

Correlations between weights and overlap in ensembles of weighted multiplex networks

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Multiplex networks describe a large number of systems ranging from social networks to the brain. These multilayer structure encode information in their structure. This information can be extracted by measuring the correlations present in the multiplex networks structure, such as the overlap of the links in different layers. Many multiplex networks are also weighted, and the weights of the links can be strongly correlated with the structural properties of the multiplex network. For example, in multiplex network formed by the citation and collaboration networks between PRE scientists it was found that the statistical properties of citations to coauthors differ from the one of citations to noncoauthors, i.e., the weights depend on the overlap of the links. Here we present a theoretical framework for modeling multiplex weighted networks with different types of correlations between weights and overlap. To this end, we use the framework of canonical network ensembles, and the recently introduced concept of multilinks, showing that null models of a large variety of network structures can be constructed in this way. In order to provide a concrete example of how this framework apply to real data we consider a multiplex constructed from gene expression data of healthy and cancer tissues.

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I. INTRODUCTION

Recently, multilayer networks [1,2] describing systems as different as social networks [3], collaboration networks [4], transportation networks [5,6], climate networks [7], or the brain [8,9] are attracting large interest. In fact it has become clear that in order to understand the complexity of a large variety of systems is not enough to consider single networks, but it is necessary to describe the complex set of interactions between different networks by adopting the framework of multilayer networks. For example, the biological functionality of the cells can be described by a multilayer network involving at least metabolic, protein interaction and transcription network layers. Similarly, social networks cannot be fully understood if the nature of the different ties is not taken into account distinguishing among friendship, collaboration, family ties, and so on. Multilayer networks are formed by a set M of layers constituted by single networks and by interlinks linking the nodes in the different layers. Multilayer networks can be distinguished in multiplex networks [3–7] and interacting networks of networks [10,11]. In interacting networks of networks the nodes in the different layers represent different elements of the system. For example, in the cell, metabolites, proteins, and transcription factors remain distinct biological entities. In a multiplex, instead, the same set of nodes forms M networks, one in each layer corresponding to different types of interactions. Examples of multiplex networks are social networks [3] where people can interact in different ways, transportation [5,6] networks where the same location can be reached by different means of transportation, or collaboration networks [4,6]. Here we will provide a multilayer network analysis of a gene network extracted using the gene expression of a pool of cancer patients and a pool of healthy subjects respectively for each layer.

Recently large attention has been given to multiplex network structure [3–7,12–19] and dynamics [20–23]. In particular it has been found that multiplex networks encode in their structure important correlations: we can distinguish, for

example, between degree correlations [14,15,17] determining whether a hub in a network is also an hub in another network, overlap determining to what extent any two nodes of the network are linked in several networks at the same time [3,5,16,19], or pairwise activity correlations measuring if the presence of a node in one network is correlated with the presence of another node in the same network [6]. Many multiplex networks are also weighted, i.e., the links between the nodes not only are distinguished by the type of interaction linking the nodes but also by the intensity of these interactions. In Ref. [4] different multiplex networks have been extracted from the American Physical Society data set in order to investigate the correlation between the weights of the links and the overlap of the links in different layers. In particular, the multiplex networks formed by the PRE authors in which the scientists are linked if they collaborated with each other and if they cite each other has been shown to display a statistical significant difference between the way scientists cite their collaborators and the way scientists cite noncollaborators. This result shows that in this as in other systems it is possible that the weights of the links are correlated with the pattern of overlap observed between the links of different layers. It is therefore very important to propose maximal entropy weighted multiplex networks (based on the theory of network ensembles [24–37]) models that can be used to generate multiplex networks with different types of correlations. These models, on one side, can be used to simulate dynamical processes on different multiplex network topologies, and, on the other side, similarly to what happens for single networks, their entropy [26,34] can be used to evaluate the information content of some of their properties [4,38]. Here we provide the theoretical framework to generate null models for these weighted multiplex networks, using the combined tools of canonical network models (exponential random graphs) and the recently introduced concept [16] of multilinks that is able to distinguish between different patterns of overlap of the links in the multiplex network. In fact, in order to reveal the correlations between the weights distribution and

overlap of the links it is fundamental to consider the weighted properties of the multilinks indicated by the multistrength and inverse multiplicity ratio. The multilinks enumerate exhaustively all the types of connections between two nodes of a multiplex network. Therefore the total number of possible multilinks grows exponentially with the number of layers M . For this reason the full multilink characterization of a multiplex network is numerically feasible only if the number of layers M is finite. To overcome this shortcoming here we define the ν multilinks that are only characterized by their overlap multiplicity ν , i.e., the ν multilinks are all the multilinks that connects two nodes of the multiplex with ν links in ν different layers. Building weighted multiplex ensembles with given properties of the ν multilinks allows the description and the realization of multiplex networks with large number of layers M .

The paper is structured as follows. In Sec. II we introduce the weighted multiplex networks and their weighted multilinks properties, in Sec. III we describe an application to real transcriptomics data, in Sec. IV we introduce weighted multiplex network ensembles, in Sec. V we provide the description of the most relevant weighted multiplex ensembles, considering the case of uncorrelated and correlated ensembles, in Sec. VI we show how this framework can be applied to construct null models of the biological case study, and, finally, in Sec. VII we give the conclusions.

II. WEIGHTED MULTIPLEX NETWORKS

A. Definition

A weighted multiplex is formed by N nodes connected by M weighted networks G_α , with $\alpha = 1, \dots, M$. A multiplex can be represented as $\vec{G} = (G_1, G_2, \dots, G_\alpha, \dots, G_M)$, where each network G_α is fully described by the weighted adjacency matrix of elements a_{ij}^α , with $a_{ij}^\alpha > 0$ if there is a link of weight a_{ij}^α between node i and node j in layer α , otherwise we have $a_{ij}^\alpha = 0$.

In order to simplify the treatment of the weighted multiplex, we suppose that the weight of the link between any pair of nodes (i, j) , a_{ij}^α can only assume integer values. This is a legitimate assumption because in a large number of weighted multiplexes the weights of the links can be considered as multiples of a minimal weight. Moreover, for the sake of simplicity we consider only networks without tadpoles and with a symmetric adjacency matrix $\{a_{ij}^\alpha\}$, i.e., undirected networks. The generalization of our approach to directed multiplex networks is straightforward.

Since each layer of the multiplex is a weighted network, we can introduce the so-called *total strength*, S_α , that takes into account the total weight of the links in layer α . The expression for S_α is

$$S_\alpha = \sum_{i < j} a_{ij}^\alpha. \quad (1)$$

B. Interaction between the weights and the topology of single layers

Each single layer α of the multiplex network is a weighted network [39,40], namely, a network with heterogeneous interactions between the nodes, that can show interesting weights-

topology correlations. These correlations can be revealed by measuring the following three quantities:

- (i) the degree k_i^α of a node i in layer α ,
- (ii) the strength s_i^α of node i in layer α ;
- (iii) the inverse participation ratio Y_i^α of node i in layer α .

These quantities can be expressed in terms of the adjacency matrix elements respectively as

$$k_i^\alpha = \sum_{j \neq i} \theta(a_{ij}^\alpha), \quad (2)$$

where the function $\theta(x) = 1$ if $x > 0$, otherwise $\theta(x) = 0$;

$$s_i^\alpha = \sum_{j \neq i} a_{ij}^\alpha \quad (3)$$

and

$$Y_i^\alpha = \sum_{j \neq i} \left(\frac{a_{ij}^\alpha}{s_i^\alpha} \right)^2. \quad (4)$$

Moreover, here we introduce for further convenience the quantity u_i^α ,

$$u_i^\alpha = Y_i^\alpha (s_i^\alpha)^2 = \sum_{j \neq i} (a_{ij}^\alpha)^2, \quad (5)$$

which indicates the sum of the squares of the weights incident to a node. Similarly to what happens for single networks [39,40], in any given layer α , the strength s_i^α of a node indicates the sum of the weights of the links of node i in layer α , while the inverse participation ratio Y_i^α indicates how unevenly the weights of the links of node i in layer α are distributed. The inverse of Y_i^α has a range between 1 and k_i^α . The extremes of the interval correspond respectively to a uniform weight distribution across the links of the node i in the layer α , i.e., $a_{ij}^\alpha = s_i^\alpha / k_i^\alpha$, which means $(Y_i^\alpha)^{-1} = k_i^\alpha$, and to the opposite situation, i.e., $(Y_i^\alpha)^{-1} \approx 1$, when one particular link of the node i has a prevailing weight, i.e., $a_{ir}^\alpha \gg a_{ij}^\alpha$ for every $j \neq r$. In these terms Y_i^α characterises the effective number of links of node i in layer α .

It is a standard procedure in network theory to evaluate the averages of the strength and the partition ratio of the weights of the links conditioning on the degree of the node. In a multiplex, we will then consider the following quantities:

$$s_\alpha(k) = \langle s_i^\alpha \delta(k_i^\alpha, k) \rangle = \frac{1}{N_k^\alpha} \sum_i s_i^\alpha \delta(k_i^\alpha, k), \quad (6)$$

$$Y_\alpha(k) = \langle Y_i^\alpha \delta(k_i^\alpha, k) \rangle = \frac{1}{N_k^\alpha} \sum_i Y_i^\alpha \delta(k_i^\alpha, k),$$

where N_k^α indicates the number of nodes of degree k in layer α . When considering s_k^α , similarly to what happens in general on single networks, we can expect a scaling of the type

$$s_\alpha(k) \propto k^{\beta_\alpha}, \quad (7)$$

with $\beta_\alpha \geq 1$. We can distinguish [39] between two main scenarios depending on the value of the exponent. For $\beta_\alpha = 1$ the average strength of nodes of degree k increases linearly with k . This means that the average weight of the links incident to a node does not depend on the degree of the node, at least if we consider only distinguishable links (for a treatment of the

case of undistinguishable links see Refs. [32,33]). For $\beta_\alpha > 1$ hubs tend to have in average links with greater weight than low connectivity nodes. In a multiplex, we might have that the weights in the different layers are distributed differently. Therefore we might observe in some layers a superlinear growth of the $s_\alpha(k)$ with the degree in that layer, while in other layers we can observe a linear dependence of the strengths on the degree. When considering single weighted networks it has been observed that in many cases the inverse participation ratio scales as an inverse power law of the degree of the node [40]. In the multiplex scenario, this would imply

$$Y_\alpha(k) \propto \frac{1}{k^{\xi_\alpha}}, \quad (8)$$

where the exponent $\xi_\alpha \leq 1$ might change from one layer to another layer. The exponent $\xi_\alpha = 1$ indicates that all the weights incident to any node are equal, while the exponent $\xi_\alpha = 0$ would imply the opposite scenario where for every node, one of the weights incident to them is significantly higher than the other weights.

C. Weights-topology correlations in multiplex networks with overlap: multilink \vec{m} , multistrength \vec{m} , and inverse multipartition ratio \vec{m}

It has been recently shown [16] that *multilinks* are the most natural way to describe and generate multiplex networks with overlap of the links. We say that two nodes are connected by a multilink $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ with $m_\alpha = 0, 1$ if they are connected in every layer α such that $m_\alpha = 1$ and not connected in every layer α , where $m_\alpha = 0$. In Fig. 1 we show an example of a multiplex formed by two layers where each pair of nodes is linked by a given multilink. In order to indicate if a multilink \vec{m} is present or not between two given nodes i and j we can introduce a multiadjacency matrix $\mathbf{A}^{\vec{m}}$ with elements $A_{ij}^{\vec{m}}$ equal to 1 if there is a multilink \vec{m} between node i and node j and zero otherwise.

In terms of the weighted adjacency matrices \mathbf{a}^α of the multiplex the elements $A_{ij}^{\vec{m}}$ of the multiadjacency matrix $\mathbf{A}^{\vec{m}}$

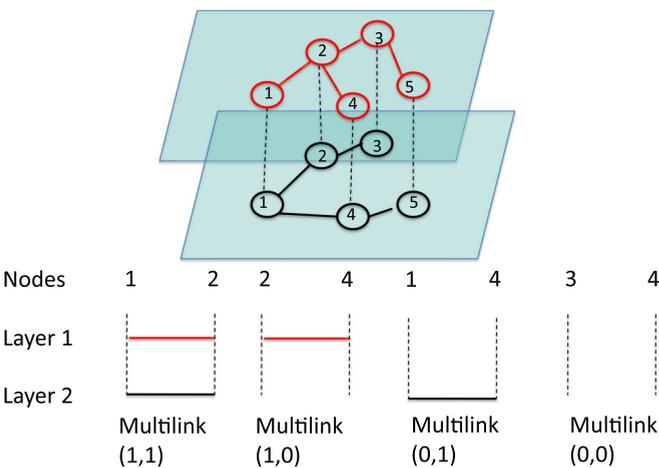


FIG. 1. (Color online) Schematic view of a duplex (multiplex) formed with two networks where any pair of nodes is linked by a different multilink \vec{m} .

are given by

$$A_{ij}^{\vec{m}} = \prod_{\alpha=1}^M [\theta(a_{ij}^\alpha) m_\alpha + (1 - \theta(a_{ij}^\alpha))(1 - m_\alpha)], \quad (9)$$

where $\theta(x) = 1$ if $x > 0$, otherwise $\theta(x) = 0$. The multilink $\vec{m} = \vec{0}$ between two nodes represents the situation in which all the layers of the multiplex the two nodes are not directly linked.

The multiadjacency matrices are 2^M but there are only $2^M - 1$ independent multiadjacency matrices because the normalization condition

$$\sum_{\vec{m}} A_{ij}^{\vec{m}} = 1 \quad (10)$$

is satisfied for any pair of nodes (i, j) . Furthermore, since the multiadjacency matrices have elements $A_{ij}^{\vec{m}} = 0, 1$, the above condition implies that between any pair of nodes (i, j) there can be only one multilink \vec{m} . We indicate the type of this multilink as

$$\vec{m} = \vec{m}^{ij} = (\theta(a_{ij}^1), \theta(a_{ij}^2), \dots, \theta(a_{ij}^\alpha), \dots, \theta(a_{ij}^M)), \quad (11)$$

where $\theta(x) = 1$ if $x > 0$ and otherwise $\theta(x) = 0$. The multilink \vec{m} is characterized by the *overlap multiplicity* $v(\vec{m}) = \sum_\alpha m_\alpha$, indicating that the multilink \vec{m} links two pair of nodes by $v(\vec{m})$ links. Using the multiadjacency matrices it is possible to define the *multidegree* \vec{m} , $k_i^{\vec{m}}$ of node i , given by

$$k_i^{\vec{m}} = \sum_{j \neq i} A_{ij}^{\vec{m}}, \quad (12)$$

indicating how many multilinks \vec{m} are connected to node i . Consider, for example, the social multiplex network where people interact by two means of communication (mobile phone and email). The multidegree $k_i^{(1,1)}$ indicates the number of friends of node i that communicate with node i both by email and mobile phone, $k_i^{(1,0)}$ indicates the number of friends of node i that only communicate with node i by mobile phone, and $k_i^{(0,1)}$ indicates the number of friends of node i that only communicate with node i by email.

For a given weighted multiplex network we can study the relation between weights and multilinks introducing, at first, the *total multistrength* \vec{m} , $S_\alpha^{\vec{m}}$ in a layer α such that $m_\alpha > 0$ as

$$S_\alpha^{\vec{m}} = \sum_{i < j} a_{ij}^\alpha A_{ij}^{\vec{m}}. \quad (13)$$

Given a particular multilink \vec{m} , this quantity indicates the total weight in layer α of multilinks \vec{m} and it is properly defined whenever $m_\alpha > 0$. The number of total multistrengths \vec{m} that we can define in a multiplex of M layers is given by $K = M2^{M-1}$. In fact, we have that the total multistrength $S_\alpha^{\vec{m}}$ is nontrivial only for multilinks \vec{m} , where $m_\alpha = 1$, while for the remaining layers β the value of m_β can be either zero or 1.

Moreover, we can define the *multistrength* \vec{m} , $s_{i,\alpha}^{\vec{m}}$ of node i in layer α such that $m_\alpha > 0$, as

$$s_{i,\alpha}^{\vec{m}} = \sum_{j \neq i} a_{ij}^\alpha A_{ij}^{\vec{m}} \quad (14)$$

and the *inverse multiparticipation ratio* \bar{m} , $Y_{i,\alpha}^{\bar{m}}$ of node i in layer α such that $m_\alpha > 0$ as

$$Y_{i,\alpha}^{\bar{m}} = \sum_{j \neq i} \left(\frac{a_{ij}^\alpha A_{ij}^{\bar{m}}}{\sum_r a_{ir}^\alpha A_{ir}^{\bar{m}}} \right)^2. \quad (15)$$

Using the same argument used to evaluate the number of total multistrengths \bar{m} , it is easy to prove that the number of local multistrength \bar{m} and the number of multiparticipation ratio \bar{m} are given by $N \cdot M \cdot 2^{M-1}$. Moreover, here we introduce $u_i^{\alpha, \bar{m}}$, the sum of the squares of the weights incident to a node i in layer α and belonging to a certain type of multilink, as

$$u_{i,\alpha}^{\bar{m}} = Y_{i,\alpha}^{\bar{m}} (s_{i,\alpha}^{\bar{m}})^2 = \sum_{j \neq i} (a_{ij}^\alpha A_{ij}^{\bar{m}})^2. \quad (16)$$

In multiplex weighted networks, it was found that multistrengths and inverse multiparticipation ratio can have a different scaling behavior depending on the type of multilink. In fact, the average quantities

$$\begin{aligned} s_\alpha^{\bar{m}}(k^{\bar{m}}) &= \langle s_i^{\alpha, \bar{m}} \delta(k_i^{\bar{m}}, k^{\bar{m}}) \rangle, \\ Y_\alpha^{\bar{m}}(k^{\bar{m}}) &= \langle Y_i^{\alpha, \bar{m}} \delta(k_i^{\alpha, \bar{m}}, k^{\bar{m}}) \rangle, \end{aligned} \quad (17)$$

are expected to scale like

$$\begin{aligned} s_\alpha^{\bar{m}}(k^{\bar{m}}) &\propto (k^{\bar{m}})^{\beta_{\alpha, \bar{m}}}, \\ Y_\alpha^{\bar{m}}(k^{\bar{m}}) &\propto (k^{\bar{m}})^{-\xi_{\alpha, \bar{m}}}, \end{aligned} \quad (18)$$

with $\beta_{\alpha, \bar{m}} \geq 1$ and positive $\xi_{\alpha, \bar{m}} \leq 1$. The significance dependence of these exponents as a function of the multilink type \bar{m} , i.e., on the presence of a certain pattern of overlap or absence of it, indicates the rich interplay between the topology of the weighted networks and their weights. For example, in the CoCi-PRE duplex described in Ref. [4], formed by authors of PRE that in one layer are connected by collaborations and on the other layer are connected by citations of each other work, the weight-topology correlation is revealed by the different exponent of the multistrength in the citation network calculated either in presence of the overlap of the links in the two layers or in absence of it. This reveals the tendency of scientific authors of PRE to cite more the scientists of high multidegree that are their co-authors than the scientists with the same multidegree that are not their coauthors. These correlations between weights and overlap patterns are a very general type of correlation likely to exist in large set of multiplex data set with significant overlap of the links. It is therefore very important to be able to construct null models for multiplex networks with the desired level of correlations between weights and overlap of the links, i.e., with given weighted properties of the multilinks.

D. Weights-topology correlations in multiplex networks with overlap: ν -total strength, the ν -multistrength sequence, and the ν -inverse multiparticipation ratio

Using multilinks \bar{m} can be numerically viable only for weighted multiplex networks with a number M of layers such that $M \ll \log(N)$. As long as this condition is not met, it is more efficient to study the properties of the ν multilinks. The ν multilinks are any type of multilink \bar{m} with multiplicity of

overlap $\nu(\bar{m}) = \nu$. Therefore in a multiplex social networks, where the layers correspond to the means of communication between two people, node i and node j are linked by a ν multilink if they can communicate by a maximum of ν means of communication, independently on the identity of these. For example, two people that communicate in Twitter and Facebook are linked by a ν multilink with $\nu = 2$, and the same is true for two people interacting by mobile phone and email.

We can therefore define the ν -multiadjacency matrices \mathbf{A}^ν with elements $A_{ij}^\nu = 0, 1$ given by

$$\begin{aligned} A_{ij}^\nu &= \sum_{\bar{m} | \nu(\bar{m}) = \nu} A_{ij}^{\bar{m}} \\ &= \sum_{\bar{m} | \nu(\bar{m}) = \nu} \prod_{\alpha=1}^M [\theta(a_{ij}^\alpha) m_\alpha + (1 - \theta(a_{ij}^\alpha))(1 - m_\alpha)], \end{aligned}$$

and $\nu = 0, 1, 2, \dots, M$. The ν -adjacency matrices are not all independent, since between any two nodes there can be just one type of ν multilink, i.e.,

$$\sum_{\nu=0}^M A_{ij}^\nu = 1. \quad (19)$$

Therefore we can consider as independent variables only the ν -adjacency matrices corresponding to the nontrivial ν multilinks with $\nu = 1, 2, \dots, M$. Moreover, we call with ν^{ij} the type of ν multilink connecting node i with node j , i.e., we have

$$A_{ij}^{\nu^{ij}} = 1 \quad (20)$$

for all pairs of nodes (i, j) . The number of distinct and nontrivial ν multilinks with $\nu \neq 0$ is given by M , hence the ν properties of the networks are only polynomial with M while the full multilink properties are growing exponentially with M . Modelling networks with given ν multilinks properties is therefore convenient when considering multiplex networks with large number of layers M . Given the definition of ν -multiadjacency matrices it is straightforward to define the ν -multidegree k_i^ν of node i , given by

$$k_i^\nu = \sum_{j=1}^N A_{ij}^\nu, \quad (21)$$

indicating the number of neighbors of node i that are connected to node i by a ν multilink, with $\nu = 0, 1, 2, \dots, M$. If we consider the weighted properties of the ν multilink for a given layer α , we can define the ν -total strength S_α^ν , the ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$, and the ν -inverse multi participation ratio $\{Y_{i,\alpha}^\nu\}$, as in the following:

$$\begin{aligned} S_\alpha^\nu &= \sum_{i < j} a_{ij}^\alpha A_{ij}^\nu, \\ s_{i,\alpha}^\nu &= \sum_{j \neq i} a_{ij}^\alpha A_{ij}^\nu, \end{aligned} \quad (22)$$

$$Y_{i,\alpha}^\nu = \sum_{j \neq i} \left(\frac{a_{ij}^\alpha A_{ij}^\nu}{\sum_r a_{ir}^\alpha A_{ir}^\nu} \right)^2. \quad (23)$$

Moreover, we can introduce the quantities $u_i^{\alpha,v}$, indicating the sum of the squares of the weights incident to a node i in layer α and belonging to a certain type of v multilink, as

$$u_{i,\alpha}^v = Y_{i,\alpha}^v (s_{i,\alpha}^v)^2 = \sum_{j \neq i} (a_{ij}^\alpha A_{ij}^v)^2. \quad (24)$$

Similarly to what we described in the previous paragraph, we can evaluate the correlations between the weights and the pattern of overlap between the links by measuring the exponents $\beta_{\alpha,v}$ and $\xi_{\alpha,v}$, determining the scaling

$$\begin{aligned} s_\alpha^v(k^v) &\propto (k^v)^{\beta_{\alpha,v}}, \\ Y_\alpha^v(k^v) &\propto (k^v)^{-\xi_{\alpha,v}}, \end{aligned} \quad (25)$$

of the average quantities $s_\alpha^v(k^v)$ and $Y_\alpha^v(k^v)$ given by

$$\begin{aligned} s_\alpha^v(k^v) &= \langle s_i^{\alpha,v} \delta(k_i^v, k^v) \rangle, \\ Y_\alpha^v(k^v) &= \langle Y_i^{\alpha,v} \delta(k_i^{\alpha,v}, k^v) \rangle. \end{aligned} \quad (26)$$

III. A BIOLOGICAL CASE STUDY

Here we analyze a data set of gene expression profiles from human cancer and healthy subjects, using the framework of multilayer networks. For this analysis, we construct a duplex based on whole-genome gene expression data, as taken from Geo Omnibus Database ([41], *GSE4183* data set). From this data set, a subset of 2835 genes was chosen, known to have a clear biological role (i.e., belonging to known functional pathways as annotated in the KEGG database [42]) and with potential interactions between each other (as annotated in PathwayCommons Protein-Protein Interaction network database [43]). In one layer, the network is reconstructed from gene expression correlation of $M_1 = 8$ normal colon samples, while in the other layer $M_2 = 15$ cancer samples are considered. Nonparametric Kendall's τ is used in order to evaluate the correlation between genes, and in each layer a network is obtained by a thresholding on the absolute value of τ that keeps about $\approx 10\%$ of the possible links ($\tau_1 = 0.5$ and $\tau_2 = 0.4$ for normal and cancer samples, respectively).

We also associate a weight a_{ij}^α to each duplex link, obtained from gene expression values of the normal and cancer groups. Namely we calculate the average value over all samples of each gene in both layers,

$$\langle e_i^\alpha \rangle = \frac{1}{M_\alpha} \sum_{k=1}^{M_\alpha} e_{ik}^\alpha, \quad (27)$$

with $\alpha = 1, 2$ indicating the two layers of the network (1 = Normal, 2 = Cancer) and e_{ik}^α indicating the expression of gene i in the sample k belonging to the layer $\alpha = 1, 2$. Finally, we define the weights on each layer as the absolute difference between all gene couples,

$$a_{ij}^\alpha = |\langle e_i^\alpha \rangle - \langle e_j^\alpha \rangle| \quad \forall i, \quad j = 1, \dots, 2,835. \quad (28)$$

The weights have been discretized as follows: given the minimum and maximum over all values of a_{ij}^α (from the union of cancer and normal samples distance matrices), we performed a uniform binning with 100 bins in this interval, thus obtaining 100 possible values for the weights a_{ij}^α . This duplex encodes in its topology all the connections among those

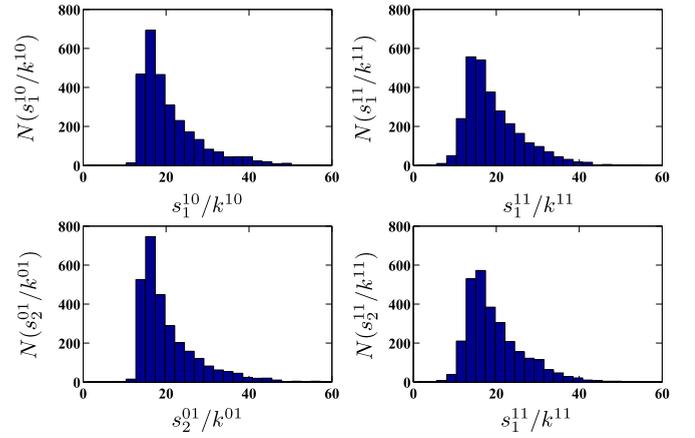


FIG. 2. (Color online) Biological case study: We display the distributions $\{s_{i,\alpha}^m/k_i^m\}$, i.e., the average weight of each node's interactions, classified according to the multilinks.

genes with highly correlated or anticorrelated gene expression profiles. Moreover, the weight distribution describes their distances in terms of mean gene expression values. These kinds of information essentially differ: For example, two genes can be highly correlated in their trends across the samples but one could be much more expressed than the other one.

We can integrate different aspects of gene expression data sets thanks to network approaches, and, furthermore, we can investigate different experimental setups thanks to multiplex networks tools. The analysis of the multiplex network we have constructed, formed by one layer for the normal samples and one layer for those patients with colorectal cancer, can help us understand if there is a backbone of highly correlated genes that are conserved after the onset of the cancer disease. Moreover, we can characterize all the interactions that are specific for the two conditions.

In order to understand how the weights of the links in a selected layer are related to different multilinks we consider the distributions $\{s_{i,\alpha}^m/k_i^m\}$, i.e., for each node we calculate the average weight of its interactions, classified according to the multilinks. In Fig. 2 we show these distributions for a given layer $\alpha = 1, 2$ and a given multilink \bar{m} . In both layers, the distribution of average weights related to multilink (1,1) differs significantly from that one of the specific layer [i.e., multilink (1,0) or (0,1)], with a lower mean value and median of the distribution. For layer 1, we compared the distributions $\{s_{i,1}^{(1,1)}/k_i^{(1,1)}\}$ and $\{s_{i,1}^{(1,0)}/k_i^{(1,0)}\}$ using a Wilcoxon rank sum test, a nonparametric test for equality of population medians. The p value is highly significant (3.88×10^{-22}) and the two mean values are, respectively, $\langle \{s_{i,1}^{(1,1)}/k_i^{(1,1)}\} \rangle = 19.36$ and $\langle \{s_{i,1}^{(1,0)}/k_i^{(1,0)}\} \rangle = 20.92$. For layer 2, the layer related to cancer samples, the rank sum test is always significant but with a less dramatic p value (5.23×10^{-8}). The mean values for this layer are, respectively, $\langle \{s_{i,2}^{(1,1)}/k_i^{(1,1)}\} \rangle = 19.54$ and $\langle \{s_{i,2}^{(0,1)}/k_i^{(0,1)}\} \rangle = 20.46$.

We studied the relation between the weights of the set of overlapping links, $\{a_{ij,1}^{(1,1)}\}$ and $\{a_{ij,2}^{(1,1)}\}$. A linear fitting shows that these weights are almost identical, with a relation $a_{ij,2}^{(1,1)} = 0.94a_{ij,1}^{(1,1)} + 3.30$ ($R^2 = 0.92$). This result is not

trivial, since genes could be correlated (preserving the links) but expressed in a different way (i.e., with different weights) in healthy and cancer samples, and highlights the existence of a backbone of genes (and related biological processes) that are conserved during the disease progression, possibly due to their fundamental functional role.

The focus here in this paper is on the possibility to generate a null model for such a multiplex real instance, in order to provide an example of possible application of the theoretical framework here developed to model real data sets. In order to generate a null model, we will construct a network ensemble with given multidegree sequence and multistrength sequence and generate multiplex networks out of this ensemble with the desired structural properties. Sampling multiplex networks from their ensembles will offer the opportunity of comparing our real biological structure with some compatible instances. Moreover, the entropy measure gives us the logarithm of the number of “typical” duplex networks in the ensemble, a value that can be used to compare different experimental setups and clinical conditions, evaluating what is the level of information encoded in the selected structural properties of biological networks.

IV. CANONICAL WEIGHTED MULTIPLEXES ENSEMBLES OR EXPONENTIAL WEIGHTED MULTIPLEXES

Null models for weighted multiplex networks can be constructed using the formalism of canonical network ensembles also known as exponential random graphs [24,25,27,28]. These ensembles of networks generate the least biased set of networks satisfying a set of constraint on average. In fact, these ensembles are derived by a maximal entropy approach conditioned to a series of structural constraints. The entropy of these ensembles and of the correspondent microcanonical ensembles enforcing the corresponding hard constraints [26,38] can be used to quantify the level of information encoded in the structural constraints that are imposed to the networks. In Refs. [16,19] this approach was taken to model simple multiplex networks. Here we show how this framework can be applied to model weighted multiplex networks.

A weighted multiplex ensemble is defined once the probability $P(\vec{G})$ of any possible weighted multiplex is given. We can build a canonical multiplex ensemble by maximizing the entropy \mathcal{S} of the ensemble given by

$$\mathcal{S} = - \sum_{\vec{G}} P(\vec{G}) \log P(\vec{G}) \quad (29)$$

under the condition that the soft constraints we want to impose are satisfied. We assume to have K of such constraints determined by the conditions

$$\sum_{\vec{G}} P(\vec{G}) F_{\mu}(\vec{G}) = C_{\mu} \quad (30)$$

for $\mu = 1, 2, \dots, K$, where $F_{\mu}(\vec{G})$ determines one of the structural constraints that we want to impose to the multiplex. Therefore, the maximal-entropy multiplex ensemble satisfying the constraints given by Eqs. (30) is the solution of the

following system of equations:

$$\frac{\partial}{\partial P(\vec{G})} \left[\mathcal{S} - \sum_{\mu=1}^K \lambda_{\mu} \sum_{\vec{G}} F_{\mu}(\vec{G}) P(\vec{G}) - \Lambda \sum_{\vec{G}} P(\vec{G}) \right] = 0, \quad (31)$$

where the Lagrangian multiplier Λ enforces the normalization of the $P(\vec{G})$ probability distribution and the Lagrangian multiplier λ_{μ} enforces the constraint μ .

Therefore we get that the probability of a multiplex $P(\vec{G})$ in a canonical multiplex ensemble is given by

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\mu} \lambda_{\mu} F_{\mu}(\vec{G}) \right], \quad (32)$$

where the normalization constant $Z = \exp(1 + \Lambda)$ is called the “partition function” of the canonical multiplex ensemble and is fixed by the normalization condition on $P(\vec{G})$. The values of the Lagrangian multipliers λ_{μ} are determined by imposing the constraints given by Eq. (30), assuming for the probability $P(\vec{G})$ the structural form given by Eq. (32). From the definition of the partition function Z and Eq. (32), it can be easily shown that the Lagrangian multipliers λ_{μ} can be expressed as the solutions of the following set of equations:

$$C_{\mu} = - \frac{\partial \log Z}{\partial \lambda_{\mu}}. \quad (33)$$

We call the entropy \mathcal{S} of the canonical multiplex ensemble the *Shannon entropy* of the ensemble.

We can define the marginal probability for a specific value of the element a_{ij}^{α} as

$$\pi_{ij}^{\alpha}(a_{ij}^{\alpha} = w) = \sum_{\vec{G}} P(\vec{G}) \delta(a_{ij}^{\alpha}, w), \quad (34)$$

where $\delta(x, y)$ stands for the Kronecker delta. The marginal probabilities $\pi_{ij}^{\alpha}(a_{ij}^{\alpha})$ sum up to 1,

$$\sum_{a_{ij}^{\alpha}=0}^{\infty} \pi_{ij}^{\alpha}(a_{ij}^{\alpha}) = 1. \quad (35)$$

We can compute also the average weight $\langle a_{ij}^{\alpha} \rangle$ between node i and node j that is

$$\langle a_{ij}^{\alpha} \rangle = \sum_{\vec{G}} P(\vec{G}) a_{ij}^{\alpha} = \sum_{a_{ij}^{\alpha}=0}^{\infty} a_{ij}^{\alpha} \pi_{ij}^{\alpha}(a_{ij}^{\alpha}). \quad (36)$$

In the layer α a link between two nodes i and j exists with probability π_{ij}^{α} that is related with all the possible weights that differ from zero,

$$\pi_{ij}^{\alpha} = \sum_{\vec{G}} P(\vec{G}) \theta(a_{ij}^{\alpha}) = \sum_{a_{ij}^{\alpha} \neq 0}^{\infty} \pi_{ij}^{\alpha}(a_{ij}^{\alpha}). \quad (37)$$

A. Uncorrelated and correlated canonical multiplex ensembles

The multiplex ensembles can be distinguished between uncorrelated and correlated multiplex ensembles. For uncorrelated multiplex ensembles, the probability of a multiplex

$P(\vec{G})$ is factorizable into the probability $P_\alpha(G_\alpha)$ of each single network G_α at layer α , i.e.,

$$P(\vec{G}) = \prod_{\alpha=1}^M P_\alpha(G_\alpha). \quad (38)$$

Therefore, the entropy \mathcal{S} of any uncorrelated multiplex ensemble given by Eq. (29) with $P(\vec{G})$ given by Eq. (38) is additive in the number of layers, i.e.,

$$\mathcal{S} = \sum_{\alpha=1}^M \mathcal{S}_\alpha = - \sum_{\alpha=1}^M \sum_{G_\alpha} P_\alpha(G_\alpha) \log P_\alpha(G_\alpha). \quad (39)$$

As a consequence of these relations, when each constraint depends on a single network G_α in a layer α the resulting multiplex ensemble is uncorrelated.

Example of these types of constraints are the total strengths S^α in each layer α , the strength s_i^α of the generic node i in layer α , or the degree k_i^α of the node i in layer α .

In these ensembles of multiplex networks we have that the presence of a link in a layer α is uncorrelated with the presence of a link between the same two nodes in a layer $\beta \neq \alpha$. Therefore we have

$$\langle a_{ij}^\alpha a_{ij}^\beta \rangle = \langle a_{ij}^\alpha \rangle \langle a_{ij}^\beta \rangle. \quad (40)$$

In correlated multiplex networks, instead the probability of a multiplex does not factorize into the probabilities of the single networks that constitute the multiplex network. We have in this case

$$P(\vec{G}) \neq \prod_{\alpha=1}^M P_\alpha(G_\alpha), \quad (41)$$

and as a consequence of this there is at least a pair of nodes (i, j) and layers α, β such that the weights of the links connecting node i and node j in layer α and layer β are correlated, i.e.,

$$\langle a_{ij}^\alpha a_{ij}^\beta \rangle \neq \langle a_{ij}^\alpha \rangle \langle a_{ij}^\beta \rangle. \quad (42)$$

Example of constraints that generate correlated multiplex ensembles are constraints on the multidegree sequence or the multistrength sequence.

V. EXAMPLES OF CORRELATED AND UNCORRELATED MULTIPLEX NETWORK ENSEMBLES

Here we provide three example of uncorrelated and correlated multiplex network ensemble. The case of uncorrelated multiplex networks (case treated in Sec. V A) is very closely related to the treatment of weighted ensembles of single networks [29–31], nevertheless the case of uncorrelated multiplex networks (cases treated in Secs. V B and V C) provides a novel framework to understand correlations between weights and multidegrees in a model. In the main text of the article we will present only few examples of multiplex network ensembles, while a longer set of ensembles is discussed in the appendix.

A. Multiplex ensembles with given expected strength sequence and degree sequence in each layer

This is an example of uncorrelated network ensemble. We fix the expected strength s_i^α and the expected degree k_i^α of

every node i , in each layer α . We have $K = M2N$ constraints in the system. These constraints are given by

$$\begin{aligned} \sum_{\vec{G}} F_{i,\alpha}(\vec{G}) P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha \right) P(\vec{G}) = s_i^\alpha, \\ \sum_{\vec{G}} F_{i,\alpha}(\vec{G}) P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} \theta(a_{ij}^\alpha) \right) P(\vec{G}) = k_i^\alpha, \end{aligned} \quad (43)$$

with $\alpha = 1, 2, \dots, M$. We introduce the Lagrangian multipliers $\lambda_{i,\alpha}$ for the first set of $N \cdot M$ constraints and the Lagrangian multipliers $\omega_{i,\alpha}$ for the second set of $N \cdot M$ constraints. Therefore, the probability $P(\vec{G})$ of a multiplex in this ensemble, of general expression given by Eq. (32), in this specific example is given by

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\alpha=1}^M \sum_i \lambda_{i,\alpha} \sum_{j \neq i} a_{ij}^\alpha - \sum_{\alpha=1}^M \sum_i \omega_{i,\alpha} \sum_{j \neq i} \theta(a_{ij}^\alpha) \right],$$

where the partition function Z can be expressed explicitly as

$$\begin{aligned} Z &= \sum_{\vec{G}} \exp \left[- \sum_{\alpha=1}^M \sum_i \sum_{j \neq i} (\lambda_{i,\alpha} a_{ij}^\alpha + \omega_{i,\alpha} \theta(a_{ij}^\alpha)) \right] \\ &= \prod_{\alpha=1}^M \prod_{i < j} \left[1 + \frac{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha}) - (\lambda_{i,\alpha} + \lambda_{j,\alpha})}}{1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}} \right], \end{aligned} \quad (44)$$

and the Lagrangian multipliers are fixed by the conditions

$$\begin{aligned} s_i^\alpha &= - \frac{\partial \log Z}{\partial \lambda_{i,\alpha}}, \\ k_i^\alpha &= - \frac{\partial \log Z}{\partial \omega_{i,\alpha}}. \end{aligned} \quad (45)$$

The average weight of the link (i, j) in layer α , i.e., $\langle a_{ij}^\alpha \rangle$, is given by Eq. (36) that in this case reads

$$\langle a_{ij}^\alpha \rangle = \frac{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha}) + (\lambda_{i,\alpha} + \lambda_{j,\alpha})}}{(e^{\lambda_{i,\alpha} + \lambda_{j,\alpha}} - 1)(e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} + e^{\lambda_{i,\alpha} + \lambda_{j,\alpha}} - 1)}. \quad (46)$$

From Eq. (34) we write the marginal probabilities $\pi_{ij}^\alpha(a_{ij}^\alpha)$ for this specific ensemble that is given by

$$\pi_{ij}^\alpha(a_{ij}^\alpha) = \frac{e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha}) a_{ij}^\alpha - (\omega_{i,\alpha} + \omega_{j,\alpha}) \theta(a_{ij}^\alpha)} [1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}]}{1 + e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})} [e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} - 1]}. \quad (47)$$

Moreover, from Eq. (37) the probability p_{ij}^α that the link (i, j) in layer α has weight different from zero is given by

$$p_{ij}^\alpha = \frac{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})}}{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} + e^{\lambda_{i,\alpha} + \lambda_{j,\alpha}} - 1}. \quad (48)$$

We observe that we can write the Eq. (32) in terms of marginal probabilities $\pi_{ij}^\alpha(a_{ij}^\alpha)$, namely

$$P(\vec{G}) = \prod_{\alpha=1}^M \prod_{i < j} \pi_{ij}^\alpha(a_{ij}^\alpha). \quad (49)$$

Therefore the entropy \mathcal{S} of this canonical multiplex ensemble is given by Eq. (29) and in this special case can be written as

$$\mathcal{S} = - \sum_{\alpha=1}^M \sum_{i<j} \sum_{a_{ij}^\alpha=0}^{\infty} \pi_{ij}^\alpha(a_{ij}^\alpha) \log(\pi_{ij}^\alpha(a_{ij}^\alpha)). \quad (50)$$

B. Multiplex ensembles with given expected multidegree sequence $\{k_i^{\vec{m}}\}$ and given expected multistrength sequence $\{s_{i,\alpha}^{\vec{m}}\}$

In many applications it is important to consider the weighted multiplex networks in which we fix at the same time the average multidegree sequence $k_i^{\vec{m}}$ and the average multistrength sequence $s_{i,\alpha}^{\vec{m}}$. The number of independent constraints is therefore $K = (2^M - 1)N + (2^{M-1})M \cdot N$.

In particular, the constraints we are imposing are the following:

$$\sum_{\vec{G}} F_{i,\alpha}^{\vec{m}}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^{\vec{m}} a_{ij}^\alpha \right) P(\vec{G}) = s_{i,\alpha}^{\vec{m}}, \quad (51)$$

$$\sum_{\vec{G}} F_i^{\vec{m}}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^{\vec{m}} \right) P(\vec{G}) = k_i^{\vec{m}}.$$

The canonical probability $P(\vec{G})$ of the multiplex in the ensemble becomes

$$\begin{aligned} P(\vec{G}) &= \frac{1}{Z} \exp \left[- \sum_{\vec{m} \neq \vec{0}} \sum_i \sum_{j \neq i} \left(\omega_i^{\vec{m}} A_{ij}^{\vec{m}} + \sum_{\alpha=1}^M \lambda_{i,\alpha}^{\vec{m}} A_{ij}^{\vec{m}} a_{ij}^\alpha \right) \right] \\ &= \frac{1}{Z} \exp \left[- \sum_{i<j} \sum_{\vec{m} \neq \vec{0}} (\omega_i^{\vec{m}} + \omega_j^{\vec{m}}) A_{ij}^{\vec{m}} \right] \\ &\quad \times \exp \left[- \sum_{i<j} \sum_{\vec{m} \neq \vec{0}} \sum_{\alpha=1}^M (\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}}) A_{ij}^{\vec{m}} a_{ij}^\alpha \right]. \quad (52) \end{aligned}$$

The partition function Z can be expressed explicitly as

$$Z = \prod_{i<j} \mathcal{Z}_{ij}, \quad (53)$$

where \mathcal{Z}_{ij} is given by

$$\mathcal{Z}_{ij} = 1 + \sum_{\vec{m} \neq \vec{0}} e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})} \prod_{\alpha=1}^M \left(\frac{e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right)^{a_{ij}^\alpha}. \quad (54)$$

The Lagrangian multipliers are fixed by the conditions

$$\begin{aligned} - \frac{\partial \log Z}{\partial \lambda_{i,\alpha}^{\vec{m}}} &= s_{i,\alpha}^{\vec{m}} = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle, \\ - \frac{\partial \log Z}{\partial \omega_i^{\vec{m}}} &= k_i^{\vec{m}} = \sum_{j \neq i} \langle A_{ij}^{\vec{m}} \rangle. \end{aligned} \quad (55)$$

We now indicate with \vec{a}_{ij} the vector $(a_{ij}^1, a_{ij}^2, \dots, a_{ij}^\alpha, \dots, a_{ij}^M)$. The probability of a multiplex $P(\vec{G})$ can be

rewritten as

$$P(\vec{G}) = \prod_{i<j} \pi_{ij}(\vec{a}_{ij}), \quad (56)$$

with

$$\pi_{ij}(\vec{a}_{ij}) = \frac{e^{-(\omega_i^{\vec{m}^{ij}} + \omega_j^{\vec{m}^{ij}})}}{\mathcal{Z}_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i,\alpha}^{\vec{m}^{ij}} + \lambda_{j,\alpha}^{\vec{m}^{ij}}) a_{ij}^\alpha}, \quad (57)$$

where $\vec{m}^{ij} = (m_1^{ij}, \dots, m_\alpha^{ij}, \dots, m_M^{ij})$ with $m_\alpha^{ij} = \theta(a_{ij}^\alpha)$. With $\pi_{ij}(\vec{a}_{ij})$ we define, for a position ij , the probability of a particular sequence of weights on the layers. The normalization condition is fulfilled,

$$\sum_{\vec{a}_{ij}} \pi_{ij}(\vec{a}_{ij}) = 1. \quad (58)$$

Later we can compute the average weight of the link ij on the multilink \vec{m} , in the layer α , and the probability of a multilink \vec{m} between node i and node j , $p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle$, respectively,

$$\begin{aligned} \langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle &= \frac{e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})}}{\mathcal{Z}_{ij}} \left[\frac{1}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right] \\ &\quad \times \prod_{\beta=1}^M \left[\frac{e^{-(\lambda_{i,\beta}^{\vec{m}} + \lambda_{j,\beta}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\beta}^{\vec{m}} + \lambda_{j,\beta}^{\vec{m}})}} \right]^{m_\beta}, \quad (59) \end{aligned}$$

$$p_{ij}^{\vec{m}} = \frac{e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})}}{\mathcal{Z}_{ij}} \prod_{\alpha=1}^M \left[\frac{e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right]^{m_\alpha}, \quad (60)$$

where the normalization condition is fulfilled, namely,

$$\sum_{\vec{m}} p_{ij}^{\vec{m}} = 1. \quad (61)$$

Moreover, the relationship between $p_{ij}^{\vec{m}}$ and the probabilities $\pi_{ij}(\vec{a}_{ij})$ is

$$\sum_{\vec{a}_{ij}} A_{ij}^{\vec{m}} \pi_{ij}(\vec{a}_{ij}) = p_{ij}^{\vec{m}}. \quad (62)$$

Finally, the probability of a multiplex $P(\vec{G})$ is given by Eq. (56) and the entropy \mathcal{S} of this ensemble can be calculated starting from its definition Eq. (29), giving

$$\mathcal{S} = - \sum_{i<j} \sum_{\vec{a}_{ij}} \pi_{ij}(\vec{a}_{ij}) \log \pi_{ij}(\vec{a}_{ij}). \quad (63)$$

C. Multiplex ensembles with given expected ν -multidegree sequence $\{k_i^\nu\}$ and expected ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$

In a multiplex networks formed by many layers, an efficient way to consider both topological and weighted properties of the multilayer structure is to construct multiplex networks with given expected ν -multidegree sequence $\{k_i^\nu\}$ and expected ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$. The $N \cdot M \cdot (M + 1)$ constraints are given by

$$\sum_{\vec{G}} F_{i,\alpha}^\nu(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha A_{ij}^\nu \right) P(\vec{G}) = s_{i,\alpha}^\nu, \quad (64)$$

$$\sum_{\vec{G}} F_i^\nu(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^\nu \right) P(\vec{G}) = k_i^\nu,$$

with $i = 1, 2, \dots, N$, $\alpha = 1, 2, \dots, M$, and $\nu = 1, 2, \dots, M$. The canonical probability $P(\vec{G})$ of the multiplex in this ensemble can be expressed in terms of the Lagrangian multipliers $\lambda_{j,\alpha}^\nu$ and ω_i^ν , i.e.,

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{i < j} \sum_{\nu=1}^M (\omega_i^\nu + \omega_j^\nu) A_{ij}^\nu \right] \times \exp \left[- \sum_{i < j} \sum_{\nu=1}^M \sum_{\alpha=1}^M (\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu) A_{ij}^\nu a_{ij}^\alpha \right], \quad (65)$$

where the partition function Z is given by

$$Z = \prod_{i < j} \mathcal{Z}_{ij}, \quad (66)$$

with

$$\mathcal{Z}_{ij} = 1 + \sum_{\nu=1}^M e^{-(\omega_i^\nu + \omega_j^\nu)} \sum_{\vec{m} | \nu(\vec{m}) = \nu} \prod_{\alpha=1}^M \left[\frac{e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right]^{m_\alpha}. \quad (67)$$

The Lagrangian multipliers are fixed by the conditions Eq. (64) that can be also written in terms of the partial derivatives of the partition function as

$$-\frac{\partial \log Z}{\partial \lambda_{i,\alpha}^\nu} = s_{i,\alpha}^\nu = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^\nu \rangle, \quad (68)$$

$$-\frac{\partial \log Z}{\partial \omega_i^\nu} = k_i^\nu = \sum_{j \neq i} \langle A_{ij}^\nu \rangle.$$

As in the previous cases, the probability $P(\vec{G})$ of a multiplex network \vec{G} is given by Eq. (56). The entropy of this ensemble takes the same expression given by Eq. (63) with $\pi_{ij}(\vec{a}_{ij})$ given by

$$\pi_{ij}(\vec{a}_{ij}) = \frac{e^{-(\omega_i^{\nu^{ij}} + \omega_j^{\nu^{ij}})}}{\mathcal{Z}_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i,\alpha}^{\nu^{ij}} + \lambda_{j,\alpha}^{\nu^{ij}}) a_{ij}^\alpha}. \quad (69)$$

The probability p_{ij}^ν that the node i and the node j are linked by a ν multilink is given by

$$p_{ij}^\nu = \frac{e^{-(\omega_i^\nu + \omega_j^\nu)}}{\mathcal{Z}_{ij}} \sum_{\vec{m} | \nu(\vec{m}) = \nu} \prod_{\alpha=1}^M \left[\frac{e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right]^{m_\alpha}. \quad (70)$$

Finally, the average weight of the link a_{ij}^α belonging to a ν multilink is given by

$$\langle a_{ij}^\alpha A_{ij}^\nu \rangle = \frac{e^{-(\omega_i^\nu + \omega_j^\nu)}}{\mathcal{Z}_{ij}} \left[\frac{1}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right] \times \sum_{\vec{m} | \nu(\vec{m}) = \nu} m_\alpha \prod_{\beta=1}^M \left[\frac{e^{-(\lambda_{i,\beta}^\nu + \lambda_{j,\beta}^\nu)}}{1 - e^{-(\lambda_{i,\beta}^\nu + \lambda_{j,\beta}^\nu)}} \right]^{m_\beta}. \quad (71)$$

VI. SAMPLING MULTIPLEX ENSEMBLES WITH GIVEN EXPECTED MULTIDEGREE SEQUENCE $\{k_i^{\vec{m}}\}$ AND GIVEN EXPECTED MULTISTRENGTH SEQUENCE $\{s_{i,\alpha}^{\vec{m}}\}$

Here we want to discuss how the theoretical framework described in the previous section can be used to generate weighted multiplex networks sampled from a multiplex network ensemble. We have chosen to focus specifically on the case of a multiplex network ensemble in which the given expected multidegree sequence $\{k_i^{\vec{m}}\}$ and the given expected multistrength sequence $\{s_{i,\alpha}^{\vec{m}}\}$ are constrained, but the framework we outline here of this case can be easily extended to the other ensembles discussed in this paper. Given Eqs. (60) and (57), the probability $\pi_{ij}(\vec{a}_{ij})$ can be expressed as a function of the probability $p_{ij}^{\vec{m}}$ of a multilink \vec{m} between node i and node j , namely

$$\pi_{ij}(\vec{a}_{ij}) = p_{ij}^{\vec{m}^{ij}} \prod_{\alpha=1}^M \left([e^{-(\lambda_{i,\alpha}^{\vec{m}^{ij}} + \lambda_{j,\alpha}^{\vec{m}^{ij}})}]^{a_{ij}^\alpha - 1} [1 - e^{-(\lambda_{i,\alpha}^{\vec{m}^{ij}} + \lambda_{j,\alpha}^{\vec{m}^{ij}})}] \right)^{m_\alpha^{ij}}. \quad (72)$$

The productory in Eq. (72) is the conditional probability of the multiweight \vec{a}_{ij} , given the multilink \vec{m}^{ij} . The new expression for $\pi_{ij}(\vec{a}_{ij})$ suggests a way for sampling networks from the distribution given by Eq. (56), with $\pi_{ij}(\vec{a}_{ij})$ given by Eq. (72). In fact for sampling a multiplex network from this particular ensemble, we draw a multilink \vec{m} with probability $p_{ij}^{\vec{m}}$ for each couple of nodes i and j . Subsequently, given a particular multilink, whenever $m_\alpha = 1$ we draw the additional weight $a_{ij}^\alpha - 1$ from a geometric distribution with parameter $1 - e^{-(\lambda_{i,\alpha}^{\vec{m}^{ij}} + \lambda_{j,\alpha}^{\vec{m}^{ij}})}$ and $a_{ij}^\alpha \geq 1$.

Following Eqs. (55) we wrote a MATLAB code [44] that produces the Lagrangian multipliers and calculates the entropy value of the ensemble. The algorithm runs until it finds convergence with precision 10^{-4} (this value can be always improved).

VII. COMPARISON BETWEEN THE NULL MODEL AND THE BIOLOGICAL CASE STUDY

Here our aim is to compare the structural properties of our biological case study with the networks with the same multidegree sequence and multistrength sequence generated by sampling the corresponding multiplex network ensemble. Starting from our biological duplex network described in Sec. III, at first we calculated the Lagrangian multipliers needed for $\{p_{ij}^{\vec{m}}\}$ and $\{\pi_{ij}(\vec{a}_{ij})\}$, and, second, we generated 100 different duplex networks. We checked the average values and fluctuations across our 100 duplexes. In Fig. 3 we compare the behavior of the average values across the duplexes

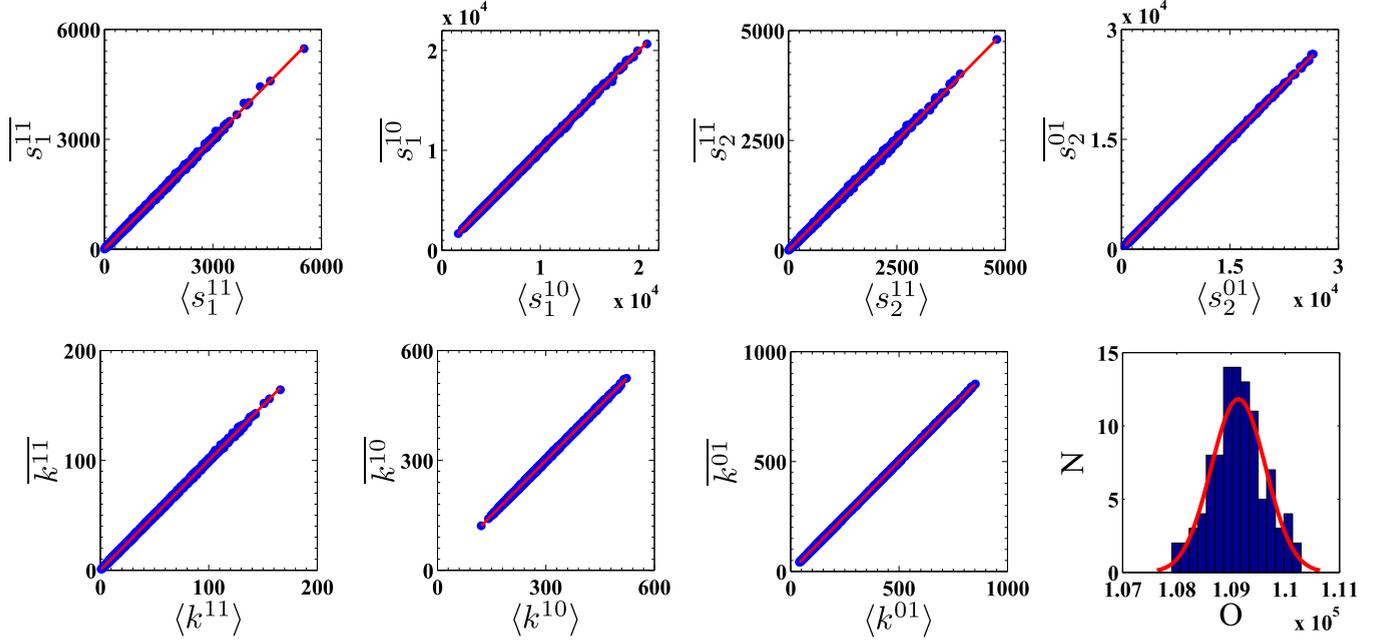


FIG. 3. (Color online) Comparison of the real values of multistrength and multidegree sequence with their related average values calculated over 100 instances. Angular brackets $\langle \dots \rangle$ indicate the real values (the fixed average values of the canonical ensemble), while overbar $\overline{(\dots)}$ defines the average measure over the 100 duplexes. Considering the relative error between the real values and the average values for each node, $\Delta E_i = (\bar{x}_i - \langle x_i \rangle) / \langle x_i \rangle$, $i = 1, \dots, 2,835$, the average absolute relative error $\langle |\Delta E| \rangle$, over all nodes for each measure, ranges from a minimum of 0.5% to a maximum of 2.4%. In the last panel we display the distribution of the 100 measures of the overlap between the two layers (in the real duplex this value was 109 056 links). The red line is a Gaussian distribution with the same mean and variance as the empirical distribution.

with the related real values, the assumed fixed average values of the canonical ensemble. We found that the multidegrees and the multistrengths are equal in average to the constrained values showing that the multiplex network framework is able to reproduce well these properties.

Nevertheless, from sample to sample the individual structural properties of the nodes (their multidegrees and their multistrengths) might fluctuate. In Fig. 4 we investigate the role of the fluctuations by plotting the histogram of the z scores of values of the multidegrees or of the multistrengths for single nodes in layer 2 of the duplex networks, the cancer layer. These distributions are calculated over the 100 multiplex networks sampled by this ensemble.

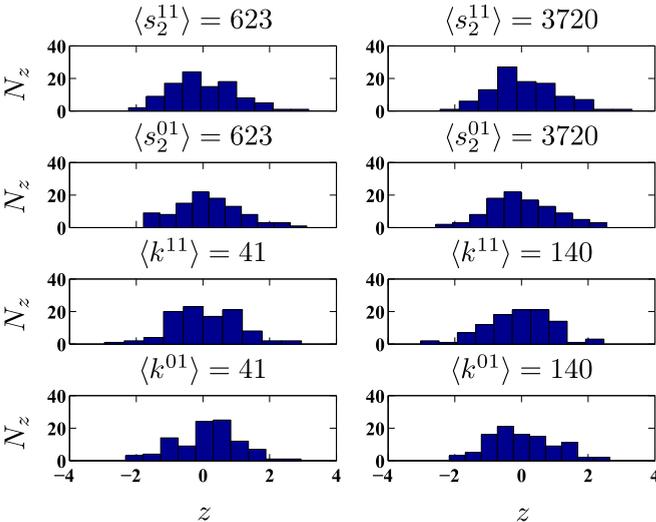


FIG. 4. (Color online) Distributions of the z scores $\{z_i\}$ related to some fixed values of multistrengths and multidegree in layer 2 (colorectal cancer layer). In each panel we display the 100 values of z across the sampled instances (gathered in 10 bins) for a chosen node with that assigned value of multistrength or multidegree. Similar results are also found for layer 1 (normal samples).

VIII. CONCLUSIONS

In conclusion, in this paper we have characterized the rich interplay between weights and the topology of multiplex networks. Multiplex networks describe a large variety of complex systems ranging from social networks to infrastructures and biological networks. Many of these multilayer structures are formed by weighted links, indicating interactions of different intensity. For example, in transportation networks different connections are characterized by a different flow of traffic, in citation and collaboration networks the interactions can be weighted by the number of collaborators or mutual citations, and in biological networks the weights can be given by the strength of chemical bonding or by mutual coexpression measurements. The correlations between weights and topology in these networks can be captured by the multistrength and multi-inverse participation ratio. As an example, we show that multiplex observables highlight significant differences and nontrivial similarities between biological processes in healthy and cancer cells in a gene expression profiling data set.

In this paper we provide a framework based on entropy of multiplex networks that can be used to construct multiplex

weighted networks with different levels of correlations between the weights and the topology of these structures. Moreover, we have shown how this framework can be applied to generate null models of complex multilayer networks. We believe that such a framework can help to develop new methods to shed light on different properties of multiplex networks that cannot be inferred if the single layers were taken separately.

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APPENDIX A: EXAMPLES OF UNCORRELATED WEIGHTED MULTIPLEX ENSEMBLES

1. Multiplex ensembles with given expected total strength in each layer

As a first example of uncorrelated weighted multiplex, we consider the case in which we fix the average strength in each layer α to be equal to S^α . In this case we have $K = M$ constraints in the system, indicated with a label $\alpha = 1, 2, \dots, M$. These constraints are given by

$$\sum_{\vec{G}} F_\alpha(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{i < j} a_{ij}^\alpha \right) P(\vec{G}) = S^\alpha. \quad (\text{A1})$$

The probability distribution of a multiplex in this ensemble is given by Eq. (32) that reads in this case,

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\alpha=1}^M \lambda_\alpha \sum_{i < j} a_{ij}^\alpha \right], \quad (\text{A2})$$

where the partition function Z can be expressed explicitly as

$$\begin{aligned} Z &= \sum_{\vec{G}} \exp \left[- \sum_{\alpha=1}^M \lambda_\alpha \sum_{i < j} a_{ij}^\alpha \right] \\ &= \prod_{\alpha=1}^M \left[\left(\frac{1}{1 - e^{-\lambda_\alpha}} \right)^{\binom{N}{2}} \right]. \end{aligned} \quad (\text{A3})$$

The Lagrangian multipliers λ_α defining the probability of the multiplex $P(\vec{G})$ are fixed by the conditions

$$S_\alpha = - \frac{\partial \log Z}{\partial \lambda_\alpha} = \binom{N}{2} \frac{e^{-\lambda_\alpha}}{1 - e^{-\lambda_\alpha}}. \quad (\text{A4})$$

Finally, the average weight $\langle a_{ij}^\alpha \rangle$ can be evaluated from Eq. (36) and is given by

$$\langle a_{ij}^\alpha \rangle = \frac{S_\alpha}{\binom{N}{2}}, \quad (\text{A5})$$

which is equivalent to say $S_\alpha = \sum_{i < j} \langle a_{ij}^\alpha \rangle$.

From Eq. (34) we write the marginal probabilities $\pi(a_{ij}^\alpha)$ in this specific multiplex ensemble as

$$\pi_{ij}^\alpha(a_{ij}^\alpha) = e^{-\lambda_\alpha a_{ij}^\alpha} (1 - e^{-\lambda_\alpha}). \quad (\text{A6})$$

Moreover, from Eq. (37) the probability p_{ij}^α of having a positive weight $a_{ij}^\alpha > 0$ of the link between node i and node j in layer α is independent on the pair of nodes (i, j) , i.e., $p_{ij}^\alpha = p^\alpha$, and is given by

$$p^\alpha = e^{-\lambda_\alpha}. \quad (\text{A7})$$

Finally, the the probability of a multiplex in this ensemble is given by Eq. (49) with the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eq. (A6). The entropy S of this canonical multiplex ensemble is given by Eq. (50). Using the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eqs. (A6) and Eq. (A4) the entropy can be rearranged as

$$\begin{aligned} S &= \sum_{\alpha=1}^M \left[\left(\binom{N}{2} + S_\alpha \right) \log \left(\binom{N}{2} + S_\alpha \right) \right. \\ &\quad \left. - S_\alpha \log S_\alpha - \binom{N}{2} \log \binom{N}{2} \right]. \end{aligned} \quad (\text{A8})$$

If the number of layers M is finite, applying the Stirling's approximation in the large N limit we get

$$S = \sum_{\alpha=1}^M \log \left[\binom{\binom{N}{2} + S^\alpha}{\binom{N}{2}} \right]. \quad (\text{A9})$$

2. Multiplex ensembles with given expected strength sequence in each layer

We consider here the multiplex ensemble in which we fix the expected strength s_i^α of every node i , in each layer α . We have $K = M \cdot N$ constraints in the system indicated with a label $\alpha = 1, 2, \dots, M$. These constraints are given by

$$\sum_{\vec{G}} F_{i,\alpha}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha \right) P(\vec{G}) = s_i^\alpha. \quad (\text{A10})$$

The probability of a multiplex $P(\vec{G})$ is given by Eq. (32) that in this case can be written as

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\alpha=1}^M \sum_i \lambda_{i,\alpha} \sum_{j \neq i} a_{ij}^\alpha \right], \quad (\text{A11})$$

where the partition function Z can be expressed explicitly as

$$\begin{aligned} Z &= \sum_{\vec{G}} \exp \left[- \sum_{\alpha=1}^M \sum_i \lambda_{i,\alpha} \sum_{j \neq i} a_{ij}^\alpha \right] \\ &= \prod_{\alpha=1}^M \prod_{i < j} [1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}]^{-1}, \end{aligned} \quad (\text{A12})$$

and the Lagrangian multipliers $\lambda_{i,\alpha}$ are fixed by the condition

$$s_i^\alpha = - \frac{\partial \log Z}{\partial \lambda_{i,\alpha}} = \sum_{j \neq i} \frac{e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}}{1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}}. \quad (\text{A13})$$

The average weight $\langle a_{ij}^\alpha \rangle$ given by Eq. (36) can be calculated explicitly as a function of the Lagrangian multipliers, giving

$$\langle a_{ij}^\alpha \rangle = \frac{e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}}{1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}}, \quad (\text{A14})$$

which implies, together with Eq. (A13), $s_i^\alpha = \sum_{j \neq i} \langle a_{ij}^\alpha \rangle$.

From Eq. (34) we write the marginal probabilities $\pi_{ij}^\alpha(a_{ij}^\alpha)$ for specific weight a_{ij}^α as

$$\pi_{ij}^\alpha(a_{ij}^\alpha) = e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})a_{ij}^\alpha} [1 - e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}], \quad (\text{A15})$$

i.e., the weight of a link is distributed exponentially, with a mean that depends both on the pair of linked nodes (i, j) and on the layer α . Moreover, from Eq. (37) we can evaluate the probability p_{ij}^α of having a weight different from zero that is given by

$$p_{ij}^\alpha = e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})}. \quad (\text{A16})$$

Finally, the the probability of a multiplex in this ensemble is given by Eq. (49) with the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eq. (A15). Therefore the entropy \mathcal{S} of this canonical multiplex ensemble is given by Eq. (50) with the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eq. (A15).

3. Multiplex ensembles with given expected strength sequence, given expected degree sequence, and given expected sequences $\{u_i^\alpha\}$ in each layer

The last example of uncorrelated multiplex that we will consider is the one in which we fix the expected strength s_i^α , the expected degree k_i^α , and the expected u_i^α of every node i in each layer α . We have $K = M \cdot 3N$ constraints in the system. These constraints are given by

$$\begin{aligned} \sum_{\vec{G}} F_{i,\alpha}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha \right) P(\vec{G}) = s_i^\alpha, \\ \sum_{\vec{G}} F_{i,\alpha}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} \theta(a_{ij}^\alpha) \right) P(\vec{G}) = k_i^\alpha, \quad (\text{A17}) \\ \sum_{\vec{G}} F_{i,\alpha}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} (a_{ij}^\alpha)^2 \right) P(\vec{G}) = u_i^\alpha, \end{aligned}$$

with $\alpha = 1, 2, \dots, M$. We introduce the Lagrangian multipliers $\lambda_{i,\alpha}$ for the first set of $N \cdot M$ constraints, the Lagrangian multipliers $\omega_{i,\alpha}$ for the second set of $N \cdot M$ constraints, and the Lagrangian multipliers $z_{i,\alpha}$ for the third set of $N \cdot M$ constraints. Therefore, the probability $P(\vec{G})$ of a multiplex in this ensemble, of general expression given by Eq. (32), in this specific example is given by

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\alpha=1}^M \sum_i \lambda_{i,\alpha} \sum_{j \neq i} a_{ij}^\alpha - \sum_{\alpha=1}^M \sum_i \omega_{i,\alpha} \sum_{j \neq i} \theta(a_{ij}^\alpha) - \sum_{\alpha=1}^M \sum_i z_{i,\alpha} \sum_{j \neq i} (a_{ij}^\alpha)^2 \right].$$

If we define as I_{ij}^α the series

$$I_{ij}^\alpha = \sum_{a_{ij}^\alpha=1}^{s_i^\alpha} \exp \left[- (\lambda_{i,\alpha} + \lambda_{j,\alpha})a_{ij}^\alpha - (z_{i,\alpha} + z_{j,\alpha})(a_{ij}^\alpha)^2 \right], \quad (\text{A18})$$

where $S^\alpha = \sum_{i=1}^N s_i^\alpha$. The sum I_{ij}^α is convergent when $(z_{i,\alpha} + z_{j,\alpha}) > 0$, the partition function Z can be expressed as

$$Z = \prod_{\alpha=1}^M \prod_{i < j} [1 + e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} I_{ij}^\alpha]. \quad (\text{A19})$$

The Lagrangian multipliers are fixed by the conditions

$$-\frac{\partial \log Z}{\partial \lambda_{i,\alpha}} = s_i^\alpha, \quad -\frac{\partial \log Z}{\partial \omega_{i,\alpha}} = k_i^\alpha, \quad -\frac{\partial \log Z}{\partial z_{i,\alpha}} = u_i^\alpha. \quad (\text{A20})$$

The average weight of the link (i, j) in layer α , i.e., $\langle a_{ij}^\alpha \rangle$, is given by Eq. (36) that in this case reads

$$\langle a_{ij}^\alpha \rangle = \frac{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})}}{[1 + e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} I_{ij}^\alpha]} \left[\sum_{a_{ij}^\alpha=1}^{s_i^\alpha} a_{ij}^\alpha \exp \left(- (\lambda_{i,\alpha} + \lambda_{j,\alpha})a_{ij}^\alpha - (z_{i,\alpha} + z_{j,\alpha})(a_{ij}^\alpha)^2 \right) \right].$$

From Eq. (34) we write the marginal probabilities $\pi_{ij}^\alpha(a_{ij}^\alpha)$ for this specific ensemble that is given by

$$\pi_{ij}^\alpha(a_{ij}^\alpha) = \frac{e^{-(\lambda_{i,\alpha} + \lambda_{j,\alpha})a_{ij}^\alpha - (\omega_{i,\alpha} + \omega_{j,\alpha})\theta(a_{ij}^\alpha) - (z_{i,\alpha} + z_{j,\alpha})(a_{ij}^\alpha)^2}}{[1 + e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} I_{ij}^\alpha]}. \quad (\text{A21})$$

Moreover, from Eq. (37) the probability p_{ij}^α that the link (i, j) in layer α has weight that differs from zero is given by

$$p_{ij}^\alpha = \frac{e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} I_{ij}^\alpha}{[1 + e^{-(\omega_{i,\alpha} + \omega_{j,\alpha})} I_{ij}^\alpha]}. \quad (\text{A22})$$

The probability of a multiplex in this ensemble is given by Eq. (49) with the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eq. (A21) while the entropy \mathcal{S} of this canonical multiplex ensemble is given by Eq. (50) with the marginals $\pi_{ij}^\alpha(a_{ij}^\alpha)$ given by Eq. (A21).

APPENDIX B: EXAMPLES OF CORRELATED WEIGHTED MULTIPLEX ENSEMBLES

1. Multiplex ensembles with given expected total multistrength $S_\alpha^{\vec{m}}$

Here we consider a correlated weighted multiplex ensemble, in which we fix the total multistrength \vec{m} , given by $S_\alpha^{\vec{m}}$ for a layer α such that $m_\alpha = 1$. Since the number of the possible multistrengths \vec{m} in layer α are given by $M \cdot 2^{M-1}$, this gives a number of constraints that is equal to $K = M \cdot 2^{M-1}$. These constraints are given by

$$\sum_{\vec{G}} F_\alpha^{\vec{m}}(\vec{G})P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{i < j} A_{ij}^{\vec{m}} a_{ij}^\alpha \right) P(\vec{G}) = S_\alpha^{\vec{m}}, \quad (\text{B1})$$

where the multiadjacency matrix element $A_{ij}^{\vec{m}}$ is defined in Eq. (9). The canonical probability $P(\vec{G})$ of the multiplex in the ensembles is given by the general expression given in Eq. (32) that in this case becomes

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\vec{m} \neq 0} \sum_{\alpha=1}^M \lambda_\alpha^{\vec{m}} \sum_{i < j} A_{ij}^{\vec{m}} a_{ij}^\alpha \right], \quad (\text{B2})$$

where the partition function Z is given by

$$Z = \mathcal{Z}^{\binom{N}{2}}, \quad (\text{B3})$$

where

$$\mathcal{Z} = \sum_{\vec{m}} \prod_{\alpha=1}^M \left(\frac{e^{-\lambda_{\alpha}^{\vec{m}}}}{1 - e^{-\lambda_{\alpha}^{\vec{m}}}} \right)^{m_{\alpha}}, \quad (\text{B4})$$

where now, without loss of generality, if $m_{\alpha} = 0$ we put $\lambda_{\alpha}^{\vec{m}} = 1/2$. We can do this because the probability of a multiplex does not depend on any of these values, and we need to define them only for simplifying the notation. The Lagrangian multipliers $\lambda_{\alpha}^{\vec{m}}$ with $m_{\alpha} = 1$ are fixed by the conditions

$$-\frac{\partial \log Z}{\partial \lambda_{\alpha}^{\vec{m}}} = S_{\alpha}^{\vec{m}}, \quad (\text{B5})$$

which yields

$$S_{\alpha}^{\vec{m}} = \binom{N}{2} \frac{1}{Z} \left(\frac{1}{1 - e^{-\lambda_{\alpha}^{\vec{m}}}} \right) \prod_{\beta=1}^M \left(\frac{e^{-\lambda_{\beta}^{\vec{m}}}}{1 - e^{-\lambda_{\beta}^{\vec{m}}}} \right)^{m_{\beta}}. \quad (\text{B6})$$

The probability of a multiplex $P(\vec{G})$ follows Eq. (56) with

$$\pi_{ij}(\vec{a}_{ij}) = \frac{e^{-\sum_{\alpha=1}^M \lambda_{\alpha}^{\vec{m}ij} a_{ij}^{\alpha}}}{Z}. \quad (\text{B7})$$

Later we can compute the average weight of the link ij on the multilink \vec{m} , in the layer α ,

$$\langle a_{ij}^{\alpha} A_{ij}^{\vec{m}} \rangle = \sum_{\vec{G}} a_{ij}^{\alpha} A_{ij}^{\vec{m}} P(\vec{G}) = \sum_{\vec{a}_{ij}} a_{ij}^{\alpha} A_{ij}^{\vec{m}} \pi(\vec{a}_{ij}). \quad (\text{B8})$$

Using Eq. (B7) for the explicit expression of $\pi(\vec{a}_{ij})$ and comparing the results with Eq. (B6) it is easy to show that

$$\langle a_{ij}^{\alpha} A_{ij}^{\vec{m}} \rangle = \frac{S_{\alpha}^{\vec{m}}}{\binom{N}{2}}. \quad (\text{B9})$$

The probability of a multilink \vec{m} between node i and node j , $p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle$ in this ensemble is independent on the pair of nodes (i, j) . Therefore we have $p_{ij}^{\vec{m}} = p^{\vec{m}}$ with

$$p^{\vec{m}} = \frac{\prod_{\alpha=1}^M \left(\frac{e^{-\lambda_{\alpha}^{\vec{m}}}}{1 - e^{-\lambda_{\alpha}^{\vec{m}}}} \right)^{m_{\alpha}}}{Z}. \quad (\text{B10})$$

Finally, the entropy \mathcal{S} of this ensemble follows Eq. (63).

2. Multiplex ensembles with given expected ν -total strength S_{α}^{ν}

In presence of many layers M we can consider as constraints the average ν -total strength S_{α}^{ν} with $\nu = 1, 2, \dots, M$. With respect to the previous case, now the number of constraints is sensibly reduced and is given by M^2 constraints,

$$\sum_{\vec{G}} F_{\alpha}^{\nu}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{i < j} a_{ij}^{\alpha} A_{ij}^{\nu} \right) P(\vec{G}) = S_{\alpha}^{\nu}. \quad (\text{B11})$$

The probability $P(\vec{G})$ of the multiplex network is therefore given in terms of M^2 Lagrangian multipliers λ_{α}^{ν} , i.e.,

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{\nu=1}^M \sum_{\alpha=1}^M \lambda_{\alpha}^{\nu} \sum_{i < j} A_{ij}^{\nu} a_{ij}^{\alpha} \right], \quad (\text{B12})$$

where the partition function Z is given by $Z = \mathcal{Z}^{\binom{N}{2}}$ with

$$\mathcal{Z} = \sum_{\nu=0}^M \sum_{\vec{m} | \nu(\vec{m})=\nu} \prod_{\alpha=1}^M \left(\frac{e^{-\lambda_{\alpha}^{\nu}}}{1 - e^{-\lambda_{\alpha}^{\nu}}} \right)^{m_{\alpha}}. \quad (\text{B13})$$

The Lagrangian multipliers λ_{α}^{ν} are fixed by the constraints Eq. (B12) that can be also expressed as

$$-\frac{\partial \log Z}{\partial \lambda_{\alpha}^{\nu}} = S_{\alpha}^{\nu}. \quad (\text{B14})$$

The probability $P(\vec{G})$ of the multiplex network is given by Eq. (56) and the entropy of the ensemble takes the simple expression given by Eq. (63), where $\pi_{ij}(\vec{a}_{ij})$ is given by

$$\pi_{ij}(\vec{a}_{ij}) = \frac{e^{-\sum_{\alpha=1}^M \lambda_{\alpha}^{\nu} a_{ij}^{\alpha}}}{Z}. \quad (\text{B15})$$

Finally, the probability p^{ν} of a ν multilink between any two nodes of the multiplex network is given by

$$p^{\nu} = \frac{1}{Z} \prod_{\alpha=1}^M \left(\frac{e^{-\lambda_{\alpha}^{\nu}}}{1 - e^{-\lambda_{\alpha}^{\nu}}} \right)^{m_{\alpha}}, \quad (\text{B16})$$

while we have that the average weight of a ν multilink is given by

$$\begin{aligned} \langle a_{ij}^{\alpha} A_{ij}^{\nu} \rangle &= \frac{S_{\alpha}^{\nu}}{\binom{N}{2}} = \frac{1}{Z} \left(\frac{1}{1 - e^{-\lambda_{\alpha}^{\nu}}} \right) \\ &\times \sum_{\vec{m} | \nu(\vec{m})=\nu} m_{\alpha} \prod_{\beta=1}^M \left(\frac{e^{-\lambda_{\beta}^{\nu}}}{1 - e^{-\lambda_{\beta}^{\nu}}} \right)^{m_{\beta}}. \end{aligned} \quad (\text{B17})$$

3. Multiplex ensembles with given expected multistrength sequence $\{s_{i,\alpha}^{\vec{m}}\}$

Here we consider another level of coarse-graining for the multiplex network and we study correlated weighted multiplex in which we fix the average strength sequence $s_{i,\alpha}^{\vec{m}}$ for each node i , in each layer α such that $m_{\alpha} = 1$, for a given multilink \vec{m} . Following the previous line of reasoning, we can express properly just $N \cdot M \cdot 2^{M-1}$ constraints.

These constraints are given by

$$\sum_{\vec{G}} F_{i,\alpha}^{\vec{m}}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^{\vec{m}} a_{ij}^{\alpha} \right) P(\vec{G}) = s_{i,\alpha}^{\vec{m}}, \quad (\text{B18})$$

with $i = 1, \dots, N$, $\vec{m} = (m_1, m_2, \dots, m_{\beta}, \dots, m_M)$ with $m_{\beta} = 0, 1$ and, finally, $\alpha = 1, \dots, M$ with the condition $m_{\alpha} = 1$. The canonical probability $P(\vec{G})$ of the multiplex in the ensemble is

$$\begin{aligned} P(\vec{G}) &= \frac{1}{Z} \exp \left[- \sum_{\vec{m} \neq \vec{0}} \sum_{\alpha=1}^M \sum_i \lambda_{i,\alpha}^{\vec{m}} \sum_{j \neq i} A_{ij}^{\vec{m}} a_{ij}^{\alpha} \right] \\ &= \frac{1}{Z} \prod_{i < j} \exp \left[- \sum_{\vec{m} \neq \vec{0}} \sum_{\alpha=1}^M (\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}}) A_{ij}^{\vec{m}} a_{ij}^{\alpha} \right], \end{aligned} \quad (\text{B19})$$

where the partition function Z can be expressed explicitly as

$$Z = \prod_{i < j} \mathcal{Z}_{ij}, \quad (\text{B20})$$

where

$$\mathcal{Z}_{ij} = \sum_{\vec{m}} \prod_{\alpha=1}^M \left(\frac{e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right)^{m_\alpha}, \quad (\text{B21})$$

where now, without loss of generality, if $m_\alpha = 0$ we put $\lambda_\alpha^{\vec{m}} = 1/2$. We can do this because the probability of a multiplex and the partition function do not depend on any of these values, and we need to define them only for simplifying the notation. The Lagrangian multipliers $\lambda_{i,\alpha}^{\vec{m}}$, with α such that $m_\alpha = 1$, are fixed by the conditions

$$-\frac{\partial \log Z}{\partial \lambda_{i,\alpha}^{\vec{m}}} = s_{i,\alpha}^{\vec{m}} = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle, \quad (\text{B22})$$

where $\langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle$ is the average weight of the link between node i and node j on the multilink \vec{m} , in the layer α . This quantity can be computed as

$$\langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle = \frac{1}{\mathcal{Z}_{ij}} \left[\frac{1}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right] \prod_{\beta=1}^M \left[\frac{e^{-(\lambda_{i,\beta}^{\vec{m}} + \lambda_{j,\beta}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\beta}^{\vec{m}} + \lambda_{j,\beta}^{\vec{m}})}} \right]^{m_\beta}.$$

We can calculate the probability of a vector $\vec{a}_{ij} = (a_{ij}^1, a_{ij}^2, \dots, a_{ij}^M)$ characterizing the weights of the links between node i and node j in all the layers, getting

$$\pi_{ij}(\vec{a}_{ij}) = \frac{1}{\mathcal{Z}_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i,\alpha}^{\vec{a}_{ij}} + \lambda_{j,\alpha}^{\vec{a}_{ij}}) a_{ij}^\alpha}. \quad (\text{B23})$$

These probabilities satisfy the normalization condition given by Eq. (58). The probability $p_{ij}^{\vec{m}}$ of a multilink \vec{m} between the node i and the node j is given by

$$p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle = \frac{1}{\mathcal{Z}_{ij}} \prod_{\alpha=1}^M \left[\frac{e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}}{1 - e^{-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})}} \right]^{m_\alpha}, \quad (\text{B24})$$

where these probabilities satisfy the normalization condition given by Eq. (61) and are related to the probabilities $\pi_{ij}^{\vec{m}}(\vec{a}_{ij})$ given by Eq. (B23) and by Eq. (62).

Probability $P(\vec{G})$ and entropy \mathcal{S} follow Eqs. (56) and (63), respectively.

4. Multiplex ensembles with given expected ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$

In the case in which one wants to describe multiplex networks with many layers M , one can consider to fix the average ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$ with $i = 1, 2, \dots, N$ and $\nu = 1, 2, \dots, M$. Therefore, the number of constraints of the previous example is reduced to just $N \cdot M^2$ soft constraints given by

$$\sum_{\vec{G}} F_{i,\alpha}^\nu(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha A_{ij}^{\vec{G}} \right) P(\vec{G}) = s_{i,\alpha}^\nu. \quad (\text{B25})$$

In this case, the probability $P(\vec{G})$ of a multiplex network \vec{G} in this ensemble is expressed in terms of the $N \times M^2$ Lagrangian

multipliers $\lambda_{i,\alpha}^\nu$ and is given by

$$P(\vec{G}) = \frac{1}{Z} \exp \left[- \sum_{i < j} \sum_{\nu=1}^M \sum_{\alpha=1}^M (\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu) A_{ij}^\nu a_{ij}^\alpha \right],$$

where the partition function Z can be expressed as

$$Z = \prod_{i < j} \mathcal{Z}_{ij} \quad (\text{B26})$$

with

$$\mathcal{Z}_{ij} = \sum_{\nu=0}^M \sum_{\vec{m} | \nu(\vec{m})=\nu} \prod_{\alpha=1}^M \left(\frac{e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right)^{m_\alpha}. \quad (\text{B27})$$

The Lagrangian multipliers are fixed by the conditions in Eq. (B25) or, equivalently, by

$$-\frac{\partial \log Z}{\partial \lambda_{i,\alpha}^\nu} = s_{i,\alpha}^\nu = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^\nu \rangle. \quad (\text{B28})$$

Therefore the probability $P(\vec{G})$ of a multiplex network \vec{G} in this ensemble is given by Eq. (56) and the entropy of the ensemble takes the simple expression given by Eq. (63), where $\pi_{ij}(\vec{a}_{ij})$ is given by

$$\pi_{ij}(\vec{a}_{ij}) = \frac{1}{\mathcal{Z}_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i,\alpha}^{\vec{a}_{ij}} + \lambda_{j,\alpha}^{\vec{a}_{ij}}) a_{ij}^\alpha}. \quad (\text{B29})$$

Finally, the probability p_{ij}^ν that the node i and the node j are linked by a ν multilink is given by

$$p_{ij}^\nu = \frac{1}{\mathcal{Z}_{ij}} \sum_{\vec{m} | \nu(\vec{m})=\nu} \prod_{\alpha=1}^M \left[\frac{e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right]^{m_\alpha}, \quad (\text{B30})$$

while the average weight of the link a_{ij}^α belonging to a ν multilink is given by

$$\begin{aligned} \langle a_{ij}^\alpha A_{ij}^\nu \rangle &= \frac{1}{\mathcal{Z}_{ij}} \left[\frac{1}{1 - e^{-(\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu)}} \right] \\ &\times \sum_{\vec{m} | \nu(\vec{m})=\nu} m_\alpha \prod_{\beta=1}^M \left[\frac{e^{-(\lambda_{i,\beta}^\nu + \lambda_{j,\beta}^\nu)}}{1 - e^{-(\lambda_{i,\beta}^\nu + \lambda_{j,\beta}^\nu)}} \right]^{m_\beta}. \end{aligned} \quad (\text{B31})$$

5. Multiplex ensembles with given expected multidegree sequence $\{k_i^{\vec{m}}\}$, given expected multistrength sequence $\{s_{i,\alpha}^{\vec{m}}\}$, and given expected sequence $\{u_{i,\alpha}^{\vec{m}}\}$

As a fourth case of correlated weighted multiplex ensemble, we consider the case in which we fix the average multidegree $k_i^{\vec{m}}$ of node i , for each node $i = 1, \dots, N$, for $\vec{m} \neq \vec{0}$. Moreover, for each node i in layer α we impose the average multistrength $s_{i,\alpha}^{\vec{m}}$ and the second moment of the weights incident to it and belonging to a multilink \vec{m} , i.e., $u_{i,\alpha}^{\vec{m}}$. The number of independent constraints is therefore $K = (2^M - 1)N + 2^M \cdot M \cdot N$.

In particular, the constraints we are imposing are the following:

$$\begin{aligned}\sum_{\vec{G}} F_{i,\alpha}^{\vec{m}}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^{\vec{m}} a_{ij}^\alpha \right) P(\vec{G}) = s_{i,\alpha}^{\vec{m}}, \\ \sum_{\vec{G}} F_i^{\vec{m}}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^{\vec{m}} \right) P(\vec{G}) = k_i^{\vec{m}}, \quad (\text{B32}) \\ \sum_{\vec{G}} F_{i,\alpha}^{\vec{m}}(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} (A_{ij}^{\vec{m}} a_{ij}^\alpha)^2 \right) P(\vec{G}) = u_{i,\alpha}^{\vec{m}}.\end{aligned}$$

The canonical probability $P(\vec{G})$ of the multiplex in the ensembles is

$$\begin{aligned}P(\vec{G}) &= \frac{1}{Z} \exp \left[- \sum_{i < j} \sum_{\vec{m} \neq \vec{0}} (\omega_i^{\vec{m}} + \omega_j^{\vec{m}}) A_{ij}^{\vec{m}} \right] \\ &\times \exp \left[- \sum_{i < j} \sum_{\vec{m} \neq \vec{0}} \sum_{\alpha=1}^M (\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}}) A_{ij}^{\vec{m}} a_{ij}^\alpha \right] \\ &\times \exp \left[- \sum_{i < j} \sum_{\vec{m} \neq \vec{0}} \sum_{\alpha=1}^M (z_{i,\alpha}^{\vec{m}} + z_{j,\alpha}^{\vec{m}}) A_{ij}^{\vec{m}} (a_{ij}^\alpha)^2 \right]. \quad (\text{B33})\end{aligned}$$

The partition function Z can be expressed explicitly as

$$\begin{aligned}Z &= \prod_{i < j} Z_{ij} \\ &= \prod_{i < j} \left(1 + \sum_{\vec{m} \neq \vec{0}} e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})} \prod_{\alpha=1}^M (I_{ij}^{\vec{m},\alpha})^{m_\alpha} \right), \quad (\text{B34})\end{aligned}$$

where $I_{ij}^{\vec{m},\alpha}$ is given by

$$I_{ij}^{\vec{m},\alpha} = \sum_{a_{ij}^\alpha=1}^{S_{i,\alpha}^{\vec{m}}} \exp \left[-(\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}}) a_{ij}^\alpha - (z_{i,\alpha}^{\vec{m}} + z_{j,\alpha}^{\vec{m}}) (a_{ij}^\alpha)^2 \right],$$

where $S_{i,\alpha}^{\vec{m}} = \sum_{i=1}^N s_{i,\alpha}^{\vec{m}}$. The Lagrangian multipliers are fixed by the conditions

$$\begin{aligned}-\frac{\partial \log Z}{\partial \lambda_{i,\alpha}^{\vec{m}}} &= s_{i,\alpha}^{\vec{m}} = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle, \\ -\frac{\partial \log Z}{\partial \omega_i^{\vec{m}}} &= k_i^{\vec{m}} = \sum_{j \neq i} \langle A_{ij}^{\vec{m}} \rangle, \\ -\frac{\partial \log Z}{\partial z_{i,\alpha}^{\vec{m}}} &= u_{i,\alpha}^{\vec{m}} = \sum_{j \neq i} \langle (a_{ij}^\alpha)^2 A_{ij}^{\vec{m}} \rangle. \quad (\text{B35})\end{aligned}$$

The average weight $\langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle$ of the multilink \vec{m} between nodes i and j in the layer α and the probability $p_{ij}^{\vec{m}}$ of a

multilink \vec{m} between node i and node j are given, respectively, by

$$\begin{aligned}\langle a_{ij}^\alpha A_{ij}^{\vec{m}} \rangle &= -\frac{e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})}}{Z_{ij}} \left[\frac{\partial I_{ij}^{\vec{m},\alpha}}{\partial (\lambda_{i,\alpha}^{\vec{m}} + \lambda_{j,\alpha}^{\vec{m}})} \right] \\ &\times \prod_{\beta \neq \alpha}^M (I_{ij}^{\vec{m},\beta})^{m_\beta} \\ p_{ij}^{\vec{m}} &= \frac{e^{-(\omega_i^{\vec{m}} + \omega_j^{\vec{m}})}}{Z_{ij}} \prod_{\alpha=1}^M (I_{ij}^{\vec{m},\alpha})^{m_\alpha}. \quad (\text{B36})\end{aligned}$$

The probability of a specific multiweight \vec{a}_{ij} in the between the nodes (i, j) is

$$\begin{aligned}\pi_{ij}(\vec{a}_{ij}) &= \frac{e^{-(\omega_i^{\vec{m}^{ij}} + \omega_j^{\vec{m}^{ij}})}}{Z_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i,\alpha}^{\vec{m}^{ij}} + \lambda_{j,\alpha}^{\vec{m}^{ij}}) a_{ij}^\alpha} \\ &\times e^{-\sum_{\alpha=1, M} (z_{i,\alpha}^{\vec{m}^{ij}} + z_{j,\alpha}^{\vec{m}^{ij}}) (a_{ij}^\alpha)^2}. \quad (\text{B37})\end{aligned}$$

As previously, probability $P(\vec{G})$ and entropy S follow Eqs. (56) and (63), respectively.

6. Multiplex ensembles with given expected ν -multidegree sequence $\{k_i^\nu\}$, given expected ν -multistrength sequence $\{s_{i,\alpha}^\nu\}$, and given expected sequence $\{u_{i,\alpha}^\nu\}$

Finally, we consider the case in which we fix the given expected ν -multidegree sequence k_i^ν of node i , for each node $i = 1, \dots, N$, for $\nu = 1, \dots, M$. In addition, for each node i in layer α we fix the average ν -multistrength sequence $s_{i,\alpha}^\nu$ and the second moment of the weights incident to it for each ν multilink, i.e., $u_{i,\alpha}^\nu$. The $N \cdot M \cdot (2M + 1)$ constraints are given by

$$\begin{aligned}\sum_{\vec{G}} F_{i,\alpha}^\nu(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} a_{ij}^\alpha A_{ij}^\nu \right) P(\vec{G}) = s_{i,\alpha}^\nu, \\ \sum_{\vec{G}} F_i^\nu(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} A_{ij}^\nu \right) P(\vec{G}) = k_i^\nu, \\ \sum_{\vec{G}} F_{i,\alpha}^\nu(\vec{G})P(\vec{G}) &= \sum_{\vec{G}} \left(\sum_{j \neq i} (a_{ij}^\alpha A_{ij}^\nu)^2 \right) P(\vec{G}) = u_{i,\alpha}^\nu, \quad (\text{B38})\end{aligned}$$

with $i = 1, 2, \dots, N, \alpha = 1, 2, \dots, M$ and $\nu = 1, 2, \dots, M$. The canonical probability $P(\vec{G})$ of the multiplex in this ensemble can be expressed in terms of the Lagrangian multipliers $\lambda_{j,\alpha}^\nu$, ω_i^ν and $z_{j,\alpha}^\nu$, i.e.,

$$\begin{aligned}P(\vec{G}) &= \frac{1}{Z} \exp \left[- \sum_{i < j} \sum_{\nu=1}^M (\omega_i^\nu + \omega_j^\nu) A_{ij}^\nu \right] \\ &\times \exp \left[- \sum_{i < j} \sum_{\nu=1}^M \sum_{\alpha=1}^M (\lambda_{i,\alpha}^\nu + \lambda_{j,\alpha}^\nu) A_{ij}^\nu a_{ij}^\alpha \right] \\ &\times \exp \left[- \sum_{i < j} \sum_{\nu=1}^M \sum_{\alpha=1}^M (z_{i,\alpha}^\nu + z_{j,\alpha}^\nu) A_{ij}^\nu (a_{ij}^\alpha)^2 \right], \quad (\text{B39})\end{aligned}$$

where the partition function Z is given by

$$Z = \prod_{i < j} \mathcal{Z}_{ij}, \quad (\text{B40})$$

with

$$\mathcal{Z}_{ij} = 1 + \sum_{\nu=1}^M e^{-(\omega_i^\nu + \omega_j^\nu)} \sum_{\vec{m} | \nu(\vec{m}) = \nu} \prod_{\alpha=1}^M (I_{ij}^{\nu, \alpha})^{m_\alpha}, \quad (\text{B41})$$

where $I_{ij}^{\nu, \alpha}$ is given by

$$I_{ij}^{\nu, \alpha} = \sum_{a_{ij}^\alpha=1}^{S^{\nu, \alpha}} \exp \left[-(\lambda_{i, \alpha}^\nu + \lambda_{j, \alpha}^\nu) a_{ij}^\alpha - (z_{i, \alpha}^\nu + z_{j, \alpha}^\nu) (a_{ij}^\alpha)^2 \right],$$

where $S^{\nu, \alpha} = \sum_{i=1}^N s_{i, \alpha}^\nu$

The Lagrangian multipliers are fixed by the conditions Eq. (B38) that can be also written in terms of the partial derivatives of the partition function as

$$\begin{aligned} -\frac{\partial \log Z}{\partial \lambda_{i, \alpha}^\nu} &= s_{i, \alpha}^\nu = \sum_{j \neq i} \langle a_{ij}^\alpha A_{ij}^\nu \rangle, \\ -\frac{\partial \log Z}{\partial \omega_i^\nu} &= k_i^\nu = \sum_{j \neq i} \langle A_{ij}^\nu \rangle, \\ -\frac{\partial \log Z}{\partial z_{i, \alpha}^\nu} &= u_{i, \alpha}^\nu = \sum_{j \neq i} \langle (a_{ij}^\alpha)^2 A_{ij}^\nu \rangle. \end{aligned} \quad (\text{B42})$$

The probability $P(\vec{G})$ of a multiplex network \vec{G} and the consequent entropy of the ensemble are given by Eq. (56) and Eq. (63) with $\pi_{ij}(\vec{a}_{ij})$ given by

$$\begin{aligned} \pi_{ij}(\vec{a}_{ij}) &= \frac{e^{-(\omega_i^{ij} + \omega_j^{ij})}}{\mathcal{Z}_{ij}} e^{-\sum_{\alpha=1, M} (\lambda_{i, \alpha}^{ij} + \lambda_{j, \alpha}^{ij}) a_{ij}^\alpha} \\ &\times e^{-\sum_{\alpha=1, M} (z_{i, \alpha}^{ij} + z_{j, \alpha}^{ij}) (a_{ij}^\alpha)^2}. \end{aligned} \quad (\text{B43})$$

The probability p_{ij}^ν that the node i and the node j are linked by a ν multilink is given by

$$p_{ij}^\nu = \frac{e^{-(\omega_i^\nu + \omega_j^\nu)}}{\mathcal{Z}_{ij}} \sum_{\vec{m} | \nu(\vec{m}) = \nu} \prod_{\alpha=1}^M (I_{ij}^{\nu, \alpha})^{m_\alpha}. \quad (\text{B44})$$

Finally, the average weight of the link a_{ij}^α belonging to a ν multilink is given by

$$\begin{aligned} \langle a_{ij}^\alpha A_{ij}^\nu \rangle &= -\frac{e^{-(\omega_i^\nu + \omega_j^\nu)}}{\mathcal{Z}_{ij}} \left[\frac{\partial I_{ij}^{\nu, \alpha}}{\partial (\lambda_{i, \alpha}^\nu + \lambda_{j, \alpha}^\nu)} \right] \\ &\times \sum_{\vec{m} | \nu(\vec{m}) = \nu} m_\alpha \prod_{\beta \neq \alpha} (I_{ij}^{\nu, \beta})^{m_\beta}. \end{aligned} \quad (\text{B45})$$

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