# Existing tools for analysis of Multilayer Networks

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## Introduction

In this Chapter, we review several structural metrics for multilayer networks, highlighting differences against definitions for single-layer networks. We start by extending the concepts of network neighbours and network path to the multilayer structure. We then proceed by considering how the presence of multiple layers requires more general definitions of local and global connectivity, centrality and community structure. We also review structural features arising from the multilayer structure that have no single-layer counterpart, such as interlayer correlations [1, 2, 3, 4, 5], structural reducibility [6] and layer clustering [6, 7]. Notice that the algorithms for multilayer community discovery [8, 9] briefly introduced here link together structure and dynamics of multilayer networks and are reviewed in more depth in the Chapter about processes on multilayer networks.

## multilayer neighbours, links and paths

Let us consider a multilayer network [1, 10, 11] with L layers and N nodes represented by the multilayer adjacency tensor  $M_{j,\beta}^{i,\alpha}$ , with  $i, j \in 1, 2, ..., N$  and  $\alpha, \beta \in 1, 2, ..., L$ . Then the neighbours of the generic node i are all the nodes connected to i across all layers. Notice that even if two nodes i and j might be disconnected in one layer  $\alpha$ , they might be adjacent on another layer  $\beta$  or being interconnected across layers. As in single-layer networks [12], neighbours of node i are classified in terms of the length of the paths connecting them to i. In the rest of this Chapter, using "neighbours" with no further attribute indicates adjacent nodes. The presence of several network layers can drastically alter the neighbourhood structure of a given node. An example is reported in Figure 0.1: Even though nodes 1 and 5 are disconnected in the left-most layer, there is a path connecting 1 and 5 in the central layer.

Let us briefly discuss the concept of path within the framework of multilayer networks. As in single layer networks [12], we define an undirected path between nodes i and j as a set of network links  $p = \{(i, \alpha, k, \alpha), (k, \alpha, k, \beta), ..., (h, \gamma, j, \gamma)\}$  where directionality is not important and the notation is such that  $(i, \alpha, k, \alpha)$  indicates an *intralayer* link between nodes i and k in layer  $\alpha$  while  $(k, \alpha, k, \beta)$  indicates an *interlayer* link between replicas of node k in layers  $\alpha$  and  $\beta$  (see Figure 0.1 for an example). The path length is then defined as the cardinality |p| of p, i.e. the number of links in a given path. The shortest path length is the cardinality of the path with the fewest inter- and intralinks connecting nodes i and j. Notice that the possibility of transitioning between layers can dramatically change the shortest path length between nodes (also called geodesic distance [12]): two nodes could be disconnected on layer  $\alpha$ , so that their distance would be  $d_{\alpha}(i, j) = \infty$ , but adjacent in another layer, consequently their distance on the multilayer structure would be  $d_M(i, j) = 1$ . A multilayer network and its aggregated single-layer counterpart display the same distances between nodes only when interlayer links are not explicitly considered, as in edge-coloured graphs [1, 13].

## Viable clusters and mutually largest connected components

In single-layer networks [12], a *connected component* is a subgraph where there is at least one path connecting any two nodes. For networks of finite size, the connected component with the largest number of nodes is called *largest connected component*. For networks of infinite size, e.g. theoretical models, the largest connected component is called *giant component*. A network is connected if it coincides with its largest connected component.

In multilayer networks, the presence of different layers of interactions allows to consider several definitions of connectedness [14, 1, 10, 11, 13, 15, 16]. The simplest approach for node-aligned multi-layer networks is to apply the single-layer notion of connectedness to



Figure 0.1: A node-aligned multilayer network with N = 7 nodes and L = 3 layers. The red arrows represent a path connecting node 1 on the left-most layer to node 2 on the right-most layer. Notice that the path considers both links between nodes in a given layer (intralayer links) and connections between replicas of nodes in different layers (interlayer links). Picture from De Domenico et al. 2014 [13].

the aggregate network [1], so that a multilayer network is fully connected if its aggregate counterpart is fully connected. According to this definition, in a connected multilayer network there exists at least one multilayer path connecting any two nodes.

Connectedness can be imposed on individual layers rather than on the aggregate network. For node-aligned multiplex networks without explicit interlinks, this requirement leads to the definition of a viable cluster [16]: a set of nodes that are mutually connected on each individual layer. The notion of viable cluster reduces to the one of largest connected component in single-layer networks. In edge-coloured graphs the viable cluster is always smaller than the intersection of largest connected components of individual layers [17], see Figure 0.2 for an example.

Viable clusters are related to mutually connected components in interdependent networks [14, 15]. Each node i on layer  $\alpha$  is in the mutually connected component if: (i) it has at least one neighbour j on  $\alpha$  that is connected to the mutually connected component and (ii) if all the replicated nodes i on other layers are also in the mutually connected component. The second requirement about interconnectedness makes the mutually connected component a more restrictive definition compared to the one of connectedness provided through the aggregate network. In case of full interdependency, the definition of largest mutually connected component corresponds to one of the largest viable cluster [16].

Notice that the way nodes are connected between layers and the presence of viable clusters or mutually connected components greatly affects the robustness properties of multilayer networks to progressive disruption [13, 18, 17] and resilience to cascading failure [14, 19].

## Centrality measures in multilayer networks

Finding the most central nodes in complex networks is fundamental in a variety of realworld scenarios [12], such as finding the most fragile agents in cascades of failure [14] or pivotal disease spreaders [20, 21] in epidemics. Centrality strongly depends on the considered network process so that a wide variety of network centrality measures have been suggested in single-layer networks over the years (for a review from the computational social sciences see [22]). Generalisations to multilayer networks are not always straightforward since nodes peripheral in one layer might be extremely central in another one [1, 10, 11]. Although attempts at producing weighted averages of centralities [23] across single layers have been successfully used in multilayer network analysis [24], many novel measures



Figure 0.2: Example of viability in an edge-coloured network with N = 6 nodes and L = 2 layers. Red nodes are the intersection of largest connected components across layers. Viability requires for all nodes to be connected among each other in every individual layer and paths combining different colours do not count. The intersection of connected components is not a viable cluster: There are no paths of dashed links only connecting the node in the upper-right corner. In order to make the nodes a viable cluster one dashed link must be added. Picture from [17].

harnessing the multilayer structure have been suggested over the last few years. Because of space constraints, our review cannot be exhaustive so we refer the interested reader to consult additional references for multiplex [25] and multilayer [1, 10, 11] networks.

## Node activity

In multilayer networks one node might be present on one layer but absent (or disconnected) on another one. In node-aligned multiplex networks this information can be encoded within a node-activity vector [4]:

$$\mathbf{b}_i = (b_i(1), b_i(2), \dots, b_i(L)), \tag{0.1}$$

with  $b_i(\alpha) = 0$  if  $k_i^{(\alpha)} = 0$  and  $b_i(\alpha) = 1$  otherwise, for  $\alpha \in 1, ..., L$ . The node activity  $B_i$  is then defined as the sum of the  $b_i(\alpha)$  across layers. The distribution of node activities provides a compact representation of the involvement of nodes across different layers [4, 25].

## Multidegree

Counting the links of a given node represents the simplest indicator of node importance at a local level, a measure called degree centrality in single-layer networks [12]. In multilayer networks *multidegree centrality* [1] is the total number of links  $k_i$  in which a node *i* is involved across all layers and it can be computed through the multilayer adjacency tensor:

$$k_i = \sum_{\alpha,\beta=1}^{L} \sum_{j=1}^{N} M_{j\beta}^{i\alpha}.$$
(0.2)

Notice that the multidegree  $k_i$  counts both inter- and intralayer links. In case interlayer links are not explicitly considered, as in edge-coloured graphs, it can be more convenient to consider the degrees coming from individual layers/colours. In formulas:

$$k_{i}^{(\alpha)} = \sum_{j=1}^{N} A_{j}^{i}(\alpha), \qquad (0.3)$$

where  $k_i^{\alpha}$  is the degree of node *i* coming from intralayer links on layer  $\alpha$  and  $A_j^i(\alpha)$  represents the adjacency tensor of layer  $\alpha$ . When interlayer links are not present, the multidegree coincides with the sum of intralayer degrees  $K_i = \sum_{\alpha} k_i^{(\alpha)}$ , which is also called *overlapping degree* in the multiplex networks literature [26, 3, 4, 25]. Notice that



Figure 0.3: Visual explanation of a multiplex cartography. Nodes are mapped into points of a 2D map displaying the participation coefficient on the x axis and multidegree on the y axis. Points can be clustered in a 2D grid for easier visualisation [4]. Picture from [28].

even in multiplex networks the multidegree of i across layers does not always coincide with the degree of i in the aggregated network as links might overlap across layers [26].

### Network cartography

Multidegree centrality  $k_i$  provides global information on the amount of interactions node *i* engages with. However, multidegree is not informative on the way *i*'s links are distributed across layers. In multiplex networks, the participation coefficient [3]  $P_i$  quantifies how uniformly node *i* distributes their own intralayer links across layers, in formulas:

$$P_{i} = \frac{L}{L-1} \left[ 1 - \sum_{\alpha=1}^{L} \left( \frac{k_{i}^{(\alpha)}}{K_{i}} \right)^{2} \right].$$
(0.4)

 $P_i$  ranges between 0 (for nodes that concentrate all their connections in one layer only) and 1 (for nodes that distribute connections over all the L layers uniformly).

The degree centrality and the participation coefficient of nodes in a multiplex network represent the coordinates of the so-called *multiplex cartography* [3], i.e. a 2D map useful for detecting central nodes. The concept of network cartography was originally introduced for community analysis in single-layer networks [27] and it was later generalised to node centrality in multiplex networks [3]. Nodes with higher multidegree centrality and higher participation coefficient tend to have more interactions present across all layers [3, 4], thus playing a more central role in processes such as epidemic spreading on multiple layers [21, 20].

## Multilayer versatility

In multilayer networks, nodes crucial for a given dynamics might not be central across all layers. Consider the case in which two distinct layers have only one node in common: Any information flow between the layers will have to pass through the common node, independently from its centrality in the layers. Hence that node will be highly central for the considered process. Multilayer versatility [1, 29] quantifies how important nodes are for diffusive processes such as information flow or spreading. Since versatility is strongly connected to diffusive processes, we hereby briefly review different types of versatility measures but refer the reader to the Chapter on the dynamics of multilayer networks for a more thorough description.

#### Eigenvector versatility

In single-layer networks, eigenvector centrality is based on an iterative procedure giving to each node a centrality score that is the weighted sum of the scores of its neighbours [12]. Therefore, the eigenvector centrality gives high centrality scores to vertices that are connected to many other well-connected vertices.

As for single-layer networks, eigenvector versatility can be defined as the solution of an eigenvalue problem given by the multilayer adjacency tensor:

$$M^{i\alpha}_{j\beta}\Theta_{i\alpha} = \lambda_1 \Theta_{j\beta}, \qquad (0.5)$$

where Einstein summation is considered for the sake of simplicity, i.e. there is summation over repeated indices. The problem of finding the eigenvector centrality consists in computing  $\Theta_{j\beta} = \lambda_1^{-1} M_{j\beta}^{i\alpha} \Theta_{i\alpha}$ , which represents the multilayer generalisation of Bonacich's eigenvector centrality per node per layer [1, 29]. Eigenvector versatility can then be condensed across layers by summing up the scores of a node across all layers  $\theta_i = \sum_{\alpha} \Theta_{i\alpha}$ . Notice that the summation across layers appears naturally through the tensorial formalism [1, 29]. Although other definitions of multilayer eigenvector centrality have been suggested in the literature, by Halu et al. [30] and Solá et al. [23], they do not provide information on how to combine centralities across layers.

#### Kats versatility

Kats centrality was introduced in the field of social network analysis for "evaluating status in a manner free from the deficiency of popularity contest procedures" [31]. This metric attributes centrality to a given node by considering contributions coming from its adjacent and more distant neighbours. Contributions coming from more distant neighbours are dampened by a factor a. Analogously to the eigenvector versatility, also Katz versatility  $\Phi_{j\beta}$  can be defined as the solution of a tensorial equation  $\Phi_{j\beta} = aM_{j\beta}^{i\alpha}\Phi_{i\alpha} + bu_{j\beta}$  [1, 29]. In formulas, the Katz centrality for a multilayer network is:

$$\Phi_{j\beta} = \left[ (\delta - aM)^{-1} \right]_{j\beta}^{i\alpha} U_{i\alpha}, \tag{0.6}$$

where  $\delta_{j\beta}^{i\alpha} = \delta_j^i \delta_{\beta}^{\alpha}$ , the dampening factor *a* has to be smaller than the reciprocal of the absolute value of the largest eigenvalue of the multilayer tensor  $M_{j\beta}^{i\alpha}$  and *b* is a constant usually equal to 1. As for the eigenvector versatility, the overall Katz centrality of a node is the sum of centrality scores  $\Phi_{j\beta}$  across layers [1, 29].

### **HITS** versatility

In single-layer networks, the Hyperlink-Induced Topic Search or HITS centrality was originally introduced for Web page rating according to their authority (e.g. their content) and their hub value (e.g. the value of their links to other web-pages) [32]. Nodes pointing to many other nodes are considered hubs while nodes receiving links by many hubs are considered authorities. The problem of computing hub and authority values for nodes translates into two coupled eigenvalue problems whose multilayer counterpart is [1, 29]:

$$\begin{cases} (MM^T)_{j\beta}^{i\alpha}\Gamma_{i\alpha} = \lambda_1\Gamma_{j\beta} \\ (M^TM)_{j\beta}^{i\alpha}\Upsilon_{i\alpha} = \lambda_1\Upsilon_{j\beta} \end{cases}$$
(0.7)

where  $\cdot^T$  indicates the transpose operation,  $\Gamma_{i\alpha}$  ( $\Upsilon_{i\alpha}$ ) is the hub (authority) centrality score of node *i* on layer  $\alpha$ . The overall HITS versatilities are then obtained by summing across layers. Notice that for undirected networks with no interlayer links the HITS versatilities coincide with the eigenvector versatility.

#### PageRank versatility

In single-layer networks PageRank centrality [33] indicates the probability that a random walker visits a given node by: (i) traversing node links and (ii) teleporting through nodes at random. For multilayer networks [1, 29], the dynamics of the random walker is regulated by a transition tensor, expressing the probability of traversing link  $(i, \alpha, j, \beta)$ :

$$R^{i\alpha}_{j\beta} = rT^{i\alpha}_{j\beta} + \frac{(1-r)}{NL}u^{i\alpha}_{j\beta}, \qquad (0.8)$$

where r is a constant expressing the probability for the random walker to teleport. In the Google Search Algorithm r is equal to 0.85 [33]. If we denote by  $\Omega_{i\alpha}$  the eigentensor of  $R_{j\beta}^{i\alpha}$ , then the PageRank versatility  $\omega_i$  of a node is obtained by summing across layers  $\sum_{\alpha} \Omega_{i\alpha}$ . Other definitions of multilayer PageRank have been proposed in the context of multiplex networks [30, 34, 35]. Multilayer PageRank resulted being more powerful than its single-layer counterpart in a wide variety of applications, including the importance [34] and tendency to incur in passenger traffic congestion [29] of airports and identifying interdisciplinary researchers in co-citation networks [36].

## Correlations in multilayer networks

Intralayer connections can be organised in correlated ways among layers. Several attempts have been made in order to quantify these interlayer dependencies [1, 3, 4, 37]. Let us briefly review quantitative measures of correlation relying on link assortment across layers.

## Link overlap and multiplexity

A simple measure of correlation among links in node-aligned multilayer networks is *link* overlap [26, 1], i.e. the number of links being simultaneously present on several layers at once between the same couple of nodes. Correlations influencing link overlap can be measured via correlation metrics [1, 25], like the conditional probability  $P(A_j^i(\alpha)|A_j^i(\beta))$ of finding a link at layer  $\alpha$  given the presence of a link between the same nodes in layer  $\beta$ :

$$P(A_j^i(\alpha)|A_j^i(\beta)) = \frac{\sum_{ij} A_j^i(\alpha) A_j^i(\beta)}{\sum_{ij} A_j^i(\beta)}.$$
(0.9)

However, such approach does not quantify the contribution that heavy-tailed degree distributions might have in boosting or altering correlations on link overlap. This might be problematic when analysing real-world networked systems with heavy-tailed degree distributions [5]. The metric called *multiplexity*  $M_{\alpha\beta}$  allows to quantify pairwise link overlap correlations between layers  $\alpha$  and  $\beta$  by considering a specific null model [5], in formulas:

$$M_{\alpha\beta} = \frac{2\sum_{i\neq j} \min\{A_j^i(\alpha), A_j^i(\alpha)\}}{L_{TOT}^{[\alpha]} + L_{TOT}^{[\beta]}}, \quad \mu_{\alpha\beta} = \frac{M_{\alpha\beta} - \langle M_{\alpha\beta} \rangle}{1 - \langle M_{\alpha\beta} \rangle}, \quad (0.10)$$

where  $L_{TOT}^{[.]}$  is the number of edges in a given layer and  $\mu_{\alpha\beta}$  is the normalised multiplexity, which is rescaled compared to a reference null model value  $\langle M_{\alpha\beta} \rangle$ . When applied to the International Trade Network [5], where nodes are countries and layers indicate traded



Figure 0.4: Some examples of possible 3-cycles on a multilayer structure. The orange node is the starting point of the cycle, intralayer links are represented as solid lines while interlayer links are dotted lines. The green line represents the second intralayer link in the cycle. Picture reproduced from Cozzo et al.[38].

commodities, strong interlayer link correlations were hugely reduced once the heavy-tailed empirical degree distribution was considered. Hence, with the proper choice of reference null model (e.g. a configuration model fixing degree but randomising links) multiplexity can discriminate between genuine link correlations and spurious effects due to interlayer degree correlations.

## Degree correlations

Degree correlations of the same node across different layers can be identified by computing the analogue of the nearest neighbour average degree  $k_{nn}(k)$  of nodes with degree k in single-layer networks. For node-aligned multilayer networks one can define [1, 25]:

$$\overline{k^{(\beta)}}(k^{(\alpha)}) = \sum_{k^{(\beta)}} k^{(\beta)} P(k^{(\beta)} | k^{(\alpha)}), \qquad (0.11)$$

which is the average degree at layer  $\beta$  of a node with degree  $k^{(\alpha)}$  on layer  $\alpha$ . Increasing (decreasing) trends of  $\overline{k^{(\beta)}}(k^{(\alpha)})$  indicate positive (negative) degree correlations among layers  $\alpha$  and  $\beta$ .

## Triadic closure and clustering coefficient

In single-layer networks the clustering coefficient measures the presence and strength of triadic closure, i.e. the tendency for three connected nodes (a triplet) to form a triangle (a closed triplet) [12]. The local clustering coefficient of node i measures how likely it is for two neighbours of i to be connected with each other, in formulas:

$$C_{i} = \frac{\sum_{j,m \neq i} A_{j}^{i}(\alpha) A_{m}^{j}(\alpha) A_{i}^{m}(\alpha)}{\sum_{i,m \neq i} A_{i}^{i}(\alpha) A_{i}^{m}(\alpha)}.$$
(0.12)

In multilayer networks there are multiple ways of considering closed triangles across layers, see Figure 0.4 for some possible examples. Consequently, there are several different ways for generalising the notion of clustering to multilayer network structures. For instance, in node-aligned multiplex networks a triangle can be formed by considering two intralayer links on layer  $\alpha$  and one intralayer link on  $\beta$  among three nodes, so that a possible generalisation of local clustering becomes [3]:

$$C_{i,1} = \frac{\sum_{\alpha} \sum_{\beta \neq \alpha} \sum_{j,m \neq i} A_j^i(\alpha) A_m^j(\beta) A_i^m(\alpha)}{(L-1) \sum_{\alpha} \sum_{j,m \neq i} A_j^i(\alpha) A_i^m(\alpha)}$$
(0.13)

Notice that this definition averages above all possible couples of layers and the denominator considers also terms j = m, so that the maximum value of local clustering coefficient is (N-1)/(N-2). Other attempts have been made in order to have measures of clustering with additional features such as: (i) naturally reducing to the single-layer definition, (ii) being bounded between 0 and 1, (iii) defined for node-layer pairs and (iv) defined also for non-node-aligned networks. All these features were encompassed in a recently suggested definition of multilayer clustering based on cycles [38] and random walks:

$$C^* = \frac{\sum_i t_{*,i}}{\sum_i d_{*,i}},\tag{0.14}$$

counting the number of 3-cycles of a given type \* (e.g. cycles being in one layer only, cycles jumping across two layers and so on) going through node *i* normalised by a factor  $d_{*,i}$ .

The analysis of multilayer clustering found a strong tendency for social networks to promote link redundancy by displaying triadic closure on every layer, an effect that would be otherwise unnoticeable by considering aggregate networks only [38]. Further investigation of multiplex configuration models [39] highlighted that degree correlations have a strong influence on the number of cycles a node participates in. This underlines the need for a comparison of clustering coefficient against suitable null models in real-world networks.

## Community discovery

A prominent problem in network science is the detection of densely connected groups of nodes known as communities [40]. For single-layer networks a variety of methods has been developed in the last twenty years, either directly maximising a given quality function of the detected community structure [41] or rather adopting information theoretic tools [42] or spectral features [43] of complex networks.

The multilayer structure challenges the concept of community in terms of tightly connected nodes, since nodes adjacent in one layer might be disconnected in another one and, in general, the meso-scale community organisation of nodes in one layer might dramatically differ across other layers [8, 37]. This difference indicates the importance of keeping into account interlayer dependencies and correlations within the definition of multilayer communities.

#### Multi-slice modularity maximisation

One of the most popular heuristics for community detection in single-layer networks is modularity maximisation [41, 40]. Modularity is a metric indicating the extent to which the distribution of links across and within a given set of communities differs compared to what one would expect in a suitable network null model. Hence, finding a network community becomes and optimisation problem of the modularity Q. A generalisation of modularity maximisation for multilayer networks is the multi-resolution method [8], which employs a specific analytical generalisation of modularity to multilayer networks. Making use of the tensorial notation [1], the multilayer modularity is written as:

$$Q_M \propto S^a_{i\alpha} (M^{i\alpha}_{j\beta} - P^{i\alpha}_{j\beta}) S^{j\beta}_a, \qquad (0.15)$$

where  $M_{j\beta}^{i\alpha}$  is the multilayer adjacency tensor,  $P_{j\beta}^{i\alpha}$  is the tensor encoding an appropriate null model for the observed network structure and  $S_a^{i\alpha}$  is defined to be 1 when node *i* in layer  $\alpha$  belongs to a given community labelled by *a* and 0 otherwise. The algorithm then proceeds with the same heuristics of single-layer networks for detecting optima in the landscape of modularity. For a more thorough discussion of the dynamical interpretation of  $Q_m$  we refer to the Chapter on dynamical processes on multilayer networks.

## InfoMAP

Spectral clustering in single-layer networks relies on the intuitive idea that a random walker tends to remain confined preferentially within a given network community rather than jumping across communities [43, 13, 44]. By defining a map equation for both single-[42] and multilayer [9] network structure, encapsulating specific types of random walkers on networks, the *InfoMAP* algorithm allows to detect multilayer communities. Since the map equation is a flow-based method operating on the network dynamics, we refer the interested reader to the Chapter on dynamical processes on multilayer networks for further details.

## Non-negative matrix factorisation for temporal networks

Temporal networks can be considered as multiplex networks with layers having a specific ordering and representing time [45]. Non-negative matrix factorisation has been suggested for detecting community structure in temporal networks [45], represented as a three-dimensional tensor  $T_{ij}^{\tau}$ . Kruskal decomposition is applied to  $T_{ij}^{\tau}$  in order to assign each node to a community across node. Notice that this methodology assumes as stationary the interdependences across replica nodes over time.

## Structural reducibility

The effort of considering more network layers does not always provide additional information about interactions among agents: Consider a node-aligned multilayer or multiplex network where all layers are copies of a single one. More in general, while individual layers can differ from each other in terms of their topology, they can also display rather high link overlap and thus contain redundant topological patterns [26, 46]. This naturally leads to the following question: What would be the optimal number of layers to consider in a trade-off between preserving the most topological information available and the least effort in terms of different layers to be considered?

To this aim, structural reducibility analysis was recently proposed [6], as a technique for quantifying how different a multiplex network is from its aggregate when its layers are kept either as distinct or rather gradually aggregated. Structural reducibility encodes the information available in the network structure through the Von Neumann entropy h [47], which is based on the spectrum  $\{\lambda_i\}_i$  of the degree-normalised<sup>1</sup> Laplacian L = (D-A)/2K, in formulas:

$$h = -\mathrm{Tr}(L\log_2 L) = -\sum_i \lambda_i \log_2 \lambda_i, \qquad (0.16)$$

where Tr indicates the trace operator on matrices. The Von Neumann entropy  $h_A$  of the aggregated network is used as a reference value. Differences between  $h_A$  and the Von Neumann entropy of multiplex structure are then used for estimating the loss of information relative to aggregating the multiplex structure [6]. The Von Neumann entropy  $h_M$  of the whole multiplex network is estimated as the average of the entropies of the individual layers, in formulas:

$$h_M(C) = \sum_{\alpha=1}^{|C|} h_{\alpha} / |C|, \qquad (0.17)$$

where the configuration index C labels a specific combination of |C| different layers, either original or aggregated. Because of the definition of entropy, the ratio  $h_M(C)/h_A$  is

<sup>&</sup>lt;sup>1</sup>Here D is a diagonal matrix having node degrees on its main diagonal, K is the number of links in the network and A is the adjacency matrix.

upper bounded by 1 ( $h_M(C) = h_A$  when all the layers have been aggregated together). Therefore the rescaled index:

$$q(C) = 1 - \frac{h_M(C)}{h_A},\tag{0.18}$$

represents a relative entropy ranging between 0 and a given maximum value. q(C) = 0when the aggregate network is equivalent to the multiplex in configuration C and this can happen if and only if |C| = 1 and all layers have been aggregated (unless the multiplex network contains identical layers).  $q(\cdot)$  is maximum when the multiplex structure in configuration C is maximally different or the most distinguishable from the aggregated network.

 $q(\cdot)$  is an entropy-based approach for defining how different a given multiplex configuration is compared to its aggregated counterpart. In general,  $q(\cdot)$  can either increase or decrease when two layers are aggregated, depending on their connectivity patterns. While  $q(\cdot)$  decreases when  $h_M(C)$  increases and this happens mainly in two cases: (i) when two layers with very different link densities are aggregated into one layer or (ii) when new structural patterns that were absent in the original layers emerge in the aggregated one. Both these cases imply a loss of topological information: This is why configurations which minimise  $h_M$  and thus maximise the relative entropy  $q(\cdot)$  are preferred, instead. This criterion identifies the multiplex configuration providing the most information about the multi-relational patterns within it. Figure 0.5 reports an example of structural reducibility analysis.

When  $q(\cdot)$  is maximum but no aggregation is performed, i.e. layers are kept as separate, then the original multiplex configuration is considered as *irreducible*: Performing any layer aggregation would imply a loss of structural information. This is an important starting point for justifying the multiplex approach [17], together with the interpretation of what individual layers represent in the irreducible network representation.

### Layer clustering

One issue of structural reducibility analysis is that the number of different configurations that have to be tested for exhaustively discovering the optimal configuration is the L-th Bell number for a multiplex with L layers, which increases super-exponentially with L. Testing a multiplex network with only L = 15 layers would require testing more than  $10^9$ configurations.

Layer clustering is a viable heuristics for solving the above issue [6]. Structural reducibility adopts a greedy-algorithm exploring the configurations were more similar layers are aggregated first. Although there are different measures of network similarity in the literature (we refer the interested reader to [48] for a review), structural reducibility employs a similarity metric based on the Von Neumann entropy h and commonly used in Quantum Mechanics, namely the Jensen-Shannon divergence:

$$\mathcal{D}_{JS}(\rho,\sigma) = h(\frac{\rho+\sigma}{2}) - \frac{h(\rho) + h(\sigma)}{2}, \qquad (0.19)$$

where  $\rho$  and  $\sigma$  are matrices. It is easy to check that  $\sqrt{D_{JS}}$  is bounded within [0, 1] and satisfies the definition of a metric. When using the degree-normalised Laplacian matrices of two distinct networks, the Jensen-Shannon distance  $\sqrt{D_{JS}}$  can be used for implementing a greedy algorithm performing structural reducibility among the most similar layers.

More in general, the Jensen-Shannon distance can be used also for performing hierarchical clustering of layers in multiplex networks, potentially unravelling community-based



Figure 0.5: Example of structural reducibility analysis of a multilayer network of L = 8 layers. Individual layers (a) are initially clustered according to how similar their Von Neumann entropies are (b), see also the subsection on Layer Clustering. A greedy algorithm selects the configurations in which the most similar layers are clustered first and it produces a hierarchy of configurations (c). The profile of the relative entropy q is maximised when only two aggregated layers are considered thus suggesting that the multilayer structure can be condensed into two layers only (d). Picture reproduced from De Domenico et al. [38].

classifications across layers of network interactions [7]. Distances between empirical network layers and families of null models can also be successfully used for quantifying how much information is needed for correctly learning the parameters of a model [7].

## Software for multilayer network structure analysis

Over the years, the network community developed several libraries and software for the analysis of the multilayer network features discussed in the previous sections. We enlist these tools here for the interested reader:

- MuxViz (http://muxviz.net/) a self-contained framework for the structural and dynamical analysis and visualisation of multilayer networks, based on R and GNU Octave [49];
- PymNet (http://www.mkivela.com/2015/12/11/multilayer-networks-library/) a Python library for multilayer network analysis integrated with NetworkX for the analysis of single-layer networks;
- MAMMULT (https://github.com/KatolaZ/mammult) a collection of libraries in C and Python focusing on multiplex networks;
- GenLouvain (http://netwiki.amath.unc.edu/GenLouvain/GenLouvain) a library in MATLAB implementing the multislice community analysis;
- InfoMAP (http://www.mapequation.org/code.html) a command line software implemented in C++ for the multilayer network analysis based on random walks;

• MultiNet (http://multilayer.it.uu.se/software.html) a set of libraries implemented in R for multilayer network analysis.

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