A factor model of multilayer network interdependence

Izabel Aguiar†, Dane Taylor‡, and Johan Ugander§

Abstract. Multilayer networks describe the rich ways in which nodes are related through different types of connections in separate layers. These multiple relationships are naturally represented by an adjacency tensor that can be interpreted using techniques from multilinear algebra. In this work we use the nonnegative Tucker decomposition (NNTuck) with KL-divergence as an expressive factor model for multilayer networks that naturally generalizes existing methods for stochastic block models of multilayer networks. We show how the NNTuck provides an intuitive factor-based perspective on layer dependence and enables linear-algebraic techniques for analyzing dependence with respect to specific layers. Algorithmically, we show that using expectation maximization (EM) to maximize this log-likelihood under the NNTuck model is step-by-step equivalent to tensorial multiplicative updates for the nonnegative Tucker decomposition under a KL loss, extending a previously known equivalence from nonnegative matrices to nonnegative tensors. Using both synthetic and real-world data, we evaluate the use and interpretation of the NNTuck as a model of multilayer networks. The ability to quantify dependencies between layers has the potential to inform survey instruments for collecting social network data, identify redundancies in the structure of a network, and indicate relationships between disparate layers. Therefore, we propose a definition of layer dependence based on using a likelihood ratio test to evaluate three nested models: the layer independent, layer dependent, and layer redundant NNTucks. We show how these definitions, paired with analysis of the factor matrices in the NNTuck, can be used to understand and interpret layer dependence in different contexts.

Key words. multilayer networks, social networks, stochastic blockmodels, factor models, Tucker decomposition, link prediction

AMS subject classifications. 91D30, 15A69

1. Introduction. Multilayer networks capture the many ways that a set of units can be connected: through different types of relationships in a social network [7, 49, 10, 53]; at different time steps [11, 22, 59]; through different types of interactions between genes or proteins [18, 40]; or by different modes of transit in a transportation network [20, 24] (see reviews [37, 9] for more examples). As more and more data take on a multilayer network form, tools for network analysis are being steadily adapted to multilayer contexts. Recent work has productively cast the study of multilayer community structure in the language of multilinear algebra [68], furnishing tensor-based definitions of multilayer stochastic block models (SBMs) [55, 16, 25, 11, 58]. In this work we extend and generalize these efforts, connecting the tensorial nonnegative Tucker decomposition with KL-divergence to the

Funding: IA acknowledges support from the NSF GRFP and the Knight-Hennessy Scholars Fellowship. DT acknowledges partial support from NSF grant DMS-2052720 and the Simons Foundation (grant #578333). JU acknowledges partial support from ARO grant 76582-NS-MUR.

†Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA (izzya@stanford.edu).
‡Department of Mathematics, University at Buffalo, The State University of New York, Buffalo, NY (danet@buffalo.edu).
§Department of Management Science and Engineering, Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA (jugander@stanford.edu).
statistical inference of multilayer SBMs. We show that minimizing the KL-divergence of the NNTuck is exactly equivalent to maximizing the log-likelihood of observing a multilayer network assumed to have been generated from a Poisson model with parameters defined by an NNTuck. In this sense the NNTuck identifies a natural generalization of existing multilayer SBMs.

In addition to the use of this multilayer SBM for community detection and link prediction, we investigate the use of the nonnegative Tucker decomposition to identify dependence amongst layers. The ability to quantify dependencies between layers has the potential to inform survey instruments for collecting social network data, identify redundancies in the structure of a network, and indicate relationships between disparate layers. We build upon these motivations from previous work [18, 56, 16] and propose the NNTuck as a natural way to identify a latent space in the dimension of the layers. Analogous to how the factor matrices in the single layer SBM identify node communities, the additional third factor matrix in the NNTuck identifies layer communities. As such, the third factor matrix of the NNTuck allows for the adjacency tensor to be low rank in the layer dimension.

Analyzing the third factor matrix is a significant focus of our work, and we propose three methods for interpreting it to quantify layer dependency. Furthermore, we propose a definition of layer dependence based on the likelihood ratio test (LRT). We use this definition to classify a variety of empirical networks as layer independent, dependent, or redundant, and find layer independence in a biological multilayer network, layer dependence in a cognitive social structure, and layer redundancy in a collection of multilayer social support networks.

The structure of this work is as follows. In Section 2 we discuss and define the notation of the stochastic block model (SBM), multilayer networks, and previous and related approaches to multilayer SBMs. In Section 3 we define the nonnegative Tucker decomposition (NNTuck) and its notation, discuss the connection of its definition under KL-divergence to block models, motivate using the multiplicative updates algorithm from [36], and offer an interpretation of the low-dimensional third factor matrix as describing the dependence between the layers of a multilayer network. In Section 4 we discuss the use of the NNTuck to empirically validate...
A The \((N \times N)\) adjacency matrix of a single-layer network with \(N\) nodes.

\(A\) The \((N \times N \times L)\) adjacency tensor of a multilayer network with \(N\) nodes and \(L\) layers. The Tucker Decomposition of \(A\) is given by \(A = G \times_1 U \times_2 V \times_3 Y\).

\(U\) The \((N \times K)\) outgoing community membership matrix in an SBM for directed networks, where \(K\) is the number of communities generating the network. For an undirected network \(U = V\) (see below) and we simply call \(U\) the community membership matrix.

\(V\) The \((N \times K)\) incoming community membership matrix in an SBM for a directed network. For an undirected network, \(U = V\).

\(Y\) The third factor matrix in the Tucker Decomposition, also referred to as the layer-dependence matrix.

\(G\) The \((K \times K)\) affinity matrix describing the rate at which nodes in different communities form edges with one another in an SBM.

\(G\) The core tensor in the Tucker Decomposition.

**Table 1**

The notation and definitions for vocabulary that will be used throughout this paper.

layer dependence and define a likelihood ratio test based definition for layer dependence.

In Section 5 we propose cross validation to select the NNTuck’s hyper-parameters \(K\) and \(C\). We discuss cross validation based on two link prediction tasks: independent link prediction, in which elements of the adjacency tensor are missing independently and according to an identical uniform distribution, and tubular link prediction, in which entire tubes of the adjacency tensor are missing (also i.i.d.). In Section 6 we use the NNTuck to analyze layer dependence in practice for: two synthetic networks; Krackhardt’s 1987 cognitive social structure dataset [39]; a biological multilayer network [40]; a social support multilayer network [7]; and 113 other multilayer social support networks [7, 8]. We conclude in Section 7 by discussing our work and indicating future directions of research.

2. **Background.** In this section we discuss related work and define notation and vocabulary. For easy reference, the primary notation has been organized in Table 1. We present stochastic block models (SBMs) in Subsection 2.1 and nonnegative matrix factorization (NMF) in Subsection 2.2. In Subsection 2.3 we introduce tensor vocabulary and notation used throughout the work and review the Tucker decomposition. In Subsection 2.4 we discuss multilayer networks and in Subsection 2.5 we present a brief survey of related work, summarized in Table 2. We conclude in Subsection 2.6 with a discussion of the novel contributions of our work situated in the literature.

2.1. **Stochastic Block Model (SBM).** Stochastic block models (SBMs) identify latent groups of nodes and the density of connections between nodes in these groups as a descriptive
and/or generative tool for analyzing networks. Introduced by White et al. (1976) [65] and expanded by Holland et al. (1983) [32], SBMs decompose a network into factors that aim to uncover group structure, identify to which groups each node belongs, and describe how nodes in these groups form connections with one another. Beyond these context-specific questions, SBMs identify low-dimensional structure in a network by grouping nodes into latent communities. Extensions of the original SBM have allowed for the model to account for heterogeneous degree distributions [34], nodes belonging to multiple overlapping communities (sometimes referred to as mixed-membership) [6], and Bayesian approaches [2]. Here, we focus on generalizing the degree-corrected, mixed-membership SBM (dc-mm-SBM) [6] to multilayer networks. Since we use much of the same framework to build our model for multilayer networks, we begin by describing the dc-mm-SBM in depth.

For a network with adjacency matrix $A \in \mathbb{Z}_{0+}^{N \times N}$, the dc-mm-SBM assumes that each node $i$ has outgoing and incoming nonnegative membership vectors, $u_i$ and $v_i$ respectively, describing node $i$’s membership to $K$ different groups when forming outgoing and incoming edges ($u_i = v_i$ when the network is undirected). A nonnegative affinity matrix $G$ describes the rate at which nodes in different groups form edges with one another. Given $U, V \in \mathbb{R}_+^{N \times K}$ and $G \in \mathbb{R}_+^{K \times K}$ the dc-mm-SBM assumes each edge is a realization of the Poisson distribution,

$$a_{ij} \sim \text{Poisson}(u_i G v_j^T), \text{ for all } i, j = 1, \ldots, N.$$  

For a more detailed discussion on the common modeling choice to use the Poisson distribution (as opposed to, e.g., a Bernoulli distribution), see Zhao et al. (2012) [70]. Written this way, we see that $u_i G v_j^T$ must be nonnegative in order to specify a valid Poisson rate. By requiring all the elements $u_i, G, v_i$ to be independently nonnegative, the parameters are all interpretable as membership weights and affinities. In matrix form, we then have,

$$(2.1) \quad A \sim \text{Poisson}(UGV^T).$$

We estimate $U, V, G$ by maximizing the log-likelihood of observing $A$ under this model. Henceforth we will assume the network is unweighted and $A \in \{0, 1\}^{N \times N}$, although a weighted network can be described using this model and the likelihood maximized all the same.

The formulation given by (2.1) incorporates both the degree-corrected SBM (dc-SBM) [34] and the mixed-membership SBM (mm-SBM) [6]. In the dc-SBM each node may only belong to one of $K$ groups but may have heterogeneous degree distribution. In the mm-SBM each node may belong, in part, to each of $K$ groups but their memberships must sum to one. To account for both, the dc-mm-SBM assumes that each node has a scalar parameter $\theta_i > 0$ describing its gregariousness. Equivalently, each node’s membership vector absorbs this degree parameter such that $u_i = \theta_i s_i$ and $v_i = \theta_i t_i$ for normalized membership vectors $\sum_k s_k = 1$ and $\sum_k t_k = 1$. We will henceforth describe this type of community membership as soft membership. Such an approach allows nodes to have membership across multiple groups while also allowing for a heterogeneous degree distribution across nodes.

There is a direct connection between the dc-mm-SBM and Poisson matrix factorization (PMF) [27]. PMF assumes that the entries of $A$ are realizations of a Poisson distribution with rate parameters given by the product of $W \in \mathbb{R}_+^{N \times K}$ and $H \in \mathbb{R}_+^{K \times N}$. That is, $a_{ij} \sim \text{Poisson}(u_i G v_j^T)$.
Poisson \( \sum_k w_{ik} h_{kj} \). The log-likelihood of observing \( A \) under this distribution is given by,

\[
\mathcal{L}(A|W, H) = \sum_{ij} a_{ij} \log \sum_k w_{ik} h_{kj} - \sum_k w_{ik} h_{kj}.
\]

**2.2. Nonnegative Matrix Factorization (NMF).** A related approach for finding latent structure in a matrix, nonnegative matrix factorization (NMF) [47, 42], aims to factor nonnegative matrix \( A \) into two nonnegative factor matrices, \( W \) and \( H \), for \( W \in \mathbb{R}^{N \times K}_+ \) and \( H \in \mathbb{R}^{K \times N}_+ \).

Not every matrix can be exactly factorized in this way, and although for these cases we are actually finding the nonnegative matrix approximation, we will henceforth refer to both problems as NMF. When estimating the NMF of a matrix \( A \) there are many loss functions with respect to which the factorization may be optimized. For reasons that will be clearly motivated in the following sections, we focus on minimizing the KL-divergence between the matrix and its factorization, defined as

\[
\text{KL}(A||WH) = \sum_{ij} \left( a_{ij} \log \frac{a_{ij}}{(WH)_{ij}} - a_{ij} + (WH)_{ij} \right).
\]

The algorithm based on multiplicative updates for minimizing KL-divergence was developed by Lee and Seung (2001) [41] and is widely used to find local optima of the non-convex optimization problem given by (2.3). This algorithm guarantees that, given nonnegative initializations, factor matrices \( W \) and \( H \) remain nonnegative throughout the optimization. Furthermore, the algorithm guarantees monotonic convergence to a local minimum.

It is known that maximizing the log-likelihood in PMF (2.2) is equivalent to minimizing the KL-divergence in NMF:

\[
\begin{align*}
\text{minimize}_{W,H} \quad & \text{KL}(A||WH) \\
\iff \text{minimize}_{W,H} \quad & \sum_{ij} (a_{ij} \log a_{ij} - a_{ij} \log (WH)_{ij} - a_{ij} + (WH)_{ij}) \\
\iff \text{minimize}_{W,H} \quad & -\sum_{ij} (a_{ij} \log (WH)_{ij} - (WH)_{ij}) \\
\iff \text{maximize}_{W,H} \quad & \mathcal{L}(A|W, H).
\end{align*}
\]

Furthermore, as was first noted in [21], using expectation maximization (EM) to find a local maximum of the log-likelihood for PMF is step-by-step equivalent to using the multiplicative updates given in [41] to minimize KL-divergence. This equivalence does not hold when comparing EM updates under a Gaussian generative model to the multiplicative updates under a Frobenius loss. This observation, in combination with the equivalence in (2.4), gives NMF with KL-divergence a strong statistical foundation. Specifically, there are two important connections to be made: (i) to factorize matrix \( A \) into a product of two nonnegative matrices by maximizing log-likelihood in PMF and minimizing KL-divergence in NMF are equivalent optimization problems, and (ii) the algorithm by which to find the model associated with a local minimum of the shared loss function is the same for PMF and NMF.
2.3. Tensor Notation and Tucker Decomposition. To facilitate a clear analysis and discussion of the tensor-based model in Section 3, we now define the tensor-specific vocabulary and notation that we will use throughout this paper. For a more thorough overview of tensor vocabulary, methods, decompositions, and definitions, see the excellent review by Kolda and Bader (2009) [38]. We focus notation and terms to third-order tensors $\mathbf{X}$ of dimension $N \times M \times L$. Our analysis in following sections will focus on “frontally square” tensors where $N = M$, but we review tensor notation in this more general setting to avoid confusion.

**Frontal slices.** The frontal slices of $\mathbf{X}$ are the $L$ matrices of size $N \times M$ that, when stacked together, form the $N \times M \times L$ tensor. A depiction of frontal slices can be found at the bottom left of Figure SM1. We denote the $t$th frontal slice of $\mathbf{X}$ as $\mathbf{X}_t$. The frontal slice of an adjacency tensor $\mathbf{A}$ corresponds to the adjacency matrix $A_{\ell}$ of a particular layer $\ell$ of the multilayer network, and thus we will make frequent references to it.

**Tensor fibers.** Analogous to rows and columns in matrices, third-order tensors have what are called row, column, and tube fibers, denoted $\mathbf{X}_{ijk}$, $\mathbf{X}_{il}$, and $\mathbf{X}_{ij}$, respectively. See Figure SM2 for a visualization of each.

**Unfoldings.** A third-order tensor has three unfoldings: the 1-unfolding, 2-unfolding, and 3-unfolding. These are higher-dimensional equivalents to vectorizing a matrix. The $n$-unfolding of a third-order tensor stacks its column, row, or tube fibers to form a matrix, and is denoted by $\mathbf{X}_{(n)}$. See Figure SM1 and Section 2 of [38] for helpful visualizations.

**The tensor $n$-mode product $(\times_n)$.** A third-order tensor can be multiplied by a matrix through a 1-, 2-, or 3-mode product. Dimensionally, for an $N \times M \times L$ tensor $\mathbf{X}$ one can take the 1-mode product with a $P \times N$ matrix, the 2-mode product with a $Q \times M$ matrix, and the 3-mode product with a $R \times L$ matrix. The resulting dimensions of these mode products would be $P \times M \times L$, $N \times Q \times L$, and $N \times M \times R$, respectively. Elementwise, the 1-mode product gives $(\mathbf{X} \times_1 \mathbf{B})_{ijk} = \sum_h x_{ihjk} b_{hk}$.

**Tucker decomposition.** Although the most prominent of the many tensor decompositions are the CP decomposition [12, 28] and the Tucker decomposition [61], other notable decompositions include RESCAL [45], DEDICOM [29], and PARATUCK2 [30], where both the CP and RESCAL decompositions are special cases of the Tucker decomposition. The Tucker decomposition decomposes an $n$th-order tensor $\mathbf{X}$ into an $n$th-order core tensor $\mathbf{G}$ and $n$ factor matrices. The Tucker decomposition of a third order $N \times M \times L$ tensor $\mathbf{X}$ is

\begin{equation}
\mathbf{X} = \mathbf{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{Y}.
\end{equation}

Here $\mathbf{G}$ is $P \times Q \times R$, $\mathbf{U}$ is $N \times P$, $\mathbf{V}$ is $M \times Q$, and $\mathbf{Y}$ is $L \times R$. A nonnegative Tucker decomposition is one where all elements of the factor matrices $\mathbf{U}$, $\mathbf{V}$, and $\mathbf{Y}$ and core tensor $\mathbf{G}$ are nonnegative. When fitting a nonnegative Tucker decomposition to a data tensor $\mathbf{X}$, two common notions of approximation are the Frobenius loss and the KL-divergence,

\begin{equation}
\text{KL}(\mathbf{X} | \mathbf{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{Y}) := \sum_{ijk} x_{ijk} \log \frac{x_{ijk}}{\hat{x}_{ijk}} - x_{ijk} + \hat{x}_{ijk},
\end{equation}

for $\hat{\mathbf{X}} = \mathbf{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{Y}$.

2.4. Multilayer Networks. Multilayer networks consist of a set of different network ‘layers’ which each encode different types of edges (sometimes called intralayer edges). In general,
the node set can differ across layers, however we focus on a subclass called *multiplex networks* in which the nodes are identical in each layer [44]. Although some multilayer network work also models connections between layers using *interlayer* edges, we do not assume or model the coupling of layers. In this case, there exists a one-to-one alignment of layers, allowing them to be encoded in a 3-dimensional adjacency tensor $A \in \mathbb{R}^{N \times N \times L}$, where $N$ and $L$ are the numbers of nodes and layers, respectively, and where each frontal slice $A_\ell$ is the adjacency matrix of a particular layer $\ell$ of the multilayer network. Here, $a_{ij\ell} > 0$ if an only if there is an edge from $i$ to $j$ in layer $\ell$, and is otherwise zero.

Multilayer networks can be either directed or undirected. In this work we assume that all layers within a given network are either directed or undirected. Extending our approach to networks that have a mixture of directed and undirected layers would be straightforward. We also assume that all edges are unweighted, $a_{ij\ell} \in \{0, 1\}$, but this assumption can easily be relaxed. For a more comprehensive review of multilayer networks, see Kivela et al. (2014) or Boccaletti et al. (2014) [37, 9]

### 2.5. Related Work.

We now discuss related work as categorized by previous approaches for (i) tensor methods for multilayer networks, (ii) stochastic block models for multilayer networks, and (iii) addressing layer dependence in multilayer networks.

**Tensor methods for Multilayer Networks.** Multilayer networks have been studied since as far back as 1939 [51], and they have been mathematically represented by tensors since at least 1987, when Krackhardt introduced the concept of *cognitive social structures* [39]. In fact, one of the foundational tensor decomposition papers by Carroll and Chang (1970) [12] was a study of multilayer relational data. Since then, tensor methods have become more prominent in analysing multilayer networks [5, 38, 45], and De Domenico et al. (2013) [19] formalized this tensorial framework by generalizing many network analysis tools to the multilayer setting.

The CP tensor decomposition [12], and even the less popular Tucker decomposition [61], have been implemented for their use in analyzing multilayer networks. The CP decomposition, for example, is implemented to interpret a fourth-order tensor of multilayer network data in [54], for community detection and analysis of activity patterns in a temporal network in [25], and to assess centrality of nodes in multilayer networks [63]. The Tucker decomposition is used for community detection in a temporal multilayer network representing brain dynamics in [3] and to cluster keywords and communities in a multilayer email network in [57].

**Stochastic block models for Multilayer Networks.** There have been a wide range of approaches to generalize the SBM to multilayer networks. In [62] a multilayer SBM is developed by fitting a new SBM to each layer, assuming that neither node-membership nor group-to-group connectivity is fixed across layers. In [11] and [16], a node’s membership vectors are held fixed across layers, but a new affinity matrix is fit for each layer. A similar model is proposed in [48] but with node membership vectors constrained to take on binary values and with a Bernoulli distribution assumption instead of Poisson. Conversely, in [58] a Tucker decomposition accounting for layer community structure is fit with the aim to predict *types* of links in a multilayer network. To do so, a new core tensor is fit for each type of link. Although layer community structure is addressed in [58], the number of node-communities is always fixed to equal the number of layer-communities: a missed opportunity to examine layer-dependence by examining the optimal number of layer-communities.
In [64], the authors propose using a Tucker decomposition as a multilayer SBM, but limit their factor matrices to only take on binary values. Thus, the extent to which layer dependence is addressed is limited to the binary clustering of layers and is more similar to the strata work of [56]. Furthermore, the core tensor is not constrained to be nonnegative, and the proposed algorithm focuses on minimizing the Frobenius norm of the difference between the tensor and the approximation given by the Tucker decomposition.

In Schein et al. (2016) [55], the authors propose the use of a Bayesian Poisson Tucker Decomposition (BPTD) as a generalization of the dc-mm-SBM to study multilayer networks. They highlight the BPTD using a fourth-order tensor to study international relations between countries over time, and show how the BPTD can group together countries, actions, and time periods into communities. Our work extends this modeling framework by introducing a technical approach to studying layer dependence in the general setting. Departing from the MCMC algorithmic approach of [55], we propose estimating the nonnegative Tucker decomposition using multiplicative updates which minimize the KL-divergence of the estimation, which also extends the expectation maximization (EM) algorithm for finding point estimates of the factors and core tensor in De Bacco et al. (2017) [16].

Because we will often reference the work and the multilayer SBM model MULTITENSOR (MT) built in [16], we define and discuss the work in more detail here. Consider a multilayer network with $N$ nodes and $L$ layers represented by adjacency tensor $A \in \mathbb{Z}^{N \times N \times L}$. Assume each node $i$ in the network has outgoing and incoming nonnegative membership vectors $u_i$ and $v_i$, respectively, representing their soft assignment to $K$ groups. The densities with which nodes in each community interact in layer $\ell$ is given by nonnegative affinity matrix $G_\ell$. The MT model then assumes the generative process whereby

\begin{equation}
A \sim \text{Poisson}(\Lambda), \text{ where } \Lambda_\ell = U G_\ell V^T \text{ for } \ell \in [1, L].
\end{equation}

Written this way we see that MT fits an SBM to each layer of the network, holding fixed the outgoing and incoming group memberships across layers. Parameters $U, V$, and $G_\ell$ are estimated by maximizing the log-likelihood of observing $A$ via an EM algorithm.

Layer Dependence. Previous work has taken on the task of assessing layer dependence in multilayer networks. In [18], tools from information theory are used to measure the difference between graphs whose edges have been aggregated from different subsets of the layers. In [56], the authors develop the strata multilayer SBM, a multilayer SBM with the goal to incorporate layer dependence into the model, done by categorizing layers into groups such that all layers were drawn from the same SBM. As we will discuss later, the NNTuck is a generalization of the strata model that is analogous to moving from fixed- to mixed-membership assignments in the SBM. In [33], the authors define a similarity measure for layers, construct a single layer network where each node is a layer and each edge is weighted by the similarity measure, and then find layer communities by doing community detection on this new network. In the MULTITENSOR (MT) work [16], layer dependence is studied through building multiple MT models using different subsets of the layers, and the models’ performance (measured by test-AUC) from a link prediction task is used to determine if there is layer dependence in the model. In this setting, layer dependence can be viewed as a specific application of transfer learning which assesses how a model built in one setting performs in an alternative one [60, 4]. Finally, while not explicitly developed for use in the multilayer setting, tools to compare
| Citation                      | Approach                                                                 |
|-------------------------------|---------------------------------------------------------------------------|
| Schein et al. (2016) [55]     | The factor matrices and core tensor are estimated using an MCMC inference algorithm.  |
| Valles-Catala et al. (2016) [62] | A separate SBM is estimated for each layer.                                    |
| DeBacco et al. (2017) [16] and Carlen et al. (2019) [11] | $Y$ is constrained so that $Y := I$.                                      |
| Paul and Chen (2016) [48]     | $U := V$ constrained to only take on binary values, $Y$ is constrained so that $Y := I$, and the model assumes a Bernoulli distribution (as opposed to Poisson). |
| Tarrés-Deulofeu et al. (2019) [58] | $U, V,$ and $Y$ have constraint $C = K$ and a new core tensor $G$ is estimated for each type of link in the network. |
| Wang and Zeng (2019) [64]     | $U, V,$ and $Y$ are constrained to only take on binary values.             |
| Stanley et al. (2016) [56]    | $Y$ is constrained to only take on binary values and $G$ can take on negative values. |

Table 2

Previous approaches to multilayer SBMs. Excepting the first citation, we write these approaches in relation to the nonnegative Tucker decomposition (NNTuck) which assumes $A \sim \text{Poisson}(G \times_1 U \times_2 V \times_3 Y)$ for $G \in \mathbb{R}^{K \times K \times C}$, $U, V \in \mathbb{R}^{N \times K}$, and $Y \in \mathbb{R}^{L \times C}$. For descriptions of our novel contributions situated in this work see Subsection 2.6 and for more details on the NNTuck see Section 3.

2.6. Contributions. Situated in this related work, the contributions of our work are as follows: (i) we use the nonnegative Tucker decomposition with KL-divergence as a natural extension of the dc-mm-SBM to multilayer networks by allowing for distinct latent structure in the nodes and layers; (ii) we propose the inspection of the third factor matrix in the NNTuck for quantifying and assessing layer dependence and discuss three specific methods for doing so; (iii) we show the equivalence in model, loss function, and algorithm between Poisson Tucker decomposition and nonnegative Tucker decomposition; (iv) we propose a definition of layer dependence based on the likelihood ratio test; (v) we define two link prediction tasks for multilayer networks to use cross validation as a tool for model selection; and (vi) we use the NNTuck to study layer dependence in a variety of empirical multilayer networks: one biological, one cognitive social structure, and 113 social support networks.

3. Nonnegative Tucker Decomposition (NNTuck). We begin this section by outlining our approach to a multilayer SBM that corresponds to a nonnegative Tucker decomposition.
with KL-divergence. We will henceforth refer to the multilayer SBM developed here as just the nonnegative Tucker decomposition (NNTuck), although it’s important to note that the SBM interpretation only corresponds to the nonnegative Tucker decomposition estimated with KL-divergence loss as in (2.6), not Frobenius loss. We present the model of the NNTuck as a multilayer SBM in Subsection 3.1, show how it generalizes MULTITENSOR (MT) in Subsection 3.2, and discuss deflation and layer dependence in the NNTuck in Subsection 3.3. We present an algorithm for estimating the NNTuck of a multilayer network and discuss the algorithm’s limitations in Subsection 3.4.

3.1. The Model. Consider a multilayer network with \( N \) nodes and \( L \) layers represented by adjacency tensor \( A \in \mathbb{Z}_{0+}^{N \times N \times L} \). We assume that each node \( i \) has nonnegative membership vectors \( u_i \in \mathbb{R}_+^{K} \) and \( v_i \in \mathbb{R}_+^{K} \) representing its soft assignment to \( K \leq N \) groups. Moreover, we assume that each layer \( \ell \) has nonnegative vector \( y_\ell \in \mathbb{R}_+^{C} \) describing the layer’s soft membership to each of \( C \leq L \) layer communities. Just as matrices \( U \) and \( V \) in the SBM describe latent community structure in the nodes of single-layer networks, the factor matrix \( Y \) in the NNTuck describes latent structure in the layers of a multilayer network. Finally, we assume tensor \( G \in \mathbb{R}_+^{K \times K \times C} \) defines \( C \) different affinity matrices. Let \( u_i, v_i, y_\ell \) be the rows of nonnegative matrices \( U, V, \) and \( Y \), respectively. The NNTuck multilayer SBM assumes

\[
A \sim \text{Poisson}(G \times_1 U \times_2 V \times_3 Y).
\]

Maximizing the log-likelihood of observing \( A \) under the model given by (3.1) is equivalent to minimizing the KL-divergence between \( A \) and \( \hat{A} = G \times_1 U \times_2 V \times_3 Y \). This is a tensorial generalization of the connection between PMF and NMF with KL-divergence referenced in (2.4) and motivates the use of the KL-divergence for determining the NNTuck.

We now define vocabulary for three types of NNTucks, each based on different assumptions of the structure and dimension of \( Y \in \mathbb{R}^{L \times C} \).

Definition 3.1 (Layer independent NNTuck). A layer independent NNTuck is a nonnegative Tucker decomposition where \( C = L \) and \( Y \) has the constraint \( Y = I \).

Definition 3.2 (Layer dependent NNTuck). A layer dependent NNTuck is a nonnegative Tucker decomposition where \( Y \) has the constraint \( C < L \).

Definition 3.3 (Layer redundant NNTuck). A layer redundant NNTuck is a nonnegative Tucker decomposition where \( C = 1 \) and we constrain \( Y \) to be the ones vector, \( Y = [1, \ldots, 1]^T \).

3.2. Relationship to MULTITENSOR (MT). If we collect the affinity matrices \( G_\ell \) from the MT model to be the frontal slices of tensor \( G \in \mathbb{R}_+^{K \times K \times L} \), then (2.7) is equivalent to

\[
A \sim \text{Poisson}(G \times_1 U \times_2 V).
\]

Note that \( G \times_1 U \times_2 V = G \times_1 U \times_2 V \times_3 I \). This model is what we define as a layer independent NNTuck in Definition 3.1 above and is sometimes called a Tucker-2 decomposition [38]. Since all factors are nonnegative, the MT model seeks to find the nonnegative Tucker-2 decomposition by maximizing the log-likelihood through EM. Given that the interpretation of the \( Y \) factor matrix is that it describes layer communities in the network, constraining \( Y = I \) as is done in MT assumes that each layer of the multilayer network was drawn from a distinct
A FACTOR MODEL OF MULTILAYER NETWORK INTERDEPENDENCE

= α + βG2
U V⊤
1001
= U V⊤𝓖
I αβ
𝓖
G1G3

Figure 2. If one or more of the frontal slices of the core tensor are linear combinations of another, there is a deflation of the core tensor. In this example, we show how a layer independent NNTuck (left) can be equivalently written as a layer dependent NNTuck (right). This figure shows how layer dependence is stored in the factor matrix Y.

SBM, albeit with common membership matrices U and V. That is, this constraint assumes that there is no latent structure in the layers of the network.

3.3. Deflation and Layer Dependence. In this section we discuss layer dependence in the NNTuck through three examples and discuss how deflation of the core tensor allows for latent structure to be identified in the layers of a multilayer network.

Definition 3.4 (Deflation). We say there is a deflation of the core tensor G ∈ ℝK×K×L of a layer independent NNTuck if there exists a tensor G′ ∈ ℝK×K×C and a factor matrix Y ∈ ℝL×C for C < L such that,

(3.3) G ×1 U ×2 V = G′ ×1 U ×2 V ×3 Y.

When the core tensor can be deflated the factor matrix Y in the NNTuck captures the interdependence between layers. We examine deflation and the Y factor matrix through the three example model instances below, respectively depicted in Figures 2, 3, and 4.

Example 3.5 (Linearly dependent core tensor). For a three-layer adjacency tensor A ∈ {0, 1}N×N×3 consider the layer independent NNTuck given by A = H ×1 U ×2 V ×3 1 where the frontal slices of core tensor H ∈ ℝK×K×3 are as follows:

H1 = [0.2 0.1 0.1], H2 = [0.3 0.01 | 0.1 0.01], H3 = [0.35 0.105 | 0.105 0.2].

As may be evident, H3 is a linear combination of H1 and H2. Specifically, H3 = H1 + βH2. In the same sense that a rank-deficient matrix has one or more columns which are a linear combination of others, we can consider the inclusion of H3 in the core tensor redundant. If we have a limited data source from which we are estimating our model, “wasting” information to fit this redundant frontal slice could lead to a less efficiently estimated model. Instead,
consider tensor $\mathcal{G}$ whose frontal slices are $G_1 = H_1$ and $G_2 = H_2$, and define
\[
Y := \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0.5 \end{bmatrix},
\]
where the third row contains the respective weights of $H_1$ and $H_2$ that sum to $H_3$. Then
\[
H \times_1 U \times_2 V \times_3 I = \mathcal{G} \times_1 U \times_2 V \times_3 Y.
\]
Note that whereas these two models are mathematically equivalent, the deflated model allows for latent structure in the layers of the network to be efficiently identified.

**Example 3.6 (strata SBM).** For $A \in \mathbb{Z}_{0+}^{N \times N \times 4}$ consider the nonnegative Tucker-2 model given by $A = H \times_1 U \times_2 V \times_3 I$. Assume that the core tensor $H \in \mathbb{R}_{+}^{K \times K \times 4}$ has frontal slices $H_3 := H_1$ and $H_4 := H_2$, for the same $H_1$ and $H_2$ in the previous example. For $\mathcal{G} = \mathbb{R}_{+}^{K \times K \times 2}$ with frontal slices $G_1 = H_1$ and $G_2 = H_2$ and factor matrix
\[
Y = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix},
\]
then $H \times_1 U \times_2 V \times_3 I = \mathcal{G} \times_1 U \times_2 V \times_3 Y$.

The interpretation of this example is that layers 1 and 3 in the multilayer network were drawn from the same SBM, one distinct from that which generated layers 2 and 4. Because membership matrices are held to be fixed across layers, this means that communities interact with the same rates in layers 1 and 3, although these rates are different from those which determine interaction in layers 2 and 4. This example clusters layers generated from the same SBM and is generatively equivalent to the strata SBM in [56].

**Example 3.7 (repeated SBMs).** For $A \in \{0,1\}^{N \times N \times 4}$ consider the layer independent NNTuck given by $A = H \times_1 U \times_2 V \times_3 I$. In this example, consider that all of the frontal
slices of $\mathcal{H}$ are equal: $H_\ell = H_1$ for $\ell = 1, 2, 3, 4$. Define $\mathcal{G} \in \mathbb{R}^{K \times K \times 1} = H_1$ and factor matrix $Y = 1 = [1, 1, 1]^T$. Then $\mathcal{H} \times_1 U \times_2 V \times_3 1 = H_1 \times_1 U \times_2 V \times_3 Y$.

The deflated model is a layer redundant NNTuck and can be interpreted by considering that all layers of the network are different realizations of the exact same SBM. That is, the underlying process which is assumed to have generated the structure observed in layer 1 is the same as that which generated the structure observed in all other layers. In this sense, a multilayer network with this multilayer SBM does not need to be represented as a multilayer network.

The following final example serves as a warning of the limitations of assessing layer interdependence using the NNTuck model.

**Example 3.8 (Linear basis as a cause for deflation.).** Consider a network for which $K = 2$, $L > 4$, and a layer independent NNTuck with $2 \times 2$ affinity matrices $G_\ell$ for $\ell = 1, \ldots, L$ for each layer of the network.

Note that there is a natural linear algebraic (as opposed to sociological or contextual) reason why this NNTuck can be deflated, or more generally why an estimated model may perform well when $C < L$ without necessarily exhibiting contextually relevant layer dependence. Specifically, any $2 \times 2$ matrix can be written as a linear combination of the following bases:

$$B_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad B_4 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$ 

For example,

$$G = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = aB_1 + bB_2 + cB_3 + dB_4.$$ 

For the NNTuck where all matrices $G_\ell$ have nonnegative entries, coefficients $a, b, c, d$ above will also be nonnegative. Thus for this $K = 2$ case, any core tensor $\mathcal{H} \in \mathbb{R}_{+}^{2 \times 2 \times L}$ can be deflated to core tensor $\mathcal{B} \in \mathbb{R}_{+}^{2 \times 2 \times 4}$ whose $\ell$th frontal slice is $B_\ell$. In this sense, we can only hope to interpret deflation as a characteristic of the network (as opposed to a characteristic of the linear algebra) when $C < K^2$. For the empirical examples we consider in the next section (where there are between $L = 7$ and $L = 21$ layers), we will need to consider this issue.
in the case where \( K = 2, 3, 4 \), depending on the network, because \( L < K^2 \) for all larger \( K \). As broader context, for the over 45 datasets provided in De Domenico’s multilayer network database \([17]\), only two datasets have more than 16 layers. Since the number of layers in common applications are typically small and \( K \) typically modestly large, \( L \geq K^2 \) is relatively uncommon, thus keeping \( C < K^2 \) as well.

### 3.4. Algorithmic Approach.

Kim and Choi (2007) \([36]\) extend Lee and Seung’s (2001) multiplicative updates for NMF \([41]\) to the nonnegative Tucker decomposition for minimizing both KL-divergence and Frobenius loss. We reproduce the updates for minimizing KL-divergence in Algorithm 3.1. The updates in \([36]\) are written for a general, \( n \)-th order tensor, so rewrite them here for a 3rd order tensor in a setting wherein some data is masked as specified by a masking tensor \( \mathcal{M} \in \{0, 1\}^{N \times N \times L} \). Note that if the data is not masked, the all ones masking tensor \( \mathcal{M} = 1^{N \times N \times L} \) recovers the original multiplicative updates. Also note that these updates are done sequentially, not in parallel.

**Algorithm 3.1 Multiplicative Updates for minimizing KL-Divergence in the NNTuck [36]**

**Input:** \( \mathcal{A}, K, C, \text{Symmetric}, \text{Masked}, \mathcal{M}, \text{Independent}, \text{Redundant} \)

**Initialize** \( U, V \in \mathbb{R}^+_N \times K, Y \in \mathbb{R}^+_L \times C \), and \( \mathcal{G} \in \mathbb{R}^{K \times K \times C} \) to have random, nonnegative entries.

if Symmetric: \( V \leftarrow U, G_\ell \leftarrow G_\ell^\top G_\ell \) for \( \ell = 1, \ldots, C \), and skip each \( V \) update step below.

if Independent: \( Y \leftarrow I \) and skip each \( Y \) update step below.

if Redundant: \( Y \leftarrow \text{ones}(C) \) and skip each \( Y \) update step below.

if not Masked: \( \mathcal{M} = 1^{N \times N \times L} \)

while \( \frac{KL(A|A_{\ell = 1}) - KL(A|A_{\ell = 1})}{KL(A|A_{\ell = 1})} < \text{rel\_tol} \):

\[
U \leftarrow U \circ \frac{[M_{(1)} \circ A_{(1)} / \hat{A}_{(1)}] \mathcal{G} \times_2 V \times_3 Y^\top_{(1)}}{M_{(1)} [\mathcal{G} \times_2 V \times_3 Y^\top_{(1)}]}
\]

\[
V \leftarrow V \circ \frac{[M_{(2)} \circ A_{(2)} / \hat{A}_{(2)}] \mathcal{G} \times_1 U \times_3 Y^\top_{(2)}}{M_{(2)} [\mathcal{G} \times_1 U \times_3 Y^\top_{(2)}]}
\]

\[
Y \leftarrow Y \circ \frac{[M_{(3)} \circ A_{(3)} / \hat{A}_{(3)}] \mathcal{G} \times_1 U \times_2 V^\top_{(3)}}{M_{(3)} [\mathcal{G} \times_1 U \times_2 V^\top_{(3)}]}
\]

\[
\mathcal{G} \leftarrow \mathcal{G} \circ \frac{\mathcal{M} \circ A / \hat{A} \times_1 U^\top \times_2 V^\top \times_3 Y^\top}{\mathcal{M} \times_1 U^\top \times_2 V^\top \times_3 Y^\top}
\]

\[
\hat{A} \leftarrow \mathcal{G} \times_1 U \times_2 V \times_3 Y
\]

Return \( U, V, Y, \mathcal{G} \).

Because these updates are derived from the multiplicative updates for NMF \([41]\), they come with guaranteed monotonic convergence to a local minima. In practice, we declare that the algorithm has found a local minima if the KL-divergence has not decreased by more than a relative tolerance of \( 10^{-5} \) in ten steps. For the case of an undirected network, we initialize
the core tensor to have symmetric frontal slices \( G_\ell = G_\ell^\top \), and initialize and fix \( U = V \) throughout the updates. We then follow the multiplicative updates above by only making updates to \( U, Y, \) and \( G \). Doing so maintains the guaranteed monotonic convergence to a local minima while preserving the symmetric structure in \( G \), and ensures the constraint for the undirected case that \( U = V \).

**Proposition 3.9.** Determining factor matrices \( U, V, \) and \( Y \) and the core tensor \( G \) in the NNTuck by maximizing the log-likelihood using expectation maximization (EM) is equivalent to using the multiplicative updates given in [36] to minimize KL-divergence.

**Proof.** See Section SM2.

The significance of this proposition is noticing that not only is minimizing KL-divergence equivalent to maximizing log-likelihood, but also that the algorithm by which to find a local minimum of the KL-divergence is the exact same as that to find a local maximum of the log-likelihood. Moreover, using EM to maximize the log-likelihood of observing \( A \) under the MT model is equivalent to minimizing the KL-divergence between \( A \) and a layer independent NNTuck. Thus, the EM steps given in [16] are equivalent to the multiplicative updates in [36], where at initialization \( Y = I \) is fixed and at each step \( Y \) is not updated.

**Algorithmic Limitations.** It is important to emphasize that the the KL-divergence given by (2.6) (and thus the log-likelihood of observing \( A \) under (3.1)) is non-convex. Therefore, although the multiplicative updates discussed above guarantee monotonic convergence, it is only to local optima. In practice, this means that the algorithm should be run multiple times with different initial conditions, and the resulting NNTuck with the maximal log-likelihood should be chosen as the “best” model. An evaluation of alternative optimization methods for nonnegative matrix and tensor factorizations, including mirror descent [31], projected gradient descent [14], and stochastic gradient descent [35], is beyond the scope of this work.

4. **Empirically Validating Layer Dependence.** The equivalence between a layer independent NNTuck and a deflated NNTuck, as discussed in Definition 3.4 and Subsection 3.3, is more difficult to identify when estimating an NNTuck for empirical multilayer networks. Thus in this section we introduce a formal definition of a layer independence test by defining a corresponding likelihood ratio test (LRT). We conclude with a presentation of three methods by which to interpret \( \hat{Y} \) of an NNTuck estimated for an empirical multilayer network.

4.1. **Layer Independence and Likelihood Ratio Tests.** Important to note in defining a layer independence test is that the theory underlying the likelihood ratio test (LRT), Wilks’ theorem [66], necessarily depends on the maximum likelihood being reached, something we cannot guarantee in our nonconvex problem context. Moreover, we propose this method for determining layer interdependence constrained to the classes of models for which the difference in the degrees of freedom \( d = (L - C)K^2 - LC > 0 \), which is not always true for certain values of \( L, K, \) and \( C \). Alternative LRTs (including a bootstrapping method that avoids asymptotics altogether) for latent variable models have been proposed [13], and address this issue as well as other common issues that arise when using the LRT to compare latent variable models.

**Definition 4.1 (Layer Independence Test).** For a multilayer network let model I be the layer independent NNTuck and let model II be the layer dependent NNTuck. A multilayer network...
has layer independence at level $\alpha$ if the likelihood ratio test with $(L-C)K^2 - LC$ degrees of freedom is significant at level $\alpha$. In this case we reject the null hypothesis that the two models fit the data equally well, and determine that model I fits the multilayer network significantly better than does model II.

**Definition 4.2 (Layer Dependence Test).** A multilayer network has layer dependence at level $\alpha$ if the LRT described above is not significant at level $\alpha$ for a pre-specified $C$.

**Definition 4.3 (Layer Redundancy Test).** A multilayer network has layer redundancy at level $\alpha$, if the LRT comparing the layer redundant NNTuck to the layer independent NNTuck with $(L-1)K^2$ degrees of freedom is not significant at level $\alpha$.

Likelihood ratio tests can be used to assess the performance of two models, where one is a nested model of the other, based on the ratio of the maximum likelihoods, a ratio that asymptotically satisfies Wilks’ theorem (assuming we’ve succeeded in maximizing the likelihood, see comment at the beginning of this section). In the context of evaluating different NNTuck models of varying latent dimension $C$, the most general model is the layer independent NNTuck and layer dependent NNTuck with $C < L$ layer communities is nested within the models with $C + 1$ layer communities. When comparing two NNTuck models, the null hypothesis of the LRT is that the two models fit the data equally well, and the alternative hypothesis is that the richer model fits the data significantly better. If the resulting $p$-value rejects the null hypothesis, then the full model should be used. Otherwise, the nested model should be used.

To use this LRT, one must determine how many parameters are in the full model and how many are in the nested model. When comparing two layer dependent NNTucks with dimensions $C_f$ and $C_n$ for $C_n < C_f$ and fixed $K$, there is a difference of $(L + K^2)(C_f - C_n)$ parameters between the two models. When comparing the layer redundant NNTuck nested under the layer independent NNTuck, the difference in number of parameters is $(L - 1)K^2$.

In comparing the layer dependent NNTuck with $C < L$, nested under the layer independent NNTuck, the difference in the number of parameters is $(L - C)K^2 - LC$.

**4.2. Investigating Layer Dependence Empirically.** If the layer dependence test determines that an empirical multilayer network has dependent layers, it is useful to investigate how they are related. Whereas in the examples in Subsection 3.3 above it is straightforward to examine layer dependency through the $Y$ factor matrix, one must use certain heuristics for empirical multilayer networks.

The main reason these approaches aid in the interpretation of $Y$ can be understood by considering that the frontal slices of the estimated core tensor are not estimated to correspond to the affinity matrix for $C$ specific layers of the multilayer network. This is evident by “reinflating” the core tensor such that $\hat{G}_{\text{inflate}} = \hat{G} \times_3 \hat{Y}$. Each frontal slice of $\hat{G}_{\text{inflate}}$ corresponds exactly to the affinity matrix for each layer of the multilayer network. Thus we offer the three following approaches for interpreting $\hat{Y}$ estimated from empirical data.

The first approach is to row-normalize $\hat{Y}$ such that $\hat{y}_t^{(1)} = \hat{y}_t/\|\hat{y}_t\|_1$ and inspect the rows of $\hat{Y}^{(1)}$ relative to one another. The second approach is to row-normalize $\hat{Y}$ such that $\hat{y}_t^{(2)} = \hat{y}_t/\|\hat{y}_t\|_2$ and inspect the entries of similarity matrix given by $\hat{Y}^{(2)}\hat{Y}^{(2)\top}$. The third approach uses reference layer bases. In this approach, $C$ reference layers are chosen, $\hat{G}$ is rewritten in the linear bases of those reference layers’ affinity matrices, and corresponding $\hat{Y}^*$
A FACTOR MODEL OF MULTILAYER NETWORK INTERDEPENDENCE

is defined in relation to the new core tensor. For specifics on this process and guidance on choosing the reference layers, see Section SM4.

5. Model Selection Through Cross Validation. In this section we discuss the use of cross validation in this work and define two link prediction tasks for tensors. We emphasize that we are more interested in how the cross validation highlights interesting model choices than by the actual predictive performance of NNTuck in these link prediction tasks. Statistical factor models of networks are generally not competitive with machine learning classifiers that use even simple topological features [15, 43, 26]. As such, the absolute performance here should not be considered a metric of primary interest, but as a means of comparative inspection.

The construction of the cross validation approach is as follows. For each link prediction task we construct five different masking tensors and estimate a model based on only observed entries of the data tensor. We select the NNTuck with the highest test set log-likelihood from 50 different runs of the multiplicative updates algorithm with random initializations. Then, test-AUC is averaged across the five different maskings. This process is repeated for varying dimensions ($K$, $C$) in the NNTuck.

We define the link prediction tasks via the structure of their masking tensors $\mathcal{M} \in \{0, 1\}^{N \times N \times L}$ where $M_{ij\ell} = 0$ indicates that the presence or absence of an edge between nodes $i$ and $j$ in layer $\ell$ is missing, and $M_{ij\ell} = 1$ otherwise. In undirected networks we enforce $M_{ij\ell} = M_{ji\ell}$ for both link-prediction tasks.

**Independent link prediction.** In this link prediction task masking is irrespective of layer. That is, we assume that for $b$-fold cross validation, elements in the tensor are missing with uniform and independent probability $1/b$. Specifically, missing entry $(i, j)$ in layer $k$ does not imply that entry $(i, j)$ is missing in all layers ($M_{ijk} = 0 \not\Rightarrow M_{ij\ell} = 0$ for $\ell \neq k$).

**Tubular link prediction.** In this link prediction task edges are always observed or missing across all layers. That is, we assume that for $b$-fold cross validation, tubes $(i, j, \cdot)$ in the tensor are missing with uniform probability $1/b$ (see Figure SM2 for a visualization of tensor tube fibers). Specifically, missing link $(i, j)$ in layer $k$ does imply that link $(i, j)$ is missing in all layers ($M_{ijk} = 0 \Rightarrow M_{ij\ell} = 0$, $\forall \ell$). We motivate this tubular task by commenting that independent link prediction is often “too easy,” in the sense that if many layers are dependent then missing elements are much easier to impute when other elements from the same tube are available. Tubular link prediction captures realistic settings where one knows nothing at all about the relationship between two units $i$ and $j$ in any layer.

Given the structure of an adjacency tensor, there are (at least) two other link prediction tasks which are representative of true missingness patterns in data: one in which an entire horizontal slice of data is missing ($M_{ijk} = 0 \Rightarrow M_{ip\ell} = 0$ for all $p, \ell$), and one in which an entire lateral slice of data is missing ($M_{ijk} = 0 \Rightarrow M_{tj\ell} = 0$ for all $r, \ell$). We limit our scope to the independent and tubular link prediction tasks above, but mention these as potentially interesting missingness patterns in the context of multilayer networks.

6. Application of the NNTuck to Synthetic and Empirical Networks. In this section we use the cross validation tools discussed in Section 5, the layer dependence tests developed in Subsection 4.1, and the $Y$ interpretability heuristics from Subsection 4.2 to use the NNTuck in application. In Subsection 6.1 we generate a synthetic network example to exhibit the interpretability of the $Y$ factor matrix when $K$ and $C$ are known. In Subsection 6.2 for
each empirical network presented we carry out the following steps: (i) use a cross validation approach to determine model hyper-parameter choices $K$ and $C$, (ii) use likelihood ratio tests with this $(K,C)$ pair to determine layer independence, redundancy, or dependence, (iii) if the network is layer dependent at level $\alpha$, examine the $Y$ factor matrix.

6.1. Synthetic network examples. In this section we define two different synthetic networks and inspect their estimated $Y$ factor matrices. For both examples, we let $N = 200$, $K = 2$, $L = 4$, and define affinity matrices

$$G_1 = \begin{bmatrix} 0.2 & 0.1 \\ 0.1 & 0.2 \end{bmatrix} \quad \text{and} \quad G_3 = \begin{bmatrix} 0.3 & 0.01 \\ 0.01 & 0 \end{bmatrix}.$$  

We set the affinity matrices $G_2$ and $G_4$ to be linear combinations of the above affinity matrices,

$$G_2 = \alpha G_1 + \beta G_3 \quad \text{and} \quad G_4 = \gamma G_1 + \eta G_3,$$

for different values of $\alpha$, $\beta$, $\gamma$, and $\eta$ between the two examples.

In both examples, we generate a multilayer network from an SBM which assumes that an edge between nodes $i$ and $j$ in layer $\ell$ is drawn from a Poisson distribution with mean $u_iG_{\ell}v_j^T$. We set $u_i = v_i$ and assign 100 nodes to the first group ($u_i = [1,0]$) and 100 nodes to the second group ($u_i = [0,1]$). Generating these synthetic networks in this way is equivalent to drawing them from $A \sim \text{Poisson}(G \times U \times V \times Y)$ for

$$Y = \begin{bmatrix} 1 & 0 \\ \alpha & \beta \\ 0 & 1 \\ \gamma & \eta \end{bmatrix}$$

and $G \in \mathbb{R}^{K \times K \times 2}$ with first and second frontal slices $G_1$ and $G_3$, respectively. For the first network we define $\alpha = 0.5$, $\beta = 0.5$, $\gamma = 0.1$, and $\eta = 0.9$, and for the second we let $\alpha = 1$, $\beta = 0$, $\gamma = 0$, and $\eta = 1$. This second synthetic network is the strata example depicted in Figure 3 and discussed in Example 3.6. As an aside, note that whereas in these two networks the entries of the rows of $Y$ sum to one, this need not be the case. Actually, by allowing the rows of $Y$ to be unnormalized we can account for heterogeneous degree distributions across layers, just as the degree-corrected single layer SBM [34] accounts for heterogeneous degree distributions across nodes.

For both networks we estimate the NNTuck with $C = 2$ and $K = 2$ and report the NNTuck with the highest log-likelihood over 20 runs with different random initializations. We threshold the values in the resulting membership matrices $\hat{U}$ and $\hat{V}$ to reflect the hard membership of the generative model. Node membership is exactly recovered for both networks and thus we focus our attention on interpreting $\hat{Y}$. In both networks, $\hat{Y}$ recovers the structural dependence between layers and we report the results of all three approaches for interpreting $\hat{Y}$ in Figure 5.

6.2. Empirical Multilayer Networks. In this section we use the NNTuck and the tools developed thus far to study: Krackhardt’s 1987 cognitive social structure dataset [39]; a biological multilayer network [40]; a social support multilayer network [7]; and 112 other
Figure 5. We reproduce the results of the methods for interpreting \( \hat{Y} \) in the NNTuck of the first and second synthetic network described above as well as for the 48th village from the Banerjee et. al (2019) [8] work (labelled “Gossip village 48” in Figure 9). For the synthetic networks, \( Y \) is the true factor matrix from which the network was generated. For all three, \( \hat{Y} \) has been estimated from the NNTuck, \( \hat{Y}^{(1)} \) has been normalized so that the entries of each row sum to one, \( \hat{Y}^{(2)} \) has been normalized so that each row has unit 2-norm. For the synthetic networks, \( \hat{Y}^{*} \) is the resulting factor matrix after rewriting \( \mathcal{G} \) in the basis of layers 1 and 3 (a process which is described in detail in Section SM3). Note that in the synthetic examples, all methods for interpreting \( \hat{Y} \), including simply inspecting \( \hat{Y} \), accurately represent how the layers of the network are related to one another. Specifically, note how \( \hat{Y}^{*} \) almost exactly recovers the ground truth of how the layers are interdependent. Focusing on \( \hat{Y}^{*} \) matrix for the gossip village, the two reference layers chosen are “Who asks you for advice?” and “Who are your relatives?”, where the remaining layers can be understood in terms of a linear combination of these.

Table 3: We include the results from the LRTs for all the data sets we introduce in the following sections. Notably, we conclude that the Malaria multilayer network has layer independence at level \( \alpha = 0.05 \), whereas and all of the other datasets have either layer redundancy or layer dependence at the same level \( \alpha \).

6.2.1. Krackhardt’s Cognitive Social Structures. Krackhardt’s (1987) Cognitive Social Structures work [39] surveys 21 people in the management team at a tech firm on their perception of the advice network within the management team. Each of the 21 people were asked to answer the question “Who would you go to for help or advice at work?” followed by a list of the 21 management employees (including themselves). The resulting 21 \( \times \) 21 multilayer network is what Krackhardt referred to as a cognitive social structure (CSS), where each layer \( \ell \) represents person \( \ell \)’s perception of who receives advice from whom in the network. The adjacency matrices for this advice CSS were transcribed from the original paper for this work, and can be accessed on GitHub [1] (the CSS for the friendship network is different and can be accessed in the R package cssTools [69]).

Interestingly, the cross validation observations are different for each link prediction task.
The $p$-values and LRT determinations for all datasets explored in the following sections. Both village support system networks are determined to be layer redundant, the Malaria network is determined to have layer independence, and the Krackhardt network is determined to have layer dependence. For the purposes of exploring an empirical \( \hat{Y} \) (see Figure 5), we perform a layer dependence test on Gossip Village 48 with \( K = 4, C = 2 \) and find that it is layer dependent at level \( \alpha = 0.05 \).

![Figure 6](image-url)

**Figure 6.** \( NNTuck \) performance on independent (left) and tubular (right) link prediction tasks with varying latent dimensions $K$ and $C$ for Krackhardt’s CSS multilayer network. Whereas the layer dependent \( NNTuck \) with $C < L$ has a higher test-AUC in the independent task, the layer independent \( NNTuck \) generally performs as well as the other models in the tubular task.

We observe a higher test-AUC associated with the layer dependent \( NNTuck \) in the independent link prediction task, and becomes more pronounced as $K$ increases. In the tubular link prediction task, however, the layer independent and layer dependent \( NNTucks \) have a similar test-AUC for nearly all values of $K$. In both link prediction tasks we observe: variation in test-AUC for different values of $K$ and $C$; the layer redundant \( NNTuck \) has a lower test-AUC than the layer dependent or layer independent \( NNTucks \); neither the independent nor tubular link prediction task is obviously harder than the other; and the observations from the independent link prediction task are not the same as those from the tubular link prediction task. One possible source of this difference is that the tubular link prediction task is the more...
difficult one, when compared to the independent task, and thus the results from this task are more representative of a model’s performance.

Based on these results, we choose $K = 3$ and $C = 4$ for the corresponding layer independence, redundancy, and dependence tests and determine that whereas the network is not layer redundant, it is layer dependent at significance level $\alpha = 0.05$ (see Table 3 for details). For the sake of brevity (and due to its size $(21 \times 4)$), we do not interpret the $\hat{Y}$ matrix here.

6.2.2. Malaria Data. This biological network was originally studied by Larremore et al. (2013) [40]. The undirected network consists of $N = 307$ malaria parasite virulence genes connected across $L = 9$ layers. Two genes are connected if they share a genetic substring of a significant length. Each layer corresponds to a different Highly Variable Region on the genes. For more information on the framework or motivating underlying biology, see [40].

In this network the test-AUC of the layer independent NNTuck is always higher than the test-AUC of either the layer dependent or layer redundant NNTuck. This performance difference indicates that the core tensor cannot be deflated without losing important information about the network’s layers. Interestingly, we observe that the layer dependent NNTuck with $C = 9$ does not perform as well as the layer independent NNTuck, even though the core tensor has the same dimension in both models. While this observation may be an artifact of the underlying optimization landscape, we do not fully understand the implications or causes and it is an interesting topic for future work. Finally, we do not observe a gap in test-AUC between the independent and tubular link-prediction tasks: predicting a missing link with information about that link in other layers is just as difficult as predicting a missing link with no other information about that link in any layer.

We therefore determine that an appropriate model choice is a layer independent NNTuck with $K = 5$ and find that this network is layer independent at significance level $\alpha = 0.05$. Layer independence in this network is supported both by a biological intuition and by the findings discussed in [16]. Therefore, $\hat{Y} = I$ and thus does not need to be interpreted.

6.2.3. Village Social Support Network. The social multilayer network we consider contains different types of social interaction within a village in Karnataka, India, one of 43
Figure 8. The test-AUC from the independent and tubular link prediction tasks for the Village 0 multilayer network. In both tasks, both the layer dependent and layer redundant NNTucks perform just as well as the layer independent NNTuck in terms of test-AUC.

Microfinance villages from Banerjee et al. (2013) [7]. We arbitrarily selected the first of the 43 villages and will henceforth refer to this village as “Village 0”. The directed network consists of $N = 843$ individuals across $L = 12$ layers. One individual is connected to another if the first indicated that they would interact in a specified way with the second. Each layer corresponds to a different type of social interaction (e.g., “Who are the people who give you advice?” and “Who are your kin?”). See Section SM5 for a full list of the questions.). For more information about the networks, survey instruments, or context of this data, see [7].

Cross validation results for the Village 0 network are shown in Figure 8. There is a slight gap in test-AUC across the two link-prediction tasks for this dataset, where the tubular link-prediction task is more difficult than the independent link-prediction task. However, in both tasks we observe that the layer redundant NNTuck and the layer dependent NNTucks (for all $C$) perform just as well as the layer independent NNTuck in terms of test-AUC.

The layer redundancy test confirms that this network is layer redundant at significance level $\alpha = 0.05$, consistent with the notion that the 12 layer network may indeed be such that all layer models are drawn from the same SBM, as we saw in Example 3.7. Considering the efforts made to collect data on these 12 different social support systems, this observation is surprising. One would expect that the distinct questions generating each layer of the network capture new information about the social network. This observation suggests otherwise, at least for the social structures that are well-modelled by stochastic block models.

6.2.4. Collection of Village Social Support Networks. We now turn our attention to two sets of multilayer social networks representing different types of interaction in 113 villages: 43 microfinance villages from Banerjee et al. (2013) [7] and 70 gossip villages from Banerjee et al. (2019) [8]. The intent in studying these large collections of village networks is to see if the observation from Subsection 6.2.3, that Village 0 is layer redundant at level $\alpha = 0.05$, is common across multiple different networks of the same type. The survey questions defining each layer for these networks are different for each data source (see Section SM5): the 12 types of social support defining the layers in the networks of Banerjee et al. (2013) [7] are different from the social support defining the 7 layers in the networks of Banerjee et al. (2019) [8].
For each of these 113 villages we fix $K = 4$ and $K = 10$ and perform cross validation under the independent link prediction task for both the layer independent and layer redundant NNTuck. We plot the test-AUCs of this multi-village link prediction task in Figure 9, where we also plot the test-AUC of the corresponding models in the Krackhardt, Village 0, and first synthetic network. Surprisingly, we note that the test-AUC for the layer redundant NNTuck is nearly equivalent to the test-AUC for the layer independent NNTuck for almost all of the village networks. Furthermore, although not included in Table 3, each of these 113 villages is layer redundant at level $\alpha = 0.05$. We highlight the village network with the biggest difference between the two test-AUCs, labeled “Gossip village 48”, and estimate a layer dependent NNTuck with $K = 4$ and $C = 2$. With this model choice, we find that the network is layer dependent at level $\alpha = 0.05$ and interpret the corresponding $\hat{Y}$ in Figure 5.

7. Conclusion. In this work we use the nonnegative Tucker decomposition (NNTuck) with KL-divergence as an extension of the stochastic block model (SBM) to multilayer networks. The NNTuck allows for layers in the network to have latent structure, just as the SBM allows for latent structure in the nodes of a single layer network. Using algebraic examples we show that the third factor matrix of the NNTuck both captures and incorporates information about layer interdependence in multilayer networks. We show that the multiplicative updates for minimizing the KL-divergence of the NNTuck are step-by-step equivalent to maximizing the log-likelihood of observing the network under the NNTuck model using expectation maximization. This equivalence generalizes a previously known result about matrices and motivates the use of this algorithm in the context of the NNTuck.

To use the NNTuck to validate layer dependence in empirical multilayer networks, we define three likelihood ratio tests (LRTs) to test layer independence, layer redundancy, and layer dependence. Furthermore, we propose three methods for interpreting the third factor matrix of an NNTuck estimated for an empirical network. We propose cross validation as a means for model selection and formalize two link prediction tasks for the multilayer setting. We use cross validation, the LRTs, and the approaches for interpreting $\hat{Y}$ to study a variety of...
synthetic and empirical multilayer networks. In doing so, we find that the Malaria multilayer network has independent layers, 113 different social support networks are layer redundant, and Krackhardt’s cognitive social structure has layer dependence.

This work also lays the groundwork for diverse future work and applications. Given the observation in Subsection 6.2.4, that for many of the village multilayer networks we study the layers seem to be noisy observations from the same SBM, it would be interesting to explore how other models of network formation (e.g., choice-based dynamic models [46]) uncover different characteristics amongst the layers that the SBM cannot identify. As discussed in Section 5, the difference in test-AUC between the layer independent NNTuck and the layer dependent NNTuck with $C = L$ is not fully understood and could be addressed in future work. Finally, another interesting future direction of this work is understanding how the NNTuck can be made more interpretable under a Varimax rotation, following recent connections between Varimax and factor model inference [52].

Understanding the layer dependencies in a multilayer network can inform the development of survey design, identify redundancies, or illuminate contextual connections. Moreover, the usefulness of finding latent structure in the layers motivates the use of latent-space models as a noise-free smoothing of the observed network, as proposed by Fisher (2021) [23]. As such, there is potential to use this work to understand layer dependence in a variety of applications where domain-specific knowledge can make use of the interpretations that the NNTuck provides.

Acknowledgments. We would like to thank Caterina De Bacco, Eleanor Power, and Dan Larremore for their helpful conversations.

REFERENCES

[1] I. P. Aguiar, Transcription of the 21 adjacency matrices in the appendix of Krackhardt’s 1987 "cognitive social structures", Jun 2021, https://github.com/izabelaguiar/krackhardt/.
[2] E. M. Airoldi, D. M. Blei, S. E. Fienberg, and E. P. Xing, Mixed membership stochastic blockmodels, Journal of Machine Learning research, 9 (2008), pp. 1981–2014.
[3] E. Al-Sharoa, M. Al-Khassaweneh, and S. Aviyente, Tensor based temporal and multilayer community detection for studying brain dynamics during resting state fMRI, IEEE Transactions on Biomedical Engineering, 66 (2018), pp. 695–709.
[4] K. M. Altenburger and J. Ugander, Which node attribute prediction task are we solving? within-network, across-network, or across-layer tasks, in Proceedings of the International AAAI Conference on Web and Social Media, vol. 15, 2021, pp. 38–48.
[5] B. W. Bader, R. A. Harshman, and T. G. Kolda, Temporal analysis of semantic graphs using ASALSAN, in Seventh IEEE International Conference on Data Mining, IEEE, 2007, pp. 33–42.
[6] B. Ball, B. Karrer, and M. E. Newman, Efficient and principled method for detecting communities in networks, Physical Review E, (2011).
[7] A. Banerjee, A. G. Chandrasekhar, E. Duflo, and M. O. Jackson, The diffusion of microfinance, Science, 341 (2013), p. 1236498.
[8] A. Banerjee, A. G. Chandrasekhar, E. Duflo, and M. O. Jackson, Using gossips to spread information: Theory and evidence from two randomized controlled trials, The Review of Economic Studies, 86 (2019), pp. 2453–2490.
[9] S. Boccaletti, G. Bianconi, R. Criado, C. I. Del Genio, J. Gómez-Gardeñes, M. Romance, I. Sendina-Nadal, Z. Wang, and M. Zanin, The structure and dynamics of multilayer networks, Physics Reports, 544 (2014), pp. 1–122.
[10] R. Breiger, S. Boorman, and P. Arabic, An algorithm for clustering relational data with applications to social network analysis and comparison with multidimensional scaling, Journal of Mathematical...
Psychology, 12 (1975), pp. 328–383.

[11] J. Carlen, J. de Dios Pont, C. Mentus, S.-S. Chang, S. Wang, and M. A. Porter, Role detection in bicycle-sharing networks using multilayer stochastic block models, Network Science, 10 (2022), pp. 46–81.

[12] J. D. Carroll and J.-J. Chang, Analysis of individual differences in multidimensional scaling via an n-way generalization of “Eckart-Young” decomposition, Psychometrika, 35 (1970), pp. 283–319.

[13] Y. Chen, I. Moustaki, and H. Zhang, A note on likelihood ratio tests for models with latent variables, Psychometrika, 85 (2020), pp. 996–1012.

[14] A. Cichocki and R. Zdunek, Multilayer nonnegative matrix factorization using projected gradient approaches, International Journal of Neural Systems, 17 (2007), pp. 431–446.

[15] A. Clauset, C. Moore, and M. E. Newman, Hierarchical structure and the prediction of missing links in networks, Nature, 453 (2008), pp. 98–101.

[16] C. De Bacco, E. A. Power, D. B. Larremore, and C. Moore, Community detection, link prediction, and layer interdependence in multilayer networks, Physical Review E, (2017).

[17] M. De Domenico, Datasets released for reproducibility, https://manliodedomenico.com/data.php.

[18] M. De Domenico, V. Nicosia, A. Arenas, and V. Latora, Structural reducibility of multilayer networks, Nature Communications, 6 (2015), pp. 1–9.

[19] M. De Domenico, A. Solé-Ribalta, E. Cozzo, M. Kivelä, Y. Moreno, M. A. Porter, S. Gómez, and A. Arenas, Mathematical formulation of multilayer networks, Physical Review X, 3 (2013), p. 041022.

[20] M. De Domenico, A. Solé-Ribalta, S. Gómez, and A. Arenas, Navigability of interconnected networks under random failures, Proceedings of the National Academy of Sciences, 111 (2014), pp. 8351–8356.

[21] C. Févotte and A. T. Cemgil, Nonnegative matrix factorizations as probabilistic inference in composite models, in 2009 17th European Signal Processing Conference, IEEE, 2009, pp. 1913–1917.

[22] K. R. Finn, M. J. Silk, M. A. Porter, and N. Pinter-Wollman, The use of multilayer network analysis in animal behaviour, Animal Behaviour, 149 (2019), pp. 7–22.

[23] D. N. Fisher and N. Pinter-Wollman, Using multilayer network analysis to explore the temporal dynamics of collective behavior, Current Zoology, 67 (2021), pp. 71–80.

[24] R. Gallotti and M. Barthelemy, The multilayer temporal network of public transport in Great Britain, Scientific Data, 2 (2015), pp. 1–8.

[25] L. Gauvin, A. Panisson, and C. Cattuto, Detecting the community structure and activity patterns of temporal networks: a non-negative tensor factorization approach, PLoS one, 9 (2014), p. e86028.

[26] A. Ghasemian, H. Hosseinzadeh, A. Galstyan, E. M. Airoldi, and A. Clauset, Stacking models for nearly optimal link prediction in complex networks, Proceedings of the National Academy of Sciences, 117 (2020), pp. 23393–23400.

[27] P. Gopalan, J. M. Hofman, and D. M. Blei, Scalable recommendation with poisson factorization, arXiv preprint arXiv:1311.1704, (2013).

[28] R. A. Harshman, Foundations of the PARAFAC procedure: Models and conditions for an explanatory multi-mode factor analysis, UCLA Working Papers in Phonetics, 16 (1970), pp. 1–84.

[29] R. A. Harshman, Models for analysis of asymmetrical relationships among N objects or stimuli, in First Joint Meeting of the Psychometric Society and the Society of Mathematical Psychology, Hamilton, Ontario, 1978, 1978.

[30] R. A. Harshman and M. E. Lundy, Uniqueness proof for a family of models sharing features of Tucker’s three-mode factor analysis and PARAFAC/CANDECOMP, Psychometrika, 61 (1996), pp. 133–154.

[31] L. T. K. Hien and N. Gillis, Algorithms for nonnegative matrix factorization with the Kullback-Leibler divergence, Journal of Scientific Computing, 87 (2021), pp. 1–32.

[32] P. W. Holland, K. B. Laskey, and S. Leinhardt, Stochastic blockmodels: First steps, Social Networks, 5 (1983), pp. 109–137.

[33] T.-C. Kao and M. A. Porter, Layer communities in multiplex networks, Journal of Statistical Physics, 173 (2018), pp. 1286–1302.

[34] B. Karrer and M. E. Newman, Stochastic blockmodels and community structure in networks, Physical Review E, 83 (2011), p. 016107.

[35] H. Kasai, Stochastic variance reduced multiplicative update for nonnegative matrix factorization, in 2018
IEEE International Conference on Acoustics, Speech and Signal Processing, 2018, pp. 6338–6342.

[36] Y.-D. Kim and S. Choi, Nonnegative Tucker decomposition, in IEEE Conference on Computer Vision and Pattern Recognition, 2007.

[37] M. Kivelä, A. Arenas, M. Barthelemy, J. P. Gleeson, Y. Moreno, and M. A. Porter, Multilayer networks, Journal of Complex Networks, 2 (2014), pp. 203–271.

[38] T. G. Kolda and B. W. Bader, Tensor decompositions and applications, SIAM Review, 51 (2009), pp. 455–500.

[39] D. Krackhardt, Cognitive social structures, Social Networks, 9 (1987), pp. 109–134.

[40] D. B. Larremore, A. Clauset, and C. O. Buckee, A network approach to analyzing highly recombinant malaria parasite genes, PLoS Computational Biology, 9 (2013), p. e1003268.

[41] D. Lee and H. S. Seung, Algorithms for non-negative matrix factorization, Advances in Neural Information Processing Systems, 13 (2000).

[42] D. Lee and H. S. Seung, Learning the parts of objects by non-negative matrix factorization, Nature, 401 (1999), pp. 788–791.

[43] D. Liben-Nowell and J. Kleinberg, The link-prediction problem for social networks, Journal of the American Society for Information Science and Technology, 58 (2007), pp. 1019–1031.

[44] P. J. Mucha, T. Richardson, K. Macon, M. A. Porter, and J.-P. Onnela, Community structure in time-dependent, multiscale, and multiplex networks, Science, 328 (2010), pp. 876–878.

[45] M. Nickel, V. Tresp, and H.-P. Kriegel, A three-way model for collective learning on multi-relational data., in International Conference on Machine Learning, vol. 11, 2011, pp. 809–816.

[46] J. Overgoor, A. Benson, and J. Ugander, Choosing to grow a graph: modeling network formation as discrete choice, in The World Wide Web Conference, 2019, pp. 1409–1420.

[47] P. Paatero and U. Tapper, Positive matrix factorization: A non-negative factor model with optimal utilization of error estimates of data values, Environmetrics, 5 (1994), pp. 111–126.

[48] S. Paul and Y. Chen, Consistent community detection in multi-relational data through restricted multilayer stochastic blockmodel, Electronic Journal of Statistics, 10 (2016), pp. 3807–3870.

[49] E. A. Power, Social support networks and religiosity in rural South India, Nature Human Behaviour, 1 (2017), pp. 1–6.

[50] M. Racz and A. Sridhar, Correlated stochastic block models: Exact graph matching with applications to recovering communities, Advances in Neural Information Processing Systems, 34 (2021).

[51] F. J. Roethlisberger and W. J. Dickson, Management and the Worker, vol. 5, Psychology Press, 1939.

[52] K. Rohe and M. Zeng, Vintage factor analysis with varimax performs statistical inference, arXiv preprint arXiv:2004.05387, (2020).

[53] S. F. Sampson, Crisis in a cloister, PhD thesis, Ph. D. Thesis. Cornell University, Ithaca, 1969.

[54] A. Schein, J. Paisley, D. M. Blei, and H. Wallach, Bayesian poisson tensor factorization for inferring multilateral relations from sparse dyadic event counts, in Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 2015, pp. 1045–1054.

[55] A. Schein, M. Zhou, D. Blei, and H. Wallach, Bayesian poisson Tucker decomposition for learning the structure of international relations, in International Conference on Machine Learning, PMLR, 2016, pp. 2810–2819.

[56] N. Stanley, S. Shai, D. Taylor, and P. J. Mucha, Clustering network layers with the strata multilayer stochastic block model, IEEE transactions on network science and engineering, 3 (2016), pp. 95–105.

[57] J. Sun, S. Papadimitriou, C.-Y. Lin, N. Cao, S. Liu, and W. Qian, Multivis: Content-based social network exploration through multi-way visual analysis, in Proceedings of the 2009 SIAM International Conference on Data Mining, SIAM, 2009, pp. 1064–1075.

[58] M. Tarrès-Deulofeu, A. Godoy-Lorite, R. Guimera, and M. Sales-Pardo, Tensorial and bipartite block models for link prediction in layered networks and temporal networks, Physical Review E, 99 (2019), p. 032307.

[59] D. Taylor, M. A. Porter, and P. J. Mucha, Tunable eigenvector-based centralities for multiplex and temporal networks, Multiscale Modeling & Simulation, 19 (2021), pp. 113–147.

[60] L. Torrey and J. Shavlik, Transfer learning, in Handbook of Research on Machine Learning Applications and Trends: Algorithms, Methods, and Techniques, IGI global, 2010, pp. 242–264.

[61] L. R. Tucker, Some mathematical notes on three-mode factor analysis, Psychometrika, 31 (1966),
pp. 279–311.

[62] T. Valles-Catala, F. A. Massucci, R. Guimera, and M. Sales-Pardo, Multilayer stochastic block models reveal the multilayer structure of complex networks, Physical Review X, 6 (2016), p. 011036.

[63] D. Wang and X. Zou, A new centrality measure of nodes in multilayer networks under the framework of tensor computation, Applied Mathematical Modelling, 54 (2018), pp. 46–63.

[64] M. Wang and Y. Zeng, Multiway clustering via tensor block models, Advances in neural information processing systems, 32 (2019).

[65] H. C. White, S. A. Boorman, and R. L. Breiger, Social structure from multiple networks. I. block-models of roles and positions, American Journal of Sociology, 81 (1976), pp. 730–780.

[66] S. S. Wilks, The large-sample distribution of the likelihood ratio for testing composite hypotheses, The Annals of Mathematical Statistics, 9 (1938), pp. 60–62.

[67] P. Wills and F. G. Meyer, Metrics for graph comparison: a practitioner’s guide, PloS one, 15 (2020), p. e0228728.

[68] M. Wu, S. He, Y. Zhang, J. Chen, Y. Sun, Y.-Y. Liu, J. Zhang, and H. V. Poor, A tensor-based framework for studying eigenvector multicentricity in multilayer networks, Proceedings of the National Academy of Sciences, 116 (2019), pp. 15407–15413.

[69] D. Yenigun, G. Ertan, and M. Siciliano, cssTools: Cognitive Social Structure Tools, 2016, https://CRAN.R-project.org/package=cssTools. R package version 1.0.

[70] Y. Zhao, E. Levina, and J. Zhu, Consistency of community detection in networks under degree-corrected stochastic block models, The Annals of Statistics, 40 (2012), pp. 2266–2292.
SUPPLEMENTARY MATERIALS: A factor model of multilayer network interdependence

Izabel Aguiar†, Dane Taylor‡, and Johan Ugander§

SM1. Code Repository. Tools for this work and an example jupyter notebook (all in python) can be found at https://github.com/izabelaguiar/NNTuck

SM2. EM and NNTuck multiplicative updates equivalence. In this section we show the equivalence between the expectation maximization (EM) updates and the multiplicative updates for the nonnegative Tucker decomposition under a KL-divergence loss.

Recall Proposition 3.9, restated below,

Proposition SM2.1. Determining factor matrices $U$, $V$, and $Y$ and the core tensor $G$ in the NNTuck by maximizing the log-likelihood using expectation maximization (EM) (SM2.2)

\[
L(A|U, V, Y, G) = \sum_{i,j,\alpha} a_{ij\alpha} \log \sum_{k,\ell,\rho} u_{ik} v_{j\ell} y_{\alpha\rho} g_{k\ell\rho} - \sum_{k,\ell,\rho} u_{ik} v_{j\ell} y_{\alpha\rho} g_{k\ell\rho},
\]

in which case the following update equations are used

\[
u_{ik} = \frac{\sum_{j,\alpha} A_{ij\alpha} \sum_{\ell} \rho_{ij\ell}^{(\alpha)}}{\sum_{j} \sum_{\rho} \sum_{\alpha} y_{\alpha\rho} g_{k\ell\rho}},
\]

\[v_{j\ell} = \frac{\sum_{i,\alpha} A_{ij\alpha} \sum_{k} \sum_{\rho} \rho_{ij\ell}^{(\alpha)} g_{k\ell\rho}}{\sum_{i} \sum_{\alpha} y_{\alpha\rho} g_{k\ell\rho}},
\]

\[g_{k\ell\rho} = \frac{\sum_{ij} A_{ij\alpha} \rho_{ij\ell}^{(\alpha)}}{\sum_{i} u_{ik} \sum_{j} v_{j\ell}}.
\]

where

\[
\rho_{ijk}^{(\alpha)} = \frac{u_{ik} v_{j\ell} y_{\alpha\rho} g_{k\ell\rho}}{\sum_{k'\ell'\rho'} u_{ik'} v_{j\ell'} y_{\alpha\rho'} g_{k'\ell'\rho'}}.
\]

Funding: IA acknowledges support from the NSF GRFP and the Knight-Hennessy Scholars Fellowship. DT acknowledges partial support from NSF grant DMS-2052720 and the Simons Foundation (grant #578333). JU acknowledges partial support from ARO grant 76582-NS-MUR.

†Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA (izzya@stanford.edu).

‡Department of Mathematics, University at Buffalo, The State University of New York, Buffalo, NY (danet@buffalo.edu).

§Department of Management Science and Engineering, Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA (jugander@stanford.edu).
Conversely, the multiplicative updates for nonnegative Tucker decomposition (NNTuck) under the KL-divergence loss as given by Kim and Choi [SM3] are,

\[
\begin{align*}
U & \leftarrow U \odot \left[A_{(1)}/\left(U G_{U}^{(1)}\right)\right] G_{U}^{(1)\top}, \\
V & \leftarrow V \odot \left[A_{(2)}/\left(V G_{V}^{(2)}\right)\right] G_{V}^{(2)\top}, \\
Y & \leftarrow Y \odot \left[A_{(3)}/\left(Y G_{Y}^{(3)}\right)\right] G_{Y}^{(3)\top}, \\
G & \leftarrow G \odot \left(\hat{A}/A\right) \times_{1} U_{\top} \times_{2} V_{\top} \times_{3} Y_{\top}, \\
z_{U} & = \sum_{j} \left(G_{U}^{(1)}\right)_{ij}, \\
z_{V} & = \sum_{j} \left(G_{V}^{(2)}\right)_{ij}, \\
z_{Y} & = \sum_{j} \left(G_{Y}^{(3)}\right)_{ij}.
\end{align*}
\] (SM2.4)

Above, \( \mathcal{E} \) is the all ones tensor of the same dimension as \( \mathcal{A} \), \( \odot \) and \( / \) denote elementwise multiplication and division, respectively, and the subscript \( _{(\ell)} \) denotes the tensor \( \ell \)-unfolding. \( G_{U}^{(1)} \), \( G_{V}^{(2)} \), and \( G_{Y}^{(3)} \) are defined as

\[
G_{U}^{(1)} = \left[\mathcal{G} \times_{2} V \times_{3} Y\right]_{(1)}, \ G_{V}^{(2)} = \left[\mathcal{G} \times_{1} U \times_{3} Y\right]_{(2)}, \ G_{Y}^{(3)} = \left[\mathcal{G} \times_{1} U \times_{2} V\right]_{(3)}.
\]

We will make use of tensor unfoldings and the tensor \( n \)-mode product in the following equivalence proofs. To help guide intuition on how tensor unfoldings are used, we provide Figure SM1 as one visualization of the three unfoldings of a third-order tensor \( \mathcal{X} \).

**Equivalence of core tensor updates.** We first show that the updates to \( \hat{\mathcal{G}} \) in (SM2.2) are equivalent to the updates to \( \mathcal{G} \) in (SM2.4). The \((i, j, \alpha)\) entry of \( \hat{\mathcal{A}} := \hat{\mathcal{G}} \times_{1} U \times_{2} V \times_{3} Y \) is

\[
\hat{A}_{i,j,\alpha} = \sum_{k'\ell'p'} u_{ik'v_{j,\alpha}y_{k',\ell',p'}} g_{k',\ell',p'}.
\]

and therefore the update to \( g_{k'\ell'p'} \) can be rewritten as,

\[
g_{k'\ell'p'} = \frac{\sum_{ij,\alpha} \left(\hat{A}_{i,j,\alpha}/\hat{A}_{i,j,\alpha}\right) u_{ik}v_{j,\alpha}y_{k'\ell',p'}}{\left(\sum_{i} u_{ik}\right) \left(\sum_{j} v_{j,\ell}\right) \left(\sum_{\alpha} y_{\alpha}\right)}
\]

\[
= g_{k'\ell'p'} \cdot \frac{\sum_{ij,\alpha} \left(\hat{A}_{i,j,\alpha}/\hat{A}_{i,j,\alpha}\right) u_{ik}v_{j,\alpha}y_{\alpha}}{\left(\sum_{i} u_{ik}\right) \left(\sum_{j} v_{j,\ell}\right) \left(\sum_{\alpha} y_{\alpha}\right)}.
\]
SUPPLEMENTARY MATERIALS: A FACTOR MODEL OF MULTILAYER NETWORK INTERDEPENDENCE

\[ x_{(1),i} = \text{vec}(\bar{A}) \]
\[ x_{(2),j} = \text{vec}(\hat{A}) \]
\[ x_{(3),\ell} = \text{vec}(\hat{A}) \]

\[ X(k) = \begin{bmatrix} x_{(k),1} \\
                        x_{(k),2} \\
                        \vdots \\
                        x_{(k),L} \end{bmatrix} \]

**Figure SM1.** The \( k \)-unfolding of a tensor can be described by vertically stacking vectorizations of one of its slices. Above, in descending order, we see the horizontal, lateral, and frontal slices of a tensor. Vectorizing each slice and vertically stacking them gives the 1-, 2-, and 3-unfolding of tensor \( X \), respectively. For \( X \in \mathbb{R}^{N \times M \times L} \), then the dimensions of the three unfoldings are \( X_{(1)} \in \mathbb{R}^{M \times NL} \), \( X_{(2)} \in \mathbb{R}^{N \times ML} \), and \( X_{(3)} \in \mathbb{R}^{L \times NM} \).

Note the \((a, b, c)\) element of the tensor mode-1 product of the following,

\[(\text{SM2.5}) \quad \left[ \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \times_1 U^T \right]_{abc} = \sum_i \left( \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \right)_{ibc} u_{ia}.

Then,

\[(\text{SM2.6}) \quad \left\{ \left[ \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \times_1 U^T \right] \times_2 V^T \times_3 Y^T \right\}_{k\ell p} = \sum_{\alpha} \left[ \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \times_1 U^T \times_2 V^T \right]_{k\ell p y_{\alpha p}}

= \sum_{j,\alpha} \left[ \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \times_1 U^T \right]_{kja} v_{j\ell y_{\alpha p}}

= \sum_{j,\alpha} \left( \sum_{i} \left( \begin{pmatrix} A \\ \bar{A} \end{pmatrix} \right)_{ija} u_{ik} \right) v_{j\ell y_{\alpha p}}

= \sum_{i,\alpha} \left( A_{ija} / \hat{A}_{ija} \right) u_{ik} v_{j\ell y_{\alpha p}}.

Now, note the \((a, b, c)\) element of the tensor mode-1 product of the following,

\[(\text{SM2.7}) \quad \left[ E \times_1 U^T \right]_{abc} = \sum_i E_{abc} u_{ia} = \sum_i u_{ia}.
Then,
\[
\{ \left[ \mathbf{E} \times_1 \mathbf{U}^\top \right] \times_2 \mathbf{V}^\top \times_3 \mathbf{Y}^\top \}_{k\ell p} = \sum_{\alpha} \left[ \mathbf{E} \times_1 \mathbf{U}^\top \times_2 \mathbf{V}^\top \right]_{k\ell \alpha} y_{\alpha p} \\
= \sum_{ja} \left[ \mathbf{E} \times_1 \mathbf{U}^\top \right]_{j\alpha} v_{j\ell} y_{\alpha p}
\]
(SM2.8)
\[
= \sum_{ja} \left( \sum_i u_{ik} \right) v_{j\ell} y_{\alpha p}
= \left( \sum_i u_{ik} \right) \left( \sum_j v_{j\ell} \right) \left( \sum_{\alpha} y_{\alpha p} \right).
\]

Therefore, focusing on the NNTuck multiplicative update of core tensor \( \mathbf{G} \), we see that the update to the \((k, \ell, \alpha)\) element of the core tensor is,
\[
g_{k\ell p} \leftarrow g_{k\ell p} \cdot \left[ \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right) \times_1 \mathbf{U}^\top \times_2 \mathbf{V}^\top \times_3 \mathbf{Y}^\top \right]_{k\ell \alpha} y_{\alpha p} \\
= \sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}
\]
(SM2.9)
\[
= \frac{\sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}}{\sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p}}.
\]
which is equivalent to the update to the \((k, \ell, \alpha)\) element of \( \mathbf{G} \) in (SM2.2).

**Equivalence of factor matrix \( \mathbf{U} \) updates.** For showing the equivalence in updates to factor matrix \( \mathbf{U} \), the following identity is used multiple times. For tensor \( \mathbf{X} \),
\[
\sum_{ja} X_{ija} = \sum_j X_{(1)ij},
\]
(SM2.10)
where \( X_{(1)} \) denotes the 1-unfolding of \( \mathbf{X} \).

Now consider the EM update to \( u_{ik} \) from SM2.2. Again,
\[
\hat{\mathbf{A}}_{ija} = \sum_{k'\ell'p'} u_{ik'} v_{j\ell'} y_{\alpha p} g_{k'\ell'p'},
\]
and so the EM update to \( u_{ik} \) can be rewritten as,
\[
u_{ik} = \frac{\sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}}{\sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}}
\]
(SM2.11)
\[
= u_{ik} \cdot \frac{\sum_{ja} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ija} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}}{\sum_{ia} \left( \frac{\mathbf{A}}{\hat{\mathbf{A}}} \right)_{ia} u_{ik} v_{j\ell} y_{\alpha p} g_{k\ell p}}.
\]
Now note that from the above equation we can identify out
\[
\sum_{\ell p} v_{j\ell} y_{\alpha p} g_{k\ell p} = [\mathbf{G} \times_2 \mathbf{V} \times_3 \mathbf{Y}]_{kja}.
\]
(SM2.12)
For vector $z$ such that $z_i = \sum_j [G \times_2 V \times_3 Y]_{(1)ij}$, note that

$$\begin{align*}
[1z^\top]_{ik} &= (1)(z_k) = \sum_j [G \times_2 V \times_3 Y]_{kja} \\
&= \sum_{ja} \sum_{lp} g_{klp}v_j \ell_{lp} \\
&= \sum_{\ell p} \sum_{ja} g_{k\ell p} v_j \ell_{lp} \\
&= \sum_{\ell p} \left( \sum_j v_j \ell \right) \left( \sum_{\ell p} y_{\ell p} g_{k\ell p} \right).
\end{align*}$$

(SM2.13)

Substituting (SM2.12) and (SM2.13) into (SM2.11), we have that

$$\begin{align*}
u_{ik} &= u_{ik} \cdot \frac{\sum_{ja} \left( A_{ij a} / \hat{A}_{ij a} \right) [G \times_2 V \times_3 Y]_{kja}}{[1z^\top]_{ik}} \\
&= u_{ik} \cdot \frac{\sum_{ja} \left( A_{ij a} / \hat{A}_{ij a} \right) [G \times_2 V \times_3 Y]_{(1)kj}}{[1z^\top]_{ik}} \\
&= u_{ik} \cdot \frac{\sum_{ja} \left( A_{ij a} / \hat{A}_{ij a} \right) [G \times_2 V \times_3 Y]_{(1)jk}^\top}{[1z^\top]_{ik}}.
\end{align*}$$

(SM2.14)

Then using (SM2.10) we have that,

$$\sum_{ja} A_{ij a} = \sum_j A_{(1)ij},$$

(SM2.15)

$$\sum_{ja} \hat{A}_{ij a} = \sum_j \hat{A}_{(1)ij} = \sum_j \left( U[G \times_2 V \times_3 Y]_{(1)ij} \right),$$

$$\sum_{ja} [G \times_2 V \times_3 Y]_{kja} = \sum_j [G \times_2 V \times_3 Y]_{(1)kj} = \sum_j [G \times_2 V \times_3 Y]_{(1)jk}^\top.$$

In the second line of (SM2.15) above, we use that

$$\hat{A} = G \times_1 U \times_2 V \times_3 Y$$

$$= G \times_2 V \times_3 Y \times_1 U$$

$$= (G \times_2 V \times_3 Y) \times_1 U,$$

and thus using the identity $Y = X \times_n B \Rightarrow Y_{(n)} = BX_{(n)}$, we get $\hat{A}_{(1)} = U[G \times_2 V \times_3 Y]_{(1)}$. 


Therefore,

\[ u_{ik} = u_{ik} \cdot \sum_j (A_{1j}/(U[G \times_2 V \times_3 Y]_{1j}))_{ij} [G \times_2 V \times_3 Y]_{1jk}^{\top} \]

\[ = u_{ik} \cdot \left[ (A_{1j}/(U[G \times_2 V \times_3 Y]_{1j}))_{ij} [G \times_2 V \times_3 Y]_{1jk}^{\top} \right]_{ik} \] \tag{SM2.16}

This is equivalent to the \( i\k \) update of \( U \) given by (SM2.4).

**Equivalence of factor matrix \( V \) updates.** In connecting the updates to factor matrix \( V \), the following identity is used multiple times. For tensor \( X \),

\[ \sum_{i\alpha} X_{i\alpha} = \sum_i X_{i(2)ji} \]

where \( X_{1j} \) denotes the \((1)-unfolding of \( X \). Now consider the EM update to \( v_{j\ell} \) given by (SM2.2). Because

\[ \hat{A}_{ij\alpha} = \sum_{k'\ell'p'} u_{ik'j\ell'p'\alpha} \]

then the EM update to \( v_{j\ell} \) can be rewritten as,

\[ v_{j\ell} = \frac{\sum_{i\alpha} (A_{ij\alpha}/\hat{A}_{ij\alpha}) \sum_{kp} u_{ikj\ell} y_{\alpha p} g_{k\ell p}}{\sum_{kp} (\sum_i u_{ik}) (\sum_{\alpha} y_{\alpha p} g_{k\ell p})} \]

\[ = v_{j\ell} \cdot \frac{\sum_{i\alpha} (A_{ij\alpha}/\hat{A}_{ij\alpha}) \sum_{kp} u_{ikj\ell} y_{\alpha p} g_{k\ell p}}{\sum_{kp} (\sum_j u_{ik}) (\sum_{\alpha} y_{\alpha p} g_{k\ell p})} \] \tag{SM2.18}

Now note that we can again identify out

\[ \sum_{kp} u_{ikj\ell} y_{\alpha p} g_{k\ell p} = [G \times_1 U \times_3 Y]_{i\alpha} \]

And again, for vector \( z \) such that \( z_{j\ell} = \sum_i [G \times_1 U \times_2 Y]_{ij\ell} \), note that

\[ [1z^{\top}]_{j\ell} = (1)(z_{\ell\ell}) = z_{\ell\ell} \]

\[ = \sum_i [G \times_1 U \times_2 Y]_{i\ell\ell} \]

\[ = \sum_{i\alpha} [G \times_1 U \times_3 Y]_{i\ell\alpha} \]

\[ = \sum_{kp} \sum_{i\alpha} u_{ikj\ell} y_{\alpha p} g_{k\ell p} \]

\[ = \sum_{kp} \sum_{i\alpha} u_{ikj\ell} y_{\alpha p} g_{k\ell p} \]

\[ \sum_{kp} \left( \sum_{i\alpha} u_{ik} \right) \left( \sum_{\alpha} y_{\alpha p} g_{k\ell p} \right) \].

\[ \text{SM6 I. AGUIAR, D. TAYLOR, AND J. UGANDER} \]
Substituting together (SM2.19) and (SM2.20) into the EM updates (SM2.18), we have that

\[(SM2.21)\]

\[v_{j\ell} = v_{j\ell} \cdot \frac{\sum_{i\alpha} \left( A_{ij\alpha} / \hat{A}_{ij\alpha} \right) [G \times_1 U \times_3 Y]_{i\ell\alpha}}{[1z^\top]_{j\ell}}.\]

Then,

\[(SM2.22)\]

\[\sum_{i\alpha} A_{ij\alpha} = \sum_{i} A^{(2)}_{ji}, \quad \sum_{i\alpha} \hat{A}_{ij\alpha} = \sum_{i} \hat{A}^{(2)}_{ji} = \sum_{i} (V[G \times_1 U \times_3 Y]^{(2)})_{ji}, \quad \sum_{i\alpha} [G \times_1 U \times_3 Y]_{i\ell\alpha} = \sum_{i} [G \times_1 U \times_3 Y]^{(2)}_{i\ell\alpha} = \sum_{i} [G \times_1 U \times_3 Y]^{(2)}_{(2)i\ell}.\]

In the second line of SM2.22 above, we use that

\[\hat{A} = G \times_1 U \times_2 V \times_3 Y = G \times_1 U \times_3 Y \times_2 V = (G \times_1 U \times_3 Y) \times_2 V,\]

and thus using the identity \(Y = X \times_n B \Rightarrow Y^{(n)} = BX^{(n)}\), we get \(\hat{A}^{(2)} = V[G \times_1 U \times_3 Y]^{(2)}.\)

Therefore,

\[(SM2.23)\]

\[v_{j\ell} = v_{j\ell} \cdot \frac{\sum_{i} (A^{(2)}_{ji} / (V[G \times_1 U \times_3 Y]^{(2)}))_{ji} [G \times_1 U \times_3 Y]^{(2)}_{j\ell\alpha}}{[1z^\top]_{j\ell}} \]

\[= v_{j\ell} \cdot \frac{[A^{(2)}_{ji} / (V[G \times_1 U \times_3 Y]^{(2)})] [G \times_1 U \times_3 Y]^{(2)}_{j\ell\alpha}}{[1z^\top]_{j\ell}}.\]

This is equivalent to the \(j\ell\) update of \(V\) given by (SM2.4).

Showing the equivalence for the updates to \(Y\) follow exactly as those above, and thus we do not reproduce it here. Therefore, we show that the EM updates given by (SM2.2) are step-by-step equivalent to the multiplicative updates given by (SM2.4).

**SM3. Masked updates.** In this section we discuss the algorithmic changes to Kim and Choi’s (2007) [SM3] multiplicative updates for the nonnegative Tucker decomposition under a KL-divergence loss to allow for masking, as used during cross validated model evaluation. This section describes the tensor completion problem wherein we wish to build the NNTuck using only observed entries.

Consider that some of the entries of adjacency tensor \(A\) are unobserved. We wish to build the NNTuck of \(A\) using only the observed entries, but we want the reconstruction \(\hat{A}\) to predict the unobserved entries. This tensor completion problem is how we train on 80% of the entries of \(\hat{A}\) for the five-fold cross validation in Section 5. Assume that there is a set \(I\) such that

\[(SM3.1)\]

\[I := \{(i, j, \alpha) \mid A_{ij\alpha} \text{ is unobserved}\}.\]
We want to rederive the update rules from [SM3] for nonnegative Tucker decomposition to only account for the observed entries of $A$. To do so, we introduce a masking tensor, $M$ such that,

$$M_{ija} = \begin{cases} 
0 & \text{if } (i, j, \alpha) \in \mathcal{I} \\
1 & \text{if } (i, j, \alpha) \notin \mathcal{I}.
\end{cases}$$

Then re-deriving the update rules from the log-likelihood and EM approach, and after re-tensorizing them, the update rules for factor matrices $U, V, Y$ and for core tensor $G$ are,

$$U = U \odot \frac{[M^{(1)} \odot A^{(1)} / \hat{A}^{(1)}] [G \times_2 V \times_3 Y]^T}{M^{(1)}[G \times_2 V \times_3 Y]^T},$$

$$V = V \odot \frac{[M^{(2)} \odot A^{(2)} / \hat{A}^{(2)}] [G \times_1 U \times_3 Y]^T}{M^{(2)}[G \times_1 U \times_3 Y]^T},$$

$$Y = Y \odot \frac{[M^{(3)} \odot A^{(3)} / \hat{A}^{(3)}] [G \times_1 U \times_2 V]^T}{M^{(3)}[G \times_1 U \times_2 V]^T},$$

$$G = G \odot \frac{[M \odot A / \hat{A}] \times_1 U^T \times_2 V^T \times_3 Y^T}{M \times_1 U^T \times_2 V^T \times_3 Y^T}.$$

In all of the above, $\odot$ denotes elementwise multiplication and $/$ denotes elementwise division.

**SM4. Interpretability of the $Y$ factor matrix.** In this section we show the steps necessary to rewrite the core tensor $G \in \mathbb{R}^{K \times K \times C}$ of the NNTuck in the basis of $C$ unique reference layers, and how to find the corresponding $\hat{Y}^*$ matrix, as discussed in Subsection 4.2.

Take as given a set of $C$ unique reference layers, denoted $r^* = \{r_1, \ldots, r_C\}$ where $r_i \in \{1, \ldots, L\}$. Define $G^*$ whose frontal slices are $G^*_\ell = \sum_{i=1}^C y_{r_i, \ell} G_{r_i, \ell}$ for $\ell = 1, \ldots, C$. Define matrix $Y^*$ such that rows $r^*$ of $Y^*$ are identity rows. Specifically, for row $\ell$ of the matrix,

$$y^*_\ell = \begin{cases} 
e_{\ell} & \text{if } \ell \in r^*, \\
y^*_\ell & \text{otherwise.}
\end{cases}$$
Define $\bar{r} := \{\ell \mid \ell \notin r^*\}$. Then row $y_\ell^*$ for $\ell \in \bar{r}$ satisfies,

$$y_{\ell,1}G_1 + y_{\ell,2}G_2 + \cdots + y_{\ell,C}G_C = y_{\ell,1}^* \left( \sum_{i=1}^{C} y_{r_1,i}G_i \right) + y_{\ell,2}^* \left( \sum_{i=1}^{C} y_{r_2,i}G_i \right) + \cdots + y_{\ell,C}^* \left( \sum_{i=1}^{C} y_{r_C,i}G_i \right).$$

This gives us the system of equations,

$$y_{\ell,1} = y_{\ell,1}^* y_{r_1,1} + y_{\ell,2}^* y_{r_2,1} + \cdots + y_{\ell,C}^* y_{r_C,1},$$

$$y_{\ell,2} = y_{\ell,2}^* y_{r_1,2} + y_{\ell,2}^* y_{r_2,2} + \cdots + y_{\ell,C}^* y_{r_C,2},$$

$$\vdots$$

$$y_{\ell,C} = y_{\ell,C}^* y_{r_1,C} + y_{\ell,C}^* y_{r_2,C} + \cdots + y_{\ell,C}^* y_{r_C,C}.$$  

Note that the first equation is the inner product between the first column of $Y$ subsetted to the rows in $r^*$ with the unknown vector $y^*$. That is,

$$y_{\ell,1} = Y_{r^*}^T y_\ell^T.$$  

Then let $Y_{r^*}$ be the matrix $Y$ subsetted to the rows in $r^*$. Then the $\ell$th row of matrix $Y^*$, denoted $y_\ell^*$, satisfies the linear system

$$(SM4.1) \quad Y_{r^*}^T y_\ell^* = y_\ell^T.$$  

Because there are $(L - C)$ unknown rows of matrix $Y^*$, there will be $(L - C)$ such linear systems for each $\ell \in \bar{r}$.

Let $Y_{\bar{r}}^*$ be the matrix $Y^*$ subsetted to the rows not in $r^*$. Then,

$$(SM4.2) \quad Y_{\bar{r}}^T Y_{\bar{r}}^* y_\ell^* = Y_\ell^T \iff Y_{\bar{r}}^* = Y_{\bar{r}}^T Y_{\bar{r}}.$$  

Note that $Y_{\bar{r}}^* \in \mathbb{R}^{C \times C}$ and is invertible if and only if the rows of $Y$ defined by $r^*$ are not linearly dependent. This highlights the importance in choosing the “correct” reference rows. Even though in practice it’s unlikely that any two rows, even if poorly chosen, will be exactly linearly dependent, if they are close then the transformed $Y^*$ matrix will not be interpretable.

The best reference layers are often determined by domain knowledge. Absent a principled approach but seeking to make the matrix interpretable, we propose the following heuristic for choosing the best reference layers: choose the $C$ layers such that $\det(Y_{r^*})$ is furthest from zero. Although searching over the entire space amounts to finding the determinant of $\binom{L}{C}$ different submatrices and isn’t practical, one can instead compare the determinant of a handful of different submatrices, where reference layers can be chosen with a combination of (perhaps weak) domain expertise and by inspection of the $Y$ matrix.

**SM5. Questions generating the social multilayer networks.** We reproduce the questions generating the multilayer social support networks from the works of Banerjee et al. (2013) [SM1] and Banerjee et al. (2019) [SM2]. For specific information about the context, original findings, or survey instruments of the research, please refer to the original papers.
**Microfinance Villages [SM1].** The 43 multilayer networks from this research, representing different villages in Karnataka, India, were the result of asking individuals about 12 different types of support. Each layer in the resulting network corresponds to the following relationships.

1. Those from whom the respondent would borrow money
2. Those to whom the respondent gives advice
3. Those from whom the respondent gets advice
4. Those from whom the respondent would borrow material goods
5. Those to whom the respondent would lend material goods
6. Those to whom the respondent would lend money
7. Those from whom the respondent receives medical advice
8. Non-relatives with whom the respondent socializes
9. Kin in the village
10. Those whom the respondent goes to pray with
11. Those who visit the respondent’s home
12. Those whose homes the respondent visits

**Gossip Villages [SM2].** The 70 multilayer networks from villages in Karnataka, India, were generated from asking individuals the following seven questions, each of which corresponds to a layer in the resulting network.

1. Whose house do you go to in your free time?
2. Who comes to your house in their free time?
3. If you urgently needed kerosene, rice other groceries or money, who do you borrow them from?
4. Who comes to your house if he or she needed to borrow kerosene, rice, other groceries or money?
5. Who do you ask for advice on matters pertaining to health/finance/farming?
6. Who asks you for advice on matters pertaining to health/finance/farming?
7. Besides people living in your household, state names of your relatives who are living in this village.

**REFERENCES**

[1] A. Banerjee, A. G. Chandrasekhar, E. Duflo, and M. O. Jackson, *The diffusion of microfinance*, Science, 341 (2013), p. 1236498.

[2] A. Banerjee, A. G. Chandrasekhar, E. Duflo, and M. O. Jackson, *Using gossips to spread information: Theory and evidence from two randomized controlled trials*, The Review of Economic Studies, 86 (2019), pp. 2453–2490.

[3] Y.-D. Kim and S. Choi, *Nonnegative Tucker decomposition*, in IEEE Conference on Computer Vision and Pattern Recognition, 2007.

[4] T. G. Kolda and B. W. Bader, *Tensor decompositions and applications*, SIAM Review, 51 (2009), pp. 455–500.