Diffusion Geometry of Multiplex and Interdependent Systems

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Complex networks are characterized by latent geometries induced by their topology or by the dynamics on the top of them. In the latter case, different network-driven processes induce distinct geometric features that can be captured by adequate metrics. Random walks, a proxy for a broad spectrum of processes, from simple contagion to metastable synchronization and consensus, have been recently used in [Phys. Rev. Lett. 118, 168301 (2017)] to define the class of diffusion geometry and pinpoint the functional mesoscale organization of complex networks from a genuine geometric perspective. Here, we firstly extend this class to families of distinct random walk dynamics – including local and non-local information – on the top of multilayer networks – a paradigm for biological, neural, social, transportation, biological and financial systems – overcoming limitations such as the presence of isolated nodes and disconnected components, typical of real-world networks. Secondly, we characterize the multilayer diffusion geometry of synthetic and empirical systems, highlighting the role played by different random search dynamics in shaping the geometric features of the corresponding diffusion manifolds.

I. INTRODUCTION

Complex networks, an abstract representation of the structural and functional backbone of complex systems, exhibit a wide spectrum of geometric features, from self-similarity to latent hidden metric spaces and topology [1–4], which have been successfully exploited to gain new insights about the structural and dynamics of social [5], neural [6], transportation [7, 8] and communication systems [9], to mention a few emblematic examples (see Ref. [10] for a review). More recently, it has been shown that even the dynamics on the top of complex networks can induce complex geometries which can not be understood from inspecting only structural ones. Such geometries have been studied in the case of a broad class of spreading phenomena: communicability distance has been introduced to study information exchange based on walks [11]; an effective distance has been introduced for contagion processes [12]; a diffusion distance has been introduced to study collective phenomena such as synchronization, consensus and random searches [13]; a temporal distance has been defined to study how perturbation spread in biological systems [14]. The common rationale is to model the propagation of information with network dynamics and investigate the corresponding distances induced between pairs of nodes.

Random walks are emblematic examples used for modeling diffusion and transport dynamics from lattices to disordered media and quantum systems, across more than a century [15–21]. They provide both an intuitive – and often analytically treatable – mathematical framework and a rich physical model that can be used to map a wide spectrum of random processes and observed features, especially in the contest of complex networks where the interplay between the underlying topology and the dynamics on the top of it is responsible for system’s function [22]. The properties of the random walks reflect particular structural features of a system: for instance, they can be used to unravel the mesoscale organization of systems from a functional perspective [23–27]: localization effects can be observed around topological defects [28]; the average number of different sites visited in a time interval by a random walker, the so-called coverage, can be used to quantify the system resilience to random failures [29]; the relative importance of system’s units can be quantified in terms of their ability to attract the overall flow, encoded by random walkers [30]; the dynamical features of the information flowing through a network can be understood [31], and even enhanced [32], in terms of the spectral entropy defined by statistical features of random walks.

Based on these dynamics, one can also define similarity measures that reflect the ability of the units to exchange information [33–35]. In [33] diffusion distance was defined for single-layer networks and it has proven to be useful for characterizing the functional structure of complex networks, e.g. identifying functional clusters, or central nodes [36]. It also provides a continuous-valued distance function which, in applications where the global information about the underlying topology is missing or partial, is more informative than the purely topological length of shortest-paths.

However, in many real systems entities interact in multiple ways, think, for example, to locations connected through different transportation modes or to metabolites in a biological network linked by various types of chemical reactions. The evolution of the traditional graph-theoretical tools allows us, nowadays, to represent this

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multifaceted information by means of layers defining multilayer networks [37, 38]. Figure 1 shows distinct representations of the multiplexity and the interdependency observed in empirical complex networks. From a mathematical perspective, taking into consideration the variety of connectivity patterns and coupling among layers and dynamics [39] requires multilinear algebra and tensors [37] to be efficiently represented and treated analytically.

![Multi-layer networks](image)

**FIG. 1.** Different multilayer networks and their supra-adjacency matrix representation [37, 40]: (a) an edge-colored multigraph, with layers corresponding to colors and no inter-layer connections; (b) a multiplex network where the replicas in the different layers are interconnected sequentially, a type of intertwining or diagonal coupling, and (c) the most general interconnected case, where inter-layer connections are not restricted to replicas (exogenous interactions). Latin letters denote nodes, while Greek letters are used for layers. 

In this study our contribution is twofold: on the one hand, we generalize multilayer random walk dynamics for the analysis of more realistic empirical systems, e.g. allowing for the existence of isolated nodes and components; on the other hand, we extend the framework of diffusion geometry [13] to realm of multilayer systems, highlighting the dependence of the diffusion manifold on the interplay between structure and dynamics within and across layers.

The paper is organized as follows: in the next section we recall the basic facts on random walks and diffusion processes on single layer networks and then generalize them to the multilayer framework. In Sec. III we extend the definition of diffusion distance to multilayer networks, presenting results obtained from the analysis of synthetic models. We conclude with applications to empirical social and transportation systems in Sec. IV, followed by Discussion and Conclusions.

II. DIFFUSION DYNAMICS IN COMPLEX NETWORKS

In a group of individuals a piece of news spreads differently if everyone knows each other or if there are subgroups of individuals that do not communicate with the others: the structure of this social network influences the diffusion of information. Similarly, one observes a strong influence of the topology on the dynamics of a broad class of empirical systems. Because of this influence of the structure on the evolution of dynamical processes, the latter are often used as a proxy for probing and uncovering structural properties of complex networks. A simple strategy to explore a network is to start from a node, to choose at random an (outgoing) edge and to follow it toward the next node, i.e., to perform a random walk on the network with transition probabilities prescribed by the network connectivity. Random walks (RWs) represent a useful model for diffusion processes. Here we will focus on node-centric continuous-time random walks (CTRWs) [22], continuous-time Markov chains (MC) on the vertex set of a network with transition rates depending on the network structure and specific navigation rules.

A. Random walks and diffusion distance on single-layer networks

Let us consider a weighted directed network \( G = (V, E) \) without isolated nodes and with (possibly weighted) adjacency matrix \( W = \{W_{ij}\} \), and two nodes \( i, j \in V \). In a discrete random walk the transition probability from \( i \) to \( j \) in one time step is given by \( p_{ij} = \frac{W_{ij}}{\sum_j W_{ij}} \). We can write it in matrix form \( p(n+1) = p(n)D^{-1}W \), where \( p \) is seen as a row vector and \( D \) is the diagonal matrix of out-strengths \( D_{ii} = s_i = \sum_j W_{ij} \). The continuous-time random walk corresponding to this jump chain (also-called its embedded Markov chain) is described by the forward equation

\[
\begin{align*}
\dot{p}(t) &= -p(t)\tilde{L} \\
p(0) &= p_0
\end{align*}
\]

where \( \tilde{L} = I - D^{-1}W \) is the random walk normalized Laplacian and \( -\tilde{L} \) is the generator of the continuous-time Markov chain with initial distribution \( p_0 \); see Appx. A for further details. The transition probabilities are given by the solution of (1), i.e., \( p_{ij}(t) = (p_0e^{-tL})_{ij} \). Rewriting (1) as a system with \( P(t) \) being a matrix and with the initial distribution given by the identity matrix, \( P(0) = I \), we obtain the unique solution \( P(t) = e^{-tL} \). Its \( i \)-th row \( (e^{-tL})_i \) is the probability vector corresponding to \( p_0 = e_i \) and \( (e^{-tL})_{ij} \) is the probability of being in \( j \) starting in \( i \) with probability 1, after time \( t \).
diffusion distance \[13\] is the \(L^2\)-norm of the difference between rows of the matrix \(e^{-tL}\).

\[
D_k(i, j) = \|p(t|i) - p(t|j)\|_2 .
\] (2)

Two nodes \(i \neq j\) are “near” w.r.t. \(D_k\) if the probability that two random walkers starting in \(i\) and \(j\) respectively, meet somewhere in the network after time \(t\).

Upon a given network, which is completely characterized by its adjacency matrix \(W\), we can define random walks with different flavors. This enables us, not only to model a wider range of physical spreading processes, but also to remove the rather restrictive assumption of connectedness, which is necessary for writing the transition matrix \(D^{-1}W\) of the classical random walk. Consequently, also the family of diffusion distances can be generalized to different types of random walks, as well as to different types of networked systems. In the remainder of this section, we extend the diffusion distance to multilayer networks, additionally exploring the varying patterns induced by different random walks dynamics \[27\] \[29\]. Of course, there are many other types of random walks that are not mentioned here, e.g., multiplicative processes \[41\] or correlated random walks \[42\], and are often defined with a specific motivation. Nevertheless, our framework is very general and, given a transition matrix \(T\), can be effortlessly extend considering the continuous-time Markov chain having exponential holding times with rate one and \(T\) as jumping matrix, see Appx. \[A\].

Before moving to the multilayer case, let us introduce the tensorial notation \[37\] for the monoplex \(G\), which allows us to generalize the formalism to multilayer networks. The adjacency matrix \(W\) can be seen as a rank-2 tensor \(W_{ij}\). In this paper, we will not use the covariant notation and the Einstein summation convention, so that \(W_{ij}\) denotes the component \((i, j)\) of the tensor. The master equation \[1\] can be re-written as

\[
\begin{align*}
\dot{p}_j(t) &= -\sum_{i=1}^{N} \tilde{L}_j^i p_i(t) \\
p_i(0) &= q_i
\end{align*}
\] (3)

with \(\tilde{L}_j^i = \delta_j^i - T_j^i\) indicating the component \((i, j)\) of the random walk normalized Laplacian tensor, \(\delta_j^i\) the Kronecker delta and \(T_j^i\) the component \((i, j)\) of the transition probability tensor.
B. Random Walks on edge-colored multigraphs

A multilayer network is defined by a set of $N$ nodes $V$ interacting with each other in multiple ways, simultaneously. The different types of interaction can be encoded by colors and grouped into layers. Each node $i \in V$ exists at least in one layer and, if it exists in multiple layers $\alpha \in \{1, \ldots, L\}$, we usually refer to $\{i, \alpha\}$ as a replica or state node, in contraposition to the physical node $i$. Interactions of the same color determine the intra-layer connectivity, while the others are called inter-layer connections. The simplest multilayer structure, depicted in Fig. 1(a), is the edge-colored multigraph, where there is no additional information (e.g., no order relation) on the set of layers $\{1, \ldots, L\}$ or, equivalently, inter-layer connectivity is not present.

There are, essentially, two ways to define random walks on these networks. One possibility is to allow the random walker to follow a sequence of edges with different colors: colored edges are then treated as multiple edges and the degrees of a node counts all the edges, regardless of their colors [44]. This choice is equivalent to aggregate the multilayer system to a single layer and perform a classical random walk on it. This approach is not desirable in general, because one does not know a priori if, and to which extent, information lost while aggregating the structure of layers will affect the results.

The second approach, used successfully in other applications [32], is to run independent dynamics on each layer (color) and then integrate the transition matrices over the layers, properly normalizing each transition probability as follows:

$$
\langle T^i_j \rangle = \sum_{\alpha=1}^L \frac{1}{\mu_i \cdot L} T^i_{j\alpha}.
$$

Indicating by $s_i(\alpha)$ the out-strength of vertex $i$ in layer $\alpha$, $\sum_{\alpha=1}^L \frac{1}{\mu_i L} \cdot 1_{s_i(\alpha) \neq 0}$ represents the multiplicity of node $i$, i.e., the fraction of layers in which $i$ is not isolated (a trapping node). This approach is more desirable than the first one, since it preserves more information related to diversity of connectivity patterns across layers. Nevertheless, the choice of adding transition matrices as in Eq. (4) can be replaced by a more general linear combination weighted by the relative importance given to each layer.

The main difference between the two approaches emerges when the edges are weighted, besides colored: a priori the scale (nominal, ordinal, ratio etc.) of the weights could be different and an inattentive summation could lead to errors. In [41], instead, for each $i \in V$, we are taking a finite mixture of probability mass functions with uniform weights $\frac{1}{\mu_i L} \geq 0$ such that $\sum_{\alpha=1}^L \frac{1}{\mu_i L} = 1$; nothing prevents one to weight layers differently, if additional information is available. In the following, we consider equal importance for all layers, thus avoiding the dependence of our results on the choice of a specific set of weights to be assigned to layers.

We now take advantage of the more involved notation of Sec. IIIA to introduce multilayer interconnected networks.

C. Random walks on multilayer networks

In the same way a monoplex can be represented by a rank-2 tensor, a multilayer network is completely characterized by its rank-4 adjacency tensor [37]. Let us indicate by $M^i_{j\alpha}$ the components of the (weighted) multilayer adjacency tensor. In this index notation $M^i_{j\alpha}$ indicates the interaction between $i$ and $j$ in the same layer, while $M^i_{j\alpha \beta}$ denotes the strength of the intertwining of the replicas of $i$ in two distinct layers. Depending on the inter-layer connectivity we can have different types of multilayers, as shown in Fig. 1. When inter-layer connections occur only between replicas of the same physical node, i.e., $M^i_{j\alpha \beta} = 0$ for $i \neq j$, the network is called a multiplex. The term $M^i_{j\alpha \beta}$ encodes the intertwining between two replicas: it is a scalar depending, in general, on $i, \alpha, \beta$ and we indicate it by $D(i; \alpha, \beta)$. For the ease of visualization we flatten the adjacency tensor into the so-called supra-adjacency matrix [37] [40], of dimension

| TABLE I. Transition probabilities for different random walks. (CRW) classical, (PRRW) PageRank, (DRW) diffusive, (MERW) maximal-entropy, and (PrRW) physical with relaxation random walks. $s_{\text{max}}$ denotes the largest eigenvalue of the adjacency tensor and $V$ is its corresponding eigentensor, satisfying $\sum_{i,\alpha} M^i_{j\alpha} V_{\alpha} = \lambda_{\text{max}} V_j$ (see [37] for details). Note that for CRW, DRW and MERW, these transition rules generalize the one introduced in [29] for the analysis of multiplex networks. The PrRW is defined as in [27], while PRRW generalizes the walk introduced in [39]. |
| CRW | PRRW | DRW | MERW | PrRW |
| $T^i_{j\beta}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ |
| $T^i_{j\beta}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ |
| $T^i_{j\beta}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ | $\frac{M^i_{j\beta}}{s_{\text{max}}}$ |
| $T^i_{j\alpha}$ | $\frac{M^i_{j\alpha}}{s_{\text{max}}}$ | $\frac{M^i_{j\alpha}}{s_{\text{max}}}$ | $\frac{M^i_{j\alpha}}{s_{\text{max}}}$ | $\frac{M^i_{j\alpha}}{s_{\text{max}}}$ |
Its diagonal blocks are the adjacency matrices of the monoplexes, while its off-diagonal blocks contain the information on the inter-layer connectivity.

We henceforth indicate by $s_i(\alpha) = \sum_{j=1}^{N} M_{j\alpha}^{i\alpha}$ the out-strength of node $i$ in layer $\alpha$ and by $s_i = \sum_{\alpha} s_i(\alpha) = \sum_{\alpha=1}^{L} \sum_{i=1}^{N} M_{j\alpha}^{i\alpha}$ its multi-layer out-strength, discarding the inter-layer edges. The inter-layer strengths are obtained as $S_i(\alpha) = \sum_{j}^{\alpha \neq \beta} M_{j\alpha}^{i\beta}$ and, consequently, $(s_i(\alpha) + S_i(\alpha))_{i=1,\alpha=1}^{N,L}$ is the out-strength supra-vector with $NL$ components obtained as the row sums of the supra-adjacency matrix.

Generally, the presence of isolated nodes or components, as well as an heterogeneous or mixed distribution of inter-layer connectivity is discarded to facilitate the analytical framework. Conversely, here we do not force any assumption on the structure of the multilayer system: if some units are not present in all layer – which is often the case for real data – we will add artificial replicas, which will appear as isolates and we will account for them adequately. We henceforth indicate by $V$ the common vertex set and by $N = |V|$ the number of physical nodes. Although the isolated nodes do not modify the connectivity of the connected component a layer, they could be troublesome for the evaluation of transition probabilities. We have to distinguish three cases (i) $S_i(\alpha) = 0$, (ii) $s_i(\alpha) = 0$, and (iii) $s_i = 0$. The latter corresponds to the trivial case, where node $i$ is isolated in every layer, so that $i$ can be simply removed from the vertex set. We can assume, without loss of generality, $s_j > 0$ for all $i \in V$. (i) and (ii) – corresponding to no inter-layer and no intra-layer connections, respectively – constitute a problem only if $S_i(\alpha) + s_i(\alpha) = 0$ for some $\alpha$. In this case one could see $\{i, \alpha\}$ as an absorbing state with the probability of remaining there equal to 1; another option is to teleport the random walker in $\{i, \alpha\}$ to any $\{j, \beta\}$ with uniform probability $\frac{1}{N_L}$. As for other approaches [23, 27, 30], we opted for the second option, since it decreases the occupation probability of the state node $\{i, \alpha\}$.

In the multilayer framework the probability transitions in one time step constitute the components $T_{j\beta}^{i\alpha}$ of a rank-4 tensor and we can expand the RW equation to highlight different contributions of jumps and switches in the dynamic

$$
p_{j\beta}(t+1) = T_{j\beta}^{i\alpha} p_{j\beta}(t) + \sum_{\alpha \neq \beta}^{L} \sum_{i=1}^{N} T_{j\beta}^{i\alpha} p_{j\alpha}(t) + \sum_{\alpha \neq \beta}^{L} \sum_{i=1}^{N} T_{j\beta}^{i\alpha} p_{i\alpha}(t) + \sum_{i=1}^{N} \sum_{\alpha \neq \beta}^{L} T_{j\beta}^{i\alpha} p_{i\alpha}(t)
$$

The continuous-time version is described by the forward equation

$$\dot{p}_{j\beta}(t) = -\sum_{i,\alpha} L_{j\beta}^{i\alpha} p_{i\alpha}(t)$$

where $L_{j\beta}^{i\alpha} = \delta_{j\beta}^{i\alpha} - T_{j\beta}^{i\alpha}$.

Upon a given network structure we can define different types of random walks, depending on the specific rules we want our random walker to explore the network. For
instance, in PageRank [30] a teleportation or jumping parameter gives the possibility to the walker to reach also nodes that are not directly connected to the current node. The flavors of the random walks are given by their transition rules, which depend on the structure of the network, as a function of the adjacency tensor. The RW presented in the monoplex case is referred to as a classical random walk (CRW). Additionally to the classical random walk, we look here at a family of diffusion distances based on four other random walk types: multilayer PageRank (PRRW) generalizing Refs. [30, 43], multilayer diffusive (DRW) generalizing the one defined in Ref. [29], maximal-entropy (MERW) generalizing Refs. [28, 29], and physical random walk with relaxation (PrRW) [27], whose transition probabilities are shown in Tab. I.

The physical random walk has been defined in [29] to describe those dynamics where the state nodes have a “common memory”, so that the information diffuses instantaneously across replicas. Think, for instance, of the system of virtual interactions among individuals, who may have a profile (an alter-ego) in different social networks. A person can then exchange information in a particular social network using the (intra-layer) connections of its alter-ego in that social system, but she/he has always a complete knowledge of the information across the layers. In this case, inter-layer connections between replicas of different physical nodes have no physical meaning and, consequently, are ignored. The physical random walk with relaxation (PrRW) [27] is a variant on the physical random walk, where the assumption on the complete knowledge of intertwining between layers is dropped. It can be seen from Tab. I that its transition probabilities contain a trade-off between intra- and inter-links, which are followed with probability $1 - r$ and $r$ respectively. If not differently stated, we consider here $r = 0.5$.

In the following section we will define a multilayer distance which reflects how nodes exchange information in and between the layers.

III. DIFFUSION DISTANCE IN MULTILAYER SYSTEMS

In the multilayer framework the probability of finding a random walker at a given node and layer is encoded in a time dependent tensor, whose component $p_{ij\beta}(t)$, corresponds to the probability of finding the random walker in the state $\{j, \beta\}$, for a given initial distribution. Similarly to Eq. (3), we can then define the diffusion distance between state nodes $\{i, \alpha\}$ and $\{j, \beta\}$ as

![FIG. 4. Comparing different types of distances among physical nodes, regardless of layers. (a) The weighted adjacency matrix of the aggregated network. The diffusion distance (w.r.t. the CRW and averaged over time) (b) of the aggregated network corresponding to the synthetic multiplex of Fig. 2(a) and (c) of the edge-colored network. (d) The equivalent diffusion distances obtained with the reduction of Eq. (7). The distances are rescaled to $[0, 1]$, normalizing by the corresponding maximum (aggregated: max($\bar{D}_t$) $\approx$ 0.13, edge-colored: max($\bar{D}_t$) $\approx$ 0.16, equivalent distances: max($\bar{D}_t$) $\approx$ 0.11).](image)
The diffusion distance is bounded in $[0, 2]$ for all $i \in V$, $\alpha \in 1, \ldots, L$, and $t > 0$, indeed, $\sum_{k, \gamma} (p_{k, \gamma}(t \{i, \alpha\}) - p_{k, \gamma}(t \{j, \beta\}))^2 \leq \sum_{k, \gamma} p_{k, \gamma}(t \{i, \alpha\}) = 1$, and it is small if there is a large probability that the random walks starting in $\{i, \alpha\}$ and $\{j, \beta\}$ meet somewhere in the multiplex by time $t$. Furthermore, as the diffusion time $t$ increases, and assuming walk is ergodic, $p_{k, \gamma}(t)$ will tend to the stationary distribution $\pi_{k, \gamma}$ and $D_t(\{i, \alpha\}, \{i, \beta\}) \to 0$.

Figure 2 shows the supra-distance matrix $D_t$ for the three more diverse RW dynamics on a synthetic multilayer network. In each layer, we have a network with $N = 30$ nodes generated from a stochastic block model with two blocks. We chose the probabilities in order to have a diverse topology: dense groups, disconnected components and isolated nodes. The coupling between the layers is $D(i; 1, 2) = D(i; 2, 1) = 1$, as shown in the supra-adjacency matrix of Fig. 2(b). The columns of panel (c) represent different diffusion times $t$. Recall that the diffusion time plays the role of a scale parameter \(13\) and that the continuous-time Markov chain has exponentially distributed holding times with rate $\lambda = 1$, i.e., the expected time occurring among each step of the RW is $1$.

$D_t(i, j) = \left( \sum_{\alpha=1}^L \frac{1}{D_t(\{i, \alpha\}, \{j, \alpha\})} \right)^{-1}$. \(7\)

Note that this is an effective distance obtained from diffusion distances across layers, and it is not related to the concept of resistance distance \(15\).

The resulting equivalent distance matrix is quite different from the one obtained evaluating the diffusion distance on the aggregated network, as shown in Fig. 4. Here the distance matrices have been rescaled in $[0, 1]$ by division through their respective maximum values, reported in the figure caption. Looking back at Fig. 2(a), we can see that the nodes from 1 to 19 are densely connected in layer 1, while node 8 and nodes from 11 to 30 form the largest connected component of the second layer. In both distance matrices there is a clear block corresponding to the last ten nodes. However, only the equivalent diffusion distance matrix captures the particular position of the first ten nodes (removing 8): in the multiplex they are distant from the last ten, because they belong to different communities in layer 1 and to disconnected components in layer 2. We also compare the aggregated network distance matrix Fig. 4(b) to the one of the edge-colored multigraph obtained removing the inter-layer links from the multilayer network, shown in Fig. 4(c). The two matrices are very similar, with only minor permutations inside the clusters.

### A. Multilayer Diffusion Manifolds

The use of different random walk dynamics to explore a system has an impact on the distances between its units and, consequently, on how the units are distributed in the induced diffusion spaces. Similarly, the diffusion time shapes the pairwise distances, highlighting local features of complex network geometry on short time scales and its more persistent structures for large diffusion times. In the multilayer setting there is an additional level of complexity given by the inter-layer connections and by the layer-layer correlations. To gain further insights, we generate 3 distinct classes of synthetic multilayer networks, with system size $N = 200$, and analyze them through the lens of diffusion geometry.

The first class consists of Barabasi-Albert scale-free networks \(10\) on each layer: we consider a linear preferential attachment with 4 edges added by each new node during the growth process, while setting at at $10\%$ the edge overlapping across layers – defined in terms of the fraction of links which are present in both layers among the same pairs of nodes \(17\).

The second class consists of Watts-Strogatz small-world network \(18\) on each layer, obtained by rewiring lattices with probability $0.2$, where edge overlapping is tuned similarly to the first class.
FIG. 5. Average diffusion distance $\bar{D}_t$ on two-layers multiplexes with different topologies, for fixed values of global average edge overlap (Barabasi-Albert and Watts-Strogatz) and partition overlap (Girvan-Newman) between layers. Dendrograms on the right-hand side of each distance matrix represents the corresponding hierarchical clustering to highlight the meso-scale organization of the system, with color encoding the planted node assignment in each layer. Distance matrices have been rescaled $\frac{\bar{D}_t}{\bar{D}_{t_{\text{max}}}}$. The Barabasi–Albert model is characterized by the presence of hubs, which are clearly recognizable in the supra-distance matrix w.r.t. the diffusive random walk, despite the small overlap between layers. The Girvan-Newman two-layers multiplex has a meso-scale organized in strong communities, partly overlapping across layers. Note that at variance with edge overlapping, here partition overlapping is defined in terms of nodes belonging to the same group without requiring those nodes to be connected by an overlapping edge.

The third class consists of layers with strong meso-scale structure organized in 4 groups, like in a Girvan-Newman model [49] on each layer: the probability that two nodes within the same group are connected is 1, whereas cross-group connections are much sparser and present with probability 0.05. Group overlapping [47] – defined in terms of the fraction of nodes planted in the same group on both layers – is again fixed at 10%.

The role of layer-layer correlations and their interplay with the distinct network topologies considered above is summarized in Fig. 5. As expected, there are relevant differences due to the type of random search dynamics and to the topological features of the underlying topologies. For instance, the diffusive walk for the Barabasi-Albert system leads to a high level of mixed pathways across layers, resulting in nodes that do not preserve in the diffusion space their original layer assignment. For the same walk, in the case of the Watts-Strogatz system the result is the opposite: nodes aggregate into functional clusters that are not well mixed up in the diffusion space. A high amount of geometric mixing is also observed when the physical random walk with relaxation is used, as expected. Overall, it is not guaranteed that multilayer diffusion pathways layers favor the geometric mixing in the diffusion manifold: the result depends on the type of dynamics and on layer-layer correlations.

To gain additional insights, we have considered a second battery of synthetic models, where we increasingly add inter-layer connectivity between layers. The absence of information pathways across layers, happening for instance when two layers are not coupled together, leads naturally to disjoint diffusion manifolds, each one corresponding to the distinct layers. When the two layers are interconnected, a trivial result is that the strength of inter-layer connectivity facilitate the flow of information across layers. However, the above process hides an interesting phenomenon, that is unveiled in Fig. 6. To better characterize it, we calculate the Frobenius norm, which is defined as follows, for a generic matrix $A$

$$
\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |A_{ij}|^2} = \sqrt{\text{trace}(A^T A)}
$$

to quantify the overall intensity of an average diffusion distance matrix. The Frobenius norm is computed when the two layers are not coupled, on the union of the two distance matrices, i.e., $\sqrt{\|A\|_F^2 + \|B\|_F^2}$, and then on the supra-distance matrices for increasing fraction of inter-layer connectivity: first state nodes corresponding to the same physical node are interconnected with each other to create an interconnected multiplex; after that this
FIG. 6. Frobenius norm of the supra-distance matrices of a synthetic two-layers network, w.r.t. a diffusive random walk. As the fraction of inter-layer links grows we move from two disconnected multiplexes to a fully inter-connected multi-layer whit all $N^2$ connections across layers. The heatmaps are four representatives of the different regimes: (a) uncoupled layers; (b) a single-inter-link between the replicas of a random nodes coupling the two layers, i.e., $[1/N, 1]$ partially interconnected multiplex; $[1/N]$ fully interconnected multiplex (all state nodes corresponding to the same physical node are interconnected); (c) $[\frac{1}{N^2}, 1]$ multilayer regime consisting of an interconnected multiplex with the addition of cross-links between state nodes of distinct physical nodes.

regime is reached, the cross-links between state nodes corresponding to all other physical nodes are created, until the total of $N^2$ connections is generated. Remarkably, when one interlink is added between the layers, the Frobenius norm increases: this is due to the fact that the new link coupling the two layers creates a bottleneck for information to be exchanged across layers, even for large values of $\tau$. Once more inter-links are added, the Frobenius norm decreases, until it tends to reach a plateau when the fraction of inter-layer links is 100%.

Our results highlight that the existence of topological correlations across layers induce changes in how information is exchanged between state nodes. Such changes alter diffusion distances and might lead to two different regimes: i) flow keeps segregated within layers and the multilayer diffusion manifold consists of two well separated sub-manifolds representing each layer separately, which are connected by weak geometric pathways; ii) flow is integrated, creating new geometric pathways for information that mix up those sub-manifolds.

IV. APPLICATIONS TO EMPIRICAL MULTILAYER SYSTEMS

We use the newly introduced family of metrics to study two real systems with multiple types of interactions: the multimodal transportation network of London [29] and the multilayer Noordin Top terrorists network [50]. The first system consists of three layers corresponding to the Tube, overground, and DLR, arranged in a multiplex with couplings $D(i; \alpha, \beta) = 1$ for $\alpha \neq \beta \in \{1, 2, 3\}$. Nodes represent stations ($N = 369$ in total) and connections between them are weighted and undirected. The network of interactions among 78 Indonesian terrorists ($N = 79$ in the data set, but actor 58 is usually removed since it is disconnected in all layers) is a four-layers multiplex, representing their pairwise trust (T), operational (O), communication (C) ties, and business (B) relations [51].

Figure 7 shows the average diffusion manifolds, projected in $\mathbb{R}^3$ through multidimensional scaling, induced
by different RW dynamics. As observed in [29], the best exploration strategy, i.e. the RW to adopt to cover efficiently the network, depends on the topology of the multilayer. This is reflected in the maps of Fig. 7 even though they are low-dimensional approximations of the true diffusion manifolds. As a matter of fact, for the London transportation network, the manifolds induced by the classical, PageRank, and diffusive random walks appear qualitatively very similar with each other, and considerably different from those induced by MERW and PrRW. Instead, the supra-distance matrices and manifolds obtained for the terrorists network appear similar in that all have a group of nodes with small pairwise distances, and another group of nodes which are distant from each other. To quantify more adequately how diverse, or similar, the manifolds are, we compare their supra-distance matrices by means of Mantel’s test [52, 53], where the null hypothesis is that the pairwise distances in one matrix are not monotonically related to the corresponding distances in the second matrix, and show the results of our test in Figs. 8-9.

V. DISCUSSION AND CONCLUSIONS

We have considered different families of random walk dynamics, adequately extended to the realm of multilayer networks, to introduce the multilayer diffusion geometry. Its classical counterpart, single-layer diffusion geometry, intimately relates metastable synchronization, consensus and random search dynamics, providing a novel framework for identifying functional clusters in complex networks.

While the framework and its validity remain the same, its natural generalization to multilayer networks – i.e., systems consisting of multiple types of relationships among their units – was missing. Here, we fill this gap and provide evidence that multilayer diffusion manifolds encode information due to the interplay between the multilayer structure and the dynamics on its top.

From the analysis of synthetic networks with overlapping edges or groups across layers, we have found that the interplay between dynamics and topology cannot be easily decoupled: e.g., the classical random walk reveals...
FIG. 8. Estimating the similarity between diffusion manifolds corresponding to different RW dynamics, evaluated on the London multimodal transportation network. We calculate the Pearson's correlation (encoded by size and color) between the entries of pairs of supra-distance matrices (Mantel's statistic) which is then tested for significance by permutation (permutation test), with $\alpha = 0.001$. The test is general, because it applies directly on distance matrices, whereas any test performed on the low-dimensional embedding of diffusion manifolds would be less precise because of the information loss during projections.

FIG. 9. Same as in Fig. 8 for the Noordin Top terrorists network.

This does not remain true in the presence of strong communities, which are not necessarily overlapping. Also the behavior of the MERW is not trivial: the top level hierarchical structure unveiled in the Barabasi-Albert is compatible with that of the Watts-Strogatz network, despite the high heterogeneity of the first, and this could be surprising since MERW is influenced by irregularities in nodes degree. In another scenario, where two layers are originally uncoupled and do not exchange information, we add inter-layer connectivity to better understand how the originally disjoint diffusion manifolds approach each other because of the presence of multilayer information pathways. Our results highlight that also in the regime of partial interconnected multiplex, where not all replicas of a physical node are interacting – which in the real world could mean a failed connection between a bus and a train station – cross-layer pathways form, allowing the interlayer information exchange. Furthermore, as we move toward the fully-interconnected multilayer, distances become smaller (as shown by the Frobenius norm), but the distinctive meso-scale structure of the Barabasi-Albert model, i.e., the presence of hubs, remains clearly visible.

Finally, we have applied our novel framework to two empirical multilayer systems, namely the public transportation of London and the social network of Noordin terrorists. The diffusion geometry corresponding to different random walk dynamics are not necessarily distinct, and we have developed a quantitative method to assess the correlation between the underlying multilayer diffusion manifolds. In the case of the transportation system, we find that the MERW, which in the synthetic networks was able to separate the layers, highlights two groups of near nodes, that are not captured by other dynamics. This may suggest that (i) the structure of this system, at different scales, has features that are characteristic of different models (e.g., heterogeneity and communities); (ii) different dynamics induce different manifolds and consequently, the analysis of networked systems embedded into space cannot exclude the analysis of the dynamics itself. Conversely, in the case of the social system, we find that the metrics have generally higher correlations, so that their latent diffusion spaces may be likewise similar. The hierarchical structure unveiled by the supra-distance matrices seems to suggest a cross-layer core-periphery functional organization, which we leave to future work.

Our work provides a novel tool for the analysis of multilayer systems from network geometry perspective [10]. Since the latent diffusion geometry is induced by network-driven processes, our framework provides also a complementary view to structural analysis, such as the one provided by hyperbolic network geometry [5, 54, 55], recently used to analyze multilayer networks [56], and higher-order analysis [57].

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Appendix A: Random walks and Markov chains

A Poisson process is a right-continuous process \((X_t)_{t \geq 0}\) with values \(\{0, 1, 2, \ldots\}\) with holding times \(S_1, S_2, \ldots\) \((S_i = J_i - J_{i-1}\) is the time occurring between the random jump times \(J_{i-1}\) and \(J_i\)) that are independent exponential random variables of rate \(0 < \lambda < \infty\). In a generalized Poisson process (or birth process) the parameter \(\lambda\) is allowed to depend on the current state of the process. Given its birth rates \(0 \leq q_i < \infty\) for \(i = 0, 1, 2, \ldots\), \((S_i)_{i \in \mathbb{N}^+}\) are independent exponential random variables with rates \(q_i\). Finally, a continuous-time Markov chain (MC) \((X_t)_{t \geq 0}\) on a finite set \(I\) with generator \(Q\) and initial distribution \(p_0\) can be described in terms of a Poisson process. Each state \(i \in I\) of the process is a chamber and doors close the passage to the other states. From time to time a single door opens (events cannot be simultaneous) allowing the process to change state and the doors open at the jump times of a Poisson process of rate \(q_{ij}\). The generator of the MC is indicated by \(Q\), because it is a particular matrix, called \(Q\)-matrix in \([58]\), satisfying three conditions

(i) \(0 \leq -q_{ii} < \infty\)

(ii) \(q_{ij} \geq 0\) \(\forall i \neq j\)

(iii) \(\sum_j q_{ij} = 0\) \(\forall i\).

To recap, a continuous-time MC can be (equivalently) defined in terms of its jump chain and holding times, or of its transition probabilities given by the solution of the forward equation \([58\text{ Thm.}2.8.2]\).

Appendix B: Maximal-entropy RW and the Perron–Frobenius theorem

An essential condition for the definition of the maximal-entropy random walk is that every component of the eigenvector \(\psi\), corresponding to the leading eigenvalue \(\lambda_{\text{max}}\), be strictly positive. This is guaranteed by the Perron–Frobenius theorem for irreducible non-negative matrices, where a matrix \(A\) is said to be irreducible if \(\forall i, j = 1, \ldots, N\) there exists an integer \(m\) such that \(A^m_{ij} > 0\), which is exactly the irreducibility of a random walk on \(\{1, \ldots, N\}\).