Entropies of complex networks with hierarchically constrained topologies

Ginestra Bianconi,[1] Anthony C. C. Coolen,[2,3] and Conrad J. Perez Vicente[4]

[1]*Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy*

[2]*Department of Mathematics, King's College London, The Strand, London WC2R 2LS, United Kingdom*

[3]*Randall Division of Cell and Molecular Biophysics, King's College London, New Hunt's House, London SE1 1UL, United Kingdom*

[4]*Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, 08028 Barcelona, Spain*

The entropy of a hierarchical network topology in an ensemble of sparse random networks, with "hidden variables" associated with its nodes, is the log-likelihood that a given network topology is present in the chosen ensemble. We obtain a general formula for this entropy, which has a clear interpretation in some simple limiting cases. The results provide keys with which to solve the general problem of "fitting" a given network with an appropriate ensemble of random networks.

I. INTRODUCTION

Entropy is a key concept in information theory [1] and in the theory of dynamical systems [2]. In information theory, the problem of inference of a probability distribution on the basis of a finite number of independent observations is usually addressed using the maximum-likelihood principle or via the minimization of the Kullback-Leibler distance between a given (empirical) distribution and an inferred one. Recently, several studies have extended the tools of information theory along these lines in order to measure the performance of filtering procedures of correlation matrices in the case of multivariate data [3,4]. In the framework of graph theory large deviations of the ensemble of random Erdös and Renyi graphs where derived by studying the free energies of statistical mechanics models defined on them [5,6]. There is now increased interest, in the community of complex networks [7–9], in the definition of entropy measures that are related to the networks' topological structure [10] or to diffusion processes defined on them [11]. The inference problem applied to complex networks can be formulated as the identification of the ensemble of networks which retains the essential structural characteristics and complexity of a given real network realization. The identification of this ensemble is an active field of research. One aims to fit a given specific network with a suitable network ensemble that retains some information on its structure. Newman and Leicht have proposed this approach to find the community structure in a given network [12]. Later, this method was extended to define ensembles of networks that have other topological characteristics in common with the real network, such as the degree sequence and/or the degree correlations. As we add further features that a desired ensemble is to have in common with a given real network, we effectively consider ensembles with decreasing cardinality. The cardinality of an ensemble of networks with a given topology has attracted the attention of the graph theory community [13–15] and more recently also of the statistical mechanics community [10].

In this paper we evaluate the entropy of a given hierarchical topology in a "canonical" or "hidden variable" ensemble; i.e., we calculate the normalized logarithm of the probability that a given topology appears in this ensemble. By hierarchical topology we will mean the set of the generalized degrees of the nodes, defined as the sequence $\boldsymbol{k}_i=(k_i^1,k_i^2,\ldots,k_i^L)$ of the number of nodes at distance $1,2,\ldots,L$ from the node i. The canonical or hidden variable [16–20] ensembles are a generalization of the $G(N,p)$ ensemble for heterogeneous nodes. The heterogeneity of the nodes is described in terms of some hidden variables x_i, defined on each node i of the network, and the probability p_{ij} of a link between a node i and a node j is not p as in $G(N,p)$, but it is a general function $Q(x_i,x_j)$ of the hidden variables at i and j nodes. These ensembles correspond to networks which satisfy soft constraints; for example, the degree of a node is not fixed, but only the average degree of each node is fixed, allowing for Poissonian fluctuations.

We derive a general formula for the entropy of a given topology in a canonical ensemble using ideas and methods from the study of diluted combinatorial optimization problems and statistical mechanical systems on sparse networks [21–41]. In the simple case where we study the likelihood of a degree distribution of a network belonging to the chosen ensemble the entropy is found to be the Kullback-Leibler distance between the probability distribution of the degrees and the expected probability of the typical topology of the network.

The paper is structured as follows: in Sec. II we introduce the definition of the problem, in Sec. III we provide the asymptotic entropy expression of the network topology in a given ensemble, in Sec. IV we study the form that the entropy takes in special and relevant cases, and the conclusions are presented in Sec. V.

II. FORMULATION OF THE PROBLEM AND DEFINITIONS

To model the essential properties of a real network it is useful to think of it as an instance of an ensemble of networks. The ensemble can be either "microcanonical" or "canonical" depending on whether the networks in the ensemble are subject to hard or soft constraints. The main example of what we call a microcanonical ensemble is $G(N,M)$ where the number of links is fixed to be exactly M, and the main example of a canonical ensemble is $G(N,p)$ in which only

the average number of links $\langle M \rangle = pN(N-1)/2$ is fixed. These ensembles can be generalized to ensembles of random graphs with a given degree sequence and with a given hidden variable distribution. In this paper we will calculate the entropy of a given network topology (defined in terms of its hierarchical structure) in a general canonical ensemble. This entropy is defined as the probability that the given network topology is found in the canonical network ensemble under consideration.

A. Canonical ensembles

We consider networks characterized by N nodes (or "sites"), labeled $i = 1, \ldots, N$, and a symmetric matrix c with entries $c_{ij} \in \{0, 1\}$ that specify whether ($c_{ij} = 1$) or not ($c_{ij} = 0$) nodes i and j are connected. We choose $c_{ii} = 0$ for all i. We write the set of all such undirected networks as $\mathcal{G} = \{0, 1\}^{N(N-1)1/2}$. On this set $\mathcal{G}$ we introduce the following probability measure, in order to define an ensemble $\{\mathcal{G}, W\}$ of random networks:

$$
W(c|\{x\}) = \prod_{i<j} \left[\frac{c}{N} Q(x_i, x_j) \delta_{c_{ij}, 1} + \left(1 - \frac{c}{N} Q(x_i, x_j) \right) \delta_{c_{ij}, 0} \right].
$$

(1)

Note that this definition obeys $\Sigma_c W(c|\{x\}) = 1$ for all $\{x\}$. In (1) the $\{x\} = (x_1, \ldots, x_N)$ represent hidden variables, drawn for each site independently with statistics $p(x)$ to be defined later, and the function $Q(x, x') \geq 0$ is chosen such that $\Sigma_{xx'} p(x)p(x')Q(x, x') = 1$. The latter condition ensures that asymptotically c represents the average connectivity—viz., $\lim_{N \to \infty} \langle N^{-1} \Sigma_{ij} c_{ij} \rangle = c$. Note that throughout this paper the hidden variables $\{x_i\}$ can be scalar, discrete, or multidimensional.

B. Hierarchical constraints topologies

Next we introduce a hierarchy of single-site observables with the objective to characterize with increasing precision the local topology of a network $c \in \mathcal{G}$. They can be interpreted as generalized degrees $k_i(c) = (k_i^1(c), \ldots, k_i^L(c))$ of individual nodes i:

$$
k_i^\ell(c) = \sum_{j_1 \cdots j_\ell} c_{ij_1} c_{j_1 j_2} \cdots c_{j_{\ell-1} j_\ell} \in \{0, 1, 2, \ldots, N^\ell\}. \quad (2)
$$

In the absence of local loops, $k_i^\ell(c)$ measures the size (measured in number of nodes) of the local environment of node i, at a distance of ℓ links. However, in this tree the nodes are counted with a multiplicity equal to their number of descendants encountered; similarly, in the case of local loops, nodes that can be visited from site i via multiple routes of length $\leq \ell$ are counted with this multiplicity. Note that $k_i^1(c) = \Sigma_j c_{ij}$ is the ordinary degree of node i and that (2) can also be written as

$$
k_i^1(c) = \sum_j c_{ij}, \quad k_i^{\ell+1}(c) = \sum_j c_{ij} k_j^\ell(c). \quad (3)
$$

By definition, if $k_i^1(c) = 0$, then $k_i^\ell(c) = 0$ for all ℓ. It is now natural to characterize the *global* topology of a network c

either by giving its N generalized degree vectors $\{k_1(c), \ldots, k_N(c)\}$ themselves or by giving the collective generalized degree statistics, conditioned on the values of the hidden variables—i.e.,

$$
P(k|x, c) = P(k_1, \ldots, k_L | x, c) = \frac{1}{Np(x)} \sum_{i=1}^N \delta_{k, k_i(c)} \delta(x - x_i),
$$

(4)

where we adopt the convention that always $k = (k_1, \ldots, k_L) \in \mathbb{N}^L$, unless indicated otherwise. Note that the definition (4) obeys $\Sigma_k P(k|x, c) = 1$ for all x and c.

C. Entropy of a network contraint topology in a given ensemble

Our goal is to quantify to what extent the above characterization of networks, by the generalized degrees $\{k\} \equiv \{k_1, \ldots, k_N\}$ or by the degree statistics $P_L(k)$, specifies their microstructure. This can be measured by the effective number of networks in the ensemble $\{\mathcal{G}, W\}$ that meet the relevant contraints—i.e., (apart from a constant) by the Boltzmann entropies:
constrain degrees:

$$
\Omega_L[\{k\}|\{x\}] = \frac{1}{N} \ln \sum_{c \in \mathcal{G}} W(c|\{x\}) \prod_i \delta_{k_i, k_i(c)}, \quad (5)
$$

constrain statistics:

$$
\Omega_L[P|\{x\}] = \frac{1}{N} \ln \sum_{c \in \mathcal{G}} W(c|\{x\}) \prod_{k, x} \delta[P(k|x) - P(k|x, c)]
$$

$$
= \frac{1}{N} \ln \sum_{k_1 \cdots k_N} \prod_{k, x} \delta \left[P(k|x) - \frac{\sum_i \delta_{k, k_i} \delta[x - x_i]}{Np(x)} \right]
$$

$$
\times e^{N \Omega_L[\{k\}|\{x\}]}. \quad (6)
$$

The larger $\Omega_L[\cdots]$, the larger the effective number of graphs with the imposed global topology—viz., $\{k_i\}$ or $P(k|x)$—so the less specific is the proposed macroscopic topology characterization. We will find that generally $\Omega_L[\cdots] = O(N^0)$ as $N \to \infty$. The remainder of this paper deals with the calculation of (5) and (6) in the limit $N \to \infty$ and their dependence on the choices made for $P(k|x)$ and the for ensemble characteristics as defined by $p(x)$ and $Q(x, x')$.

III. ASYMPTOTIC VALUES OF THE ENTROPY OF NETWORK TOPOLOGY IN A GIVEN ENSEMBLE

A. Derivation of steepest-descent extremization formulas

Since the ensemble (1) is invariant under all node permutations, the difference between the two formulas (5) and (6) should reflect only the node permutation freedom that is present in (6) but absent from (5). We evaluate (5) and (6) by writing each Kronecker δ and each δ function in integral form. Upon defining the shorthand $k_i^0 = 1$ for all i and $\omega_i \cdot k_i = \Sigma_{\ell=1}^L \omega_i^\ell k_i^\ell$, expression (3) allows us to simplify the term $\delta_{k, k_i(c)}$ to

$$\delta_{k_i,k_i(c)} = \int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}_i e^{i\boldsymbol{\omega}_i \cdot k_i}}{(2\pi)^L} \exp\left(-i\sum_j c_{ij}\sum_{\ell=1}^{L} \omega_i^\ell k_j^{\ell-1}\right). \quad (7)$$

We next define

$$D[\{\boldsymbol{\omega},\boldsymbol{k}\}|\{x\}] = \sum_{\boldsymbol{c}\in\mathcal{G}} W(\boldsymbol{c}|\{x\}) \exp\left(-i\sum_{ij} c_{ij}\sum_{\ell=1}^{L} \omega_i^\ell k_j^{\ell-1}\right) \quad (8)$$

and subsequently find out that our two entropies can be written in the form

$$\Omega_L[\{\boldsymbol{k}\}|\{x\}] = \frac{1}{N}\ln\int_{-\pi}^{\pi}\prod_i\left[\frac{d\boldsymbol{\omega}_i e^{i\boldsymbol{\omega}_i\cdot k_i}}{(2\pi)^L}\right] D[\{\boldsymbol{\omega},\boldsymbol{k}\}|\{x\}], \quad (9)$$

$$\Omega_L[P|\{x\}] = \frac{1}{N}\ln\int\prod_{\boldsymbol{k},x}\left[\frac{d\hat{P}(\boldsymbol{k}|x)e^{iN\hat{P}(\boldsymbol{k}|x)P(\boldsymbol{k}|x)}}{2\pi/N}\right]$$

$$\times\sum_{\boldsymbol{k}_1\cdots\boldsymbol{k}_N}\exp\left(N\Omega_L[\{\boldsymbol{k}\}|\{x\}] - i\sum_i \hat{P}(\boldsymbol{k}_i|x_i)\right)$$

$$= \frac{1}{N}\lim_{\Delta\to 0}\ln\int\prod_{\boldsymbol{k},x}\left[\frac{d\hat{P}(\boldsymbol{k}|x)e^{iN\Delta\hat{P}(\boldsymbol{k}|x)P(\boldsymbol{k}|x)}}{2\pi/N\Delta}\right]$$

$$\times\sum_{\boldsymbol{k}_1\cdots\boldsymbol{k}_N}\int_{-\pi}^{\pi}\prod_i\left[\frac{d\boldsymbol{\omega}_i e^{i[\boldsymbol{\omega}_i\cdot k_i - \hat{P}(\boldsymbol{k}_i|x_i)/p(x_i)]}}{(2\pi)^L}\right]$$

$$\times D[\{\boldsymbol{\omega},\boldsymbol{k}\}|\{x\}]. \quad (10)$$

The core of the problem is apparently to calculate the function $D[\{\boldsymbol{\omega},\boldsymbol{k}\}]$ in (8), which involves the introduction of a measure $W(\boldsymbol{\omega},\boldsymbol{k},x|\{\boldsymbol{\omega},\boldsymbol{k}\}) = N^{-1}\Sigma_i\delta_{\boldsymbol{k},k_i}\delta[x-x_i]\delta[\boldsymbol{\omega}-\boldsymbol{\omega}_i]$:

$$D[\{\boldsymbol{\omega},\boldsymbol{k}\}|\{x\}] = \prod_{i<j}\left\{1 + \frac{c}{N}Q(x_i,x_j)\right.$$

$$\times\left[\exp\left(-i\sum_{\ell=1}^{L}[\omega_i^\ell k_j^{\ell-1} + \omega_j^\ell k_i^{\ell-1}]\right) - 1\right]\right\}$$

$$= \exp\left\{\frac{1}{2}cN\int dx\,dx'\,Q(x,x')\int_{-\pi}^{\pi}d\boldsymbol{\omega}\,d\boldsymbol{\omega}'\right.$$

$$\times\sum_{\boldsymbol{k}\boldsymbol{k}'} W(\boldsymbol{\omega},\boldsymbol{k},x|\cdots)\times W(\boldsymbol{\omega}',\boldsymbol{k}',x'|\cdots)$$

$$\times\left[\exp\left(-i\sum_{\ell=1}^{L}[\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1}]\right) - 1\right]$$

$$\left. + O(N^0)\right\}. \quad (11)$$

We isolate $W(\cdots|\cdots)$ via suitable integrations over δ functions, using the functional measure $\{dW\} = \lim_{\Delta\boldsymbol{\omega}\to 0}\lim_{\Delta x\to 0}\Pi_{\boldsymbol{\omega},\boldsymbol{k},x}[dW(\boldsymbol{\omega},\boldsymbol{k},x)\Delta\boldsymbol{\omega}\Delta x\sqrt{N/2\pi}]$, resulting in

$$D[\{\boldsymbol{\omega},\boldsymbol{k}\}] = \int\{dW\,d\hat{W}\}\exp\left(iN\int_{-\pi}^{\pi}d\boldsymbol{\omega}dx\right.$$

$$\times\sum_{\boldsymbol{k}}\hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)W(\boldsymbol{\omega},\boldsymbol{k},x) + O(N^0)\right)$$

$$\times\exp\left(\frac{1}{2}cN\int dx\,dx'\,Q(x,x')\int_{-\pi}^{\pi}d\boldsymbol{\omega}\,d\boldsymbol{\omega}'\right.$$

$$\times\sum_{\boldsymbol{k}\boldsymbol{k}'} W(\boldsymbol{\omega},\boldsymbol{k},x)W(\boldsymbol{\omega}',\boldsymbol{k}',x')\right)$$

$$\times\left[\exp\left(-i\sum_{\ell=1}^{L}[\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1}]\right) - 1\right]$$

$$\times\exp\left(-i\sum_i\hat{W}(\boldsymbol{\omega}_i,\boldsymbol{k}_i,x_i)\right). \quad (12)$$

Now only the last line contains microscopic variables, and it factorizes fully over the nodes of the network. Upon inserting (12) into (9) and (10) this allows us to evaluate both expressions for $N\to\infty$ via steepest-descent integration over the distributions $W(\boldsymbol{\omega},\boldsymbol{k},x)$, leading to

$$\Omega_L[\{\boldsymbol{k}\}|\{x\}] = \text{extr}_{\{W,\hat{W}\}}\Psi_1[\{W,\hat{W}\}], \quad (13)$$

$$\Omega_L[P|\{x\}] = \text{extr}_{\{W,\hat{W},\hat{P}\}}\Psi_2[\{W,\hat{W},\hat{P}\}], \quad (14)$$

with the functions

$$\Psi_1[\{W,\hat{W}\}] = i\int_{-\pi}^{\pi}d\boldsymbol{\omega}\,dx\sum_{\boldsymbol{k}}\hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)W(\boldsymbol{\omega},\boldsymbol{k},x) + \Phi[\{W\}]$$

$$+ \int dx\,p(x)\sum_{\boldsymbol{k}} P(\boldsymbol{k}|x)$$

$$\times\ln\int_{-\pi}^{\pi}\frac{d\boldsymbol{\omega}}{(2\pi)^L}e^{i[\boldsymbol{\omega}\cdot k - \hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)]}, \quad (15)$$

$$\Psi_2[\{W,\hat{W},\hat{P}\}] = i\int_{-\pi}^{\pi}d\boldsymbol{\omega}\,dx\sum_{\boldsymbol{k}}\hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)W(\boldsymbol{\omega},\boldsymbol{k},x)$$

$$+ \Phi[\{W\}] + i\int dx\sum_{\boldsymbol{k}}\hat{P}(\boldsymbol{k}|x)P(\boldsymbol{k}|x)$$

$$+ \int dx\,p(x)\ln\int_{-\pi}^{\pi}\frac{d\boldsymbol{\omega}}{(2\pi)^L}$$

$$\times\sum_{\boldsymbol{k}} e^{i[\boldsymbol{\omega}\cdot k - \hat{P}(\boldsymbol{k}|x)/p(x) - \hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)]}, \quad (16)$$

where

$$\Phi[\{W\}] = \frac{1}{2}c \int dx\, dx'\, Q(x,x') \int_{-\pi}^{\pi} d\boldsymbol{\omega}\, d\boldsymbol{\omega}'$$

$$\times \sum_{\boldsymbol{k}\boldsymbol{k}'} W(\boldsymbol{\omega},\boldsymbol{k},x) W(\boldsymbol{\omega}',\boldsymbol{k}',x')$$

$$\times \left[\exp\left(-i\sum_{\ell=1}^{L} [\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1}] \right) - 1 \right]. \tag{17}$$

It will be convenient to introduce new functions $Q(\boldsymbol{k}|x) = \exp[-i\hat{P}(\boldsymbol{k}|x)/p(x)]$ and $V(\boldsymbol{\omega},\boldsymbol{k},x) = \exp[-i\hat{W}(\boldsymbol{\omega},\boldsymbol{k},x)]$ so that our saddle-point equations simplify to

$$\Omega_L[\{\boldsymbol{k}\}|\{x\}] = \mathrm{extr}_{\{V,W\}} \widetilde{\Psi}_1[\{V,W\}], \tag{18}$$

$$\Omega_L[P|\{x\}] = \mathrm{extr}_{\{Q,V,W\}} \widetilde{\Psi}_2[\{Q,V,W\}], \tag{19}$$

with the functions

$$\widetilde{\Psi}_1[\{V,W\}] = \Phi[\{W\}] - \int_{-\pi}^{\pi} d\boldsymbol{\omega}\, dx \sum_{\boldsymbol{k}} W(\boldsymbol{\omega},\boldsymbol{k},x) \ln V(\boldsymbol{\omega},\boldsymbol{k},x)$$

$$+ \int dx\, p(x) \sum_{\boldsymbol{k}} P(\boldsymbol{k}|x) \ln \int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}}{(2\pi)^L}$$

$$\times V(\boldsymbol{\omega},\boldsymbol{k},x) e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}, \tag{20}$$

$$\widetilde{\Psi}_2[\{Q,V,W\}] = \Phi[\{W\}]$$

$$- \int_{-\pi}^{\pi} d\boldsymbol{\omega}\, dx \sum_{\boldsymbol{k}} W(\boldsymbol{\omega},\boldsymbol{k},x) \ln V(\boldsymbol{\omega},\boldsymbol{k},x)$$

$$- \int dx\, p(x) \sum_{\boldsymbol{k}} P(\boldsymbol{k}|x) \ln Q(\boldsymbol{k}|x)$$

$$+ \int dx\, p(x) \ln \sum_{\boldsymbol{k}} Q(\boldsymbol{k}|x) \int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}}{(2\pi)^L}$$

$$\times V(\boldsymbol{\omega},\boldsymbol{k},x) e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}. \tag{21}$$

B. Simplification and reduction of the functional saddle-point equations

We can now do the functional variations of $\widetilde{\Psi}_1[\cdots]$ and $\widetilde{\Psi}_2[\cdots]$ and find our saddle-point equations from which to solve $\{Q,V,W\}$. For $\widetilde{\Psi}_1[\cdots]$ (referring to ensembles with constrained generalized degrees) these are found to be the following:

$$\ln V(\boldsymbol{\omega},\boldsymbol{k},x) = c \int dx'\, Q(x,x') \int_{-\pi}^{\pi} d\boldsymbol{\omega}' \sum_{\boldsymbol{k}'} W(\boldsymbol{\omega}',\boldsymbol{k}',x')$$

$$\times \left[\exp\left(-i\sum_{\ell=1}^{L} [\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1}] \right) - 1 \right], \tag{22}$$

$$W(\boldsymbol{\omega},\boldsymbol{k},x) = \frac{p(x)P(\boldsymbol{k}|x)V(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}}{\int_{-\pi}^{\pi} d\boldsymbol{\omega}'\, V(\boldsymbol{\omega}',\boldsymbol{k},x)e^{i\boldsymbol{\omega}'\cdot\boldsymbol{k}}}. \tag{23}$$

For $\widetilde{\Psi}_2[\cdots]$ (referring to ensembles with constrained distributions of generalized degrees) these are found to be the following:

$$\ln V(\boldsymbol{\omega},\boldsymbol{k},x) = c \int dx'\, Q(x,x') \int_{-\pi}^{\pi} d\boldsymbol{\omega}' \sum_{\boldsymbol{k}'} W(\boldsymbol{\omega}',\boldsymbol{k}',x')$$

$$\times \left[\exp\left(-i\sum_{\ell=1}^{L} [\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1}] \right) - 1 \right], \tag{24}$$

$$W(\boldsymbol{\omega},\boldsymbol{k},x) = \frac{p(x)Q(\boldsymbol{k}|x)V(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}}{\sum_{\boldsymbol{k}'} Q(\boldsymbol{k}'|x)\int_{-\pi}^{\pi} d\boldsymbol{\omega}'\, V(\boldsymbol{\omega}',\boldsymbol{k}',x)e^{i\boldsymbol{\omega}'\cdot\boldsymbol{k}'}}, \tag{25}$$

$$P(\boldsymbol{k}|x) = \frac{Q(\boldsymbol{k}|x)\int_{-\pi}^{\pi} d\boldsymbol{\omega}\, V(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}}{\sum_{\boldsymbol{k}'} Q(\boldsymbol{k}'|x)\int_{-\pi}^{\pi} d\boldsymbol{\omega}\, V(\boldsymbol{\omega},\boldsymbol{k}',x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}'}}. \tag{26}$$

The last equation is easily solved, viz.,

$$Q(\boldsymbol{k}|x) = \frac{P(\boldsymbol{k}|x)}{\int_{-\pi}^{\pi} d\boldsymbol{\omega}\, V(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}}, \tag{27}$$

whereas in both cases (constrained degrees versus constrained degree statistics) we can eliminate immediately the kernels $W(\boldsymbol{\omega},\boldsymbol{k},x)$, leaving us in either case with a closed problem for the kernel $V(\boldsymbol{\omega},\boldsymbol{k},x)$ only. Upon inserting the solution (27) into (26) one finds that this remaining problem is in fact *identical* for both types of constraints—namely,

$$\log V(\boldsymbol{\omega},\boldsymbol{k},x) = c \int dx' \, p(x')Q(x,x')\sum_{\boldsymbol{k}'} P(\boldsymbol{k}'|x') \frac{\int_{-\pi}^{\pi} d\boldsymbol{\omega}' V(\boldsymbol{\omega}',\boldsymbol{k}',x')e^{i\boldsymbol{\omega}'\cdot\boldsymbol{k}} \left[\exp\left(-i\sum_{\ell=1}^{L} \left[\omega_\ell k'_{\ell-1} + \omega'_\ell k_{\ell-1} \right] \right) - 1 \right]}{\int_{-\pi}^{\pi} d\boldsymbol{\omega}' V(\boldsymbol{\omega}',\boldsymbol{k}',x')e^{i\boldsymbol{\omega}'\cdot\boldsymbol{k}'}}. \quad (28)$$

In addition one finds that (23) holds in both cases. The solution of (28) is of the form

$$V(\boldsymbol{\omega},\boldsymbol{k},x) = \exp\left(-c \int dx' \, Q(x,x')p(x') \right) \exp\left[c \sum_{\boldsymbol{\xi}\in\mathbb{N}^L} \gamma(\boldsymbol{k},\boldsymbol{\xi},x)e^{-i\boldsymbol{\omega}\cdot\boldsymbol{\xi}} \right], \quad (29)$$

where $\gamma(\boldsymbol{k},\boldsymbol{\xi},x)$ then obeys

$$\gamma(\boldsymbol{k},\boldsymbol{\xi},x) = \int dx' \, p(x')Q(x,x')\sum_{\boldsymbol{k}'} P(\boldsymbol{k}'|x')\prod_{\ell=1}^{L} \delta_{\xi_\ell,k'_{\ell-1}} \frac{\int_{-\pi}^{\pi} d\boldsymbol{\omega} \exp\left[i\sum_{\ell=1}^{L} \omega_\ell(k'_\ell - k_{\ell-1}) + c\sum_{\boldsymbol{\xi}'\in\mathbb{N}^L} \gamma(\boldsymbol{k}',\boldsymbol{\xi}',x')e^{-i\boldsymbol{\omega}\cdot\boldsymbol{\xi}'} \right]}{\int_{-\pi}^{\pi} d\boldsymbol{\omega} \exp\left[i\boldsymbol{\omega}\cdot\boldsymbol{k}' + c\sum_{\boldsymbol{\xi}'\in\mathbb{N}^L} \gamma(\boldsymbol{k}',\boldsymbol{\xi}',x')e^{-i\boldsymbol{\omega}\cdot\boldsymbol{\xi}'} \right]}. \quad (30)$$

The two integrals over $\boldsymbol{\omega}$ in the latter fraction can be done. Both are of the form

$$\mathcal{I}(\boldsymbol{k},\boldsymbol{k}',x) = \int_{-\pi}^{\pi} d\boldsymbol{\omega} \exp\left[i\boldsymbol{\omega}\cdot\boldsymbol{k} + c\sum_{\boldsymbol{\xi}'\in\mathbb{N}^L} \gamma(\boldsymbol{k}',\boldsymbol{\xi}',x')e^{-i\boldsymbol{\omega}\cdot\boldsymbol{\xi}'} \right] = (2\pi)^L \sum_{m\geqslant 0} \frac{c^m}{m!} \sum_{\boldsymbol{\xi}^1\dots\boldsymbol{\xi}^m\in\mathbb{N}^L} \left[\prod_{n=1}^{m} \gamma(\boldsymbol{k}',\boldsymbol{\xi}^n,x') \right] \delta_{\boldsymbol{k},\sum_{n\leqslant m}\boldsymbol{\xi}^n}, \quad (31)$$

and hence the equation for $\gamma(\boldsymbol{k},\boldsymbol{\xi},x)$ becomes

$$\gamma(\boldsymbol{k},\boldsymbol{\xi},x) = \delta_{\xi_1,1} \int dx' \, p(x')Q(x,x')\sum_{\boldsymbol{k}'} P(\boldsymbol{k}'|x')\prod_{\ell=1}^{L-1} \delta_{\xi_{\ell+1},k'_\ell} \frac{\sum_{m\geqslant 0} \frac{c^m}{m!} \sum_{\boldsymbol{\xi}^1\dots\boldsymbol{\xi}^m\in\mathbb{N}^L} \left[\prod_{n=1}^{m} \gamma(\boldsymbol{k}',\boldsymbol{\xi}^n,x') \right] \prod_{\ell=1}^{L} \delta_{k'_\ell,k_{\ell-1}+\sum_{n\leqslant m}\xi^n_\ell}}{\sum_{m\geqslant 0} \frac{c^m}{m!} \sum_{\boldsymbol{\xi}^1\dots\boldsymbol{\xi}^m\in\mathbb{N}^L} \left[\prod_{n=1}^{m} \gamma(\boldsymbol{k}',\boldsymbol{\xi}^n,x') \right] \delta_{\boldsymbol{k}',\sum_{n\leqslant m}\boldsymbol{\xi}^n}} \quad (32)$$

$$= \delta_{\xi_1,1} \int dx' \, p(x')Q(x,x')\sum_{\boldsymbol{k}'} \frac{k'_1}{c} P(\boldsymbol{k}'|x')\prod_{\ell=1}^{L-1} \delta_{\xi_{\ell+1},k'_\ell} \frac{\sum_{\boldsymbol{\xi}^1\dots\boldsymbol{\xi}^{k'_1-1}} \left[\prod_{n=1}^{k'_1-1} \gamma(\boldsymbol{k}',\boldsymbol{\xi}^n,x') \right] \prod_{\ell=1}^{L} \delta_{k'_\ell,k_{\ell-1}+\sum_{n<k'_1}\xi^n_\ell}}{\sum_{\boldsymbol{\xi}^1\dots\boldsymbol{\xi}^{k'_1}} \left[\prod_{n=1}^{k'_1} \gamma(\boldsymbol{k}',\boldsymbol{\xi}^n,x') \right] \delta_{\boldsymbol{k}',\sum_{n\leqslant k'_1}\boldsymbol{\xi}^n}}, \quad (33)$$

where we use the conventions that $[\prod_{n=1}^{m} u_n]_{m=0} \equiv 1$, $[\sum_{n=1}^{m} u_n]_{m=0} \equiv 0$, and $[\sum_{\xi_1\dots\xi_m} u(\xi_1,\dots,\xi_m)]_{m=0} \equiv 1$. If $L=1$, we have $\boldsymbol{k} = \to k$ and $\boldsymbol{\xi}\to 1$, so $\gamma(\boldsymbol{k},\boldsymbol{\xi},x)\to\gamma(k,x)$. This describes the situation where the degrees are not generalized, but measure as usual only the number of direct links per node. Here our equation for $\gamma(\cdots)$ simplifies drastically to

$$L=1: \quad \gamma(k,x) = \int dx' \, p(x')Q(x,x')\sum_{k'} k' \frac{P(k'|x')}{c\gamma(k',x')}. \quad (34)$$

The right-hand side is clearly independent of k, so $\gamma(k,x) = \gamma(x)$ with

$$\gamma(x) = \int dx' \, p(x') \frac{Q(x,x')}{c \, \gamma(x')} \sum_k k P(k|x').$$ (35)

If $L > 1$, we can manipulate at most some further Kronecker δ's, and the final form is therefore

$$\gamma(\boldsymbol{k}, \boldsymbol{\xi}, x) = \frac{\xi_2 \delta_{\xi_1, 1}}{c} \int dx' \, p(x') Q(x, x') \sum_{k' \geqslant 0} P(\xi_2, \ldots, \xi_L, k'|x')$$

$$\times \frac{\sum_{\boldsymbol{\xi}^1 \ldots \boldsymbol{\xi}^{\xi_2 - 1}} \left[\prod_{n=1}^{\xi_2 - 1} \gamma((\xi_2, \ldots, \xi_L, k'), \boldsymbol{\xi}^n, x') \right] \delta_{k', k_{L-1} + \sum\limits_{n < \xi_2} \xi_L^n} \prod_{\ell=1}^{L-1} \delta_{\xi_{\ell+1} - k_{\ell-1}, \sum\limits_{n < \xi_2} \xi_\ell^n}}{\sum_{\boldsymbol{\xi}^1 \ldots \boldsymbol{\xi}^{\xi_2}} \left[\prod_{n=1}^{\xi_2} \gamma((\xi_2, \ldots, \xi_L, k'), \boldsymbol{\xi}^n, x') \right] \delta_{k', \sum\limits_{n \leqslant \xi_2} \xi_L^n} \prod_{\ell=1}^{L-1} \delta_{\xi_{\ell+1}, \sum\limits_{n \leqslant \xi_2} \xi_\ell^n}}.$$ (36)

C. Simplification of the asymptotic entropy formulas

At this stage we insert our previous results for the kernels $\{V, W, Q\}$ into (18)–(21) to arrive at more explicit expressions for the asymptotic entropies, which will only involve the function $\gamma(\boldsymbol{k}, \boldsymbol{\xi}, x)$ of (36). The first step is to substitute expression (27) into (21). This leads, in combination with the fact that at the relevant saddle points the kernels $\{V, W\}$ obey identical equations for the two cases (constrained generalized degrees versus constrained statistics of generalized degrees), to the simple and natural relation between our two entropies:

$$\lim_{N \to \infty} \Omega_L[P|\{x\}] = \lim_{N \to \infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}]$$
$$- \int dx \, p(x) \sum_{\boldsymbol{k}} P(\boldsymbol{k}|x) \ln P(\boldsymbol{k}|x). \quad (37)$$

The extra freedom to construct microscopic network realizations in the case where we only constrain the generalized degree distribution, as opposed to constraining the actual values of the generalized degrees, is measured by the Shannon entropy of the imposed distribution $P(\boldsymbol{k}|x)$.

Relation (37) could be also derived from the definition of $\Omega[\cdots]$, given in (5) and (6). In fact, we can observe that the probability $W(\boldsymbol{c}|\{x\})$ present in the definition (5) of $\Omega[\{\boldsymbol{k}\}|\{x\}]$ is invariant under all permutations of the labels of those nodes that have the same hidden variable x; this follows directly from definition (1). Consequently $\Omega_L[\{\boldsymbol{k}\}|\{x\}]$ must also be invariant under any permutation of the labels of nodes with same value of x. It follows that $\Omega_L[\{\boldsymbol{k}\}|\{x\}]$ is dependent on the degree sequence $\{\boldsymbol{k}\}$ only through the distributions $\{P(\boldsymbol{k}|x)\}$. Therefore, we can use this simple insight to predict the relation between $\Omega_L[\{\boldsymbol{k}\}|\{x\}]$ and $\Omega_L[P|\{x\}]$, Eq. (37). In fact, because $\Omega_L[\{\boldsymbol{k}\}|\{x\}]$ must be only dependent on the distribution $P(\boldsymbol{k}|x)$, we have that

$$\Omega_L[P|\{x\}] = \frac{1}{N} \ln \sum_{\boldsymbol{k}_1 \cdots \boldsymbol{k}_N} \prod_{\boldsymbol{k}, x} \delta \left[P(\boldsymbol{k}|x) - \frac{\sum_i \delta_{\boldsymbol{k}, \boldsymbol{k}_i} \delta[x - x_i]}{N p(x)} \right] e^{N \Omega_L[\{\boldsymbol{k}\}|\{x\}]}$$
$$= \frac{1}{N} \ln e^{N \Omega_L[\{\boldsymbol{k}\}|\{x\}]} \prod_x \frac{[N p(x)]!}{\prod_{\boldsymbol{k}}[N p(x) P(\boldsymbol{k}|x)]!},$$ (38)

where $\{\boldsymbol{k}\}$ is any generalized degree sequence with degree distributions $P(\boldsymbol{k}|x)$. Using (38) we can derive relation (37).

In order to evaluate $\lim_{N \to \infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}]$ we only need to express $\lim_{N \to \infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}]$ in terms of the function $\gamma(\boldsymbol{k}, \boldsymbol{\xi}, x)$. We first note that at the relevant saddle point the function $\Phi[\{W\}]$, Eq. (17), takes the value

$$\Phi[\{W\}] = \frac{1}{2} \int dx \int_{-\pi}^{\pi} d\boldsymbol{\omega} \sum_{\boldsymbol{k}} W(\boldsymbol{\omega}, \boldsymbol{k}, x) \ln V(\boldsymbol{\omega}, \boldsymbol{k}, x).$$ (39)

Insertion into (20), followed by elimination of $W(\boldsymbol{\omega}, \boldsymbol{k}, x)$ via (23), leads us to

$$\lim_{N \to \infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}]$$
$$= \int dx \, p(x) \sum_{\boldsymbol{k}} P(\boldsymbol{k}|x) \ln \int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}}{(2\pi)^L} V(\boldsymbol{\omega}, \boldsymbol{k}, x) e^{i\boldsymbol{\omega} \cdot \boldsymbol{k}}$$
$$- \frac{1}{2} \int dx \, p(x) \sum_{\boldsymbol{k}} P(\boldsymbol{k}|x)$$
$$\times \frac{\int_{-\pi}^{\pi} d\boldsymbol{\omega} e^{i\boldsymbol{\omega} \cdot \boldsymbol{k}} V_0(\boldsymbol{\omega}, \boldsymbol{k}, x) \ln V(\boldsymbol{\omega}, \boldsymbol{k}, x)}{\int_{-\pi}^{\pi} d\boldsymbol{\omega} V_0(\boldsymbol{\omega}, \boldsymbol{k}, x) e^{i\boldsymbol{\omega} \cdot \boldsymbol{k}}},$$ (40)

where $V_0(\boldsymbol{\omega}, \boldsymbol{k}, x) = V(\boldsymbol{\omega}, \boldsymbol{k}, x) \exp[c \int dx' \, Q(x, x') p(x')]$. The final step is the elimination of $V(\boldsymbol{\omega}, \boldsymbol{k}, x)$ via (29), followed

by integration over $\boldsymbol{\omega}$, using the property that $\gamma(\boldsymbol{k},\boldsymbol{\xi},x)=0$ unless $\xi_1=1$:

$$\int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}}{(2\pi)^L} V_0(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}$$

$$= \sum_{m\geqslant 0} \frac{c^m}{m!} \sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^m} \prod_{n\leqslant m} [\gamma(\boldsymbol{k},\boldsymbol{\xi}^n,x)]\delta_{\boldsymbol{k},\Sigma_{n\leqslant m}\boldsymbol{\xi}^n} = \delta_{\boldsymbol{k},\boldsymbol{0}}$$

$$+ \frac{c^{k_1}\theta\left[k_1-\frac{1}{2}\right]}{k_1!} \sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^{k_1}} \prod_{n\leqslant k_1} [\gamma(\boldsymbol{k},\boldsymbol{\xi}^n,x)]\delta_{\boldsymbol{k},\Sigma_{n\leqslant k_1}\boldsymbol{\xi}^n},$$

$$(41)$$

$$\int_{-\pi}^{\pi} \frac{d\boldsymbol{\omega}}{(2\pi)^L} V_0(\boldsymbol{\omega},\boldsymbol{k},x)\ln V_0(\boldsymbol{\omega},\boldsymbol{k},x)e^{i\boldsymbol{\omega}\cdot\boldsymbol{k}}$$

$$= \sum_{m>0} \frac{c^m}{(m-1)!} \sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^m} \prod_{n\leqslant m} [\gamma(\boldsymbol{k},\boldsymbol{\xi}^n,x)]\delta_{\boldsymbol{k},\Sigma_{n\leqslant m}\boldsymbol{\xi}^n}$$

$$= \frac{c^{k_1}\theta\left[k_1-\frac{1}{2}\right]}{(k_1-1)!} \sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^{k_1}} \prod_{n\leqslant k_1} [\gamma(\boldsymbol{k},\boldsymbol{\xi}^n,x)]\delta_{\boldsymbol{k},\Sigma_{n\leqslant k_1}\boldsymbol{\xi}^n}.$$

$$(42)$$

So one arrives at the compact result, where we have used the fact that if $k_1=0$, then $k_\ell=0$ for all ℓ (which follows from the definition of the generalized degrees):

$$\lim_{N\to\infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}] = \sum_{k_1} P(k_1)\ln \pi_c(k_1)$$

$$+ \frac{1}{2}\left[c - \int dx\, p(x)\sum_{\boldsymbol{k}} k_1 P(\boldsymbol{k}|x)\right]$$

$$+ \int dx\, p(x)\sum_{\boldsymbol{k}} P(\boldsymbol{k}|x)$$

$$\times\ln\left\{\sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^{k_1}} \left[\prod_{n\leqslant k_1} \gamma(\boldsymbol{k},\boldsymbol{\xi}^n,x)\right]\delta_{\boldsymbol{k},\Sigma_{n\leqslant k_1}\boldsymbol{\xi}^n}\right\},$$

$$(43)$$

with the average-c Poissonian degree distribution $\pi_c(k)$ $=c^k e^{-c}/k!$.

IV. APPLICATIONS OF THE GENERAL THEORY

A. Regular random graphs

Our first application domain is that of the r-regular degree distribution $P(\boldsymbol{k}|x)=\delta_{\boldsymbol{k},\boldsymbol{k}(r)}$, with $\boldsymbol{k}(r)=(r,r^2,\ldots,r^L)$. Here one can solve (36) explicitly:

$$\gamma(\boldsymbol{k},\boldsymbol{\xi},x) = \frac{\xi_2 \delta_{\xi_1,1}}{c} \int dx'\, p(x')Q(x,x') \sum_{k'\geqslant 0} \delta_{(\xi_2,\ldots,\xi_L,k'),\boldsymbol{k}(r)} \frac{\displaystyle\sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^{k_1(x')-1}} \left[\prod_{n=1}^{r-1} \gamma(\boldsymbol{k}(r),\boldsymbol{\xi}^n,x')\right]\delta_{k_L(r),k_{L-1}+\Sigma_{n<r}\xi_L^n}\prod_{\ell=1}^{L-1} \delta_{r^\ell-k_{\ell-1},\Sigma_{n<r}\xi_\ell^n}}{\displaystyle\sum_{\boldsymbol{\xi}^1\ldots\boldsymbol{\xi}^{k_1(x')}} \left[\prod_{n=1}^{r} \gamma(\boldsymbol{k}(r),\boldsymbol{\xi}^n,x')\right]\prod_{\ell=1}^{L} \delta_{r^\ell,\Sigma_{n\leqslant r}\xi_\ell^n}}.$$

$$(44)$$

The solution is seen to be of the form $\gamma(\boldsymbol{k},\boldsymbol{\xi},x)$ $= \gamma(\boldsymbol{k},x)\delta_{\boldsymbol{\xi},(1,r,r^2,\ldots,r^{L-1})}$ and independent of k_L. Insertion of this form into the above equation then gives

$$\gamma(\boldsymbol{k},x) = \frac{r}{c} \int dx'\, p(x')Q(x,x') \frac{\prod_{\ell=1}^{L-1} \delta_{k_\ell,r^\ell}}{\gamma(\boldsymbol{k}(r),x')}.$$

$$(45)$$

We conclude that

$$\gamma(\boldsymbol{k},\boldsymbol{\xi},x) = \gamma(x)\left[\prod_{\ell=1}^{L-1} \delta_{k_\ell,r^\ell}\right]\left[\prod_{\ell=1}^{L} \delta_{\xi_\ell,r^{\ell-1}}\right],$$

$$(46)$$

where $\gamma(x)$ is the solution of

$$\gamma(x) = \frac{r}{c} \int dx'\, p(x')\frac{Q(x,x')}{\gamma(x')}.$$

$$(47)$$

For the entropies (37) and (43) one then finds

$$\lim_{N\to\infty} \Omega_L[P|\{x\}] = \lim_{N\to\infty} \Omega_L[\{\boldsymbol{k}\}|\{x\}]$$

$$= \ln \pi_c(r) + r \int dx\, p(x)\ln \gamma(x) + \frac{1}{2}(c-r).$$

$$(48)$$

As expected, the two entropies are identical (since for regular graphs there is no entropy contribution from degree permutations) and independent of L [since upon specifying that the degrees are r-regular, the full distributions $P(\boldsymbol{k}|x)$ are uniquely specified for any L]. In the special case $Q(x,x')$

= 1 of uncorrelated degrees the above solution simplifies further. Now $\gamma(x) = \sqrt{r/c}$ and

$$\lim_{N \to \infty} \Omega_L[P|\{x\}] = \lim_{N \to \infty} \Omega_L[\{k\}|\{x\}]$$

$$= \ln \pi_c(r) + \frac{1}{2} r \ln(r/c) + \frac{1}{2}(c - r). \quad (49)$$

B. Case $L = 1$

For $L = 1$ we have already simplified our formula for the function $\gamma(k, \xi, x)$ to relation (35) for a simple function $\gamma(x)$. We can do the same for expression (43) for the entropy, which gives

$$\lim_{N \to \infty} \Omega_1[\{k\}|\{x\}] = \sum_k P(k) \ln \pi_c(k) + \frac{1}{2}(c - \bar{k})$$

$$+ \int dx \, p(x) \sum_k P(k|x) \ln \gamma^k(x), \quad (50)$$

$$\lim_{N \to \infty} \Omega_1[P|\{x\}] = \sum_k P(k) \ln \pi_c(k) + \frac{1}{2}(c - \bar{k})$$

$$- \int dx \, p(x) \sum_k P(k|x) \ln[P(k|x)/\gamma^k(x)], \quad (51)$$

with $\pi_c(k) = c^k e^{-c}/k!$, with $\bar{k} = \int dx \, p(x) \Sigma_k k P(k|x)$, $P(k) = \int dx \, p(x) P(k|x)$, and where $\gamma(x)$ is to be solved from

$$\gamma(x) = \int dx' \, p(x') \frac{Q(x,x')}{c \gamma(x')} \sum_k k P(k|x'). \quad (52)$$

We see immediately that for $Q(x,x') = 1$ (the Erdös-Rényi ensemble) and upon choosing $P(k|x) = P(k)$ [since for $Q(x,x') = 1$, the hidden variables x are obsolete] we would have had $\gamma(x) = \sqrt{\bar{k}/c} \, \forall x$. Expression (50) now becomes

$$Q(x,x') = 1: \begin{cases} \lim_{N \to \infty} \Omega_1[\{k\}|\{x\}] = \sum_k P(k) \ln \pi_c(k) + \frac{1}{2}(c - \bar{k}) + \frac{1}{2}\bar{k} \ln(\bar{k}/c), \\ \\ \lim_{N \to \infty} \Omega_1[P|\{x\}] = -\sum_k P(k) \ln[P(k)/\pi_c(k)] + \frac{1}{2}(c - \bar{k}) + \frac{1}{2}\bar{k} \ln(\bar{k}/c). \end{cases} \quad (53)$$

So, if one also chooses $\bar{k} = c$, the entropy of networks with degree distribution $P(k)$ in the Erdös-Rényi ensemble is minus the Kullback-Leibler distance between $P(k)$ and a Poisson degree distribution, provided the ensemble and $P(k)$ have the same average connectivity. An alternative derivation of Eq. (53) can also be obtained starting from the expression of the total number of graphs with given degree sequence $\mathcal{N}[\{k\}]$ derived in [10,13,15]:

$$\mathcal{N}[\{k\}] = (\bar{k}N - 1)!! \frac{e^{-\lambda/4}}{\Pi_i k_i!}, \quad (54)$$

with $\lambda = (\overline{k^2}/\bar{k})^2 - 1$ and $\overline{k^2} = \Sigma_i k_i^2/N$. The entropy $\Omega[\{k\}]$ of the degree sequence $\{k\}$ in the Erdös-Rényi ensemble is the logarithm of the probability of having one of the total number $\mathcal{N}[\{k\}]$ of possible networks in the ensemble. Since in a Erdös-Rényi network each link has a probability c/N to be present, we have

$$\lim_{N \to \infty} \Omega_1[\{k\}] = \lim_{N \to \infty} \frac{1}{N} \ln \left\{ \mathcal{N}[\{k\}] \right.$$

$$\left. \times \left(\frac{c}{N}\right)^{N\bar{k}/2} \left(1 - \frac{c}{N}\right)^{N(N-1)/2 - N\bar{k}/2} \right\}. \quad (55)$$

Upon inserting the expression of $\mathcal{N}[\{k\}]$, Eq. (54), into Eq. (55), we recover Eq. (53).

The other terms in (50) apparently represent the effect of average connectivity mismatches and of the degree correlations induced by $Q(\cdot, \cdot)$ and make matters more complicated. The simple form of our $L = 1$ equations, however, still allows us to push the analysis further for certain cases, by solving $\gamma(x)$ explicitly from Eq. (52). For instance, if the (symmetric) kernel $Q(x,x')$ has an eigenfunction $f(x) = \sqrt{p(x)k(x)}$, with $k(x) = \Sigma_k k P(k|x)$, then

$$\int dx' \, Q(x,x') f(x') = \lambda f(x), \quad f(x) = \sqrt{p(x)k(x)}:$$

$$\gamma(x) = \sqrt{\frac{\lambda}{c}} f(x). \quad (56)$$

If $Q(\cdot, \cdot)$ has this property, together with the normalization $\int dx \, dx' \, p(x) Q(x,x') p(x') = 1$, then one finds that the entropy (50) becomes

$$\lim_{N \to \infty} \Omega_1 [\{k\}|\{x\}] = \sum_k P(k) \ln \pi_c(k) + \frac{1}{2}(c - \bar{k})$$

$$+ \frac{1}{2} \int dx \, p(x) k(x) \ln[\lambda p(x) k(x)/c]$$

$$= \sum_k P(k) \ln \pi_c(k) + \frac{1}{2}(c - \bar{k})$$

$$+ \frac{1}{2} \int dx\, p(x)k(x)\ln[p(x)k(x)]$$

$$+ \frac{1}{2}\bar{k}\ln[\lambda/c], \qquad (57)$$

[where $\bar{k} = \int dx\, p(x)k(x)$]. Let us next discuss some example kernels $Q(x,x')$ for which $\gamma(x)$ can be solved explicitly, either directly, or via the above procedure based on using eigenfunctions of $Q(\cdot,\cdot)$.

(i) *First example*: Here we assume $Q(x,x')$ to be such that the conditional connectivities $k(x) = \Sigma_k k P(k|x)$ are the typical ones for the ensemble (1), which implies that

$$k(x) = c \int dx'\, Q(x,x')p(x') \qquad (58)$$

and $\bar{k} = c$. In this case Eq. (52) has the solution $\gamma(x) = k(x)/c$, which leads to the following simple expression for the entropies:

$$\lim_{N\to\infty} \Omega_1[\{k\}|\{x\}] = \int dx\, p(x)\sum_k P(k|x)\ln \pi_{k(x)}, \qquad (59)$$

$$\lim_{N\to\infty} \Omega_1[P|\{x\}] = -\int dx\, p(x)\sum_k P(k|x)\ln[P(k|x)/\pi_{k(x)}]. \qquad (60)$$

This indicates that in this case the entropy $\lim_{N\to\infty}\Omega_1[P|\{x\}]$ takes the form of an integral over $p(x)$ of the Kullback-Leibler distance between the probabilities $P(k|x)$ and the Poission distribution $\pi_{k(x)}$. We note that for the hidden variable model the typical degree distribution of the nodes with hidden variable x is indeed $\pi_{k(x)}$ [20].

(ii) *Second example*:

$$Q(x,x') = a_0 + a_1\delta(x-x'), \quad k(x) = \frac{1}{2}c/p(x), \qquad (61)$$

with $x \in [-1,1]$. Normalization of $Q(\cdot,\cdot)$ tells us that $a_0 = 1 - a_1\int dx\, p^2(x)$, and we need $0 \le a_1 \le [\int dx\, p^2(x)]^{-1}$ to ensure non-negative bond probabilities in our network ensemble. The networks in this ensemble have a nontrivial community structure. In fact, nodes with the same hidden variable have a larger probability to be connected. Here one finds a solution with $\bar{k} = c$ and $\gamma(x) = \gamma$, where

$$\gamma = \sqrt{1 - a_1\int dx\, p^2(x) + \frac{1}{2}a_1}, \qquad (62)$$

$$\lim_{N\to\infty} \Omega_1[\{k\}|\{x\}] = \sum_k P(k)\ln \pi_c(k)$$
$$+ \frac{1}{2}c\ln\left[1 - a_1\int_{-1}^{1} dx\, p^2(x) + \frac{1}{2}a_1\right]. \qquad (63)$$

(iii) *Third example*:

$$Q(x,x') = \frac{g(x)+g(x')}{2\int dx''p(x'')g(x'')}, \quad k(x) = \frac{[\sqrt{\langle g^2\rangle_0} + g(x)]^2}{p(x)}, \qquad (64)$$

with $x \in [-1,1]$, with the shorthand $\langle \phi \rangle_0 = \frac{1}{2}\int_{-1}^{1} dx\, \phi(x)$ and with $g(x) \ge 0$ for all $x \in [-1,1]$. Here one finds the solution

$$\gamma(x) = \frac{1}{\sqrt{c}}\sqrt{\frac{\langle g\rangle_0 + \sqrt{\langle g^2\rangle_0}}{\int dx'\, p(x')g(x')}}[\sqrt{\langle g^2\rangle_0} + g(x)],$$

$$\lambda = \frac{\langle g\rangle_0 + \sqrt{\langle g^2\rangle_0}}{\int dx\, p(x)g(x)}. \qquad (65)$$

C. Case $L=2$

Here we have to find first the solution of (36), which now reduces to

$$\gamma((k_1,k_2),(1,\xi),x)$$
$$= \frac{\xi}{c}\int dx'\, p(x')Q(x,x')\sum_{k'\ge 0} P(\xi,k'|x')$$
$$\times \frac{\sum_{\xi_1\cdots\xi_{\xi-1}}\left[\prod_{n=1}^{\xi-1}\gamma((\xi,k'),(1,\xi_n),x')\right]\delta_{k',k_1 + \sum_{n<\xi}\xi_n}}{\sum_{\xi_1\cdots\xi_\xi}\left[\prod_{n=1}^{\xi}\gamma((\xi,k'),(1,\xi_n),x')\right]\delta_{k',\sum_{n\le\xi}\xi_n}}. \qquad (66)$$

We observe that the right-hand side is independent of k_2, so the solution of our equation must have the form $\gamma((k_1,k_2),(1,\xi),x) = \gamma(k_1,\xi,x)$, where

$$\gamma(k,\xi,x) = \frac{\xi}{c}\int dx'\, p(x')Q(x,x')\sum_{k'\ge 0} P(\xi,k'|x')$$
$$\times \frac{\sum_{\xi_1\cdots\xi_{\xi-1}}\left[\prod_{n=1}^{\xi-1}\gamma(\xi,\xi_n,x')\right]\delta_{k',k + \sum_{n<\xi}\xi_n}}{\sum_{\xi_1\cdots\xi_\xi}\left[\prod_{n=1}^{\xi}\gamma(\xi,\xi_n,x')\right]\delta_{k',\sum_{n\le\xi}\xi_n}}. \qquad (67)$$

The entropy would become

Let us limit ourselves to the simplest scenario where there are no degree correlations—i.e., $Q(x,x') = 1$. Here we have $\gamma(k,\xi,x) = \gamma(k,\xi)$, and we need only the generalized degree statistics $P(k_1,k_2) = \int dx\, p(x)P(k_1,k_2|x)$. Our formulaes thereby reduce to

$$\gamma(k,\xi) = \frac{\xi}{c} \sum_{k' \geqslant 0} P(\xi,k') \frac{\sum_{\xi_1 \cdots \xi_{\xi-1}} \left[\prod_{n=1}^{\xi-1} \gamma(\xi,\xi_n) \right] \delta_{k',k+\sum_{n<\xi} \xi_n}}{\sum_{\xi_1 \cdots \xi_{\xi}} \left[\prod_{n=1}^{\xi} \gamma(\xi,\xi_n) \right] \delta_{k', \sum_{n \leqslant \xi} \xi_n}},$$

(69)

$$\lim_{N \to \infty} \Omega_2[\{\boldsymbol{k}\}|\{x\}] = \sum_{k_1} P(k_1)$$

$$\times \ln \pi_c(k_1) + \frac{1}{2} \left[c - \sum_{k_1 k_2} k_1 P(k_1,k_2) \right]$$

$$+ \sum_{k_1 k_2} P(k_1,k_2) \ln \left\{ \sum_{\xi_1 \cdots \xi_{k_1}} \left[\prod_{n \leqslant k_1} \gamma(k_1,\xi_n) \right] \right.$$

$$\times \delta_{k_2, \sum_{n \leqslant k_1} \xi_n} \right\}.$$

(70)

Here one observes the validity of the following simple relation:

$$\sum_{k_2} \gamma(k_1,k_2) \gamma(k_2,k_1) = \frac{k_1}{c} P(k_1).$$

(71)

V. CONCLUSIONS

In conclusion, we have calculated the entropies $\Omega_L[\{\boldsymbol{k}\}|\{x\}]$ and $\Omega_L[P|\{x\}]$ of hierarchical constrained network topologies in the "canonical" ensemble of large sparse networks described in terms of "hidden variables."

The expression of the entropy $\Omega_L[P|\{x\}]$ assumes a very clear form in the case in which the network topology under study is the degree distribution of a network of the ensemble. Here the entropy measures the large deviation of the topology of the given networks from the typical topology of networks in the chosen ensemble.

The entropy measures the likelihood that a particular network topology belongs to an ensemble; as such, it is an important quantity whenever one seeks to represent or characterize observed networks in terms of appropriate random network ensembles. We therefore believe that it may have many applications in the future in the context of community detection problems as well as other inference problems on complex networks.

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