

Evolving complex networks with conserved clique distributions

Gregor Kaczor and Claudius Gros

Institute for Theoretical Physics, Johann Wolfgang Goethe University, Frankfurt am Main, Germany

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We propose and study a hierarchical algorithm to generate graphs having a predetermined distribution of cliques, the fully connected subgraphs. The construction mechanism may be either random or incorporate preferential attachment. We evaluate the statistical properties of the graphs generated, such as the degree distribution and network diameters, and compare them to some real-world graphs.

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I. INTRODUCTION

The structural and statistical properties of networks have been studied intensively over the past decade [1,2], due to their ubiquitous importance in technology, different realms of life, and complex system theory in general [3]. With time it was realized that the topological properties of real-world networks often transcend the universality class of both the straightforward, all-random Erdős-Rényi graph [4], as well as that of random networks with arbitrary degree distributions [5].

Many real-world networks have a well defined community structure [6]. A community is, loosely speaking, a subgraph that has an intrasubgraph link density that is substantially above the average link density of the whole network. The community with link density equal to 1 is denoted in graph theory as a “clique.” A clique is a fully interconnected subgraph, the smallest clique having just two vertices.

A clique is also a specific realization of a graph motif, i.e., of subgraphs with definite topologies [7,8], and of k -cores, viz., subgraphs with at least k interconnections [9]. In a related work, Derenyi *et al.* introduced the notion of clique percolation in the context of overlapping graph communities [10]. For scale-free graphs, having a degree distribution $p_k \sim k^{-\gamma}$, the second moment $\langle k^2 \rangle$ diverges for the important case $2 < \gamma < 3$ and finite numbers of cliques of arbitrary size emerge [11].

For any graph, one can define a characteristic clique distribution $P_C(S)$, viz., the probability for a clique of size S to occur. A loopless graph exclusively has cliques of size 2 with $P_C(S) = \delta_{S,2}$ and the number of three-site cliques is related to the standard clustering coefficient [1,2]. The clustering coefficient C is a normalized measure for the occurrence of three-site loops, with every three-site loop being part of at least one clique of size $S \geq 3$.

It is therefore of interest to investigate the clique distribution of real-world graphs and to consider the problem of constructing graphs with specific clique distributions.

II. ALGORITHM

We consider a given set of cliques C_1, \dots, C_M containing $S_i = S(C_i)$ sites each, an instantiation of a certain clique distribution $P_C(S)$. We presume the clique set to be monotonically ordered,

$$S_i \geq S_{i+1}, \quad i = 1, \dots, M-1, \quad (1)$$

as illustrated in Fig. 1. We study the task to generate recursively a dense and connected graph out of the M cliques $\{C_i\}$ in such a way that the final graph has exactly the same distribution $P_C(S)$ of fully connected subgraphs, viz., of cliques. In Fig. 1, we illustrate the simplest procedure for solving this task, by concatenating the cliques C_1, C_2, \dots via a single common vertex between two consecutive cliques.

Let us digress briefly and consider what would have happened if we had used sites 4 and 7, together with a new site 9 to attach the $S_3=3$ clique in the third step for the case illustrated in Fig. 1. In this case, sites 4 and 7 would be connected and a spurious three-site clique, namely (4,5,7), would have been generated. A thoughtless attachment of cliques in general, therefore, generates spurious additional cliques, resulting in an uncontrolled clique distribution for the final graph.

A. Hierarchical algorithm

In general, one can join two cliques of sizes S_1 and S_2 via common vertices. The minimal number of common vertices is one, the maximal is

$$\min(S_1, S_2) - 1. \quad (2)$$

Using more common sites, namely more than $\min(S_1, S_2)$, would result in the destruction of the smaller clique. We can then formulate a class of hierarchical algorithms conserving

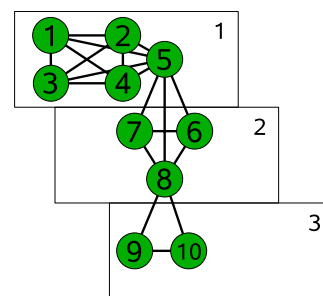


FIG. 1. (Color online) Illustration of a clique-conserving algorithm generating a connected graph out of a given set of cliques. Starting with a five-site clique (1,2,3,4,5) in step one, a four-site clique (5,6,7,8) and a three-site clique (8,9,10) are added in steps two and three via a single common vertex.

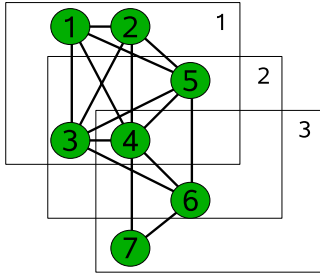


FIG. 2. (Color online) Illustration of the dense hierarchical algorithm for generating dense graphs out of a given set of cliques. Starting with the largest clique (1,2,3,4,5), here of size $S_1=5$, in step 1, cliques of size S_i ($i=2,3,\dots$) are added consecutively step by step by adding one additional vertex at each step and using $S_i - 1$ vertices from a previously added clique. The second clique is here (3,4,5,6) and the third clique (4,6,7). Both random and preferential attachment may be used.

a given, arbitrary but ordered, via Eq. (1), initial clique distribution:

(i) At step $m=1, \dots, M$ one adds the clique C_m with $S_m = S(C_m)$ sites. One starts by selecting a number $\tilde{S}_m \in [1, S_m - 1]$. Here we will mostly concentrate on the case $\tilde{S}_m = S_m - 1$.

(ii) Next one selects recursively \tilde{S}_m mutually interconnected vertices out of the graph segment constructed in the previous $m-1$ steps. The new clique is then added by mutually connecting $S_m - \tilde{S}_m$ new sites among themselves and with the \tilde{S}_m selected sites of the existing graph segment.

We call the choice $\tilde{S}_m = S_m - 1$ the “dense hierarchical algorithm;” it is illustrated in Fig. 2. Here we will study exclusively the dense algorithm, which results in quite dense networks. The opposite limit, namely the case $\tilde{S}_m = 1$ in step (i) of the hierarchical algorithm, is illustrated in Fig. 1.

Starting with M cliques, the dense hierarchical algorithm generates a network containing N sites in its final state, with

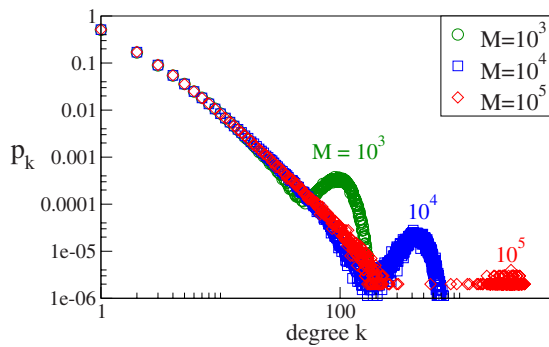


FIG. 3. (Color online) The degree distributions p_k for graphs with scale-free clique distribution, compare Eq. (5), and an exponent $\alpha=2.6$. Blue squares are for a system of $M \approx 10^5$ cliques, green stars and red diamonds show systems for 10^4 and 10^3 cliques, respectively. The data are obtained by averaging over 1000/263/19 realizations for $P_C(S)$ for clique numbers M equal to $10^3/10^4/10^5$.

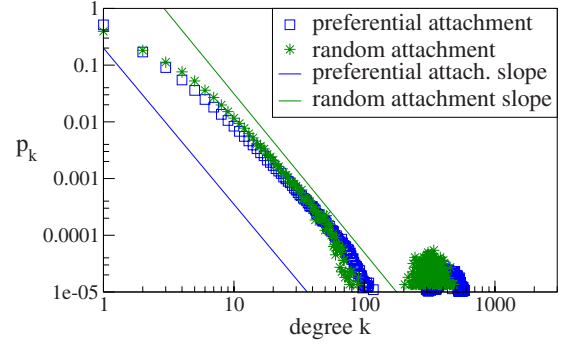


FIG. 4. (Color online) The degree distribution p_k for graphs having a scale-free clique distribution with $\alpha=2.6$ and $M \approx 10^4$ cliques. Shown are results both for random and preferential attachment with lines indicating the respective slopes -2.7 (random) and -2.5 (preferential).

$$N = S_1 + (M - 1), \tag{3}$$

with S_1 being the size of the starting clique, which is also the largest. This is so because exactly one new vertex is added at each of the $(M-1)$ steps.

B. Random versus preferential attachment

The selection of the \tilde{S}_m vertices in step (ii) can be done either randomly, by preferential attachment, or by other rules. When considering preferential attachment, we first select a single vertex i with an attachment probability $\Pi(k_i)$ proportional to the vertex-degree k_i ,

$$\Pi(k_i) = \frac{k_i}{\sum_j(k_j)} \tag{4}$$

(linear preferential attachment). We then select recursively $\tilde{S}_m - 1$ vertices out of the neighbors of i via preferential attachment. The set of possible vertices is given, at every step of this recursive selection process, by the set of vertices linked to all sites previously selected. Note that the ordering (1) of the initial clique distribution is a precondition for the hierarchical algorithm to function.

C. Decimation algorithm

For further reference we briefly mention a second clique-conserving algorithm for network construction via vertex decimation. Starting with an initial network of M unconnected cliques C_1, \dots, C_M , one selects pairs of unconnected vertices either randomly or via preferential attachment. One then attempts a decimation by merging the two selected vertices into a single vertex. One then calculates the clique distribution of the new network, which has one less site. If the new clique distribution is identical to the original distribution, the decimation is accepted, or else it is rejected.

III. SIMULATION RESULTS

We have studied the properties of the hierarchical clique-conserving graph-generation algorithm extensively using nu-

TABLE I. Statistical properties of graphs (compare Fig. 3) containing $M \approx 10^3, 10^4, 10^5$ cliques generated by the hierarchical algorithm with preferential attachment, using a scale-free clique distribution (5), with an exponent $\alpha=2.6$. C is the clustering coefficient, ℓ the average path length, $\langle \kappa \rangle$ the average degree, D the network diameter, d the link density, and N the total number of vertices. m is the slope of the degree distribution p_k measured for $k \in [10, 40]$ for $M \approx 10^3$ and $k \in [10, 100]$ for $M \approx 10^4, 10^5$.

M	C	ℓ	D	$\langle \kappa \rangle$	d	N	m
986	0.34	3.2	7.5	5.1	0.00508	1007	-2.6
9979	0.36	3.3	8.8	5.7	0.00056	10032	-2.7
99999	0.37	3.4	9.8	5.8	0.000058	100096	-2.4

merical results, evaluating their respective statistical properties and comparing them to some selected real-world graph.

A. Initial clique distribution

The hierarchical graph generation algorithm conserves per construction the initial clique distribution $P_C(S)$. We have studied two cases. In Sec. IV, we will discuss the results obtained by using the measured clique distribution of real-world networks for $P_C(S)$. Here we will concentrate on some model clique distributions, in particular of scale-free form,

$$P_C(S) \sim \left(\frac{1}{S}\right)^\alpha, \quad \alpha > 2. \tag{5}$$

We performed simulations for various exponents α and scale-free clique-distributions containing a total number M of cliques. For the simulations, a cutoff S_1 needs to be chosen for the scale-free distribution (5), i.e., the maximal clique-size S_1 . The expected number $N_{S_1}(S)$ of cliques is then

$$N_{S_1}(S) = \left(\frac{1}{S}\right)^\alpha \frac{M}{\sum_{S'=1}^{S_1} (1/S')^\alpha}, \tag{6}$$

where M is the total number of cliques. We selected S_1 by the condition

$$N_{S_1}(S_1) > 1, \quad N_{S_1}(S_1 + 1) < 1, \tag{7}$$

viz., there is at least one clique of size S_1 present on average. We compared results obtained for M ranging typical from 10^3 to 10^5 in order to extract scaling properties in the large-network limit. In order to extract reliable statistical properties, the results were averaged over N_{real} different random realizations.

TABLE II. Statistical properties of graphs (compare Fig. 5) containing $M \approx 10^5$ cliques generated by the hierarchical algorithm with preferential attachment. α denotes the scaling exponent for the clique distribution $P_C(S)$, C the clustering coefficient, ℓ the average path length, $\langle \kappa \rangle$ the average degree, D is the network diameter, d is the link density, and N the total number of vertices. m is the slope of the degree distribution p_k measured for $k \in [10, 100]$.

α	C	ℓ	D	$\langle \kappa \rangle$	d	N	m
2.1	0.51	3.2	9.2	9.9	0.000098	100099	-2.1
2.6	0.36	3.4	9.8	5.8	0.000058	100096	-2.4
3.2	0.23	3.7	11.3	3.8	0.000038	100042	-3.1
4.2	0.10	4.1	13.4	2.8	0.000027	100020	-3.2

When selecting the value S_1 for the maximal clique size, one discards all cliques with sizes $S > S_1$. This is admissible when the percentage of discarded cliques is small. With the criteria (7), the percentage of discarded cliques vanishes in the thermodynamic limit $M \rightarrow \infty$. For the system of order $10^4, 10^5$, the percentage of discarded is well below 1%.

B. System-size analysis

In Fig. 3, we present the degree distribution p_k for graphs with a scale-free clique distribution (5) and an exponent $\alpha = 2.6$, generated through the hierarchical algorithm with preferential attachment. The degree distribution results from averaging $N_{\text{real}} = 1000, 263, 10$ realizations for clique distributions containing $M \approx 10^3, 10^4, 10^5$ cliques. We note that the degree distribution approaches a well defined curve for the thermodynamic limit $M \rightarrow \infty$.

The degree distributions shown in Fig. 3 have bumps at high degrees for finite numbers of cliques M . This is due to the fact that the algorithm starts by incorporating the large cliques first so that vertices with an high initial degree see it further increased via the preferential attachment during the construction process. This effect vanishes in the thermodynamic limit as the probability of a given vertex to be chosen as a part of a new clique decreases with system size.

The statistical analysis of the networks presented in Fig. 3 is given in Table I; the number of cliques M and the number of vertices N obey the relation (3) valid for the dense hierarchical algorithm. The resulting degree distribution approaches within the numerical errors a scale-free functional dependence with an exponent $|m|$ approximately given by the exponent $\alpha=2.6$ of the conserved clique distribution $P_C(S)$.

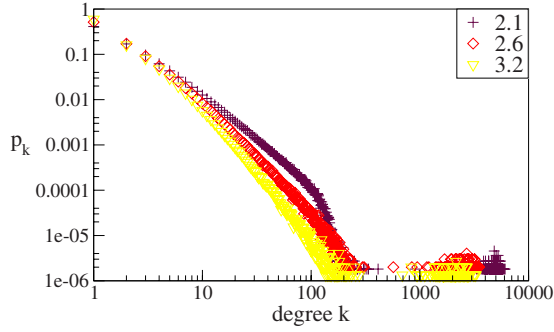


FIG. 5. (Color online) The degree distribution for three scale-free clique distributions with exponents $\alpha_1=2.1$ (maroon plus, 11 simulation runs), $\alpha_2=2.6$ (red diamonds, 26 simulation runs), and $\alpha_3=3.2$ (yellow triangles, 15 simulation runs), for $M \approx 10^5$ cliques.

In Fig. 4, we compare the degree distribution between construction rules with preferential and random attachment, respectively. The difference is quite small in the region of small to intermediate degrees k , where the finite-size corrections are minor. This is because of the algorithmic restriction that only common neighbors of the already processed vertices can be used to construct a clique iteratively. This restriction decreases the number of vertices available for the preferential attachment and results in a similar degree distribution, which is, however, slightly different from the ideal scale-free line.

C. Dependency on the scaling exponent

We have studied the properties of the graphs generated by the hierarchical algorithm for scale-free clique distributions $P_C(S)$ and several scaling exponents α . We have analyzed the corresponding graphs as a function of clique numbers $M \approx 10^3, 10^4, 10^5$, averaging over several clique-distribution realizations. The resulting degree distributions are shown in Fig. 5 for the case $M \approx 10^5$, the corresponding statistical analysis in Table II. In order to estimate the finite-size corrections, we present in Table III the corresponding results for

$M \approx 10^4$. We note, in particular, a good agreement in the estimates for the scaling exponent $|m|$ of the resulting degree distribution.

Interestingly enough, the exponent $|m|$ for the degree distribution of the graph generated by the hierarchical algorithm with preferential attachment saturates at ≈ 3.1 , close to the value 3 expected for the standard preferential attachment algorithm [1]. When $\alpha < 3$, the large tail of the degree distribution stemming directly from the clique distribution dominates the resulting exponent $|m|$ for the degree distribution, but fails to do so for $\alpha > 3$, when the preferential attachment mechanism dominates the generation of the fat tail.

Next, we comment on the size of the network diameter D of the generated graphs. With increasing α , we observe an increasing average path length ℓ and an increasing average diameter D while the clustering coefficient C decreases. The network diameter is intuitively affected by the number of low-degree vertices. A larger number of low-degree vertices for degree distributions of identical functional dependences generally results in a bigger network diameter. Alternatively, one may consider the number of trivial cliques, namely those with size $S=2$, viz., edges not forming part of any larger clique. They tend to connect to low-degree vertices, since two connected high-degree vertices would have a higher probability to belong to cliques of size 3 or larger.

In order to examine the influence of these trivial cliques on the network diameter, we have eliminated, from the graph generated by the hierarchical algorithm with $M \approx 10^4$ and $\alpha=2.1, 2.6, 3.2, 4.2$, all cliques of size $S=2$. The statistical properties of the resulting graph are given in Table III. The network diameter ℓ decreases substantially and the clustering C increases. We note that the scaling exponent m for the degree distribution remains unaffected, as it depends on the vertices with large degrees only. This result is nevertheless somewhat surprising, in view of the dramatic reduction in the number of vertices N resulting from the decimation of all trivial cliques.

IV. COMPARISON WITH REAL-WORLD DATA

We evaluated the clique distributions $P_C(S)$ for two real-world networks, a protein-protein interaction network [13]

TABLE III. Top four rows: Statistical properties of graphs with $M \approx 10^4$ cliques and various scaling exponents α for the clique distribution $P_C(S)$. C is the clustering coefficient, ℓ the average path length, $\langle \kappa \rangle$ the average degree, D the network diameter, d the link density, N the total number of vertices, and m the slope measured between degree 10 and 60. The degree distributions result from averaging $N_{\text{real}} = 86, 263, 866, 306$ realizations for clique distributions having $\alpha=2.1, 2.6, 3.2, 4.2$. Bottom four rows: The same data as for the top four rows, but with all cliques of degree $S=2$ removed from the graphs.

α	C	ℓ	D	$\langle \kappa \rangle$	d	N	m
2.1	0.51	3.1	7.5	10.5	0.00104	10093	-2.0
2.6	0.36	3.4	8.8	5.6	0.00056	10032	-2.5
3.2	0.23	3.7	10.0	3.8	0.00038	10017	-2.9
4.2	0.10	4.1	11.8	2.7	0.00027	10007	-3.1
2.1	0.94	2.73	4.1	16.7	0.0028	5885	-2.0
2.6	0.92	2.77	4.5	10.0	0.0021	4625	-2.5
3.2	0.90	2.77	4.9	7.2	0.00206	3491	-3.0
4.2	0.97	2.74	5.0	5.5	0.0024	2207	-3.0

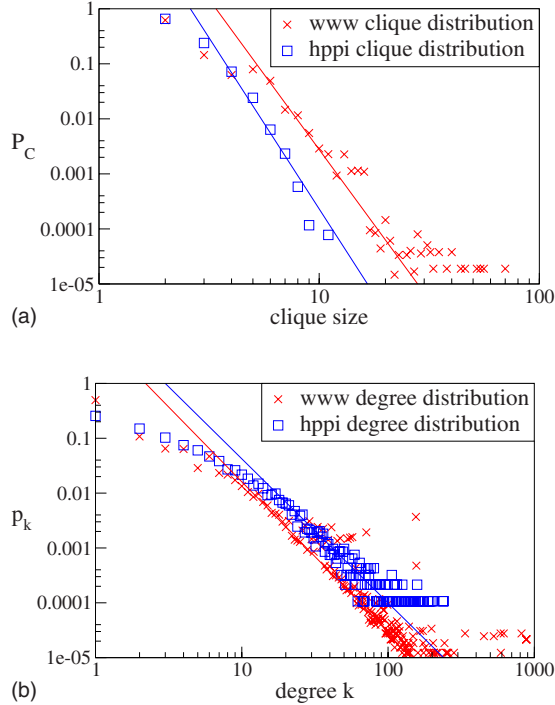


FIG. 6. (Color online) Top figure: Clique distribution $P_C(S)$ of the WWW data set [12] and Human Protein Protein Interaction Database (HPPI)[13]. The distributions have the exponents $\alpha_{\text{www}} = -5.5$, $\alpha_{\text{hppi}} = -6.2$. The statistical properties are given in Table IV. Bottom figure: Degree distribution p_k of the same data shown in the top figure. Continuous lines show the respective slope of $m_{\text{www}} = -2.8$, $m_{\text{hppi}} = -2.5$. The statistical properties are given in Table IV.

and a WWW graph [12]. We then used the resulting clique distributions $P_C(S)$ as the starting point for the hierarchical algorithm with preferential attachment and compared the generated graphs with the properties of the original real-world networks [13].

Figure 6 shows the clique and the degree distributions of the respective original graphs, with their corresponding statistical properties given in Table IV. We note that the protein-interaction graph contains cliques of up to ten sites, where a typical clique size is slightly larger in the WWW net. The scaling of the degree distribution p_k is clearly observable for the WWW net, but only indicative for the protein-interaction networks, due to the limited number of vertices it contains.

In Table IV, we have also included the properties of the graphs generated by the hierarchical algorithm using prefer-

ential attachment. The main difference between the generated networks analyzed in Table IV and those previously discussed is the fact that they are not averaged over an ensemble of realizations of a clique distribution. The reason is that the exact experimental clique distributions for the protein-interaction network and for the WWW network have been taken as an input for the hierarchical algorithm, which is per construction conserved with respect to the clique distribution.

Next we note two caveats with respect to the protein interaction graph. First, it is not complete, being updated continuously as new experimental results become available [13]. Secondly, the protein-interaction network contains unconnected subsets of vertices. The largest component does not encompass the entire graph but 8972 sites out of a total of 9362 vertices. We have used this largest component for the data analysis.

While analyzing the data presented in Table IV, we note substantial differences between the properties of the real-world graphs with respect to the one generated by the hierarchical clique-conserving algorithm. These differences involve essentially all key statistical quantities, such as the total number of vertices, the average degree, the network diameter, and the large- k falloff of degree distribution.

This leaves us with two possible conclusions, the first being that the clique distribution $P_C(S)$ is probably not a good quantity for the purpose of characterizing a given graph, at least in the two examples considered here. The second is the possibility that an altogether different clique-conserving algorithm may be needed for the clique distribution to be used as a characterizing quantity.

The data presented in Table IV were generated using the hierarchical algorithm with preferential attachment, however, as discussed above (see Fig. 4), the difference between random and preferential attachment is actually quite small for clique distributions having a fat tail.

V. DISCUSSION

In this paper, we presented an algorithm, the hierarchical algorithm, by which one can generate graphs having a predetermined distribution of cliques, viz., of fully connected subgraphs. We have studied, in a first step, the degree distribution of the resulting networks for scale-free clique distribution as a function of the scaling exponent.

In a second step, we used two selected real-world graphs, a protein-interaction network and a WWW network, and ex-

TABLE IV. Statistical properties of a HPPI and of a WWW graph. C is the clustering coefficient, ℓ the average path length, $\langle \kappa \rangle$ the average degree, D the diameter, d the link density, N the total number of vertices, and m the slope measured for $k \in [10, 44]$ for the real data ($k \in [10, 20]$ for the generated graph and $k \in [10, 100]$ for generated WWW data).

Data	Source	C	ℓ	D	$\langle \kappa \rangle$	d	N	m
HPPI	real	0.11	4.3	14	7.8	0.00085	8972	-2.5
	gener.	0.20	3.8	11	3.0	0.00016	25747	-3.5
WWW	real	0.23	7.2	46	3.0	0.000009	325729	-2.8
	gener.	0.27	3.751	12	4.1	0.0000086	475588	-3.6

amined the relation between their degree and clique distributions relative to those of graphs generated via the hierarchical algorithm having the same respective clique distribution. We find no good agreement, and this leads us to the conclu-

sion that either the clique distribution is insufficient for an in-depth characterization of real-world networks, or that the hierarchical algorithms need further development.

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