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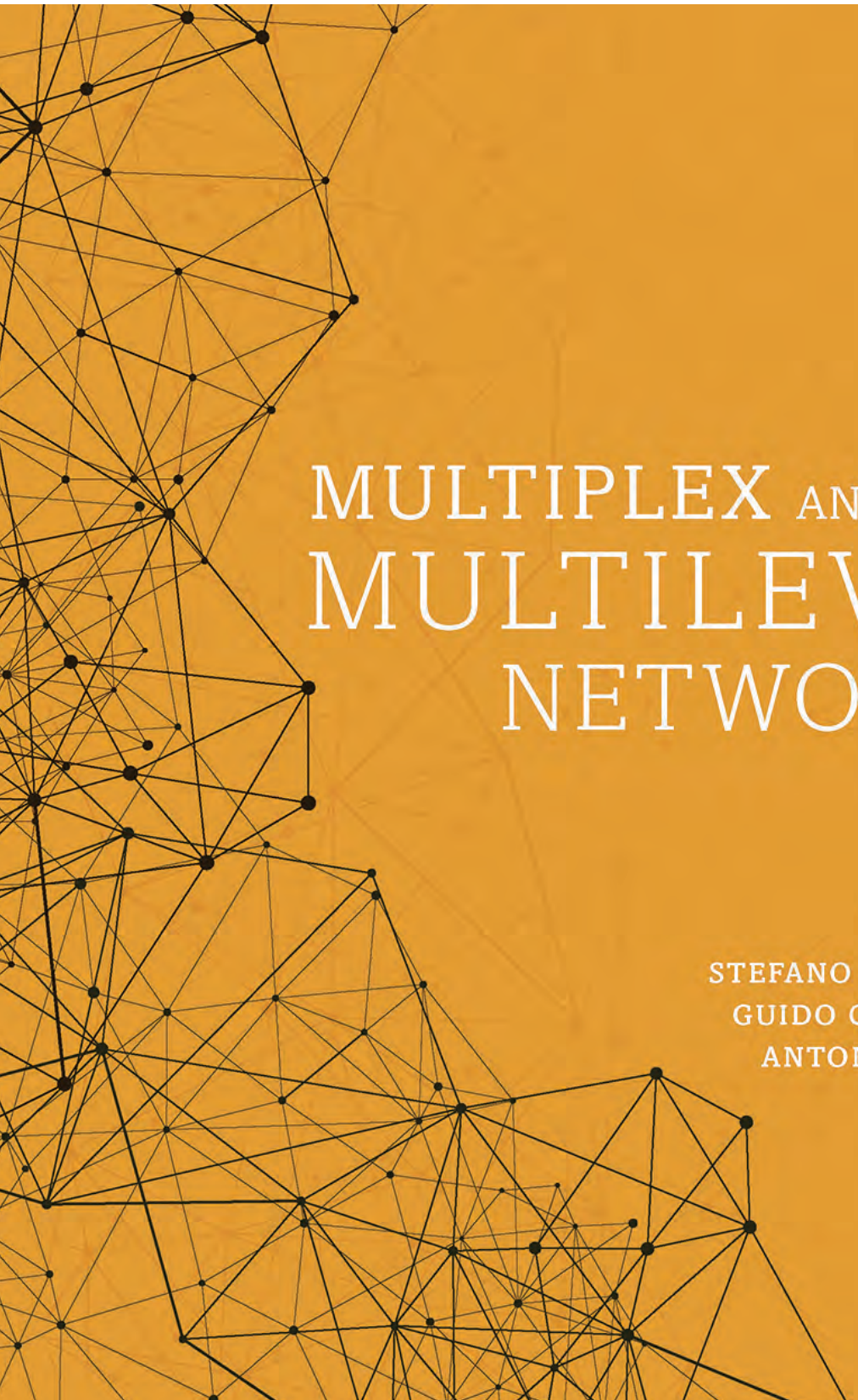

MULTIPLEX AND MULTILEVEL NETWORKS

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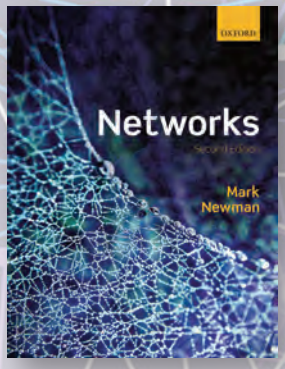

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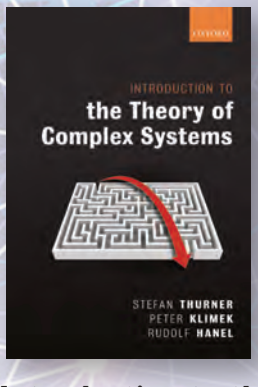

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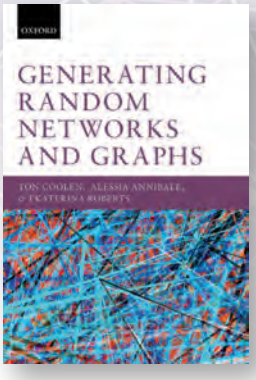

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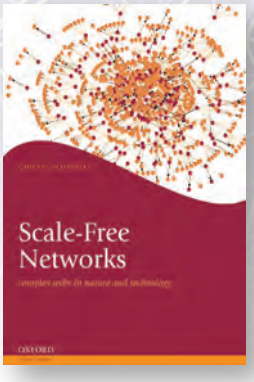

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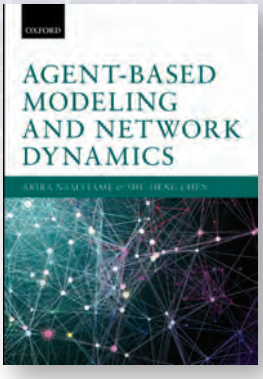

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Preface

As the field of complex networks entered its maturity phase, most scientists working in this field thought that the established methodology could deal with all cases of networked systems. However, as is usually the case in the scientific enterprise, some novel observations showed that what we already know is only a limited case, and network theory has still long way to go until we can make any definitive claim. The ever-increasing availability of data in fields ranging from computer science to urban systems, medicine, economics, and finance showed that networks that were usually perceived as distinct and isolated are, in reality, interacting with other networks. While this sounds like a trivial observation, it was shown that interactions of different networks can lead to unexpected behaviors and allow systemic vulnerabilities to emerge. Nowadays, a whole series of papers, conferences, and activities has been devoted to the analysis and modeling of the so-called network of networks.

Since the early days when this novel view of complex networks first highlighted these issues, the European Commission has engaged this challenge by financing research in the area of multilevel complex systems. This book summarizes the outcome of this engagement, as the scientific contribution for each chapter is based on a large collaborating effort that was part of the MULTIPLEX project (http://www.multiplexproject.eu). This project utilized 23 distinct research teams across Europe and, from 2012 to 2016, explored this new area of research.

The starting point of the MULTIPLEX project has been the science of complex systems. In mathematical terms, the signature of complexity is the appearance of regularities at multiple scales, for example, spatial and temporal correlations between topological quantities, such as the nodes' degree. For example, in spreading phenomena such as diseases or information exchange in a population, the hubs of the contact networks between individuals take a preponderant role in the various waves of the spreading. At a higher correlation level, two-point degree correlations determine the topological mixing (i.e., assortativity) properties of the network, which may slow down or enhance such spreading phenomena. Moreover, from a dynamical perspective, a process taking place on the network might coevolve with the network itself: a feedback loop can take place between the structure of the network and what happens on it. This problem, which is hard to solve even for simple cases, becomes much more complicated by the presence of different layers at which the dynamics can operate. It is thus clear that further progress in domains dominated by multilevel networks, such as the ICT domain, will certainly benefit from an understanding of how multilevel complex systems organize and operate.

As mentioned earlier, many works have shown that networks with interactions at different levels behave in a significantly different way than when in isolation. For example, dependencies between networks may induce cascading failures and sudden collapses

of the entire system, as, indeed, was observed in recent large-scale electricity blackouts. Thus, a better understanding of the structure of such systems is essential for future information technology and for improving and securing everyday life in an increasingly interconnected and interdependent world. This makes the science of complex networks particularly suitable for the exploration of the many challenges that we face today, including critical infrastructures and communication systems, as well as techno-social and socioeconomic networks.

In this book, we summarize results on the development of a mathematical, computational and algorithmic framework for the study of multilevel complex networks. These results represent a noteworthy paradigm shift, beyond which a significant progress in the understanding, prediction, control, and optimization of the dynamics and robustness of complex multilevel systems can be made. Through a combination of mathematical analysis, modeling approaches, and the use of huge heterogeneous datasets, several relevant aspects related to the topological and dynamical organization and evolution of multilevel complex networks have been addressed. Additionally, the theories, models, and algorithms produced within MULTIPLEX have been tested and validated in real-world systems of relevance in economic, technological and societal arenas.

With this book, we aim to build a guide for this fascinating novel view of complex networks, by providing to scientists, practitioners, and, most importantly, students, the basic knowledge that is necessary to pursue research in this field. Closing this short preface, we would like to thank all authors for their contributions and for their fruitful collaboration.

Stefano Battiston, Guido Caldarelli, and Antonios Garas

Contents

1

Multilayer Networks

Sergio Gómez[1], Manlio De Domenico[1], Elisa Omodei[1], Albert Solé-Ribalta[1,2], and Alex Arenas

[1]Departament d'Enginyeria Informàtica i Matemàtiques, Universitat Rovira i Virgili, Tarragona (Catalonia)
[2]Currently at Internet Interdisciplinary Institute, Universitat Oberta de Catalunya, Castelldefels, Barcelona (Catalonia).

1.1 Multilayer, multiplex, and interconnected networks

The development of *network science* has provided researchers and practitioners with the necessary theory and tools for the analysis of complex networks (see, e.g., [38, 210, 88, 15]). After an initial phase in which the focus was on simple and static networks, the field has evolved in the last years toward the consideration of more involved and dynamic topological structures. Thus, the literature is now full of references to evolving networks, interdependent networks, multilayer networks, multiplex networks, simplicial complexes, and hypergraphs. Here, we are going to introduce interconnected multilayer networks, analyzing them from just a few fronts: types of multilayer networks, their mathematical description, the dynamics of random walkers, and the centrality (versatility) of nodes. This selection emphasizes how the interconnected multilayer structure differs from that of the standard single-layer networks, and its influence on dynamics on top of them. For a broader review of this field, see Ref. [37].

Multilayer networks appear naturally in real data when we realize that, in many cases, the relationships (links) between the elements (nodes) can be of different kinds. For example, people are connected through friendship, family, or work relations. We may represent this structure with a network formed by three layers, one for each type of relationship, and with the same nodes repeated in all layers. This multilayer network allows for an explicit consideration of the different characteristics the dynamics may have in each layer, and the interactions between them. For instance, confidential information for a company may flow easily within the work layer, should have difficulties in jumping

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to the other layers, and could spread slowly to family or friends due to lack of interest. Thus, we have different behaviors in each layer, and interactions between them, which result in more realistic but, at the same time, more complex dynamics.

It is important to discuss the difference between the topological structure which represents the core of this study, namely *interconnected multilayer networks* [200, 119, 236, 72, 277, 122, 253], and other multilayer structures which have been named *multiplexes* in the past and have been the subject of recent studies [170, 213, 33, 27, 274]. Note that interconnected multilayer networks are not simply a special case of or equivalent to interdependent networks [106]: in multilayer systems, many or even all the nodes have a counterpart in each layer, so one can associate a vector of states to each node. This feature has no counterpart in *interdependent networks*, which were conceived as interconnected communities within a single, larger network [48, 77]. In fact, interdependent networks are characterized by having different types of nodes, instead of links.

Historically, the term *multiplex* has been adopted to indicate the presence of more than one relationship between the same actors of a social network [221]. This type of network is well understood in terms of "coloring" (or labeling) the edges corresponding to interactions of different nature. For instance, the same individual might have connections with other individuals based on financial interests (indicated by, say, a red line) and connections with the same or different individuals based on friendship (indicated by, say, a blue line). This type of network is represented by a *noninterconnected multiplex*.

Conversely, in other real-world systems, like the transportation network of a city, the same geographical position can be part, for instance, of the network of subway or the network of bus routes, simultaneously. In this specific case, an edge-colored graph would not capture the full structure of the network, because it is missing information about the cost to *move* from the subway network to the bus route. This cost can be economic

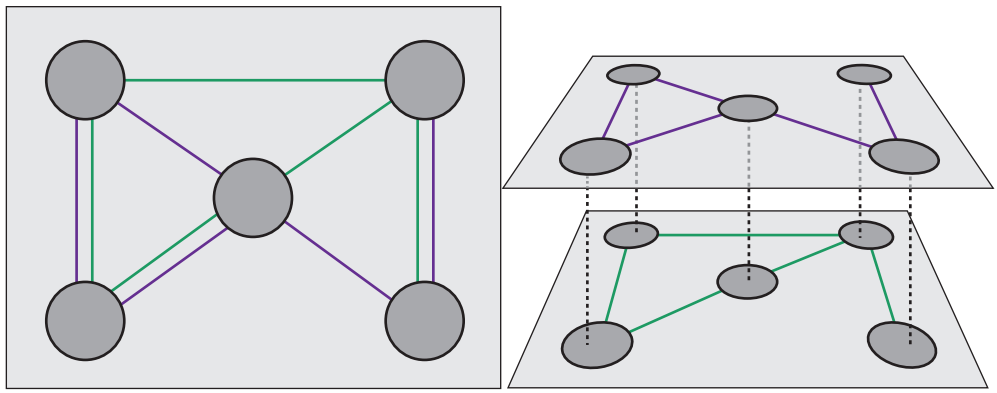

Figure 1.1 *Edge-colored versus interconnected multilayer networks. (Left) Edge-colored graph representing two different types of interactions (purple, and green) between five actors. (Right) An interconnected multiplex representing the same actors exhibiting the same relationships but on different levels which are separated by a cost (dotted vertical lines) to move from one layer to the other.*

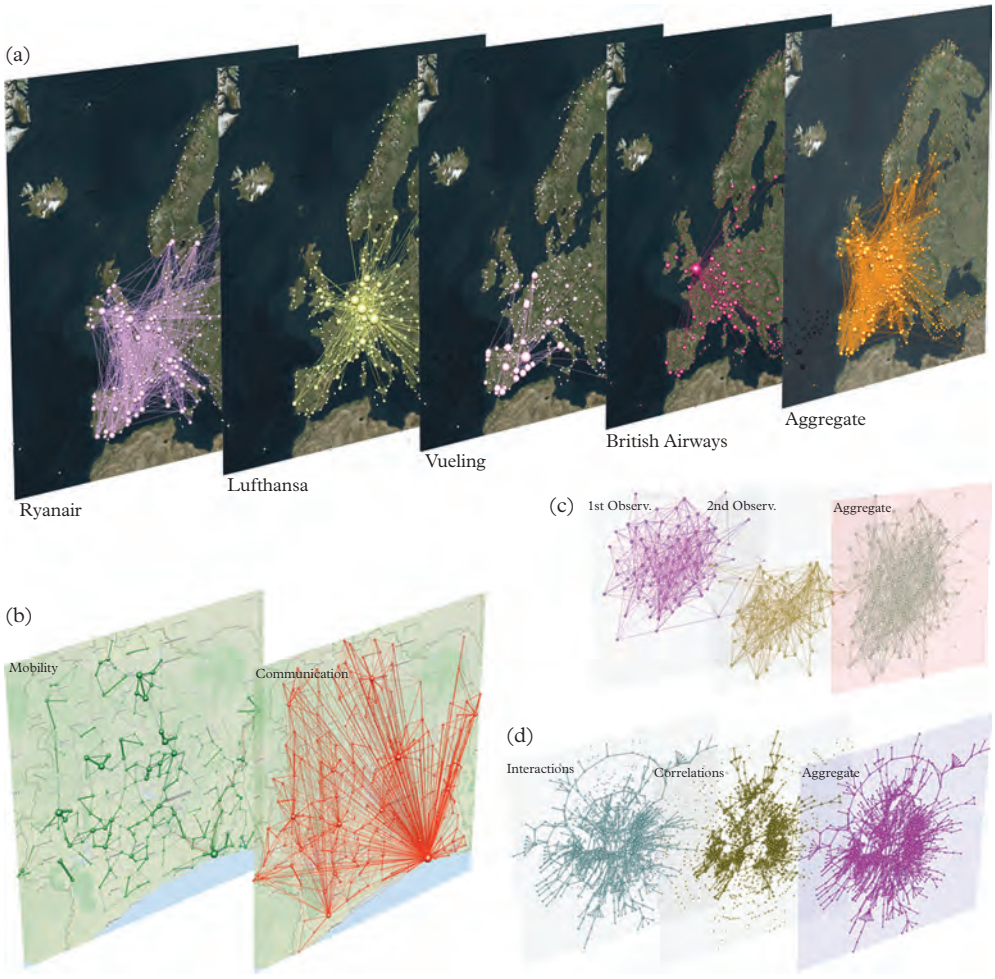

Figure 1.2 *Multilayered visualization of empirical interconnected multiplex networks. Interlayer connections not shown for simplicity. (a) Flight routes operated by different air companies between European airports [56]. (b) Mobility and the communication networks of sub-prefectures in the Ivory Coast, built from mobile phone calls data [233, 176]. (c) Two different observations (separated by 3 weeks) of one ant colony [36]. (d) Interaction network (left) of genes in* Saccharomyces cerevisiae*, obtained through synthetic genetic array methodology, and correlation-based network (middle) connecting genes with similar genetic interaction profiles [65]. We show in each layer the largest connected component, where only pairs with high genetic interaction scores and highly correlated genetic profiles are considered. The resultant aggregated network (right) is shown, to highlight the information loss. Visualization made with MuxViz [71].*

or might account for the time required to physically commute between the two layers. Therefore, the interconnected multilayer topology presented in this section provides a better representation of the system. Figure 1.1 shows an illustration of an edge-colored graph (left) and an interconnected multiplex (right). It is evident that a simple projection of the latter—mathematically equivalent to summing up the corresponding adjacency matrices—would provide a network where the information about the colors is lost. On the other hand, an edge-colored graph cannot account for interconnections, keeping irreconcilable the two structures in Figure 1.1, which should be used to represent very different networked systems.

For further details about the classification of such multilayer networks, we refer to Ref. [149] and references therein.

A real-world example of a multiplex network is provided by the transportation network of a city, where the same geographical position can be part, for instance, of the network of a subway or the network of bus routes, simultaneously. We show in Figure 1.2(a) the case of flight routes operated by different air companies between European airports. In other examples, layers encode the human mobility and the mobile communication networks of different geographical areas (Figure 1.2(b)), or physical contacts over time between ants in a colony (Figure 1.2(c)). In biological systems, such as genetic networks, two genes might exhibit different interactions (e.g., allelic or nonallelic) or be related because of their chemical interactions or their functional roles (Figure 1.2(d)).

1.2 Mathematical description of multilayer networks

A first step in the analysis of multilayer networks is the development of an adequate mathematical framework. While most single-layer networks can be described with adjacency and/or weights matrices, multilayer networks have to account for intralayer edges, interlayer edges, and the possibility of having replicas of the same node in several layers. Depending on the problem at hand, the use of a set of adjacency layers, one per layer, is enough to describe the system [27]. However, this option makes sense only for edge-colored graphs, not for interconnected multilayer networks. A more powerful approach consists in describing the multilayer networks with *supra-adjacency* matrices [119, 149], which are block matrices formed by diagonal blocks to describe the intralayer adjacency matrices, and off-diagonal blocks for the interlayer connections between every pair of layers. They represent faithfully all the edges in any multilayer network, but have problems when nodes in different layers represent the same "real" node. The most general framework is provided by *tensor algebra* [72].

1.2.1 Tensorial formalism

Edge-colored graphs can be represented by a set of adjacency matrices [56, 213, 33, 27]. However, standard matrices, used to represent networks, are inherently limited in the complexity of the relationships that they can capture, that is, they do not represent a suitable framework in the case of interconnected multiplexes. This is the case of

increasingly complicated types of relationships—which can also change in time—between nodes. Such a level of complexity can be characterized by considering tensors and higher-order algebras [72].

A great advantage of tensor formalism also relies on its compactness. An adjacency tensor can be written using a more compact notation that is very useful for the generalization to *multilayer tensor* networks. In this notation, a row vector $\mathbf{a} \in \mathbb{R}^N$ is given by a covariant vector a_α $(\alpha = 1, \ldots, N)$, and the corresponding contravariant vector a^α (i.e., its dual vector) is a column vector in Euclidean space. A canonical vector is assigned to each node, and the corresponding interconnected multilayer network is represented by a rank-4 adjacency tensor.

However, in the majority of applications, it is not necessary to perform calculations using canonical vectors and tensors explicitly. Consequently, a classical single-layer network represented by a rank-2 mixed adjacency tensor W^α_β [72] can be simply indicated by W^i_j, where the "abuse of notation" consists in interpreting the indices i and j as nodes, and W^i_j indicates the intensity of the relationship between them. Hence, W^i_j represents the well-known adjacency matrix of a graph, and the classical notation for the weight w_{ij} of the link between i and j corresponds to W^i_j. The "abuse of notation" also consists in treating W^i_j as a rank-2 tensor, although it explicitly indicates the entry of a matrix, while keeping the algebraic rules governing covariant and contravariant tensors. This "abuse of notation" dramatically reduces the complexity of some tensorial equations, although it is worth remarking that it should be used only when calculations do not involve canonical tensors explicitly.

To distinguish simple networks from the more complicated situations (e.g., interconnected multiplex networks) that we use in this paper, we will use the term *monoplex networks* to describe such standard networks, which are time independent and possess only a single type of edge to connect its nodes.

In general, there might be several types of relationships between pairs of nodes and a more general system represented as a multilayer object—in which each type of relationship is encompassed in a single *layer* α $(\alpha = 1, 2, \ldots, L)$ of a system—is required. Note that α no longer has the same meaning of the index in the adjacency tensor discussed above. To avoid confusion, in the following we refer to nodes with Latin letters and to layers with Greek letters, allowing us to distinguish indices that correspond to nodes from those that correspond to layers in tensorial equations.

We use an *intralayer adjacency tensor* for the second-order tensor $W^i_j(\alpha)$ that indicates the relationships between nodes within the *same* layer α. We take into account the possibility that a node i from layer α can be connected to any other node j in any other layer β. To encode information about relationships that incorporate multiple layers, we introduce the second-order *interlayer adjacency tensor* $C^i_j(\alpha\beta)$. Note that $C^i_j(\alpha\alpha) = W^i_j(\alpha)$.

It has been shown that the mathematical object accounting for the whole interconnected multilayer structure is given by a fourth-order (i.e., rank-4) *multilayer adjacency tensor* $M^{i\alpha}_{j\beta}$. This tensor might be simply thought as a higher-order matrix with four indices. It is the direct generalization of the adjacency matrix in the case of monoplexes, encoding the intensity of the relationship (which may not be symmetric) between a node

i in layer α and a node j in layer β [72]. This object is very general and can be used to represent structures where an actor is present in some layers but not in all of them. This is the case, for instance, when considering a network of online social relationships, of an individual with an account on Facebook but not on Twitter. The algebra still holds for these situations without any formal modification. In fact, one simply introduces "empty nodes" and assigns the value 0 to the associated edges, although the calculations of network diagnostics should carefully account for the presence of such nodes (e.g., for a proper normalization) [72].

Often, to reduce the notational complexity in the tensorial equations, the Einstein summation convention is adopted. It is applied to repeated indexes in operations that involve tensors. For example, we use this convention in the left-hand sides of the following equations:

$$A_i^i = \sum_{i=1}^{N} A_i^i,$$

$$A_j^i B_i^j = \sum_{i=1}^{N}\sum_{j=1}^{N} A_j^i B_i^j,$$

$$A_{j\beta}^{i\alpha} B_{i\gamma}^{k\beta} = \sum_{i=1}^{N}\sum_{\beta=1}^{L} A_{j\beta}^{i\alpha} B_{i\gamma}^{k\beta},$$

whose right-hand sides include the summation signs explicitly. It is straightforward to use this convention for the product of any number of tensors of any order. In the following, we will use the tth power of rank-4 tensors, defined by multiple tensor multiplications:

$$(A^t)_{j\beta}^{i\alpha} = (A)_{j_1\beta_1}^{i\alpha} (A)_{j_2\beta_2}^{j_1\beta_1} \cdots (A)_{j\beta}^{j_{t-1}\beta_{t-1}}. \tag{1.1}$$

Using repeated indexes, where one index is a subscript and the other is a superscript, is equivalent to performing a tensorial operation known as a *contraction*. Note that one should be very careful in performing tensorial calculations. For instance, using traditional notation, the product $a^i b^j$ would be a number, that is, the product of the components of two vectors. However, in our formulation, the same calculation denotes a Kronecker product between two vectors, resulting in a rank-2 tensor, that is, a matrix.

An interesting network that can be derived from the interconnected structure is the aggregated network, where the edges between two actors are summed up across all layers. The superposition of the different layers is equivalent to summing up the adjacency tensor of each layer. The corresponding aggregated network G_j^i is a monoplex and is obtained by contracting the layer indexes of the multilayer adjacency tensor, that is, $G_j^i = M_{j\alpha}^{i\alpha}$. This aggregation loses the information about inter-layer connections. If such information is important for the application of interest, then the tensor should be contracted with the 1-tensor u_α^β (the rank-2 tensor with all components equal to 1), that is, $\bar{G}_j^i = M_{j\beta}^{i\alpha} u_\alpha^\beta$.

This formalism is extremely useful for showing how topological descriptors of interconnected networks differ from the ones corresponding to their aggregated graphs [72, 66]. Moreover, it is particularly suitable for performing compact calculations.

As a representative example, let us consider the number of paths of length 2 from a node in a certain layer to any other node in any other layer of the system. Taking advantage of the extended algebra, it is straightforward to show that the resulting rank-4 tensor accounting for such paths is given by $H^{i\alpha}_{j\beta} = M^{i\alpha}_{k\gamma} M^{k\gamma}_{j\beta}$. If only the number of paths between any pair of nodes is required, regardless of the layer, then the corresponding rank-2 tensor of paths is simply obtained by contracting with the 1-tensor u^{β}_{α}, that is, $X^{i}_{j} = H^{i\alpha}_{j\beta} u^{\beta}_{\alpha}$. Conversely, in the case of the aggregate, we first contract the multilayer adjacency tensor to obtain the aggregation $\mathcal{J}^{i}_{j} = M^{i\alpha}_{j\beta} u^{\beta}_{\alpha}$, where interlayer connections are included as self-loops, and then square the resulting tensor to obtain $Y^{i}_{j} = \mathcal{J}^{i}_{k} \mathcal{J}^{k}_{j}$. Of course, a similar argument can be used to calculate the number of longer paths. From these tensorial equations, it is evident that the aggregated graph cannot be considered, in general, a good proxy of the interconnected topology.

Summarizing, the tensorial formulation provides a suitable framework for several real-world networked systems, from transportation networks to social ones. It is also worth noting that special cases of multilayer adjacency tensors are time-dependent (i.e., "temporal") networks [72, 149]. More specifically, in the case of social sciences, the multilayer adjacency tensor can be used, for instance, to model the structural changes of a social network over time, or to define the topology of actors involved in several different levels of relationships and for whom it is indispensable to define an interconnection between such levels. For these networked systems, it is desirable to adopt descriptors (e.g., clustering coefficient, modularity, etc.) that are the natural extension of their well-known counterparts in monoplex networks.

1.2.2 Tensorial nature of adjacency tensors

Although we have already shown in Ref. [72] the advantages of using the tensor formalism to deal with multilayer networks, the assignment of the indices as covariant or contravariant may seem arbitrary. The problem arises from the absence of natural basis transformations which could guide us in this decision. The idea is that, if we perform a change of basis governed by a matrix Q^{α}_{β}, each contravariant index of any tensor is transformed using Q, while covariant indices change with Q^{-1}, the inverse of Q. Thus, an object with three indexes which transforms with two Q and one Q^{-1} is bounded to be 1-covariant and 2-contravariant. However, these transformations are not the origin but the consequence of the "meaning" of the object. For example, inner products, metric tensors, and symplectic forms must be 2-covariant, since they are bilinear functions which assign two vectors to a number, while linear transformations are 1-covariant and 1-contra variant because they have to convert a vector (or 1-form) in another vector (or 1-form).

In the case of monoplex networks, the adjacency tensor may be viewed as a linear transformation which, given a vector (or 1-form) representing a node, returns the set

of their adjacent nodes. Thus, the only acceptable representation for the monoplex adjacency object is a 1-covariant and 1-contravariant tensor. Likewise, the multilayer adjacency tensor transforms a node in one layer into the set of adjacent nodes, keeping also the information of which layer they belong to; thus, a 2-covariant and 2-contravariant tensor is needed.

Once we know the order of the adjacency tensor, its transformation under a change of coordinates is completely determined. First, we show how this works for a single-layer network and, afterwards, for a full multilayer network.

By following Ref. [72], the adjacency tensor W_β^α of a network can be represented as a linear combination of tensors of the canonical basis by

$$W_\beta^\alpha = \sum_{i,\, j=1}^{N} w_{ij} e^\alpha(i) e_\beta(j) = \sum_{i,\, j=1}^{N} w_{ij} E_\beta^\alpha(ij), \tag{1.2}$$

where $E_\beta^\alpha(ij) \in \mathbb{R}^{N\times N}$ indicates the tensor of the canonical basis corresponding to the tensorial product of the canonical vectors $\mathbf{e}(i)$ and $\mathbf{e}^\dagger(j)$ (defined in $\mathbb{R}^N$) assigned to nodes $i(e^\alpha(i))$ and $j(e_\beta(j))$, respectively.

Let

$$Q_\beta^\alpha = \sum_{i=1}^{N} e'^\alpha(i) e_\beta(i) \tag{1.3}$$

be the change of basis tensor which transforms the basis vector set $\{e^\alpha(i), i = 1,\ldots,N\}$ into a second set $\{e'^\alpha(i), i = 1,\ldots,N\}$. Here, Q_β^α is expressed in terms of the basis vectors from both bases, and it is straightforward to show that $e'^\alpha(i) = Q_\beta^\alpha e^\beta(i)$ and $e'_\beta(i) = e_\alpha(j)(Q^{-1})_\beta^\alpha$. By remarking that a change of basis should not affect the intensity of the relationship between nodes n_i and n_j, by following the above prescription, we obtain

$$\begin{aligned} W'^\gamma_{\ \delta} &= \sum_{i,\, j=1}^{N} w_{ij} e'^\gamma(i) e'_\delta(j) = \sum_{i,\, j=1}^{N} w_{ij} Q_\alpha^\gamma e^\alpha(i) e_\beta(j) (Q^{-1})_\delta^\beta \\ &= Q_\alpha^\gamma \left[\sum_{i,\, j=1}^{N} w_{ij} e^\alpha(i) e_\beta(j) \right] (Q^{-1})_\delta^\beta = Q_\alpha^\gamma W_\beta^\alpha (Q^{-1})_\delta^\beta, \end{aligned} \tag{1.4}$$

providing the desired tensor transformation law.

In the following, we use the same notation as in Ref. [72], to avoid confusion. In the same spirit, we introduce the vectors $e^{\tilde{\gamma}}(k)$ $(\tilde{\gamma}, k = 1,\ldots,L)$ of the canonical basis in the space $\mathbb{R}^L$, where the Greek index indicates the components of the vector, and the Latin index indicates the kth canonical vector. Therefore, it is straightforward to build the

second-order tensors $E_{\tilde{\delta}}^{\tilde{\gamma}}(hk) = e^{\tilde{\gamma}}(h)e_{\tilde{\delta}}(k)$ representing the canonical basis of the space $\mathbb{R}^{L\times L}$.

The representation of the multilayer object $M_{\beta\tilde{\delta}}^{\alpha\tilde{\gamma}}$ in terms of the Kronecker product of canonical vectors is given by [72]

$$M_{\beta\tilde{\delta}}^{\alpha\tilde{\gamma}} = \sum_{i,\,j=1}^{N}\sum_{h,k=1}^{L} w_{ij}(hk)e^{\alpha}(i)e_{\beta}(\,j)e^{\tilde{\gamma}}(h)e_{\tilde{\delta}}(k). \tag{1.5}$$

Proceeding as in the case of a single-layer network, we obtain

$$\begin{aligned} M'^{\alpha\tilde{\gamma}}_{\beta\tilde{\delta}} &= \sum_{i,\,j=1}^{N}\sum_{h,k=1}^{L} w_{ij}(hk)Q_{\rho}^{\alpha}e^{\rho}(i)(Q^{-1})_{\beta}^{\sigma}e_{\sigma}(\,j)\tilde{Q}_{\tilde{\phi}}^{\tilde{\gamma}}e^{\tilde{\phi}}(h)(\tilde{Q}^{-1})_{\tilde{\delta}}^{\tilde{\epsilon}}e_{\tilde{\epsilon}}(k) \\ &= Q_{\rho}^{\alpha}\tilde{Q}_{\tilde{\phi}}^{\tilde{\gamma}}M_{\sigma\tilde{\epsilon}}^{\rho\tilde{\phi}}(Q^{-1})_{\beta}^{\sigma}(\tilde{Q}^{-1})_{\tilde{\delta}}^{\tilde{\epsilon}}, \end{aligned} \tag{1.6}$$

providing the desired transformation law of the multilayer adjacency tensor under a change of coordinates.

1.2.3 Eigenvalue problem with tensors

The eigenvalue problem for a rank-2 tensor, that is, a standard matrix, is defined by $W_j^i v_i = \lambda v_j$. The extension of this problem to rank-4 tensors leads to the equation

$$M_{j\beta}^{i\alpha}V_{i\alpha} = \lambda V_{j\beta}. \tag{1.7}$$

To solve this problem, it is worth noting that any tensor can be *unfolded* to lower-rank tensors [154]. For instance, a rank-2 tensor like W_j^i, with N^2 components, can be flattened to a vector w_k with N^2 components. In the case of the rank-4 multilayer adjacency tensor $M_{j\beta}^{i\alpha}$, although any unfolding is allowed, it is particularly useful for some applications to choose the ones flattening to a squared rank-2 tensor $\tilde{M}_l^k$ with $NL \times NL$ components, where L indicates the number of layers [119]. In fact, this unfolding produces as many block adjacency matrices, named *supra-adjacency matrices* in some applications [119, 149, 73, 66], as the number of permutations of diagonal blocks of size N^2, that is, $L!$. However, such unfoldings do not alter the spectral properties of the resulting supra-matrix and can be used to solve the eigenvalue problem for rank-4 tensors. In fact, the solution of the eigenvalue problem

$$\tilde{M}_l^k\tilde{v}_k = \tilde{\lambda}_1\tilde{v}_l, \tag{1.8}$$

is a *supra-vector* with NL components which corresponds to the unfolding of the eigentensor $V_{i\alpha}$. We will make use of this eigenvalue formalism for tensors in Section 1.4.

1.3 Random walks in multiplex networks

Random walks constitute one of the simplest dynamics one can define on top of graphs or complex networks [311, 290, 180]. They can be used to approximate other types of diffusion [61, 210]. Random walks on monoplex networks [61, 214, 210] have attracted considerable interest because they are both important and easy to interpret. They have yielded important insights into a huge variety of applications and can be studied analytically. For example, random walks have been used to rank Web pages [46] and sports teams [55], optimize searches [304], investigate the efficiency of network navigation [313, 68], characterize cyclic structures in networks [247], and coarse-grain networks to illuminate mesoscale features such as community structure [115, 242, 167].

In a random walk process, the walker is initially positioned in any node and then starts to navigate the network, following the available edges. At each step, the edge is selected at random between the outgoing links of the current node, hence the name "random walker." If the network is undirected and connected, all nodes have a nonnull probability of being visited, and these probabilities are proportional to the degrees of the nodes (in the limit of paths of infinite length). The analysis of random walks for specific complex network topologies, such as networks with power-law degree distributions or small-world architectures, has revealed the different ways in which the networks are explored [214, 313].

When the network is structured in layers, the navigation of the random walker is formed by two kinds of movements: intralayer steps, in which the walker jumps between nodes within the same layer, and interlayer steps, where the walker switches from one layer to another one. In what follows, we will consider multiplex networks, the particular case of general multilayer networks in which the same nodes are present in all layers, and interlayer connections appear only between the different instances of the same node (see Figure 1.3). The multiplex networks can be weighted, thus converting the random walks in biased random walks, as we will specify below. The analysis of random walks in multiplex networks we are going to describe can be found in [73].

Given a multiplex network with N nodes in each of the L layers, we use $W_{ij}^{(\alpha)}$ to indicate the weighted intralayer connection between two vertices i and j in layer α, where Latin letters refer to vertices ($i,j = 1,2,...,N$), and Greek letters indicate layers ($\alpha = 1,2,...,L$). Similarly, $D_{(i)}^{\alpha\beta}$ denotes the weight of switching from layer α to layer β when located in a vertex i. Without loss of generality, we may suppose that $W_{ii}^{(\alpha)} = 0$ for all nodes i, since these self-loops can be accounted for in the terms $D_{(i)}^{\alpha\alpha}$. The corresponding weighted $NL \times NL$ supra-adjacency matrix becomes[1]

$$\mathcal{A} = \begin{pmatrix} \mathbf{D}^{11} + \mathbf{W}^{(1)} & \mathbf{D}^{12} & \dots & \mathbf{D}^{1L} \\ \mathbf{D}^{21} & \mathbf{D}^{22} + \mathbf{W}^{(2)} & \dots & \mathbf{D}^{2L} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{D}^{L1} & \mathbf{D}^{L2} & \dots & \mathbf{D}^{LL} + \mathbf{W}^{(L)} \end{pmatrix}, \tag{1.9}$$

[1] In this section, we (partly) adopt the supra-adjacency formalism and notation instead of the tensorial one in order to emphasize the difference in role between intralayer and interlayer links.

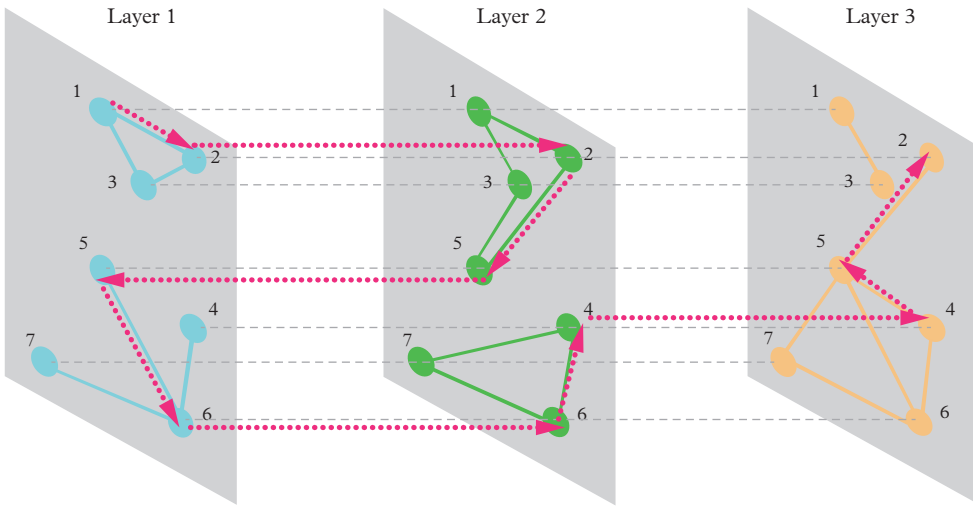

Figure 1.3 *Example of the navigation on a multiplex network. Path (dotted pink line) of a random walker through the multiplex structure. Note how the walker is able to visit disconnected components. In this example, there are no intralayer links between Layers 1 and 3.*

where we have used boldface to represent the matrices $\mathbf{W}^{(\alpha)}$ (intralayer weights of layer α) and $\mathbf{D}^{\alpha\beta}$ (a diagonal matrix with the weights of switching from layer α to layer β). A commonly studied particular case is the one in which the switching-layer weight is the same for all nodes, so that $\mathbf{D}^{\alpha\beta} = D^{\alpha\beta}\mathbf{I}$, where $\mathbf{I}$ is the $N \times N$ identity matrix:

$$\mathcal{A} = \begin{pmatrix} D^{11}\mathbf{I} + \mathbf{W}^{(1)} & D^{12}\mathbf{I} & \dots & D^{1L}\mathbf{I} \\ D^{21}\mathbf{I} & D^{22}\mathbf{I} + \mathbf{W}^{(2)} & \dots & D^{2L}\mathbf{I} \\ \vdots & \vdots & \ddots & \vdots \\ D^{L1}\mathbf{I} & D^{L2}\mathbf{I} & \dots & D^{LL}\mathbf{I} + \mathbf{W}^{(L)} \end{pmatrix}. \tag{1.10}$$

It is advantageous to distinguish between the strength $s_{i\alpha} = \sum_j W_{ij}^{(\alpha)}$ of a node i with respect to its connections with other nodes j in the same layer α, and the strength $S_{i\alpha} = \sum_\beta D_{(i)}^{\alpha\beta}$ of the same vertex with respect to connections to its counterparts in different layers.

1.3.1 Navigation on a multiplex network

The description of the random walk navigation on a multiplex network is completely specified by the transition probabilities $\mathcal{P}_{j\beta}^{i\alpha}$, which account for the probabilities that a random walker at node i in layer α moves to vertex j in layer β. The master equation of this process reads[2]

[2] For convenience, we will not use the Einstein summation convention throughout Section 1.3.

$$p_{j\beta}(t+\Delta t) = \sum_{\alpha=1}^{L}\sum_{i=1}^{N} \mathcal{P}_{j\beta}^{i\alpha} p_{i\alpha}(t), \tag{1.11}$$

where $p_{i\alpha}(t)$ represents the probability of the random walker being in node i of layer α at time t. Equation 1.11 expresses that the probability of being in (j,β) at time $t+\Delta t$ is equal to the probability of being in any other (i,α) at time t, and then jumping to (j,β). The double sum in Eq. 1.11 can be separated into four terms:

$$\begin{aligned} p_{j\beta}(t+\Delta t) = \mathcal{P}_{j\beta}^{j\beta} p_{j\beta}(t) + \sum_{\substack{\alpha=1 \\ \alpha\neq\beta}}^{L} \mathcal{P}_{j\beta}^{j\alpha} p_{j\alpha}(t) \\ + \sum_{\substack{i=1 \\ i\neq j}}^{N} \mathcal{P}_{j\beta}^{i\beta} p_{i\beta}(t) + \sum_{\substack{\alpha=1 \\ \alpha\neq\beta}}^{L}\sum_{\substack{i=1 \\ i\neq j}}^{N} \mathcal{P}_{j\beta}^{i\alpha} p_{i\alpha}(t), \end{aligned} \tag{1.12}$$

which take into account that, in the previous time step, the random walker could have already been in node j and/or layer β.

Equation 1.11 can be put in a more compact form if we define $\mathbf{p}_\alpha$ as the row vector with N components $p_{i\alpha}$ with respect to layer α and introduce the supra-vector $\mathbf{p} \equiv (\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_L)$ with NL components. Now, Eq. 1.11 can be written as

$$\dot{\mathbf{p}}(t) = -\mathbf{p}(t)\mathcal{L}, \tag{1.13}$$

hereafter referred to as the "random walk equation." In this equation, $\mathcal{L}$ refers to the $NL \times NL$ normalized supra-Laplacian matrix, whose structure is similar, although not identical, to the (unnormalized) supra-Laplacian matrix proposed in [119] to model the diffusion process in multiplex networks (see also [277]). The structure of the random walk equation is the same regardless of the transition probabilities $\mathcal{P}_{j\beta}^{i\alpha}$ adopted in Eq. 1.12. In particular, we are going to analyze four different prescriptions for the random walk dynamics: classical, diffusive, physical, and maximum entropy random walks.

1.3.2 Classical random walks

The classical description of random walkers on a graph (i.e., monoplex networks) is already present in [311, 290, 180], although applications to networks with complex topologies are more recent [214, 313].

In monoplex networks, the random walker has probability $1/k_i$ of moving from vertex i to vertex j in the neighborhood of i, where k_i indicates the degree of a vertex i. The direct extension of such walks to the case of multiplex networks is considering the interlayer connections as additional edges available in vertex i. It follows that the probability of moving from vertex i to vertex j within the same layer α or of switching to the counterpart of vertex i in layer β is uniformly distributed. In such a scenario, the normalizing factor

for obtaining the correct probability is the total strength $s_{i\alpha} + S_{i\alpha}$ of vertex i. The resulting transition probabilities for this classical random walker in a multiplex (RWC) are given in Table 1.1. For sake of completeness, the Laplacian matrix corresponding to this process in monoplex networks is generally referred to as the normalized Laplacian.

1.3.3 Diffusive random walks

In monoplex networks, this type of random walk has been studied in detail in [252]. Here, the random walker stays at vertex i with a rate that depends on i. In fact, if $k_{\max} = \max_i\{k_i\}$ is the maximum degree in the network, the walker is allowed to wait in vertex i with rate $1 - k_i/k_{\max}$ and to jump to any neighbor with rate $1/k_{\max}$. This procedure is equivalent to adding a weighted self-loop to each node in such a way that all nodes have the same strength. It can be shown that the corresponding random walk equation depends on the unnormalized Laplacian matrix, as in the classical diffusive process, hence the name "diffusive random walk."

We extend this walk to the case of multiplex networks by considering interlayer connections as additional edges to estimate the maximum vertex strength, $s_{\max} = \max_{i,\alpha}\{s_{i\alpha} + S_{i\alpha}\}$. The resulting transition rules for this random walker in a multiplex (RWD) are given in Table 1.1.

1.3.4 Physical random walks

Here, we propose a new type of random walk dynamics in the multiplex, which reduces to the classical random walk in the case of monoplex. The transition rules are the same,

Table 1.1 *Transition probability for four different random walk processes on multiplex networks. We account for jumping between vertices (Latin letters) and switching between layers (Greek letters). When appearing in pairs, $j \neq i$ and $\beta \neq \alpha$ must be considered. See text for further detail.*

Transition Probability	**RWC**	**RWD**	**RWP**	**RWME**
$\mathcal{P}_{i\alpha}^{i\alpha}$	$\dfrac{D_{(i)}^{\alpha\alpha}}{s_{i\alpha} + S_{i\alpha}}$	$\dfrac{s_{\max} + D_{(i)}^{\alpha\alpha} - s_{i\alpha} - S_{i\alpha}}{s_{\max}}$	0	$\dfrac{D_{(i)}^{\alpha\alpha}}{\lambda_{\max}}$
$\mathcal{P}_{i\beta}^{i\alpha}$	$\dfrac{D_{(i)}^{\alpha\beta}}{s_{i\alpha} + S_{i\alpha}}$	$\dfrac{D_{(i)}^{\alpha\beta}}{s_{\max}}$	0	$\dfrac{D_{(i)}^{\alpha\beta}}{\lambda_{\max}} \dfrac{\psi_{(\beta-1)N+i}}{\psi_{(\alpha-1)N+i}}$
$\mathcal{P}_{j\alpha}^{i\alpha}$	$\dfrac{W_{ij}^{(\alpha)}}{s_{i\alpha} + S_{i\alpha}}$	$\dfrac{W_{ij}^{(\alpha)}}{s_{\max}}$	$\dfrac{W_{ij}^{(\alpha)}}{s_{i\alpha}} \dfrac{D_{(i)}^{\alpha\alpha}}{S_{i\alpha}}$	$\dfrac{W_{ij}^{(\alpha)}}{\lambda_{\max}} \dfrac{\psi_{(\alpha-1)N+j}}{\psi_{(\alpha-1)N+i}}$
$\mathcal{P}_{j\beta}^{i\alpha}$	0	0	$\dfrac{W_{ij}^{(\beta)}}{s_{i\beta}} \dfrac{D_{(i)}^{\alpha\beta}}{S_{i\alpha}}$	0

Abbreviations: RWC, classical random walker; RWD, random walker in a multiplex; RWME, maximal entropy random walker in a multiplex; RWP, physical random walker in a multiplex.

except that we assume that the timescale for switching layers is negligible with respect to the timescale required to move from one vertex to another one in its neighborhood. Therefore, in the same time step, the random walker is allowed to both switch layers and jump to another vertex, with the layer-switching and vertex-jumping actions being independent. This is a fundamental difference from the random walkers described so far, because they were not allowed to both switch and jump in the same time unit. Moreover, another major difference lies in treating interlayer connections as another type of edge, one that does not compete with the intralayer edges.

As an example of this dynamics, one might imagine the case of online social networks where each layer corresponds to a different social structure (e.g., Facebook and Twitter), and users play the role of vertices. In this case, the time required by a user to switch from one layer to the other one requires less than a few seconds.

The resulting transition rules for this physical random walker in a multiplex (RWP) are given in Table 1.1. It is straightforward to show that this process is equivalent to the classical random walker in the case of monoplexes.

1.3.5 Maximal entropy random walks

In classical random walks, a walker jumps from a vertex to a neighbor with uniform probability that depends only on the local structure, namely, the vertex strength. However, a walk dynamics has recently been proposed where the transition rate of jumps is influenced by the global structure of the network [49], or only local information is available [267]. More specifically, the walkers choose the next vertex to jump into so as to maximize the entropy of their path at a global level, whereas classical random walkers maximize the entropy of their path at neighborhood level. To achieve such maximal entropy paths, the transition rates are governed by the largest eigenvalue of the adjacency matrix, and the components of the corresponding eigenvector [49].

In the case of multiplex networks, we use the supra-adjacency matrix Eq. 1.9 to achieve the same result. We indicate with $\lambda_{\max}$ the largest eigenvalue of this matrix and with ψ the corresponding eigenvector. Therefore, according to the prescription given in [49], the resulting transition rules for this maximal entropy random walker in a multiplex (RWME) are given in Table 1.1.

1.3.6 Comparison of types of random walkers

A representative example of each walk is shown in Figure 1.4, where vertices and layers visited by one random walker up to 100 time steps are reported. We show two different cases, corresponding to different choices of interlayer weights, to make evident the differences in the dynamics.

In the top panels of Figure 1.5, we show the transition probabilities in the case of a multiplex of 20 vertices embedded in two different realizations of a Watts–Strogatz small-world network [308]. The probability of finding a random walker in a certain vertex on a certain layer is also shown in the same figure, considering one walk starting from the first vertex only (middle panels) and from any other vertex with uniform probability (bottom

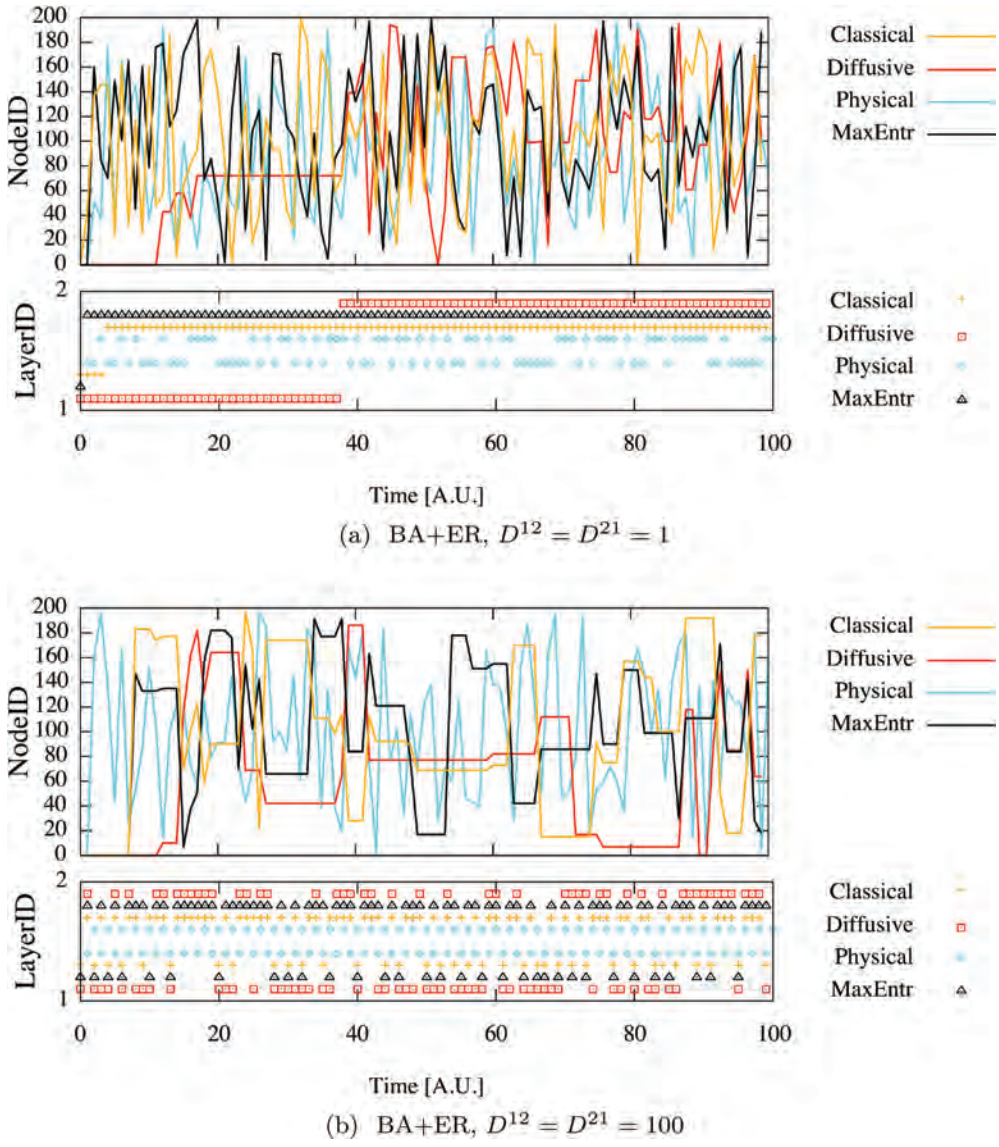

Figure 1.4 *Random walks realizations on different multiplex structures. Vertices (top panels) and layers (bottom panels) visited by one random walker in 100 time steps. The four types of walk considered in this study are shown. The multiplex is built with one Barabási–Albert (BA, Layer 1) and one Erdős–Rényi (ER; Layer 2) network with 200 vertices, while interlayer weights are specified above.*

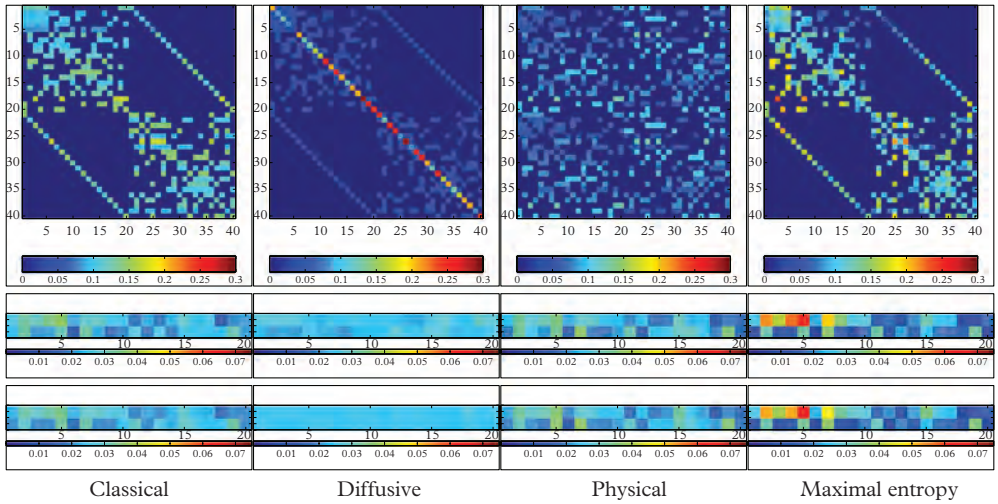

Figure 1.5 *Probabilities governing four random walk strategies on multiplex networks. (Top) Transition probabilities for walks considered in this study. Note that we have rescaled by a factor of 2 the transition matrix of the diffusive walk for better visualization and to allow comparisons. (Middle) Occupation probability, for each vertex in each layer, considering one random walk starting only from the first vertex. (Bottom) As in the middle panels, but considering one random walk starting with uniform probability from any other vertex. Multiplex of 20 vertices embedded in two different realizations of a Watts–Strogatz small-world network (rewiring probability is 0.2), where* $D^{11} = D^{12} = D^{21} = D^{22} = 1$. *Different exploration strategies are responsible for the different probability that a vertex is visited and occupied by a random walker.*

panels). As expected, different exploration strategies result in different occupation probabilities, where some vertices in a certain layer might be explored more (or less) frequently, as in the case of RWC, RWP, and RWME, or uniformly, as in the case of RWD.

Figures 1.4 and 1.5 clearly highlight the different dynamics and how navigation strategy influences the exploration of the multiplex.

1.3.7 Occupation probability of random walkers

We define the occupation probability of node i in layer α as the probability of finding the random walker in that location of the multiplex, in the limit of large time, $\Pi_{i\alpha} = \lim_{t\to\infty} p_{i\alpha}(t)$. We also indicate with Π the corresponding supra-vector. In general, Π is the left eigenvector of the supra-transition matrix corresponding to the unit eigenvalue. In some cases, the occupation probability can be estimated from the detailed balance equation

$$\Pi_{i\alpha}\mathcal{P}^{i\alpha}_{j\beta} = \Pi_{j\beta}\mathcal{P}^{j\beta}_{i\alpha}, \tag{1.14}$$

obtaining

$$\Pi_{i\alpha} = \frac{s_{i\alpha} + S_{i\alpha}}{\sum_{\beta}\sum_{j}(s_{j\beta} + S_{j\beta})} \tag{1.15}$$

for RWC, generalizing the well-known result obtained for walks in a monoplex network,

$$\Pi_{i\alpha} = \frac{1}{NL} \tag{1.16}$$

for RWD, as expected for a purely diffusive walk, and

$$\Pi_{i\alpha} = \psi^2_{(\alpha-1)N+i} \tag{1.17}$$

for RWME, generalizing the results obtained in [49] for monoplex networks.

Indeed, following the approach proposed in [214] for random walks on monoplexes, it is possible to show that the time required for a random walker starting from vertex i to arrive back to the same vertex, that is, the mean return time, is given by

$$\langle T_{ii}\rangle = \frac{1}{\sum\limits_{\alpha=1}^{L}\Pi_{i\alpha}}. \tag{1.18}$$

It is straightforward to verify that distributions expected in the case of monoplex are recovered for $L = 1$. It is worth noting that for classical random walks, the occupation probability of vertex i is proportional to its supra-strength, that is, intra- plus interlayer strengths, whereas for diffusive walks, such a probability is the same for any vertex, regardless of multiplex topology.

1.3.8 Random walks coverage

The coverage of a random walk is an important measure which quantifies how difficult (or easy) is to visit all the nodes in a network. There are two main approaches for defining the coverage: (i) calculate the expected time the random walker takes to visit all the nodes; (ii) calculate the average fraction of visited nodes as a function of the length of the walk. Here, we adopt the second option, which is computationally friendlier, and denote the coverage as $\rho(t)$. In multiplex networks, one has to take into account that the same node is present in all layers; thus, the logical approach is to consider a node to have been "visited" if the random walker visited that node at least once in any of the layers. For example, in a multiplex transportation network consisting of buses, trains, and a metro, it is not important if you have arrived at a location by bus or metro; what counts is having been there.

First, the probability of finding the random walker at node i at time t, regardless of the layer, is given by $p_i(t) = \sum_{\alpha} p_{i\alpha}(t)$. Introducing the supra-vector $\mathbf{E}_i \equiv (\mathbf{e}_i, \mathbf{e}_i, \ldots, \mathbf{e}_i)$, where $\mathbf{e}_i$ is the ith canonical vector, we may write

$$p_i(t+1) = \mathbf{p}(t)\mathcal{P}\mathbf{E}_i^{\dagger}. \tag{1.19}$$

We have set $\Delta t = 1$ to make t equivalent to the walk length. Next, we define the probability $\sigma_{ij}(t)$ of not finding the random walker at node i after t time steps, assuming that it started at vertex j. This probability satisfies the recursive relation

$$\sigma_{ij}(t+1) = \sigma_{ij}(t)\,[1 - p_i(t+1)], \tag{1.20}$$

which can be written as

$$\dot{\sigma}_{ij}(t) = -\sigma_{ij}(t)\mathbf{p}(t)\mathcal{P}\mathbf{E}_i^{\dagger} \tag{1.21}$$

and whose solution is

$$\sigma_{ij}(t) = \sigma_{ij}(0)\exp\Big[-\mathbf{p}_j(0)\mathbb{P}\mathbf{E}_i^{\dagger}\Big], \quad \mathbb{P} = \sum_{\tau=0}^{t}\mathcal{P}^{\tau+1}, \tag{1.22}$$

where $\mathbf{p}_j(0) \equiv (\mathbf{e}_j, \mathbf{0}, \ldots, \mathbf{0})$ explicitly indicates that at time $t = 0$, the walker started at vertex j in the first layer, without loss of generality. The matrix $\mathbb{P}$ accounts for the probability of reaching each vertex through any path of length $1, 2, \ldots, t+1$. Note also that $\sigma_{ij}(0) = 1 - \delta_{ij}$, where δ_{ij} is the Kronecker delta, since a walk starting at node i cannot also at the same time be at node j unless $i = j$. Finally, a good approximation of the coverage is given by double averaging over all vertices the probability $1 - \sigma_{ij}(t)$, obtaining

$$\rho(t) = 1 - \frac{1}{N^2}\sum_{\substack{i,j=1 \\ i\neq j}}^{N}\exp\Big[-\mathbf{p}_j(0)\mathbb{P}\mathbf{E}_i^{\dagger}\Big], \tag{1.23}$$

which can be solved numerically to obtain the coverage at each time step. Comparisons between the predicted coverage using Eq. 1.23 and Monte Carlo simulations show a perfect agreement, thus confirming the validity of our theoretical development (see [73]). It must be pointed out that this expression for the coverage is applicable not only to multiplex networks but also to standard single-layer networks.

We show in Figure 1.6 the coverage versus time in the case of RWP only, for some representative multiplexes where $D_{(i)}^{12} = D_{(i)}^{21} = D_{(i)}^{11} = D_{(i)}^{22} = 1, \forall i = 1, \ldots, N$. Results for different combination of topologies (indicated by double acronyms in the figure) are shown, together with results for walks in a single layer (indicated by single acronyms in the figure). The topologies analyzed include Erdős–Rényi (ER), Barabási–Albert (BA), and Watts–Strogatz (WS) networks. The abbreviation "diff" indicates that the layers have the same topology but different random realizations, while "same" indicates that the same topology and same random realization is present in both layers. The inset shows the relative difference of coverages with respect to the case of an ER monoplex.

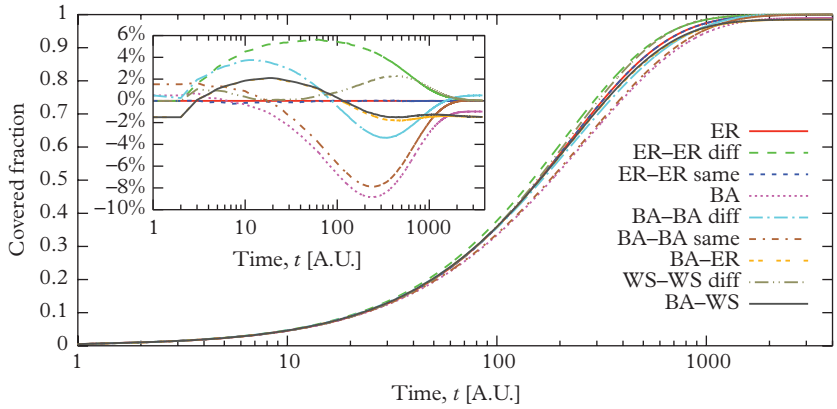

Figure 1.6 *Dependence of the coverage on multiplex topology: number of visited vertices versus time for monoplex and multiplex topologies (see the text for further details). The inset shows the relative difference of each curve with respect to the coverage obtained for an ER monoplex, showing that vertices in different topologies are visited with different timescales.*

The multiplex topology has an evident impact on the walk process, delaying or accelerating the exploration of the network with respect to a random search in a monoplex random network. This is a genuine effect of the multilayer structure, and it is not related to the finite size of the considered networks, as shown in Figure 1.7, where multiplexes of 2,000 nodes and many different topologies are considered.

In Figure 1.8, for each random walk considered, we show the inverse of the time τ_C required to cover 50% of a BA+ER multiplex with 200 vertices as a function of the interlayer weight $D_X = D^{12} = D^{21}$, with $D^{11} = D^{22}$. It is worth mentioning that the final result depends quantitatively, but not qualitatively, on the choice of the covered fraction. This representative example shows the impact of transition rules on the exploration of the multiplex, providing evidence that the best strategy to use to cover the network depends on the topology and on the weight of inter-layer connections. Moreover, in this specific experiment, the walk in the multiplex is *infra-diffusive* (*sub-diffusive*), depending on the value of D_X, that is, the time to cover the multiplex lies between (is smaller than) the times required to cover each layer separately. It is worth noting that in other cases, like RWME on BA+BA multiplexes, walks show *enhanced diffusion*, that is, the time to cover the multiplex is smaller than the time to cover each layer separately. This is shown, for instance, in Figure 1.9.

1.4 Centrality and versatility

In this section, we focus on the definition of node centrality in multilayer networks. We obtain these properties using algebraic operations involving the multilayer adjacency tensor, canonical vectors, and canonical tensors, achieving the natural extension of the

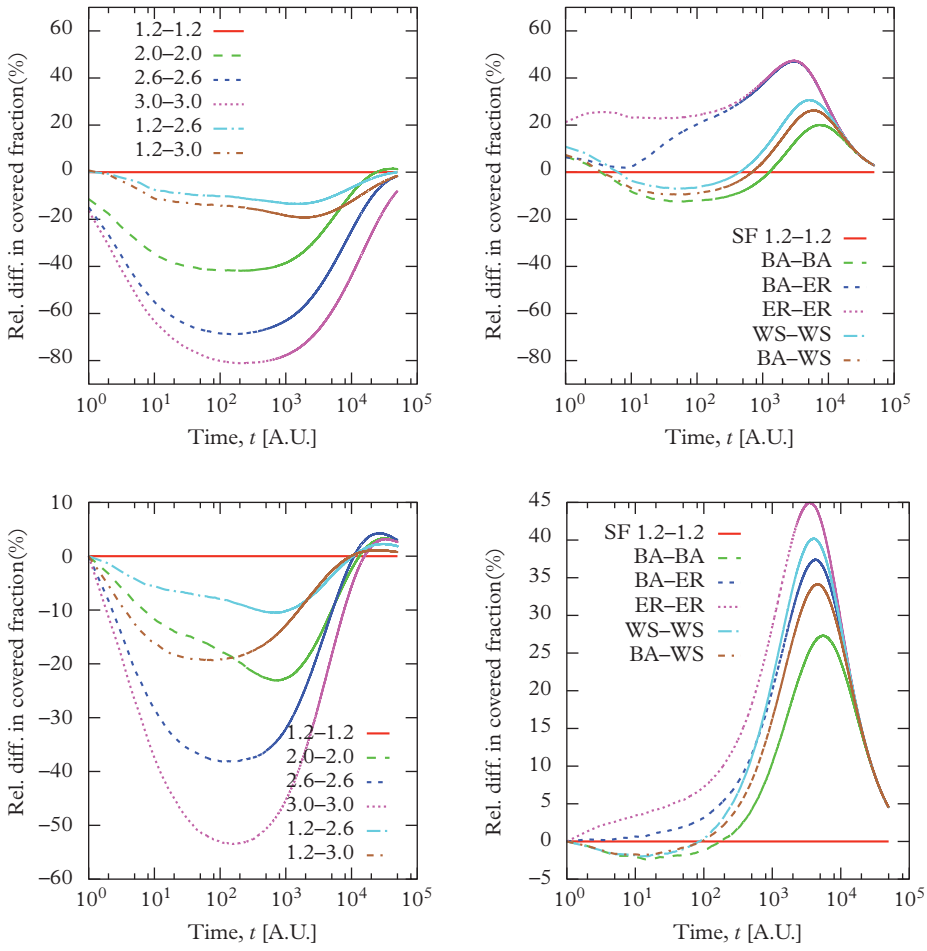

Figure 1.7 *Dependence of the coverage on multiplex topology: same as the inset of Figure 1.6, where the relative difference of each curve is calculated with respect to the coverage obtained for a multiplex of two different scale-free (SF) networks with exponent 1.2. Top panels refer to RWC, whereas bottom panels refer to RWP. Left panels (top and bottom) refer to multiplexes of different scale-free networks with other degree distributions, whose exponents are specified in the legend. Right panels (top and bottom) refer to multiplexes of other topologies.*

concept of centrality in single-layer networks. We refer the reader to Ref. [72] for other multilayer network diagnostics.

In practical applications, one is often interested in assigning a global measure of importance to each node, aggregating the information obtained from the different layers. A naive choice could be to combine the centrality of the nodes—obtained from the different layers separately—according to some heuristic choice. This is a viable

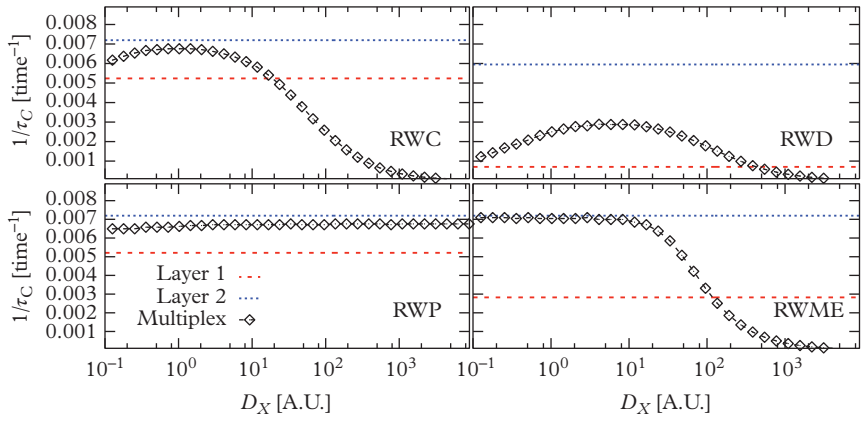

Figure 1.8 *Critical dependence of the coverage on navigation strategy and interlayer connection strength. Different random walks are used to calculate the inverse of the time τ_C required to cover 50% of a BA+ER multiplex with 200 vertices, as a function of $D_X = D^{12} = D^{21}$. The values for walks in each layer are shown for comparison and make clear how different exploration strategies have a strong effect on the coverage timescale.*

solution when there is no interconnection between layers, that is, in the case of edge-colored graphs [274, 125]. However, the main drawback of applying this approach to interconnected multilayer networks is that the measure will depend on the choice of the heuristics and might not evaluate the real importance of nodes. Conversely, our approach capitalizes on the tensorial formulation of interconnected multilayer networks and accounts for the higher level of complexity of such systems without relying on external assumptions and naturally extending the well-known centrality measures adopted for several decades in the case of monoplexes.

1.4.1 Eigenvector centrality

Among the numerous notions of centrality introduced to quantify the importance of nodes (and other components) in a network [307], eigenvector centrality is among the oldest ones [43, 42]. The eigenvector centrality of a node is defined to be proportional to the sum of the eigenvector centralities of its neighbors. The recursive nature of this notion yields a vector of centralities that satisfies an eigenvalue problem. In the case of monoplexes, the eigenvector centrality vector $\mathbf{v}$, whose components are the centralities of nodes according to [43, 42], is a solution of the eigenvector equation $W^i_j v_i = \lambda_1 v_j$, where λ_1 is the largest eigenvalue of W^i_j, and v_i indicates the eigenvector centrality of node i (note the use of the Einstein summation convention).

A naive approach for the calculation of the importance of each node in an interconnected network might be to project the interconnected topology to an aggregated monoplex and to associate to each node the centrality that node has in such an aggregated

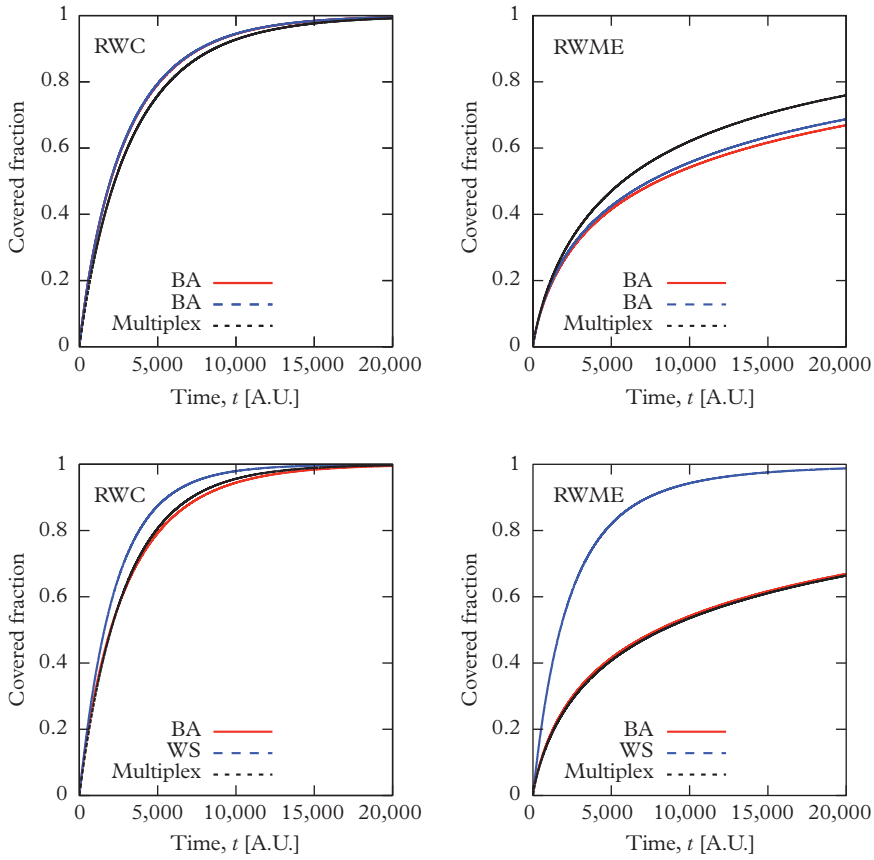

Figure 1.9 *Different types of diffusion characterize different topological structures and navigation strategies. Coverage versus time for two different multiplex topologies (BA+BA on the top panels, and BA+WS on the bottom panels) and two different walk rules (RWC on the left panels, and RWME on the right panels). While the diffusion on single layers separately and that on the multiplex are similar for RWC on BA+BA, this is not the case for RWME on BA+BA, where enhanced diffusion is shown in the multiplex. In the other cases, the diffusion is* infra-*diffusive.*

network. The main drawback of this approach is that it mixes the information from all layers, with uncontrollable effects, as shown in Ref. [74] for both synthetic and empirical networks. Another attempt to extend this calculation to the case of multilayer networks might be to calculate the eigenvector centralities for each layer separately, to build the tensor $\bar{V}_{i\alpha}$ encoding the centrality of each node in each layer. The final step would be to choose a heuristic aggregation of such centralities to assign a unique centrality measure to each node, regardless of the layer. However, the tensor $\bar{V}_{i\alpha}$ is not the solution of a unique eigenvalue problem but the combination of the solutions of L different eigenvalue problems treated separately; therefore, it is not a natural extension of the notion of eigenvector centrality to the realm of interconnected multilayer networks.

Instead, according to Ref. [72], this descriptor can be obtained as the solution of the tensorial equation

$$M^{i\alpha}_{j\beta}\Theta_{i\alpha} = \lambda_1 \Theta_{j\beta}, \tag{1.24}$$

where λ_1 is the largest eigenvalue, and $\Theta_{i\alpha}$ is the corresponding *eigentensor* encoding the centrality of each node in each layer when accounting for the whole interconnected structure. The eigentensor can be obtained by means of an iterative procedure, as the power method in the case of monoplexes. An analysis of this eigentensor problem is provided in Section 1.2.3. Thus, the multilayer generalization of Bonacich's eigenvector centrality [43, 42] is given by Eq. 1.24.

This centrality, like others in the rest of this section, assigns a measure of importance to each node in each layer, accounting for the full interconnected structure of the multilayer network. However, in practical applications, one is often interested in assigning a global measure of importance to each node, aggregating the information obtained from the different layers. The choice of the aggregation method is not trivial; it strongly influences the final estimation and might lead to wrong results. However, this is not case for the tensorial framework discussed so far. In fact, the centrality $\Theta_{i\alpha}$ is calculated by inherently accounting for the interconnected structure of the whole system. We do not need to arbitrarily combine the information from different separate measures. In our framework, the most intuitive type of aggregation, that is, summing up over layers, represents the unique and correct choice. Thus, the eigenvector centrality of each node becomes $\theta_i = \Theta_{i\alpha} u^{\alpha}$, where u^{α} is the tensor with all components equal to 1.

1.4.2 Katz centrality

It is a well-known fact that eigenvector centrality can lead to incorrect results in the case of directed networks. In fact, nodes with only outgoing edges have an eigenvector centrality of 0 if Bonacich's definition is adopted. Moreover, in this case, there are two leading eigenvectors, for incoming centrality and outgoing centrality, requiring distinguishing between covariant and contravariant calculations. The Katz centrality [144] solves the above problem by assigning a small amount b of centrality to each node before calculating centrality. For monoplexes, the Katz centrality is given by $v_j = aW^i_j v_i + bu_j$, where a must be smaller than the reciprocal of the largest eigenvalue λ_1 of W, and one often chooses $b = 1$.

Following a similar idea, we define the centrality tensor for each node in each layer as the solution of the tensorial equation

$$\Phi_{j\beta} = aM^{i\alpha}_{j\beta}\Phi_{i\alpha} + bu_{j\beta}, \tag{1.25}$$

corresponding to the natural extension of the equation proposed by Katz to the case of interconnected multilayer networks. The solution is given by $\Phi_{j\beta} = [(\delta - aM)^{-1}]^{i\alpha}_{j\beta} U_{i\alpha}$, where $\delta^{i\alpha}_{j\beta} = \delta^i_j \delta^{\alpha}_{\beta}$. As for the eigentensor centrality, this *Katz centrality tensor* accounts for

the whole interconnected topology and it is enough to contract it with the 1-vector to obtain the Katz centrality for each node, that is, $\phi_i = \Phi_{i\alpha} u^{\alpha}$.

1.4.3 Hubs and authorities centrality

In directed networks, such as Web sites, we can rank nodes differently according to their importance as senders or receptors of links, respectively. The Hyperlink-Induced Topic Search (HITS) approach, also known as the hubs and authorities' algorithm [150], assigns two different descriptors for each node, namely, hub and authority. In fact, Web pages that point to an important page generally also point to other important pages, building a structure similar to a bipartite topology where relevant pages—that is, authorities—are pointed by special Web pages—that is, hubs. It follows that nodes with high authority centrality are linked by nodes with high hub centrality, while very influent hubs point to nodes that are very authoritative. Such a mechanism is described by two coupled equations which reduce to the two eigenvalue problems $(WW^{\dagger})^{i}_{j} v_i = \lambda_1 v_j$ and $(W^{\dagger}W)^{i}_{j} z_i = \lambda_1 z_j$, where $W^{\dagger}$ denotes the transpose of the adjacency matrix, λ_1 indicates the leading eigenvalue, and v_i and z_i indicate hub and authority scores, respectively. The natural extension of the equations proposed by Kleinberg to the case of interconnected multilayer networks is given by

$$(MM^{\dagger})^{i\alpha}_{j\beta} \Gamma_{i\alpha} = \lambda_1 \Gamma_{j\beta}, \tag{1.26}$$

$$(M^{\dagger}M)^{i\alpha}_{j\beta} \Upsilon_{i\alpha} = \lambda_1 \Upsilon_{j\beta}, \tag{1.27}$$

where $\Gamma_{i\alpha}$ and $\Upsilon_{i\alpha}$ indicate hub and authority centrality, respectively. It is worth remarking that for undirected interconnected multiplexes, hub and authority scores are the same as and equal to the corresponding eigenvector centrality. The hub and authority tensors should be contracted with the 1-vector to obtain the scores corresponding to each node regardless of the layer, that is, $\gamma_i = \Gamma_{i\alpha} u^{\alpha}$, and $\upsilon_i = \Upsilon_{i\alpha} u^{\alpha}$, respectively.

1.4.4 Random walk centralities

Random walks can also be used to calculate the centrality of actors in complex networks, for example, when there is no knowledge of the full topology, and only local information is available. In such cases, centrality descriptors based on the shortest paths, for example, betweenness and closeness centrality, should be substituted by centrality notions based on random walks [214, 211].

As we have seen in Section 1.3, a random walk on a multilayer network induces nontrivial effects because the presence of interlayer connections affects its navigation of a networked system [73]. Let $\mathcal{P}^{i\alpha}_{j\beta}$ denote the tensor of transition probabilities for jumping between pairs of nodes and switching between pairs of layers, and let $p_{i\alpha}(t)$ be the time-dependent tensor that gives the probability of finding a walker at a particular node in a particular layer. Hence, the covariant master equation that governs the discrete-time

evolution of the probability from time t to time $t+1$ is given by Eq. 1.11, which reads $p_{j\beta}(t+1) = \mathcal{P}^{i\alpha}_{j\beta} p_{i\alpha}(t)$.

The steady-state solution of this equation is given by $\Pi_{i\alpha}$, quantifying the probability of finding a walker in the node i of layer α in the infinite-time limit. In the case of monoplexes, the steady-state solution can be obtained by solving the eigenvalue problem for the rank-2 transition tensor and calculating the leading eigenvector corresponding to the unitary eigenvalue. Similarly, in the case of multilayer networks, the solution can be obtained by calculating the leading *eigentensor*, solution of the higher-order eigenvalue problem

$$\mathcal{P}^{i\alpha}_{j\beta} \Pi_{i\alpha} = \lambda \Pi_{j\beta}. \tag{1.28}$$

We refer to Section 1.2.3 for the mathematical details to solve this problem. The probability $\Pi_{i\alpha}$, which we define as *random walk occupation centrality*, depends on the full interconnected structure of the multilayer network and, likewise, the previously described multilayer centralities. Finally, we may aggregate by layer to obtain the corresponding node centralities, $\pi_i = \Pi_{i\alpha} u^{\alpha}$.

Although different exploration strategies can be adopted to walk in a multilayer network [73], we first focus on the classical random walks (RWC) as previously described in Section 1.3.2. Let us indicate with $\Omega_{i\alpha}$ the strength of node i in layer α, including the interlayer connections, that is, $\Omega_{i\alpha} = s_{i\alpha} + S_{i\alpha}$, where $s_{i\alpha}$ and $S_{i\alpha}$ are the intralayer and interlayer strengths, respectively. The multi-strength vector, whose components indicate the strength of each node accounting for the full multilayer structure, is given by summing up its strengths across all layers, that is, by $\omega_i = \Omega_{i\alpha} u^{\alpha}$. We indicate with $D^{i\alpha}_{j\beta}$ the strength tensor whose entries are all zeros, except for the $i=j$ and $\alpha=\beta$ entries, which are given by $\Omega_{i\alpha}$. This tensor represents the multilayer extension of the well-known diagonal strength matrix in the case of monoplexes. Therefore, the transition tensor is given by $\mathcal{P}^{i\alpha}_{j\beta} = M^{k\gamma}_{j\beta} \tilde{D}^{i\alpha}_{k\gamma}$, where $\tilde{D}^{i\alpha}_{j\beta}$ is the tensor whose entries are the reciprocals[3] of the non-zero entries of the strength tensor. For this classical random walk, it can be easily shown that $\Pi_{i\alpha} \propto \Omega_{i\alpha}$ [73].

It is worth noting that, in this specific case, the computation of the centrality by means of the aggregated network would provide the same centralities for the interconnected multiplex, if interlayer edges were replaced by self-loops. In the more specific case that the interlayer edges have the same strength for all nodes, the random walk centrality will be just a linear function of the strengths in the aggregated network, without the necessity of accounting for the self-loops, thus recovering the traditional *degree centrality* [265, 101] for unweighted, undirected monoplex networks. However, this is no longer the case for the other centrality measures discussed in this section, where calculating the diagnostics from the aggregate might lead to wrong conclusions.

[3] It is worth remarking that, in general, this is different from the inverse of a tensor $A^{i\alpha}_{j\beta}$, which is defined as the tensor $B^{i\alpha}_{j\beta}$ such that $A^{i\alpha}_{k\gamma} B^{k\gamma}_{j\beta} = \delta^{i\alpha}_{j\beta}$, where $\delta^{i\alpha}_{j\beta} = \delta^{i}_{j} \delta^{\alpha}_{\beta}$.

For the other types of random walkers, namely diffusive (RWD), physical (RWP), and maximal entropy (RWME), see Section 1.3 and, in particular, Section 1.3.7, which provide the different occupation probabilities, leading to the respective alternative definitions of random walk occupation probability centralities.

Apart from centralities derived from random walk occupation probabilities, it is possible to define additional centralities based on other properties of the random walkers. The most relevant are *PageRank* [46], which will be described in Section 1.4.5, *random walk betweenness centrality* and *random walk closeness centrality* [211]. Random walk betweenness measures the net flow of random walkers through nodes, and random walk closeness is related to the mean first passage time needed to reach a node from the rest of locations in the network. See Ref. [276] for their extension to multilayer interconnected networks.

1.4.5 PageRank centrality

We capitalize on the previous analysis of random walkers to extend to interconnected networks a widely adopted measure of centrality, that is, the *PageRank centrality* [46]. A recent study in this direction has been reported in [125], in the case of edge-colored graphs, where the authors, exploiting the random walk interpretation of PageRank centrality, define the PageRank of a multiplex network by means of a random walk subject to teleportation. In that study, the PageRank for nodes in the first layer is computed using the standard definition for a monoplex [46], whereas the PageRank for nodes in the second layer is computed using the centrality information obtained from the first one. It is worth noting that this definition is limited to edge-colored graphs with only two layers, with any extension to a larger number of layers being possible but very complicated from the mathematical point of view.

Here, we exploit the fact that PageRank centrality can be seen as the steady-state solution of the equation $p_j(t+1) = R^i_j p_i(t)$ in the case of monoplexes, where R^i_j is the transition matrix of a random walk where the walker jumps to a neighbor with rate r and then teleports to any other node in the network with another rate, $1-r$. In the case of interconnected multilayer networks, the teleportation might occur to any other node in any layer. Depending on the application of interest, the walker can be teleported to other nodes with a rate that is specific to each layer. However, to keep the study as simple as possible, we consider the case with the same teleportation rate for all layers. Let $\mathcal{R}^{i\alpha}_{j\beta}$ be the corresponding transition tensor, where the walker jumps to a neighbor with rate r and teleports to any other node in the network with the rate $1-r$. This rank-4 tensor is given by

$$\mathcal{R}^{i\alpha}_{j\beta} = r\mathcal{P}^{i\alpha}_{j\beta} + \frac{1-r}{NL} u^{i\alpha}_{j\beta}, \tag{1.29}$$

where $u^{i\alpha}_{j\beta}$ is the rank-4 tensor with all components equal to 1. The steady-state solution of the master equation corresponding to this transition tensor provides the PageRank centrality for interconnected multiplex networks. This definition is valid for

all multiplexes where all nodes have outgoing edges. If this is not the case, as in several real-world networks, Eq. (1.29) reduces to $\mathcal{R}^{i\alpha}_{j\beta} = \frac{1}{NL} u^{i\alpha}_{j\beta}$ for all nodes i with no outgoing connections, ensuring the correct normalization of the transition tensor $\mathcal{R}^{i\alpha}_{j\beta}$. We set $r = 0.85$, as in the classical PageRank algorithm.

To compute the aggregate centrality of a node, accounting for the whole interconnected topology, we proceed as for the random walk occupation centrality previously discussed. Let $\Pi_{i\alpha}$ be the eigentensor of the transition tensor $\mathcal{R}^{i\alpha}_{j\beta}$ (see Section 1.2.3 for details), denoting the steady-state probability of finding the walker in node i and layer α. The multilayer PageRank is obtained by simply contracting the layer index of the eigentensor with the 1-vector: $\pi_i = \Pi_{i\alpha} u^{\alpha}$, that is, by summing up over layers.

1.4.6 Centrality measures based on shortest path

For the sake of completeness, we briefly consider here centrality measures based on shortest paths, namely, betweenness and closeness.

The extension of the *shortest-path betweenness centrality*, defined in the case of monoplex networks in Refs [12, 100, 45], is obtained by counting the number of shortest paths between any pair of *origin* and *destination* nodes (o, d) that go through node j in the interconnected structure [275, 73].

Equivalently to the case of a monoplex, we define a path $\ell_{[o\sigma \to d\gamma]} \in \mathcal{P}_{[o\sigma \to d\gamma]}$, in the interconnected multilayer network, as an ordered sequence of nodes which starts from node o in layer σ and finishes in node d in layer γ. We require that there exists an edge between all pairs of consecutive nodes in ℓ. Here, $\mathcal{P}_{[o\sigma \to d\gamma]}$ indicates the set of all possible paths between node o in layer σ and node d in layer γ. For every path $\ell_{[o\sigma \to d\gamma]}$, it is possible to define a cost function $c(\ell_{[o\sigma \to d\gamma]})$, usually depending on the weight of the edges the path traverses and on the application of interest, to account for the "goodness" of the path. Hence, the shortest path from node o in layer σ to node d in layer γ is the path

$$\ell^{*}_{[o\sigma \to d\gamma]} = \min_{\ell'_{[o\sigma \to d\gamma]} \in \mathcal{P}_{[o\sigma \to d\gamma]}} c(\ell'_{[o\sigma \to d\gamma]}), \tag{1.30}$$

which minimizes the cost function. Using Eq. (1.30), we define the shortest path from node o to node d, regardless of the layer, as

$$\ell^{*}_{[o \to d]} = \min_{\sigma,\gamma \in \{1,\ldots,L\}} \ell^{*}_{[o\sigma \to d\gamma]}. \tag{1.31}$$

The shortest-path betweenness centrality τ_j of node j is defined to be proportional to the number of times that node j, regardless of the layer, belongs to the set $\ell^{*}_{[o \to d]}$ for every possible origin–destination pair (o, d). We must remark that betweenness centrality is crucial for understanding congestion in networks [278].

On the other hand, in the same spirit of monoplex networks, we define the *shortest-path closeness centrality* (see [28, 249]) of a node j in an interconnected multilayer topology as the average of the inverse of the cost of the shortest paths that start from any other node o

in the network [73]. Thus, given the cost of a shortest path $c(\ell^*_{[o\to i]})$ between node i and node o, the shortest-path closeness centrality ξ_i can be easily computed by considering all possible origin nodes o.

Note that the shortest paths contributing to betweenness and closeness centralities may start and/or end in only a few of the available layers, and that they may contain interlayer edges. This means that, once again, it is impossible to derive the correct centralities by just considering the aggregated network or the individual layers of the multilayer network.

1.4.7 Centrality becomes versatility

The calculation of centrality in several empirical multilayer interconnected networks shows that the highly ranked nodes are not those with large importance in the aggregated network or in individual layers, but the nodes responsible for the cohesion of the whole structure, bridging together different types of relations [73]. Thus, they can be called *versatile nodes*, and we can safely say that centrality becomes a measure of *versatility* for this kind of networks.

Table 1.2 contains the 25 nodes with largest PageRank versatility of a Wikipedia multilayer interconnected network consisting of biologists, chemists, computer scientists, economists, inventors, mathematicians, philosophers, and physicists [73]. The multilayer network is the largest connected component, formed by 5,513 nodes and 8 layers. Weighted links are established according to the hyperlinks found in the corresponding Web pages and can be either intralayer or interlayer links (see [73] for all the details).

The top-rated scientist is Edmund F. Robertson, due to his being one of the creators of the MacTutor History of Mathematics Archive, a Web site containing biographies of many mathematicians, whose corresponding pages point to this Web site and the Wikipedia page of Edmund F. Robertson. Thus, this node could be considered spurious, one which should have been removed from the network during the preprocessing of the data. Anyway, this is not important for assessing the meaning of versatility. For example, Milton Friedman made contributions to economics, statistics, international finance, risk/insurance, and microeconomic theory: Hilary Putnam is a computer scientist and mathematician with outstanding contributions in the philosophy of mind, of mathematics and of science; E. O. Wilson is the father of sociobiology; Harold Clayton Urey won the Nobel Prize in Chemistry and is well known for theories on the development of organic life from nonliving matter and for playing a significant role in the development of the atomic bomb; and Kurt Gödel is one of the greatest logicians of all time, with impacts on several different disciplines, from pure mathematics to physics and philosophy. Out of this distinguished group, Wilson and Clayton are ranked among the highest (with scores ranging from 300 to almost 1,000) in the aggregated network, and with respect to the average centrality of the separated layers. In contrast, despite being still highly rated, Albert Einstein and Plato are not as highly ranked when the full structure of the network is considered.

In summary, we have seen how taking into account the full structure of multilayer interconnected networks has important consequences for their structural properties and

Table 1.2 *Top ranked nodes of Wikipedia dataset by PageRank versatility. For comparison purposes, the table also shows the corresponding ranks according to the PageRank in the aggregated network, and the ranks after averaging the PageRank at every single layer as independent networks. In parentheses, the variation of rank with respect to versatility is shown. Global diversity stands for the number of layers sending or receiving links to the considered node.*

		PageRank Centrality Ranking				Diversity
Name	**Versatility**	**Aggregate**		**Average**		**Global**
Edmund F. Robertson	1	1	(+0)	18	(+17)	2
Milton Friedman	2	16	(+14)	22	(+20)	8
Hilary Putnam	3	34	(+31)	1,302	(+1,299)	4
E. O. Wilson	4	332	(+328)	996	(+992)	8
Harold Clayton Urey	5	537	(+532)	451	(+446)	8
Kurt Gödel	6	43	(+37)	325	(+319)	8
Avicenna	7	30	(+23)	8	(+1)	4
Ernst Mayr	8	191	(+183)	582	(+574)	8
Herbert A. Simon	9	48	(+39)	14	(+5)	8
Charles Stark Draper	10	1,196	(+1,186)	1,169	(+1,159)	8
Ivan Pavlov	11	423	(+412)	56	(+45)	6
Aristotle	12	3	(−9)	2	(−10)	5
Paul Samuelson	13	26	(+13)	43	(+30)	8
Immanuel Kant	14	2	(−12)	19	(+5)	2
Norbert Wiener	15	68	(+53)	407	(+392)	8
Chien-Shiung Wu	16	100	(+84)	599	(+583)	6
George Dantzig	17	217	(+200)	1,244	(+1,227)	8
Ronald Ross	18	1,602	(+1,584)	5,472	(+5,454)	5
John C. Slater	19	1,242	(+1,223)	1,627	(+1,608)	8
Porphyry (philosopher)	20	311	(+291)	1,063	(+1,043)	3
Peter Mansfield	21	1,502	(+1,481)	2,914	(+2,893)	5
Rosalyn Yalow	22	888	(+866)	1,580	(+1,558)	7
Samuel Goudsmit	23	1,364	(+1,341)	1,960	(+1,937)	8
Albert Einstein	24	10	(−14)	11	(−13)	4
Plato	25	4	(−21)	15	(−10)	2

the dynamics from them, and these have boosted the interest in this kind of system and yielded an enormous amount of scientific literature.

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