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Detection of topological patterns in complex networks: correlation profile of the internet

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Abstract

A general scheme for detecting and analyzing topological patterns in large complex networks is presented. In this scheme the network in question is compared with its properly randomized version that preserves some of its low-level topological properties. Statistically significant deviation of any topological property of a network from this null model likely reflects its design principles and/or evolutionary history. We illustrate this basic scheme using the example of the correlation profile of the Internet quantifying correlations between degrees of its neighboring nodes. This profile distinguishes the Internet from previously studied molecular networks with a similar scale-free degree distribution. We finally demonstrate that the clustering in a network is very sensitive to both the degree distribution and its correlation profile and compare the clustering in the Internet to the appropriate null model.

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Networks have emerged as a unifying theme in complex systems research. It is in fact no coincidence that networks and complexity are so heavily intertwined. Any future definition of a complex system should reflect the fact that such systems consist of many mutually interacting components. These components are not identical as say electrons

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in condensed matter physics. Instead each of them has a unique identity separating it from others. The very basic question one may ask about a complex system is which other components a given component interacts with? Systemwide this information can be visualized as a graph whose nodes correspond to individual components and edges to their mutual interactions. Such a network can be thought of as a backbone of the complex system along which propagate various signals and perturbations.

Living organisms provide us with a quintessential paradigm for a complex system. Therefore, it should not be surprising that in biology networks appear on many different levels: from genetic regulation and signal transduction in individual cells, to neural system of animals, and finally to food webs in ecosystems. However, complex networks are not limited to living systems: in fact they lie at the foundation of an increasing number of artificial systems. The most prominent example of this is the Internet and the World Wide Web being correspondingly the “hardware” and the “software” of the network of communications between computers.

An interesting common feature of many complex networks is an extremely broad, often scale-free, distribution of degrees (defined as the number of immediate neighbors) of their nodes [1]. While the majority of nodes in such networks are each connected to just a handful of neighbors, there exist a few hub nodes that have a disproportionately large number of interaction partners. The distribution of degrees is an example of a low-level topological property of a network. The degree of a node counts how many neighbors it has, but, being a single node property, it contains no information about the identity of those neighbors. It is clear that most of non-trivial properties of networks lie in the coordinated way in which their nodes are connected to each other. However, such multi-node patterns are rather difficult to identify and quantify. By just looking at many large complex networks one gets the impression that they are wired in a rather haphazard way. One may wonder which topological properties of a given network are indeed random, and which arose due to evolution and/or fundamental design principles and limitations? Such non-random features can then be used to identify the network and better understand the underlying complex system.

In this work we propose a universal recipe for how such information can be extracted. To this end we first construct a properly randomized null model of a given network. As was pointed out in Ref. [2], broad distributions of degrees observed in most complex networks indicate that in such networks the degree is an important individual characteristic of a node and as such it should be preserved in any meaningful randomization process. In addition to degrees one may choose to preserve some other low-level topological properties of the network. Any higher level topological property, such as e.g. the pattern of correlations between degrees of neighboring nodes, the number of loops of a certain type, the number and sizes of components, the diameter of the network, spectral properties of its adjacency matrix, can then be measured in the real complex network and separately in an ensemble of its randomized counterparts. Dealing with the whole ensemble allows one to put error bars on any quantity measured in the randomized network. One then concentrates only on those topological properties of the complex network that significantly deviate from the null model, and, therefore, are likely to reflect its basic design principles and/or evolutionary history.

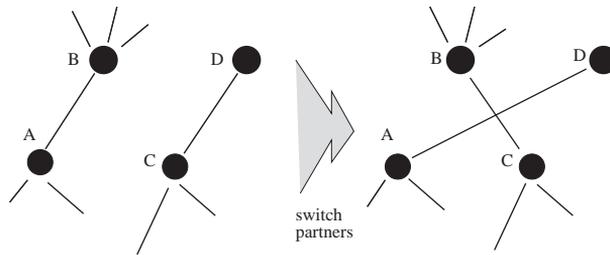


Fig. 1. One elementary step of the local rewiring algorithm. A pair of edges A–B and C–D is randomly selected. They are then rewired in such a way that A becomes connected to D, and C to B, provided that none of these edges already exist in the network, in which case the rewiring step is aborted, and a new pair of edges is selected. The last restriction prevents the appearance of multiple edges connecting the same pair of nodes.

The *local rewiring algorithm* that randomizes a network yet strictly conserves degrees of its nodes [3]¹ consists of repeated application of the elementary rewiring step shown and explained in detail in Fig. 1. It is easy to see that the number of neighbors of every node in the network remains unchanged after an elementary step of this randomization procedure. The directed network version of this algorithm separately conserves the number of upstream and downstream neighbors (in- and out-degrees) of every node. The matlab programs for both directed and undirected versions of this algorithm can be downloaded at our webpage.²

Another simple numerical algorithm generating such a random network “from scratch” was proposed in Ref. [2].³ It starts with assigning to each node a number k_i of “edge stubs” equal to its desired degree. A random network is then constructed by randomly picking two such edge stubs and joining them together to form a real edge connecting these two nodes. One of the limitations of this “stub reconnection” algorithm is that for broad distribution of degrees, which is usually the case in complex networks [1], the algorithm generates multiple edges joining the same pair of hub nodes. This problem cannot be avoided by simply not allowing multiple edges to form during the reconnection process as in this case the whole algorithm would get stuck in a configuration in which the remaining edge stubs have no eligible partners.⁴ Fortunately the local rewiring algorithm [3] (see footnote 1) instead of completely deconstructing a network and then randomly putting it back together, only gradually

¹ These algorithms first appeared in the context of random matrices in Gale [4]. More recently they were used in the graph-theoretical context of Kannan et al. [4].

² The matlab programs simulating several versions of the local rewiring algorithm can be downloaded for non-commercial purposes at <http://www.cmth.bnl.gov/~maslov/matlab.htm>

³ This algorithm also first appeared in the mathematical literature [5].

⁴ We have numerically studied this question for the scale-free network of the Internet, described in details later on in the text. The edge reconnection algorithm not allowing for the formation of multiple links got stuck every time we tried it. It, was found that in the resulting network the average number of unconnected edge stubs is 23 times its standard deviation, which completely precludes even the occasional completion of this algorithm.

changes its wiring pattern. Hence, any topological constraint such as e.g. that of no multiple edges, or no disconnected components, can be maintained at each step of the way.

Once an ensemble of randomized versions of a given complex network is generated, the abundance of any topological pattern is compared between the real network and characteristic members of this ensemble. This comparison can be quantified using two natural parameters: (1) the ratio $R(j) = N(j)/\overline{N_r(j)}$, where $N(j)$ is the number of times the pattern j is observed in the real network, and $\overline{N_r(j)}$ is the average number of its occurrences in the ensemble of its random counterparts; (2) the Z-score of the deviation defined as $Z(j) = [N(j) - \overline{N_r(j)}]/\Delta N_r(j)$, where $\Delta N_r(j)$ is the standard deviation of $N_r(j)$ in the randomized ensemble. This general idea was recently applied to protein networks in yeast [3] and *E. coli* [6].

We now illustrate our general methods using the example of the Internet, defined on the level of autonomous systems (AS). Autonomous Systems are large groups of workstations, servers, and routers usually belonging to one organization such as e.g. a university, or a business enterprise. The data on direct connections between Autonomous Systems is regularly updated and is available on the website of the National Laboratory for Applied Network Research.⁵ Such coarse-grained structure of the Internet was the subject of several recent studies [7–10]. In the following analysis we use the millennium snapshot of the Internet (data from January 2, 2000), when $N = 6474$ Autonomous Systems were linked by $E = 12572$ bi-directional edges.

It was recently reported [7] that the Internet is characterized by a scale-free distribution of AS degrees $p(K) \propto 1/K^\gamma = 1/K^{2.1 \pm 0.2}$. One can show that for such a scale-free network the above mentioned constraint of no multiple connections between nodes is extremely important. Indeed, degrees of the two highest connected hubs in a scale-free network scale as $k_{\max} \sim N^{1/(\gamma-1)}$. In an uncorrelated random network with no constraints on edge multiplicity the expected number of edges connecting these two hubs scales as $k_{\max}^2/(2E) \sim N^{2/(\gamma-1)-1}$ (here we assumed that $E \sim N$). When $\gamma < 3$ it increases indefinitely as N to ∞ . For the Internet that corresponds to the two largest hubs with degrees of respectively $K_0 = 1458$ and $K_1 = 750$ being connected by as many as $K_0 K_1 / (2E) = 1458 \cdot 750 / (2 \cdot 12572) = 43.5$ edges! Hence, in this case a random network ensemble generated by our local rewiring algorithm is very different from the one generated by the stub reconnection algorithm and analytically studied in Ref. [2].

Fig. 2 shows the average degree $\langle K_1 \rangle_{K_0}$ of neighbors of nodes with the degree K_0 in the real Internet (squares) as well as in a typical random network with no multiple connections between nodes generated by our local rewiring algorithm (circles). From this figure it is clear that most of the $\langle K_1 \rangle_{K_0} \propto K_0^{-0.5}$ dependence reported in Ref. [8] is reproduced in our random ensemble and hence can be attributed to the effective repulsion between hubs due to the constraint of having no more than one edge directly connecting them to each other. In the absence of correlations between degrees of neighboring nodes by definition one has $\langle K_1 \rangle_{K_0} = \text{const} = \langle K^2 \rangle / \langle K \rangle$ [2]. This expression, shown as a horizontal line in Fig. 2, applies only to a randomized network in which multiple edges between a pair of nodes are allowed. In a random scale-free network

⁵ Website maintained by the NLANR Measurement and Network Analysis Group at <http://moat.nlanr.net/>

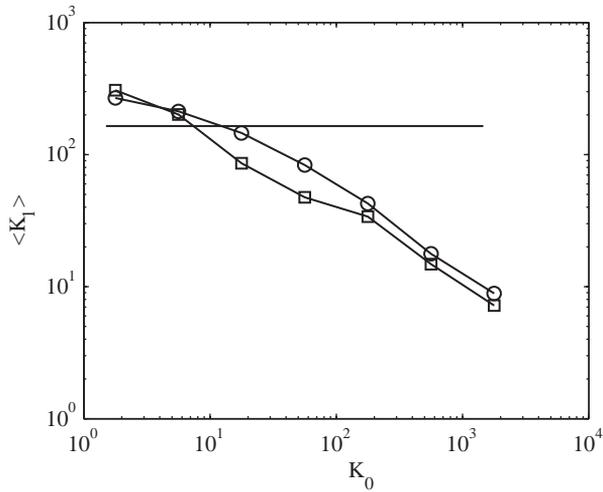


Fig. 2. The average degree $\langle K_1 \rangle_{K_0}$ of neighbors of nodes with degree K_0 in the Internet (squares) and its typical randomized counterpart (circles). Error bars in multiple realizations of the randomized network are smaller than symbol sizes. The horizontal line is the analytical result $\langle K_1 \rangle_{K_0} = \text{const} = \langle K^2 \rangle / \langle K \rangle \simeq 165$ valid for a random network in which multiple edges between pairs of nodes are allowed [2].

with no multiple edges the conditional probability distribution $P(K_1|K_0)$ crosses over from K_1/K_1^γ for $K_1 \ll K_1^* = 2E/K_0$ to $1/K_1^\gamma$ power law tail for $K_1 \gg K_1^*$. Such a crossover results in an asymptotic scaling $\langle K_1 \rangle_{K_0} \sim K_0^{\gamma-3}$. We have confirmed numerically that $P(K_1|K_0)$ in our randomized ensemble is very similar to that measured in the real Internet [10].

From the above discussion one may get the impression that the topology of the Internet is in perfect agreement with its randomized version. This is however not true. Let $N(K_0, K_1)$ to denote the total number of edges connecting nodes with degrees K_0 , and K_1 .⁶ This is an example of a higher level topological property of a complex network, which can be compared to its average value $\overline{N_r(K_0, K_1)}$ in the appropriate null-model network. By comparing $N(K_0, K_1)$ and $\overline{N_r(K_0, K_1)}$ one studies the correlation profile of the complex network, quantifying the correlations in degrees of neighboring nodes. In Fig. 3 we visualize the correlation profile of the Internet by plotting the ratio $R(K_0, K_1) = N(K_0, K_1) / \overline{N_r(K_0, K_1)}$. Regions on the $K_0 - K_1$ plane, where $R(K_0, K_1)$ is above (below) 1 correspond to enhanced (suppressed) connections between nodes with degrees K_0 and K_1 in the Internet compared to its randomized counterpart. The statistical significance of these deviations, measured by the Z-score $Z(K_0, K_1) = (N(K_0, K_1) - \overline{N_r(K_0, K_1)}) / \Delta N_r(K_0, K_1)$, is shown in Fig. 4. To improve the statistics, in all correlation profiles studied in this paper we logarithmically binned the degrees K_0 and K_1 at two bins per decade. In Figs. 3 and 4 one can see several

⁶ This quantity was analytically studied in several model networks in Ref. [11].

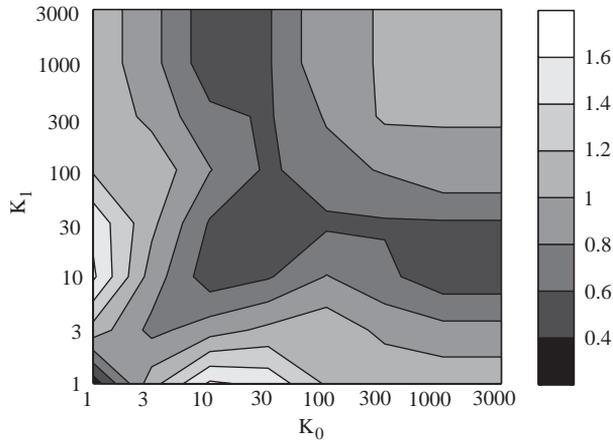


Fig. 3. Correlation profile of the Internet. The ratio $R(K_0, K_1) = N(K_0, K_1) / \overline{N_r(K_0, K_1)}$, where $N(K_0, K_1)$ is the total number of edges in the Internet connecting pairs of Autonomous Systems with degrees K_0 and K_1 , while $\overline{N_r(K_0, K_1)}$ is its average value in the ensemble of randomized versions of the Internet, generated by the local rewiring algorithm described in the text.

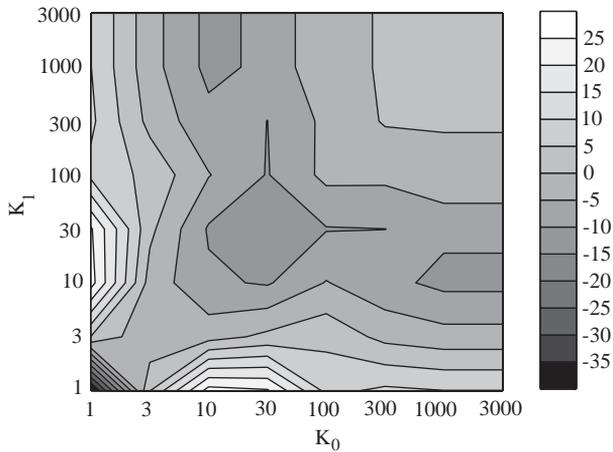


Fig. 4. Statistical significance of correlations in the Internet. The Z-score of correlation patterns in the Internet $Z(K_0, K_1) = (N(K_0, K_1) - \overline{N_r(K_0, K_1)}) / \Delta N_r(K_0, K_1)$. Here $\Delta N_r(K_0, K_1)$ is the standard deviation of $N_r(K_0, K_1)$ measured in an ensemble of 1000 randomized networks.

prominent features:

- Strong suppression of edges between nodes of low degrees $3 \geq K_0, K_1 \geq 1$.
- Suppression of edges between nodes of intermediate degrees $100 > K_0, K_1 \geq 10$,
- Strong enhancement of the number of edges connecting a node of a low degree $3 \geq K_0 \geq 1$ to that of an intermediate degree $100 > K_1 \geq 10$.

On the other hand any pair among the 5 highest degree nodes with $K_0, K_1 > 300$ was found to be connected by an edge, both in the real network, and in a typical random network. Hence $R(K_0, K_1)$ is close to 1 in the upper right corner of Fig. 3.

The strong suppression of connections between pairs of nodes with low degrees can in part be attributed to the constraint that all AS on the Internet have to be connected to each other by at least one path. For example, this constraint explicitly forbids links between a pair of nodes with the degree of 1. However, when we used an ensemble of random networks in which the formation of isolated clusters was prevented at every rewiring step, we found very little change in the observed correlation profile. The division of all nodes on the Internet into three distinct groups of low-, intermediate-, and highly-connected ones visible in its correlation profile may be due to its hierarchical structure of, correspondingly, users, low-level (possibly regional) Internet service providers (ISP), and high-level (global) ISP. Similar hierarchical picture was recently suggested in Ref. [12] on the basis of the traceroute data.

It is worthwhile to note that the correlation profile of the Internet measured in this work makes it qualitatively different from yeast protein networks analyzed by us earlier [3]. Those molecular networks are characterized by suppressed connections between nodes of very high degree, and increased number of links between nodes of intermediate degree. Thus correlation profile allows one to differentiate between complex networks with very similar (scale-free) degree distributions.

The correlation profile is by no means the only topological pattern one can investigate in a given complex network, with other examples being its spectral dimension [13], the betweenness of its edges and nodes [14,8], feedback, feed-forward loops, and other small network motifs [6]. In the rest of this paper we analyze the level of clustering [15] of the Internet, quantified by its number of loops of length 3 (triangles). The real Internet contains 6584 such loops, while its random counterparts, generated by our local rewiring algorithm, have 8636 ± 224 triangles (this and all future results were measured in an ensemble of 100 randomized networks.) Thus the clustering of the real Internet is some 9 standard deviations *below* its value in a randomized network! This result is surprising because there are good reasons for the Internet to have above average level of clustering. Indeed, one expects its nodes to preferentially link according to their geographical location [8,9], general type of business or academic enterprises they represent, etc. All these factors usually tend to increase clustering [15]. On the other hand, the correlation profile of the Internet visualized in Fig. 3 naturally leads to the reduction in clustering. Indeed, the suppression of connections from nodes with intermediate degrees to other such nodes in favor of nodes with low degrees reduces the number of triangles in the network.

In order to explore the interplay between the level of clustering in the network and its correlation profile we studied two “extremal” random networks with the same degrees of individual nodes as the real Internet. The first network contained no triangles, while the second one had 59144 triangles. Both networks were generated using a simple modification of our basic local rewiring algorithm in which a rewiring step was accepted only if it did not increase (in the first case) or decrease (in the second case) the number of triangles in the network. This adds a zero-temperature Metropolis

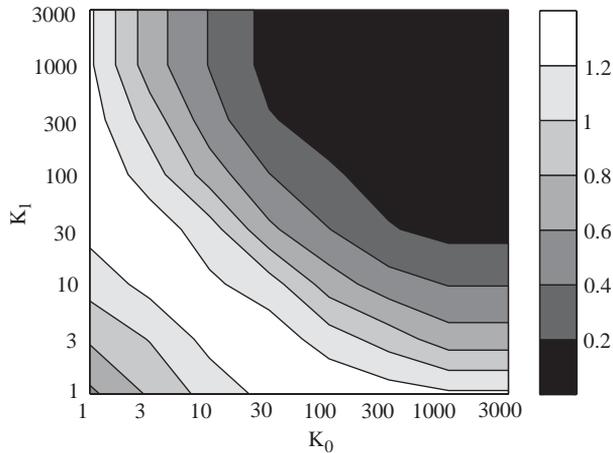


Fig. 5. The correlation profile $R(K_0, K_1)$ of a network with the same set of degrees as the Internet but with no triangles. Note the suppression of connections between different hubs in favor of connections between hubs and nodes of low degree.

dynamics [16] to the elementary “edge swapping” step of our algorithm,⁷ in which the energy function is the number of triangles taken with an appropriate sign. In the first case after some transient time all triangles have disappeared from the network, at which point we measured its correlation profile (Fig. 5). In the second case our algorithm was designed to generate a network with the largest possible number of triangles. Computer time limitations have forced us to stop the program when we reached 59144 triangles, which as will be shown later is rather close to the absolute maximum of 63844 triangles for a given set of node degrees. The correlation profile of this very clustered network is shown in Fig. 6. From Fig. 5 one concludes that the correlation profile in which connections between hubs are suppressed in favor of connections between hubs and nodes of low degree favors a reduced number of triangles. If instead nodes with similar degrees (including hubs) prefer to connect to each other (the light-colored area on and around the diagonal in Fig. 6) the number of triangles increases. This can be demonstrated analytically. Consider an edge connecting a pair of nodes with degrees K_0 and K_1 . The maximal number of triangles containing this edge is $\min(K_0 - 1, K_1 - 1)$. Indeed, in the best case scenario all $K - 1$ remaining neighbors of the smaller degree node are also neighbors of the larger degree node. Therefore, given a correlation profile specified by $N(K_0, K_1)$ —the number of edges connecting nodes with degrees K_0, K_1 —the absolute maximum number of triangles in the network is given by $N_{\Delta}^{\max} = \sum_{K_0, K_1} N(K_0, K_1) \min(K_0 - 1, K_1 - 1) / 6$. Here the factor $\frac{1}{6}$ corrects for the fact that in our counting scheme each triangle would be counted 2 times along each of its

⁷ A different Metropolis dynamics in which edges are rewired one at time was used to generate random networks in Ref. [17].

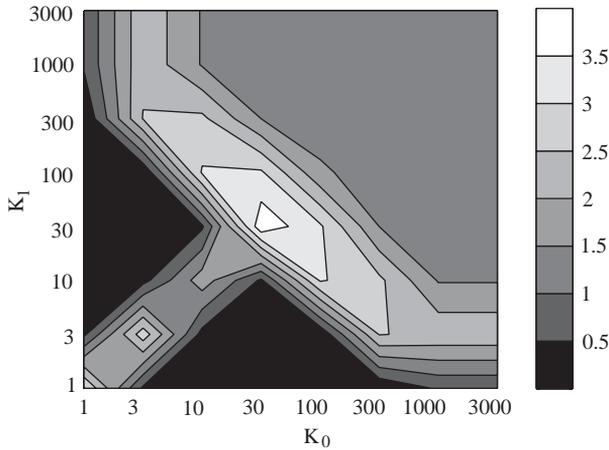


Fig. 6. The correlation profile $R(K_0, K_1)$ of a network with the same set of degrees as the Internet but with a very large number of triangles (59144). Note the tendency of nodes with similar degrees to connect to each other.

three sides. Using identities $\min(K_0 - 1, K_1 - 1) = (K_0 - 1 + K_1 - 1)/2 - |K_0 - K_1|/2$ and $\sum_{K_0, K_1} N(K_0, K_1)(K_0 - 1) = \sum_{K_0, K_1} N(K_0, K_1)(K_1 - 1) = N\langle K(K - 1) \rangle$ one finally gets:

$$N_{\Delta}^{\max} = \frac{N\langle K(K - 1) \rangle}{6} - \frac{1}{12} \sum_{K_0, K_1} N(K_0, K_1)|K_0 - K_1|. \tag{1}$$

The first part of this expression corresponds to a hypothetical situation of the maximal cliquishness in which all neighbors of every node are connected to each other. It is easy to see that except for some very special cases of the distribution of degrees such maximal cliquishness can never be realized. Indeed, whenever a pair of nodes of unequal degrees K_0, K_1 are connected to each other the second term in the Eq. (1) decreases the maximal number of triangles. Given the set of node degrees K_i , one can easily construct the network with the largest possible number of triangles. One starts by connecting the largest hub node to other nodes in the order of decreasing degrees. In the second round of this algorithm one selects the remaining neighbors of the second largest hub in the order of decreasing degree. The process continues round by round until neighbors of all nodes are specified. When a node reaches its desired degree it will be simply skipped during later rounds of this algorithm. One can show that the network generated by this algorithm has the smallest value of $\sum_{K_0, K_1} N(K_0, K_1)|K_0 - K_1|$ and the largest number of triangles among all networks with a given set of node degrees. In case of the Internet such network has 63,884 triangles just below the $N_{\Delta}^{\max} = 64,702$ specified by its correlation profile. These numbers of triangles are an order of magnitude below the naive estimate $N\langle K(K - 1) \rangle/6 \simeq 690,000$ traditionally used as a normalization factor in the formula for the clustering coefficient of a network [15]. Hence, based on

the traditional definition even the “loopiest” network with the same node degrees as the Internet has a clustering coefficient of only 0.09! For the “native” correlation profile of the Internet Eq. (1) predicts the maximal number of triangles close to 24,000, which sets the observed level of clustering (6584 triangles) around 27% of its maximal value for this correlation profile.

In order to check if degree correlations visible in the correlation profile of the Internet (Fig. 3) fully account for the observed number of triangles we generated an ensemble of random networks that preserves not only degrees but also the correlation profile of the complex network. To this end we used a modification of our main local rewiring algorithm. There are two principal ways in which this can be done. In the first scheme, reminiscent of generating a microcanonical ensemble in statistical physics, one allows only for those local rewiring steps that strictly conserve the number of edges $N(K_0, K_1)$ between nodes with degrees K_0, K_1 . This is achieved by constraining the selection of pairs of edges for the rewiring step of Fig. 1 only to those connecting nodes with degrees K_0, K_1 , and K_0, K_1' . It is easy to see that such a local rewiring step strictly conserves $N(K_0, K_1)$. In practice we softened randomization constraints by coarse-graining the logarithm of degree to half-decade bins. Using this “microcanonical algorithm” we generated an ensemble of networks with 4132 ± 75 loops. The fact that the number of loops in the real Internet (6584) is now significantly larger than in these random networks, confirms the intuitive notion that the Internet is indeed characterized by a significant degree of clustering. We have also found that this 60% increase in the level of clustering is equally spread over the whole spectrum of degrees.

As is always the case with microcanonical algorithms one should worry if the above algorithm is ergodic. In other words there is no guarantee that in this algorithm the system does not get trapped in a disconnected component of the phase space. This is easily checked by annealing the network using a *canonical* Metropolis [16] version of our algorithm with the energy function or Hamiltonian given by $H = \sum_{K_0, K_1} [N(K_0, K_1) - N_r(K_0, K_1)]^2 / N(K_0, K_1)$, and sampling networks at a finite temperature T . Local moves lowering the Hamiltonian are always accepted, while those increasing it by ΔH are only accepted with the probability $\exp(-\Delta H/T)$. As seen in Fig. 7 the above algorithm nicely extrapolates between the microcanonical algorithm for small T and the unrestricted local rewiring algorithm for large T . This confirms that our microcanonical algorithm is indeed ergodic.

Another conceivable use of the Metropolis algorithm described above is to generate an artificial network with a given distribution of degrees $p(K)$ and a given correlation profile $R(K_0, K_1)$. To achieve this one first generates a seed network with a given $p(K)$, e.g. by the stub reconnecting algorithm of Ref. [2] (see footnote 3). This network is first annealed using the Metropolis algorithm with the energy functional punishing multiple connections between nodes. The resulting network, containing no multiple connections is subsequently annealed with another energy functional favoring the desired correlation profile. This results in an ensemble of random networks with no multiple connections between nodes and the desired correlation profile.

In summary we have proposed a general algorithm to detect characteristic topological features in a given complex network. In particular, we introduced the concept of the *correlation profile*, which allowed us to quantify differences between different complex

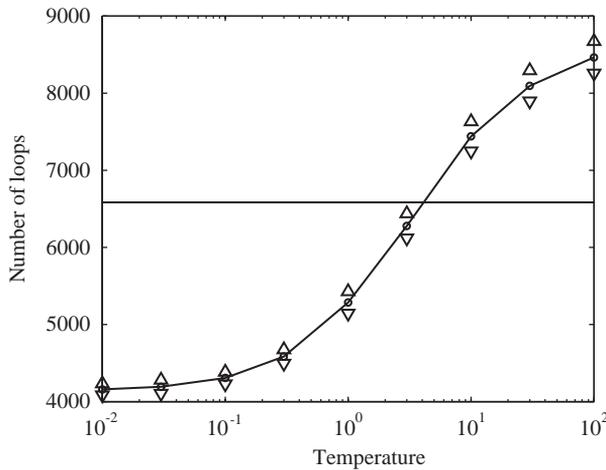


Fig. 7. The number of loops as a function of the Metropolis temperature observed in an ensemble of random versions of the Internet. Random networks were generated by the Metropolis [19] version of the local rewiring algorithm with the energy function $H = \sum_{K_0, K_1} [N(K_0, K_1) - N_r(K_0, K_1)]^2 / N(K_0, K_1)$. Upper and lower triangles represent the standard deviation within an ensemble. The horizontal line shows the actual number of triangles (6584) in the Internet.

networks even when their degree distributions are similar to each other. Applied to the Internet, this profile identifies hierarchical features of its structure, and helps to account for the level of clustering in this network.

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