Structure of Triadic Relations in Multiplex Networks

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Recent advances in the study of networked systems have highlighted that our interconnected world is composed of networks that are coupled to each other through different "layers" that each represent one of the many possible subsystems or types of interactions. Nevertheless, it is traditional to aggregate multilayer data into a single weighted network in order to take advantage of existing tools. This is admittedly convenient, but it is also extremely problematic, as important information can be lost as a result. It is therefore important to develop multilayer generalizations of network concepts. In this paper, we analyze triadic relations and generalize the idea of transitivity to multiplex networks. We focus on triadic relations (which yield the simplest type of transitivity) and thus generalize the concept and computation of clustering coefficients to multiplex networks. We show how the layered structure of such networks introduces a new degree of freedom that has a fundamental effect on transitivity. We compute multiplex clustering coefficients for several real multiplex networks and illustrate why generalizing standard network concepts to multiplex networks must be done with great care. We also derive analytical expressions for our clustering coefficients in a family of random multiplex networks. Our analysis illustrates that social networks have a strong tendency to promote redundancy by closing triads at every layer and that they thereby have a different type of multiplex transitivity from transportation networks, which do not exhibit such a tendency. These insights are invisible if one only studies aggregated networks.

The computation of triadic relations—that is, relationships between triplets of nodes—using a clustering coefficient is one of the central ideas in network theory. Triadic relations are the smallest structural patterns that produce transitivity in a network, and counting them and analyzing them is thus crucial to have a proper understanding of clustering in networks. To measure transitivity in a network, one computes a clustering coefficient by comparing the number of connected triples of nodes to the number of triangles. In the present paper, we generalize the ideas of triadic relations and transitivity to multiplex networks, in which entities are connected to each other via multiple types of edges. To do this, we take into account the many possible types of cycles that can occur in multiplex networks, and we show that different types of real networks have different types of clustering patterns that cannot be detected using traditional measures of transitivity in networks. Our results thus suggest that clustering mechanisms are likely to be very different in different types of networks, as we have demonstrated for social and transportation networks.

The quantitative study of networks is fundamental for investigations of complex systems throughout the biological, social, information, engineering, and physical sciences [1–3]. The broad applicability of networks, and their success in providing insights into the structure and function of both natural and designed systems, has generated considerable excitement across myriad scientific disciplines. Numerous tools have been developed to study networks, and the realization that several common features arise in a diverse variety of networks has facilitated the development of theoretical tools to study them. For example, many networks constructed from empirical data have heavy-tailed degree distributions, satisfy the small-world property, and/or possess modular structures; and such structural features can have important implications for information diffusion, robustness against component failure, and more.

Traditional studies of networks generally assume that nodes are connected to each other by a single type of static edge that encapsulates all connections between them. This assumption is almost always a gross oversimplification, and it can lead to misleading results and even the fundamental inability to address certain problems. Instead, most real systems have multilayer structures [4], as there are almost always multiple types of ties or interactions that can occur between nodes, and it is crucial to take them into account. For example, transportation systems include multiple modes of travel, biological systems include multiple signaling channels that operate in parallel, and social networks include multiple types of relationships and multiple modes of communication. We will represent such systems using the formalism of *multiplex networks*, which allow one to incorporate multiple types of edges between nodes.

The notion of multiplexity was introduced years ago in fields such as engineering [5, 6] and sociology [1, 7–9], but such discussions included few analytical tools to accompany them. This situation arose for a simple reason: although many aspects of single-layer networks are well understood, it is very challenging to properly generalize even the simplest concepts for multiplex networks. Theoretical developments on multilayer networks (including both multiplex networks and interconnected networks) have gained steam only in the last few years [10–19], and even basic notions like centrality and diffusion have barely been studied in multiplex settings [20–28]. Moreover, new degrees of freedom arise from the multilayer structure of multiplex networks, and this brings both new challenges [4, 29] and new phenomena. This includes multiplexity-induced correlations [18], new types of dynamical feedbacks [25], and "costs" of inter-layer connections [30]. For reviews about networks with multiple layers, see Refs. [4, 31].

In the present article, we focus on one of the most important structural properties of networks: triadic relations, which are used to describe the simplest and most fundamental type of transitivity in networks [1, 3, 32, 33]. We develop multiplex generalizations of clustering coefficients, which can be done in myriad ways, and (as we will illustrate) the most appropriate generalization depends on the application under study. Such considerations are crucial when developing multiplex generalizations of any single-layer (i.e., "monoplex") network diagnostic. There have been several attempts to define multiplex clustering coefficients [34–38], but there are severe shortcomings in these definitions. For example, some of them do not reduce to the standard single-layer clustering coefficient or are not properly normalized (see *SI Appendix*).

The fact that existing definitions of multiplex clustering coefficients are mostly *ad hoc* makes them difficult to interpret. In our definitions, we start from the basic concepts of walks and cycles to obtain a transparent and general definition of transitivity. This approach also guarantees that our clustering coefficients are always properly normalized. It reduces to a weighted clustering coefficient [39] of an aggregated network for particular values of the parameters; this allows comparison with existing single-layer diagnostics. We also address two additional, very important issues: (1) Multiplex networks have many types of connections, and our multiplex clustering coefficients are (by construction) decomposable, so that the contribution of each type of connection is explicit; (2) because our notion of multiplex clustering coefficients builds on walks and cycles, we do not require every node to be present in all layers, which removes a major (and very unrealistic) simplification that is used in existing definitions.

Using the example of clustering coefficients, we illustrate how the new degrees of freedom that result from the existence of a structures across layers of a multiplex network yield rich new phenomena and subtle differences in how one should compute key network diagnostics. As an illustration of such phenomena, we derive analytical expressions for the expected values of our clustering coefficients on multiplex networks in which each layer is an independent Erdős-Rényi (ER) graph. We find that the clustering coefficients depend on the intra-layer densities in a nontrivial way if the probabilities for an edge to exist are heterogeneous across the layers. We thereby demonstrate for multiplex networks that it is insufficient to generalize existing diagnostics in a naïve manner and that one must instead construct their generalizations from first principles (e.g., as walks and cycles in this case).

Mathematical Representation

We use the formalism of supra-adjacency matrices [20] to represent the multiplex network structure. Let $\mathcal{A}$, $\mathcal{C}$, and $\bar{\mathcal{A}}$, respectively, denote the intra-layer supra-adjacency matrix, coupling supra-adjacency matrix, and supra-adjacency matrix (see *Materials and Methods*). Supra-adjacency matrices satisfy $\bar{\mathcal{A}} = \mathcal{A} + \mathcal{C}$ and $\mathcal{A} = \bigoplus_\alpha \mathbf{A}^{(\alpha)}$, where $\mathbf{A}^{(\alpha)}$ is the adjacency matrix of layer α and $\bigoplus$ denotes the direct sum of the matrices. We consider undirected networks, so $\mathcal{A} = \mathcal{A}^T$. Additionally, $\mathcal{C} = \mathcal{C}^T$ represents the set of connections between corresponding nodes (i.e., between the same entity) on different layers. For clarity, we denote nodes in a given layer and in monoplex networks with the symbols u, v, w; and we denote indices in a supra-adjacency matrix with the symbols i, j, h. We also define $l(u) = \{(u, \alpha) \in V | \alpha \in L\}$ as the set of supra-adjacency matrix indices that correspond to node u.

The local clustering coefficient C_u of node u in an unweighted monoplex network is the number of triangles that include node u divided by the number of connected triples with node u in the center [3, 33]. The local clustering coefficient is a measure of transitivity [32], and it can be interpreted as the density of the focal node's neighborhood. For our purposes, it is convenient to define a local clustering coefficient C_u as the number of 3-cycles t_u that start and end at the focal node u divided by the number of 3-cycles d_u such that the second step occurs in a complete graph (i.e., assuming that the neighborhood of the focal node is as dense as possible). In mathematical terms, $t_u = (\mathbf{A}^3)_{uu}$ and $d_u = (\mathbf{AFA})_{uu}$, where $\mathbf{A}$ is the adjacency matrix of the graph and $\mathbf{F}$ is the adjacency matrix of a complete network with no self-loops (i.e., $\mathbf{F} = \mathbf{J} - \mathbf{I}$, where $\mathbf{J}$ is a complete square matrix of 1s and $\mathbf{I}$ is the identity matrix).

The *local clustering coefficient* is then $C_u = t_u/d_u$. This is equivalent to the usual definition of the clustering coefficient: $C_u = t_u/(k_u(k_u-1))$, where k_u is the degree of node u. One can obtain a single global clustering coefficient for a monoplex network either by averaging C_u over all nodes or by computing $C = \frac{\sum_u t_u}{\sum_u d_u}$. Henceforth, we will use the term *global clustering coefficient* for the latter quantity.

Triads on Multiplex Networks

In addition to 3-cycles (i.e., triads) that occur within a single layer, multiplex networks also contain cycles that can traverse different additional layers but still have 3 intra-layer steps. Such cycles are important for analysis of transitivity in multiplex networks. In social networks, for example, transitivity involves social ties across multiple social environments [1, 40]. In transportation networks, there typically exist several transport means to return to one's starting location, and different combinations of transportation modes are important in different cities [41]. For dynamical processes on multiplex networks, it is important to consider 3-cycles that traverse different numbers of layers, so we need to take them into account when defining a multiplex clustering coefficient. We define a *supra-walk* as a walk on a multiplex network in which, either before or after each intra-layer step, a walk can either continue on the same layer or change to an adjacent layer. We represent this choice using the following matrix:

$$\widehat{\mathcal{C}} = \beta\mathcal{I} + \gamma\mathcal{C}\,, \tag{1}$$

where the parameter β is a weight that accounts for the walker staying in the current layer and γ is a weight that accounts for the walker stepping to another layer. In a supra-walk, a *supra-step* then consists either of only a single intra-layer step or of a step that implies changing between a pair of layers (either before or after having an intra-layer step). In the latter scenario, we impose a further constraint that two consecutive inter-layer steps are not allowed. The number of 3-cycles for node i is then

$$t_{M,i} = [(\mathcal{A}\widehat{\mathcal{C}})^3 + (\widehat{\mathcal{C}}\mathcal{A})^3]_{ii}\,, \tag{2}$$

where the first term corresponds to cycles in which the inter-layer step is taken after an intra-layer one and the second term corresponds to cycles in which the inter-layer step is taken before an intra-layer one. We can simplify Eq. **2** by exploiting the fact that both $\mathcal{A}$ and $\mathcal{C}$ are symmetric. This yields

$$t_{M,i} = 2[(\mathcal{A}\widehat{\mathcal{C}})^3]_{ii}\,. \tag{3}$$

It is useful to decompose multiplex clustering coefficients that are defined in terms of multilayer cycles into so-called *elementary cycles* by expanding Eq. **3** and writing it in terms of the matrices $\mathcal{A}$ and $\mathcal{C}$. That is, we write $t_{M,i} = \sum_{\mathcal{E}\in\mathscr{E}} w_{\mathcal{E}}(\mathcal{E})_{ii}$, where $\mathscr{E}$ denotes the set of elementary cycles. We can use symmetries in our definition of cycles and thereby express all of the elementary cycles in a standard form with terms in the set $\mathscr{E} = \{\mathcal{AAA}, \mathcal{AACAC}, \mathcal{ACAAC}, \mathcal{ACACA}, \mathcal{ACACAC}\}$. See Fig. 1 for an illustration of elementary cycles and the *SI Appendix* for details on deriving the elementary cycles. Note that the above definition of 3-cycle is not the only possible one in multiplex networks. In the *SI Appendix*, we discuss alternative definitions, some of which lead to more elementary cycles than the ones that we just enumerated.

To define multiplex clustering coefficients, we need both the number of cycles $t_{*,i}$ and a normalization $d_{*,i}$, where $*$ stands for any type of cycle. To determine the normalization, it is natural to follow the same procedure as with monoplex clustering coefficients and use a complete multiplex network $\mathcal{F} = \bigoplus_\alpha \mathbf{F}^{(\alpha)}$, where $\mathbf{F}^{(\alpha)} = \mathbf{J}^{(\alpha)} - \mathbf{I}^{(\alpha)}$ is the adjacency matrix for a complete graph on layer α. We can then proceed from any definition of $t_{*,i}$ to $d_{*,i}$ by replacing the second intra-layer step with a step in the complete multiplex network. We obtain $d_{M,i} = 2(\mathcal{A}\widehat{\mathcal{C}}\mathcal{F}\widehat{\mathcal{C}}\mathcal{A}\widehat{\mathcal{C}})_{ii}$ for $t_{M,i} = 2[(\mathcal{A}\widehat{\mathcal{C}})^3]_{ii}$. Similarly, one can use any other definition of a cycle (e.g., any of the elementary cycles or the cycles discussed in the *SI Appendix*) as a starting point for defining a clustering coefficient.

The above formulation allows us to define local and global clustering coefficients for multiplex graphs analogously to monoplex networks. We can calculate natural multiplex analog to the usual monoplex local clustering coefficient for any node i of the supra-graph. Additionally, in a multiplex network, a node u of an intra-layer network allows an intermediate description for clustering between local and the global clustering coefficients. We define

$$c_{*,i} = \frac{t_{*,i}}{d_{*,i}}\,, \tag{4}$$

$$C_{*,u} = \frac{\sum_{i\in l(u)} t_{*,i}}{\sum_{i\in l(u)} d_{*,i}}\,, \tag{5}$$

$$C_* = \frac{\sum_i t_{*,i}}{\sum_i d_{*,i}}\,, \tag{6}$$

where $l(u)$ is as defined before.

We can decompose the expression in Eq. **6** in terms of the contributions from cycles that traverse exactly one, two, and three layers ($m = 1, 2, 3$ respectively) to give

$$t_{*,i} = t_{*,1,i}\beta^3 + t_{*,2,i}\beta\gamma^2 + t_{*,3,i}\gamma^3\,, \tag{7}$$

$$d_{*,i} = d_{*,1,i}\beta^3 + d_{*,2,i}\beta\gamma^2 + d_{*,3,i}\gamma^3\,, \tag{8}$$

$$C_*^{(m)} = \frac{\sum_i t_{*,m,i}}{\sum_i d_{*,m,i}}\,. \tag{9}$$

We can similarly decompose Eqs. **4** and **5**. Using the decomposition in Eq. **7** yields an alternative way to average over contributions from the three types of cycles:

$$C_*(\omega_1, \omega_2, \omega_3) = \sum_{m}^{3} \omega_m C_*^{(m)}\,, \tag{10}$$

where $\vec{\omega}$ is a vector that gives the relative weights of the different contributions. There are also analogs of Eq. **10** for the clustering coefficients defined in Eqs. **4** and **5**. The clustering coefficients in Eqs. **4–6** all depend on the values of the parameters β and γ, but the dependence vanishes if $\beta = \gamma$. Unless we explicitly indicate otherwise, we assume in our calculations that $\beta = \gamma$.

Results and Discussions

We investigate transitivity in empirical multiplex networks by calculating clustering coefficients. In Table I, we give the values of layer-decomposed global clustering coefficients for multiplex networks (four social networks and two transportation networks) constructed from real data. To help give context to the values, the table also includes the clustering-coefficient values that we obtain for ER networks with matching edge densities in each layer. Additionally, note that the two transportation networks have different numbers of nodes in different layers (i.e., they are not "node-aligned" [4]). As we will now discuss, multiplex clustering coefficients give insights that are impossible to infer by calculating weighted clustering coefficients for aggregated networks or even by calculating them separately for each layer of a multiplex network.

For each social network in Table I, note that $C_M < C_M^{(1)}$ and $C_M^{(1)} > C_M^{(2)} > C_M^{(3)}$. Consequently, the primary contribution to the triadic structure of these multiplex networks arises from 3-cycles that stay within a given layer. To check that the ordering of the different clustering coefficients is not an artifact of the heterogeneity of densities of the different layers, we also calculate the expected values of the clustering coefficients in ER networks with identical edge densities to the data. We observe that all clustering coefficients exhibit larger inter-layer transitivities than would be expected in a ER networks with identical edge densities, and that the same ordering relationship is also true. We speculate that the reason for this observation is simple one: individuals that close triads between different layers are likely also to "meet" and then establish relations in a single layer.

Conversely, the transportation networks that we examine exhibit the opposite pattern. For the London Underground metro ("Tube") network, for example, we observe that $C_M^{(3)} > C_M^{(2)} > C_M^{(1)}$. This reflects the fact that single lines in the Tube are designed to avoid redundant connections. A single-layer triangle would require a line to make a full loop within 3 stations. Two-layer triangles, which are a bit more frequent than single-layer ones, entail that two lines run in almost parallel directions and that one line jumps over a single station. For 3-layer triangles, the geographical constraints do not matter because one can construct a triangle with three straight lines.

We also analyze the triadic local closure of the Kapferer tailor shop social network by examining the local clustering-coefficient values. In Fig. 2A, we show a comparison of the layer-decomposed local clustering coefficients (also see Fig. 6a of [38]). Observe that the condition $c_{M,i}^{(1)} > c_{M,i}^{2} > c_{M,i}^{(3)}$ holds for most of the nodes. In Fig. 2B, we subtract the expected values of the clustering coefficients of nodes in a network generated with the configuration model from the corresponding clustering-coefficient values observed in the data to discern whether the relative order of the local clustering coefficients is to be expected from an associated random network (with the same layer densities and degree sequences as the data). Similar to the results for the global clustering coefficients, we see that taking a null model into account lessen the difference between the coefficients counting different numbers of layers but does not completely remove it.

We investigate the dependence of local triadic structure on degree for one social and one transportation network. In Fig. 3A, we show how the different multiplex clustering coefficients depend on the unweighted degrees of the nodes in the aggregated network in the Kapferer tailor shop. Note that the relative order of the mean clustering coefficients is independent of the degree. In Fig. 3B, we illustrate that the aggregated network for the airline transportation network exhibits a non-constant difference between the curves of $C_{M,u}$ and the weighted clustering coefficient $C_{Z,u}$ (see *Materials and Methods*). Using a global normalization $-$for $C_{Z,u}$, see *Materials and Methods*$-$ thus reduces the clustering coefficient around the small airports much more than it does for the large airports. That, in turn, introduces a bias.

The airline network is organized differently from the London Tube network: each layer encompasses flights from a single airline. We observe that the two-layer global clustering coefficient is larger than the single-layer one for hubs (high-degree nodes) in the airline network, but it is smaller for small airports (low-degree nodes), as seen from Fig. 3B. However, the global clustering coefficient counts the total number of 3-cycles and connected triplets and it thus gives more weight to high-degree nodes than low-degree nodes, and we find that the global clustering coefficients for the airline network satisfy $C_M^{(2)} > C_M^{(1)} > C_M^{(3)}$. The intra-airline clustering coefficients have small values, presumably because it is not in the interest of an airline to introduce new flights between two airports that can already be reached by two flights via the same airline through some major airport. The two-layer cycles correspond to cases in which an airline has a connection from an airport to two other airports and a second airline has a direct connection between those two airports. Completing a three-layer cycle requires using three distinct airlines, and this type of congregation of airlines to the same area is not frequent in the data: the three-layer cycles are more likely than the single-layer ones only for few of the largest airports.

Conclusions

We derived measurements of transitivity for multiplex networks by developing multiplex generalizations of triad relations and clustering coefficients. By using examples from empirical data in diverse settings, we showed that different notions of multiplex transitivity are important in different situations. For example, the balance between intra-layer versus inter-layer clustering is different in social versus transportation networks (and even in different types of networks within each category, as we illustrated explicitly for transportation networks), reflecting the fact that multilayer transitivity can arise from different mechanisms. Such differences are rooted in the new degrees of freedom that arise from inter-layer connections and are invisible to calculations of clustering coefficients on single-layer networks obtained via aggregation. In other words, this is inherently a multilayer phenomenon: all of these diverse flavors of transitivity reduce to the same phenomenon when one throws away the multilayer information. Generalizing clustering coefficients for multiplex networks makes it possible to explore such phenomena and to gain deeper insights into different types of transitivity in networks. The existence of multiple types of transitivity also has important implications for multiplex network motifs and multiplex community structure. In particular, our work on multiplex clustering coefficients demonstrates that definitions of all clustering notions for multiplex networks need to be able to handle such features.

MATERIALS AND METHODS

Supra-Adjacency Matrices

We represent a multiplex network using a finite sequence of graphs $\{G^\alpha\}_\alpha$, with $G^\alpha = (V^\alpha, E^\alpha)$, where $\alpha \in L$ is the set of layers. Without loss of generality, we assume that $L = \{1, \ldots, b\}$ and $V^\alpha \subseteq \{1, \ldots, n\}$. For simplicity, we examine unweighted and undirected multiplex networks. We define the intra-layer supra-graph as $G_A = (V, E_A)$, where the set of nodes is $V = \sqcup_\alpha V^\alpha = \bigcup_\alpha \{(u, \alpha) : u \in V^\alpha\}$ and the set of edges is $E_A = \bigcup_\alpha \{((u, \alpha), (v, \alpha)) : (u, v) \in E^\alpha\}$. We also define the coupling supra-graph $G_C = (V, E_C)$ using the same sets of nodes and the edge set $E_C = \bigcup_{\alpha,\beta} \{((u, \alpha), (u, \beta)) : u \in V^\alpha, u \in V^\beta, \alpha \neq \beta\}$. If $((u, \alpha), (u, \beta)) \in E_C$, we say that (u, α) and (u, β) are "interconnected." We say that a multiplex network is "node-aligned" [4] if all layers share the same set of nodes (i.e., if $V^\alpha = V^\beta$ for all α and β). The supra-graph is $\bar{G} = (V, \bar{E})$, where $\bar{E} = E_A \cup E_C$; its corresponding adjacency matrix is the supra-adjacency matrix.

Clustering Coefficients on Aggregated Networks

A common way to study multiplex systems is to aggregate layers to obtain either multi-graphs or weighted networks, where the number of edges or the weight of an edge is the number of different types of edges between a pair of nodes [4]. One can then use any of the numerous ways to define clustering coefficients on weighted monoplex networks [42, 43] to calculate clustering coefficients on the aggregated network.

One of the weighted clustering coefficients is a special case of the multiplex clustering coefficient that we defined. References [39, 44, 45] calculated the weighted clustering coefficient as

$$C_{Z,u} = \frac{\sum_{vw} W_{uv} W_{vw} W_{wu}}{w_{\max} \sum_{v \neq w} W_{uv} W_{uw}} = \frac{(\mathbf{W}^3)_{uu}}{((\mathbf{W}(w_{\max}\mathbf{F})\mathbf{W})_{uu}}\,, \quad (11)$$

where $W_{uv} = \sum_{i \in l(u), j \in l(v)} A_{ij}$ is the weighted adjacency matrix $\mathbf{W}$. The elements of $\mathbf{W}$ are the weights of the edges, the quantity $w_{\max} = \max_{u,v} W_{uv}$ is the maximum weight in $\mathbf{W}$, and $\mathbf{F}$ is the adjacency matrix of the complete unweighted graph. We can define the global version C_Z of $C_{Z,u}$ by summing over all of the nodes in the numerator and the denominator of Eq. **11** (analogously to Eq. **6**).

The coefficients $C_{Z,u}$ and C_Z are related to our multiplex coefficients in node-aligned multiplex networks. Letting $\beta = \gamma = 1$ and summing over all layers yields $\sum_{i \in l(u)} ((\mathcal{A}\widehat{\mathcal{C}})^3)_{ii} = (\mathbf{W}^3)_{uu}$. That is, in this special case, the weighted clustering coefficients $C_{Z,u}$ and C_Z are equivalent to the corresponding multiplex clustering coefficients $C_{M,u}$ and C_M. That is, $C_{M,u}(\beta = \gamma) = \frac{w_{\max}}{b} C_{Z,u}$ and $C_M(\beta = \gamma) = \frac{w_{\max}}{b} C_Z$. We need the term $w_{\max}/b$ to match the normalizations because aggregation removes the information about the number of layers b, so the normalization must be based on the maximum weight instead of the number of layers. That is, a step in the complete weighted network is described by using $w_{\max}\mathbf{F}$ in Eq. **11** instead of using $b\mathbf{F}$. Note that this relationship between our multiplex clustering coefficient and the weighted clustering coefficient is only true for node-aligned multiplex networks. The normalization of our multiplex clustering coefficient depends on how many nodes are present in the local neighborhood of the focal node if all nodes are not shared between all layers. This is in contrast to the "global" normalization by $w_{\max}$ that the weighted clustering coefficient uses.

Clustering Coefficients in Erdős-Rényi (ER) networks

Almost all real networks contain some amount of transitivity, and it is often desirable to know if a network contains more transitivity that would be expected by chance. In order to answer this question, one typically compares clustering-coefficient values of a network to what would be expected from some random network that acts as a null model. The simplest random network to use is an Erdős-Rényi (ER) network.

The clustering coefficient in an unweighted monoplex ER network is equal to the probability p of an edge to exist. That is, the density of a neighborhood of a node, measured by the clustering coefficient, is the same as the density of the whole network for ER networks. In node-aligned multiplex networks with ER intra-layer graphs with connection probabilities p_α, we have the same result only if all of the layers are statistically identical (i.e., $p_\alpha = p$ for all α). However, heterogeneity among layers complicates the behavior of clustering coefficients; if the layers have different connection probabilities, then the expected value of the mean clustering coefficient is a nontrivial function of the connection probabilities (e.g., it is not always equal to the mean of the connection probabilities). For example, the formulas for the expected global layer-decomposed clustering coefficients are

$$\langle C_M^{(1)} \rangle = \frac{\sum_\alpha p_\alpha^3}{\sum_\alpha p_\alpha^2} \equiv \frac{\overline{p^3}}{\overline{p^2}}\,, \tag{12}$$

$$\langle C_M^{(2)} \rangle = \frac{3\sum_{\alpha\neq\beta} p_\alpha p_\beta^2}{(b-1)\sum_\alpha p_\alpha^2 + 2\sum_{\alpha\neq\beta} p_\alpha p_\beta}\,, \tag{13}$$

$$\langle C_M^{(3)} \rangle = \frac{\sum_{\alpha\neq\beta,\beta\neq\gamma,\gamma\neq\alpha} p_\alpha p_\beta p_\gamma}{(b-2)\sum_{\alpha\neq\beta} p_\alpha p_\beta}\,. \tag{14}$$

See the *SI Appendix* for the local clustering coefficients and for the empirical validation of our theoretical results.

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TABLE I: Clustering coefficients C_M, $C_M^{(1)}$, $C_M^{(2)}$, $C_M^{(3)}$ corresponding, respectively, to the global, one-layer, two-layer, and three-layer clustering coefficients for various networks. "Tailor shop": Kapferer tailor shop network ($n = 39$, $b = 4$) [46]. "Management": Krackhardt office cognitive social structures ($n = 21$, $b = 21$) [47]. "Families": Padgett Florentine families social network ($n = 16$, $b = 2$) [48]. "Bank": Roethlisberger and Dickson bank wiring room social network ($n = 14$, $b = 6$) [49]. "Tube": The London Underground (i.e., "The Tube") transportation network ($n = 314$, $b = 14$) [50]. "Airline": Network of flights between cities, in which each layer corresponds to a single airline ($n = 3108$, $b = 530$) [51]. The rows labeled "orig." have the clustering coefficients for the original networks, and the rows labeled "ER" have the expected value and the standard deviation of the clustering coefficient in an ER random network with exactly as many edges on each layer as in the original network. For the original values, we perform a two-tailed Z-test to test if the observed clustering coefficients could have been produced by the ER networks. Our notation is as follows: *: $p < 0.05$, **: $p < 0.01$ for Bonferroni-corrected tests with 24 hypothesis; ': $p < 0.05$, ": $p < 0.01$ for uncorrected tests. We symmetrize directed networks by considering two nodes to be connected if there is at least one edge between them. The social networks above are node-aligned multiplex graphs, but the transport networks are not. Reported values are averages over different numbers of realizations: 1.5×10^5 for Tailor shop, 1.5×10^3 for Airline, 1.5×10^4 for Management, 1.5×10^5 for Families, 1.5×10^4 for Tube, 1.5×10^5 for Bank.

		Tailor shop	Management	Families	Bank	Tube	Airline
C_M	orig.	0.319**	0.206**	0.223'	0.293**	0.056	0.101**
	ER	0.186 ± 0.003	0.124 ± 0.001	0.138 ± 0.035	0.195 ± 0.009	0.053 ± 0.011	0.038 ± 0.000
$C_M^{(1)}$	orig.	0.406**	0.436**	0.289'	0.537**	0.013"	0.100**
	ER	0.244 ± 0.010	0.196 ± 0.015	0.135 ± 0.066	0.227 ± 0.038	0.053 ± 0.013	0.064 ± 0.001
$C_M^{(2)}$	orig.	0.327**	0.273**	0.198	0.349**	0.043	0.150**
	ER	0.191 ± 0.004	0.147 ± 0.002	0.138 ± 0.040	0.203 ± 0.011	0.053 ± 0.020	0.041 ± 0.000
$C_M^{(3)}$	orig.	0.288**	0.192**	-	0.227**	0.314**	0.086**
	ER	0.165 ± 0.004	0.120 ± 0.001	-	0.186 ± 0.010	0.051 ± 0.043	0.037 ± 0.000

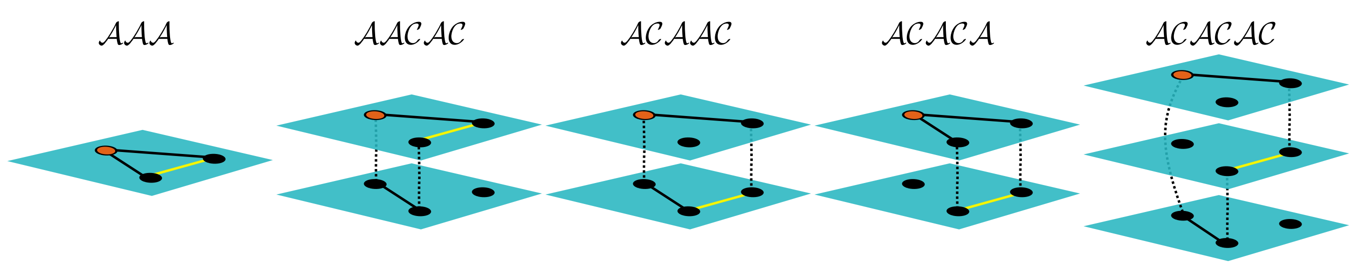

FIG. 1: Sketch of elementary cycles $\mathcal{AAA}$, $\mathcal{AACAC}$, $\mathcal{ACAAC}$, $\mathcal{ACACA}$, and $\mathcal{ACACAC}$. The orange node is the starting point of the cycle. The intra-layer edges are the solid lines, the intra-layer edges are the dotted lines, and the second intra-layer step is the yellow line.

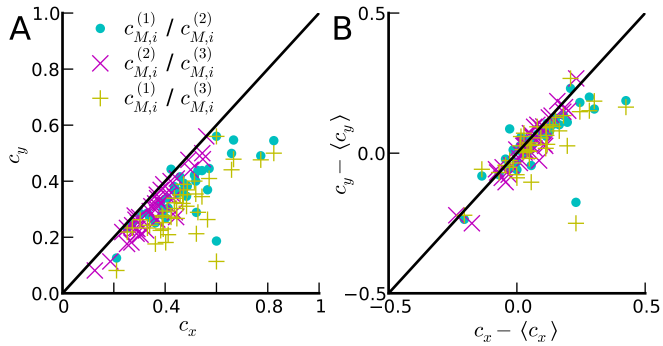

FIG. 2: Comparison of different local clustering coefficients in the Kapferer tailor-shop network. Each point corresponds to a node. (A) The raw values of the clustering coefficient. (B) The value of the clustering coefficients minus the expected value of the clustering coefficient for the corresponding node from a mean over 1000 realizations of a configuration model with the same degree sequence on each layer as in the original network. In a realization of the multiplex configuration each intra-layer network is an independent realization of monoplex configuration model.

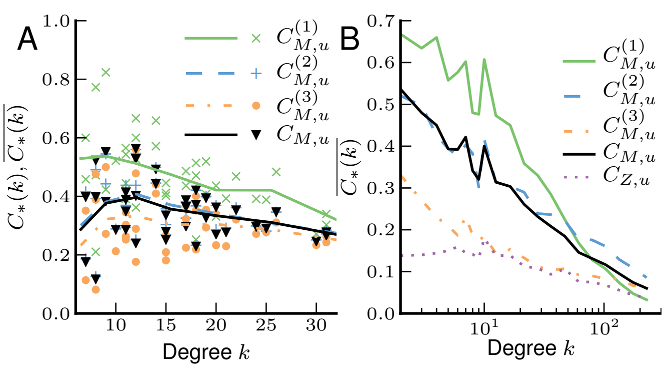

FIG. 3: Local clustering coefficients versus unweighted degree of the aggregated network for (A) the Kapferer tailor-shop network and (B) the airline network. The curves give the mean values of the clustering coefficients for a degree range (i.e., binning similar degrees). Note that the x-axe in panel (B) is in log scale.

SUPPLEMENTARY INFORMATION FOR "STRUCTURE OF TRIADIC RELATIONS IN MULTIPLEX NETWORKS"

Weighted Clustering Coefficients

There are two primary weighted clustering coefficients for monoplex networks that provide alternatives to the one that we discussed in the main text [52, 53]. They are

$$C_{O,u} = \frac{1}{w_{\max} k_u (k_u - 1)} \sum_{v,w} (W_{uv} W_{uw} W_{vw})^{1/3} \,, \quad (15)$$

$$C_{Ba,u} = \frac{1}{s_u (k_u - 1)} \sum_{v,w} \frac{(W_{uv} + W_{uw})}{2} A_{uv} A_{uw} A_{vw} \,, \quad (16)$$

where $\mathbf{A}$ is the unweighted adjacency matrix associated with the weighted adjacency matrix $\mathbf{W}$, the degree of node u is $k_u = \sum_v A_{uv}$, the strength of u is $s_u = \sum_v W_{uv}$, and the quantity $w_{\max} = \max_{u,v} W_{uv}$ is the maximum weight in $\mathbf{W}$.

Multiplex Clustering Coefficients in the Literature

Let $\mathbf{A}^{(\alpha)}$ denote the intra-layer adjacency matrix for layer α. If the multiplex network is weighted $\mathbf{W}^{(\alpha)}$ is used to denote the weight matrix (i.e., the weighted intra-layer adjacency matrix) for layer α. The weight matrix of the aggregated network is denoted by $\mathbf{W}$ (see *Materials and Methods* in the main text). The clustering coefficient that was defined in [34] for node-aligned multiplex networks is

$$C_{Be,u} = \frac{\sum_{v,w} \sum_\alpha A^{(\alpha)}_{uv} \sum_\beta A^{(\beta)}_{uw} \sum_\gamma A^{(\gamma)}_{uw}}{\sum_{v,w} \sum_\beta A^{(\beta)}_{uv} \sum_\alpha \max(A^{(\alpha)}_{uw}, A^{(\alpha)}_{vw})} \,, \quad (17)$$

which can be expressed in terms of the aggregated network as

$$C_{Be,u} = \frac{\sum_{v,w} W_{uv} W_{uw} W_{vw}}{\sum_{v,w} W_{uv} \sum_\alpha \max\left(A^{(\alpha)}_{uw}, A^{(\alpha)}_{vw}\right)} \,. \quad (18)$$

The numerator of Eq. (18) is the same as the numerator of the weighted clustering coefficient $C_{Z,u}$, but the denominator is different. Because of the denominator in Eq. (18), the values of the clustering coefficient $C_{Be,u}$ do not have to lie in the interval $[0, 1]$. For example, $C_{Be,u} = (n-2)b/n$ for a complete multiplex network (where n is the number of nodes in the multiplex network), so $C_{Be,u} > 1$ when $b > \frac{n}{n-2}$.

References [35, 36] defined a family of local clustering coefficients for directed and weighted multiplex networks:

$$C_{Br,u,t} = \frac{\sum_\alpha \sum_{v,w \in N(u,t)} (W^{(\alpha)}_{wv} + W^{(\alpha)}_{vw})}{2|N(u,t)|b} \,, \quad (19)$$

where $N(u,t) = \{v : |\{\alpha : A^{(\alpha)}_{uv} = 1 \quad \text{and} \quad A^{(\alpha)}_{vu} = 1\}| \geq t\}$, L is the set of layers, and t is a threshold. The clustering coefficient (19) does not yield the ordinary monoplex local clustering coefficient for unweighted (i.e., networks with binary weights) and undirected networks when it is calculated for the special case of a monoplex network (i.e., a multiplex network with one layer). Furthermore, its values are not normalized to lie between 0 an 1. For example, consider a complete multiplex network with n nodes and an arbitrary number of layers. In this case, the clustering coefficient (19) takes the value of $n-2$ for each node. If a multiplex network is undirected (and unweighted), then $C_{Br,u,t}$ can always be calculated when one is only given an aggregated network and the total number of layers in the multiplex network. As an example, for the threshold value $t = 1$, one obtains

$$C_{Br,u,1} = \frac{1}{k_u b} \sum_{v,w} \frac{W_{vw}}{2} A_{uv} A_{uw} A_{vw} \,, \quad (20)$$

where $\mathbf{A}$ is the binary adjacency matrix corresponding to the weighted adjacency matrix $\mathbf{W}$ and $k_u = \sum_v A_{uv}$ is the degree of node u.

Reference [37] defined a clustering coefficient for multiplex networks that are not necessarily node-aligned as

$$C_{Cr,u} = \frac{2 \sum_\alpha |\overline{E}_\alpha(u)|}{\sum_\alpha |\Gamma_\alpha(u)|(|\Gamma_\alpha(u)| - 1)} \,, \quad (21)$$

where L is again the set of layers, $\Gamma_\alpha(u) = \Gamma(u) \cap V_\alpha$, the quantity $\Gamma(u)$ is the set of neighbors of node u in the aggregated network, V_α is the set of nodes in layer α, and $\overline{E}_\alpha(u)$ is the set of edges in the induced subgraph of the aggregated network that is spanned by $\Gamma_\alpha(u)$. For a node-aligned multiplex network, $V_\alpha = V$ and $\Gamma_\alpha(u) = \Gamma(u)$, so one can write

$$C_{Cr,u} = \frac{\sum_{vw} A_{uv} W_{vw} A_{wu}}{b \sum_{v \neq w} A_{uv} A_{wu}} \,, \quad (22)$$

which is a local clustering coefficient of the aggregated network.

Battiston et al. [38] defined two versions of clustering coefficients for node-aligned multiplex networks:

$$C_{Bat1,u} = \frac{\sum_\alpha \sum_{\beta \neq \alpha} \sum_{v \neq u, w \neq u} A^{(\alpha)}_{uv} A^{(\beta)}_{vw} A^{(\alpha)}_{wu}}{(b-1) \sum_\alpha \sum_{v \neq u, w \neq u} A^{(\alpha)}_{uv} A^{(\alpha)}_{wu}} \,, \quad (23)$$

$$C_{Bat2,u} = \frac{\sum_\alpha \sum_{\beta \neq \alpha} \sum_{\gamma \neq \alpha,\beta} \sum_{v \neq u, w \neq u} A^{(\alpha)}_{uv} A^{(\gamma)}_{vw} A^{(\beta)}_{wu}}{(b-2) \sum_\alpha \sum_{\beta \neq \alpha} \sum_{v \neq u, w \neq u} A^{(\alpha)}_{uv} A^{(\beta)}_{wu}} \,. \quad (24)$$

The first definition, $C_{Bat1,u}$, counts the number of $\mathcal{ACACA}$-type elementary cycles and the second definition, $C_{Bat2,u}$, counts the 3-layer elementary cycles $\mathcal{ACACAC}$. In both of these definitions, note that the sums in the denominators allow terms in which $v = w$, so a complete multiplex network has a local clustering coefficient of $(n-1)/(n-2)$ for every node.

Reference [29] proposed definitions for global clustering coefficients using a tensorial formalism for multilayer networks; when representing a multiplex network as a third-order tensor, the formulas in [29] reduce to clustering coefficients that we propose in the present article (Eq. (6) of the main text). Parshani et al. [54] defined an "inter-clustering coefficient" for two-layer interdependent networks that can be interpreted as multiplex networks [4, 55–57]. Their definition is similar to edge "overlap" [38]; in our framework, it corresponds to counting 2-cycles of type $(\mathcal{A}\mathcal{C})^2$. A few other scholars [58, 59] have also defined generalizations of clustering coefficients for multilayer networks that cannot be interpreted as multiplex networks [4].

In Table II, we show a summary of the properties satisfied by several different (local and global) clustering coefficients. In particular, we check the following properties: (1) The value of the clustering coefficient reduces to the values of the associated monoplex clustering coefficient for a single-layer network. (2) The value of the clustering coefficient is normalized so that it takes values that are less than or equal to 1. (All of the clustering coefficients are nonnegative.) (3) The clustering coefficient has a value of p in a large (i.e., when the number of nodes $n \to \infty$) node-aligned multiplex network in which each layer is an independent ER network with an edge probability of p in each layer. (4) Suppose that we construct a multiplex network by replicating the same given monoplex network in each layer. The clustering coefficient for the multiplex network has the same value as for the monoplex network. (5) There exists a version of the clustering coefficient that is defined for each node-layer pair separately. (6) The clustering coefficient is defined also for multiplex networks that are not node-aligned.

Other Possible Definitions of Cycles

There are many possible ways to define cycles in multiplex networks. If we relax the condition of disallowing two consecutive inter-layer steps, then we can write

$$t_{SM,i} = [(\widehat{\mathcal{C}}\mathcal{A}\widehat{\mathcal{C}})^3]_{ii}\,, \tag{25}$$

$$t_{SM',i} = [(\widehat{\mathcal{C}}'\mathcal{A} + \mathcal{A}\widehat{\mathcal{C}}')^3]_{ii}\,, \tag{26}$$

where $\widehat{\mathcal{C}}' = \frac{1}{2}\beta\mathcal{I} + \gamma\mathcal{C}$. Unlike the matrices in definition Eq. (2) in the main text, the matrices $\widehat{\mathcal{C}}\mathcal{A}\widehat{\mathcal{C}}$ and $\widehat{\mathcal{C}}'\mathcal{A} + \mathcal{A}\widehat{\mathcal{C}}'$ are symmetric. We can thus interpret them as weighted adjacency matrices of symmetric supra-graphs, and we can then calculate cycles and clustering coefficients in these supra-graphs.

One might want to forbid the option of staying inside of a layer in the first step of the second term of Eq. (26). We can then write

$$t_{M',i} = [(\mathcal{A}\widehat{\mathcal{C}})^3 + \gamma\mathcal{C}\mathcal{A}(\widehat{\mathcal{C}}\mathcal{A})^2]_{ii}\,. \tag{27}$$

With this restriction, cycles that traverse two adjacent edges to the focal node i are only calculated two times instead of four times. Similar to Eq. (3) in the main text, we can simplify Eq. (27) to obtain

$$t_{M',i} = [2(\mathcal{A}\widehat{\mathcal{C}})^2\mathcal{A}\widehat{\mathcal{C}}']_{ii}\,. \tag{28}$$

In Table III, we show the values of the clustering coefficient calculated using this last definition of cycle for the same networks studied in the main text.

Defining Multiplex Clustering Coefficients Using Auxiliary Networks

An elegant way to generalize clustering coefficients for multiplex networks is to define a new (possibly weighted) auxiliary supra-graph G_M so that one can define cycles of interest as weighted 3-cycles in G_M. Once we have a function that produces the auxiliary supra-adjacency matrix $\mathcal{M} = \mathcal{M}(\mathcal{A}, \mathcal{C})$, we can define the auxiliary complete supra-adjacency matrix $\mathcal{M}^F = \mathcal{M}(\mathcal{F}, \mathcal{C})$. One can then define a local clustering coefficient for node-layer pair i with the formula

$$c_i = \frac{(\mathcal{M}^3)_{ii}}{(\mathcal{M}\mathcal{M}^F\mathcal{M})_{ii}}\,. \tag{29}$$

As for a monoplex network, the denominator written in terms of the complete matrix is equivalent to that usual one written in terms of connectivity. We thereby consider the connectivity of a node in the supra-graph induced by the matrix $\mathcal{M}$. We refer to the matrix $\mathcal{M}$ as the *multiplex walk matrix* because it encodes the permissible steps in a multiplex network. When $\mathcal{M}$ is equal to $\mathcal{A}\widehat{\mathcal{C}}$ or $\widehat{\mathcal{C}}\mathcal{A}$, the induced supra-graph is directed, so one needs to distinguish between the in-connectivity and out-connectivity degrees.

A key advantage of defining clustering coefficients using an auxiliary supra-graph is that one can then use the it to calculate other diagnostics (e.g., degree or strength) for nodes. One can thereby investigate correlations between clustering-coefficient values and the size of the multiplex neighborhood of a node. (The size of the neighborhood is the number of nodes that are reachable in a single step via connections defined by matrix $\mathcal{M}$.)

The symmetric multiplex walk matrices of Eqs. (25) and (26) are

$$\mathcal{M}_{SM} = \widehat{\mathcal{C}}\mathcal{A}\widehat{\mathcal{C}}\,, \tag{30}$$

$$\mathcal{M}_{SM'} = (\widehat{\mathcal{C}}'\mathcal{A} + \mathcal{A}\widehat{\mathcal{C}}')\,. \tag{31}$$

To avoid double-counting intra-layer steps in the definition of $\mathcal{M}_{SM'}$, we need to rescale either the intra-layer weight parameter β (i.e., we can write $\widehat{\mathcal{C}}' = \beta'\mathcal{I} + \gamma\mathcal{C} = \frac{1}{2}\beta\mathcal{I} + \gamma\mathcal{C}$) or the inter-layer weight parameter γ [i.e., we can write $\widehat{\mathcal{C}}' = \beta\mathcal{I} + \gamma'\mathcal{C} = \beta\mathcal{I} + 2\gamma\mathcal{C}$ and also define $\mathcal{M}_{SM'} = \frac{1}{2}(\mathcal{A}\widehat{\mathcal{C}}' + \widehat{\mathcal{C}}'\mathcal{A})$].

Consider a supra-graph induced by a multiplex walk matrix. The distinction between the matrices $\mathcal{M}_{SM}$ and $\mathcal{M}_{SM'}$ is that $\mathcal{M}_{SM}$ also includes terms of the form $\mathcal{C}\mathcal{A}\mathcal{C}$ that take into account walks that have an inter-layer step ($\mathcal{C}$) followed by an intra-layer step ($\mathcal{A}$) and then another inter-layer step ($\mathcal{C}$). Therefore, in the supra-graph induced by $\mathcal{M}_{SM}$, two nodes in

TABLE II: Summary of the properties of the different multiplex clustering coefficients. The notation $C_{*(,u)}$ means that the property holds for both the global version and the local version of the associated clustering coefficient.

Property	$C_{M(,u)}$	$C_{Be,u}$	$C_{Z(,u)}$	$C_{Ba,u}$	$C_{O,u}$	$C_{Br,u}$	$C_{Cr,u}$	$C_{Bat(1,2),u}$
(1) Reduces to monoplex c	✓	✓	✓	✓	✓		✓	
(2) $C_* \leq 1$	✓		✓	✓	✓		✓	✓
(3) $C_* = p$ in multiplex ER	✓						✓	
(4) Monoplex C for copied layers	✓		✓	✓	✓		✓	
(5) Def. for node-layer pairs	✓							
(6) Def. for non-node-aligned	✓						✓	

TABLE III: Clustering coefficients (rows) for the same networks (columns) from Table 1 in the main text. For the Tube and the Airline networks, we only calculate clustering coefficients for non-node-aligned networks.

CC	Families	Bank	Tailor shop	Management	Tube	Airline
$C_{M'}$	0.218	0.289	0.320	0.206	0.070	0.102
$C_{M'}^{(1)}$	0.289	0.537	0.406	0.436	0.013	0.100
$C_{M'}^{(2)}$	0.202	0.368	0.338	0.297	0.041	0.173
$C_{M'}^{(3)}$	-	0.227	0.288	0.192	0.314	0.086
$C_{M'}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$	0.164	0.377	0.344	0.309	0.123	0.120
$\overline{C_{Cr,u}}$	0.342	0.254	0.308	0.150	0.038	0.329
$\overline{C_{Ba,u}}$	0.195	0.811	0.612	2.019	-	-
$\overline{C_{Br,u}}$	0.674	1.761	4.289	1.636	-	-
$\overline{C_{O,u}}$	0.303	0.268	0.260	0.133	-	-
$\overline{C_{Be,u}}$	0.486	0.775	0.629	0.715	-	-
$\overline{C_{Bat1,u}}$	0.159	0.199	0.271	0.169	-	-
$\overline{C_{Bat2,u}}$	-	0.190	0.282	0.179	-	-

the same layer that are not connected in that layer can be connected nodes if the same nodes are connected in another layer.

The matrix $\widehat{\mathcal{C}}$ sums the contributions of all node-layer pairs that share the same node when $\beta = \gamma = 1$. In other words, if we associate a vector of the canonical basis e_i to each node-layer pair i and denote by $\Gamma_C((u,\alpha)) = \{(u,\beta)|\beta \in L\}$ all node-layer pairs sharing the same node, then

$$\widehat{\mathcal{C}} e_i = \sum_{j \in \Gamma_C(i)} e_j \tag{32}$$

produces a vector with entries equal to 1 for nodes that belong to the basis vector and 0 for nodes that do not. Consequently, $\mathbf{M}_{SM}$ is particularly interesting, because it is related to the weighted adjacency matrix of the aggregated graph for $\beta = \gamma = 1$. That is,

$$(\widehat{\mathcal{C}}\mathcal{A}\widehat{\mathcal{C}})_{ij} = W_{uv}, \qquad i \in l(u), j \in l(v). \tag{33}$$

One can also write the multiplex clustering coefficient induced by Eq. (2) in terms of the auxiliary supra-adjacency matrix by considering Eq. (3), which is a simplified version of the equation that counts cycles only in one direction:

$$\mathcal{M}_M = \sqrt[3]{2}\mathcal{A}\widehat{\mathcal{C}}\,. \tag{34}$$

The matrix $\mathcal{M}_M$ is not symmetric, which implies that the associated graph is a directed supra-graph. Nevertheless, the clustering coefficient induced by $\mathcal{M}_M$ is the same as that induced by its transpose $\mathcal{M}_M^T$ if $\mathcal{A}$ is symmetric.

Expressing Clustering Coefficients Using Elementary 3-Cycles

We now give a detailed explanation of the process of decomposing any of our walk-based clustering coefficients into elementary cycles. An elementary cycle is a term that consists of products of the matrices $\mathcal{A}$ and $\mathcal{C}$ (i.e., there are no sums) after one expands the expression for a cycle (which is a weighted sum of such terms). Because we are only interested in the diagonal elements of the terms and we consider only undirected intra-layer supra-graphs and coupling supra-graphs, we can transpose the terms and still write them in terms of the matrices $\mathcal{A}$ and $\mathcal{C}$ rather than also using their transposes. There are also multiple ways of writing non-symmetric elementary cycles [e.g., $(\mathcal{AACAC})_{ii} = (\mathcal{CACAA})_{ii}$].

We adopt a convention in which all elementary cycles are transposed so that we select the one in which the first element is $\mathcal{A}$ rather than $\mathcal{C}$ when comparing the two versions of the term from left to right. That is, for two equivalent terms, we choose the one that comes first in alphabetical order. To calculate the clustering coefficients that we defined in the present supplement, we also need to include elementary cycles that start and end in an inter-layer step. The set of elementary 3-cycles is thus $\mathscr{E} = \{\mathcal{AAA}, \mathcal{AACAC}, \mathcal{ACAAC}, \mathcal{ACACA}, \mathcal{ACACAC}, \mathcal{CAAAC}, \mathcal{CAACAC}, \mathcal{CACACAC}\}$.

We now write our clustering coefficients using elementary 3-cycles. We obtain the normalization formulas by using the elementary 3-cycles, but replacing the second $\mathcal{A}$ term with $\mathcal{F}$. This yields a standard form for any of our local multiplex clustering coefficients:

$$c_{*,i} = t_{*,i}/d_{*,i}\,, \tag{35}$$

where

$$\begin{aligned} t_{*,i} = [&w_{\mathcal{AAA}}\mathcal{AAA} + w_{\mathcal{AACAC}}\mathcal{AACAC} + w_{\mathcal{ACAAC}}\mathcal{ACAAC} \\ &+ w_{\mathcal{ACACA}}\mathcal{ACACA} + w_{\mathcal{ACACAC}}\mathcal{ACACAC} \\ &+ w_{\mathcal{CAAAC}}\mathcal{CAAAC} + w_{\mathcal{CAACAC}}\mathcal{CAACAC} \\ &+ w_{\mathcal{CACACAC}}\mathcal{CACACAC}]_{ii} \end{aligned} \tag{36}$$

$$\begin{aligned} d_{*,i} = [&w_{\mathcal{AAA}}\mathcal{AFA} + w_{\mathcal{AACAC}}\mathcal{AFCAC} + w_{\mathcal{ACAAC}}\mathcal{ACFAC} \\ &+ w_{\mathcal{ACACA}}\mathcal{ACFCA} + w_{\mathcal{ACACAC}}\mathcal{ACFCAC} \\ &+ w_{\mathcal{CAAAC}}\mathcal{CAFAC} + w_{\mathcal{CAACAC}}\mathcal{CAFCAC} \\ &+ w_{\mathcal{CACACAC}}\mathcal{CACFCAC}]_{ii}\,, \end{aligned} \tag{37}$$

where i is a node-layer pair and the $w_{\mathcal{E}}$ coefficients are scalars that correspond to the weights for each type of elementary cycle. (These weights are different for different types of clustering coefficients; one can choose whatever is appropriate for a given problem.) Note that we have absorbed the parameters β and γ into these coefficients (see below and Table IV). We illustrate the possible elementary cycles in Fig. 1 of the main text and in Fig. 4 of the present supplement.

One can even express the cycles that include two consecutive inter-layer steps in the standard form of Eqs. (36)–(37) for node-aligned multiplex networks, because $\mathcal{CC} = (b-1)\mathcal{I} + (b-2)\mathcal{C}$ in this case. Without the assumption that $\beta = \gamma = 1$, the expansion for the coefficient c_{SM} is cumbersome because it includes coefficients $\beta^k\gamma^h$ with all possible combinations of k and h such that $k + h = 6$ and $h \neq 1$. Furthermore, in the general case, it is not possible to infer the number of layers in which a walk traverses an intra-layer edge based on the exponents of β and γ for c_{SM} and $c_{SM'}$. For example, in $c_{SM'}$, the intra-layer elementary triangle $\mathcal{AAA}$ includes a contribution from both β^3 (i.e., the walk stays in the original layer) and $\beta\gamma^2$ (i.e., the walk visits some other layer but then comes back to the original layer without traversing any intra-layer edges while it was gone). Moreover, all of the terms with b arise from a walk moving to a new layer and then coming right back to the original layer in the next step. Because there are $b-1$ other layers from which to choose, the influence of cycles with such transient layer visits is amplified by the total number of layers in a network. That is, adding more layers (even ones that do not contain any edges) changes the relative importance of different types of elementary cycles.

In Table IV, we show the values of the coefficients $w_{\mathbf{E}}$ for the different ways that we defined 3-cycles in multiplex networks. In Table V, we show their corresponding expansions in terms of elementary cycles for the case $\beta = \gamma = 1$. These cycle decompositions illuminate the difference between $c_{M.i}$, $c_{M',i}$, $c_{SM,i}$, and $c_{SM',i}$. The clustering coefficient $c_{M,i}$ gives equal weight to each elementary cycle, whereas $c_{M',i}$ gives half of the weight to $\mathcal{AAA}$ and $\mathcal{ACACA}$ cycles (i.e., the cycles that include an implicit double-counting of cycles) as compared to the other cycles.

A Simple Example

We now use a simple example (see Fig. 5) to illustrate the differences between the different notions of a multiplex clustering coefficient. Consider a two-layer multiplex network with three nodes in layer a and two nodes in layer b. The three node-layer pairs in layer a form a connected triple, and the two exterior node-layer pairs of this triple are connected to the two node-layer pairs in layer b; these last two node-layer pairs are connected to each other.

The adjacency matrix $\mathcal{A}$ for the intra-layer graph is

$$\mathcal{A} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \tag{38}$$

and the adjacency matrix $\mathcal{C}$ of the coupling supra-graph is

$$\mathcal{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}. \tag{39}$$

Thus, the supra-adjacency matrix is

$$\bar{\mathcal{A}} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}. \tag{40}$$

The multiplex walk matrix $\mathcal{M}_M$ is

$$\mathcal{M}_M = \sqrt[3]{2} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix}, \tag{41}$$

and we note that it is not symmetric. For example, node-layer pair $(2, b)$ is reachable from $(1, a)$, but node-layer pair $(1, a)$

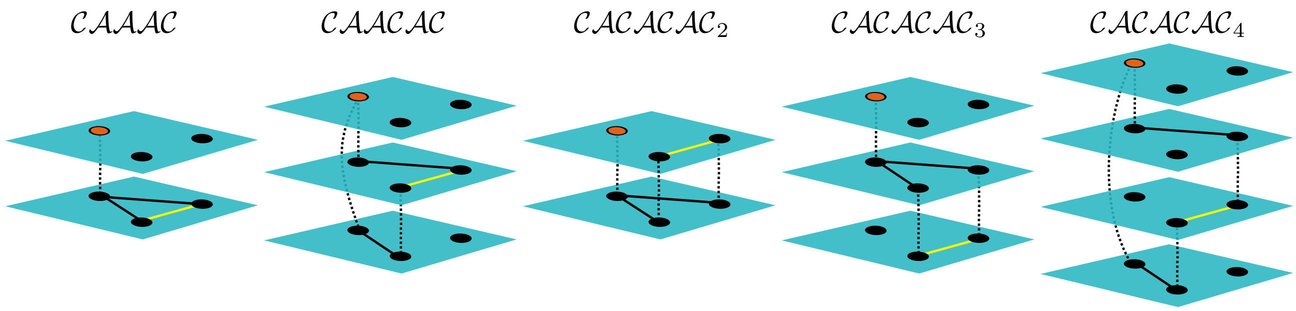

FIG. 4: Sketches of elementary cycles for which both the first and the last step are allowed to be an inter-layer step. These elementary cycles are $\mathcal{CAAAC}$, $\mathcal{CAACAC}$, and $\mathcal{CACACAC}$. The orange node is the starting point of the cycle; we show intra-layer edges as solid lines, intra-layer edges as dotted curves, and the second intra-layer step as a yellow line. Note that the elementary cycle $\mathcal{CACACAC}$ also includes three "degenerate" versions, in which the 3-cycle returns to a previously-visited layer.

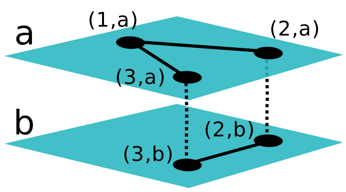

FIG. 5: A simple, illustrative example of a multiplex network.

is not reachable from $(2, b)$. The edge $[(1, a), (2, b)]$ in this supra-graph represents the walk $\{(1, a), (2, a), (2, b)\}$ in the multiplex network. The symmetric walk matrix $\mathcal{M}_{SM'}$ is

$$\mathcal{M}_{SM'} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix} . \tag{42}$$

The matrix $\mathcal{M}_{SM'}$ is the sum of $\mathcal{M}_M$ and $\mathcal{M}_M^T$ with rescaled diagonal blocks in order to not double-count the edges $[(1, a), (2, a)]$ and $[(1, a), (3, a)]$. Additionally,

$$\mathcal{M}_{SM} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix} , \tag{43}$$

which differs from $\mathcal{M}_{SM'}$ in the fact that node-layer pairs $(2, a)$ and $(3, a)$ are connected through the multiplex walk $\{(2, a), (2, b), (3, b), (3, a)\}$.

The adjacency matrix of the aggregated graph is

$$\mathcal{W} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} . \tag{44}$$

That is, it is a complete graph without self-loops.

We now calculate $c_{*,i}$ using the different definitions of a multiplex clustering coefficient. To calculate $c_{M,i}$, we need to compute the auxiliary complete supra-adjacency matrix $\mathcal{M}_M^F$ according to Eq. 34:

$$\mathcal{M}_M^F = \sqrt[3]{2}\mathcal{F}\widehat{\mathcal{C}} = \sqrt[3]{2} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix} . \tag{45}$$

The clustering coefficient of node-layer pair $(1, a)$, which is attached to two triangles that are reachable along the directions of the edges, is

$$c_{M,(1,a)} = \frac{1}{2} . \tag{46}$$

For node-layer pair $(2, a)$, we get

$$c_{M,(2,a)} = 1 , \tag{47}$$

which is the same as the clustering-coefficient values of the remaining node-layers.

To calculate $c_{SM',i}$, we need to compute $\mathcal{M}_{\mathcal{SM}'}^{\mathcal{F}}$, which we obtain using equation (31)

$$\mathcal{M}_{SM'}^F = (\mathcal{F}\widehat{\mathcal{C}} + \widehat{\mathcal{C}}\mathcal{F}) = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix} . \tag{48}$$

In the supra-graph associated with the supra-adjacency matrix $\mathcal{F}\widehat{\mathcal{C}} + \widehat{\mathcal{C}}\mathcal{F}$, all node-layers are connected to all other node-layers except those that correspond to the same nodes. The clustering coefficient of node-layer pair $(1, a)$, which is attached to six triangles, is

$$c_{SM',(1,a)} = \frac{1}{2} = c_{M,(1,a)} . \tag{49}$$

TABLE IV: Coefficients of elementary multiplex 3-cycle terms $w_{\mathcal{E}}$ [see Eqs. (36,37)] for different multiplex clustering coefficients. For example, $w_{\mathcal{AAA}}$ for type M clustering coefficients (i.e., C_M, $C_{M,u}$ and $c_{M,i}$) is equal to $2\beta^3$. For type SM' and SM clustering coefficients, we calculate the expansions only for node-aligned multiplex networks.

C.C.	$\beta^h\gamma^k$	$\mathcal{AAA}$	$\mathcal{AACAC}$	$\mathcal{ACAAC}$	$\mathcal{ACACA}$	$\mathcal{ACACAC}$	$\mathcal{CAAAC}$	$\mathcal{CAACAC}$	$\mathcal{CACACAC}$
	β^3	2							
M	$\beta\gamma^2$		2	2	2				
	γ^3					2			
	β^3	1							
M'	$\beta\gamma^2$		2	2	1				
	γ^3					2			
	β^3	1							
SM'	$\beta\gamma^2$	$2(b-1)$	2	4	3		1		
	γ^3			$2(b-2)$	$2(b-2)$	2		2	
	β^6	1							
	$\beta^4\gamma^2$	$2(b-1)$	4	4	4		1		
SM	$\beta^3\gamma^3$		$2(b-2)$	$2(b-2)$	$4(b-2)$	8		4	
	$\beta^2\gamma^4$	$(b-1)^2$	$4(b-1)$	$4(b-1)$	$(b-2)^2$	$8(b-2)$	$2(b-1)$	$2(b-2)$	4
	$\beta^1\gamma^5$		$2(b-2)(b-1)$	$2(b-2)(b-1)$		$2(b-2)^2$		$4(b-1)$	$4(b-2)$
	γ^6						$(b-1)^2$	$2(b-2)(b-1)$	$(b-2)^2$

TABLE V: Coefficients of the elementary multiplex 3-cycle terms $w_{\mathcal{E}}$ [see Eqs. (36,37)] for different multiplex clustering coefficients when $\beta = \gamma = 1$. For type SM' and SM clustering coefficients, we calculate the expansions only for node-aligned multiplex networks.

C. C.	$\mathcal{AAA}$	$\mathcal{AACAC}$	$\mathcal{ACAAC}$	$\mathcal{ACACA}$	$\mathcal{ACACAC}$	$\mathcal{CAAAC}$	$\mathcal{CAACAC}$	$\mathcal{CACACAC}$
M	2	2	2	2	2	0	0	0
M'	1	2	2	1	2	0	0	0
SM	$1b^2$	$2b^2$	$2b^2$	b^2	$2b^2$	b^2	$2b^2$	b^2
SM'	$2b-1$	2	$2b$	$2b-1$	2	1	2	0

The clustering coefficient of node-layer pair $(2, a)$, which is attached to one triangle, is

$$c_{SM',(2,a)} = 1\,. \tag{50}$$

To calculate $c_{SM,i}$, we compute $\mathcal{M}^F_{SM}$ using equation (30)

$$\mathcal{M}^F_{SM} = \widehat{\mathcal{C}}\mathcal{F}\widehat{\mathcal{C}} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 2 & 0 & 2 \\ 1 & 2 & 0 & 2 & 0 \\ 1 & 0 & 2 & 0 & 2 \\ 1 & 2 & 0 & 2 & 0 \end{pmatrix}\,. \tag{51}$$

The only difference between the graphs $\widehat{\mathcal{C}}\mathcal{F}\widehat{\mathcal{C}}$ and $(\mathcal{F}\widehat{\mathcal{C}} + \widehat{\mathcal{C}}\mathcal{F})$ is the weight of the edges in $\widehat{\mathcal{C}}\mathcal{F}\widehat{\mathcal{C}}$ that take into account the fact that intra-layer edges might be repeated in the two layers.

The clustering coefficient of node-layer pair $(1, a)$, which is attached to eight triangles, is

$$c_{SM,(1,a)} = \frac{8}{12} = \frac{2}{3}\,. \tag{52}$$

The clustering coefficient of node-layer pair $(2, a)$, which is attached to four triangles, is

$$c_{SM,(2,a)} = \frac{4}{6} = \frac{2}{3}\,. \tag{53}$$

Because we are weighting edges based on the number of times an edge between two nodes is repeated in different layers among a given pair of nodes in the normalization, none of the node-layer pairs has a clustering coefficient equal to 1. By contrast, all nodes have clustering coefficients with the same value in the aggregated network, for which layer information has been lost. In particular, they each have a clustering-coefficient value of 1, independent of the definition of the multiplex clustering coefficient.

Further Discussion of Clustering Coefficients in Erdős-Rényi (ER) Multiplex Networks

The expected values of the local clustering coefficients in ER multiplex networks are

$$\langle c_{\mathcal{AAA},i} \rangle = \frac{1}{b}\sum_{\alpha} p_\alpha \equiv \overline{p} \tag{54}$$

$$\langle c_{\mathcal{AACAC},i} \rangle = \frac{1}{b}\sum_{\alpha} p_\alpha \equiv \overline{p} \tag{55}$$

$$\langle c_{\mathcal{ACAAC},i} \rangle = \frac{1}{b}\sum_{\alpha} \frac{\sum_{\beta\neq\alpha} p_\beta^2}{\sum_{\beta\neq\alpha} p_\beta} \tag{56}$$

$$\langle c_{\mathcal{ACACA},i} \rangle = \frac{1}{b}\sum_{\alpha} p_\alpha \equiv \overline{p} \tag{57}$$

$$\langle c_{\mathcal{ACACAC},i} \rangle = \frac{1}{b(b-1)}\sum_{\alpha} \frac{\sum_{\beta\neq\alpha;\gamma\neq\beta,\alpha} p_\beta p_\gamma}{\sum_{\gamma\neq\alpha} p_\gamma}. \tag{58}$$

Note that $c^{(1)}_{M,i} = c_{\mathcal{AAA},i}$ and $c^{(3)}_{M,i} = c_{\mathcal{ACACAC},i}$, but the 2-layer clustering coefficient $c^{(2)}_{M,i}$ arises from a weighted sum of contributions from three different elementary cycles.

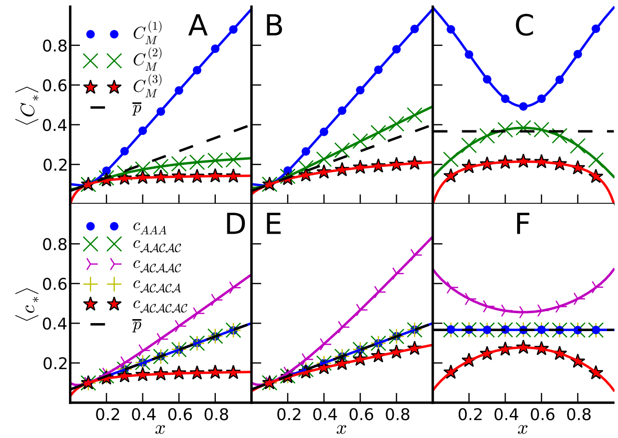

FIG. 6: (A, B, C) Global and (D, E, F) local multiplex clustering coefficients in multiplex networks that consist of ER layers. The markers give the results of simulations of 100-node ER node-aligned multiplex networks that we average over 10 realizations. The solid curves are theoretical approximations (Eqs 12-14 of main text). Panels (A, C, D, F) show the results for three-layer networks, and panels (B, E) show the results for six-layer networks. The ER edge probabilities of the layers are (A, D) $\{0.1, 0.1, x\}$, (B, E) $\{0.1, 0.1, 0.1, 0.1, x, x\}$, and (C, F) $\{0.1, x, 1-x\}$.

In Fig. 6, we illustrate the behavior of the global and local clustering coefficients in multiplex networks in which the layers consist of ER networks with varying amounts of heterogeneity in the intra-layer edge densities. Although the global and mean local clustering coefficients are equal to each other when averaged over ensembles of monoplex ER networks, we do not obtain a similar result for multiplex networks with ER layers unless the layers have the same value of the parameter p. The global clustering coefficients give more weight to denser layers than the mean local clustering coefficients. This is evident for the intra-layer clustering coefficients, $c^{(1)}_{M,i}$ and $C^{(1)}_M$, for which the mean local clustering coefficient is always equal to the mean edge density, but the global clustering coefficient has values that are greater than or equal to the mean edge density. This effect is a good example of a case where the situation in multiplex networks departs from the results and intuition from monoplex networks.

In particular, failing to take into account the heterogeneity of edge densities in multiplex networks can lead to incorrect or misleading results when trying to distinguish among values of a clustering coefficient that are what one would expect from an ER random network versus those that are the signature of a triadic-closure process (see Fig. 6).