Edge Correlations in Multilayer Networks

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Many recent developments in network analysis have focused on multilayer networks, which one can use to encode time-dependent interactions, multiple types of interactions, and other complications that arise in complex systems. Like their monolayer counterparts, multilayer networks in applications often have mesoscale features, such as community structure. A prominent type of method for inferring such structures is the employment of multilayer stochastic block models (SBMs). A common (but inadequate) assumption of these models is the sampling of edges in different layers independently, conditioned on community labels of the nodes. In this paper, we relax this assumption of independence by incorporating edge correlations into an SBM-like model. We derive maximum-likelihood estimates of the key parameters of our model, and we propose a measure of layer correlation that reflects the similarity between connectivity patterns in different layers. Finally, we explain how to use correlated models for edge prediction in multilayer networks. By taking into account edge correlations, prediction accuracy improves both in synthetic networks and in a temporal network of shoppers who are connected to previously-purchased grocery products.

I. INTRODUCTION

A network is an abstract representation of a system in which entities called nodes interact with each other via edges, typically in a pairwise fashion [1]. Networks arise in many domains and are useful for numerous practical problems, such as detecting bot accounts on Twitter [2], finding vulnerabilities in electrical grids [3], and identifying potentially harmful interactions between drugs [4]. A common feature of many networks is mesoscale (i.e., intermediate-scale) structures. Detecting such structures amounts to a type of coarse-graining, providing representations of a network that are more compact than listing all of the nodes and edges. Types of mesoscale structures include community structure [5], core–periphery structure [6, 7], role similarity [8], and others. An increasingly popular approach for modeling and detecting such structures is by using stochastic block models (SBMs) [9], a generative model that can produce networks with community structure or other mesoscale structures.

For many applications of network analysis, it is important to move beyond ordinary graphs (i.e., “monolayer networks”) to examine more complicated network structures, such as collections of interrelated networks. One can study such structures through the flexible lens of multilayer networks [10–13]. Similar to monolayer networks, a multilayer network consists of a collection of ‘state nodes’ that are connected pairwise by edges. A ‘state node’ is a manifestation of a ‘physical node’ (which we will also sometimes call simply a ‘node’), which represents some entity, in a specific layer. Different layers may correspond to interactions in different time periods, yielding a temporal network; different types of relations, yielding a multiplex network; or other possibilities. As in the monolayer setting, modeling and inferring mesoscale structures in multilayer networks is a prominent research area.

A key assumption of almost all existing models of multilayer networks with mesoscale structure is that edges are generated independently, conditioned on a multilayer partition [14–21]. This independence condition applies both within each layer (which is inconsistent with the fact that real networks often include 3-cliques and other small-scale structures) and across layers (which is inconsistent with the fact that the same nodes often are often adjacent to each other in multiple layers). In this paper, we focus on relaxing the edge-independence assumption that applies to edges between the same two physical nodes in different layers. (We still consider each pair of nodes independently.) In Fig. 1 we show an example of a two-layer network with both strong positive and strong negative edge correlations. Incorporating such correlations into a network model is beneficial for many applications. For example, a multiplex network of air routes, where each layer corresponds to one airline, is likely to include some popular routes that appear in multiple layers, while unpopular routes appear only in one [22]. In a temporal social network, we expect people to have repeated interactions with other people [23]; this is a stronger statement than just saying that they tend to interact more within the same community over time. Such edge persistence is also common in many bipartite user–item networks: shoppers tend to buy the same grocery products over time [24], customers of a music-streaming platform listen repeatedly to their favorite songs [25], and Wikipedia users edit specific pages several times [26].

Multilayer network models that incorporate edge correlations have many important applications. One is the task of edge prediction (also called link prediction), where one seeks to assign probabilities of occurrence to unob-
graph matching application is to data. We discuss this in more detail in Sec. III. Another approach over related studies [34, 38, 39] include the fact that correlation values cover an intuitive range (between −1 and 1) and that they work equally well for quantifying layer similarity and dissimilarity.

Our proposed edge-correlated network models are also useful for community detection. Given a multilayer network, one can design an inference algorithm that determines both the parameters that describe the edge probabilities (and correlations) and a multilayer community structure that underlies these probabilities. Solving this inference problem then enables the detection of “correlated communities”. Because of the additional complexity in the model, this is bound to be more difficult than standard multilayer community detection, so we leave this inference problem for future work. Instead, for the rest of the paper, we assume that we know the block structure of a network, and we infer the remaining parameters, including the correlations that are the core element of our model [40]. Additionally, we assume that the block assignments $g$ are the same for all layers; the case in which communities can vary arbitrarily across layers is significantly more difficult [41], and we leave its consideration for future work. With this restriction, one can determine $g$ using any method of choice.

Some existing models of multilayer networks incorporate interlayer dependencies by prescribing joint degree distributions [42, 43], by incorporating edge overlaps [44, 45], or by modeling the appearance of new edges through preferential-attachment mechanisms [46]. The models that we describe in this paper are similar to those that were introduced in [30–32] for graph-matching purposes. Another noteworthy paper is one by Barucca et al. [47] that described a generalized version of the temporal SBM by Ghasemian et al. [17]. This generalization includes an “edge persistence” parameter $\xi$, which gives the probability that an edge from one layer also occurs in the next temporal layer. For several reasons, we take a different approach. First, the model of [17] is specific to temporal networks, whereas we are also interested in other types of multilayer networks. Second, their model does not easily incorporate degree correction. Third, we want to include correlations explicitly in the model, rather than implicitly using the edge persistence parameter $\xi$.

Our paper proceeds as follows. In Sec. II, we describe our models of multilayer networks with edge correlations. We start with a simple example of correlated Erdős-Rényi (ER) graphs in Sec. II A to make our exposition for more complicated models easier to follow. In Sec. II B we integrate mesoscale structures by incorporating correlations in an SBM-like model. We then introduce degree correction in Sec. II C. For all of these models, we derive maximum likelihood (ML) estimates both of the marginal edge-existence probabilities in each layer and of the interlayer correlations. In Sec. III, we describe how to use these models for edge prediction, and we provide some results for synthetic networks. We then proceed with applications in Sec. IV. In Sec. IV A, we use our models to estimate pairwise layer correlations in several empirical networks. In Sec. IV B we use our correlated models for edge prediction in a temporal network of grocery purchases. We summarize our results in Sec. V and discuss a few ideas for future work.
II. CORRELATED MODELS

In this paper, our derivations consider just two network layers at a time. Although this may seem limiting, we can apply this framework to generate correlated networks with more than two layers in a sequential manner (see the discussion in Sec. [II A]), and we can determine pairwise layer correlations for a network with arbitrarily many layers (see the applications in Sec. [IV]). In Sec. [V], we briefly discuss the challenges that arise when modeling three or more layers simultaneously, rather than in a sequential pairwise fashion.

Let $A^1$ and $A^2$ denote the adjacency matrices of our two network layers. As in many generative models of networks, we assume that edges in these two layers are generated by some random process, so the entries $A^1_{ij}$ and $A^2_{ij}$ are random variables. Imposing some statistical correlation between these two sets of random variables then introduces interlayer correlations in the resulting multilayer network structure.

Our goal is to propose a model of correlated networks in which each layer is, marginally, a degree-corrected stochastic block model (DCSBM) [33]. However, it is instructive to first consider the simpler cases in which each layer is marginally an Erdős–Rényi random graph (see Sec. [II A]) or an SBM without degree correction (see Sec. [II B]). Correlated ER models and correlated SBMs have been studied previously, most notably in work by Lyzinski et al. [33] on the graph-matching problem. However, our use of these models for estimating layer correlations is novel, as are the correlated DCSBMs that we propose in Sec. [II C].

In monolayer SBMs, it is common to use either Bernoulli or Poisson random variables to generate edges between nodes. The former is generally more accurate, because it does not yield multiedges; but the latter is more common, as it often simplifies calculations considerably [48, 49]. However, we have found that Bernoulli models are simpler when incorporating correlations [24]. They also have several other advantages, including the fact that they work for both sparse and dense networks and that they can handle the entire correlation range between $-1$ and $1$. Therefore, we consider only Bernoulli models in this paper.

A. Correlated Erdős–Rényi Layers

1. Forward model

Consider a network with two layers and identical sets of nodes in each layer. Assume that our two intralayer networks are ER graphs (from the $G(n, p)$ ensemble [1]) with edge probabilities $p_1$ and $p_2$. For each pair of nodes $(i, j)$, we therefore have

\begin{align}
\mathbb{P}(A^1_{ij} = 1) &= p_1, \\
\mathbb{P}(A^2_{ij} = 1) &= p_2.
\end{align}

To couple edges that connect the same pair of nodes in different layers, let

\[ q := \mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) \]

denote the joint probability for an edge to occur in both layers. Unless $q = p_1 p_2$, this construction implies that the random variables $A^1_{ij}$ and $A^2_{ij}$ are not independent.

The parameters $p_1$, $p_2$, and $q$ (which lie in the interval $[0, 1]$) fully specify our first forward model of networks with correlated ER layers. To generate a network from this model, one considers each pair of nodes $(i, j)$ and, independently of all other node pairs, assigns values to $A^1_{ij}$ and $A^2_{ij}$ according to the following probabilities:

\begin{align}
\mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) &= q, \\
\mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 0) &= p_1 - q, \\
\mathbb{P}(A^1_{ij} = 0, A^2_{ij} = 1) &= p_2 - q, \\
\mathbb{P}(A^1_{ij} = 0, A^2_{ij} = 0) &= 1 - p_1 - p_2 + q.
\end{align}

These expressions follow from the laws of probability and from the definitions of $p_1$, $p_2$, and $q$. For these probabilities to be well-defined, it is both necessary and sufficient that $0 \leq q \leq \min(p_1, p_2)$ and $p_1 + p_2 \leq 1 + q$. In Fig. 2, we illustrate the feasible region for $p_1$ and $p_2$, given a value of $q$. 

![FIG. 2: Visualization of the feasible region (gray area) for $p_1$ and $p_2$, given a value of $q$. The boundaries of this region are defined by the inequalities $q \leq p_1 \leq 1$, $q \leq p_2 \leq 1$, and $p_1 + p_2 \leq 1 + q$. The hyperbola $p_1 p_2 = q$ specifies the boundary between regimes with positive layer correlation and regimes with negative layer correlation.](image)
It is also possible to generate a correlated ER network in a sequential manner. First, one generates the adjacency matrix $A^1$ by placing edges with probability $p_1$. One then determines the probabilities of edges in the second layer by conditioning on the first layer:

$$
P(A^2_{ij} = 1 | A^1_{ij} = 1) = \frac{P(A^1_{ij} = 1, A^2_{ij} = 1)}{P(A^1_{ij} = 1)} = \frac{q}{p_1},$$

$$
P(A^2_{ij} = 1 | A^1_{ij} = 0) = \frac{P(A^1_{ij} = 0, A^2_{ij} = 1)}{P(A^1_{ij} = 0)} = \frac{p_2 - q}{1 - p_1},$$

$$
P(A^2_{ij} = 0 | A^1_{ij} = 1) = \frac{P(A^1_{ij} = 1, A^2_{ij} = 0)}{P(A^1_{ij} = 1)} = \frac{p_1 - q}{p_1},$$

$$
P(A^2_{ij} = 0 | A^1_{ij} = 0) = \frac{P(A^1_{ij} = 0, A^2_{ij} = 0)}{P(A^1_{ij} = 0)} = \frac{1 - p_1 - p_2 + q}{1 - p_1}. \quad (5)$$

With this approach, it is possible to generate networks with arbitrarily many layers by first sampling edges in the first layer, and then sampling edges in each subsequent layer by conditioning on the previous one. This kind of process is especially well-suited for temporal networks, in which layers have a natural ordering. For multiplex networks, an extension of equations (4) to more than two layers is more appropriate.

It is also possible to parametrize this model in terms of the marginal Bernoulli probabilities $p_1$ and $p_2$ and the Pearson correlation

$$
\rho = \frac{\mathbb{E}[A^1_{ij}A^2_{ij}] - \mathbb{E}[A^1_{ij}]\mathbb{E}[A^2_{ij}]}{\sigma[A^1_{ij}]\sigma[A^2_{ij}]} = \frac{q - p_1p_2}{\sqrt{p_1(1-p_1)p_2(1-p_2)}}, \quad (6)
$$

We now derive ML estimates of the parameters $p_1$, $p_2$, and $q$. Let $E$ denote the set of node pairs that can form edges. For undirected networks without self-edges, there are $|E| = N(N - 1)/2$ such node pairs to consider, where $N$ is the number of physical nodes. By contrast, $|E| = N(N - 1)/2$ when generating directed networks without self-edges. With this general notation, all our derivations in Sec. II are valid for both directed and undirected networks, with or without self-edges. (They are also valid for bipartite networks.) We consider each pair of nodes $(i, j) \in E$ independently when generating edges, so the likelihood of observing adjacency matrices $A^1$ and $A^2$ is

$$
P(A^1, A^2 | p_1, p_2, q) = \prod_{(i,j) \in E} q^{A^1_{ij}}(1-q)^{1-A^1_{ij}}(p_2 - q)^{A^2_{ij}}(1-p_2) + q)^{1-A^2_{ij}}(1-A^2_{ij}) \cdot \quad (7)
$$

It is helpful to introduce the following notation:

$$
e_{11} := |\{(i,j) \in E : A^1_{ij} = 1, A^2_{ij} = 1\}|,$$

$$
e_{10} := |\{(i,j) \in E : A^1_{ij} = 1, A^2_{ij} = 0\}|,$$

$$
e_{01} := |\{(i,j) \in E : A^1_{ij} = 0, A^2_{ij} = 1\}|,$$

$$
e_{00} := |\{(i,j) \in E : A^1_{ij} = 0, A^2_{ij} = 0\}|.$$

These quantities correspond, respectively, to the number of node pairs that are adjacent in both layers, are adjacent in the first layer but not in the second, are adjacent in the second layer but not in the first, and are not adjacent in either layer. Using this notation and taking the logarithm of (7), we arrive at the following expression for the log-likelihood:

$$
\mathcal{L} = e_{11} \log q + e_{10} \log(p_1 - q) + e_{01} \log(p_2 - q) + e_{00} \log(1 - p_1 - p_2 - q) . \quad (8)
$$

When fitting our model to network data, the quantities $e_{11}$, $e_{10}$, $e_{01}$, $e_{00}$ are all known; and we seek to determine the values of $p_1$, $p_2$, and $q$ that are best explained by the data. To do so, we maximize the log-likelihood (8) by
setting its partial derivatives to 0 \[50\]. We obtain

\[
\begin{align*}
\hat{p}_1 &= \frac{e_{11} + e_{10}}{e_{11} + e_{10} + e_{01} + e_{00}}, \\
\hat{p}_2 &= \frac{e_{11} + e_{01}}{e_{11} + e_{10} + e_{01} + e_{00}}, \\
\hat{q} &= \frac{e_{11}}{e_{11} + e_{10} + e_{01} + e_{00}}.
\end{align*}
\]

In all three expressions, the denominator is equal to the number of potential edges (i.e., the cardinality of \(E\)). Additionally, let \(m_1 = e_{11} + e_{10}\) and \(m_2 = e_{11} + e_{01}\), respectively, denote the number of observed edges in the first and the second layers. It follows that the ML estimate \(\hat{p}_1\) is equal to the number of observed edges in layer 1 divided by the number of potential edges, and an analogous relation holds for \(\hat{p}_2\). The estimate \(\hat{q}\) is equal to the number of node pairs that are adjacent in both layers divided by the total number of node pairs. These results match our intuition.

We obtain an estimate of the Pearson correlation \(\rho\) between the two layers by substituting the ML estimates \(\hat{p}_1, \hat{p}_2, \) and \(\hat{q}\) into Eqn. [10] to obtain

\[
\hat{\rho} = \frac{e_{00}e_{11} - e_{10}e_{01}}{\sqrt{(e_{11} + e_{10})(e_{11} + e_{01})(e_{10} + e_{00})(e_{01} + e_{00})}}.
\]

(12)

One can show that maximizing the log-likelihood \[5\] with respect to \(p_1, p_2,\) and \(\rho\) (rather than \(p_1, p_2,\) and \(q\)) gives the same expression for \(\hat{\rho}\), confirming that this is indeed an ML estimate of the correlation. Note that \(\hat{\rho}\) is not defined when either layer is an empty or a complete graph, as the corresponding Bernoulli random variable has a standard deviation of 0.

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### B. Correlated SBMs

One of the ways in which real-world networks differ from ER random graphs is that they have mesoscale structures, such as communities \[5\]. We use stochastic block models (SBMs) to incorporate such structures into our correlated models.

Let \(g\) be a vector of block assignments, which we take to be identical for both network layers; and let \(K\) be the number of blocks. As we explained in Sec. [I], we assume throughout this paper that we are given \(g\), and we aim to estimate the remaining model parameters. Following terminology from \[27\], let \(B = \{1, \ldots, K\} \times \{1, \ldots, K\}\) be the set of “edge bundles" \((r, s)\), each of which is described by its own set of parameters \(p_{r,s}^1, p_{r,s}^2,\) and \(q_{r,s}\). The \(K \times K\) matrices \(p^1, p^2,\) and \(q\) play an analogous role to \(p_1, p_2,\) and \(q\) for ER layers.

Let \(g_i\) denote the block assignment of node \(i\). A correlated two-layer SBM is described by the following set of equalities:

\[
\begin{align*}
\mathbb{P}(A_{ij}^1 = 1) &= p_{g_i g_j}^1, \\
\mathbb{P}(A_{ij}^2 = 1) &= p_{g_i g_j}^2, \\
\mathbb{P}(A_{ij}^1 = 1, A_{ij}^2 = 1) &= q_{g_i g_j},
\end{align*}
\]

Lyzinski and collaborators proposed this forward model in \[31\] to study the graph-matching problem. By contrast, we focus on the inverse problem of estimating the parameters \(p^1, p^2,\) and \(q\), given some network data.

#### 1. Maximum-likelihood parameter estimates

As in Sec. [IA], suppose that we consider each node pair \((i, j)\) independently. The likelihood of observing adjacency matrices \(A^1\) and \(A^2\) is then

\[
\begin{align*}
\mathbb{P}(A^1, A^2|g, p^1, p^2, q) &= \prod_{(i,j) \in E} \left[ q_{g_i g_j}^1 A_{ij}^1 (p_{g_i g_j}^1 - q_{g_i g_j}) A_{ij}^2 (1 - A_{ij}^1) A_{ij}^2 (1 - A_{ij}^2) \\
&\quad \times (1 - p_{g_i g_j}^1 - p_{g_i g_j}^2) A_{ij}^1 (1 - A_{ij}^2) \right].
\end{align*}
\]

(13)

In this product, each factor depends on \(i\) and \(j\) only via their block memberships \(g_i\) and \(g_j\), so can combine several terms. First, define

\[
\epsilon_{rs}^{ab} := \left| \{(i,j) \in E : A_{ij}^1 = a, A_{ij}^2 = b, g_i = r, g_j = s\} \right|
\]

for \((a, b) \in \{(1, 1), (1, 0), (0, 1), (0, 0)\}\), in analogy with \(\epsilon_{11}, \epsilon_{10}, \epsilon_{01},\) and \(\epsilon_{00}\) from Sec. [IA]. We can then write the log-likelihood as

\[
\mathcal{L} = \sum_{(r,s) \in B} \left[ \epsilon_{rs}^{11} \log q_{rs} \\
+ \epsilon_{rs}^{10} \log (p_{rs}^1 - q_{rs}) + \epsilon_{rs}^{01} \log (p_{rs}^2 - q_{rs}) \\
+ \epsilon_{rs}^{00} \log (1 - p_{rs}^1 - p_{rs}^2 + q_{rs}) \right].
\]

(14)

The advantage of writing the log-likelihood as in (14) is that it clearly separates the contribution from different edge bundles. Using the results for ER layers from
two node indices $I$ way to define an "effective correlation" is to first sample for one of the purposes that we outlined in Sec. I. One example, one may wish to use such a network diagnostic single correlation measurement for a given network. For ent edge bundles can be useful, it is also helpful to have a (19) by conditioning on the block assignments of the ran-
to emphasize that they are random variables.
where we use capital letters for the node indices compute the Pearson correlation of the random variables although having different correlation values for differ-
We can calculate each term on the right-hand side of (19) to obtain correlation estimates between networks layers, even for networks with nontrivial mesoscale structure.
which recovers the value in (12) for ER layers without any block structure. We stress that there is no reason a priori to expect this outcome. In fact, the analogous result does not hold for Poisson models [23]. In the present case, the fact that there is such a correspondence between models is convenient for practical reasons, as it implies that one can perform the simpler calculations from Sec. II B to incorporate degree correction.

C. Correlated DCSBMs
The models that we have discussed thus far generate networks in which nodes in the same block have the same expected degree. SBMs that make this kind of assumption tend to perform poorly when used to infer mesoscale structure in real networks, many of which have highly heterogeneous degree distributions. This observation led to the development of degree-corrected SBMs (DCSBMs) [33]. We expect that such adjustments can also make a difference when modeling edge correlations, so we now extend the model from Sec. II B to incorporate degree correction.

We continue to work with two-layer networks, which we again specify in terms of two intralayer adjacency matrices $A^1$ and $A^2$, with a common block structure that is specified by a vector $g$. For each node pair $(i, j) \in \mathcal{E}$, we place edges in the two layers according to the probabilities $\mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) = \sqrt{\frac{m_1}{|E|} \left(1 - \frac{m_1}{|E|}\right)}$.

Lastly, $\mathbb{E}[A^1_{ij}A^2_{ij}] = \mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) = \sum_{(r,s) \in B} \hat{q}_{rs} \frac{e_{rs}}{|E|} = \sum_{(r,s) \in B} \frac{e_{rs}}{|E|} = \frac{e_{11}}{|E|}$.

The estimated value of the effective correlation is thus
\[
\hat{\rho} = \frac{\rho^{ corr \{ A^1_{ij}, A^2_{ij} \} }}{\sqrt{\frac{m_0 e_{11} - e_{10} e_{01}}{(e_{11} + e_{10})(e_{11} + e_{01})(e_{10} + e_{00})(e_{01} + e_{00})}}},
\]
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We continue to work with two-layer networks, which we again specify in terms of two intralayer adjacency matrices $A^1$ and $A^2$, with a common block structure that is specified by a vector $g$. For each node pair $(i, j) \in \mathcal{E}$, we place edges in the two layers according to the probabilities $\mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) = \sqrt{\frac{m_1}{|E|} \left(1 - \frac{m_1}{|E|}\right)}$.

Lastly, $\mathbb{E}[A^1_{ij}A^2_{ij}] = \mathbb{P}(A^1_{ij} = 1, A^2_{ij} = 1) = \sum_{(r,s) \in B} \hat{q}_{rs} \frac{e_{rs}}{|E|} = \sum_{(r,s) \in B} \frac{e_{rs}}{|E|} = \frac{e_{11}}{|E|}$.
We will justify the expression in [24] shortly. The quantities \( \theta^l_i \) and \( \theta^l_j \), with \( l \in \{1, 2\} \), are the degrees of nodes \( i \) and \( j \), normalized by the mean degrees. We calculate these quantities directly from an input degree sequence, so they are not model parameters. For undirected and unipartite networks, \( \theta^l_i = d^l_i / \langle d^l \rangle \), where \( i \in \mathcal{N} \) and \( \langle d^l \rangle \) is the mean degree in layer \( l \). This normalization recovers the model in Sec. II B when \( \theta^l = 1 \) (i.e., when all nodes have the same degree).

The probabilities in equations (22)–(23) ensure that, marginally, \( A^1 \) and \( A^2 \) are generated according to monolayer degree-corrected SBMs [33]. It is not obvious how to model the joint probability \( P(A^1_{ij} = 1, A^2_{ij} = 1) \). In particular, it is not clear how it should depend on the observed degrees of nodes \( i \) and \( j \) in layers 1 and 2. Part of the complication is that there are four such quantities for each node pair \((i, j)\). The choice from [24] works particularly well when \( \rho = 1 \) and the normalized degree sequences \( \theta^1 \) and \( \theta^2 \) are the same, as it reduces to a single degree-corrected SBM that generates two identical network layers. Another sensible option is to set \( P(A^1_{ij} = 1, A^2_{ij} = 1) = \theta^1_i \theta^1_j \theta^2_i \theta^2_j q_{\theta^1, \theta^2} \). This choice has the nice property that edges in a particular edge bundle \((r, s) \in \mathcal{B}\) are independent if and only if \( q_{rs} = p_{rs}^1 p_{rs}^2 \), which matches the independence condition from Sec. II B for the non-degree-correcting setting. However, this second model underperforms the one from [22], [24] for edge prediction (see Sec. III and [24]). Consequently, for the rest of this paper, we use the model from equations (22)–(24) as our correlated DCSBM.

\[ L = \sum_{(r,s) \in \mathcal{B}} \sum_{(i,j) \in \mathcal{E}} \left[ A^1_{ij} A^2_{ij} \log q_{rs} + A^1_{ij} (1 - A^2_{ij}) \log \left( p^1_{rs} - \frac{\theta^2_i \theta^2_j}{\theta^1_i \theta^1_j} q_{rs} \right) + (1 - A^1_{ij}) A^2_{ij} \log \left( p^2_{rs} - \frac{\theta^1_i \theta^1_j}{\theta^2_i \theta^2_j} q_{rs} \right) \right] + \left(1 - A^1_{ij}\right) \left(1 - A^2_{ij}\right) \log \left(1 - \theta^1_i \theta^1_j p^1_{rs} - \theta^2_i \theta^2_j p^2_{rs} + \sqrt{\theta^1_i \theta^1_j \theta^2_i \theta^2_j q_{rs}}\right) \delta(g_i, r) \delta(g_j, s) + \text{(const.)}. \]  

As in Sec. II B, we seek to maximize \( L \) with respect to the parameters \( p^1_{rs}, p^2_{rs}, \) and \( q_{rs} \) by setting the corresponding derivatives to 0. However, degree-corrected models have the crucial complication that node pairs \((i, j)\) in the same edge bundle \((r, s)\) are no longer stochastically equivalent (i.e., the corresponding entries of the adjacency matrix are no longer sampled from independent, identically distributed random variables), so their contributions to the log-likelihood are no longer the same. Consequently, the ML equations for correlated DCSBMs involve \( O(N^2 / K^2) \) terms, making them more difficult to solve efficiently.

We are able to make some approximations that make these ML equations easier to solve. Recall that \( \theta^l_i = 1 \) if the degree of node \( i \) is equal to the mean degree in layer \( l \). For \((i,j) \in \mathcal{E}\), we write

\[ \theta^1_i \theta^1_j = 1 + \varepsilon^1_{ij}, \]

\[ \theta^2_i \theta^2_j = 1 + \varepsilon^2_{ij}. \]

Assuming that most deviations from the mean degree are small, \( \varepsilon^1_{ij} \) and \( \varepsilon^2_{ij} \) are small parameters (which can be either positive or negative) for most choices of \((i,j)\). Additionally, as we aim to combine all terms that correspond to the same edge bundle \((r, s)\) in the log-likelihood (25), some of the errors from our approximation will cancel each other out.

Assuming that \( \varepsilon^1_{ij} \) and \( \varepsilon^2_{ij} \) are small,

\[ \sqrt{\frac{\theta^1_i \theta^1_j \theta^2_i \theta^2_j}{\theta^1_i \theta^1_j}} = \sqrt{(1 + \varepsilon^1_{ij})(1 + \varepsilon^2_{ij})} \approx 1 + \frac{\varepsilon^1_{ij} + \varepsilon^2_{ij}}{2}, \]

where we use a Taylor expansion for the approximation and ignore the quadratic term. We also calculate

\[ \sqrt{\frac{\theta^1_i \theta^1_j}{\theta^2_i \theta^2_j}} \approx 1 + \frac{\varepsilon^1_{ij} - \varepsilon^2_{ij}}{2} \]

and

\[ \sqrt{\frac{\theta^2_i \theta^2_j}{\theta^1_i \theta^1_j}} \approx 1 + \frac{\varepsilon^2_{ij} - \varepsilon^1_{ij}}{2}. \]

Using the approximations (26)–(28), we expand the first derivatives of \( L \) to first order in \( \varepsilon^1_{ij} \) and \( \varepsilon^2_{ij} \); see [24] for details. This calculation yields the following system of equations:
algorithm to solve (29) for the parameters. These terms provides a good initialization of a numerical
zeroth-order solution that we obtain from ignoring perturbations of the degrees from their mean values).
node pairs \((i, j)\) have the same Pearson correlation \(\rho_{rs}\). This no longer holds for degree-corrected models. Instead, each node pair \((i, j)\)

\[
\begin{align*}
\frac{e_{rs}^{10}}{p_{rs} - q_{rs}} - \frac{e_{rs}^{00}}{1 - p_{rs}^2 - q_{rs}^2 + q_{rs}} + \frac{g_{rs}^{10}}{2 (p_{rs} - q_{rs})^2} q_{rs} - f_{rs}^1 & = 0,
\frac{e_{rs}^{01}}{p_{rs}^2 - q_{rs}} - \frac{e_{rs}^{00}}{1 - p_{rs}^2 - p_{rs}^2 + q_{rs}} + \frac{g_{rs}^{01}}{2 (p_{rs}^2 - q_{rs})^2} p_{rs} - f_{rs}^1 & = 0,
\frac{e_{rs}^{11}}{q_{rs} - p_{rs}} - \frac{e_{rs}^{00}}{1 - p_{rs}^2 - p_{rs}^2 + q_{rs}} + \frac{g_{rs}^{10}}{2 (p_{rs}^2 - q_{rs})^2} q_{rs} - f_{rs}^1 & = 0.
\end{align*}
\] (29)

In these equations, \(e_{rs}^{11}, e_{rs}^{10}, e_{rs}^{01}\), and \(e_{rs}^{00}\) are defined as in Sec. III. Additionally, we set

\[
\begin{align*}
g_{rs}^{10} & = \sum_{(i,j) \in E} A_{ij}^1 (1 - A_{ij}^2) (\varepsilon_{ij}^2 - \varepsilon_{ij}^1) \delta(g_i, r) \delta(g_j, s), \\
g_{rs}^{01} & = \sum_{(i,j) \in E} (1 - A_{ij}^1) A_{ij}^1 (\varepsilon_{ij}^1 - \varepsilon_{ij}^2) \delta(g_i, r) \delta(g_j, s), \\
f_{rs}^1 & = \sum_{(i,j) \in E} (1 - A_{ij}^1) (1 - A_{ij}^2) \varepsilon_{ij}^1 \delta(g_i, r) \delta(g_j, s), \\
f_{rs}^2 & = \sum_{(i,j) \in E} (1 - A_{ij}^1) (A_{ij}^2) \varepsilon_{ij}^2 \delta(g_i, r) \delta(g_j, s).
\end{align*}
\]

We can efficiently calculate all of these quantities from the matrices \(A^1\) and \(A^2\).

The system of equations (29) reduces to the analogous equations for correlated SBMs if we ignore all the terms that depend on \(\varepsilon_{ij}^1\) (i.e., the terms that correspond to perturbations of the degrees from their mean values). The zeroth-order solution that we obtain from ignoring these terms provides a good initialization of a numerical algorithm to solve (29) for the parameters \(p_{rs}^1, p_{rs}^2,\) and \(q_{rs}\). In practice, when using correlated DCSBMs for edge prediction (see Sec. III), we find that using a first-order approximation to determine \(p_{rs}^1, p_{rs}^2,\) and \(q_{rs}\) gives results that are almost identical to those from the zeroth-order approximation. Given that the latter is significantly easier to determine than the former, we suggest using the zeroth-order parameter in most cases.

2. Correlation values

For the non-degree-corrected SBMs from Sec. III node pairs \((i, j)\) from a given edge bundle \((r, s)\) have the same Pearson correlation \(\rho_{rs}\). This no longer holds for degree-corrected models. Instead, each node pair \((i, j)\)

\[
\begin{align*}
\rho_{ij} = \frac{\mathbb{E}[A_{ij}^1 A_{ij}^2] - \mathbb{E}[A_{ij}^1] \mathbb{E}[A_{ij}^2]}{\sigma[A_{ij}^1] \sigma[A_{ij}^2]} & = \frac{\sqrt{\theta_1^1 \theta_1^2 \theta_2^1 \theta_2^2} p_{rs}^1 p_{rs}^2}{\sqrt{\theta_1^1 \theta_1^2 (1 - \theta_1^2 p_{rs}^1) \theta_2^1 \theta_2^2 (1 - \theta_2^2 p_{rs}^2)}}.
\end{align*}
\] (30)

As in our earlier expansions of the ML equations, we approximate \(\rho_{ij}\) to first order in \(\varepsilon_{ij}^1\) and \(\varepsilon_{ij}^2\). We obtain

\[
\rho_{ij} \approx \rho_{rs} + \rho_{rs} \left( \frac{\varepsilon_{ij}^1}{2} \frac{p_{rs}^1}{1 - p_{rs}^1} + \frac{\varepsilon_{ij}^2}{2} \frac{p_{rs}^2}{1 - p_{rs}^2} - \frac{\varepsilon_{ij}^1 + \varepsilon_{ij}^2}{2} \frac{p_{rs}^1 p_{rs}^2}{q_{rs} - p_{rs}^1 p_{rs}^2} \right).
\] (31)

Ignoring terms that depend on \(\varepsilon_{ij}^1\) and \(\varepsilon_{ij}^2\) (i.e., terms that correspond to perturbations of the degrees from their mean values), we have \(\rho_{ij} \approx \rho_{rs}\). This approximation works especially well when \(p_{rs}^1\) and \(p_{rs}^2\) are also small, such that the respective network layers are sparse.

The case \(q_{rs} = p_{rs}^1 p_{rs}^2\) requires separate consideration 51 to avoid dividing by 0. First-order approximations in \(\varepsilon_{ij}^1\) and \(\varepsilon_{ij}^2\) for this case give

\[
\rho_{ij} \approx \frac{-\varepsilon_{ij}^1 + \varepsilon_{ij}^2}{2} \sqrt{\frac{p_{rs}^1}{1 - p_{rs}^1} \frac{p_{rs}^2}{1 - p_{rs}^2}}.
\] (32)

In particular, the zeroth-order solution gives \(\rho \approx 0\), in agreement with the non-degree-corrected SBM from Sec. III.

III. EDGE PREDICTION

The aim of edge prediction (also called “link prediction”) in networks is to infer likely missing edges and/or spurious edges 52. Edge prediction is useful for filling in incomplete data sets, such as protein-interaction networks (in which edges are often established as a result
of costly experiments) \cite{53} or terrorist-association networks (which are typically constructed based on partial knowledge) \cite{54}. In the context of bipartite user-item networks, edge-prediction techniques provide candidates for personalized recommendations.

Edge prediction is often model-driven \cite{4, 9, 15, 53, 54, 55}, and the first step typically consists in computing probabilities for node pairs \((i, j)\) to have edges between them. For example, one can use a monolayer degree-corrected Bernoulli SBM for this task. Having inferred some block structure \(q\) and edge propensities \(p\), the probability that two nodes \(i\) and \(j\) are adjacent according to the model is

\[
P(A_{ij} = 1) = \theta q_i \theta q_j p_{g_i, g_j}. \tag{33}
\]

The pairs \((i, j)\) for which these probabilities are relatively large, but which are not adjacent in the actual network (i.e., with \(A_{ij} = 0\)), produce a list of likely candidates for missing edges. Similarly, pairs \((i, j)\) for which these probabilities are small but which are adjacent in the actual network (i.e., with \(A_{ij} = 1\)) are possible spurious edges.

### A. Edge Prediction Using Correlated Models

There have been several recent attempts to perform edge prediction in multilayer networks \cite{15, 20, 25}. All these methods use multilayer information to infer mesoscale structures in networks, but then they perform edge prediction independently in each layer, conditioned on the inferred mesoscale structure. In particular, when using one of these approaches, two nodes being adjacent in one layer has no bearing on their probability to be adjacent in another layer. We aim to use our correlated models to overcome this limitation.

As in our prior discussions, consider a network with two layers with intralayer adjacency matrices \(A^1\) and \(A^2\), and let \(g\) be the shared block structure of these layers. Our goal is to predict edges in the second layer, conditioned on the adjacency structure of the first layer. For each node pair \((i, j) \in \mathcal{E}\), the key quantities to calculate are the probabilities \(P(A^2_{ij} = 1|A^1_{ij} = 1)\) and \(P(A^2_{ij} = 1|A^1_{ij} = 0)\) for \(i\) and \(j\) to be adjacent in the second layer, conditioned on them either being adjacent or non-adjacent in the first layer. For example, using the correlated Bernoulli SBM from Sec. II.B (which has no degree correction), we have

\[
P(A^2_{ij} = 1|A^1_{ij} = 1) = \frac{q_i q_j}{p_{g_i, g_j}}, \tag{34}
\]

\[
P(A^2_{ij} = 1|A^1_{ij} = 0) = \frac{p_{g_i, g_j}^1 - q_i q_j}{1 - p_{g_i, g_j}^1}. \tag{35}
\]

This set of probabilities is the same across all node pairs \((i, j)\) from the same edge bundle \((r, s)\). Now suppose that we have a positive correlation in this edge bundle, so \(p_{rs} > 0\). From the definition of the Pearson correlation, it follows that \(q_{rs} > p_{rs} p_{rs}\). We then find that

\[
P(A^2_{ij} = 1|A^1_{ij} = 1) > p_{rs}^2, \quad P(A^2_{ij} = 1|A^1_{ij} = 0) < p_{rs}^2. \tag{36}
\]

The pairs \((i, j)\) for which these probabilities are relatively large, but which are not adjacent in the actual network (i.e., with \(A_{ij} = 0\)), produce a list of likely candidates for missing edges. Similarly, pairs \((i, j)\) for which these probabilities are small but which are adjacent in the actual network (i.e., with \(A_{ij} = 1\)) are possible spurious edges.

### B. Tests on Synthetic Networks

We use \(K\)-fold \cite{56} cross-validation to assess the performance of the models from Table I on the edge-prediction task. In machine learning, this is a robust way to measure predictive performance \cite{52}. After partitioning a given data set into \(K\) parts, one then fits a model to \(K - 1\) of these subsets and uses it to make predictions on the remaining (i.e., “holdout”) set, repeating the process \(K\) times (using each subset once as a holdout). For our problem, we perform 5-fold cross-validation (which is a standard choice in the machine-learning literature) by splitting the data in the second layer of a given network into 5 subsets. Effectively, this consists in hiding 20% of the entries of the adjacency matrix \(A^2\), such that we do not know whether they are edges or not. We then train a model on 100% of the entries of \(A^1\) and 80% of the entries of \(A^2\) and use it to make predictions about the 20% holdout data. We do this 5 times, to cover each choice of holdout data.

A common way to assess the performance of a binary classification model (i.e., a model that assigns one of two possible values to test data) is using a receiver operating characteristic (ROC) curve. An ROC curve plots the true-positive rate (TPR) of a classifier versus the false-positive rate (FPR) for various choices of a threshold. Many models — including those that are used for edge prediction in networks — make probabilistic predictions, so specifying a threshold is necessary to convert these into binary predictions. Lowering the threshold increases both the TPR and the FPR. A model has predictive power if the former grows faster than the latter.
TABLE I: Edge-prediction probabilities for various correlated and monolayer network models

| Model   | $P(A_{ij}^c = 1 | A_{ij}^c = 1)$ | $P(A_{ij}^c = 1 | A_{ij}^c = 0)$ |
|---------|----------------------------------|----------------------------------|
| Corr. ER | $q/p_1$                          | $(p_2 - q)/(1-p_1)$               |
| Corr. SBM | $q_{rs}/p_{rs}^2$                | $(p_{rs}^2 - q_{rs})/(1-p_{rs}^2)$ |
| Corr. CM | $\sqrt{\theta_1^2 \theta_2^2 q/(\theta_1^2 \theta_1^2 p_1)}$ | $(\theta_2^2 \theta_2^2 p_2 - \sqrt{\theta_1^2 \theta_1^2 q})/(1-\theta_1^2 \theta_1^2 p_1)$ |
| Corr. DCSBM | $\sqrt{\theta_1^2 \theta_2^2 q_{rs}/(\theta_1^2 \theta_1^2 p_{rs}^2)}$ | $(\theta_2^2 \theta_2^2 p_{rs}^2 - \sqrt{\theta_1^2 \theta_1^2 q_{rs}})/(1-\theta_1^2 \theta_1^2 p_{rs}^2)$ |
| SBM     | $p_{rs}^2$                       | $\theta_2^2 \theta_2^2 p_{rs}^2$ |
| DCSBM   | $\theta_2^2 \theta_2^2 p_{rs}^2$ | $\theta_2^2 \theta_2^2 p_{rs}^2$ |

such that the entire ROC curve lies above the diagonal line TPR = FPR, which gives the performance of a random classifier. As a single summary measure of a model’s predictive performance, it is common to report the area under an ROC curve (AUC). Larger AUC values are better, with a value of AUC = 0.5 indicating equal success as random guessing and AUC = 1 corresponding to perfect prediction. Even in the latter case, one still needs to determine a choice of threshold that completely separates true positives from false positives.

We now describe how to generate synthetic networks that are suitable for testing the models in Table I. We construct these networks so that they have two tunable parameters: the Pearson correlation $\rho \in [-1, 1]$ and a community-mixing parameter $\mu \in [0, 1]$ which controls the strength of the planted mesoscale structure. (See Bazzi et al. [14] for more details about the definition of $\mu$.) One can also explicitly control the degree distribution, for example by including a third parameter $\tau$ for the slope of a truncated power law (e.g., as used in [14] to sample a degree sequence in each layer). For the experiments in this section, we fix $\tau = -2$ and use a minimum degree of $k_{\text{min}} = 10$ and a maximum degree of $k_{\text{max}} = 50$. It would be interesting to explore the performance gap between degree-corrected and non-degree-corrected models as one varies $\tau$, $k_{\text{min}}$, and $k_{\text{max}}$, although we do not do so in the present paper. Lastly, for the numerical experiments in this section, there are $N = 2000$ nodes in each layer and $n_c = 5$ communities, with community sizes sampled from a flat Dirichlet distribution (i.e., one with $q = 1$ and $\theta = 1$ in the notation of [14]).

We examine two versions, which we call CorrSBM and CorrDCSBM, of a correlated benchmark that is parametrized by the correlation $\rho$ and the community-mixing parameter $\mu$. For both versions, we generate the (undirected and unipartite) adjacency matrix $A_1$ of the first layer in the same way. Specifically, given $\mu$ and degree-distribution parameters $\tau$, $k_{\text{min}}$, and $k_{\text{max}}$, we use the code from [57] to generate $A_1$ and its associated block structure $q$. We fit a monolayer model — either an SBM or a DCSBM, depending on the selected version of the benchmark — to $A_1$ to obtain the marginal edge propensities $p_1$ for the first layer. We then choose $p_2$ in one of two ways. For $\rho \in [0,1]$, we set $p_2^2 = p_1$, which ensures that we can generate networks with correlations that cover the entire range from 0 to 1. For $\rho \in [-1,0]$, we set $p_2^2 = J - p_1$, where $J$ is a matrix with all entries equal to 1; this ensures that we can generate networks with correlations that cover the entire range from -1 to 0. Given $p_1$, $p_2$, and $\rho$, we then determine $q$ using either the correlated SBM of Sec. II B or the correlated DCSBM of Sec. II C. For the CorrDCSBM benchmark with $\rho \geq 0$, we set the normalized degrees $\theta_i^2$ to be equal to the corresponding quantities $\theta_i$ from the first layer. Again, this choice ensures that we can generate networks all the way to $\rho = 1$. (We also implemented a version of this benchmark that samples degrees independently in the second layer, and we found qualitatively similar results.) The final step consists in generating $A^2$ given $A^1$, parameter values $p_2$ and $q$, and — for the CorrDCSBM benchmark only — the normalized degree sequences $\theta_1$ and $\theta_2$ for both layers. To do this, we first compute edge probabilities using either of the correlated models from Secs. II B and II C and we then generate edges independently according to these probabilities.

We now present results for the two variants of the benchmark. In Fig. 3, we show sample ROC curves for one network sampled from the CorrDCSBM benchmark with $\mu = 0.3$ and $\rho = 0.5$. We compare the performance of our correlated models with a monolayer DCSBM baseline, which performs edge prediction using only information from the second network layer. Two of the correlated models outperform this baseline, and the correlated CM performs equally well (i.e., it has a similar AUC). In Fig. 4, we show results for the CorrSBM benchmark for two choices of the community-mixing parameter $\mu$ and several values (both positive and negative) of the Pearson correlation $\rho$. As expected, the AUC values for monolayer SBMs are independent of $\rho$, whereas the predictive performance of correlated ER models and correlated SBMs improves as we increase $|\rho|$. In particular, when $|\rho| = 1$, the two correlated models make perfect predictions. When $\rho = 0$, the performance of the correlated ER model is indistinguishable from chance (because AUC = 0.5), whereas correlated SBMs perform at the same level as monolayer SBMs. The gap between the two correlated models is progressively smaller for progressively larger $\mu$, because the underlying block structure is progressively weaker. The AUC of the monolayer base-
(a) Models without mesoscale structure

(b) Models with mesoscale structure

FIG. 3: ROC curves from 5-fold cross-validation for a network sampled from the CorrDCSBM benchmark with community-mixing parameter $\mu = 0.3$ and correlation $\rho = 0.5$. (a) Correlated models that do not incorporate any mesoscale structure compared to a monolayer DCSBM baseline (AUC $\approx 0.83$). The AUC values for the two correlated models are approximately 0.76 (correlated ER) and 0.83 (correlated CM). (b) Correlated models that incorporate mesoscale structure compared to a monolayer DCSBM baseline (AUC $\approx 0.83$). The AUC values for the two correlated models are approximately 0.89 (correlated SBM) and 0.91 (correlated DCSBM).

One striking feature in Fig. 4 is that all curves are approximately straight lines (to within sampling error). It makes sense that the performance of monolayer SBMs does not vary with $\rho$, as these models do not use any information from the other layer, but the linear dependence on $\rho$ of the other two curves is less obvious. For the correlated ER model, we can establish rigorously (see Appendix A) that the AUC is approximately equal to $(1 + |\rho|)/2$ when $p_1 \approx p_2$ or when $p_1 \approx 1 - p_2$. Given that the correlated SBM curves from Fig. 4 also exhibit a linear dependence on $\rho$, we believe that it is possible to establish similar results for correlated models that incorporate mesoscale structure. These results have practical importance, as they allow one to quickly estimate the additional benefits of using correlated models instead of monolayer SBMs for edge prediction.

In Fig. 5, we show results for the CorrDCSBM benchmark for two choices of the community-mixing parameter $\mu$ and nonnegative values of the Pearson correlation $\rho$. As expected, when $\rho = 0$, correlated DCSBMs perform similarly to monolayer DCSBMs. As in Fig. 4, the performance of the monolayer model is roughly independent of $\rho$, whereas the two correlated models do better as $\rho$ increases. The gap between the two correlated models narrows substantially as one increases $\mu$ from 0.3 to 0.8.

IV. APPLICATIONS

We discuss two applications of correlated models to the analysis of empirical networks. In Sec. IV A, we report pairwise layer correlations for several multiplex networks of different sizes. In Sec. IV B, we consider a temporal bipartite network of customers and products. Using an approach similar to that from Sec. III, we demonstrate that correlated models have a better edge-prediction performance than their monolayer counterparts.

A. Layer Correlations in Empirical Networks

In this section, we calculate pairwise layer correlations using the formula (21). Recall that this expression gives the effective correlation between two layers, assuming that they have identical block structures (although their edge-propensity parameters can be different). Crucially, this calculation does not require that one first determines the underlying block structure. In fact, as we demonstrated in Sec. II B, the effective correlation for a correlated SBM recovers the correlation for a correlated ER graph, which is straightforward to compute. Accounting for node degrees, as we did in Sec. II C for correlated DCSBMs, significantly increases the complexity of such a calculation. Additionally, as we showed in Sec. II C, correlations using a degree-corrected model are rather similar to those that one obtains without degree correction.

In Table II, we report the mean pairwise layer corre-
FIG. 4: Edge-prediction results on synthetic networks from the CORR-SBM benchmark with (left) $\rho \leq 0$ and (right) $\rho \geq 0$ using two choices of the community-mixing parameter $\mu$. We use $\mu = 0.3$ in the top row and $\mu = 0.8$ in the bottom row. In all plots, along the horizontal axis, we vary the correlation $\rho$ that we use to generate network instances. On the vertical axis, we indicate the AUC for 5-fold cross-validation using a monolayer SBM (dashed curves) or a correlated SBM or ER model (solid curves). Each data point is a mean across 10 trials, and the error bars correspond to one standard deviation from that mean. As expected, the AUC does not change with $\rho$ for the monolayer model, but it increases with $|\rho|$ for the two correlated models. For progressively larger $\mu$, such that the sampled networks have progressively weaker mesoscale structure, there is a smaller performance gap between correlated ER models and correlated SBMs.

We make a few observations about some of the results in Table II. For the C. elegans connectome, the layers that correspond to two types of chemical synapses are highly correlated with each other, and their correlation to the layer of electrical synapses is comparatively lower. For the EU air transportation network, the two most correlated layers are those that correspond to Scandinavian Airlines and Norwegian Air Shuttle Flights; this is consistent with the findings in [38], which were based on a different method for quantifying layer similarity. For the network of arXiv collaborations among network scien-
FIG. 5: Edge-prediction results on synthetic networks from the CorrDCSBM benchmark with correlation \( \rho \geq 0 \) with community-mixing parameter (a) \( \mu = 0.3 \) and (b) \( \mu = 0.8 \). In both panels, along the horizontal axis, we vary the correlation \( \rho \) that we use to generate network instances. On the vertical axis, we indicate the AUC for 5-fold cross-validation using a monolayer DCSBM (dashed curves) or a correlated DCSBM or CM (solid curves). Each data point is a mean across 10 trials, and the error bars correspond to one standard deviation from that mean. As expected, the AUC is roughly independent of \( \rho \) for the monolayer model, but it increases with \( \rho \) for the two correlated models. As we increase \( \mu \), such that the sampled networks have progressively weaker mesoscale structure, there is a substantial narrowing of the performance gap between correlated CMs and correlated DCSBMs.

B. Edge Prediction in Shopping Networks

The data-science company dunnhumby gave us access to “pseudonymized” transaction data from stores belonging to a major grocery retailer in the UK. The data were pseudonymized by replacing personally identifiable information with numerical IDs, rendering it impossible to identify any individual shoppers. For our analysis, we aggregate transactions over fixed time windows to construct bipartite networks of customers and products. We refer to these structures as “shopping networks”. Because some purchases occur in higher volumes than others, it is useful to add weights to the edges. Given a customer \( i \) and a product \( j \), the item-penetration weight is equal to the fraction of all of the items bought by customer \( i \) that are product \( j \). The basket-penetration weight is equal to the fraction of all baskets (i.e., distinct shopping trips) of customer \( i \) that include product \( j \). See the PhD dissertation [24] for more details about these weighting schemes.

We now apply the edge-prediction methodology from Sec. [III] to temporal shopping networks, in which edges can change from changes in shopping behavior, with a fixed set of customers and a fixed set of products. We construct networks with two layers, which cover the three-month time periods of March–May 2013 and June–August 2013, respectively. Using the same underlying transaction data, we construct two networks which we then analyze further. For the first network (which we call SHOPPINGMOD), we use basket-penetration weights on the edges and apply multilayer modularity maximization [66, 67] to the weighted network to determine community assignments \( g \), which we fix for the rest of our analysis [68]. For the second network (which we call SHOPPINGSBM), we initially calculate item-penetration weights, and we then apply a threshold to remove 50% of the edges (the half with the smallest weights). We fit a degree-corrected SBM to the resulting unweighted network using the belief-propagation algorithm from [69] to infer \( g \). We expect better edge-prediction performance on the second network, because we detect its block structure using an SBM (as opposed to using modularity max-
TABLE II: Pairwise layer correlations in several multiplex networks.

| Domain       | Network                                  | Number of layers | Mean correlation | Largest correlation (corresponding layers) |
|--------------|------------------------------------------|------------------|------------------|-------------------------------------------|
| Social       | CS Aarhus [59]                           | 5                | 0.27             | 0.45 (“work” and “lunch” layers)           |
|              | Lazega law firm [60]                    | 3                | 0.39             | 0.48 (“advice” and “co-work” layers)       |
|              | YouTube [61]                            | 5                | 0.12             | 0.20 (“shared subscriptions” and “shared subscribers”) |
| Biological   | C. elegans connectome [62]              | 3                | 0.47             | 0.85 (“MonoSyn” and “PolySyn” layers)      |
|              | P. falciparum genes [28]                | 9                | 0.08             | 0.25 (“HVR7” and “HVR9” layers)            |
|              | Homo sapiens proteins [63]              | 7                | 0.04             | 0.29 (“direct interaction” and “physical association”) |
| Other        | FAO international trade [64]            | 364              | 0.13             | 0.74 (“Pastry” and “Sugar confectionery”)   |
|              | EU air transportation [65]              | 37               | 0.03             | 0.39 (“Scandinavian Airlines” and “Norwegian Air Shuttle”) |
|              | ArXiv collaborations [66]               | 13               | 0.07             | 0.73 (“physics.data-an” and “cs.SI”)       |

TABLE III: Predictive performance of different models on the shopping data set, as measured by the AUC.

| Model                  | AUC (ShoppingMod) | AUC (ShoppingSBM) |
|------------------------|-------------------|-------------------|
| Monolayer SBM          | 0.549             | 0.633             |
| Correlated ER          | 0.724             | 0.743             |
| Correlated SBM         | 0.742             | 0.793             |
| Monolayer DCSBM        | 0.725             | 0.797             |
| Correlated CM          | 0.817             | 0.870             |
| Correlated DCSBM       | 0.818             | 0.875             |

As with our tests on synthetic networks in Sec. [III], we use 5-fold cross-validation to assess edge-prediction performance. We summarize the AUC values of our various correlated models and the monolayer baselines in Table III and we show sample ROC curves in Fig. 6. We make a few observations about these results. First, our approximation AUC ≈ (1 + ρ)/2 for correlated ER models is very accurate for these two networks, whose correlations are approximately 0.44 and 0.48, respectively. Second, our correlated multilayer models outperform the monolayer baselines for both networks. In particular, the very simple correlated ER model — which assigns one of two probabilities to edges, as indicated in Table I — performs about as well as the more sophisticated monolayer DCSBM for the SHOPPINGMod network. Third, as expected, AUC values are systematically larger for SHOPPINGSBM than for SHOPPINGMod. Finally, although incorporating mesoscale structure leads to better performance when there is no degree correction, this does not seem to be the case for degree-corrected models, as correlated DCSBMs do not perform significantly better than correlated CMs. This is also apparent in Figs. 6(b,d), where the ROC curves for the two models are almost identical. This result suggests that, for some networks, taking into account layer correlations and degree heterogeneity alleviates the need to also consider mesoscale structure when performing edge prediction. This observation has practical implications, as a correlated CM is much easier than a correlated DCSBM to fit to data and to use for edge prediction. However, for recommendation systems, there are situations in which fitting a correlated DCSBM is beneficial, even if its edge-prediction performance is similar to that of a correlated CM. For instance, one may wish to identify relevant customers for a chosen product, irrespective of how much they buy (i.e., their degree). CMs are able to distinguish between customers with equal degrees and identify those with the greatest predisposition to buy a particular product, whereas CMs are not.

V. CONCLUSIONS AND DISCUSSION

We have introduced models of multilayer networks in which edges that connect the same nodes in different layers are not independent (in contrast to previous work). These models offer an improved representation of many empirical networks, as interlayer correlations are a common phenomenon: flights between major airports are serviced by multiple airlines, individuals interact repeatedly with the same people, consumers often buy the same products over time, and so on. Among other potential applications, our models can be used to improve edge prediction, to study the graph-matching problem on more realistic benchmark networks, and to calculate layer correlations as new summary statistics for networks. To model layer correlations, we used bivariate Bernoulli random variables to generate edges simultaneously in two network layers. (See [24] for derivations using Poisson random variables.) Correlated Bernoulli stochastic block models have been proposed previously [31], although only as forward models for generating networks, rather than for performing inference given empirical data. Another key contribution of our work is a degree-corrected variant of such a model. The maximum-likelihood equations are significantly more difficult to solve in this case, but we were able to make useful simplifications with suitable approximations. Notably, these simplified equations closely approximate those for non-degree-corrected models for networks with homogeneous degree distributions.

The models in this paper that incorporate some mesoscale structure $g$ assume that such structure is given. This setup has the benefit that one can use any de-
FIG. 6: ROC curves for the edge-prediction task using 5-fold cross-validation on two temporal networks, ShoppingMod and ShoppingSBM. We consider models without degree correction as well as models with degree correction. The dotted diagonal line in each plot indicates the expected ROC curve for a random classifier. All other curves lie above this diagonal line, suggesting that they have predictive power. In all cases, correlated multilayer models outperform their monolayer counterparts. For both networks, correlated SBMs outperform correlated ER models, whereas correlated DCSBMs perform similarly to correlated CMs (as illustrated by the almost overlapping curves in panels (b) and (d)).

desired algorithms to produce a network partition, including ones that operate on weighted or annotated networks or that use nonstandard null models in a modularity objective function. This makes our approach for analyzing correlations suitable for a wide variety of applications.

Fitting a correlated SBM to network data yields a correlation value $\rho_{rs}$ for each edge bundle $(r,s)$. We have defined an effective correlation that combines all of these values into a single measure of similarity between two layers. Notably, the value of the effective correlation is independent of a network’s mesoscale structure, making it extremely easy to compute (see Eqn. (12)). We illustrated this method of assessing layer similarity on multiplex networks from social, biological, and other domains.

Another application of our work is to edge prediction in multilayer networks. Our numerical experiments revealed that simple correlated models (e.g., a correlated configuration model or a correlated SBM without degree...
correction) can outperform monolayer DCSBMs even for moderate correlation values. We also observed such improved performance for consumer–product networks, which have significant layer correlations \( \rho \approx 0.45 \). We expect that a correlated multilayer DCSBM will typically outperform a monolayer DCSBM for most empirical networks, even when there are lower levels of correlation.

There are many interesting ways to build further on our work. For example, it would be useful to be able to model all layers simultaneously, rather than in a pairwise fashion, especially for multiplex networks, in which layers do not have a natural ordering. One challenge is that a multivariate Bernoulli distribution of dimension \( L \) has \( 2^L - 1 \) parameters; this grows quickly with the number \( L \) of layers. For a temporal setting, we have proposed generating correlated networks in a sequential way by conditioning each layer on the previous one. In some cases, it will be useful to relax this “memoryless” assumption and condition a layer on all previous layers, rather than only on the most recent layer. For example, the purchases of shoppers in December one year are strongly related not only to their purchases in November, but also to what they bought in December during the previous year.

In this paper, we have not considered the case of non-identical mesoscale structure across layers; see [24] for a possible approach. Additionally, although one can account for edge weights when fitting a block structure \( g \) to use with our models, the rest of our derivations apply only to unweighted networks. Modeling correlated weighted networks entails prescribing both edge-existence and edge-weight correlations. Yet another idea is to derive correlated models for networks with overlapping communities. Previous research [15] suggests that this can substantially improve edge-prediction performance.

Lastly, our work is a starting point for designing an algorithm for detecting correlated communities in networks by inferring \( g \) alongside other model parameters. A practical outcome of such an algorithm would be a set of communities that persist across layers if and only if the edges in those communities are sufficiently highly correlated with each other. This approach would offer a new interpretation of what it means for a community to span multiple layers [11, 70].

In summary, our work highlights the importance of relaxing edge-independence assumptions in statistical models of network data. Doing so provides richer insights into the structure of empirical networks, improves edge-prediction performance, and yields more realistic models on which to test community-detection, graph-matching, and other types of algorithms.

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Appendix A: Edge-Prediction AUC as a Function of the Pearson Correlation \( \rho \)

We establish the following result.

**Proposition.** The AUC for a correlated ER model is an affine function of \( \rho \). In particular, when \( p_1 \approx p_2 \) or \( p_1 \approx 1 - p_2 \), we have \( \text{AUC}_{\text{ER}} \approx (1 + |\rho|)/2 \).

**Proof.** Suppose that \( \rho > 0 \). (The case \( \rho \leq 0 \) is similar.) With a correlated ER model, all unobserved interactions \( (i, j) \) in the second layer have one of two probabilities: \( q/p_1 \) if \( A_{ij}^1 = 1 \) and \( (p_2 - q)/(1 - p_1) \) if \( A_{ij}^1 = 0 \). Because \( \rho > 0 \), we have \( q > p_1 p_2 \), which implies that \( q/p_1 > (p_2 - q)/(1 - p_1) \). Selecting a threshold between these two probabilities amounts to predicting that everything that is an edge in the first layer is also an edge in the second layer, and that everything that is not an edge in the first layer is also not an edge in the second layer. Let \( a \) and \( b \) denote the TPR and FPR, respectively, at such an intermediate threshold. In this case, \( a \) and \( b \) are the coordinates of the point where the slope of the ROC curve changes. See our illustration in Fig. 7.

![Diagram of the ROC curve for an ER model](attachment:fig7.png)

**FIG. 7:** Diagram of the ROC curve for an ER model, which assigns one of two possible edge probabilities to each pair of nodes.

By straightforward geometry,

\[
\text{AUC}_{\text{ER}} = 1 - \frac{ab}{2} - \frac{(1 - a)(1 - b)}{2} - (1 - a)b = \frac{1}{2} + \frac{a - b}{2}
\]

is the area under this ROC curve. The next step is to estimate \( a \) and \( b \). The correlated ER model is set up such that the number of true positives is proportional [71] to \( e_{11} \); the model’s prediction is correct every time that an edge that is present in the first layer is also present in the second layer. To find the TPR, one needs to divide
this quantity by the number of edges in the second layer, which is equal to \( e_{11} + e_{01} \). Therefore,
\[
a \approx \frac{e_{11}}{e_{11} + e_{01}} \approx \frac{q}{p_2} = p_1 + \rho \sqrt{\frac{1-p_2}{p_2} p_1 (1-p_1)}. \tag{A1}
\]
Similarly, every time an edge that is present in the first layer is not present in the second counts as an incorrect prediction by the model. Therefore, the number of non-edges in the second layer, we obtain
\[
b \approx \frac{e_{10}}{e_{10} + e_{00}} \approx \frac{p_1 - q}{1-p_2} = p_1 - \rho \sqrt{\frac{p_2}{1-p_2} p_1 (1-p_1)}. \tag{A2}
\]
From (A1) and (A2), it follows that
\[
\text{AUC}_{ER} \approx \frac{1}{2} + \frac{\rho}{2} \sqrt{p_1 (1-p_1)} \left( \sqrt{\frac{1-p_1}{p_2}} + \sqrt{\frac{p_2}{1-p_2}} \right),
\]
which is an affine function of \( \rho \). When \( p_1 \approx p_2 \) or \( p_1 \approx 1-p_2 \), as is the case in Fig. 3, we get \( \text{AUC}_{ER} \approx (1+|\rho|)/2 \), as desired. Using a similar argument, one can show that the same result holds (with the same assumptions on \( p_1 \) and \( p_2 \)) for the case with \( \rho \leq 0 \).

Given that the correlated SBM curves from Fig. 4 also depend linearly on \( \rho \), we believe that it is possible to establish similar results for correlated models that incorporate mesoscale structure.

### Appendix B: Data Sets

We provide brief descriptions of the multiplex networks that we analyzed in Sec. IV A. For weighted networks, we disregard edge weights when calculating layer correlations. We downloaded all networks, aside from the YouTube and Malaria data sets, from

\[ \text{https://comunelab.fbk.eu/data.php} \]

#### 1. CS Aarhus

This is an undirected and unweighted social network of offline and online relationships among \( N = 61 \) members of the Computer Science department at Aarhus University [59]. There are \( T = 5 \) layers: (1) regularly eating lunch together; (2) friendship on Facebook; (3) co-authorship; (4) leisure activities; and (5) working together.

#### 2. Lazega Law Firm

This directed, unweighted network encompasses interactions between \( N = 71 \) partners and associates who work at the same law firm [60]. The network has \( T = 3 \) layers that encode co-work, friendship, and advice relationships.

#### 3. YouTube

This is an undirected, weighted network of interactions among \( N = 15088 \) YouTube users [61]. There are \( T = 5 \) types of interactions: (1) direct contact (“friendship”); (2) shared contacts; (3) shared subscriptions; (4) shared subscribers; and (5) shared favorites.

#### 4. C. elegans Connectome

This is a directed, unweighted network of synaptic connections between \( N = 279 \) neurons of the nematode \( C. \) elegans [62]. There are \( T = 3 \) layers, which correspond to electric, chemical monadic (“MonoSyn”), and chemical polyadic (“PolySyn”) junctions.

#### 5. P. falciparum Genes

This is an undirected, unweighted network of recombinant genes from the parasite \( P. falciparum \), which causes malaria [63]. There are \( T = 9 \) layers that correspond to distinct highly variables regions (HVRs), in which these recombinations occur. Two genes are adjacent in a layer if they share a substring whose length is statistically significant.

#### 6. Homo sapiens Proteins

This is a directed, unweighted network of interactions among \( N = 18222 \) proteins in \( Homo sapiens \) [72]. There are \( T = 7 \) layers, which correspond to the following types of interactions: (1) direct interaction; (2) physical association; (3) suppressive genetic interaction; (4) association; (5) colocalization; (6) additive genetic interaction; and (7) synthetic genetic interaction. The original data is from BioGRID [64], a public database of protein interactions (for humans as well as other organisms) that is curated from different types of experiments.

#### 7. FAO Trade

This is a weighted, directed network of food imports and exports during the year 2010 between \( N = 214 \) countries [34]. There are \( T = 364 \) layers, which correspond to different food products. We ignore edge weights when we estimate layer correlations.

#### 8. EU Air Transportation

This is an undirected, unweighted network of flights between \( N = 450 \) airports in Europe. There are \( T = 37 \) layers, each of which corresponds to a different airline [22].
9. ArXiv Collaborations

This is an undirected, weighted coauthorship network between $N = 14489$ network scientists [65]. There are $T = 13$ layers, which correspond to different arXiv subject areas: “physics.soc-ph”, “physics.data-an”, “physics.bio-ph”, “math-ph”, “math.OC”, “cond-mat.dis-nn”, “cond-mat.stat-mech”, “q-bio.MN”, “q-bio”, “q-bio.BM”, “nlin.AO”, “cs.SI”, and “cs.CV”.

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The Hessian is negative definite at the critical point that one obtains by setting these derivatives to 0, so this point is a local maximum (as opposed to a local minimum or saddle point) of the log-likelihood function.

The cases when one or more of the denominators in Eqn. (31) are $O(\varepsilon)$ also require separate derivations. However, we do not treat these exceptional cases here.

Note that this $K$ is different from the one that denotes the number of blocks elsewhere in this paper.

We use GenLouvain to perform multilayer modularity maximization. This algorithm requires the specification of (at least) two parameters $[41, 66]$, which we set to $\gamma = 1.2$ and $\omega = 5.0$.