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978-1-009-08730-8 — Multilayer Network Science: From Cells to Societies
Oriol Artime , Barbara Benigni , Giulia Bertagnolli , Valeria d'Andrea ,
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1 Introduction

What is a complex system? It is a *network* of actors or units related by special types of interactions that, together, form a whole. Whether involving two proteins within a cell or two individuals within a social group, relationships and interactions tie these units together in such a way that “the whole is larger than the sum of its parts,” a concept initially introduced by the Greek philosopher Aristotle and later exploited by Gestalt psychologists, at the end of the nineteenth century, to explain human perception beyond the traditional atomistic view.

In fact, the “whole” exhibits features that each actor or unit, in isolation, does not and could not. Therefore, it is usually difficult, if not impossible, to understand a system from the analysis of its components alone, as in atomistic or other reductionist theories [309]. The framework required to study such relationships and interactions is known as network science.[1]

The foundations of network science can be found in the pioneering work of Leonhard Euler in 1736, when the famous mathematician provided the first mathematically grounded proof to definitively solve the problem of the Seven Bridges of Königsberg. He mapped the empirical problem of traversing the city of Königsberg – under the constraint that one should use each one of its seven bridges only one time – onto the abstract problem of performing a special walk through a graph. After Euler’s solution, graph theory quickly developed in the successive two centuries, culminating in the groundbreaking contributions by Paul Erdős and Alfréd Rényi on random graphs and their statistical analysis at the end of the 1950s.

For decades, social scientists and (systems) biologists have widely used graph theory to map connections between individuals and biological units, respectively, to gain novel insights about the *properties of a system*, the relevance of a *unit within the system*, and the *organization of units within the system*. In 1974, François Jacob, the winner of the 1965 Nobel Prize in Physiology or Medicine, described biology as a science effectively dealing with systems within systems [280], well before the age of genomics and large-scale biology. He recognized that biological systems also can be mapped onto units of systems at a larger scale: in fact, proteins interact with each other to make cells function, cells interact with each other to construct tissues and organs, which in turn interact with each other to build an organism. Finally, at the top of this hierarchical web of interactions, organisms interact with each other to define a population, like our society. In the same decade, similar ideas regarding the

[1] We refer the reader to this interesting, nontechnical, and recent introduction to the basic concepts characterizing complex systems [96].

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nontrivial interdependencies between scales were laid out by the 1977 Nobel Laureate in Physics, Phillip Anderson, in the context of natural sciences [14].

Social scientists, as biologists, were among the first to face the existence of multiple levels (or scales) as well as multiple *layers* of descriptions for the units of a social system. In the early 1970s, Wayne W. Zachary observed the interactions within a group of individuals belonging to a karate club over three years [304] in order to understand the dynamics of conflicts, which allowed him to predict the outcome of the group split that happened later. He annotated interactions across eight distinct contexts, from “the association in and between academic classes at the university” to “attendance at intercollegiate karate tournaments held at local universities.” However, at that time, the mathematical framework required to study a network with multiple *layers of complexity* – such as the eight contexts – was not yet developed and Zachary opted for an approximation: aggregating the multiple interactions across contexts into a single representative number denoting the intensity of the relationship between a pair of actors.

In this work, we seek to better understand the challenges faced by systems biologists and social scientists between the 1970s and the past decade, while introducing the basic concepts required to define the framework of *multilayer network science* with an interdisciplinary language that should be familiar to biologists, social scientists, computer scientists, applied mathematicians, and physicists. Therefore, it will become clear that, for instance, Zachary’s approach was a possible model to study the karate club network, but likely neither the most accurate nor the most predictive one. We will discuss under which conditions a system admits a multilayer representation, providing examples such as the ones shown in Figures 1 and 2, where units are individuals and geographic areas, respectively, and interactions represent coauthorship of scientific papers and transportation routes, respectively. Another emblematic example, accounting for the temporal and socio-spatial interdependence typical of many systems, concerns the organization of ecological systems [225]. Finally, very recently, multilayer modeling in systems biology and medicine has been used to integrate information about biological processes, drug targets, genotype, and phenotype to the subset of the human interactome targeted by SARS-CoV-2, the COVID-19 virus [288] (see Figure 3). This work is full of examples like these, and we hope to make clear the broad spectrum of potential interdisciplinary applications of the multilayer framework.

Our ultimate goal is to guide the reader through the potential applications of multilayer modeling, which nowadays provides a well-established paradigm for the analysis of systems characterized by multiple levels and layers of

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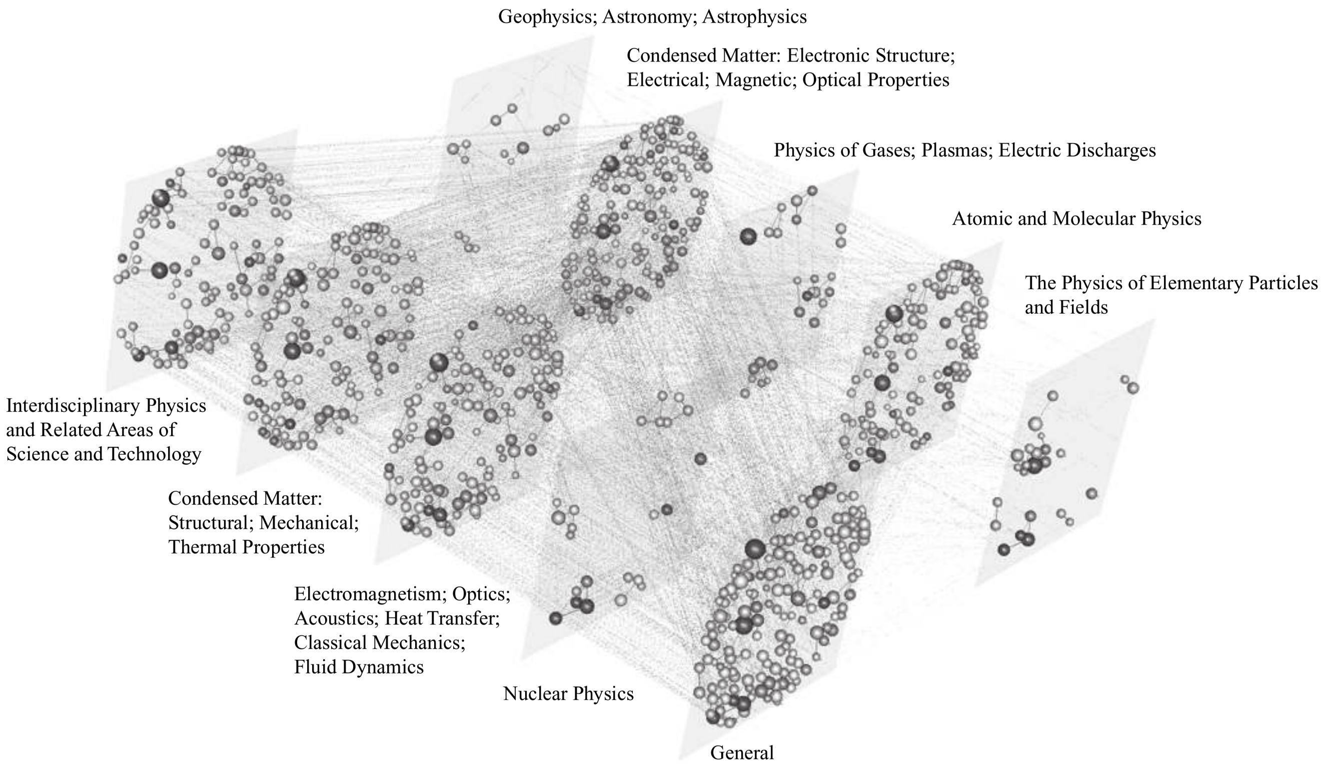

Figure 1 Multilayer representation of a coauthorship network. Nodes represent authors publishing papers in the journals of the American Physical Society, and links connect two authors if they have published a paper together. Layers encode distinct subtopics of physics (e.g., geophysics or nuclear physics). Links within the same layer represent coauthorship of one paper about the same topic, while links between layers indicate coauthorship of one paper categorized simultaneously across distinct topics. Figure from [93] under Creative Commons Attribution-ShareAlike 4.0 International License.

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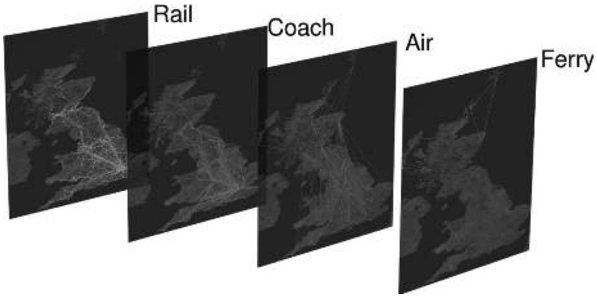

Figure 2 A multilayer transportation network where connections using a particular means of transport are associated with intralayer links and intermodal exchanges are represented by the interlayer links. Here, the national public transportation network for Great Britain [125, 126] as rendered by MuxViz [101]. Figure from [126].

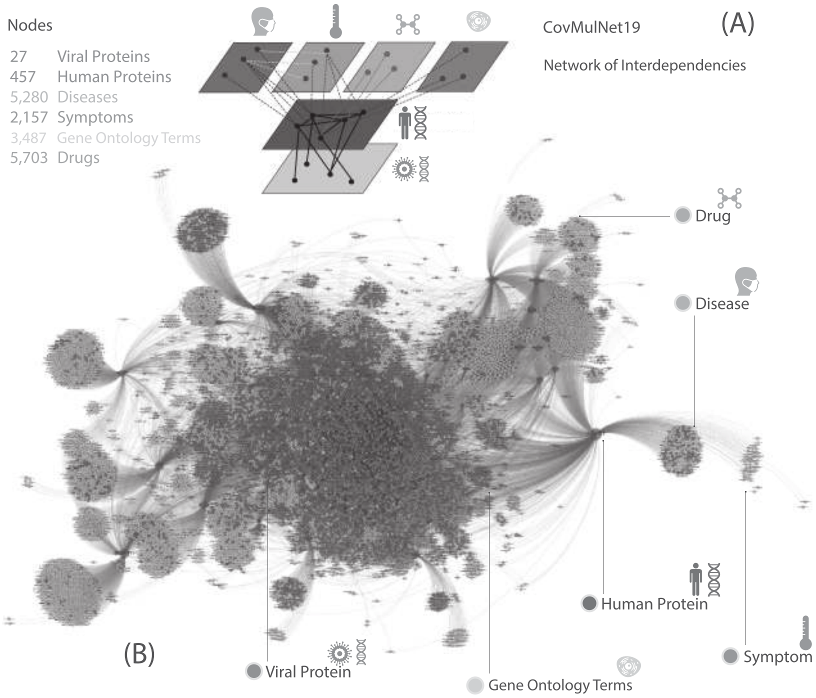

Figure 3 Illustration of CovMulNet19, the multilayer network encoding COVID-19 genotype-phenotype-drug interactions. A schematic map of intra- and interlayer interdependencies between diseases, symptoms, drugs, gene ontology terms, human proteins, and viral proteins of SARS-CoV-2, the COVID-19 virus. Figure from [288].

description, including systems whose structure changes over time. The aim is to provide the reader with the tools required to model and analyze systems in terms

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of coupled layers, as well as with the conditions under which this approach is plausible.

It is worth remarking here that this work should be considered as an extended introduction to the field but not the most complete one. For this reason, we point the reader to the first reviews [36, 53, 103, 161, 295] and recent books [51, 83] on this topic or more specifically on analysis and visualization of multilayer networks [94], which, taken together with our work, will provide a more comprehensive view of the field.

In Section 2, we will introduce the representation of multilayer networks based on the tensorial formulation [97], providing the mathematical ground for the analytical techniques for structure (Section 3) and dynamics (Section 4), allowing the reader to find a reference for the analysis of versatility (or multilayer centrality) and mesoscale organization (or community detection), as well as for percolation, synchronization, competition, and modeling of intertwined phenomena. Toward the end (Section 5), we will discuss a few selected advances in network science – namely the latent geometry of a complex network based on network-driven processes and the statistical theory of information dynamics leading to the formalism of network density matrices – and their recent generalization and application to multilayer networks. Finally (Section 6), we will show how multilayer networks are ubiquitous and can be used for modeling complex systems, from cells to societies.

2 Representation of Multilayer Systems

2.1 Tensorial Representation of a Complex Network

One convenient way to mathematically represent a complex network is by means of its adjacency matrix [30, 31, 114, 173, 203]. However, to deal with multilayer networks, it might be more convenient to introduce first the more general concept of the tensor, a multilinear function that maps objects defined in a vector space into other objects of the same type, regardless of the choice of a coordinate system. For instance, a simple scalar x is also a rank-0 tensor, a vector x_i is a rank-1 tensor, and a matrix X_{ij} is a rank-2 tensor. More generally, given a vector space $\mathcal{V}$ with algebraic dual space[2] $\mathcal{V}^\star$ over the real numbers $\mathbb{R}$, we can define the tensor M as the multilinear function

$$M\colon \mathcal{V}^\star \times \mathcal{V}^\star \times \ldots \mathcal{V}^\star \times \mathcal{V} \times \mathcal{V} \times \ldots \mathcal{V} \longrightarrow \mathbb{R}, \tag{2.1}$$

[2] This is the space of all the possible linear transformations that map an object of $\mathcal{V}$ into a real number. For instance, think about $\mathcal{V} = \mathbb{R}^2$ and the linear functional $f\colon \mathbb{R}^2 \longrightarrow \mathbb{R}$: it follows that $f(x, y) = ax + by$, with a, b two integer numbers, is an element of $\mathcal{V}^\star$.

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where the number of products is m for the vector space and n for its dual. This definition formally characterizes a rank-mn tensor $M^{i_1 i_2 \dots i_n}_{j_1 j_2 \dots j_m}$ that is m-covariant and n-contravariant. In fact, under a change of basis B, m components transform as the same linear mapping of the change of basis (B), whereas n components transform as the inverse one (B^{-1}). Therefore, in general, there are two types of canonical basis: the covariant basis denoted by $e_i(a)$ ($a = 1, 2, \dots, m$), which is defined in $\mathcal{V}$, and the contravariant (or dual) basis denoted by $e^i(b)$ ($b = 1, 2, \dots, n$), which is defined in $\mathcal{V}^\star$. If the vector space is Euclidean, the coordinates of the canonical vectors and their duals are the same, whereas this is not the case in general. In the following, to define an adjacency matrix, or a rank-2 adjacency tensor, we will work in the Euclidean space but we will keep the covariant and contravariant notation, since it will allow us to generalize the results to the case of non-Euclidean spaces. The interested reader can find more about the tensorial framework in any good linear algebra textbook, while for the purpose of this work it is sufficient to understand how we can use tensors in practice in a few key situations.

Let us start by better defining the canonical vectors in the case of networks. For a graph with N nodes, the canonical covariant vectors $e_i(a)$ defined in the space of nodes $\mathbb{R}^N$ are N rank-1 tensors of dimension N with all entries equal to 0 except for the a-th entry, which is equal to 1. Similarly for canonical contravariant vectors. The product of canonical vectors gives canonical matrices – for example, $E_{ij}(ab) = e_i(a)e_j(b)$ is a rank-2 covariant tensor with all components equal to 0 except for the one corresponding to the a-th row and the b-th column, equal to 1. Similarly, we can build contravariant tensors and mixed tensors – that is, tensors obtained by the product between the covariant and contravariant vectors.

The careful reader has noticed at this point that we have defined the *outer* product of two canonical vectors, also known as the Kronecker product, which gives a rank-2 tensor as a result. This result is general: the outer product of two tensors X and Y is a new tensor Z with a number of covariant (contravariant) indices given by the sum of the number of covariant (contravariant) indices of X and Y. Therefore, the outer product of two tensors is always a tensor of higher order than the original ones – for example, $X^k_{ij} Y^{mn}_l = Z^{kmn}_{ijl}$.

It is possible to define also an *inner* product: in this case, we talk about a contraction because the rank of resulting tensor is reduced by two units. For instance, this is the case in the product $X^k_{ij} Y^{mn}_k = Z^{mn}_{ij}$, where the index k is covariant for X and contravariant for Y. This operation corresponds to summing over the components of X and Y identified by the index k. The careful reader has noticed that we have omitted the summation symbol: this choice – known as

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Einstein summation convention – is optional and often adopted for simplicity. In the following, we will make use of this convention.

At this point, we are ready to define the adjacency tensor of a complex network in terms of canonical vectors [97] as

$$W^i_j = \sum_{a,b=1}^{N} w_{ab} e^i(a) e_j(b) = \sum_{a,b=1}^{N} w_{ab} E^i_j(ab), \tag{2.2}$$

where w_{ab} is a real number, usually nonnegative, used to encode the intensity of the interaction between nodes a and b, while $E^i_j(ab) \in \mathbb{R}^{N\times N}$ are the mixed canonical rank-2 tensors. We might wonder if W^i_j is a true tensor, or just a matrix. To this end, it is enough to understand how it transforms under a change of basis

$$B^i_j = \sum_{a=1}^{N} e'^i(a) e_j(a), \tag{2.3}$$

a linear function that transforms the basis vector set $\{e^i(a)\}$ into a second set $\{e'^i(a)\}$. By noting that w_{ab} must be invariant with respect to the change of basis, we have:

$$\begin{aligned} W'^k_l &= \sum_{a,b=1}^{N} w_{ab} e'^k(a) e'_l(b) = \sum_{a,b=1}^{N} w_{ab} B^k_i e^i(a) e_j(b) (B^{-1})^j_l \\ &= B^k_i \left[\sum_{a,b=1}^{N} w_{ab} e^i(a) e_j(b) \right] (B^{-1})^j_l = B^k_i W^i_j (B^{-1})^j_l \end{aligned} \tag{2.4}$$

– that is, the adjacency object W^i_j transforms like a tensor [102]. This result is important since a tensor is an object with features that, in general, are not shared by a matrix or, at higher orders, a hypermatrix. In fact, the components of a tensor can always be arranged into hypermatrices, while the opposite is not necessarily true.

Since we work in the Euclidean space, we might wonder why we use this notation and not a simpler one. In general, this is convenient because of the presence of directed relationships between nodes: to distinguish between incoming and outgoing directions, it is sufficient to map this information into covariant and contravariant indices in such a way that the adjacency tensor W^i_j represents a linear transformation that maps nodes into a function of their incoming or outgoing flow. For instance, node a is represented by $e_i(a)$ in the space of nodes and $W^i_j e_i(a) = w_j(a)$ provides a rank-1 tensor encoding the set of nodes linked by a, while $W^i_j u_i = s_j$, with u_i the rank-1 tensor with all components equal to 1, provides a rank-1 tensor encoding the outgoing strength of

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all nodes. Similarly, $W^i_j e^j(a) = w^i(a)$ gives the set of nodes linking to a, while $W^i_j u^j = s^i$ gives the incoming strength of nodes.

Before moving to the next section, it is useful to define some tensors used throughout this work. We have just seen the rank-1 1–tensor in action: similarly we can define the rank-2 1–tensor $U^i_j = u^i u_j$ or higher-order tensors. Another fundamental tensor is the Kronecker one, defined by δ^i_j, with components equal to 1 if $i = j$ and equal to 0 otherwise.

2.2 Tensorial Representation of a Multilayer Network

In the previous section, we introduced the fundamental procedure required to build an adjacency tensor to represent a classical network (a monoplex). Using a similar procedure, we can build a *multilayer adjacency tensor* to represent a multilayer network, as shown in Figure 4. A multilayer system is characterized by N physical nodes interacting in L distinct ways simultaneously. Each type of interaction defines a *layer*. At variance with single-layer networks, there are more edge sets to encode: as many as the number (L) of layers and, in general, as many as the number ($L(L-1)$) of directed pairwise connections between layers, since we have to specify which node i in a layer α is connected to which node

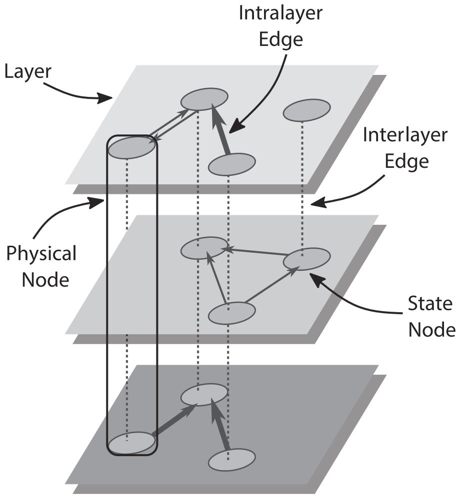

Figure 4 A system where nodes are characterized by three distinct types of interactions, encoded by colored layers. Overall, the system is a multilayer network because to describe relationships we need to specify more than one network. Units are physical nodes: each one is a set of *state nodes* or *replicas*, each one encoding the identity of the corresponding physical node in each layer separately. *Intralayer* edges define connectivity within each layer, whereas *interlayer* edges define connectivity across layers. Reproduced with permission from [93].

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j in a layer β ($i,j = 1,2,\ldots,N$, $\alpha,\beta = 1,2,\ldots,L$).[3] Note that, for simplicity, we are indicating with Greek letters the indices related to layers and with Latin letters the indices related to nodes.

There are different types of multilayer networks depending on the presence or absence of links between layers and on the way nodes are defined (see Figure 5). In the following, we will mostly deal with the class of systems characterized by interlayer connectivity since it is not possible to define a meaningful multilayer adjacency tensor for the class of edge-colored multigraphs.[4]

Let us introduce the canonical rank-1 vectors $e^{\alpha}(p)$ $(\alpha, p = 1,\ldots,L)$ in the space of layers $\mathbb{R}^L$, and the corresponding canonical rank-2 tensors $E^{\alpha}_{\beta}(pq) = e^{\alpha}(p)e_{\beta}(q)$, similarly to what we have done for monoplexes. It is straightforward to show [97] that the linear combination of

$$M^{i\alpha}_{j\beta} = \sum_{a,b=1}^{N}\sum_{p,q=1}^{L} w_{ab}(pq)e^{i}(a)e_{j}(b)e^{\alpha}(p)e_{\beta}(q) \tag{2.5}$$

fully characterizes a multilinear object in the space $\mathbb{R}^{N\times L\times N\times L}$. This object is, in fact, the desired multilayer adjacency tensor since, under a change of coordinates, it transforms like a tensor:

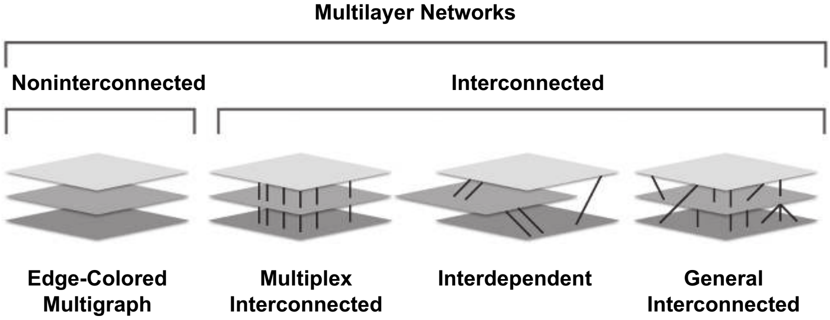

Figure 5 Multilayer networks include a broad spectrum of possible models. Edge-colored networks are useful models when interlayer connectivity is not well defined: this is the case of a social network where edges can represent different types of social relationships (e.g., trust, family, business, etc.) [73, 100, 205]. Conversely, in interconnected networks, interlayer connectivity is well defined and allows us to model a variety of systems [98, 102, 214, 232], including those with interdependencies where nodes control and/or are controlled by nodes in another network [68, 129, 230, 236, 289]. Reproduced with permission from [93].

[3] This simple observation suggests that a good candidate for multilayer adjacency tensor should be a rank-4 tensor.

[4] Note that, instead, it is possible to define a valid hypermatrix encoding this object, and this hypermatrix can be thought of as an array of matrices [49].

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$$M'^{i\alpha}_{j\beta} = \sum_{a,b=1}^{N}\sum_{p,q=1}^{L} w_{ab}(pq) B^i_k e^k(a)(B^{-1})^l_j e_l(b) \tilde{B}^\alpha_\gamma e^\gamma(p)(\tilde{B}^{-1})^\delta_\beta e_\delta(q)$$
$$= B^i_k \tilde{B}^\alpha_\gamma M^{k\gamma}_{l\delta}(B^{-1})^l_j(\tilde{B}^{-1})^\delta_\beta. \quad (2.6)$$

By indicating with $E^{i\alpha}_{j\beta}(ab;pq) = E^i_j(ab)E^\alpha_\beta(pq)$ the canonical rank-4 tensors, we can simply reduce the definition of the multilayer adjacency tensor to

$$M^{i\alpha}_{j\beta} = \sum_{a,b=1}^{N}\sum_{p,q=1}^{L} w_{ab}(pq)E^{i\alpha}_{j\beta}(ab;pq), \quad (2.7)$$

where $w_{ab}(pq)$ encodes the intensity of the interaction between node a in layer p and node b in layer q. Note that $w_{ab}(pp)$ indicates the weights of the links in layer p.

It is worth noticing that, as for the space of nodes, in the space of layers, we can define multilayer 1–tensors and Kronecker tensors as $U^{i\alpha}_{j\beta} = U^i_j U^\alpha_\beta$ and $\delta^{i\alpha}_{j\beta}$, respectively. Another important tensor, representing a complete multilayer network without self-edges, will be used later in this work to characterize multilayer triadic closure: for consistency, we prefer to introduce it here as $F^{i\alpha}_{j\beta} = U^{i\alpha}_{j\beta} - \delta^{i\alpha}_{j\beta}$.

At this point, the reader should be familiar enough with tensors to note that different decompositions are possible. Here, we are not referring to operations like Tucker decomposition – the higher-order generalization of singular value decomposition (SVD) [281] – but to a linear decomposition to highlight the fundamental components of a multilayer system. In fact, we can identify four tensors that encode distinct structural information:

$$m^{j\beta}_{i\alpha} = \underbrace{m^{j\beta}_{i\alpha}\delta^\beta_\alpha\delta^j_i + m^{j\beta}_{i\alpha}\delta^\beta_\alpha(1-\delta^j_i)}_{\text{intralayer relationships}} + \underbrace{m^{j\beta}_{i\alpha}(1-\delta^\beta_\alpha)\delta^j_i + m^{j\beta}_{i\alpha}(1-\delta^\beta_\alpha)(1-\delta^j_i)}_{\text{interlayer relationships}}$$
$$= \underbrace{m^{i\alpha}_{i\alpha}}_{\text{self-relationships}} + \underbrace{m^{j\alpha}_{i\alpha}}_{\text{endogenous}} + \underbrace{m^{j\beta}_{i\alpha}}_{\text{exogenous}} + \underbrace{m^{i\beta}_{i\alpha}}_{\text{intertwining}}$$
$$= \mathbb{S}_{i\alpha}(M) + \mathbb{N}^j_{i\alpha}(M) + \mathbb{X}^{j\beta}_{i\alpha}(M) + \mathbb{I}^\beta_{i\alpha}(M). \quad (2.8)$$

Here, the components of the tensor are indicated by $m^{j\beta}_{i\alpha}$ ($i,j = 1,2,\ldots,N$ and $\alpha,\beta = 1,2,\ldots,L$), while δ^j_i and δ^β_α indicate the Kronecker delta function in the space of nodes and layers, respectively. The four tensors encode the following relationships:

- **Intralayer interactions**:
  - **self-interactions** ($\mathbb{S}$): from a node to itself;
  - **endogeneous interactions** ($\mathbb{N}$): between distinct nodes belonging to the same layer;

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