A statistical mechanics approach for scale-free networks and finite-scale networks

Ginestra Bianconi

The Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy

We present a statistical mechanics approach for the description of complex networks. We first define an energy and an entropy associated to a degree distribution which have a geometrical interpretation. Next we evaluate the distribution which extremize the free energy of the network. We find two important limiting cases: a scale-free degree distribution and a finite-scale degree distribution. The size of the space of allowed simple networks given these distribution is evaluated in the large network limit. Results are compared with simulations of algorithms generating these networks.

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Universality features of the structure of complex networks are very good candidate for a statistical mechanics treatment. While non-equilibrium aspects of these networks was first elucidated, later attention has been addressed to equilibrium properties of these graphs. In this paper we reveal some new property of finite-scale and scale-free networks. We characterize their different degree distribution as equilibrium degree distribution of a statistical mechanics problem written in terms of an energy and an entropy having a graphical interpretation. We observe that scale-free degree distribution for uncorrelated networks and in the large size limit correspond to structure in which the space of distinguishable simple graphs is strongly suppressed respect to the finite-scale distribution case.

Complex networks describe the intertwine relations between the elements of a variety of complex systems as different as the Internet and the biological networks of the cell [1,2,3]. To understand the interplay between their functions and their structure it is natural to study how far from optimal performance are these networks. Consequently optimal networks have been defined respect to the finite-scale distribution case.

A statistical mechanics approach for scale-free networks and finite-scale networks. In this paper we reveal some new property of finite-scale and scale-free networks. We characterize their different degree distribution as equilibrium degree distribution of a statistical mechanics problem written in terms of an energy and an entropy having a graphical interpretation. We observe that scale-free degree distribution for uncorrelated networks and in the large size limit correspond to structure in which the space of distinguishable simple graphs is strongly suppressed respect to the finite-scale distribution case.

In particular in [21] an energy of the type $E = -\sum k_i \log(k_i)$ was considered. The Montecarlo probability for a single move at $T = 1$ involve a linear preferential attachment mechanism with nodes of higher degree attracting links with higher probability. As a function of the temperature of the graph the model has two phase transitions. At the boundary between a sparse phase and a connected phase at a critical temperature $T_c \sim 1$ a scale-free network with exponent $\gamma = 3$ is found. In [13] the authors define a minifield theory whose Feynman diagrams are the networks of the ensemble. The networks of these ensemble map to a urn or “ball in the box” model [24] in which the “boxes” map to the nodes, the “balls” map to the edges of the graph and the probability of having $k$ edges at node $i$ is given by $p(k) \propto k^{-\gamma+1}$. The scale-free network ensemble is recovered in the case of trees or networks with finite number of cycles. The same approach is extend further to graphs with cycles in [15,19], in which the authors show that the mapping to the “ball in the box” model regards a distribution $p(k) \propto k^{-\gamma}$. In the canonical ensemble of Ref. [20], the authors describe an equilibrium network in which there is preferential attachment of nodes of high degree. The model again map to the urn model [24] with the probability $p(k) \sim k^{-\gamma}$. Finally another urn (“ball in the box” model ) is presented in [23] in which the same mapping between the network and the “ball/boxes” is made but the probability $p(k) = (k!)^3$ is chosen. This choice of the $p(k)$ probability involve some preferential attachment of the
dynamics when the heat-bath rule \[^2\] is considered. A finite scale network if recovered when \(\beta = 1\) for each node of the graph while a scale-free degree distribution with exponent \(\gamma = 2\) plus logarithmic corrections is obtained in the case of uniform distribution of effective \(\beta_i\) on each node \(i\) of the network.

In the following paper we will present a statistical mechanics treatment of complex networks in which we consider as thermodynamic quantities two terms having a precise graphical interpretation. The “energy” associated with the degree distribution will the logarithm of the number of allowed equivalent simple networks is possible to draw given a degree sequence. The “entropy” associated with a degree distribution will be the logarithm of the number of ways in which we can distribute \(L\) edges among the \(N\) nodes of the graph following the distribution \(\{N_k\}\). From this statistical mechanics approach we observe the emergence either of scale-free networks or finite-scale networks without been close to a phase transition in the network. The models is very closed related to the urn (“balls in the box”) models but with urn (“boxes”) mapping to the degree of the nodes and not to the nodes themselves. On the same time the dynamical rules which give rise to the network directly derives from the choice of the energy function we make. The appearance of scale-free degree distribution in the opposite limit of some finite-scale degree distributions can be put in relation with the findings of Ref. \[^26\, 27\, 28\].

where the normalization factor \((2L)!\) is chosen for convenience and the sum is extended over all distributions \(\{s_e\}\) with \(e = 1,\ldots,2L\) such that satisfy the conditions

\[
kN_k = \sum_e \delta_{s_e,k} \\
\sum_k N_k = N.
\]

In the following we will consider an the energy \(E(\{s_e\}) = E(\{N_k\})\) associated to the degree distribution of the network given by the logarithm of the number \(N_G\) of indistinguishable simple networks it is possible to draw given the degree sequence, i.e.

\[
E(\{N_k\}) = \log(N_G),
\]

(where simple networks are networks without tadpoles and double links). The number \(N_G\) can be expressed as

\[
N_G = e^{E(\{N_k\})} = \prod_k k^{N_k}.
\]

In fact, for every simple graph associated with the given distribution every permutation of the edges departing from each node generates the same set of links. These permutations are given by \(\prod_k k!N_k\), and consequently we derive Eq. \[^1\]. For \(z > 0\) low energy configurations are weighted more while for \(z < 0\) high energy configurations are more weighted in the partition function \(Z\) defined in Eq. \[^1\]. Consequently we expect that in the system for \(z < 0\) we should bound the energy per particle and therefore the maximal connectivity to a finite value \(K\). Since the energy associated to the distribution \(\{s_e\}\) only depends on the degree distribution \(\{N_k\}\) we can write the partition function as a sum over the distributions \(\{N_k\}\) with given energy \(E(\{N_k\})\) and entropy \(S(\{N_k\})\), i.e.

\[
Z = \frac{1}{(2L)!} \sum_{\{N_k\}} e^{-\frac{1}{2}E(\{N_k\})+S(\{N_k\})}.
\]

The entropic term \(S(\{N_k\})\) is equal to the logarithm of the number of ways \(N_{(N_k)}\) in which we can distribute \(2L\) edges into any degree sequence \(\{k_1,\ldots,k_N\}\) of distribution \(\{N_k\}\), or equivalently the number of sequences \(\{s_e\}\) which correspond to a degree distribution \(\{N_k\}\) and is given by

\[
e^{S(\{N_k\})} = N_{(N_k)} = \frac{(2L)!}{\prod_k (kN_k)!}.
\]
For $z > 0$ the equilibrium degree distribution $\{N_k\}$ will minimize the free energy of the network $F(\{N_k\}) = E(\{N_k\}) - zS(\{N_k\})$. For $z < 0$ the equilibrium distribution will maximize the free energy $E(\{N_k\}) - zS(\{N_k\})$.

The role of the parameter $z$ is to measure a tradeoff between the ‘energetic’ and the ‘entropic’ term in the definition of the free energy, as well as the temperature $T$ in classical statistical mechanics. Respect for the other statistical mechanics problems described in the introduction, this model can be cast into a “ball in the box” model with ball mapping to edges and “boxes” mapping to connectivity values and a weight $p(k) = (k!)^{-\beta/k}$ associated to each edge of the graph linked to a node of degree $k$ with $p(k) \propto k^{-\beta}$ for large values of $k$. In equation (5) the sum $\sum$ over the $\{N_k\}$ distributions is extended only to $\{N_k\}$ for which the total number of nodes $N$ and the total number of links $L$ in the network is fixed, i.e.

$$\sum_k N_k = N$$
$$\sum_k kN_k = 2L. \quad (7)$$

To enforce these conditions we introduce in (5) the delta functions in the integral form obtaining the expression

$$Z = \frac{1}{(2L)!} \int \frac{d\lambda}{2\pi} \int \frac{d\nu}{2\pi} \left. \sum_{\{N_k\}} \exp \left[ -\frac{1}{z} E(\{N_k\}) + S(\{N_k\}) \right] \right|_{\sum_k N_k = N}$$
$$-i\lambda (2L - \sum_k kN_k) - i\nu(N - \sum_k N_k) \right.$$  

$$= \int \frac{d\lambda}{2\pi} \int \frac{d\nu}{2\pi} \exp \left[ -i\lambda 2L - i\nu N + \sum_k \log G_k(\lambda, \nu) \right]$$
$$= \int \frac{d\lambda}{2\pi} \int \frac{d\nu}{2\pi} \exp[Nf(\lambda, \nu)] \quad (8)$$

where

$$G_k(\lambda, \nu) = \sum_{N_k} \frac{1}{(kN_k)!} \exp \left[ kN_k \left( i\lambda + i\nu/k - \frac{1}{zk} \log(k!) \right) \right]. \quad (9)$$

Assuming the sum over all $N_k$ can be approximated by the sum over all $L_k = kN_k = 1, 2, \ldots \infty$ we get

$$\log G_k(\lambda, \nu) = \exp \left[ i\lambda + i\nu/k - \frac{1}{zk} \log(k!) \right]$$

and

$$f(\lambda, \nu) = -i\langle k \rangle \lambda - i\nu + \frac{1}{N} \sum_k e^{\lambda + i\nu/k - \frac{1}{zk} \log(k!)}, \quad (10)$$

where $< k > = 2L/N$ indicates the average degree of the network. By evaluating (5) at the saddle point, deriving the argument of the exponential respect to $\lambda$ and $\nu$, we obtain

$$\langle k \rangle = \frac{1}{N} \sum_k e^{i\lambda + i\nu/k - \frac{1}{zk} \log(k!)}$$

and the marginal probability that $L_k = kn = \ell$ is given by

$$P(L_k = \ell = nk) = \frac{1}{\ell!} e^{-\ell/k \log(k)} Z_k(L, \ell, N)$$

with

$$Z_k(L, \ell, N) = \int \frac{d\lambda}{2\pi} \int \frac{d\nu}{2\pi} \exp[Nf(\lambda, \nu, \ell)] \quad (13)$$

and $f(\lambda, \nu, \ell) = i\langle k \rangle - \ell/N \lambda - i\nu(1 - \ell/(kN)) + \frac{1}{N} \sum_{k \neq k} \exp[i\lambda + i\nu/s - \frac{1}{zk} \log(s!)].$ If we develop (12) for $\ell \ll L$ and we use the Stirling approximation for factorials, we get that each variable $L_k$ is a Poisson variable with mean $< L_k >$ satisfying

$$\frac{< L_k >}{k} = < N_k > = k^{\gamma - 1} e^{\lambda + \nu/k}. \quad (14)$$

If we restrict ourself to the networks with finite average degree in the thermodynamic limit, the allowed values of $z$ are $z \in (-1, 1)$. From the expression (12) for $< N_k >$, if $z \in (0, 1)$ the equilibrium degree distribution is scale-free with a power-law tail characterized by the exponent $\gamma = \frac{1}{2} + 1$. The parameter $\nu \neq 0$ modulates the average degree of the graph constituting for $\nu > 0$ an effective lower cutoff of the distribution whereas the upper cutoff $K$ of the degrees is the natural cutoff of the distribution (14). A different scenario arises if $z < 0$, when the equilibrium network, in average (14) has a power-law degree distribution increasing with the degree $k$. In this case the Lyapunov functions $\nu$ and $\lambda$ cannot fix the average degree unless one introduces by hand an upper cutoff $K$ in the degree of the nodes of the order of magnitude of the average degree $\langle k \rangle$. We note here that also for $z \in (0, 1)$ it could be convenient to set by hand a structural cutoff $K \sim N^{1/2}$ for $z > 1/2$ in order to obtain an uncorrelated network.
The system of equations is solvable provided \( \langle k \rangle > 0 \) and the parameter of the distribution satisfying Eqs. (15), or with \( z < 0 \) and the parameter of the distribution satisfying Eqs. (16), are significantly different. In fact, for \( z > 0 \) there are highly connected nodes in the network and the degree distribution for large degrees \( k \) decays as a power-law with an exponent \( \gamma \) fixed by the value of \( z \). On the contrary, for \( z < 0 \) the predicted distribution (14) has a finite-scale and there are no highly connected nodes. Furthermore the topology of the network is very different from the one of the power-law case since the most connected nodes are also more abundant than less connected ones. In Figure 2 we show the distributions \( < N_k > \) which solve these equations for \( z > 0 \) positive and negative at different values of the average connectivity \( \langle k \rangle \) taking \( K = (1 + z) \langle k \rangle \) for \( z < 0 \).

Given the distributions (14) we can calculate the energy of the network as a function of \( z \) at fixed average connectivity \( \langle k \rangle \), always fixing the upper cutoff to \( K = (1 + z) \langle k \rangle \). In Figure 3 we present the energy of the network such that \( N_k = < N_k > \) as a function of \( z \) for different average connectivities.

The energy has a minimum in the limit \( z \to 0 \) when the equilibrium degree distribution is such that \( < N_k > \) is infinitely peaked around the average connectivity. On the contrary, in the limit \( z \to 1 \) where the degree distribution has a power-law exponent \( \gamma \to 2 \) the energy \( E(<N_k>) \) is at the maximum. We note here that the energy \( E(<N_k>) \) of complex networks calculated on the equilibrium degree distribution (14) is an extensive quantity in both cases \( z > 0 \) and \( z < 0 \).

In the case \( z < 0 \) and in the case \( z > 0 \) where we introduce by hand a structural cutoff \( K \sim N^{1/2} \) we can assume that the networks described in this paper are ran-
In our approach the "boxes" map to the degree of the connection with "ball in the box" problems [23, 24, 30]. In fact the total number of wiring it is possible to draw given 2L edges is given by (2L)!!. This number include all type of possible wiring of the edges including the ones which give rise to graphs which are not simple. Assuming that the graph is randomly wired, i.e. that the probability that a node with $k_i$ edges connect to a node with $k_j$ edges is a Poisson variable with average $k_i k_j/(<k>N)$ the probability II that the graph is simple is equal to [31]

$$\Pi = \prod_{i,j} \left(1 + \frac{k_i k_j}{<k>N} \right) e^{-k_i k_j/k} \sim e^{-\frac{1}{z} \left(\frac{k^2}{<k>}\right)^2}.$$  \hfill (18)

Finally in the expression (17) for $N_{SG}$ there is an additional terms which takes into account the equivalent wiring of the edges which is given by $e^{-E(N_k)}$. The term $\frac{<k^2>}{<k>^2}$ for scale-free graphs with cutoff $K \propto N^{1/2}$ is subleading respect to the energetic term $E(N_k)$ which dominates for large network sizes $N$. Consequently the number $N_{SG}$ of distinguishable simple graphs given a degree sequence is maximal for the graph with $z = 0$ and minimal for the scale-free graph with $\gamma \to 2$.

**I. ALGORITHMS**

From the derivation of our model it is evident the connection with "ball in the box" problems [23, 24, 30]. In our approach the "boxes" map to the degree of the nodes and the "balls" map to the edges of the graph. This makes a crucial difference respect with the models [15, 23], in which the "boxes" map to the nodes of the graph. The model, as well as a urn model can be simulated using a heat-bath rule [25] which then suggest the following algorithm:

- **Algorithm I**-
  - Choose randomly a "ball" randomly, i.e. choose a link $(i,j)$;
  - Choose a "box" randomly, i.e. chose a node $j'$ with a random value of its degree $k_j'$. This choice is implemented by choosing a node $j'$ with probability proportional to $1/N_{k(j')}$. 
  - Swap link $(i,j)$ with link $(i,j')$ with the heat bath rule algorithm, i.e. with probability $\Pi = (k_j' + 1)^{-1/z}$

From the shape of the linking probability $\Pi$ we infer that this algorithm, include some sort of inverse preferential attachment since rewiring to nodes with lower degree are more frequents. In Figure 4 we report the resulting degree distributions as a function of $\gamma$. The resulting distribution differ from the theoretical prediction for the presence of sharp lower cutoff. Nevertheless the distribution for large $k$ decays with power-law exponents close to the expectation (see Inset Figure 4) with the difference depending on finite size effects. We checked that the upper cutoff $K$ scale with the network size as $K \propto N^\alpha$ and $\alpha \propto z$.

For the case $z < 0$ the algorithm follow a rule similar to the one used in the case $z > 0$ with the further introduction of the ad hoc upper cutoff $K$ which is needed for the stability of the algorithm. Consequently the algorithm is as following:

- **Algorithm II**-

![FIG. 4: MonteCarlo results for networks of $N = 1000$ nodes and $L = 4000$ links for different value of $z$. The Inset report the power-law exponent $\gamma$ of the distribution as a function of $z$ (empty circles) and the predicted behavior (solid lines).](image1)

![FIG. 5: Degree distribution of the network evolving following algorithm II with different values of zeta. The networks have $N = 500$ nodes $L = 1000$ links have been evolved in 5000 L timesteps for 10 runs and have a maximal cutoff $K$ taken to be $K = [\langle k \rangle(1+z)]$.](image2)
• Choose randomly a link \((i, j)\);
• Choose node \(j'\) with a random value of its degree \(k_{j'}\), i.e. choose a node \(j'\) with probability proportional to \(1/Nk_{j'}\).
• Swap link \((i, j)\) with link \((i, j')\) only if \(k_{j'} < K\) and in this case with probability \(\Pi\) with
\[
\Pi = \frac{(k_{j'} + 1)^{-1/z}}{\sum_{r=1}^{N}(k_{r} + 1)^{-1/z}}. \tag{19}
\]
The results of the simulations following algorithm II are reported in Fig. 5. The algorithm requires a very long equilibration time respect to the case with \(z > 0\). Consequently we consider relatively small networks sizes up to 500 nodes. In the Inset we report the value the best value of the power-law fit to data together with the theoretical expectations.

In conclusion, the statistical mechanics treatment of complex networks shown in this paper is able to put in a similar context, but in opposite limits, the emergence of scale-free networks and finite-scale networks. Scale-free degree distribution correspond to higher energy states of the network respect to finite-scale networks. Especially homogeneous random graphs obtained for \(z = 0\) have minimal energy. Heterogenous scale-free networks correspond to higher energy states. We have shown that this implies that uncorrelated simple scale-free networks live in a space of allowed networks relatively small. We believe that correlations present in various complex networks describing many technological, biological and social systems can only further reduce this space. Consequently the evolutionary rule by which this degree distribution is selected reveal a tendency of minimizing this space.

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