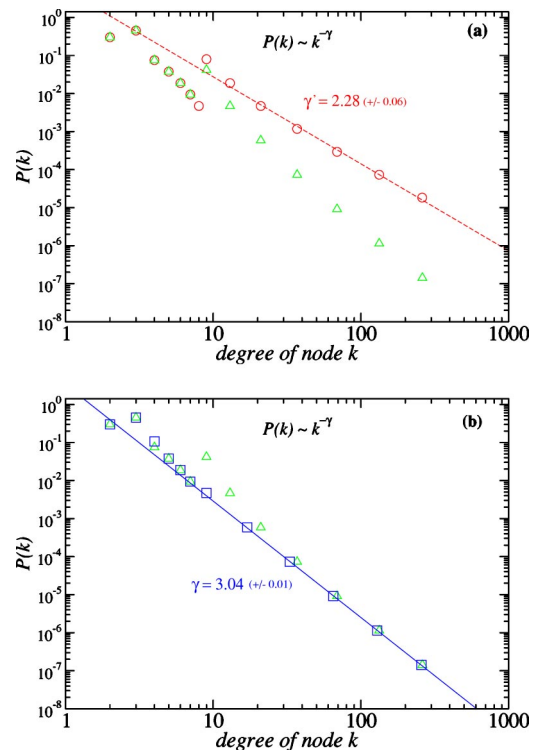


FIG. 3. (a) Circles: Distribution of nodes with degree k , $N(k)$, normalized to the total number of nodes, N_{tot} [i.e., $N(k)/N_{tot}$]. The network is constructed with the configuration (2+2) up to $i=8$ (54 613 nodes) and three nodes as initial cluster (triangles as building blocks). Dashed line: Fit to the circles (only the main and intermediate hubs). It shows a power law with exponent $\gamma'=2.28$. Triangles: Probability distribution $P(k)=(1/N_{tot})[N(k)/\Delta k]$, where Δk means that hubs with degree k are binned into intervals $\Delta k_{j+1}=k_{j+1}-k_j=2^j \approx k^j$ (i.e., $k_j < k \leq k_{j+1}$). We note that for degrees $k=8$ and 9 we used $\Delta k=2^1$. From $1 < k \leq 7$, there are values for each k , and the binning is not required. (b) Triangles: same as (a). Squares: In order to prove that the numerical results provide the same results given by Eq. (4), we subtract five units of the degree of node k [in the general case $(l+m)+1$ units] for each triangle (only the main and intermediate hubs). The difference between triangles and squares comes from the approximation made from $k_j=2^j+5$ to $\ln k_j \approx j \ln 2$. Continuous line: Fit to the squares. It shows a power law with exponent $\gamma \approx 3$.

difference between the numerical values of γ and the predicted ones by using Eqs. (8) and (9) is very small. In addition, as we will show in Fig. 4 with a simple simulation, if the network is very large both results are exactly the same. It is also important to remark that nonhub nodes do not follow a power-law distribution with exponent given by Eq. (8). This tendency of nonhub nodes is also found in the RSMOB model.

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 the nonhub nodes are connected to the main hub, and (ii) the basic building blocks (e.g., triangle, tetrahedron). The former determines the value γ and the latter affects the structure of network architecture.

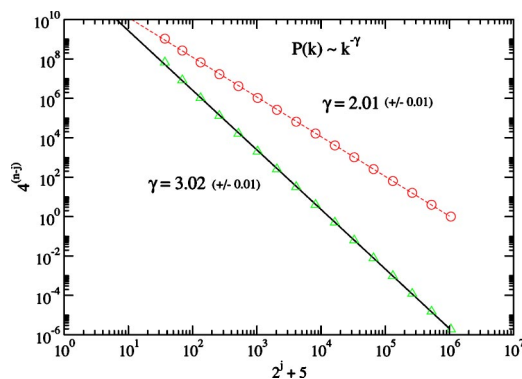


FIG. 4. Values of 2^j+5 (degree of hubs) versus the values of $4^{(n-j)}$ (the number of copies) for $j=1, \dots, n$ and $n=20$.

C. Advantages of the model

From this construction of the hierarchical network we have several advantages if we compare with the RSMOB model [2]. First, γ can be arbitrarily close to any specified value above 2, far from the restraints of the RSMOB model. Second, 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 four initial nodes, and in Fig. 1(c) we show our model up to $i=2$. Figure 1(b) shows a reorganization of Fig. 1(a) to point out the 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 $N_j \propto k_j^{-(\ln 4/\ln 3)}$, 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 $N_j \propto k_j^{-(1+\ln 2/\ln 3)}$ 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 [2,15].

Evidence for hierarchical organization in many real networks (biological and non-biological networks) has recently been reported. On the biological side, the metabolic network was analyzed 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 the yeast *Saccharomyces cerevisiae* 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 nonbiological networks, we can also find some examples that hold a scale-free topology integrated in a hierarchical organization [4]. Here, we only mention the type of network and the corresponding value of γ : $\gamma=2.3$ for the actor network [10], $\gamma_{out}=2.45$ and $\gamma_{in}=2.1$ (denoting the out- and in-degree distribution respectively) for the worldwide web [10], $\gamma=2.1-2.2$ [21] for the internet at the AS level (interdomain level), and $\gamma=3.25$ for a language network [4]. In all these cases the scaling of $C(k)$ suggests a hierarchical organization [4]. For

these examples with $\gamma > 2$, our model is able to generate a scale-free topology with exponents arbitrarily close to the values shown above.

It is interesting to note that our model holds a similarity with the model in [9,10], in particular with the preferential attachment feature. In that model, new nodes are added at 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 nonhubs but only to those that have higher degree [22]. In that sense, a remanence of the preferential attachment concept is held in our model though the degree distribution for the nonhub nodes does not follow a power law as in the RSMOB model.

III. NUMERICAL RESULTS OF DEGREE DISTRIBUTION AND PROBABILITY DISTRIBUTION

A. (2+2) configuration

In Fig. 3(a) 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. The dashed line fits the degree of the hubs of our generated network. The meaning of this line is just the distribution of nodes normalized to the total number of nodes. We see that the value of γ' is slightly different from the theoretical value of 2, but the difference comes from the approximation made from $k_j=(2^j+4)+1=2^j+5$ to $\ln k_j \approx j \ln 2$. If we plot the dots after subtracting five units [in the general case $(l+m)+1$ units] on the axis of the degree of node k and fit them, we can find exactly $\gamma'=2$, indicating that the difference between the two results came from that approximation.

We will illustrate more clearly the above issue with the following numerical simulation. For example, 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 $j=1, \dots, n$ and $n=20$, we can obtain a power law corresponding to $\gamma'=2$ for the distribution of nodes and $\gamma=3$ for the probability distribution after binning (see Fig. 4). This indicates that by generating a large number of iterations in our model we are able to obtain exactly the exponents predicted by Eq. (9).

We have explained that the degree distribution follows a power-law; however, we are interested in the probability distribution of node degree $P(k)=(1/N_{tot})[N(k)/\Delta k]$. In Fig. 3(b) we show the probability distribution (triangles) after binning is applied for the hubs. In addition, in order to obtain the same value predicted by Eq. (9), we plot the probability distribution of the hubs after subtracting five units on the axis of k (squares). The continuous line is fitted to the squares and it shows a power-law probability distribution with exponent $\gamma=3$.

B. Other configurations

In order to verify Eqs. (8) and (9) by using more numerical data, we plot the degree and probability distributions ob-

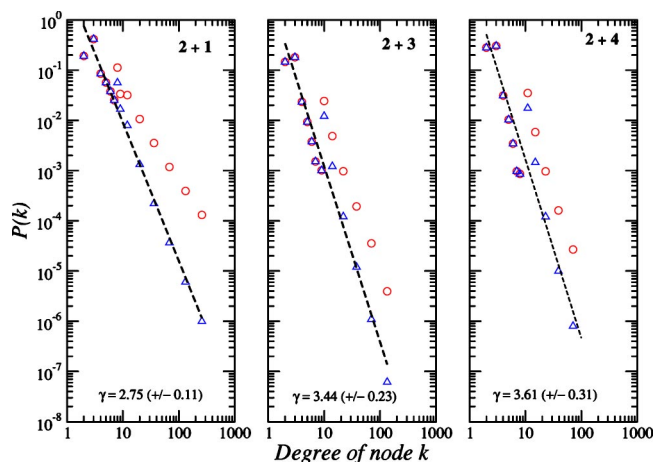


FIG. 5. Circles: Distribution of nodes with degree k , $N(k)$, normalized to the total number of nodes, N_{tot} [i.e., $N(k)/N_{tot}$]. The network is constructed with different configurations. These configurations are indicated at the top right of each figure: (2+1) (7654 nodes) and (2+3) (253 906 nodes) up to $i=8$ iterations and (2+4) (149 299 nodes) up to $i=7$ iterations. Networks were generated by using three nodes as the initial cluster (triangles as building blocks). Triangles: Probability distribution $P(k)=(1/N_{tot})[N(k)/\Delta k]$, where Δk means that hubs with degree k are binned into intervals $\Delta k_{j+1}=k_{j+1}-k_j=2^j=k^l$ (i.e., $k_j < k \leq k_{j+1}$). The dashed line is fitted to the triangles and it shows power-law probability distributions. The exponents of the distributions are shown at the bottom of each figure. For comparison, the predicted exponents given by Eq. (9) after binning (i.e., $\gamma=1+\gamma'$) are (2+1) $\gamma=2.58$, (2+3) $\gamma=3.32$, and (2+4) $\gamma=3.58$.

tained with our proposed model for some different configurations. In Fig. 5, we show the results of $P(k)$ by using (2+1) and (2+3) up to $i=8$ iterations and (2+4) up to $i=7$ iterations. We plot the degree distribution with circles. Probability distributions (triangles) are obtained after binning the degree distributions. Exponents of the power laws are indicated at the bottom of each figure. These values are in the vicinity of those obtained by Eq. (9).

C. γ vs l and m

In Fig. 6, we plot the general expression $\gamma=1+\ln(l+m)/\ln l$. This expression gives the value of the exponent γ in terms of the parameters l and m . For each value l , we have evaluated γ up to $m=8$. In Fig. 6, we can see that the range of values of γ can be arbitrarily close to any specified value above 2, by tuning l and m . In addition, we can see in Fig. 6 that for $l=2$, the predicted values of γ for $m=1$ ($\gamma=2.58$), $m=3$ ($\gamma=3.32$), and $m=4$ ($\gamma=3.58$) are in agreement with those ones obtained by numerical computation of the model shown in Fig. 5 for $m=1,3,4$.

IV. HIERARCHY AND STRUCTURAL ORGANIZATION OF THE MODEL

Some topological quantities are usually studied in order to provide signatures of hierarchy and structural organization of

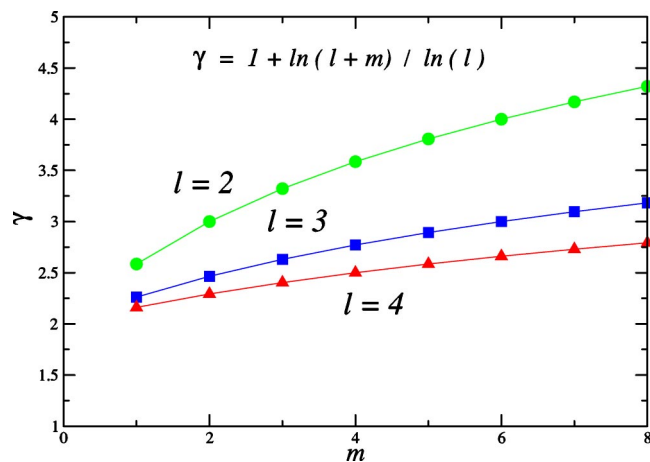


FIG. 6. General expression of γ in terms of the parameters of our proposed model l and m .

networks. In particular, we have analyzed the clustering dependence and the assortativity of our model.

A. Clustering dependence

A key signature of a hierarchical network is provided by analyzing the clustering of the network. The local clustering 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 . The average of C_i over the vertices of degree k gives the *degree-dependent local clustering* $C(k)$, and it reads as

$$C(k) = \left(\sum_{i:k_i=k} C_i(k_i) \right) / N(k), \quad (10)$$

where $N(k)$ is the number of nodes of degree k . This quantity indicates the probability that two nearest neighbors of a node of degree k are linked to each other. A scaling law of $C(k)$ as k^{-1} is a fingerprint of hierarchical organization in networks.

In our model, we can also obtain a general expression of the clustering coefficient $C(k)$. In Fig. 1(e), we show a sketch of our model with the $(l+m)$ configuration considering only the main hub with k' ($k'=k-l-m$) edges to nonhub nodes. It is seen that there are $k'/2$ edges among the nonhub nodes. From this, it is straightforward to see that the clustering coefficient for nonhub nodes is

$$C(k) = (k'/2) / \{[k(k-1)]/2\} \approx 1/k, \quad (11)$$

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 $C(k)$ [23], in agreement with the observed properties in metabolic networks [2].

In Fig. 7, we calculate $C(k)$ for the (2+1), (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.

It is worth noticing that, although this is a deterministic model, the power law for $C(k)$ shows a noisy signal for a low degree of nodes in Fig. 7. The reason is because the nonhub

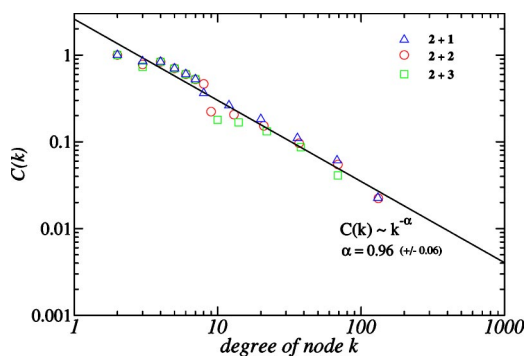


FIG. 7. The clustering coefficient $C(k)$ evaluated with the configurations (2+1), up to $i=8$ iterations (7654 nodes) (triangles), (2+2), up to $i=7$ iterations (13 653 nodes) (circles), and (2+3), up to $i=6$ iterations (10 156 nodes) (squares). In all these cases, the building blocks are triangles.

nodes (small degrees) do not follow a power law, and the power-law distribution is generated by only the hub nodes. This is not an exclusive feature of our model because the deterministic RSMOB model also shows this behavior.

B. Assortativity k_{nn}

Another interesting quantity used to uncover the structural organization and to characterize a network is the average degree of nearest neighbors $k_{nn}(k)$ for nodes of degree k . This quantity is related to the degree correlations between nodes [24–27], and it can be written as

$$k_{nn}(k) = \sum_{k'} k' P(k'|k), \quad (12)$$

where $P(k'|k)$ is the conditional probability that a given node with degree k is connected to a node of degree k' . When some correlations are present, the behavior of $k_{nn}(k)$ characterizes a network. For example, when $k_{nn}(k)$ grows with k , it means that nodes of high degree are likely to have nearest neighbors of high degree. This property is called *assortative mixing* [28]. In contrast, a decreasing behavior of $k_{nn}(k)$ means that nodes of high degree are likely to have nearest neighbors of low degree. This property is called *disassortative mixing*. If correlations are not present, $k_{nn}(k) = \text{const}$.

We have evaluated $k_{nn}(k)$ for the proposed model with configurations (2+1), (2+2), and (2+3) and the values are as shown in Fig. 8.

These results show an assortative behavior for small degree, and an uncorrelated behaviour for large degree of nodes. The assortative tendency found for small degree corresponds to the nonhub nodes, and the uncorrelated tendency is related to the hub nodes. Interestingly, a similar plot for k_{nn} was shown in [24], where the hierarchy and structural organization of the world-wide airport network was analyzed. There, it is shown that high-degree nodes (airports with many nonstop connections, or international airports) tend to have an uncorrelated structure, and low-degree nodes (airports with few nonstop connections or domestic airports)

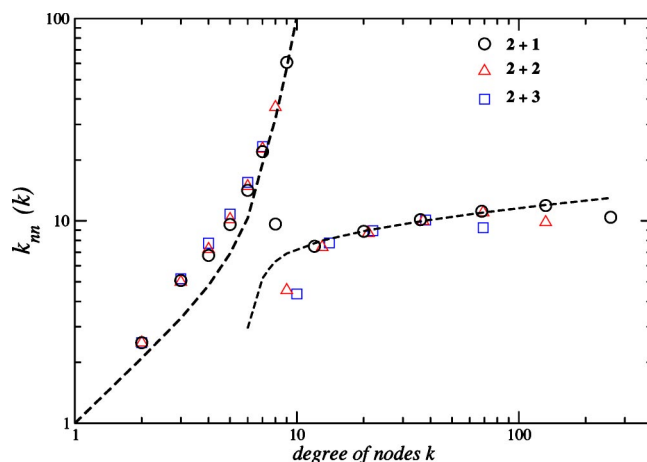


FIG. 8. Numerical results of $k_{nn}(k)$ calculated by using the proposed model with configurations (2+1) up to $i=8$ iterations (circles), (2+2) up to $i=7$ iterations (triangles), and (2+3) up to $i=6$ iterations (squares). Dashed lines: Results of Eq. (14) (high degree of nodes) and Eq. (15) (low degree of nodes). For each configuration, the symbol with highest degree k indicates the contribution from the main hub. We also note that the degree of the main hub does not follow the approximate equation because this top node does not have a parent. A small deviation from the analytical line around degree $k=8$ is found only for the (2+1) configuration. In this case, some nonhub nodes and some hubnodes have the same degree.

tend to be connected with nonhub nodes.

Furthermore, we have derived the approximate mathematical expression of k_{nn} for our proposed model. The derivation of k_{nn} in our proposed model is as follows.

(1) *For hub nodes j* (j means the j th intermediate hub), the degree reads as $k_j = l^j + (l+m) + 1$. Therefore, by using Eq. (12) we can write

$$k_{nn}(k_j) \approx \frac{[(j+1)l^j + (l^{j-1})(m+l) + l^{j+1}]}{l^j + (l+m) + 1}. \quad (13)$$

The first contribution of the numerator comes from the conditional probability of nonhub nodes. The number of nonhub nodes connected to the j th intermediate hub node is l^j , and we multiply it by the degree of nonhub nodes, which is around $j+1$. The second term comes from $(j-1)$ th intermediate hubs, and the third term comes from the $(j+1)$ th hub. The denominator is the degree of the j th intermediate hub. In addition, for a large number of intermediate hubs j , the previous equation can be read as

$$k_{nn}(k_j) \approx (j+1) + \frac{(l+m)}{l} + l. \quad (14)$$

(2) *For nonhub nodes with degree k* , we can write

$$k_{nn}(k) \approx \frac{k + l + l^2 + l^3 + \dots + l^{(k-1)}}{k} \approx \frac{l(l^{(k-1)} - 1)}{k(l-1)}. \quad (15)$$

The first term j comes from the degree of the nonhub nodes shown at the bottom of Fig. 2(d) (dark color), which are also connected to the main hub. The series in terms of l comes from the connectivity of these nonhub nodes to the j th intermediate hubs (for each j).

From Eqs. (14) and (15), we can see that nonhub nodes and hub nodes have different behavior. These equations are plotted in Fig. 8 (dashed lines) for the case $l=m=2$ (i.e., $2+2$). It is worth noticing that the degree of the main hub does not follow the approximate equation because this top node does not have a parent. For example, it is straightforward to see that the circle (configuration $2+1$) with highest degree corresponds to the main hub with degree given by $k=2^i+(2+1)$. As the number of iteration is $i=8$, the degree of the main hub is $k=259$. We see that a circle with that high degree is seen in Fig. 8 and slightly below the analytical line. Finally, we remark that, although the equations proposed for nonhub nodes [Eq. (15)] and hub nodes [Eqs. (13) and (14)] are an approximate estimation, the analytical expressions capture quite well the behavior of the results obtained by numerical calculation of the model shown in Fig. 8.

V. CONCLUSIONS

In summary, we have presented here a 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 such 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 [2]. Therefore, our model might be a useful tool to uncover the hierarchical features in biological and nonbiological networks in a broader scope. As future work, it would be interesting to analyze the community structure or modularity in the proposed network by using the quantitative measures provided by a recent work of Newman and Girvan [29].

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- [1] L. H. Hartwell, J. J. Hopfield, S. Leibler, and A. W. Murray, *Nature (London)* **402**, C47 (1999).
 - [2] E. Ravasz, A. L. Somera, D. A. Mongru, Z. N. Oltvai, and A.-L. Barabási, *Science* **297**, 1551 (2002).
 - [3] A.-L. Barabási and Z. N. Oltvai, *Nat. Rev. Genet.* **5**, 101 (2004).
 - [4] E. Ravasz and A.-L. Barabási, *Phys. Rev. E* **67**, 026112 (2003).
 - [5] M. Girvan and M. E. J. Newman, *Proc. Natl. Acad. Sci. U.S.A.* **99**, 7821 (2002).
 - [6] A. Vazquez, R. Pastor-Satorras, and A. Vespignani, *Phys. Rev. E* **65**, 066130 (2002).
 - [7] P. Erdős and P. A. Rényi, *Publ. Math. Inst. Hung. Acad. Sci.* **5**, 17 (1960).
 - [8] D. J. Watts and S. H. Strogatz, *Nature (London)* **393**, 440 (1998).
 - [9] A.-L. Barabási and R. Albert, *Science* **286**, 509 (1999).
 - [10] A.-L. Barabási, R. Albert, and H. Jeong, *Physica A* **272**, 173 (1999).
 - [11] R. Albert and A.-L. Barabási, *Rev. Mod. Phys.* **74**, 47 (2002).
 - [12] L. A. N. Amaral, A. Scala, M. Barthelemy, and H. E. Stanley, *Proc. Natl. Acad. Sci. U.S.A.* **97**, 11149 (2000).
 - [13] A.-L. Barabási, E. Ravasz, and T. Vicsek, *Physica A* **299**, 559 (2001).
 - [14] S. Jung, S. Kim, and B. Kahng, *Phys. Rev. E* **65**, 056101 (2002).
 - [15] It is worth noticing that although our proposed model is much more flexible than the RSMOB model, our model cannot reproduce hierarchical networks with $\gamma < 2$. In our model, in order to control the value of γ , edges are connected from hubs to nonhub nodes. To reproduce hierarchical networks with $\gamma < 2$, too many edges from hubs to nonhub nodes would be required, which increases the complexity of the model. In addition, the fractalness of the network would be lost in this process.
 - [16] H. Jeong, B. Tombor, R. Albert, Z. N. Oltvai, and A.-L. Barabási, *Nature (London)* **407**, 651 (2000).
 - [17] A. Wagner and D. A. Fell, *Proc. R. Soc. London, Ser. B* **268**, 1803 (2001).
 - [18] S. Wuchty, *Mol. Biol. Evol.* **18**, 1694 (2001).
 - [19] A. Wagner, *Mol. Biol. Evol.* **18**, 1283 (2001).
 - [20] A.-L. Barabási, Z. Deszo, E. Ravasz, S. H. Yook, and Z. Oltvai, in *Sitges Proceedings on Complex Networks (2005)*, Lecture Notes in Physics (Springer-Verlag, Berlin, in press).
 - [21] M. Faloutsos, P. Faloutsos, and C. Faloutsos, *Comput. Commun. Rev.* **29**, 251 (1999).
 - [22] Though nonhub nodes with the highest degree in m copies are connected to the main hub, we can modify the construction such that the required number of nonhub nodes is 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 an appropriate number of pairs of adjacent nonhub nodes. In such a case, the exponent will be more flexible. However, the fractalness of the network will be lost.
 - [23] J. C. Nacher, N. Ueda, T. Yamada, M. Kanehisa, and T. Akutsu, *BMC Bioinf.* **5**, 207 (2004).
 - [24] A. Barrat, M. Barthelemy, R. Pastor-Satorras, and A. Vespignani, *Proc. Natl. Acad. Sci. U.S.A.* **101**, 3747 (2004).
 - [25] R. Pastor-Satorras, A. Vazquez, and A. Vespignani, *Phys. Rev. Lett.* **87**, 258701 (2001).
 - [26] S. Maslov and K. Sneppen, *Science* **296**, 910 (2001).
 - [27] M. Catanzaro, G. Caldarelli, and L. Pietronero, *Phys. Rev. E* **70**, 037101 (2004).
 - [28] M. E. J. Newman, *Phys. Rev. Lett.* **89**, 208701 (2002).
 - [29] M. E. J. Newman and M. Girvan, *Phys. Rev. E* **69**, 026113 (2004).
 - [30] J. F. Mendes, S. N. Dorogovtsev, and A. F. Ioffe, *Evolution of Networks: From Biological Nets to the Internet and WWW* (Oxford Press, New York, 2003).