Gibbs entropy of network ensembles by cavity methods

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The Gibbs entropy of a microcanonical network ensemble is the logarithm of the number of network configurations compatible with a set of hard constraints. This quantity characterizes the level of order and randomness encoded in features of a given real network. Here, we show how to relate this entropy to large deviations of conjugated canonical ensembles. We derive exact expression for this correspondence using the cavity methods for the configuration model, for the ensembles with constraint degree sequence and community structure and for the ensemble with constraint degree sequence and number of links at a given distance.

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I. INTRODUCTION

The evolution of complex networks is usually described by nonequilibrium stochastic dynamics [1–5]. However, a networks' specific topological structure may reveal relevant organizational principles, such as a universality for the large-scale structure or hierarchical communities [6] that is sure to impact dynamical processes taking place on the network [7,8].

Extracting relevant statistical information encoded in the networks' structure is a fundamental concern of community detection algorithms [6] and other inference problems. To study these problems, several authors have suggested entropy based methods [9–11], which are grounded in the information theory of networks [11–16]. These methods have proved to be very useful. In fact, in a series of recent papers [11–19] it has been shown that one may extend ideas and concepts of statistical mechanics and information theory to complex network ensembles.

In this paradigm, one generalizes the typical random graph ensembles studied in the mathematical literature [20] to ensembles characterized by an extensive number of constraints that fix, for example, the degree sequence [21], number of links between different communities the number of links at a given distance [12,13], degree correlations between linked nodes [11], acyclic networks [17], or even network with a given number of triangles [18] and generalized motifs [19].

It is well known that in statistical mechanics we distinguish between microcanonical ensembles describing all sets of microscopic configurations compatible with a given value of the total energy and canonical ensembles that correspond to microscopical configurations in which the total energy fluctuates around a given mean. A pivotal result of statistical mechanics is the equivalence of these ensembles in the thermodynamic limit, i.e., in the limit where the number of particle in the system is very large. Similarly, in the theory of random graphs we distinguish between the $G(N,L)$ ensemble, which consists of all networks with N nodes and a total of exactly L links, and the $G(N,p)$ ensemble, which is formed by all networks of N nodes and the total number of links being a Poisson distributed random variable with average $\langle L\rangle = p(N-1)$. Exploiting the parallelism between statistical mechanics and theory of random graphs we can call the random graph ensemble $G(N,L)$ a *microcanonical network ensemble* and the $G(N,p)$ graph ensemble a *canonical network ensemble*. Similarly to statistical mechanics, the random graph ensembles $G(N,L)$ and $G(N,p)$ are, in the thermodynamic limit, asymptotically equivalent as long as L of the $G(N,L)$ ensemble and p of the $G(N,p)$ ensemble are related by the equality $L=p(N-1)$.

It was shown in [12,13,15] that the parallel construction between network ensembles can be extended to much more complex networks. In fact it is possible to define microcanonical network ensembles by imposing a set of hard constraints that must be satisfied by each network in the ensemble and canonical network ensembles, which satisfy soft constraints, i.e., the constraints are satisfied on average. The set of constraints might fix, for example, the degree sequence, the community structure, or the spatial structure of networks embedded in space.

A widely studied example of the microcanonical network ensemble is the configuration model [21] that fixes the degree sequence, i.e., degrees for all nodes in the networks. On the other hand, canonical network ensembles that impose soft constraints on the degree sequence have been studied under different names ("hidden variable model" and "fitness model") by the physics [22–24] and statistics [25] communities.

In a recent work [15] it has been shown that if the number of constraints is extensive the microcanonical ensemble and its conjugate canonical ensemble are no longer equivalent. In particular, using a network entropy measure, it was shown that a microcanonical ensemble has lower entropy than the conjugate canonical ensemble, even though the marginal probabilities take the same expression. An example of this difference was given by comparing the microcanonical ensemble of regular networks with fixed degree $k_i=c\in\mathbb{N}$ for all nodes $i=1,\ldots,N$ and the canonical Poisson network ensemble with average degree $\bar{k}_i=c$, for every $i=1,2,\ldots,N$, where the overbar refers to the ensemble average. It is easy to check that in this paradigmatic case, the entropy of the regular networks is smaller than the entropy of the Poisson networks with the same average degree. The importance of such a topological difference is also revealed by the observation that dynamical models defined on microcanonical network ensembles or corresponding canonical ones display different critical behaviors.

The calculation for the entropy of arbitrary microcanonical ensembles was performed in [12,13] using a Gaussian approximation, and in [14,16] by exact path integral approaches restricted to sparse networks and constraint degree sequence. Here, we show an extension of the exact results found in [14,16] using the more transparent cavity method [26,27] and derive the correspondence between the entropies of microcanonical and conjugate canonical ensembles.

II. ENTROPY OF SIMPLE CANONICAL NETWORK ENSEMBLES

We first consider a canonical ensemble of *simple* networks, each consisting of N nodes and characterized by an adjacency matrix $\{\boldsymbol{a}\}\in\{0,1\}^{N\times N}$. A link between two nodes i and j may be present ($a_{ij}=1$) or absent ($a_{ij}=0$). The network is simple in that self-interactions are not permitted and that the adjacency matrix is symmetric.

Each network is described by its probability distribution $\mathcal{P}(\{a\})=\Pi_{i<j}\pi_{ij}(a_{ij})$. The link between nodes i and j is present with probability $p_{ij}=\pi_{ij}(1)$ and is otherwise absent with probability $(1-p_{ij})=\pi_{ij}(0)$. The ensemble is subject to $\kappa=1,\ldots,M$ structural constraints of the type

$$f_\kappa(\mathbf{p})=F_\kappa, \tag{1}$$

where $f_\kappa(\mathbf{p})$ is a constraint function on the probability matrix $\{\mathbf{p}\}$, which consists of matrix elements p_{ij}, and $F_\kappa\in\mathbb{R}$ is the constraining value.

In accordance with the principle of maximal entropy [28], the link probabilities for this canonical ensemble are provided by the maximization of the Shannon entropy of network ensembles [9,15],

$$\begin{aligned} S[\mathbf{p}] &= -\sum_{i<j}\sum_{\alpha=\{0,1\}}\pi_{ij}(\alpha)\ln[\pi_{ij}(\alpha)] \\ &= -\sum_{i<j}[p_{ij}\ln p_{ij}+(1-p_{ij})\ln(1-p_{ij})], \end{aligned} \tag{2}$$

subjected to the constraints of Eq. (1). This optimization exercise gives rise to the maximal entropy canonical network ensemble, which is a generalization of the $G(N,p)$ random network ensemble [1]. The marginal probabilities p_{ij} are given as the solution to the system of equations

$$\frac{\partial}{\partial p_{ij}}\left\{S[\mathbf{p}]+\sum_{\kappa=1}^{M}\lambda_\kappa f_\kappa(\mathbf{p})\right\}=0, \tag{3}$$

where $\lambda_\kappa\in\mathbb{R}$ are the Lagrange multipliers enforcing the constraints.

Let us consider the simple case of constraints on the expected degree of each node, i.e., we select $\bar{k}_i$, such that our $M=N$ constraints given by Eq. (1) take the form

$$\sum_{j=1}^{N}p_{ij}=\bar{k}_i,\quad i=1,\ldots,N. \tag{4}$$

The marginal probabilities p_{ij} that satisfy Eq. (4) are given as

$$p_{ij}=\frac{e^{-\lambda_i-\lambda_j}}{1+e^{-\lambda_i-\lambda_j}}=\frac{\theta_i\theta_j}{1+\theta_i\theta_j}, \tag{5}$$

with the Lagrange multipliers λ_i fixed by Eq. (4) and the variables $\theta_i=e^{-\lambda_i}$, which are commonly referred to as hidden variables [22–24]. In Table I we generalize this procedure to network ensemble satisfying a number of different structural constraints.

III. LARGE DEVIATIONS OF CANONICAL ENSEMBLES SOLVED BY THE CAVITY METHOD

The constraints for canonical ensembles are satisfied only on average; it is therefore relevant to investigate the probability of large fluctuations in these ensembles. The entropy for large deviations $\Omega[\{G_\kappa\}]$ of canonical ensembles is defined as

$$\begin{aligned} \Omega[\{G_\kappa\}] = -\lim_{N\to\infty}\frac{1}{N}\ln\Bigg[&\sum_{\{a_{ij}\}}p_{ij}^{a_{ij}}(1-p_{ij})^{1-a_{ij}} \\ &\times\prod_{\kappa=1}^{M}\delta(G_\kappa-g_\kappa(\mathbf{a}))\Bigg], \end{aligned} \tag{6}$$

where the delta function $\delta(\cdots)$ enforces the $\kappa=1,\ldots,M$ hard constraint,

$$g_\kappa(\mathbf{a})=G_\kappa, \tag{7}$$

with $g_\kappa(\mathbf{a})$ being the constraining function specified on the adjacency matrix and $G_\kappa\in\mathbb{N}$ as the constrained value. The quantity $\Omega[\{G_\kappa\}]\geq 0$ measures the probability that networks in canonical ensembles satisfy Eq. (7). If $\Omega[\{G_\kappa\}]$ is large, then this implies that the probability that the number of networks in the canonical ensemble satisfy the topological constraints is large. Small values of $\Omega[\{G_\kappa\}]$, on the other hand, correspond to the large deviations of the canonical ensemble, i.e., there the networks satisfying the hard constraints are rare. The exact calculation of $\Omega[\{G_\kappa\}]$ has been performed using path integral methods [14,16] with linear hard constraints that fix the degree sequence.

Using the cavity method, we now demonstrate how to compute Eq. (6) for more general cases of canonical ensemble and hard constraints fixing, for example, the (i) degree sequence, (ii) community structure, and (iii) number of links at a given distance. In order to apply the cavity method to the calculation of $\Omega[\{G_\kappa\}]$ it is first necessary to describe the factor graph we will consider, which is depicted in Fig. 1. Following recent efforts to evaluate the number of loops in networks [29–31] we take the variables of the factor graph to be the matrix elements a_ℓ of the adjacency matrix, where the index $\ell=1,\ldots,N(N-1)/2$ identifies each possible link of the undirected network [33]. The factor nodes, which are identified by Greek letters, $\alpha=1,2\ldots,M$, denote the M topological constraints imposed on the network. In particular, each factor

TABLE I. Maximum-entropy network ensembles with given set of constraints. The probability p_{ij} of each link (i,j) is given for network ensembles in which we imposed different types of constraints. These probabilities are expressed in terms of "hidden variables" of the ensembles $\{\theta_i\}$, $W(q,q')$, $W(d)$, and $\{\alpha_i\}$, which are determined by the respective "conditions" specified in the table. In the network ensembles with given community structure, the community of each node is associated with a Potts variable $q_i=1,\ldots,Q=\mathcal{O}(\sqrt{N})$. In the network ensemble embedded in a physical space the distance between the nodes is binned in L intervals $I_s\in[d_s,d_s+\Delta d_s)$ and it is indicated by a discrete variable $s_{ij}=s$ if the distance d_{ij} between the nodes i and j satisfies $d_{ij}\in I_s$. The functions $\chi_s(d)$ are indicator functions of the intervals I_s, i.e., $\chi_s(d)=0,1$ and $\chi_s(d)=1$ if and only if $d\in I_s$.

Constraints	Probabilities $p_{ij}/(1-p_{ij})$	Conditions
Given expected number of links L	$p/(1-p)$	$pN(N-1)/2=L$
Given expected community structure $\{A_{q,q'}\}$	$W(q_i,q_j)$	$A(q,q')\|_{q\neq q'}=\Sigma_{ij}p_{ij}\delta_{q_i,q}\delta_{q_j,q'}$ $A(q,q)=\Sigma_{i<j}p_{ij}\delta_{q_i,q}\delta_{q_j,q}$
Given expected degree sequence $\{\kappa_i\}$	$\theta_i\theta_j$	$\kappa_i=\Sigma_j p_{ij}$
Given expected degree sequence $\{\kappa_i\}$ community structure $\{A(q,q')\}$	$\theta_i\theta_j W(q_i,q_j)$	$\kappa_i=\Sigma_j p_{ij}$ $A(q,q')\|_{q\neq q'}=\Sigma_{ij}p_{ij}\delta_{q_i,q}\delta_{q_j,q'}$ $A(q,q)=\Sigma_{i<j}p_{ij}\delta_{q_i,q}\delta_{q_j,q}$
Spatial networks		
Given expected degree sequence $\{\kappa_i\}$ and number of link at distance $d\in I_s, B_s$	$\theta_i\theta_j W(s_{ij})$	$\kappa_i=\Sigma_j p_{ij}$ $B(s)=\Sigma_{ij}p_{ij}\chi_s(d_{ij})$
Given expected degree sequence $\{\kappa_i\}$ and number of triangles for each node $\{T_i\}$	$\theta_i\theta_j e^{f_{ij}(\alpha_i+\alpha_j)+g_{ij}}$	$\kappa_i=\Sigma_j p_{ij}$ $T_i=\Sigma_{jk}p_{ij}p_{jk}p_{ki}$ $f_{ij}=\Sigma_k p_{ik}p_{kj}$ $g_{ij}=\Sigma_k p_{ik}\alpha_k p_{kj}$

node α is linked to a list of variables, which are identified by the set $\partial\alpha$. Likewise, variable ℓ is connected to a set of constraints, which is indicated as $\partial\ell$. In our ensemble we assume that the number of constraints connected to a variable ℓ is equal for each variable of the factor graph and is given by $|\partial\ell|$. The cavity method remains valid even for $M=\mathcal{O}(N^2)$ but the scaling $M=\mathcal{O}(N)$ is necessary (as will become clear in the following derivation) to ensure that the entropy $\Omega[\{G_\kappa\}]$ remains finite.

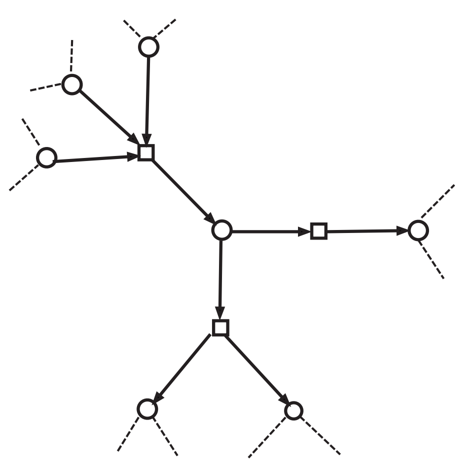

FIG. 1. Factor graph used for the cavity calculations. The variable nodes ℓ are indicated with circles and have a fixed connectivity $|\partial\ell|=3$ in the figure. The factor nodes, instead, are indicated by squares. Their role is to impose the hard constraints defined in Eq. (7).

A. Large deviations of canonical ensembles with linear constraints

The constraint given by Eq. (7) now fixes the degrees of the factor nodes, i.e.,

$$K_\alpha=\sum_{\ell\in\partial\alpha}a_\ell, \tag{8}$$

with $\alpha=1,\ldots,M$ and factor node degree $K_\alpha\in\mathbb{N}$. Correspondingly, we can write Eq. (6) as

$$\Omega[\{K_\alpha\}]=-\lim_{N\to\infty}\frac{1}{N}\ln\left[\sum_{\{a_\ell\}}p_\ell^{a_\ell}(1-p_\ell)^{1-a_\ell}\times\prod_{\alpha=1}^{M}\delta\left(K_\alpha-\sum_{\ell'\in\partial\alpha}a_{\ell'}\right)\right], \tag{9}$$

Within the summation term on the first line of Eq. (9) and for each value a_ℓ, we introduce the unity identity $1=x^{a_\ell}x^{-a_\ell}$, which is parametrized by $x\geq 0$. We can then define $\Omega_N[\{K_\alpha\},x]$ as

$$\Omega_N[\{K_\alpha\},x]=-\frac{1}{N}\ln\left[\sum_{\{a_\ell\}}(p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell}\times\prod_{\alpha=1}^{M}\delta\left(K_\alpha-\sum_{\ell'\in\partial\alpha}a_{\ell'}\right)\right]+\frac{L}{N}\ln(x), \tag{10}$$

where L is the total number of distinguishable links constraint by the constraint in Eq. (8). The introduction of the parameter x at this stage is completely irrelevant and in fact the relation

$$\Omega[\{K_\alpha\}] = \lim_{N\to\infty} \Omega_N[\{K_\alpha\},x] \tag{11}$$

holds for all values of x. However, in what follows, we will focus on the particular limiting case where x tends to zero. Thus, we write

$$\Omega[\{K_\alpha\}] = \lim_{x\to 0}\lim_{N\to\infty} \Omega_N[\{K_\alpha\},x]. \tag{12}$$

The calculation of $\Omega[\{K_\alpha\},x]$ may be formulated in terms of the cavity method or the belief propagation (BP) algorithm [26,27], aimed at determining $\ln \mathcal{Z}$ with $\mathcal{Z}$ defined as in the following:

$$\mathcal{Z} = \sum_{\{a_\ell\}} (p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell} \tag{13}$$

$$\times \prod_{\alpha=1}^{M} \delta\left(K_\alpha - \sum_{\ell'\in\partial\alpha} a_{\ell'}\right), \tag{14}$$

where the entropy $\Omega_N[\{K_\alpha\},x]$ is given by

$$N\Omega_N[\{K_\alpha\},x] = -\ln \mathcal{Z} + L\ln(x). \tag{15}$$

The "messages" of this BP algorithm are sent between variable and factor nodes. In particular, we may define $\nu_{\ell\to\alpha}(a_\ell)$ as the message sent from variable node ℓ to factor node α indicating the probability that matrix element ℓ takes value a_ℓ, in the absence of constraint α. We correspondingly define $\hat{\nu}_{\alpha\to\ell}(a_\ell)$ as the message that the factor node α sends to variable ℓ for the distribution of all variables connected to α, except variable ℓ. The BP update rules [26,27] take the form

$$\nu_{\ell\to\alpha}(a_\ell) = \frac{1}{\mathcal{C}_{\ell,\alpha}}(p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell}\prod_{\beta\in\partial\ell\setminus\alpha}\hat{\nu}_{\beta\to\ell}(a_\ell), \tag{16}$$

$$\hat{\nu}_{\alpha\to\ell}(a_\ell) = \sum_{\{a_{\ell'}\}_{\ell'\in\partial\alpha\setminus\ell}} \delta\left(K_\alpha - a_\ell - \sum_{\ell'\in\partial\alpha\setminus\ell} a_{\ell'}\right) \times \prod_{\ell'\in\partial\alpha\setminus\ell} \nu_{\ell'\to\alpha}(a_{\ell'}), \tag{17}$$

where $\mathcal{C}_{\ell,\alpha}>0$ are normalization constants. To proceed, we make the ansatz that the cavity distribution satisfies a binomial form

$$\nu_{\ell\to\alpha}(a_\ell) = h_{\ell,\alpha}^{a_\ell}(1-h_{\ell,\alpha})^{1-a_\ell}, \tag{18}$$

which is parametrized by fields $h_{\ell,\alpha}\in\mathbb{R}$. Using integral representations of delta functions, we calculate the cavity messages given by Eq. (17) as

$$\hat{\nu}_{\alpha\to\ell}(a_\ell) = \int_{-\infty}^{\infty}\frac{dz}{2\pi}e^{-\mathrm{i}z[K_\alpha - a_\ell]}\prod_{\ell'\in\partial\alpha\setminus\ell}[1-h_{\ell',\alpha}(1-e^{\mathrm{i}z})]. \tag{19}$$

Assuming self-consistently that $h_{\ell'\alpha}$ are small, we approximate the product in the above equation as

$$\hat{\nu}_{\alpha\to\ell}(a_\ell) = \int_{-\infty}^{\infty}\frac{dz}{2\pi}\exp\left(-\mathrm{i}z[K_\alpha - a_\ell] - \sum_{\ell'\in\partial\alpha\setminus\ell} h_{\ell',\alpha}(1-e^{\mathrm{i}z})\right), \tag{20}$$

which on suitable transformation of variables takes the form of Hankel's contour integral, giving

$$\hat{\nu}_{\alpha\to\ell}(a_\ell) = \frac{1}{\Gamma(K_\alpha+1-a_\ell)}\exp\left(h_{\ell,\alpha} - \sum_{\ell'\in\partial\alpha} h_{\ell',\alpha}\right) \times\left(-h_{\ell,\alpha} + \sum_{\ell'\in\partial\alpha} h_{\ell',\alpha}\right)^{K_\alpha - a_\ell}. \tag{21}$$

Finally, inserting the above result into Eq. (16), we get that $h_{\ell,\alpha}$ satisfied the recursion equation

$$h_{\ell,\alpha} = \frac{p_\ell x \prod_{\beta\in\partial\ell\setminus\alpha}\dfrac{K_\beta}{\left(-h_{\ell,\beta}+\sum_{\ell'\in\partial\alpha} h_{\ell',\beta}\right)}}{1-p_\ell + p_\ell x\prod_{\beta\in\partial\ell\setminus\alpha}\dfrac{K_\beta}{\left(-h_{\ell,\beta}+\sum_{\ell'\in\partial\beta} h_{\ell',\beta}\right)}}. \tag{22}$$

Provided that every link exists with probability $p_\ell \neq 1$, we can choose the value of x to be sufficiently small so as to approximate $h_{\ell,\alpha}$ by

$$h_{\ell,\alpha} = \frac{p_\ell x}{1-p_\ell}\prod_{\beta\in\partial\ell\setminus\alpha}\frac{K_\beta}{\left(-h_{\ell,\beta}+\sum_{\ell'\in\partial\beta} h_{\ell',\beta}\right)}. \tag{23}$$

Since we have assumed that every variable ℓ is linked to exactly $|\partial\ell| = 2,3,\ldots$ factor nodes, Eq. (23) is solved for every value of $x \ll 1$ by the cavity field

$$h_{\ell,\alpha} = x^{1/|\partial\ell|}\hat{h}_{\ell,\alpha}, \tag{24}$$

where the cavity fields $\hat{h}_{\ell,\alpha}$ satisfy the equation

$$\hat{h}_{\ell,\alpha} = \frac{p_\ell}{1-p_\ell}\prod_{\beta\in\partial\ell\setminus\alpha}\frac{K_\beta}{\left(-\hat{h}_{\ell,\beta}+\sum_{\ell'\in\partial\beta}\hat{h}_{\ell',\beta}\right)}. \tag{25}$$

Equations (24) and (25) define the cavity distributions $h_{\ell,\alpha}$ which are indeed small for sufficiently small values of x, as previously assumed. Finally, using the BP algorithm [26,27] we can derive the marginal distributions for the factor graph which are given by

$$P_\ell(a_\ell) = C_\ell^{-1}(p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell}\prod_{\beta\in\partial\ell}\hat{\nu}_{\beta\to\ell}(a_\ell),$$

$$P_\alpha(\{a_{\ell'}\}_{\ell'\in\partial\alpha}) = C_\alpha^{-1}\delta\left(K_\alpha - \sum_{\ell'\in\partial\alpha} a_{\ell'}\right) \times \prod_{\ell'\in\partial\alpha}\left[(p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell} \times \prod_{\beta\in\partial\ell'\in\backslash\alpha} \hat{\nu}_{\beta\to\ell'}(a_{\ell'})\right],$$

where C_ℓ and C_α are normalization constants that satisfy

$$C_\ell = \prod_{\alpha\in\partial\ell}\hat{\nu}_{\alpha\to\ell}(0)\left[p_\ell x\prod_{\beta\in\partial\ell}\frac{K_\beta}{\sum_{\ell'\in\partial\beta\backslash\alpha} h_{\ell',\beta}} + 1 - p_\ell\right],$$

$$C_\alpha = \pi_{(\Sigma_{\ell\in\partial\alpha}h_{\ell,\alpha})}(K_\alpha)\prod_{\ell'\in\partial\alpha}(1-p_{\ell'})\prod_{\beta\in\partial\ell'\backslash\alpha}\hat{\nu}_{\beta\to\ell'}(0). \tag{26}$$

The term $\pi_x(y)$ gives the probability for Poisson distributed random variable y with average x. Following [26,27], in terms of our marginal distributions, the quantity $-\ln\mathcal{Z}$, with $\mathcal{Z}$ defined in Eq. (14), may be expressed as the minimum of the Bethe free energy,

$$G_{\text{Bethe}}[\{K_\alpha\}] = \sum_{\alpha=1}^{M}\sum_{\{a_\ell\}_{\ell\in\partial\alpha}} P_\alpha(\{a_\ell\})\ln\left(\frac{P_\alpha(\{a_\ell\})}{\psi_\alpha(\{a_\ell\})}\right) - \sum_{\ell=1}^{N(N-1)/2}(|\partial\ell|-1)\sum_{a_\ell=\{0,1\}} P_\ell(a_\ell)\ln\left(\frac{P_\ell(a_\ell)}{\phi_\ell(a_\ell)}\right), \tag{27}$$

where $|\partial\ell|$ indicates the number of factor nodes connected to variable ℓ and

$$\psi_\alpha(\{a_\ell\}) = \prod_{\ell\in\partial\alpha}(p_\ell x)^{a_\ell}(1-p_\ell)^{a_\ell}, \tag{28}$$

$$\phi_\ell(a_\ell) = (p_\ell x)^{a_\ell}(1-p_\ell)^{1-a_\ell}. \tag{29}$$

Inserting the expression for the marginal distributions [Eq. (26)] into Eq. (27) we obtain the result [27,29,30] that

$$-\ln\mathcal{Z} = -\sum_{\alpha=1}^{M}\ln C_\alpha + (|\partial\ell|-1)\sum_{\ell=1}^{N(N-1)/2}\ln C_\ell. \tag{30}$$

Using the definition of entropy of large deviations [Eq. (10)] and the expressions in Eq. (27) for C_α and C_ℓ, together with Eqs. (24) and (25) for the cavity fields, we get, for $x \ll 1$,

$$\begin{aligned} N\Omega_N[\{K_\alpha\},x] &= -\sum_{\alpha=1}^{M}\ln C_\alpha + (|\partial\ell|-1)\sum_{\ell=1}^{N(N-1)/2}\ln C_\ell + L\ln(x) \\ &= -\sum_{\alpha=1}^{M}\ln\left[\frac{1}{K_\alpha!}\left(x^{1/|\partial\ell|}\sum_{\ell\in\partial\alpha}\hat{h}_{\ell,\alpha}\right)^{K_\alpha}\exp\left(-x^{1/|\partial\ell|}\sum_{\ell\in\partial\alpha}\hat{h}_{\ell,\alpha}\right)\prod_{\ell\in\partial\alpha}(1-p_\ell)\right] \\ &\quad + (|\partial\ell|-1)\sum_{\ell=1}^{N(N-1)/2}\ln\left[p_\ell\prod_{\beta\in\partial\ell}\frac{K_\beta}{\sum_{\ell'\in\partial\beta\backslash\alpha}\hat{h}_{\ell',\beta}} + 1 - p_\ell\right] + L\ln(x). \end{aligned} \tag{31}$$

Finally, going in the limit $x\to 0$ and $N\to\infty$ we get, according to Eq. (11)

$$\begin{aligned} \Omega[\{K_\alpha\}] = \lim_{N\to\infty}\frac{1}{N}\Bigg\{ &-\sum_{\alpha=1}^{M}\ln\left[\frac{1}{K_\alpha!}\left(\sum_{\ell\in\partial\alpha}\hat{h}_{\ell,\alpha}\right)^{K_\alpha}\right] \\ &+ (|\partial\ell|-1)\sum_{\ell=1}^{N(N-1)/2}\ln\left[p_\ell\prod_{\beta\in\partial\ell}\frac{K_\beta}{\sum_{\ell'\in\partial\beta\backslash\alpha}\hat{h}_{\ell',\beta}} + 1 - p_\ell\right] - |\partial\ell|\sum_{\ell}\ln(1-p_\ell)\Bigg\}, \end{aligned} \tag{32}$$

where the cavity fields $\hat{h}_{\ell,\alpha}$ are the solution of the BP [Eq. (25)].

B. Specific hard constraints

We now consider a few specific cases for the hard constraints, which allow us to simply our expression (32) further.

1. Degree sequence

Also known as the configuration model [21], we consider constraints that fix the degree sequence

$$(k_1, k_2, \ldots, k_N) \in \mathbb{N}^N$$

for the network, where

$$k_i = \sum_{j=1}^{N} a_{ij}, \tag{33}$$

with $i=1,\ldots,N$. In terms of the factor graph, each factor node α fixes the degree for a specific node i in the undirected network. Recalling that variable ℓ represents the tuple (i,j) in the adjacency matrix, the variable is linked to $|\partial\ell|=2$ constraints that fix the degrees for nodes i and j. Finally, the cavity fields $h_{\ell,\alpha}$ can be written as $h_{j,i}$, as we have identified factor node α with node index i and, similarly, variable ℓ with nodes i and j.

To simplify expression (32) for $\Omega[\{k_i\}]$ we introduce

$$\gamma_i = \sum_{j\neq i}^{N} \hat{h}_{j,i}. \tag{34}$$

Using Eq. (25) it is easy to show that the variables $\{\gamma_i\}$ satisfy the following equation:

$$\gamma_i = \sum_{j\neq i}^{N} \left(\frac{p_{ij}}{1-p_{ij}}\right)\frac{k_j}{\gamma_j - \hat{h}_{i,j}}, \tag{35}$$

where $\hat{h}_{i,j}$ is given by the solution to Eq. (25). Finally, in the limit $x\to 0$, we get the exact result for the entropy of the large deviation of canonical network ensembles to be

$$\Omega[\{k_i\}] = \lim_{N\to\infty}\frac{1}{N}\left\{-\sum_{i=1}^{N}\ln\left[\frac{1}{k_i!}\gamma_i^{k_i}\right] + \sum_{\langle i,j\rangle}\ln\left[\frac{p_{ij}}{1-p_{ij}}\frac{k_ik_j}{\gamma_i\gamma_j}+1\right] - \sum_{\ell}\ln(1-p_\ell)\right\}, \tag{36}$$

where $\langle i,j\rangle$ indicates the sum over all links in the adjacency matrix. If $h_{j,i}\ll\gamma_i$ Eq. (35) simplifies to

$$\gamma_i = \sum_{j\neq i}^{N}\frac{p_\ell}{1-p_\ell}\frac{k_j}{\gamma_j}, \tag{37}$$

which then gives in the diluted limit $p_\ell\ll 1$ the result [14,16]

$$\Omega[\{k_i\}] = \lim_{N\to\infty}\left\{-\frac{1}{N}\left(\sum_{i=1}^{N}\ln\left[\frac{1}{k_i!}\gamma_i^{k_i}e^{-k_i}\right]\right)\right\}, \tag{38}$$

for the configuration model.

2. Community structure and degree sequence

Suppose we assign to node i a Pott's index $q_i=1,\ldots,Q$ that indicates the community to which the node i belongs. In addition to the degree constraint given by Eq. (33), we also impose on the level of the adjacency matrix that

$$A(q,q') = \sum_{i<j=1}^{N}\left(1-\frac{1}{2}\delta_{q,q'}\right)\delta_{q,q_i}\delta_{q',q_j}a_{ij}, \tag{39}$$

where $q<q'=1,\ldots Q$. The total number of constraints is $M=N+Q(Q-1)/2$.

Each variable node ℓ in our factor graph is now linked to three factor nodes—two for constraining the degrees of nodes i and j, separately, in the undirected network and a third one to enforce the community structure q_i,q_j. Similarly to the previous case we introduce

$$\gamma_\alpha = \sum_{\ell\in\partial\alpha}\hat{h}_{\ell,\alpha}, \tag{40}$$

where $\alpha\in\{i,j,(q_i,q_j)\}$ indicated the type of constraint. Given the cavity equations (25), it can be shown that the variables $\{\gamma_i\}$ satisfy the following equation:

$$\gamma_\alpha = \sum_{\ell\in\partial\alpha}\frac{p_\ell}{1-p_\ell}\prod_{\beta\in\partial\ell\setminus\alpha}\frac{K_\beta}{\gamma_\beta-\hat{h}_{\ell,\beta}}, \tag{41}$$

where $K_\beta\in\{k_i,k_j,A(q_i,q_j)\}$, depending on the value of α and the cavity fields $\hat{h}_{\ell,\alpha}$ satisfy the cavity equations (25). The entropy of large deviations $\Omega[\{K_\alpha\}]$ given by Eq. (32) can be expressed as

$$\Omega[\{K_\alpha\}] = \lim_{N\to\infty}\frac{1}{N}\left\{-\sum_{\alpha=1}^{M}\ln[\pi_{\gamma_\alpha}(K_\alpha)] + \sum_{i,j=1}^{N}\frac{p_{ij}}{1-p_{ij}}\left[\frac{k_ik_jA(q_i,q_j)}{\gamma_i\gamma_j\gamma_{(q_i,q_j)}}+1\right] - \sum_\alpha\gamma_\alpha - 2\sum_\ell\ln(1-p_\ell)\right\}. \tag{42}$$

In the case in which $\hat{h}_{\ell,\beta}\ll\gamma_\beta$ and the network is diluted, i.e., $p_\ell\ll 1$ we get

$$\Omega[\{K_\alpha\}] = \lim_{N\to\infty}\frac{1}{N}\left\{-\sum_{\alpha=1}^{M}\ln\left[\frac{1}{K_\alpha!}\gamma_\alpha^{K_\alpha}e^{-K_\alpha}\right]\right\}. \tag{43}$$

The value of $\Omega[\{K_\alpha\}]$ converges to a finite value in the limit of $N\to\infty$ only if the number of constraints M is of the same order of magnitude as N, i.e., $M=\mathcal{O}(N)$, in other words if the number of communities $Q=\mathcal{O}(\sqrt{N})$. For $M=\mathcal{O}(N^\xi)$, with $\xi\in(1,2)$, we have $\Omega[\{K_\alpha\}]\sim N^{\xi-1}$.

3. Links at a given distance and degree sequence

Let us embed the N nodes in a metric space, such that two nodes i and j are a distance $d_{ij}<D$ apart. We divide the interval $[0,D]$ into $L=\mathcal{O}(N)$ intervals $I_s=[d_s,d_s+\Delta d_s)$ with $s=1,2,\ldots,L$ and $d_{s+1}=d_s+\Delta d_s$. The constraint for the number of links at a given distance is given by specifying a sequence of integers $B_1,B_2,\ldots,B_L$ that satisfy

$$B_s = \sum_{i<j}^{N}\chi_s(d_{ij})a_{ij}, \tag{44}$$

where $\chi_s(d_{ij})=1$ if $d_{ij}\in I_s$ and $\chi_s(d_{ij})=0$, otherwise. The total number of constraints is in this case $M=N+L$.

Once again each variable ℓ is linked to $|\partial\ell|=3$ factor node constraints—two for fixing the degrees of node i and j and a third for the number of links B_s in the interval I_s. We introduce the variables γ_α according to the definition

$$\gamma_\alpha = \sum_{\ell \in \partial\alpha} \hat{h}_{\ell,\alpha}, \tag{45}$$

with $\alpha \in \{i,j,s_{i,j}\}$. These parameters satisfy the following equation:

$$\gamma_\alpha = \sum_{\ell \in \partial\alpha} \frac{p_\ell}{1-p_\ell} \prod_{\beta \in \partial\ell \setminus \alpha} \frac{K_\beta}{\gamma_\beta - \hat{h}_{\ell,\beta}}, \tag{46}$$

where the cavity field solve the cavity equation (25). The entropy of large deviations $\Omega[\{K_\alpha\}]$ given by Eq. (32) can be expressed as

$$\Omega[\{K_\alpha\}] = \lim_{N\to\infty} \frac{1}{N}\left\{ -\sum_{\alpha=1}^{M} \ln[\pi_{\gamma_\alpha}(K_\alpha)] + \sum_{i,j=1}^{N} \frac{p_{ij}}{1-p_{ij}}\left(\frac{k_i k_j B_{s_{i,j}}}{\gamma_i\gamma_j\gamma_{s_{i,j}}} - p_{ij}\right) - \sum_\alpha \gamma_\alpha - 2\sum_\ell \log(1-p_\ell)\right\}, \tag{47}$$

where the subscript $s_{i,j}$ denotes the interval s such that $d_{ij} \in I_s$. Using Eq. (46) in the limit of sparse networks with $p_\ell \ll 1$ the entropy of large deviations simplifies and takes the form

$$\Omega[\{K_\alpha\}] = \lim_{N\to\infty} \frac{1}{N}\left\{ -\sum_{\alpha=1}^{M} \ln\left[\frac{1}{K_\alpha!}\gamma_\alpha^{K_\alpha} e^{-K_\alpha}\right]\right\}. \tag{48}$$

The value of $\Omega[\{K_\alpha\}]$ converges to a finite limit for $N\to\infty$ only if the number of constraints M is of the same order of magnitude as N, i.e., $M=\mathcal{O}(N)$, i.e., only if $L=\mathcal{O}(N)$. If $M \simeq N^\xi$ with $\xi \in (1,2)$ then $\Omega[\{K_\alpha\}] \sim N^{\xi-1}$.

C. Special case for constraining degrees in sparse networks

Further simplifications for the expressions obtained in the previous section are possible when the constraining degrees K_α of sparse networks are the expected degrees over the canonical ensembles, i.e., $K_\alpha = \sum_{\ell \in \partial\alpha} p_\ell = k_\alpha$. The BP equations simplify to give

$$h_{\ell,\alpha} = p_\ell. \tag{49}$$

Thus, Eq. (32) reduces to

$$\Omega[\{k_\alpha\}] = -\lim_{N\to\infty}\frac{1}{N}\sum_{\alpha=1}^{M} \ln \pi_{k_\alpha}(k_\alpha). \tag{50}$$

Since this is the minimum value of Ω, we obtain, for $M = \mathcal{O}(N)$, the limit $\lim_{N\to\infty} \Omega > 0$ and therefore the canonical ensemble is not self-averaging in the thermodynamic limit.

1. Degree sequence

In the situation wherein only the degree sequence of the network is constrained, we have $K_i = \sum_{j=1}^{N} p_{ij} = k_i$, for all $i = 1,\ldots,N$. The entropy $\Omega[\{k_i\}]$ of the expected degrees in the configuration model $\Omega[\{k_i\}]$ takes the form

$$\Omega[\{k_i\}] = -\sum_{k>0} p_k \ln[\pi_k(k)], \tag{51}$$

where p_k is the probability for a node to have degree k.

2. Community structure and degree sequence

As in Sec III B 2, each node i is assigned a Pott's index $q_i = 1,\ldots,Q$ that indicates the community to which the node belongs, with $Q = \mathcal{O}(\sqrt{N})$. The expected degree constraints take the form

$$k_i = \sum_{j=1}^{N} p_{ij}, \tag{52}$$

$$A(q,q') = \sum_{i<j}^{N}\left(1 - \frac{1}{2}\delta_{q,q'}\right)\delta_{q,q_i}\delta_{q',q_j} p_{ij}, \tag{53}$$

for $i=1,\ldots,N$ and $q<q'=1,\ldots Q$ The total number of constraints is in this case $M = N + Q(Q-1)/2 = \mathcal{O}(N)$. The entropy $\Omega[\{k_i\},\{A(q,q')\}]$ takes the value

$$\Omega[\{k_i\},\{A(q,q')\}] = -\sum_{k>0} p_k \ln[\pi_k(k)] - \lim_{N\to\infty}\frac{1}{N} \times \sum_{q<q'}^{Q} \ln[\pi_{A(q,q')}(A(q,q'))]. \tag{54}$$

3. Links at a given distance and degree sequence

Following the setup of Sec. III B 3, the constraints in terms of expected degrees are given by Eq. (52) and

$$B_s = \sum_{i<j}^{N} \chi_s(d_{ij}) p_{ij}, \tag{55}$$

where $i=1,\ldots,N$ and $s=1,\ldots L$, and where $\chi_s(d_{ij})=1$ if $d_{ij} \in I_s$ and $\chi_s(d_{ij})=0$, otherwise. We now express $\Omega[\{k_i\},\{B_p\}]$ as

$$\Omega[\{k_i\},\{B_p\}] = -\sum_{k>0} p_k \ln[\pi_k(k)] - \lim_{N\to\infty}\frac{1}{N}\sum_{s=1}^{L} \ln[\pi_{B_s}(B_s)]. \tag{56}$$

IV. ENTROPY OF SIMPLE MICROCANONICAL NETWORK ENSEMBLES

So far we have investigated the entropy of simple canonical network ensembles and large deviations therein. In this section we derive an expression for the entropy Σ of a microcanonical ensemble with linear constraints. Moreover, using the result of Eq. (32) we relate Σ to the entropy Ω of the most likely configuration of a canonical ensemble when linear constraints are imposed.

Specifying $\kappa = 1,\ldots,M$ hard constraints on the adjacency matrix, as in Eq. (7), the microcanonical ensembles' entropy Σ is given by

$$\Sigma = \lim_{N\to\infty}\frac{1}{N}\ln Z_N, \tag{57}$$

where the partition function Z_N is given by

$$Z_N = \sum_{\{a_{ij}\}} \prod_{\kappa=1}^{M} \delta(G_\kappa(\mathbf{a}) - g_\kappa). \tag{58}$$

In what follows we shall prove the following relationship:

$$\Sigma = S^\star[\mathcal{P}] - \Omega^\star(\{G_\kappa\}), \tag{59}$$

where $S^\star[\mathcal{P}]$, given by Eq. (2), is the Shannon entropy of the conjugated canonical ensemble. The term $\Omega^\star[\{G_\kappa\}]$ is the logarithm of the probability that a network in the conjugated canonical ensemble satisfies the hard constraints.

Physically, Eq. (59) implies that a network satisfying the hard constraints of Eq. (7) belongs, with probability 1, to the conjugated canonical ensemble. However, such networks make up only a fraction $e^{N\Omega^\star[\{G_\kappa\}]}$ of the total canonical ensemble measure.

A. Proof of correspondence between canonical and microcanonical entropies

We now prove the relationship of Eq. (59), for the case of hard constraints specifying the degree sequence. In order to evaluate Eq. (58) in this case we use the integral representation of the Dirac-delta functions, and we get

$$Z_N = \int \prod_{i=1}^{N} \frac{d\omega_i}{2\pi} \exp\left(-\sum_{i=1}^{N} \mathrm{i}\omega_i k_i + \sum_{i<j} \ln[1 + e^{\mathrm{i}\omega_i + \mathrm{i}\omega_j}] \right), \tag{60}$$

where with the change of variables $z_i = \omega_i - \omega_i^\star$,

$$Z_N = \int \prod_{i=1}^{N} \frac{dz_i}{2\pi} e^{F_N(\{z,\omega^\star\})}, \tag{61}$$

with

$$F_N(\{z,\omega^\star\}) = -\sum_{i=1}^{N} (\mathrm{i}\omega_i^\star + \mathrm{i}z_i)k_i + \sum_{i<j} \ln[1 + e^{\mathrm{i}\omega_i^\star + \mathrm{i}\omega_j^\star}] + \sum_{i<j} \ln[1 + p_{ij}(e^{\mathrm{i}z_i + \mathrm{i}z_j} - 1)], \tag{62}$$

and the $\omega^\star$ variables are chosen so as to satisfy the marginal probabilities for the canonical ensemble, i.e.,

$$p_{ij} = \frac{e^{\mathrm{i}\omega_i^\star + \mathrm{i}\omega_j^\star}}{1 + e^{\mathrm{i}\omega_i^\star + \mathrm{i}\omega_j^\star}}. \tag{63}$$

We observe that Eq. (62) can be expressed as

$$F_N(\{z,\omega^\star\}) = S[\mathcal{P},\{\omega^\star\}] - \sum_i \mathrm{i}z_i k_i + \sum_{i<j} \ln[1 + p_{ij}(e^{\mathrm{i}z_i + \mathrm{i}z_j} - 1)]. \tag{64}$$

Therefore, with simple manipulations it can be shown that the partition function can be written as

$$Z_N = e^{NS^\star[\mathcal{P}]} \sum_{\{a_{ij}\}} p_{ij}^{a_{ij}} (1 - p_{ij})^{1 - a_{ij}} \prod_{i=1}^{N} \delta_{k_i, \Sigma_j a_{ij}} = \exp(N\{S^\star[\mathcal{P}] + \Omega_N[\{k_i\},1]\}). \tag{65}$$

Given definition (57), this proves the relationship [Eq. (59)] between entropies of microcanonical and conjugate canonical ensembles.

B. Special cases for constraining degrees

Following the simplification of Sec. III C we assume that the constraining degrees K_α are expectation values of the canonical ensemble. Using Eq. (59) we get

$$\Sigma = S^\star[\mathcal{P}] - \Omega^\star[\{k_\alpha\}]. \tag{66}$$

where $\Omega[\{k_\alpha\}]$ is given by Eq. (32), where k_α are the expected degrees of the canonical ensembles. For sparse networks, we can use Eq. (50) and Σ takes the simple form

$$\Sigma = S^\star[\mathcal{P}] + (|\partial\ell| - 1) \sum_{k>0} n_k \ln \pi_k(k), \tag{67}$$

where n_k is the probability that a random constraint enforces the degree k.

We note that when using a Gaussian approximation [12,13] for network models with linear constraints, the value for the entropy Σ_G obtained for the microcanonical ensembles is reasonably good, with an estimated error equal to

$$|\Sigma - \Sigma_G| = \left| \frac{1}{N} \sum_{\alpha=1}^{M} \ln \frac{[k_\alpha e^{-1}]^{k_\alpha} \sqrt{2\pi k_\alpha}}{k_\alpha!} \right| \leq \frac{M}{N} |\ln e^{-1} \sqrt{2\pi}| = \frac{M}{N} 0.08. \tag{68}$$

We conclude this section with the expressions for Σ for a few specific constraints.

1. Degree sequence

From Eq. (66) we get in the case of the sparse configuration model

$$\Sigma = S^\star[\mathcal{P}] + \sum_{k>0} p_k \ln[\pi_k(k)], \tag{69}$$

where p_k is the probability of observing a node with degree k.

2. Community structure and degree sequence

In the ensemble with a given degree sequence and a constraint on the number of links within and between communities $q = 1, \ldots, Q$, the total number of communities $Q = \mathcal{O}(\sqrt{N})$. Here, we obtain for sparse networks

$$\Sigma = S^\star[\mathcal{P}] + \sum_{k>0} p_k \log[\pi_k(k)] + \lim_{N\to\infty} \frac{1}{N} \sum_{q,\leq q'=1}^{Q} \log[\pi_{A_{q,q'}}(A_{q,q'})], \tag{70}$$

where $A_{q,q'}$ is given by Eq. (39).

3. Links at a given distance and degree sequence

When the constraints are on the number of links at a specific distance and the degree sequence, the expression for the entropy of the microcanonical ensemble takes the form

$$\Sigma = S[\mathcal{P}] + \sum_{k>0} p_k \log[\pi_k(k)] + \lim_{N\to\infty}\frac{1}{N}\sum_{s=1}^{L} \log[\pi_{B_s}(B_s)], \tag{71}$$

where B_s is given by Eq. (55) valid for sparse networks.

V. CONCLUSIONS

In conclusion we have derived exact results for the large deviation properties of canonical network ensembles and for the entropy of microcanonical network ensembles in the case of simple networks with linear constraints. Our results apply to simple networks with given degree sequence and community structure, and to networks embedded in a metric space. Our approach makes use of the transparent cavity method, which can also be extended to other types of constraints or directed networks.

Our calculations are valid even when the number of constraints scales like $M=\mathcal{O}(N^2)$. Nevertheless, only in the case of a linear number of constraints, i.e., $M=\mathcal{O}(N)$, can we ensure that the entropy $\Omega[\{K_\alpha\}]$ remains finite in the limit $N\to\infty$.

Further inquiry will be directed toward the exact evaluation of the entropy of weighted networks and networks wherein the number of loops passing through each node is constrained. Moreover, the relation between the information entropy of network ensembles studied here and the von Neumann entropy, as introduced in [32], presents further scope for investigation.

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