

Grand canonical ensemble of weighted networks

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The cornerstone of statistical mechanics of complex networks is the idea that the links, and not the nodes, are the effective particles of the system. Here, we formulate a mapping between weighted networks and lattice gases, making the conceptual step forward of interpreting weighted links as particles with a generalized coordinate. This leads to the definition of the grand canonical ensemble of weighted complex networks. We derive exact expressions for the partition function and thermodynamic quantities, both in the cases of global and local (i.e., node-specific) constraints on the density and mean energy of particles. We further show that, when modeling real cases of networks, the binary and weighted statistics of the ensemble can be disentangled, leading to a simplified framework for a range of practical applications.

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Introduction. What distinguishes a network from the systems typically studied in physics is the complex heterogeneous pattern of interactions (links) among its constituent elements (nodes). Indeed, the statistical mechanics approach to networks has been developed by treating the interactions themselves as the degrees of freedom of the system, leading to the interpretation of links as the actual particles of the system [1].¹ Under this view, the maximum number of particles V (i.e., the maximum number of links) is the equivalent of the volume of a physical system. For binary networks with a fixed number N of nodes, a series of seminal works [3–5] defined the canonical ensemble by fixing the number of links L , and the grand canonical ensemble by letting L fluctuate around its expected value. For instance, in the Erdős-Rényi model these two cases correspond to $G(L)$, obtained by fixing L , and $G(p)$, obtained by setting the link probability $p = L/V$. The microcanonical ensemble is retrieved in this framework upon defining an energy function associated with network configurations, whose definition—differently from physical systems—cannot be derived from first principles [6,7]. This difficulty led the statistical mechanics of networks to be reframed more closely to information theory, according to Jayne’s interpretation [8]. Within this more general framework, the microcanonical ensemble is defined by assigning equal probability to the network configurations that exactly satisfy a given set of structural constraints, whereas in the canonical ensemble, network probabilities are such that the constraints are met on average over the ensemble [9,10]. Notably, this framework naturally incorporates networks with discrete weighted interactions [11], by treating links as multiple particle states. In particular, the canonical ensemble has been derived for networks with links assuming integer

weights [12,13] and approximately for networks with (distinguishable) multilinks [14,15].

Building on this idea of considering links as particles, here we put forward the paradigm that the weights of existing links are generalized coordinates (e.g., energy or magnetic moment) associated with such particles.² This analogy allows defining a rigorous mapping between networks and lattice gases in an appropriate space, and consequently a statistical mechanics framework corresponding to the grand canonical ensemble of networks.

Here, for simplicity, we discuss the case of undirected networks with links assuming continuous weights. We define a mapping between a network G of this kind with N nodes and a lattice gas as follows. First, we note that each link of G corresponds to an edge of K_N , the complete simple graph of N nodes. Thus we define a lattice using the *line graph* of K_N , also called in this case the *triangular graph* T_N of order N [17].³ This is the graph obtained by associating a vertex with each edge of K_N , and connecting two vertices with an edge if and only if the corresponding edges of K_N have a vertex in common. We can now map each link of G with weight w into a particle with internal coordinate w occupying the corresponding vertex (lattice site) of the graph T_N (see Fig. 1). Therefore we have that the binary adjacency matrix $\mathbf{A} = \{a_{ij}\}_{(i,j) \in \mathcal{V}}$ of the network fixes the positions of the gas particles on the lattice T_N , whereas its weighted adjacency matrix $\mathbf{W} = \{w_{ij}\}_{(i,j) \in \mathcal{V}}$ defines the internal coordinates of the existing particles. Here, \mathcal{V} denotes the set of all unordered node pairs (i, j) , with $|\mathcal{V}| = V = N(N - 1)/2$ being the volume of the system.

²A different analogy between evolving networks and equilibrium Bose gases consists in treating nodes as energy levels and links as noninteracting particles [16].

³See Ref. [18] for a recent application of line graphs to community detection in networks.

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¹Links also represent the primary statistical units of observation when extracting networks of interactions from data [2].

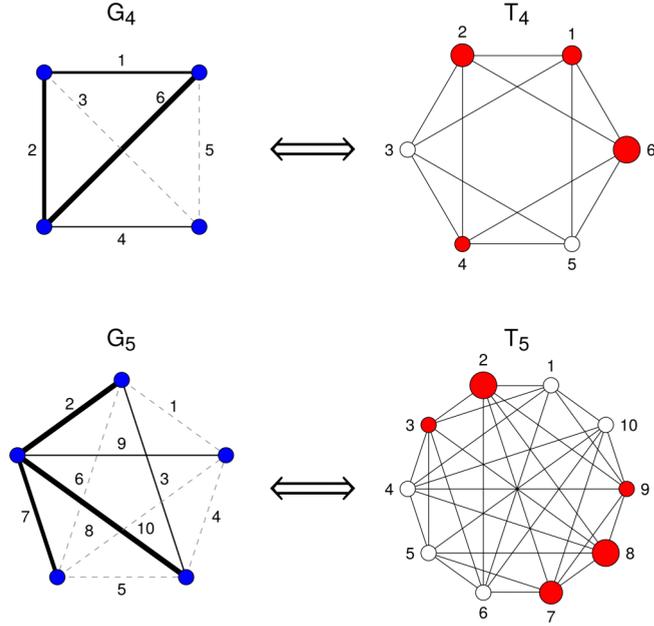


FIG. 1. Mapping between an undirected graph G_N and a lattice gas on the corresponding triangular graph T_N of K_N (we report the illustrative examples $N = 4, 5$). Only the existing links of G_N (represented as solid black lines) are placed as particles on the lattice sites (represented as solid dots), and the weight of such links (given by the lines' thickness) corresponds to the generalized coordinates of particles (given by the dots' size). Note that two particles in the lattice gas are neighbors if the corresponding links in G_N have a node in common.

This mapping allows formulating in a rigorous way the grand canonical ensemble of complex weighted networks. We first define the configuration \mathcal{C} of the undirected weighted network G as the pair (\mathbf{A}, \mathbf{W}) : the set of existing links $(i, j) \in \mathcal{L}_A \subseteq \mathcal{V}$ with $|\mathcal{L}_A| = L$ (i.e., the set of node pairs with $a_{ij} = 1$) and the set of weights $\{w_{ij}\}_{(i,j) \in \mathcal{L}_A}$ associated with them—meaning that only existing links (particles) contribute to the statistics of the system. Therefore, the grand canonical probability distribution is $P(\mathcal{C}) = P(\mathbf{A}, \mathbf{W}) \equiv P(\mathcal{L}_A, \{w_{ij}\}_{(i,j) \in \mathcal{L}_A})$, and the sum over configuration involves integrating out the weights over all existing links and then summing over all possible adjacency matrices. The average operator is thus

$$\sum_{\mathcal{C}} P(\mathcal{C}) \cdot \iff \sum_{\mathbf{A}} \prod_{i < j}^{\mathcal{L}_A} \int_0^{\infty} dw_{ij} P(\mathcal{L}_A, \{w_{ij}\}_{(i,j) \in \mathcal{L}_A}), \quad (1)$$

where to have a compact notation we use $\prod_{i < j}^{\mathcal{U}}$ to mean $\prod_{(i,j) \in \mathcal{U} | i < j}$ and analogously $\sum_{i < j}^{\mathcal{U}}$ to mean $\sum_{(i,j) \in \mathcal{U} | i < j}$, with \mathcal{U} being either \mathcal{L}_A or \mathcal{V} . The information entropy associated with the probability measure $P(\mathcal{C})$ is as usual $S = -\sum_{\mathcal{C}} P(\mathcal{C}) \log P(\mathcal{C})$, and the shape of $P(\mathcal{C})$ is found by maximizing S under given constraints. This connects us with the framework of exponential random graph models [4, 12, 19].

Global constraints. The simplest nontrivial ensemble is obtained by imposing the mean total number of links (particles) $\langle L \rangle \equiv \langle \sum_{i < j}^{\mathcal{V}} a_{ij} \rangle = L^*$ and the mean total weight (e.g., energy) $\langle W \rangle \equiv \langle \sum_{i < j}^{\mathcal{L}_A} w_{ij} \rangle = W^*$, where the average is de-

finied by the measure $P(\mathbf{A}, \mathbf{W})$. This is the weighted version of the Erdős-Rényi model. We get $P(\mathbf{A}, \mathbf{W}, \alpha, \beta) = Z_G^{-1}(\alpha, \beta) e^{-H(\mathbf{A}, \mathbf{W}, \alpha, \beta)}$ with the Hamiltonian

$$H(\mathbf{A}, \mathbf{W}, \alpha, \beta) = \alpha \sum_{i < j}^{\mathcal{V}} a_{ij} + \beta \sum_{i < j}^{\mathcal{L}_A} w_{ij}, \quad (2)$$

where α and β are the Lagrange multipliers related to L and W , respectively. $Z_G(\alpha, \beta)$ is, in analogy with statistical mechanics, the grand canonical partition function

$$Z_G(\alpha, \beta) = \sum_{\mathcal{C}} e^{-H(\mathbf{A}, \mathbf{W}, \alpha, \beta)} = \sum_{\mathbf{A}} e^{-\alpha \sum_{i < j}^{\mathcal{V}} a_{ij}} Z_{\mathcal{C}}(\beta), \quad (3)$$

where $Z_{\mathcal{C}}(\beta) = \prod_{i < j}^{\mathcal{L}_A} \int_0^{\infty} dw_{ij} e^{-\beta w_{ij}} = \beta^{-\sum_{i < j}^{\mathcal{V}} a_{ij}} = \beta^{-L}$ is the canonical partition function. The sum in Eq. (3) is easily performed by noting that $\sum_{\mathbf{A}} e^{-\alpha \sum_{i < j}^{\mathcal{V}} a_{ij}} \beta^{-\sum_{i < j}^{\mathcal{V}} a_{ij}} = \sum_{L=0}^{\mathcal{V}} n_{\mathcal{C}}(L) e^{-\alpha L} \beta^{-L}$, where $n_{\mathcal{C}}(L) = \binom{\mathcal{V}}{L}$ is the number of binary configurations with exactly L links. We finally have

$$Z_G(\alpha, \beta) = \sum_{L=0}^{\mathcal{V}} \binom{\mathcal{V}}{L} \frac{e^{-\alpha L}}{\beta^L} = \left[1 + \frac{e^{-\alpha}}{\beta} \right]^{\mathcal{V}}. \quad (4)$$

The equations determining the values of α and β are then

$$\langle L \rangle \equiv -\partial_{\alpha} \log Z_G(\alpha, \beta) \equiv \frac{\mathcal{V}}{\beta e^{\alpha} + 1} = L^*, \quad (5)$$

$$\langle W \rangle \equiv -\partial_{\beta} \log Z_G(\alpha, \beta) \equiv \frac{\mathcal{V} \beta^{-1}}{\beta e^{\alpha} + 1} = W^*, \quad (6)$$

from which we immediately find $\beta^{-1} = W^*/L^* = w^*$, i.e., the mean weight, and $1 + e^{\alpha}/w^* = \mathcal{V}/L^*$. We thus see that while β controls the mean weight (energy) of existing links (particles), α controls the mean density of links (particles).⁴ Note that since between each pair of nodes there can be only a single link (particle), the system can be represented with \mathcal{V} copies of a Fermi system having a single energy level $\varepsilon = 1$. Under this analogy, $\log \beta$ plays the role of the inverse absolute temperature $1/T$, whereas $-\alpha$ is the ratio μ/T between the chemical potential and temperature. Therefore we can write $Z_G(\mu, T) = [1 + e^{-(\varepsilon - \mu)/T}]^{\mathcal{V}}$.

Remarkably, we can perform the parameter transformation $\alpha' = \alpha + \log \beta$, so that α' alone determines the mean link density and, given this density, β alone sets the mean weight of existing links: We have

$$P(\mathbf{A}, \mathbf{W}) = \left[\prod_{i < j}^{\mathcal{V}} \frac{e^{-\alpha' a_{ij}}}{1 + e^{-\alpha'}} \right] \left[\prod_{i < j}^{\mathcal{L}_A} \beta e^{-\beta w_{ij}} \right]. \quad (7)$$

This shows that individual link occupations are all mutually independent events and that, given a binary configuration \mathbf{A} , the weight values of individual existing links are also independent events. Besides, moments of link occupation and of link weight probability distributions can be independently set in order to satisfy the constraints. As explicitly shown below, this property is due to the global nature of the constraints. Note

⁴See Ref. [20] for a recent model of social balance with a chemical potential capturing the cost of link activation.

that as for equilibrium statistical mechanics with short-range interactions, if the system is homogeneous, then local and global measures coincide.

Local constraints. We now impose for each node i the mean degree or number of incident links $\langle k_i \rangle \equiv \langle \sum_{j(\neq i)}^{\mathcal{V}} a_{ij} \rangle = k_i^*$ and the mean strength or total weight of incident links $\langle s_i \rangle = \langle \sum_{j(\neq i)}^{\mathcal{L}_A} w_{ij} \rangle = s_i^*$. This grand canonical ensemble can be seen as the continuous version of the *enhanced configuration model* [13], for which we use the acronym CECM. We have $P(\mathbf{A}, \mathbf{W}, \{\alpha_i, \beta_i\}_{i=1}^N) = Z_G^{-1}(\{\alpha_i, \beta_i\}_{i=1}^N) e^{-H(\mathbf{A}, \mathbf{W}, \{\alpha_i, \beta_i\}_{i=1}^N)}$ with

$$H(\mathbf{A}, \mathbf{W}, \{\alpha_i, \beta_i\}_{i=1}^N) = \sum_{i < j}^{\mathcal{V}} (\alpha_i + \alpha_j) a_{ij} + \sum_{i < j}^{\mathcal{L}_A} (\beta_i + \beta_j) w_{ij}, \quad (8)$$

$$\begin{aligned} Z_G(\{\alpha_i, \beta_i\}_{i=1}^N) &= \sum_{\mathbf{c}} e^{-H(\mathbf{A}, \mathbf{W}, \{\alpha_i, \beta_i\}_{i=1}^N)} \\ &= \sum_{\mathbf{A}} e^{-\sum_{i < j}^{\mathcal{V}} (\alpha_i + \alpha_j) a_{ij}} Z_C(\{\beta_i\}_{i=1}^N), \end{aligned} \quad (9)$$

and $Z_C(\{\beta_i\}_{i=1}^N) = \prod_{i < j}^{\mathcal{L}_A} (\beta_i + \beta_j)^{-1}$ being the canonical partition function. Performing the sum over all binary configurations leads to

$$\begin{aligned} Z_G(\{\alpha_i, \beta_i\}_{i=1}^N) &= \sum_{\mathbf{A}} \frac{e^{-\sum_{i < j}^{\mathcal{V}} (\alpha_i + \alpha_j) a_{ij}}}{\prod_{i < j}^{\mathcal{L}_A} (\beta_i + \beta_j)} = \sum_{\mathbf{A}} \prod_{i < j}^{\mathcal{L}_A} \frac{e^{-(\alpha_i + \alpha_j)}}{\beta_i + \beta_j} \\ &= 1 + \sum_{\mathcal{U} \subset \mathcal{V}} \prod_{i < j}^{\mathcal{U}} \frac{e^{-(\alpha_i + \alpha_j)}}{\beta_i + \beta_j} = \prod_{i < j}^{\mathcal{V}} \left(1 + \frac{e^{-(\alpha_i + \alpha_j)}}{\beta_i + \beta_j} \right), \end{aligned} \quad (10)$$

where $\sum_{\mathcal{U} \subset \mathcal{V}}$ is the sum over all distinct nonempty subsets \mathcal{U} of \mathcal{V} (that is, \mathcal{U} is a generic set of possible links of the network), while the empty subset $\mathcal{U} = \emptyset$ contributes for 1. The values of the multipliers are found through the constraints equations for all $1 \leq i \leq N$,

$$\begin{aligned} \langle k_i \rangle &\equiv -\partial_{\alpha_i} \log Z_G(\{\alpha_l, \beta_l\}_{l=1}^N) \\ &\equiv \sum_{j(\neq i)}^{\mathcal{V}} \frac{1}{1 + (\beta_i + \beta_j) e^{\alpha_i + \alpha_j}} = k_i^*, \end{aligned} \quad (11)$$

$$\begin{aligned} \langle s_i \rangle &\equiv -\partial_{\beta_i} \log Z_G(\{\alpha_l, \beta_l\}_{l=1}^N) \\ &\equiv \sum_{j(\neq i)}^{\mathcal{V}} \frac{(\beta_i + \beta_j)^{-1}}{1 + (\beta_i + \beta_j) e^{\alpha_i + \alpha_j}} = s_i^*. \end{aligned} \quad (12)$$

Note that after some algebra we can rewrite $P(\mathbf{A}, \mathbf{W})$ as

$$\begin{aligned} P(\mathbf{A}, \mathbf{W}) &= \left[\prod_{i < j}^{\mathcal{V}} \frac{e^{-[\alpha_i + \alpha_j + \log(\beta_i + \beta_j)] a_{ij}}}{1 + e^{-[\alpha_i + \alpha_j + \log(\beta_i + \beta_j)]}} \right] \\ &\times \left[\prod_{i < j}^{\mathcal{L}_A} (\beta_i + \beta_j) e^{-(\beta_i + \beta_j) w_{ij}} \right] = \pi(\mathbf{A}) q(W_{\mathcal{L}_A}), \end{aligned} \quad (13)$$

with $\pi(\mathbf{A})$ being the unconditional probability distribution of the binary configuration \mathbf{A} , and $q(W_{\mathcal{L}_A})$ the probability density function of the weights of the existing links (i.e., the set \mathcal{L}_A) conditional to \mathbf{A} . The form of $q(W_{\mathcal{L}_A})$ is exponential, differently from the geometric and Poissonian forms obtained in Refs. [13, 15], respectively, due to the continuous nature of the weights.

At this point some considerations are in order. (I) Both $\pi(\mathbf{A})$ and $q(W_{\mathcal{L}_A})$ factorize into the product of single link probability distributions: Occupations of different links are independent events and, conditional to the binary configuration, the weights of different links are also independent. (II) However, the parameters defining single link probabilities and weights are entangled, which means that local link densities cannot be set independently of local weights, because of the simultaneous conservation of mean node degrees and strengths. Such an interplay helps to clarify the role of nodes (and in particular of node heterogeneity) in terms of the interaction between links (particles). Indeed, only if the node properties are homogeneous, such as when we impose global constraints, these topological interactions disappear: The system is spatially homogeneous in terms of the density of particles and of energy, which can be thus set independently. The statistical mechanical case analogous to a heterogeneous network situation instead arises when we constrain the local mean particle and energy densities $n(\mathbf{x})$ and $\varepsilon(\mathbf{x})$ to be heterogeneous, i.e., both dependent on \mathbf{x} . This case is typically not encountered in ordinary equilibrium statistical mechanics, with the possible exception of glassy disordered systems and long-range interactions. (III) If we look at the generic link occupation probability

$$p_{ij} = \frac{e^{-[\alpha_i + \alpha_j + \log(\beta_i + \beta_j)]}}{1 + e^{-[\alpha_i + \alpha_j + \log(\beta_i + \beta_j)]}} \quad (14)$$

from the viewpoint of statistical mechanics, we can again interpret the single link problem as a single state local Fermi system with energy level $\varepsilon = 1$, inverse local temperature $T_{ij}^{-1} = \log(\beta_i + \beta_j)$, and local chemical potential $\mu_{ij} = -T_{ij}(\alpha_i + \alpha_j)$. However, at stake with the homogeneous case, different links are not independent copies of the same problem, but topologically interacting single-level Fermi systems with different local temperatures and chemical potentials—which are mutually related by local heterogeneous constraints. We thus have $Z_G(\{\mu_{ij}, T_{ij}\}_{i,j=1}^N) = \prod_{i < j}^{\mathcal{V}} [1 + e^{-(\varepsilon - \mu_{ij})/T_{ij}}]$.

Separability of binary and weighted statistics. We finally explore the separability of local link densities and weight distributions also for the case of local constraints [24]. To this end we introduce a two-step entropy maximization procedure, the *separable enhanced configuration model* (SECM):

(1) We first constrain the mean node degrees only, obtaining the probability of the binary configuration \mathbf{A} as for the standard configuration model [4],

$$\pi(\mathbf{A}) = \prod_{i < j}^{\mathcal{V}} \frac{e^{-(\alpha'_i + \alpha'_j) a_{ij}}}{1 + e^{-(\alpha'_i + \alpha'_j)}}. \quad (15)$$

(2) Then, for each \mathbf{A} , we constrain the mean node strengths, obtaining the probability density of the link weights

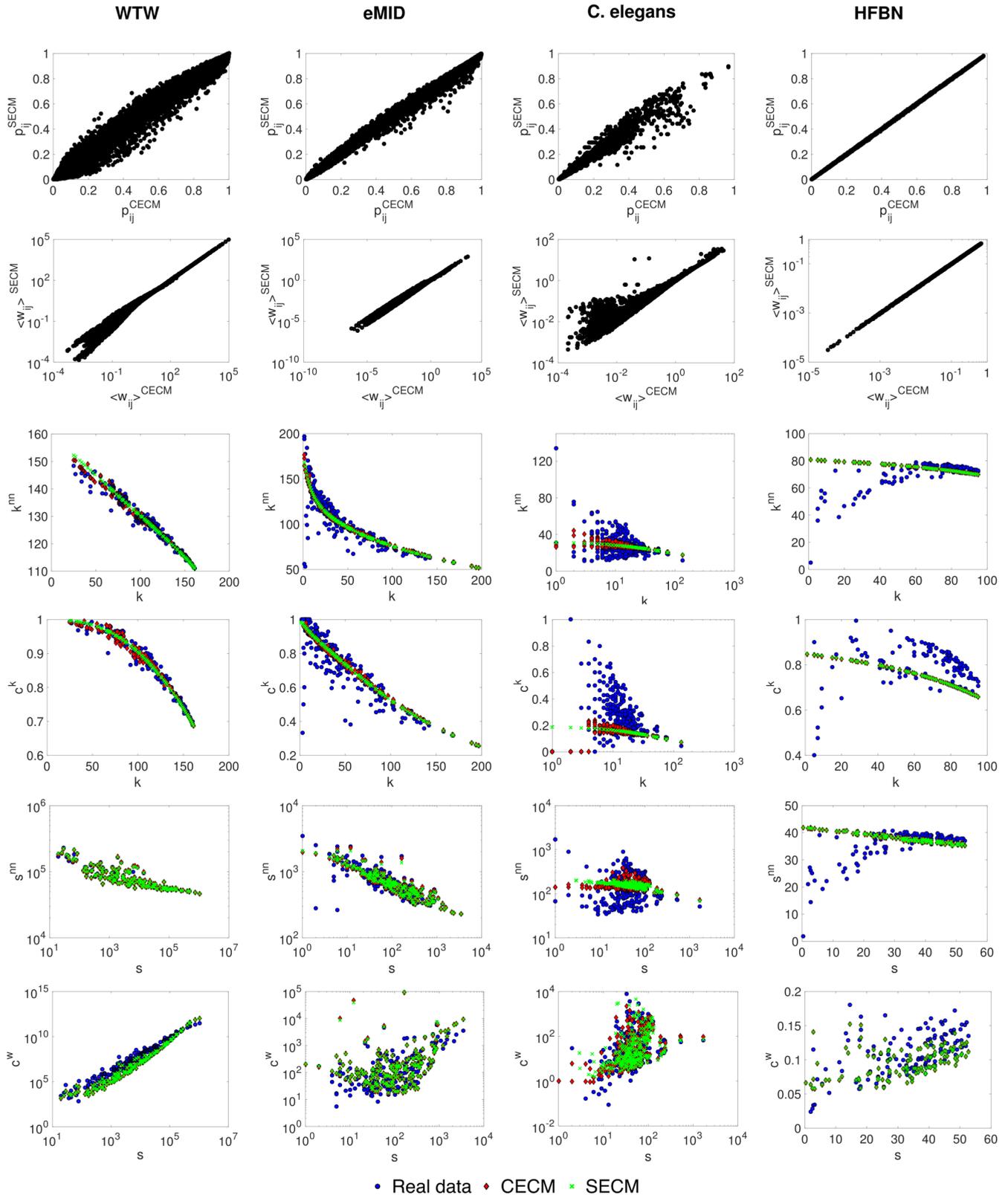


FIG. 2. Properties of CECEM and SECEM ensembles in four real networks: the World Trade Web [13], the eMID interbank network [13], the neural network of *C. elegans* [21], and the human functional brain network (HFBN) [22]. The upper part of the figure shows the comparison of link probabilities (first row) and of expected weights (second row) obtained by CECEM and SECEM. The lower part of the figure instead shows how the two ensembles reproduce higher-order statistics of the real networks (defined in Refs. [12,23]): nearest-neighbor degree k^{nn} (third row), clustering coefficient c^k (fourth row), nearest-neighbor strength s^{nn} (fifth row), and weighted clustering c^w (sixth row).

conditional to \mathbf{A} (coinciding with that of the CECM),

$$q(W_{\mathcal{L}_A}) = \prod_{i < j} (\beta_i + \beta_j) e^{-(\beta_i + \beta_j)w_{ij}}. \quad (16)$$

The SECM is thus defined by the constraint equations for all $1 \leq i \leq N$,

$$\langle k_i \rangle \equiv \sum_{j(\neq i)}^{\nu} \frac{1}{1 + e^{\alpha'_i + \alpha'_j}} = k_i^*, \quad (17)$$

$$\langle s_i \rangle \equiv \sum_{j(\neq i)}^{\nu} \frac{(\beta_i + \beta_j)^{-1}}{1 + e^{\alpha'_i + \alpha'_j}} = s_i^*, \quad (18)$$

and by the joint probability distribution

$$P(\mathbf{A}, \mathbf{W}) = \left[\prod_{i < j}^{\nu} \frac{e^{-(\alpha'_i + \alpha'_j)\alpha_{ij}}}{1 + e^{-(\alpha'_i + \alpha'_j)}} \right] \left[\prod_{i < j}^{\mathcal{L}_A} (\beta_i + \beta_j) e^{-(\beta_i + \beta_j)w_{ij}} \right]. \quad (19)$$

By definition, in the SECM the parameters defining link probabilities and weights are disentangled, so that the local statistics for these quantities can be set independently. In the CECM instead the parameters controlling the link weights also play a role in determining the connection probabilities—see Eq. (14). Indeed, in the latter case, a link (i, j) with a high expected weight ($\beta_i + \beta_j \rightarrow 0$) is forced to be realized ($p_{ij} \rightarrow 1$), and vice versa a link with a low expected weight ($\beta_i + \beta_j \rightarrow \infty$) becomes unlikely ($p_{ij} \rightarrow 0$). Owing to the interplay of its parameters, the CECM better captures the dispersion of higher-order properties of the network with respect to the SECM, as shown in Fig. 2. However, in the CECM connection probabilities, the contribution of parameters $\{\beta_i\}_{i=1}^N$ is logarithmic with respect to that of parameters $\{\alpha_i\}_{i=1}^N$: Weighted properties in general give only small

perturbations to the Lagrange multipliers of node degrees. As such, CECM and SECM define similar link probabilities and expected weights (Fig. 2), and are almost interchangeable for all practical purposes—the advantage of SECM being an easier numerical implementation. Finally, it is noteworthy that CECM and SECM coincide when, for all $1 \leq i \leq N$, the constraints on strengths and degrees satisfy $s_i^* = \gamma k_i^*$ for constant γ . Indeed, in this case $\beta_i = \beta_0$, and thus we have the exact correspondence $\alpha'_i \equiv \alpha_i + \frac{1}{2} \log(2\beta_0)$. This is for instance the HFBN case of Fig. 2.

Final remarks. Ensembles of random graphs with given structural properties such as those discussed here typically find a twofold application [1,25]. On one hand, they can be taken as null models for networks and thus used to assess the significance of patterns observed in real networked systems. On the other hand, when details on the microscopic structure of a real network are unknown, they can be used to reconstruct the most likely network configuration. The grand canonical ensemble introduced here represents, both in its rigorous version and separable approximation, a very versatile tool for these tasks in the most general class of networks with weights assuming continuous values.⁵ For instance, the *fitness-induced configuration model* [23] used to reconstruct networks without degree information is easily implemented in our grand canonical ensemble formulation [26]. More generally, the mathematical framework introduced in this Rapid Communication opens the possibility to study (possibly multilayer [27]) network ensembles defined by higher-order terms and interactions of generalized coordinates, introducing an appropriate grand canonical Hamiltonian and then using the toolbox of statistical mechanics for particle systems.

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⁵Note that the mathematical derivation of the ensembles works for a definition domain of link weights given by any finite or semi-infinite interval with arbitrary extremes (positive and negative).

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