Exactly scale-free scale-free networks

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Abstract

Many complex natural and physical systems exhibit patterns of interconnection that conform, approximately, to a network structure referred to as scale-free. Preferential attachment is one of many algorithms that have been introduced to model the growth and structure of scale-free networks. With so many different models of scale-free networks it is unclear what properties of scale-free networks are typical, and what properties are peculiarities of a particular growth or construction process. We propose that a maximum entropy process provides the best representation of what are typical properties of scale-free networks, and provides a standard against which real and algorithmically generated networks can be compared. We find that preferential attachment growth models do not yield typical realizations of scale-free networks because there is a latent structure, which we term “hub-centric”. We provide a method to generate or remove this latent hub-centric bias — thereby demonstrating exactly which features of preferential attachment networks are atypical of the broader class of scale-free networks. We are also able to statistically demonstrate whether real networks are typical realizations of scale-free networks; using a new surrogate generation method for complex networks, exactly analogous the the widely used surrogate tests of nonlinear time series analysis.
I. INTRODUCTION

The notion of scale-free networks has been around for a while \cite{3}. The introduction of the preferential attachment (PA) algorithm for generating random scale-free graphs was a significant step in understanding the properties of scale-free networks, and the physical processes that create them \cite{1}. PA has spawned a good deal of subsequent algorithms and analysis.

The purpose of this paper is to highlight that not all scale-free networks have the same properties, and that algorithms, like PA, do not capture the full richness of scale-free networks, nor do they necessarily display properties that may be termed typical of all scale-free networks.

To achieve our aim, we first briefly recall in this introduction the principal processes that have been proposed to describe and generate scale-free networks, and indicate deficiencies of these processes when employed as models of typical scale-free networks. We then propose a maximum entropy process that provides an unbiased sample of the set of all scale-free networks. A maximum entropy process provides a better representation of expected properties of scale-free networks, both in terms of richness and typicality. A maximum entropy process also provides an unbiased standard against which other processes that generate scale-free networks can be compared.

In section \[II\] we make a careful comparison of PA with our unbiased standard to illustrate how PA has a significant bias in the structural properties of the networks it generates. We demonstrate it has a hub-centric bias.

In section \[III\] we use a surrogate data approach to examine a selection of real-world networks claimed to be scale-free, and analyse in what sense these networks are typical of scale-free networks and how they differ.

A. Scale-free networks from processes

In this section we briefly review the notion of scale-free networks, and the principal models of the physical processes that generate scale-free networks. These models can be broadly divided into growth models and configuration models.

Scale-free networks are usually identified by the histogram of node degrees having a
power-law tail. Many naturally occurring networks have been identified as having a scale-
free property: citation and collaboration networks [4–6], airline networks [7], protein-protein
interaction [8], metabolic pathways [9], the world-wide web and internet [10].

To understand the formation of scale-free networks various models have been proposed to
mimic the physical or conceptual processes that build and shape these networks. One of the
first, proposed by Barabási and Albert, is preferential attachment [1], which is a restatement
of the process described by de Solla Price [3] as a model of observed scale-free networks of
citations [4].

Preferential attachment is an unchanging, additive growth process, where nodes of a fixed
degree are added to the network, with links preferentially attached to existing nodes depend-
ing on their degree; usually proportional to the degree. Although this was suggested as a
model of the process that grows the world-wide web (seen as hyperlinks between webpages),
it was recognised that there is an additional aging process (AOL is replaced by Facebook,
yahoo looses popularity to Google) so that attachment preferences change as the network
growth procedes [12, 15, 16].

Other processes can be introduced into a network growth model, such as shuffling parts of
the network, and deletion of links and nodes [12, 21], such that these actions do not change
the underlying scale-free property of the networks produced. Moreover, scale-free networks
can be produced by processes that are not growth processes. Configuration models proceed
by choosing nodes to have prescribed degrees, then connecting these together to form a
scale-free network [17]; although care is needed to ensure the networks obtained satisfy
other expected properties, such as, being simple (no self-links or multiple edges between
nodes) and connected [14, 18, 21].

B. Not all scale-free networks are the same

With so many different processes generating scale-free networks, the question arises: do
they generate the same networks? The simple answer is no. Many differences in the scale-
networks generated by different processes have been noted; some particular differences are
outlined in the following.

Consider a preferential attachment process PA(m, A) that attaches nodes of degree m with
the probability of linking a new node to a node of degree k is $k + A - 1$, where $A \geq 1$ is
a constant called the initial attractiveness \[19\]. The minimum degree \( m \) clearly effects the robustness of the networks generated, and it effects other properties too \[21\]. It can be shown that \( \text{PA}(m, A) \) the power-law tail has an exponent \( \gamma = 2 + A/m \). This type of preferential attachment process restricts the power-law exponent to \( \gamma > 2 \). Some real-world networks have \( \gamma < 2 \), and network growth models can be modified to shape networks and allow such power-laws \[20\] \[21\].

When other network statistics are considered (such as diameter, node-degree assortativity, clustering coefficients), then the differences between scale-free networks found in the real-world and generated by different models become more apparent.

For example, consider the node-degree assortativity of scale-free networks generated by preferential attachment. These networks have low assortativity, but many natural networks are found to have very high assortativity \[22\]. Although these natural networks are not small-world (they are scale-free but estimates of the exponent are much smaller than observed for most processes that generate scale-free networks: \( \gamma < 2 \)), it can be shown that other processes can generate scale-free networks with high node-degree assortativity \[23\]. Newman \[24\] observed systematic biases in the assortativity of real-world scale-free networks: technological networks tended to be dis-assortative, social networks assortative. Newman also showed that networks generated by preferential attachment have a definite bias compared to real-world networks; on the other hand, altruistic attachment does not \[25\]. Other issues with the assortativity of preferential attachment networks have been observed elsewhere \[12\] \[26\].

More generally, it has been noted that growth models have systematic biases (of network statistics) relative to configuration models \[11\] \[27\]. Indeed, networks of growth models usually only attain the scale-free property asymptotically, and small networks display systematic biases \[22\] \[26\]; configuration models need not have biases.

C. Maximum entropy processes

In this section we aim to define a process that generates scale-free networks in as pure form as possible, that is, without any biases. This process is a maximum entropy process, which can serve as a standard to which other processes can be compared to both recognise and understand the nature of their biases.

As previously noted, scale-free is usually taken to mean that the node-degree histogram
has a power-law tail. We need to make this definition more precise. Let $G$ be the set of connected simple graphs with $N$ nodes, and let $\mathbf{n}(G) = (n_1, \ldots, n_{N-1})$, $n_k \in \mathbb{Z}$, be the degree histogram of $G \in G$, that is, $n_k$ is the number of nodes of degree $k$.

**Definition 1.** If $p = (p_1, \ldots, p_{N-1})$, where $p_k \in [0, 1]$ and $\sum_{k=1}^{N-1} p_k = 1$, then $p$ has a power-law tail if $p_k \propto (k - \alpha)^{-\gamma}$ for $k \geq \beta$, where $\alpha, \beta \in \mathbb{Z}$, $\gamma \in \mathbb{R}$, $\alpha, \beta \geq 0$ and $\gamma > 1$.

In this definition $\alpha$ shifts the power-law tail relative to $k$, $\beta$ is where the power-law tail is deemed to begin, and $\gamma$ is the power-law of the tail. For the special case of preferential attachment $\text{PA}(m, A)$, the key parameters $\alpha$, $\beta$ and $\gamma$ are implicitly defined by $m$ and $A$.

**Definition 2.** $G \in G$ is a scale-free graph if $\mathbf{n}(G) \simeq Np$, where $p$ has a power-law tail.

Although Defn. 2 is apparently what most literature means by scale-free, what approximately equal means in $\mathbf{n}(G) \simeq Np$ is not always clear. It is usually taken to mean that the form $(k - \alpha)^{-\gamma}$ fits $\mathbf{n}(G)$, in the sense of least-squares curve-fitting of $\log n_k$ against $\log k$, or a multinomial fit of $\mathbf{n}$ against $\mathbf{p}$.

Of interest are processes generating independent random scale-free graphs. A stationary stochastic process $\mathcal{P}$ generating independent random graphs in $G$ is equivalent to selecting graphs according to a fixed probability mass function $\mathcal{P}: \mathcal{G} \to [0, 1]$, where $\sum_{G \in \mathcal{G}} \mathcal{P}(G) = 1$. Write $G \sim \mathcal{P}$ to denote that $G \in \mathcal{G}$ is selected according to process $\mathcal{P}$. (Since the process is completely defined by its probability mass function, use the same symbol $\mathcal{P}$ to denote the process and its probability mass function.)

**Definition 3.** A process $\mathcal{P}$ generates scale-free graphs (on average), if

$$\mathbb{E}[\mathbf{n}(G) \mid G \sim \mathcal{P}] = Np,$$

where $p$ has a power-law tail.

Such a process generates scale-free graphs, as Defn. 2 with the notion of approximately equal, $\mathbf{n}(G) \simeq Np$, implicitly defined by $\mathcal{P}$. For example, one can compute the variance $\mathbb{E}[\sum_{k=1}^{N-1} (n_k - Np_k)^2 \mid G \sim \mathcal{P}]$, or compute the probability of a histogram $\mathbf{n}(G)$ deviating from $Np$ in some norm by more than a threshold $\epsilon$, that is, $\Pr(\|\mathbf{n}(G) - Np\| > \epsilon \mid G \sim \mathcal{P})$.

Preferential attachment $\text{PA}(m, A)$ is one example of such a process; a network is grown by random preferential attachment until a graph with $N$ nodes is obtained. This process
implicitly defines the probability mass function for $G \in \mathcal{G}$, which depends on $m$ and how the seed network is chosen. Other growth models (with link aging, initial attractiveness, shuffling) will usually obtain different probability mass functions.

A difficulty with growth processes, including PA($m$, $A$), is although they satisfy Defn. 3 of scale-free processes, the power-law $\gamma$ is implicitly defined. In some cases (although not for PA) it is not clear that $\gamma$ is necessarily the same for all graphs generated for fixed growth parameters. Depending on the initial seed graph, it is possible to imagine growth processes which would converge to different power-laws. In contrast, one of the advantages of configuration models is the mean histogram $Np$ is prescribed: the process combines nodes with pre-defined degrees into a network \cite{17}.

Even if two processes generate scale-free graphs by Defn. 3 or have the same power-law $\gamma$, or have the same expected histogram $Np$, the expected value of other graph statistics such as assortativity, clustering, diameter, may be quite different as noted in the previous section.

If we are to understand the nature of scale-free graphs, and the nature of the processes that generate them, then it is useful to establish some benchmark or standard against which processes are compared. To some extent PA($m$, $A$) has served that propose, principally because it is a simple growth process. Unfortunately, it is not a satisfactory standard for many reasons we already indicated: it has a limited range of $\gamma$; $p$ and $\gamma$ are implicitly defined; it has known biases of statistics like assortativity.

We propose that the best standard against which to compare processes that generate scale-free networks is a maximum entropy process $ME(p)$ with prescribed mean histogram $Np$. A maximum entropy process samples all graphs with mean histogram $Np$ with the least bias or emphasis of structures and features that are not common features of all such graphs.

**Definition 4.** The maximum entropy process $ME(p)$ uniformly samples $n$ by the multinomial distribution of $p$, and uniformly samples graphs with the histogram $n$. That is, $Pr(G \mid G \sim \mathcal{P}_{ME(p)}) = Pr(G \mid n) Pr(n \mid p)$, where

$$Pr(G \mid n) = \frac{1}{\{|G \in \mathcal{G} \mid n(G) = n\}}; \quad (2)$$

and

$$Pr(n \mid p) = N! \prod_{k=1}^{N-1} \frac{p_k^{n_k}}{n_k!}; \quad (3)$$
The process $ME(p)$ has maximum entropy for the following reasons. It partitions all graphs in $G$ into equivalence classes by histogram $n$, and uniformly samples these [2], hence, achieving maximum entropy within these equivalence classes. The sampling of $n$ uses a multinomial distribution [3], which is the maximum entropy process for filling a histogram with frequencies $p$. Hence, even though the degrees of nodes within a graph are not independent, the degrees of nodes of successive randomly generated graphs behave as though they were independent.

For details on how to efficiently implement $ME(p)$, see Algorithm 1 in Appendix A. A maximum entropy process $ME(p)$ can be implemented by as a Monte Carlo Markov Chain (MCMC) [21], however, a naive MCMC implementation could converge slowly and not be effective for large graphs [31–33]. The key ideas of Algorithm 1 are that the equivalence class of graphs with the same degree histogram can be sampled uniformly by a process of edge switching [34, 35], and a canonical graph with a given degree histogram can be constructed by the Havel-Hakimi process [37, 38]. Combining these key ingredients with a test for connectivity [21] provides a sufficient algorithm.

**Definition 5.** Let $SF(\gamma, m)$ denote the maximum entropy process $ME(p)$, where $p$ has a power-law tail $\gamma$, with $\alpha = \beta = m$ and $p_k = 0$ for $k < m$.

In the following $SF(\gamma, m)$ will serve as our standard against which scale-free graphs and scale-free graph generators are compared.

**II. A HUB OF HUBS IS MORE THAN A RICH CLUB**

In this section we use algorithm 1 to explore what are the typical properties of scale-free networks, and moreover, infer that PA networks exhibit an atypical “hub-centric” structure. Power-law distributions alone imply that the degree distribution has a long tail and some nodes in the tail must have high degree, but the presence of “hubs” implies something more and are often said to “hold the network together”. What we observe in the following is something more than this. There are three properties to which we refer with the term “hub-centric” (which we define later in an algorithmic sense): (i) the distribution of hubs throughout the network, (ii) their interconnection, and (iii) their connection with low-degree nodes. The presence or absence of these three properties determine, to a very great extent,
many of the global properties of a scale-free network. Moreover, we observe that PA networks exhibit properties which are atypical of the broader class.

However, before moving to the conclusion that the difference between these two types of networks is due to the hub-centric properties of PA networks, we first present a numerical study of the various main measures of network geometry: assortativity, clustering coefficient and diameter. We apply these measures to various different families of scale-free networks to highlight the wide variation which is possible. We will also explore other prominent features — most importantly: (i) the robustness to targeted worst-case attacks (i.e. “attack vulnerability” \[39\]) on hubs; and (ii) a detailed motif analysis.

For our comparison experiments we generate four types of PA($m, A$) networks, with $m = 1, 2, 3, 4$ and $A = 0$. For given $N$ and $m$ we generate a sample from PA($m, A$) of $M$ graphs $G_i, i = 1, \ldots, M$. From a degree histogram $n(G)$ we use the following formula \[28\] to estimate the power-law tail exponent $\gamma$ of $G$, as

$$\hat{\gamma}(G) = 1 + N \left( \sum_{k=1}^{N-1} n_k \log \frac{k}{m - \frac{2}{\gamma}} \right)^{-1}. \quad (4)$$

Letting $\gamma = \frac{1}{M} \sum_{i=1}^{M} \hat{\gamma}(G_i)$ we use Algorithm 1 and generate an sample of $M$ graphs from $SF(\gamma, m)$. Results reported in the following are for $N = 2000, m = 1, 2, 3, 4$, and $M = 40$. Computation with other values produced comparable results. In the following subsections we examine each of the network properties outlined above, starting with motif rank and then robustness.

A. Comparison of motif rank

The motif, defined as a small connected subgraph that recurs in a graph, is the basic building block, or functional unit, of complex networks \[40\]. In real-world networks (e.g. gene regulatory networks), the relative frequencies of different motifs often represent different functions of the network \[41, 42\]. Moreover, it sheds light on the structure of the whole network. We restrict our analysis here to the four-node motifs, and classify them into three groups: \{$A, D\}, \{B, E\}, \{C, F\}$ (shown in Fig. 1), which suggests they are the building blocks of the sparse, moderate, and dense networks. The result of the motif analysis is also shown in Fig. 1.
FIG. 1. Each figure shows the frequencies of six types of four-node motifs, for a corresponding networks with $m \in \{1, 2, 3, 4\}$. On the left, are the results for preferential attachment, on the right, the uniform sampling algorithm.

From Fig.1, there is an apparent difference between the motif distribution of these two type of networks: as $m$ increases, the motif frequencies of PA networks become larger, and the “dense” motifs of type $C$ occur more frequently than the less dense type $E$ — suggesting that the PA networks are denser than the corresponding $SF(\gamma, m)$ networks. This would be a natural consequence of the PA networks becomes more hub-centric (more cross links between hubs) as $m$ increases, while the hubs of the $SF(\gamma, m)$ network remain more evenly distributed (less cross-links between hubs, and correspondingly fewer “dense” motifs).

**B. Robustness and attack vulnerability**

Due to the long tail of the power-law distribution, scale-free networks are often claimed to be simultaneously robust to the random loss of nodes (i.e. “error tolerance”) and fragile to targeted worst-case attacks [39]. The robustness is seen to be a consequence of the extremely high number of (“unimportant”) low degree nodes, the fragility is due to the extremely important role of the hubs. This property is also called the “Achilles’ heel” of PA networks, or the “robust yet fragile” feature. Intuitively, the inhomogeneous connectivity distribution of many networks caused by the power-law distribution would possess these two properties. However, from our analysis, $SF(\gamma, m)$ networks generated by sampling uniformly
from the family of all scale free networks do not exhibit this second property. Again, we may attribute this to the hub-centric nature of PA networks.

We quantify the robustness to targeted attacks by specific removal of the most highly connected (or important) nodes until the network is disconnected. We then take the number of the nodes removed as a measure. In Fig. 2 (a), we use degree to quantify relative importance of a vertex, while in (b), we use the betweenness centrality (BC) of a vertex as a measure, which is roughly defined as the number of geodesics (shortest paths) going through a vertex:

\[
BC(v) = \sum_{i \neq j, i \neq v, j \neq v} g_{ivj}g_{ij},
\]

where \( g_{ij} \) is total number of shortest paths between node \( i \) and \( j \), and \( g_{ivj} \) is the number of those paths that pass through \( v \).

The case of targeted attack is trivial for \( m = 1 \), in which situation the networks are highly likely to be trees. Hence, we restrict our analysis for the case where \( m = 2, 3, 4 \). these results are shown in Fig. 2. From Fig. 2 it is safe to conclude that \( SF(\gamma, m) \) network is much more robust than the corresponding PA network when facing targeted attack. This is the consequence of the fact that PA networks are more hub-centric, while the \( SF(\gamma, m) \) networks are not. The fragility of the PA networks is due to the placement of hubs within the network — not the scale-free-ness of the network per se.

C. Numerical statistics of network

In this section we present the difference between the PA networks and \( SF(\gamma, m) \) networks by computing the widely quoted numerical network properties:

- **diameter**: the maximal shortest path length.
- **global clustering coefficient**: the proportion of the number of closed triplets divided by the number of connected triples of vertices, which is a measure of degree to which nodes in a graph tend to cluster together.
- **local clustering coefficient**: the proportion of links between the vertices within its neighborhood divided by the number of links that could possibly exist between them, which quantifies how close its neighbors are to being a clique.
- **assortativity**: the Pearson correlation coefficient of degree between pairs of linked
FIG. 2. Numerical estimates of histograms showing the number of nodes required to be removed to induce collapse of the network giant component. Nodes are selected for removal via node degree or node betweenness centrality (there is very little differences between the two selection criteria — here we plot removal via node degree). Panels (from top to bottom) are for different minimum degrees $m = 1, 2, 3$. Results for PA are plotted as a solid blue line and and results for $SF(\gamma, m)$ are plotted as a red dashed line. Histograms are computed with logarithmically equally space bins — the same binning is used for both network construction methods. Clearly, $SF(\gamma, m)$ networks are, for $m > 1$, an order of magnitude more robust to targeted attack than typical PA networks.

The application of these four statistics is summarise in Fig. 3

We select cases with $m = 2$ and $m = 3$ to visualize the curve of these statistics for the pair of networks in Fig. 4. Although not shown, we note here that the case with $m = 1$ is similar to the case $m = 2$, while $m = 4$ is similar to $m = 3$. 

nodes, which measures the preference for a network’s nodes to attach to others that are similar in degree.
From the curves of various network statistics depicted above, we find that PA networks are atypical. In particular, PA networks have: (i) more negative assortativity compared with corresponding $SF(\gamma, m)$ networks; (ii) increasing clustering coefficient as $m$ increases; and, (iii) in the case $m = 3$ and $m = 4$ the two clustering coefficient curves separate from each other. All these discrepancies point to the fact that as $m$ increases, the PA network becomes more and more hub-centric, while the $SF(\gamma, m)$ network remain highly uniform – and the high degree nodes remain evenly distributed throughout the $SF(\gamma, m)$ networks.
FIG. 4. Distribution of the statistics of networks with $m = 2$ (upper four panels) and $m = 3$ (lower four panels)
| $m$ | PA | $\gamma,m$ | diameter | global_cc | local_cc | assortativity | motif rank |
|-----|-----|-------------|----------|-----------|----------|---------------|------------|
| 1   | 19.47(1.71) | 0.0037(0.0033) | 0.67(0.01) | -0.095(0.017) | BECFD |
| 2   | 7.05(0.22) | 0.0059(0.0005) | 0.061(0.011) | -0.14(0.014) | FCEBDA |
| 3   | 9.45(1.53) | 0.014(0.004) | 0.093(0.14) | -0.095(0.052) | FCEBDA |
| 4   | 5.28(0.45) | 0.011(0.0004) | 0.12(0.014) | -0.19(0.015) | FCEBDA |
| 5   | 7.57(0.54) | 0.0087(0.0021) | 0.017(0.014) | -0.038(0.019) | FCEBDA |
| 6   | 4.93(0.27) | 0.014(0.0004) | 0.18(0.017) | -0.24(0.019) | FCEBDA |
| 7   | 6.67(0.47) | 0.0072(0.0019) | 0.011(0.011) | -0.021(0.017) | FCEBDA |

TABLE I. Summary of numerical statistics for the four pairs of networks ($m = 1, 2, 3, 4$).

We now introduce algorithms to modify the specific aspects of the network which contribute to this hub-centric property. Note that the hub-centric structure is a global property of the network, since only modification on a small portion of PA networks (such as the case with the so-called “rich-club” phenomena [43]) is not sufficient: when we only make the modification described in [43] to manipulate rich-club connections the PA and $SF(\gamma,m)$ network statistical distributions remain disparate. Therefore, the modification scheme we propose in the following applies across the entire network structure — from super-rich nodes and hubs, to the poorest nodes. To maintain conciseness and focus, we present the brief idea of our modifications scheme here; for details see Algorithm 3 of Appendix B. In the following paragraphs we outline these two modification schemes — one to remove what we call the hub-centric features of PA networks and a second scheme to add these features to $SF(\gamma,m)$ realisations. The aim of these computations is to show that these modifications alone are sufficient to align the corresponding distributions of network structural properties (assortativity and so on).

The modification scheme for an initial PA network is the following. First, we cut the links within the group of rich nodes and between rich nodes and the group of poor nodes as far as possible while preserving the connectivity of the network. Then, we use the algorithm described in [43] among the giant nodes (which we define as the nodes whose degree is even larger than the typical rich nodes), to reconstruct the structure of the rich nodes. That is, we obtain networks with minimal interconnection between hubs, minimal connection from...
FIG. 5. (Modification on PA) The curve of the statistics for $SF(\gamma, m)$ networks (solid lines), PA networks (bold dotted gray lines), modified PA networks (termed PA' with bold dotted black lines) and modified fitted PA networks (termed PA' ' with dotted black lines), where $m = 3$.

hubs to low degree nodes, but a similar rich-club structure (the interconnection among the super hubs). After setting the thresholds $\alpha_1 = 60\%$, $\alpha_2 = 5\%$ and $\alpha_3 = 0.5\%$ in Alg. 2 (Appendix B), we apply this modification to the case with $m = 3$ and $m = 4$. The result with $m = 3$ is shown in Fig. 5, and for conciseness, the result with $m = 4$, although similar, are omitted.

From Fig. 5, the range of the distributions for the modified graphs overlap with the unmodified target distribution $SF(\gamma, m)$ — indicating that our modification provides a good fit to the distribution of PA networks, with the additional of hub-centric links. Moreover, we test the modified curves of the PA networks and the curves of $SF(\gamma, m)$ networks. For this purpose, we add the following random factors. First, we choose $\alpha_1$ randomly from the set $[50\%, 80\%]$, and then the result for $m = 3$ is also depicted in Fig. 5. The results for $m = 4$ are similar, but omitted for conciseness.
From the calculations of Fig. 5 we see that the modification of the PA scheme (removing the hub-centric properties of such networks) allows us to produce network statistics which have a distribution similar to the unmodified uniform sampling scheme (for the local clustering coefficient and assortativity, at least) or bracketing the expected distribution for $SF(\gamma, m)$ (for the maximum diameter). Although this bracketing — by modifying the hub-centric nature of the PA network we go from smaller than $SF(\gamma, m)$ to larger that $SF(\gamma, m)$ — does not immediately provide indistinguishable statistical distributions, it is clear that this is due only to the unselective manner in which we choose the threshold parameters for this algorithm. Changing these parameters effects a continuous change in these statistical distributions. This is sufficient to make our case that these hub-centric groups of nodes are what causes the PA networks to be atypical. We do note, however, that the parametric changes we have explored are insufficient to modify the PA network to reproduce the full distribution of observed global clustering coefficients for the $SF(\gamma, m)$ network: there appears to be still further unexplored richness in the variety of these networks — scale-free networks with close to zero clustering (very tree-like networks [21]).

To further support our claim, we also present here a reverse modification algorithm on $SF(\gamma, m)$ networks to generate interconnection among hubs, which would result in the adjusted curves of the statistics for $SF(\gamma, m)$ networks approaching that of the PA networks. Leaving the details to Appendix B (Alg. 3), we again introduce the idea briefly here. At first, we delete the edges among the poor nodes and relink these edges to rich nodes with probability proportional to the degree of the rich nodes. Moreover, we use the algorithm described in [43] to make a club of super-rich (“giant”) nodes (the definition is similar to the one in the first modification) connected. By this way, we are able generate the hub-centric structure in networks. Setting $\alpha_1 = 80\%$, $\alpha_2 = 5\%$ and $\alpha_3 = 0.5\%$ for Alg. 2, the result for $m = 3$ is shown in Fig. 6. The calculation for $m = 4$ is similar and omitted for conciseness.

From Fig. 6, after generating hubs by artificially reconstructing the structure of networks, the numerical analysis of $SF(\gamma, m)$ networks indicates statistical distributions of structural properties which approach that of PA networks — supporting our claim that hub-centric structure in PA networks makes them atypical of random scale-free graphs.

By modifying the properties of a uniformly sampled network we are able to produce distributions of maximum diameter and global clustering coefficient very similar to that observed for the PA. That is, we add hub-centric structure to the $SF(\gamma, m)$ network and
FIG. 6. (Modification on $SF(\gamma, m)$) The curve of the $SF(\gamma, m)$ networks (solid lines), PA networks (bold dotted gray lines) and modified $SF(\gamma, m)$ networks (termed $SF(\gamma, m)'$ with dotted lines) in the case $m = 3$

achieve statistical features similar to that typical of PA networks. We do not achieve such good agreement for assortativity and local clustering coefficient. Nonetheless, taken together Fig. 5 and 6 show that matching distributions can be achieved by either adding or removing the hub-centric features in each of the four statistics that we examine here. Hence, the features which we modify with the algorithms described in the appendix are exactly the properties of PA networks that are atypical of the broader distribution of properties scale free networks when sampled by a maximum entropy process. The only caveat being that the two algorithms are not exactly inverses of one another, and, in particular, measures of global clustering hint at further unexplored diversity in the global structure of typical scale free networks (as the networks become progressively more tree like, even for $m > 1$).
D. Hub-centric structure in PA networks

To conclude this section, we now collate the results of our analysis. We see that the hubs of a PA network “hold” that network together. The strength of interconnection among hubs (and connection with low degree nodes) may be explained by the preferential attachment itself. In that growth model, once nodes and links are added, they will never be altered again. This, we claim, causes inhomogeneity in PA networks. The largest hubs will always (with probability approaching one) be the earliest nodes in the growing network and these nodes are necessarily closely interlinked. Conversely, the last nodes added to the network will have minimal degree and yet these nodes will (with very high probability) be directly connect to the hubs. In fact, it is clear that the last nodes added (those with the lowest degree) are most likely to be connected directly to the hubs \[2\]. These are precisely the properties we alluded to earlier with our description of “hub-centric” networks, and, these are precisely the properties which are adjusted by the modification algorithms \[3\] and \[2\] of Appendix B.

The consequences of this hub-centric structure of PA networks is two-fold. First, since PA is an elegant and intuitive way to generate graphs, there may exist some generation procedures in the real world which are similar to preferential attachment, and thus we can use this claim to illustrate the hub-centric structure in such growth networks. This observation has potential for practical use — for example, with hub detection in control of disease transmission, or, to control of a network by manipulating the hubs. Second, such a claim also indicates that there is systematic bias with PA networks. This bias will lead to difficulty when using PA networks to explain real world networks which do not result from such a constrained growth process — even when the degree sequence of each network satisfies the power law distribution.

III. APPLICATION TO PARTICULAR PUTATIVE SCALE-FREE SYSTEMS

In this section, we introduce a variant of the surrogate data test, proposed for nonlinear time series analysis, to interpret real world networks. We proceed by generating an ensemble of random networks, both similar to the observed data-based network (in that they share the same degree distribution) and yet, at the same time, random. By comparing the properties of
the real network with the corresponding distribution of $SF(\gamma, m)$ networks we can determine whether the particular network is typical. Our observations here are both a consequence of the previous section and a motivation for the development of a network surrogate test.

We will start with a brief discussion of robustness. As we saw above, PA networks are vulnerable to targeted attack, while $SF(\gamma, m)$ networks don’t have such an evident “Achilles' heel”. Recent research into the structure of several important complex networks shows that, even if their degree distribution could have an approximately power-law tail, the networks in question is robust to targeted attack to some degree: the most highly connected nodes do not necessarily represent an “Achilles’ heel”. In particular, recent results of modeling the router-level Internet has shown that the core of that network is constructed from a mesh of highbandwidth, low-connectivity routers, and [44] concludes that although power-law degree distributions imply the presence of high-degree vertices, they do not imply that such nodes form a necessarily “crucial hub”. A related line of research into the structure of biological metabolic networks has shown that claims of SF structure fail to capture the most essential biochemical as well as “robust yet fragile” features of cellular metabolism and in many cases completely misinterpret the relevant biology — for example, [45] indicates the removal of high degree nodes leaves the biosynthetic pathways fully intact. Hence, real-world scale-free networks do, indeed, exhibit absence of the much-touted “robustness” properties. Our model provides an explanation for that absence.

In the following, we will probe the limitation of the explanative power of PA networks via numerical statistics. We find that many real complex networks appear more “uniform” under our surrogate test. Also, based on this result, we propose a simplistic classification of real world networks.

Our surrogate tests are developed in this way: for a real world network which satisfies the power-law distribution, we estimate its minimum vertex degree and power law exponent by using the algorithm described in [28]. We then use the relation $\gamma = 2 + A/m$ in Section 1 to estimate its initial attractiveness, and then generate PA networks with controlled $\gamma$ and $m$. We then substitute $\gamma$ and $m$ into Algorithm 1 to generate the $SF(\gamma, m)$ networks. For each set of parameter values, we generate 40 networks for $SF(\gamma, m)$ and PA networks respectively. In Fig. 7 we draw the boxplot of numerical statistics of the real networks, as well as its corresponding PA and $SF(\gamma, m)$ networks.

From Fig. 7 we can conclude that, in terms of interpretation of real networks, $SF(\gamma, m)$

FIG. 7. Network characteristics: (a) diameter; (b) global clustering coefficient; (c) local clustering coefficient; and, (d) assortativity. Boxplot analysis for collaboration and information networks, depicting maximum, minimum, upper quantile (75%), median and lower quantile (25%) of the data. 1. CS PhD collaboration 2. Erdös collaboration 3. a symmetrized snapshot of the structure of the Internet at the level of autonomous systems 4. a metabolic pathway network, 5. the *S.cerevisiae* protein-protein interaction network 6. US Airport connection.
FIG. 8. The first panel shows the motif distribution and the lower panels the curves of statistics of the $SF(\gamma, m)$ networks (solid lines), PA networks (dotted lines) and Erdős collaboration network (bold mixed lines). The motif rank in ascending order is shown below the graph.
networks provides a significantly better model for data from the Internet topology, and metabolic and protein interaction networks. For CS PhD collaboration and US airport connection networks, $SF(\gamma, m)$ is slightly better than PA. However, for Erdős collaboration network, neither $SF(\gamma, m)$ nor PA networks is good, although the statistics of PA networks are closer to that of the Erdős network than $SF(\gamma, m)$ networks.

To examine the case of Erdős collaboration network more closely, we plot the motif rank and various other statistics of the Erdős collaboration networks in Fig.8. This figure suggests that the hub-centric structure in the Erdős collaboration network is much more significant than PA allows: the Erdős collaboration network is a densely connected core along with loosely coupled radial branches reaching out from that core. Erdős practiced what he preached – he was a weaver of social networks and thus a builder of social capital. Moreover, this collaboration network is specifically Erdős-centric — it is specifically focussed on that one unique hub and its connections. Hence, the nodes closer to Erdős benefit most and become the strongest hubs (after Erdős himself) in the resultant network.

The cases where $SF(\gamma, m)$ provides better representations would suggest, for instance, that the structure of protein interaction networks is more uniform, because the cellular ecosystem necessitates such stableness; and, in the case of the the Internet on the level of automatic system, the system is balanced and distributed in a rather deliberate way. Both these systems have been “engineered” for robustness. Finally, we note that neither the $SF(\gamma, m)$ nor PA networks performs well in reproducing the diameter of the biological networks. It is curious that biological networks present abnormally large diameters — we speculate that this more spread-out tree-like structure is a consequence of the components of biological systems having specific functional roles.

Based on our results, we also note (via analysis of robustness, motif and numerical statistics of a network, and comparison with its corresponding PA and $SF(\gamma, m)$ networks) that one can classify the real network in the sense of hub-structure: if its property is closer to the PA networks, we can conclude it is hub-centric and typically the result of a growth process. Conversely, networks that are not PA are more likely to be purposefully widely distributed.
IV. CONCLUSION AND DISCUSSION

We have proposed a new algorithm which allows us to make maximum-entropy random-samples of finite size graphs with degree histogram being probabilistic realisations of a specified degree distribution. We focus on scale free networks and use this method to generate random networks with power-law tail degree distributions of arbitrary $\gamma$ (exponent) and $m$ (minimum degree). This provides a simple alternative to the various generative processes in the literature. However, our approach has the benefit that it makes no particular biasing assumptions (such as preferential attachment). To emphasise the need for this algorithm we compare our results to distributions of networks obtained from the widely applied PA scheme of [1]. PA provides an excellent model of growth of a static network, however, we find that many real world networks do not conform to this model.

We found the high-degree nodes in PA networks are hub-centric, and that this hub-centric-ness has a greater influence on the overall structure than attributable only to the high-degree nodes themselves. This result helps us assess the contribution of hubs in real world networks to the overall network structure.

Appendix A: Implementing $ME(p)$

A maximum entropy process $ME(p)$ can be implemented by as a Monte Carlo Markov Chain (MCMC) [21]. However, a naive MCMC implementation could converge slowly and not be effective for large graphs [31–33]. Here we state an alternative algorithm; the key ingredients being edge switching [34, 35], connectivity testing [21], and constructing graphs by the Havel-Hakimi process [37, 38].

For $G \in \mathcal{G}$ let $d(G) = (d_1, \ldots, d_N)$ denote the degree sequence, that is, $d_i > 0$ is the degree of node $i$. An arbitrary degree sequence $d \in \mathbb{Z}^N$ is called graphical if there exists $G \in \mathcal{G}$ such that $d(G) = d$.

Algorithm 1. Let $p$ be a target probability mass (with power-law tail).

1. Generate a sample $n$ from the multinomial distribution of $p$.

2. Generate a uniformly sampled random degree sequence $d$ from $n$. 
3. Use the Havel-Hakimi process to test $d$ is graphical and construct the canonical graph $G$ with $d(G) = d$. If $d$ is not graphical, then return to step 2.

4. Test $G$ is connected; if not, then return to step 2.

5. Apply edge-switching to $G$ to uniformly sample the equivalence class of $n(G)$.

Although this algorithm is generally efficient for large graphs, when $m = 1$ and $\gamma$ sufficiently large ($\gamma > \gamma_1$, [21]) the Havel-Hakimi process often constructs disconnected graphs, and so step 3 becomes a bottle-neck. Fortunately, in this case a MCMC algorithm [21], that employs edge switching [34, 35] is efficient.

Step 1 requires a sample $n$ from the multinomial distribution of $p$, and step 2 a uniformly sampled degree sequence $d$ for $n$. Let $q_k = \sum_{i=1}^{k} p_i$, $q_0 = 0$, and $I_k = [q_{k-1}, q_k]$. Choose uniform random variants $x_i \in (0, 1), i = 1, \ldots, N$. Then let $d_i = k$ if $x_i \in I_k$ and $n_k = |\{x_i \in I_k\}|$.

With step 3 we must determine whether a given $d$ is graphical. Havel [37] and Hakimi [38] independently developed a test of $d$ being graphical. The following Havel-Hakimi test implicitly constructs a canonical graph $G$ if $d$ is graphical. Let $N \geq 2$ and $\tilde{d} = d$.

1. Choose $i$ such that $\tilde{d}_i > 0$.

2. If $\tilde{d}$ does not have at least $\tilde{d}_i$ entries $\tilde{d}_j > 0, j \neq i$, then $d$ is not graphical.

3. Subtract 1 from the $\tilde{d}_i$ entries $\tilde{d}_j, j \neq i$, of highest degree. Set $\tilde{d}_i = 0$.

4. If $d = 0$, then $d$ is graphical. Else return to step 1.

The canonical realisation of $G \in G$ for a graphical $d$ is implied by step 3 of the test: the node $i$ is connected to those other nodes $j$ selected in step 3. The graph $G$ can be built as the test proceeds by constructing its adjacency matrix $A$.

Step 4 of Algorithm [I] requires testing whether a graph $G$ is connected. Let $A$ be the adjacency matrix of $G$, and define $C_p = I + A + \cdots + A^p$. Then $G$ is connected if $C_p$ has no zero elements for some $p \leq N - 1$.

Step 5 requires modifying a graph $G$ by edge switching. Let $A$ be the adjacency matrix of $G$. Let $i, j, k, l$ be distinct nodes, such that $A_{ij} = A_{kl} = 1$ and $A_{il} = A_{kj} = 0$. Then the edges are switched by setting $A_{ij} = A_{kl} = 0$ and $A_{il} = A_{kj} = 1$. Edge switching does
not change \( n(G) \), and if repeated sufficiently often the resulting graph is uniformly sampled from its equivalence class \([35, 36]\).

**Appendix B: Modification algorithms**

In this section we provide the detailed modification algorithms described in the main text. These algorithms are presented here to separate them from the more central \( SF(\gamma, m) \) network generation algorithm (Alg. 1). The first modification algorithm (Alg. 2) changes the distribution of PA networks' statistics, by “spreading hubs”, to make it closer to the \( SF(\gamma, m) \) networks. Moreover, after adding random factors on the first modification, we can fit the curve of the \( SF(\gamma, m) \) networks. We also present the contrary modification algorithm (Alg. 3) to change the curve of \( SF(\gamma, m) \) networks to approach that of PA networks by “concentrating hubs”.

The following algorithm decentralises hubs by spreading the hubs of a network.

**Algorithm 2.** 1. Start with a simply connected network \( G \) (presumably generated with a PA process).

2. Select three percentages \( \alpha_1, \alpha_2, \alpha_3 \) for the definition of the poor, rich and giant nodes in the algorithm.

3. Sort the degree sequence, select the \( \alpha_1 \) lowest degree, and define the corresponding vertices as the poor nodes. Similarly, select the \( \alpha_2 \) and \( \alpha_3 \) highest degree, define them as the rich and giant nodes.

4. Delete all the links between the poor nodes and rich nodes.

5. Add the minimal number of links among the rich nodes to make them connected, and define them as a “club”.

6. Check the poor nodes sequentially, if one is not linked to the club, random choose one member in club and link this member to the poor node and add the poor node to the club, until the members of club includes all the vertices of \( G \).

7. Randomly pick up 2 linked giant nodes \( g_1, g_2 \), and 2 linked non-giant nodes \( v_1, v_2 \) which are not linked to \( g_1, g_2 \).
8. Apply the edge-switching method among $v_1, v_2, g_1, g_2$ \[43\]. (At least one of the possible edge switches will result in a connected graph.)

9. Repeat Step 7 and Step 8 until there is no links among the giant nodes.

In brief, Steps 4-6 cut the links between the group of rich nodes and group of poor nodes, and Step 7-9 change the structure among the rich nodes, since it is this group of rich nodes possess most of the edges. Steps 7-9 preserve the degree sequence. The result is that the PA networks become less hub-centric. We also note that, in Step 5, there is often no need to add links, since the group of rich nodes is often already connected.

We choose $\alpha_1 = 60\%$, $\alpha_2 = 5\%$, $\alpha_3 = 0.5\%$ for our modification algorithm, and apply it to the case with $m = 3$ and $m = 4$. The result with $m = 3$ is shown in Fig. 5, other results are similar, but omitted for conciseness.

The following algorithm concentrates hubs by modifying the initial network to make the hubs more strongly centralised.

**Algorithm 3.**

1. Start with a simply connected network $G$ (presumably generated with the SF($\gamma, m$) process).

2. Select three percentage $\alpha_1, \alpha_2, \alpha_3$ for the definition of the poor rich and giant nodes in the algorithm.

3. Sort the degree sequence, select the $\alpha_1$ lowest degree, and define the corresponding vertices as the poor nodes. Similarly, select the $\alpha_2$ and $\alpha_3$ highest degree, define them as the rich and giant nodes.

4. Traverse the poor nodes of $G$.

   (a) For each poor node $v_i$, if there exists another poor node among its adjacent nodes, then select randomly one node among them, and delete the links between them. Otherwise go to Step 5.

   (b) For $v_i$, select one node from the group of rich nodes with the assigned probability proportional to their degree, link $v_i$ with it.

5. Randomly pick up 2 not linked to giant nodes $g_1, g_2$, and 2 not linked to non-giant nodes $v_1, v_2$ which are connected with $g_1$ and $g_2$. 26
6. Apply the edge-switching method among $v_1, v_2, g_1, g_2$ [43]. (At least one of the possible edge switches will result in a connected graph.)

7. Repeat Step 5 and Step 6 until the subgraph induced by giant nodes is complete.

This reverse modification algorithm on $SF(\gamma, m)$ networks aims to generate interconnected hubs. Step 4 deletes the edges between the poor nodes and rich nodes as far as possible under the constraint of connectivity, and relinks these edges among rich nodes, and Step 5 forces the giant nodes to connect with each other. Hence, we can generate the hub-centric structure in networks, which results in the adjusted curves of the statistics for $SF(\gamma, m)$ networks approaching that of the PA networks.

Setting $\alpha_1 = 80\%, \alpha_2 = 5\%$ and $\alpha_3 = 0.5\%$ on this modification, the result for $m = 3$ is shown in Fig.6.

Appendix C: Acknowledgements

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