APPENDIX I OF 'THE USE OF MULTILAYER NETWORK ANALYSIS ACROSS SOCIAL SCALES IN ANIMAL BEHAVIOUR'

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The mathematical formalism of *multilayer networks* [Kivelä et al., 2014, Newman, 2018], a generalization of ordinary graphs (i.e., 'monolayer networks'), was developed recently to help study multitudinous types of networks and to unify them into one framework. In this appendix, we complement the main text with an introduction to this formalism. We follow the mathematical approach of the review article [Kivelä et al., 2014], including most of their terminology and much of their notation. Another useful resource is [Porter, 2018], which is an expository summary of multilayer networks for mathematics students.[1]

1. Mathematical Formalism

A multilayer network $M = (V_M, E_M, V, \mathtt{L})$ has an underlying set $V = \{1, \ldots, N\}$ of N entities (i.e., 'physical nodes') that occur on layers in $\mathtt{L}$, which we construct as a sequence, $\mathtt{L} = \{L_a\}_{a=1}^{d}$, of sets $L_1, \ldots, L_d$ of elementary layers, where d is the number of 'aspects' (i.e., types of layering). One 'layer' in $\mathtt{L}$ is thus a combination, through the Cartesian product $L_1 \times \cdots \times L_d$, of 'elementary layers' from all aspects. Therefore, each layer in a multilayer network includes one elementary layer from each aspect. For example, if the sets of elementary layers of a multilayer network are $L_1 = \{1, 2\}$ (so 1 and 2 are each elementary layers, perhaps representing different points in time) and $L_2 = \{X, Y, Z\}$, then the network's layers are $(1, X)$, $(1, Y)$, $(1, Z)$, $(2, X)$, $(2, Y)$, and $(2, Z)$. In a multilayer network, the set of node-layer tuples (i.e., 'state nodes' that correspond to the same entity) in M is $V_M \subseteq V \times L_1 \times \cdots \times L_d$, and the set of multilayer edges is $E_M \subseteq V_M \times V_M$. The edge $((i, \alpha), (j, \beta)) \in E_M$ indicates that there is an edge from node i on layer α to node j on layer β (and vice versa, if M is undirected). Each aspect of M represents a type of layering: a type of social interaction, a point in time, and so on. For example, a multirelational network that does not change in time has one aspect; a multirelational network that has layers that encompass multiple time points has two aspects; and so on. To consider weighted edges, one proceeds as in monolayer networks by assigning a weight to each edge using a function $w : E_M \longrightarrow X$, where $X = \mathbb{R}_{\geq 0}$ if all weights are nonnegative real numbers. In Fig. S1, we show an example of a multilayer network with one aspect.

1.1. Adjacency Structure.

Each multilayer network with the same number of nodes in each layer has an associated adjacency tensor[2] $\mathcal{A}$ of order $2(d + 1)$. See [Kivelä et al., 2014] for details. Analogous to the case of monolayer networks, each unweighted (and directed[3]) edge in E_M is associated with a 1 entry of $\mathcal{A}$, and the other entries are 0. To incorporate edge weights, one uses the values of the weights

[1] We draw on some exposition from [Porter, 2018] in our section on mathematical formalism.

[2] A tensor is a linear-algebraic object that generalizes a matrix. See [De Domenico et al., 2013, Kivelä et al., 2014] for discussions of tensors in the context of multilayer networks.

[3] An undirected edge in E_M is associated with two 1 entries of $\mathcal{A}$.

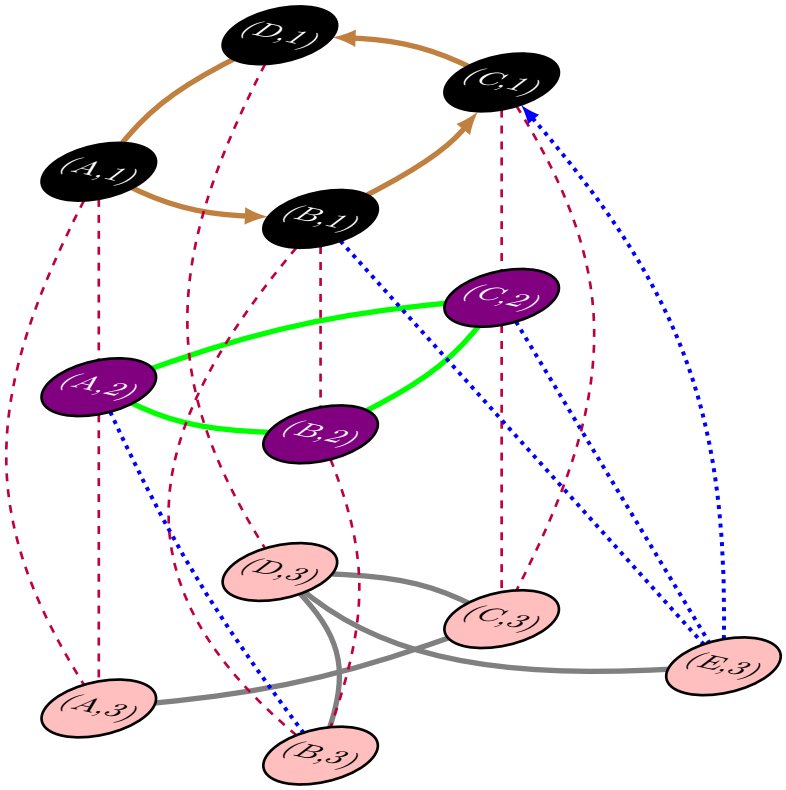

FIGURE S1. An example of a multilayer network with three layers. We label each layer using different colours for its state nodes and its edges: black nodes and brown edges (three of which are unidirectional) for layer 1, purple nodes and green edges for layer 2, and pink nodes and grey edges for layer 3. Each state node (i.e., node-layer tuple) has a corresponding physical node and layer, so the tuple $(A, 3)$ denotes physical node A on layer 3, the tuple $(D, 1)$ denotes physical node D on layer 1, and so on. We draw intralayer edges using solid arcs and interlayer edges using broken arcs; an interlayer edge is dashed (and magenta) if it connects corresponding entities and dotted (and blue) if it connects distinct ones. We include arrowheads to represent unidirectional edges. [We drew this network using TIKZ-NETWORK, by Jürgen Hackl and available at `https://github.com/hackl/tikz-network`), which allows one to draw multilayer networks directly in a LaTeX file.]

instead of 1. As discussed in [Kivelä et al., 2014], multilayer networks can have different numbers of nodes in different layers. To ensure that the dimensions are consistent in $\mathcal{A}$, one adds empty state nodes when necessary. Edges attached to such state nodes are 'forbidden' (these yield 'structural zeros' in $\mathcal{A}$), and this needs to be taken into account when doing calculations.

For convenience[4], it is common to flatten $\mathcal{A}$ into a 'supra-adjacency matrix' $\mathbf{A}_M$, which is the adjacency matrix of the graph G_M associated with M. Intralayer edges (the solid arcs in Fig. S1) are on the diagonal blocks of a supra-adjacency matrix

[4]Several developments in multilayer network analysis, including particular choices for how to generalize ideas from monolayer network analysis, have exploited the tensorial structure of multilayer networks. Readers who wish to ignore this structure are free to start with supra-adjacency matrices.

$$\mathbf{A}_M = \left(\begin{array}{ccccc|ccccc|ccccc}
0 & 1 & 0 & 1 & 0 & \omega_{A1,A2} & 0 & 0 & 0 & 0 & \omega_{A1,A3} & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & \omega_{B1,B2} & 0 & 0 & 0 & 0 & \omega_{B1,B3} & 0 & 0 & \omega_{B1,E3} \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & \omega_{C1,C2} & 0 & 0 & 0 & 0 & \omega_{C1,C3} & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega_{D1,D3} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\omega_{A2,A1} & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \omega_{A2,A3} & \omega_{A2,B3} & 0 & 0 & 0 \\
0 & \omega_{B2,B1} & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \omega_{B2,B3} & 0 & 0 & 0 \\
0 & 0 & \omega_{C2,C1} & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & \omega_{C2,C3} & 0 & \omega_{C2,E3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\omega_{A3,A1} & 0 & 0 & 0 & 0 & \omega_{A3,A2} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & \omega_{B3,B1} & 0 & 0 & 0 & \omega_{B3,A2} & \omega_{B3,B2} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & \omega_{C3,C1} & 0 & 0 & 0 & 0 & \omega_{C3,C2} & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & \omega_{D3,D1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\
0 & \omega_{E3,B1} & \omega_{E3,C1} & 0 & 0 & 0 & 0 & \omega_{E3,C2} & 0 & 0 & 0 & 0 & 0 & 1 & 0
\end{array}\right)$$

FIGURE S2. Supra-adjacency matrix corresponding to the multilayer network in Fig. S1. Entries in diagonal blocks correspond to intralayer edges, whereas entries in off-diagonal blocks correspond to interlayer edges. We follow the colouring scheme in Fig. S1: entries that correspond to intralayer edges in layer 1 are in brown, those in layer 2 are in green, and those in layer 3 are in grey. Magenta entries correspond to interlayer edges between state nodes that represent the same entity, and blue entries correspond to interlayer edges between state nodes that represent distinct entities. We use subscripts to identify the weights of the specific interlayer edges; for example, $\omega_{A1,A2}$ denotes the weight of the edge from state node $(A, 1)$ to state node $(A, 2)$, and $\omega_{A2,A1}$ denotes the weight of the edge from $(A, 2)$ to $(A, 1)$. As in monolayer networks, intralayer edges can also be weighted, but we do not indicate any such weights in $\mathbf{A}_M$.

(see Fig. S2), and interlayer edges (the dashed magenta arcs and dotted blue arcs in Fig. S1) are on the off-diagonal blocks. For this illustration, we suppose that the intralayer edges are unweighted; these are the 1 entries (which we colour based on layer) in $\mathbf{A}_M$. We show interlayer edges between state nodes that represent the same entity in magenta, and we show interlayer edges between state nodes that represent distinct entities in blue. We suppose that the interlayer edge from state node (i, α) to (j, β) has weight $\omega_{i\alpha,j\beta}$, which we take to be a nonnegative real number (although one can use negative values for antagonistic interlayer interactions).

1.2. **Types of Multilayer Networks.** Multilayer networks allow one to investigate a diverse variety of complicated network architectures and to integrate different types of data into one mathematical object. One can then use a common toolkit to study these diverse scenarios.

Two key types of multilayer networks arise from (i) labeling edges or (ii) labeling nodes. When one labels edges, one thinks of edges in different layers as representing different types of interactions. This is the case for a *multiplex network*, a type of multilayer network in which the only permitted types of interlayer edges are those that connect replicates of the same entity in different layers. We show such edges, which correspond to diagonal elements of off-diagonal blocks in a supra-adjacency matrix, as dashed magenta arcs in Fig. S1 and as magenta matrix elements in Fig. S2. A special case of a multiplex network is an edge-coloured multigraph, which has multiple layers but does not have any interlayer edges. In this case, only the diagonal blocks in a supra-adjacency matrix can have nonzero elements (such that all $\omega_{i\alpha,j\beta} = 0$ in Fig. S2). By contrast, when one labels nodes, one can think

of different layers as representing different subsystems (in *interconnected networks* and 'networks of networks'), and there can be interlayer edges with nonzero supra-adjacency matrix elements in both the diagonal and off-diagonal entries of the off-diagonal blocks. In this case, there are interlayer edges between different entities, as we indicate using the dotted blue arcs in Fig. S1 and the blue matrix elements in Fig. S2. To emphasize the fact that different layers in Fig. S1 can represent different subsystems, we use different colours for the nodes from different layers in this network diagram.

For further details on types of multilayer networks, see [Kivelä et al., 2014].

1.3. **Weights of Interlayer Edges.** An important idea is that interlayer edges are fundamentally different from intralayer edges, and it is often less straightforward to determine weights from data for interlayer edges than for intralayer ones. In the context of the supra-adjacency matrix in Fig. S2, for most applications, it is easier to determine weights that are associated with the 1 entries in the diagonal blocks than to assign appropriate values to the weights $\omega_{i\alpha,j\beta}$. As in monolayer networks, larger weights correspond to stronger interactions.

A conceptually easy situation is a multimodal transportation network, in which one might determine interlayer edge weights based on how long it takes to change modes of transportation (with larger weights for shorter times). Suppose, for example, that entity A represents Oxford, entity B represents Cambridge, layer 1 represents coach transportation, and layer 2 represents train transportation. We determine interlayer edge weights from the time it takes to change transportation modes, with larger weights for shorter times. If it takes longer to walk from the coach station to the train station in Oxford than it does in Cambridge, then $\omega_{A1,A2} > \omega_{B1,B2}$.

A harder scenario to model is communication between people in a social network. We will use ourselves—with nodes called Mason, Noa, Kelly, and Matt—to provide an example. One possibility is to construe an interlayer edge that connects an entity to itself as encoding a transition probability between different modes of communication. Therefore, $\omega_{i\alpha,j\beta} \in [0, 1]$ because it represents a probability. One can also include interlayer edges between distinct entities (in blue in Fig. S2), as Mason can send a message to Noa using one mode of communication (i.e., in one layer), such as via an e-mail that he typed on his laptop, but she may read the contents of that message using some other mode of communication (i.e., in another layer), such as on a mobile phone. Noa may then subsequently text the message to Kelly and Matt. Additionally, because the four of us have different usage patterns for different modes of communication, we also have different transition probabilities between layers, and our associated interlayer edge weights thus differ from each other. For example, Mason is almost always on his computer and almost never on his phone, so his transition probability from communicating via computer to communicating via phone is small, whereas the probability of the reverse transition is very large. By contrast, during proverbial work hours, Noa spends a similar amount of time on her computer and her phone, and her transition probabilities for changing between these two modes of communication are similar to each other.

For other applications, including in animal behaviour, interlayer edges can run into significant conceptual difficulties, and researchers struggle with how to make sense of them. There are dependencies across layers and interlayer edges can encode such dependencies, but how does one determine meaningful values for the weights of those edges? In some applications, it may be useful to think of interlayer edges as transition probabilities, as in the above example involving humans. In others, it may be useful to construe an interlayer edge as representing a dependency between one layer (e.g., proximity associations) and a second layer (e.g., grooming interactions, which require proximity to occur). A larger weight for such an edge encodes

a stronger dependency, thereby entailing a stronger dependence of one layer on another. Additionally, different individual animals can have different values for such weights (as in the example above), corresponding to individual differences.

There are numerous possibilities for applying multilayer network analysis in animal behaviour (and in other applications), because it is very flexible, but it can also be very challenging to interpret the results of such analysis. As we have illustrated in this subsection, a key issue that requires careful thought is determining the weights of interlayer edges (or whether to use such edges at all). In different disciplines and for different systems and research questions, one can use interlayer edges to represent qualitatively different things (e.g., communication ties, correlations, or transition probabilities), and how to determine interlayer edge weights depends on the application domain, the system of interest, and one's particular research question.

2. Eigenvector Versatility: An Example of a Multilayer Versatility Measure

In this section, we illustrate the formalism of calculating a 'versatility' measure [De Domenico et al., 2015] in a multilayer network to supplement our conceptual discussion in the main text. For simplicity, we consider eigenvector versatility, which is a generalization of eigenvector centrality from monolayer networks, but one can also generalize other monolayer centrality measures (such as PageRank) into associated versatility measures for multilayer networks.

To calculate eigenvector centralities in a monolayer network, one calculates the leading eigenvector $\mathbf{v}_1$ (which is associated with the largest positive eigenvalue λ_1) of the equation $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$, where $\mathbf{A}$ is the network's adjacency matrix. For this type of centrality, we assume that the network associated to $\mathbf{A}$ is strongly connected (or just that it is connected, for an undirected network), so that—by the Perron–Frobenius theorem—the eigenvector $\mathbf{v}_1$ has strictly positive entries [Newman, 2018]. These entries give the eigenvector centralities of the corresponding nodes in the network.

Calculating eigenvector versatility proceeds in a similar way. One first calculates the leading eigenvector $\mathbf{v}_{M,1}$ of the equation $\mathbf{A}_M\mathbf{v}_M = \lambda\mathbf{v}_M$. The eigenvector $\mathbf{v}_{M,1}$ gives multilayer eigenvector centralities for each state node (i.e., for each node in each layer). Importantly, we need to use the whole multilayer structure to calculate the multilayer eigenvector centrality for each state node. For each entity, one then aggregates the centrality values over all layers to determine its eigenvector versatility. The article [De Domenico et al., 2015] used a maximum-entropy principle for their choice of aggregation, but other ways of weighting different layers are also possible [Kivelä et al., 2014].

3. Similarity of Layers: An Example Measure

In this section, we present one example measurement of similarity of layers in a multilayer network. As we suggested in the main text, such calculations can be helpful for exploring overlaps of individuals and/or social interactions across layers, including for discerning task specialists and generalists. For simplicity, we consider the special case of multiplex networks. See [Kao and Porter, 2018] and several references therein for a discussion of several types of similarity measures and comparisons between them.

One way to quantify the similarity of two layers is to count the number of intralayer edges that occur in both layers. There is an overlapping edge between nodes i and j in layers α and β if and only if there is an edge between nodes i and j in both α and β. That is, $\theta(A^{\alpha}_{ij}) = 1$ and $\theta(A^{\beta}_{ij}) = 1$, where A^{α}_{ij} is the intralayer adjacency element between entities i and j on layer α (and A^{β}_{ij} is defined analogously), and $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ otherwise.

Usually, one wants to be a bit more sophisticated than using a raw count of overlapping edges, and there are many possible ways to proceed. One example is 'local overlap' [Cellai et al., 2013]

$$o_i^{\alpha\beta} = \sum_j \theta(w_{ij}^{\alpha})\theta(w_{ij}^{\beta}) \,,$$

which counts the number of overlapping edges that are attached to node i in both layer α and layer β. In an undirected multiplex network, the local overlap $o_i^{\alpha\beta}$ quantifies the similarity between the connection patterns of node i in layer α and node i in layer β, although it does not take into account that the intralayer degrees of a state node contributes to the amount of overlap that involves it. One way to do this is with 'local similarity' [Kao and Porter, 2018]

$$\phi_i^{\alpha\beta} = \frac{o_i^{\alpha\beta}}{k_i^{\alpha} + k_i^{\beta} - o_i^{\alpha\beta}} \in [0,1] \,, \tag{1}$$

where $k_i^{\alpha} = \sum_j \theta(w_{ij}^{\alpha})$ is the degree of node i in layer α (and k_i^{β} is defined analogously). Local similarity $\phi_i^{\alpha\beta}$ calculates the number of overlapping edges that are attached to node i in layers α and β as a proportion of the number of unique edges that are attached to node i in the two layers.

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