Emergence of large cliques in random scale-free networks

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In a network cliques are fully connected subgraphs that reveal which are the tight communities present in it. Cliques of size $c > 3$ are present in random Erdős and Rényi (ER) random graphs in which every couple of nodes have the same probability $p$ to be linked. In fact while scale-free graphs have a power-law degree distribution $P(k) \sim k^{-\gamma}$ and a diverging second moment $\langle k^2 \rangle$ when $\gamma < 3$, ER graphs have a Poisson degree distribution and consequently finite fluctuations of the node degrees. The degree distribution strongly affects the statistical properties of processes defined on the graph. For example, percolation and epidemic spreading which have very different phenomenology when defined on a ER graph or on a scale-free graphs 4 10.

The occurrence of a skewed degree distribution has also striking consequences regarding the frequency of particular subgraphs present in the network. For example, ER graphs with finite average connectivity have a finite number of finite loops 4 5. On the contrary scale-free graphs have a number of finite loops which increases with the number $N$ of vertices, provided that $\gamma \leq 3$ 5 8. The abundance of some subgraphs of small size – the so-called motifs – in biological networks has been shown to be related to important functional properties selected by evolution 10 11 12. Among subgraphs, cliques play an important role. A clique of size $c$ is a complete subgraph of $c$ nodes, i.e. a subset of $c$ nodes each of which is linked to any other. The maximal size $c_{\text{max}}$ of a clique in a graph is called the clique number. Finding the clique number of a generic network is an NP-complete problem 13, even though it is relatively easy to find upper ($c_{\text{+}}$) and lower ($c_{\text{-}}$) bounds 14. The clique number also provides a lower bound for the chromatic number of a graph, i.e. the minimum number of colors needed to color the graph 15. Finally, cliques and overlapping succession of cliques have been recently used to characterize the community structure of networks 16 17.

In ER graphs it is very easy to show that cliques of size $3 < c \ll N$ appear in the graph only when the average degree diverges as $\langle k \rangle \sim N^{1/\gamma}$ with $N$ 4. On the other hand, real scale-free networks, such as the Internet at the autonomous system level, contain cliques of size much larger than $c = 3$. For example, Fig. 1 reports upper and lower bounds $c_{\text{+}}, c_{\text{-}}$ 14 for the size of the maximal clique of the Internet and protein interaction networks of c.elegans and yeast 18. This shows that scale-free networks can have large cliques and that the clique number of the Internet graphs increase with the network size $N$.

Is the presence of such large cliques a peculiar property of how these networks are wired or is this a typical property of networks with such a broad distribution of degrees? This letter addresses this question and shows that scale free random networks do indeed contain cliques of size much larger than $c = 3$. We shall do this by computing the first two moments of the number $N_c$ of cliques of size $c$ in a network of $N$ nodes. These provide upper and lower bounds for the probability $P(N_c > 0)$ of finding cliques of size $c$ in a network through the inequalities 4

$$\frac{\langle N_c \rangle^2}{\langle N_c^2 \rangle} \leq P(N_c > 0) \leq \langle N_c \rangle.$$ (1)

Here and in the following the notation $\langle \ldots \rangle$ will be used for statistical averages. Eq. 1 in turn provide upper and lower bounds for the clique number $c \leq c_{\text{max}} \leq \tau$. Indeed if $\langle N_c \rangle \rightarrow 0$ for $c > \tau$ as $N \rightarrow \infty$, we can conclude that no clique of size larger than $\tau$ can be found. Likewise if for $c = \underline{c}$ the ratio $\langle N_c \rangle^2 / \langle N_c^2 \rangle$ stays finite, then cliques of size $c \leq \underline{c}$ can be found in the network with at least a finite probability. The results indicate that the finding in Fig. 1 are expected, given the scale free nature of these graphs. Our predictions are summarized in Table I. We find that the ER result $c_{\text{max}} = 3$ extends to random scale free networks with $\gamma > 3$ whereas for $\gamma < 3$ the clique number $c_{\text{max}}$ diverges with the network size $N$ in a way which is extremely sensitive of the degree distribution of mostly connected nodes, i.e. to the precise definition of the cutoff.

The results of Table I are expected, given the scale free nature of these graphs. Our predictions are summarized in Table I. We find that the ER result $c_{\text{max}} = 3$ extends to random scale free networks with $\gamma > 3$ whereas for $\gamma < 3$ the clique number $c_{\text{max}}$ diverges with the network size $N$ in a way which is extremely sensitive of the degree distribution of mostly connected nodes, i.e. to the precise definition of the cutoff.

The results of Table I are derived for the hidden variable ensemble proposed in Ref. 15 20, where the link probability $p$ between two nodes is replaced by a function $r(q_i, q_j)$ which depends on the fitness $q_i$ and $q_j$ of...
FIG. 1: The lower bound $c_-$ (filled symbols) and the upper bound $c_+$ (empty symbols) of the clique number of the Internet graphs (circles) and the protein interaction networks of e.coli and yeast (triangles) are shown as a function of the network size $N$. The lines (null hypothesis on Internet data) and the triangles pointing down (null hypothesis on protein interaction networks) indicate the upper bound (dashed line and empty symbols) and the lower bound (solid line and filled symbols) computed from Eq. (9) for random graphs constructed with the same properties of the considered real graphs.

The average degree $\langle k \rangle = \langle q \rangle$ is equal to the average fitness, and it diverges as $N \to \infty$ for $\gamma < 2$. Likewise, the degree $k_i$ of node $i$ follows a Poisson distribution with average $q_i$. Notice that a cutoff is needed in $\rho(q)$ to keep the linking probability $r(q, q')$ smaller than one. In particular, we will take require

$$Q = (1 - \epsilon) \sqrt{(q)/N}$$

so that $r(Q, Q) = 1 - \epsilon$. For $\gamma > 3$, values of $q_i \approx Q$ will never occur, as the maximal $q_i \approx N^{1/(\gamma - 1)} \ll Q$. We shall see that this is immaterial for the clique number, however. Instead, for $\gamma < 2$, $\langle q \rangle$ diverges with the cutoff, and hence $Q \sim N^{1/\gamma}$.

Average number of cliques. A clique of size $c$ is a set of $c$ distinct nodes $C = \{i_1, \ldots, i_c\}$, each one connected with all the others. For each choice of the nodes, the probability that they are connected in a clique is

$$\prod_{i \neq j \in C} r(q_i, q_j) = \prod_{i \in C} \left( \frac{q_i}{\langle q \rangle N} \right)^{c-1}$$

The precise definitions of $\bar{c}$ and $\bar{c}$ together with the expression for the constants $b, b'$ are given in the text.

The end nodes $i$ and $j$. Apart from its close relation with the ER ensemble, this choice is also convenient because it allows for a simple generalization of the results to networks with a correlated degree distribution. Quite similar results can be derived for the Molloy-Reed ensemble with the same approach (provided a cutoff is chosen appropriately to avoid double links among mostly connected nodes). Other ensembles, such as that of Ref. 22, instead implicitly introduce a degree correlations for highly connected nodes and therefore require a different approach. Given the extreme sensitivity of the clique number on details of the cutoff of the degree distribution, we also expect quite different results.

Hidden variable network ensemble As in Ref. 19, we generate a realization of a scale-free networks by the following procedure: i) assign to each node $i$ of the graph a hidden continuous variable $q_i$ distributed according a $\rho(q)$ distribution. Then ii) each pair of nodes with hidden variables $q_i, q_j$ are linked with probability $r(q_i, q_j)$. For random scale-free networks with uncorrelated degree distribution, we take $\rho(q) = \rho_0 q^{-\gamma}$ for $q \in [m, Q]$ and

$$r(q, q') = \frac{qq'}{\langle q \rangle N}.$$  

(2)

Table I: Scaling of the theoretically estimated upper and lower bound of the clique number of random scale-free networks with different exponents $\gamma$ of the degree distribution.

| $\gamma$ | $\epsilon = 0$ | $\epsilon \neq 0$ |
|---|---|---|
| $\gamma > 3$ | $c_{\max} = 3$ & $c_{\max} = \epsilon$ |
| $2 < \gamma < 3$ | $c \lesssim c_{\max} \leq \epsilon$ & $c \lesssim c_{\max} \leq \epsilon$ |
| $1 < \gamma \leq 2$ | $c \lesssim \sqrt{\beta} N^{1/\beta}$ & $c \lesssim \sqrt{\beta} N^{1/\beta}$ |

where $\Delta q \approx \sum_{\{n(q)\}} n(q)$ satisfying $\sum_{n(q)} n(q) = c$. Introducing such constraint by a delta function, we can perform the resulting integral by saddle point method, i.e.

$$\langle N_c \rangle = \int_{-\pi}^{\pi} \frac{\omega}{2\pi} e^{Nf(\omega)} \propto \frac{e^{Nf(y^*)}}{\sqrt{2\pi N f''(y^*)}}$$

where $f(y) = y^\gamma + \langle \log [1 + Q^c \epsilon - y] \rangle$, and we have taken the limit $\Delta q \to 0$. In Eq. 6, $y^*$ is fixed by the
saddle point condition
\[
\frac{c}{N} = \left\langle \frac{Q^{c-1}e^{-y^*}}{1 + Q^{c-1}e^{-y^*}} \right\rangle. \tag{7}
\]

We present here an asymptotic estimate of \(\langle N_c \rangle\). Slightly more refined arguments, which do not add much to the understanding given here, can be used to derive an upper bound \(2\). In the limit \(N \to \infty\), the left hand side of Eq. (7) is small hence to a good approximation \(c \approx N(Q^{c-1})e^{-y^*} \). Inserting this in Eq. (8) we find
\[
\langle N_c \rangle \approx \left( \frac{Ne(Q^{c-1})}{c} \right)^c \sqrt{\frac{2\pi c}{c}}. \tag{8}
\]

Therefore, in order to have \(\langle N_c \rangle \to 0\) it is sufficient to take \(c > \bar{c}\), where \(\bar{c}\) is the solution of
\[
Ne(Q^{c-1}) = c. \tag{9}
\]

We consider now separately the case of scale-free networks with different exponents \(\gamma\) of the degree distribution.

- **Networks with \(\gamma > 3\)**
  Eq. (4) has no solution for \(c > \gamma\). Indeed \(N(Q^{c-1}) \sim N^{(3-\gamma)/2} \to 0\) in this range. For \(c < \gamma\), the integral in \(\langle Q^{c-1} \rangle\) is no longer dominated by the upper cutoff, and it is hence finite. Therefore \(N(Q^{c-1}) \sim N^{(3-\gamma)/2}\) which implies that \(\bar{c} = 3\). It is easy to see that this conclusion holds also if we take the natural cutoff \(Q = aN^{-1}\).

- **Network with \(2 < \gamma < 3\)**
  Using Eq. (3), Eq. (9) becomes
  \[
  \frac{\bar{c}(\bar{c} - \gamma)}{(1 - \epsilon)e^{\gamma}} \approx bN^{(3-\gamma)/2} \tag{10}
  \]
  for \(b = (\gamma - 1)m(\gamma - 1)e(1-\gamma)/2\). The solution depends crucially on whether \(\epsilon = 0\) or not. In the former case \(\bar{c} \approx N^{(3-\gamma)/4}\) increases as a power law of the system size, whereas for \(\epsilon > 0\) it increases only as \(\log N/\log(1 - \epsilon)\), as detailed in Table 1.

- **Network with \(1 < \gamma < 2\)**
  Taking into account the divergence of \(\langle q \rangle\) and \(Q \sim N^{1/\gamma}\), Eq. (9) becomes
  \[
  \frac{\bar{c}(\bar{c} - \gamma)}{(1 - \epsilon)e^{\gamma}} \approx b'N^{1/\gamma} \tag{11}
  \]
  with \(b' = ((\gamma - 1)m(2 - \gamma))(\gamma - 1))^{1/\gamma}\). Again, for \(\epsilon = 0\) and \(\epsilon > 0\) we find different results, \(\bar{c} \sim N^{1/(2\gamma)}\) and \(\bar{c} \sim \log N/\log(1 - \epsilon)\) respectively (see Table 1).

\begin{center}
\textbf{Second moment of the average number of cliques.}
\end{center}

When computing the average number of some particular subgraphs in a random network ensemble the result might be dominated by extremely rare graphs with an anomalously large number of such subgraphs. In this case, the average number of a subgraph does not provide a reliable indication of its value. In order to have more insight on the characteristics of typical networks we use the classical relation Eq. (11) of probability theory \(4\) which provides a lower bound for the probability that a typical graph contains at least one clique of size \(c\). This requires us to compute the second moment \(\langle N_c^2 \rangle\) of the number of cliques of size \(c\) in the random graph ensemble. In order to do this calculation we are going to count the average number of pairs of cliques of size \(c\) present in the graph with an overlap of \(o = 0, \ldots, c\) nodes. We use the notation \(\{n(q)\}\) to indicate the number of the nodes with fitness \(q\) belonging to the first clique, \(\{n_o(q)\}\) to indicate the number of nodes belonging to the overlap and \(\{n'(q)\}\) to indicate the number of nodes belonging to the second clique but not to the overlap. We consider only sequences \(\{n(q)\}, \{n'(q)\}, \{n_o(q)\}\) which satisfy \(\sum_q n(q) = c, \sum_q n_o(q) = o\) and \(\sum_q n'(q) = c - o\). With these conditions, following the same steps as for \(\langle N_c \rangle\) we get
\[
\langle N_c^2 \rangle = \sum_{o=0}^{c} \int dy \int dy' \int dy'' \int dy''' e^{N(f(y,y',y'',y'))} \tag{12}
\]

where
\[
\int (y,y',y'',Q) = \left[ \frac{1}{N}[yc + y'(c-o) + y'''o] + \log\left[ 1 + e^{-(y''-y)}Q^{(c-1)} + e^{-(y+y'')}Q^{2c-o-1} \right] \right]. \tag{13}
\]

The evaluation of this integral by saddle point is straightforward. The key idea is that, in order to have \(\langle N_c^2 \rangle\) of the same order as \(\langle N_c \rangle^2\) one needs to require that the sum is dominated by configurations with non-overlapping cliques \((o \sim 0)\). Using the estimate of \(\langle N_c \rangle\) derived above and the definition of \(\bar{c}\), for \(\gamma < 3\) we arrive at
\[
P(N_c > 0) \geq \frac{\langle N_c^2 \rangle}{\langle N_c^2 \rangle} \geq \left[ 1 + \frac{4(c-o)(1-c)(c-o)e}{\bar{c}(\bar{c}-\gamma)} \right]^{-c}. \tag{14}
\]

The lower bound for the clique number will depend on \(\epsilon\) and \(\bar{c}\).

In the case \(\epsilon = 0\) let define the clique size \(\xi\) satisfying
\[
\frac{\bar{c}(\bar{c} - \gamma)e}{\epsilon(\bar{c} - \gamma)} = \frac{1}{\xi}. \tag{15}
\]

i.e. \(\xi \sim \bar{c}^{2/3}\). From Eq. (14) and the definition of \(\xi\) it follows that as \(N, \bar{c} \to \infty\) the probability to have at least a clique of size \(c = \xi\) is finite, i.e.
\[
P(N_\xi > 0) \geq \frac{1}{\epsilon}. \tag{16}
\]
Instead in the case $\epsilon > 0$ for any $\alpha > 0$ the r.h.s. of Eq. 14 is very close to 1 for and clique sizes $\zeta = (1 - \alpha)\bar{c}$ and $\bar{c} \ll 1/(\alpha \epsilon)$, i.e.

$$P(N_\zeta > 0) \to 1.$$  \hspace{1cm} (17)

This implies that for $\epsilon > 0$ the lower bound is very close to the upper bound $\zeta = (1 - \alpha)\bar{c}$ for very large networks.

**Conclusions** In conclusion we have calculated upper and lower bounds for the maximal clique size $c_{\text{max}}$ in uncorrelated scale-free network, showing that $c_{\text{max}}$ diverges with the network size $N$ as long as $\gamma < 3$. In particular large cliques are present in scale-free networks with $\gamma \in (2, 3)$ and finite average degree. It is suggestive to put the emergence of large cliques for $\gamma < 3$ in relation with the persistence up to zero temperature of long range order in spin models defined on these graphs 24. These results were derived within the hidden variable ensemble 10,20, but the same method can be extended to other ensembles 21,22 including those with a correlated degree.

In Fig. 11 we compare the upper and lower bounds derived here for random scale-free graphs with the estimated clique number of real networks. These networks have many nodes with degree larger than that of the structural cutoff. Networks with such highly connected nodes cannot be considered as uncorrelated. The best approximation, within the class of uncorrelated networks discussed here, is provided by those with maximal cutoff ($\epsilon = 0$). The bounds of Fig. 11 have been derived from Eq. 9 and 15, assuming a random network with an exponent $\gamma$ as measured from real data ii) the same number of nodes and links (i.e. the same average degree) and iii) a structural cutoff given by Eq. 3 with $\epsilon = 0$. Also notice that $\epsilon = 0$ yields the least stringent bounds.

Fig. 11 shows that generally the largest clique size $c_{\text{max}}$ of real networks falls well within our bounds. Of course, accounting for the presence of correlations in the degree of highly connected nodes in these networks may provide more precise estimates. We saw that our estimates are very sensitive to the tails of the degree distribution and we expect it to depend also strongly on the nature of degree correlations. Preliminary results, extending the present calculation to correlated networks 22 where $r(q, q') = 1 - e^{-\alpha q q'}$ with the natural cutoff $Q \approx N^{1/(\gamma - 1)}$, indicates that the clique number can take values a factor two bigger than in real data 23. These preliminary results underline the importance of extending this approach to correlated networks.

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[\text{References}]

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