Graph matching between bipartite and unipartite networks: to collapse, or not to collapse, that is the question.

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Abstract

Graph matching consists of aligning the vertices of two unlabeled graphs in order to maximize the shared structure across networks; when the graphs are unipartite, this is commonly formulated as minimizing their edge disagreements. In this paper we address the common setting in which one of the graphs to match is a bipartite network and one is unipartite. Commonly, the bipartite networks are collapsed or projected into a unipartite graph, and graph matching proceeds as in the classical setting. This potentially leads to noisy edge estimates and loss of information. We formulate the graph matching problem between a bipartite and a unipartite graph using an undirected graphical model, and introduce methods to find the alignment with this model without collapsing. In simulations and real data examples, we show how our methods can result in a more accurate matching than the naive approach of transforming the bipartite networks into unipartite, and we demonstrate the performance gains achieved by our method in simulated and real data networks, including a co-authorship-citation network pair and brain structural and functional data.

1 Introduction

The problem of inferring the correspondence between the vertices of two or more graphs, commonly referred as graph matching, has received recent interest in the literature, motivated by multiple applications in social and biological network analysis, image and document processing, pattern recognition, among others (Conte et al., 2004; Foggia et al., 2014; Yan et al., 2016). Myriad approximate matching methods and random graph models have been developed for studying this problem, mostly focusing on the setting where the practitioner seeks to align a pair of unipartite graphs that represent two sets relationships between a common set of entities (Pedarsani and Grossglauser, 2011; Narayanan and Shmatikov, 2009; Lyzinski et al., 2014, 2016; Korula and Lattanzi, 2014; Fan et al., 2019). In many scenarios, the available network structures are more complex and can consists of different classes of vertices and/or edges that cannot be well represented using unipartite graphs. In these settings, often the existing approaches are inapplicable directly, and significant data processing is needed to rend the problem amenable to existing analysis.
The goal of this paper is to study the graph matching problem where the pair of graphs consist of one unipartite and one bipartite network. Bipartite networks are often used to encode relationships between entities in two different classes, for example, transactions of customers with businesses (Bennett et al., 2007), authorship of publications by scientist (Ji et al., 2016), occurrence of words within a set of documents (Dhillon, 2001), protein-gene interactions (Pavlopoulos et al., 2018), among many other examples. A convenient approach when dealing with bipartite data is to collapse into a unipartite network over one class of entities by defining some edges using a measure of connectivity, for example one-mode projections (Zhou et al., 2007; Arora et al., 2012), correlation (MacMahon and Garlaschelli, 2013) or inverse covariance (Narayan et al., 2015; Lo and Marculescu, 2017). Although by doing this it is possible to proceed with inference using methods for unipartite networks, this approach has multiple disadvantages. Having to estimate these edges requires the definition of a proper measure, which is difficult to assess in practice and might be different depending of the inference goals. Moreover, this process results in noisy estimates that can induce errors in subsequent inference. Additionally, this estimation process often requires algorithmic and parameter decisions, and the results of subsequent analysis can be sensitive to those choices. Developing inference methods for bipartite network data directly is an important problem to address, and the analysis of bipartite network data has attracted significant interest, particularly in problems such as community detection (Larremore et al., 2014; Zhou and Amini, 2019; Razae et al., 2019), co-clustering (Dhillon, 2001; Choi, 2017) and topic modeling (Blei et al., 2003), for which methods specifically tailored for this type of data have been developed.

In particular, here we consider the graph matching problem when one of the graphs is a bipartite network between two disjoint sets of vertices $U$ and $V$, and the other graph is a unipartite graph with edges between elements in $U$. An example of this setting is given in Figure 1.1 with data from Ji et al. (2016), in which $U$ represents a group of statisticians and $V$ is a set of papers written by them. An edge in the unipartite graph connects two statisticians if they are coauthors in one paper, and the edges of the bipartite graph link the authors with all the papers that they have cited. Typically, joint graph inference across such a network pair usually requires a priori knowledge of the correspondence between the vertices of the graphs. In the more traditional setting when both graphs are unipartite (or both bipartite (Koutra et al., 2013)), if the correspondence is unknown then graph matching is commonly used to recover an estimate of the latent correspondence (Chen et al., 2016).

The problem of graph matching between bipartite and unipartite networks presents a more challenging setting than the classical graph matching problem, as the edges of the graphs cannot be directly related. For example, if matching a friendship network to a purchasing network, it need not be the case that two vertices that are friends need have correlated purchasing habits. To address this problem, we introduce a new formulation of graph matching based on a novel joint model for the pair of graphs. We model the edges of the bipartite network using an undirected graphical model based on the information contained in a permuted version of the unipartite graph. The unshuffling permutation and the parameters of the model are then jointly estimated, yielding (demonstrably) superior performance over methods that perform this estimation in different stages. Moreover, using simulations and real data we show that our approach yields superior performance over classical graph matching strategies that first collapse the bipartite network onto one of its parts.
2 Graph matching problem formulation

Given a pair of simple graphs $G_1 = (U_1, E_1)$ and $G_2 = (U_2, E_2)$ with the same number of vertices $n := |U_1| = |U_2|$ and edge sets $E_i \subseteq U_i \times U_i, i = 1, 2$, the classical graph matching problem consists in finding a bijection between the vertices of the two graphs to maximize a measure of their induced similarity. If the graphs are isomorphic, then there exists an exact matching that makes the aligned edges identical, but usually, in practice, there is no such isomorphism (and finding it if it exists is notoriously difficult in practice Babai (2016)). The inexact graph matching aims to minimize the number of edge disagreements between the aligned graphs, and can be formally defined using the adjacency matrices $A_1, A_2 \in \{0, 1\}^{n \times n}$ of $G_1$ and $G_2$ respectively, as solving a quadratic assignment problem to find the permutation $\tilde{P}$ such that

$$
\tilde{P} \in \arg\min_{P \in \Pi_n} \|A_1 - PA_2P^T\|_F^2,
$$

where $\Pi_n := \{P \in \{0, 1\}^{n \times n} : PP^T = I_n\}$ is the set of $n \times n$ permutation matrices, with $I_n$ the $n \times n$ identity matrix, and $\| \cdot \|_F$ is the Frobenius norm. Typically, it is assumed that the vertex sets $U_1$ and $U_2$ represent the same set of entities $U$, and the graphs $G_1$ and $G_2$ represent their relationships in two different views, so the edges of the aligned graphs would be similar/correlated. The formulation in Equation (2.1) aims to capture this similarity, and has been justified in different random graph models (Pedarsani and Grossglauser, 2011; Lyzinski et al., 2016; Lyzinski, 2018; Cullina and Kiyavash, 2016, 2017; Arroyo et al., 2018; Fan et al., 2019).

In this paper, we consider a different setting, in which instead of observing two views of the interactions between the vertices in $U$, in one of the views we observe the interaction between $U$ and a different set of vertices $V$, with $|V| = m$, which are encoded in a bipartite
graph. Denote by $G = (U_1, E)$ and $H = (U_2, V, F)$ the unipartite and bipartite graphs that are observed, where $U_1$ and $U_2$ are two different orderings of $U$, and $E \subset \binom{U_1}{2}$ and $F \subset U_2 \times V$ their corresponding edges. We assume that the unipartite graph $G$ is unweighted and undirected with no self loops, while the bipartite graph $H$ is allowed to have weighted edges. Define $A \in \{0, 1\}^{n \times n}$ and $B \in \mathbb{R}^{n \times m}$ as the adjacency matrices for $G$ and $H$ respectively, so $A_{ij} = 1$ indicates that $\{i, j\} \in E$, for $u_i, u_j \in U_1$, and $B_{ik} = 1$ indicates an edge between $u_i \in U_2$ and $v_j \in V$ (or in general, $B_{ij} \in \mathbb{R}$ represents the weight of the relationship between these vertices). The goal of this paper is to find a bijection between the vertices $U_1$ and $U_2$ that uncover the latent correspondence between these vertex sets.

### 2.1 The bipartite–to–unipartite graph matching problem

Formulating a graph matching problem between a unipartite and a bipartite graph in the setting just described is not immediate, as this problem is not immediately compatible to the traditional graph matching formulation in Equation (2.1). Indeed, in the bipartite–to–unipartite setting it is not possible to define a correspondence between the edges of both graphs. Similarly, this setting is also different from other formulations of graph matching across two bipartite graphs (Koutra et al., 2013).

A popular approach when dealing with bipartite graphs is to collapse the graph into a (possibly weighted) unipartite graph with a new adjacency matrix $\tilde{B} \in \mathbb{R}^{n \times n}$ that uses an appropriate measure to define the edges. This is commonly done via one-mode projections (Zhou et al., 2007; Zweig and Kaufmann, 2011), such as the co-occurrence matrix $\tilde{B} := \frac{1}{m} BB^T$. Once this matrix is constructed, one can proceed in matching the two matrices $A$ and $\tilde{B}$ by minimizing $\|A - P\tilde{B}P^T\|_F^2$, as in Equation (2.1). However, this approach faces several issues. On one hand, the matching solution depends on the collapsing method employed, and while multiple approaches for collapsing a graph are commonly used, none of them are constructed having the goal of graph matching in mind. Choosing the appropriate projection of the bipartite network among different options available, sometimes with parameter choices, is a complicated problem, and it is difficult to know a priori if a projection method is appropriate for subsequent graph matching. Finally, the estimated edges are amplifying noise in the original $B$, which makes the graph matching problem yet more challenging.

To formulate the unipartite to bipartite matching problem directly, we first consider a model for the edges of the bipartite graph given $A$. We posit $B$ to be a random bipartite graph with a distribution depending on $A$ via an undirected graphical model (Lauritzen, 1996; Wainwright and Jordan, 2008). Let $P^* \in \Pi_n$ be the permutation matrix associated with the mapping of the vertices in $U_1$ to the vertices in $U_2$, and let $W := W(A, P^*) = (P^*)^T AP^*$ be the adjacency matrix obtained by permuting $A$ to match the order of the vertices in $B$. We model the columns of $B$ with a distribution that forms a Markov random field (MRF) with respect to $W$. Formally, a positive probability distribution $F$ on $\mathbb{R}^n$ forms a MRF with respect to $W$ if a random vector $X \sim F$ satisfies the local Markov property of conditional independence

$$X_i \perp X_{[n]\setminus \mathcal{N}_i(W)\cup \{i\}} \mid X_{\mathcal{N}_i(W)}, \quad \forall i \in [n],$$

where $\mathcal{N}_i(W) = \{j \in [n] : W_{ij} = 1\}$ is the set of neighbors of vertex $i$ in $W$. In other words, the distribution of $X_i$ can only be directly affected by other entries of $X$ that are connected
to $i$ in the underlying graph $W$. We assume that the columns of $B$ are independent and identically distributed with distribution $F$, denoted by $B_1, \ldots, B_m \sim F$, where $B_k \in \mathbb{R}^n$ represents the $k$-th column of $B$, and we write the likelihood of $B$ as

$$f(B) := \prod_{k=1}^{m} f_X(B_k). \quad (2.2)$$

If the graphical model $W$ is known, the (exact) graph matching problem in the MRF model just introduced can be formulated as finding the unshuffling permutation $P$ that aligns $A$ and $W$. In practice, however, $W$ is unobserved and some estimation process needs to be incorporated into the graph matching formulation. To make the problem more tractable, we focus in a subclass of graphical models in which the conditional distribution of each node can be expressed as a generalized linear model (GLM) (McCullagh and Nelder, 1989; Yang et al., 2012). For a vector $X \sim F$, the conditional distribution of $X_i = x_i$ given the rest of the variables is expressed as

$$f_X(x_i | x_{[n]\setminus\{i\}}) \propto \exp \left( \beta_i x_i + \sum_{j \in \mathcal{N}_i(W)} \Theta_{ij} x_i x_j - 2 \Theta_{ii} C(x_i) \right), \quad (2.3)$$

where $C(\cdot)$ is a known function, and $\gamma, \beta \in \mathbb{R}^n$ and $\Theta \in \mathbb{R}^{n \times n}$ are parameters of the model. Because of the local Markov property, only the entries $(i, j)$ of $\Theta$ for which $W_{ij} = 1$ participate in the model, so by imposing the constraint

$$\Theta_{ij}(1 - W_{ij}) = 0, \quad i, j \in [n], i \neq j, \quad (2.4)$$

the likelihood of the model for a given $x \in \mathbb{R}^n$ can be expressed as

$$f_X(x) \propto \exp \left( \beta^T x + \sum_{i \neq j} \Theta_{ij} x_i x_j - 2 \sum_{i=1}^{n} \Theta_{ii} C(x_i) \right). \quad (2.5)$$

This MRF framework allows us to model different edge distributions in the bipartite graph, and in this paper we focus on two special cases.

- **Binary Bernoulli distribution.** The Ising model (Ising, 1925) is popularly used in modeling binary-valued data. The distribution of this model can be obtained by setting $C(X_i) = 0$, in which case, the node-wise distribution in Equation (2.3) takes the form of a logistic regression model, and the joint distribution of a binary random vector $X$ taking a value $x \in \{0, 1\}^n$ is

$$P(X = x) := \frac{1}{Z(\Theta, \beta)} \exp \left( \sum_{i=1}^{n} \beta_i x_i + \sum_{i \neq j} \Theta_{ij} x_i x_j \right), \quad (2.6)$$

where $Z(\Theta, \beta)$ is the partition function or normalizing constant, given by

$$Z(\Theta, \beta) := \sum_{y \in \{0, 1\}^n} \exp \left( \sum_{i=1}^{n} \beta_i y_i + \sum_{i \neq j} \Theta_{ij} y_i y_j \right). \quad (2.7)$$
The above expression requires the calculation of the sum over all the possible elements in \( \{0, 1\}^n \), which has cardinality \( 2^n \), and hence it is not computable for a general \( \Theta \). It is therefore sometimes more convenient to work with the pseudo-likelihood (Bhattacharyya and Mukherjee, 2018; Ravikumar et al., 2010), which is defined as the product of the conditional likelihoods of each variable, given by

\[
\tilde{f}_X(x) = \prod_{i=1}^{n} \left( \frac{1}{1 + \exp(-x_i (\beta_i + \sum_{i \neq j} \Theta_{ij} x_j))} \right) . \tag{2.8}
\]

- **Weighted Gaussian distribution.** By setting \( C(X_i) = X_i^2 \), the entries of \( X \) can be modeled using a multivariate Gaussian distribution via a Gaussian graphical model (Speed and Kiiveri, 1986). The matrix \( \Theta \) is required to be positive definite, denoted by \( \Theta \succ 0 \), so \( \Theta^{-1} \) is a proper covariance matrix. Set \( \mu = \Theta^{-1} \beta \). The likelihood of the model is given by

\[
f_X(x) = (2^n \pi^n \det \Theta^{-1})^{-1/2} \exp\left( -\frac{1}{2} (x - \mu)^T \Theta (x - \mu) \right) , \tag{2.9}
\]

and this matrix is constrained to satisfy Equation (2.4) and \( \Theta \succ 0 \).

Having defined the distribution of the edges in the bipartite graph, we now proceed to formulate the graph matching problem in this setting. The model imposes constraints in \( \Theta \) that depend on \( W \) according to Equation (2.4), and this matrix \( W = (P^*)^T A P^* \) is a function of the unknown permutation \( P^* \). Therefore, it is natural to define the solution of the graph matching problem as the permutation matrix \( \hat{P} \) that constrains the zero-entries of the matrix \( \Theta \) in such a way that it produces the best fit to the bipartite graph \( B \) over all possible permutations \( P \in \Pi_n \). The fit to the data can be measured using a loss function \( \hat{\ell}(\Theta, \beta) \), such as the log-likelihood of \( B \)

\[
\hat{\ell}(\Theta, \beta) = \frac{1}{m} \sum_{k=1}^{m} \left( \beta^T B_k + \sum_{i \neq j} \Theta_{ij} B_{ik} B_{jk} - 2 \sum_{i=1}^{n} \Theta_{ii} C(B_{ik}) \right) - \log(Z(\Theta, \beta)), \tag{2.10}
\]

and the graph matching problem from a unipartite to a bipartite graph can then be defined as

\[
(\hat{P}, \hat{\Theta}, \hat{\beta}) = \arg\max_{P, \Theta, \beta} \hat{\ell}(\Theta, \beta) \\
\text{subject to } \Theta_{ij}(1 - (P^T A)_{ij}) = 0, \quad i \neq j, \tag{2.11}
\]

\[
P \in \Pi_n, \quad \Theta \in \mathbb{R}^{n \times n}, \quad \beta \in \mathbb{R}^n .
\]

The variables \( \Theta \) and \( \beta \) are nuisance parameters for graph matching, but as a by-product, this problem formulation also produces estimates for these parameters in the model.

### 2.2 Inexact graph matching

In the previous formulation, we assumed that the edges of \( A \) and the underlying graphical model for \( B \) can be perfectly matched, so, in a sense, the formulation of the graph matching problem in Equation (2.11) corresponds to an exact matching. In some situations, the
edges of \( A \) are noisy, and the correspondence with the edges of \( W \) might not be exact. To account for this noise, the graph \( A \) can be modeled as an errorful observation of the underlying unshuffled graph \( P^* W (P^*)^T \), in which the edges are independently perturbed with some probability \( p \in [0, 1] \). Given \( p, W \) and \( P \), the likelihood of an adjacency matrix \( A \in \{0, 1\}^{n \times n} \) can be written as

\[
P(A) = \prod_{i > j} (1 - p)^{1 \{A_{ij} = (PWP^T)_{ij}\}} p^{1 \{A_{ij} \neq (PWP^T)_{ij}\}}.
\]

By taking logarithms and arranging the terms, the log-likelihood can be written in a form that is more akin to the classical graph matching formulation (2.1), given by

\[
\ell_A(W, P) = \log(p) \sum_{i > j} 1 \{A_{ij} \neq (PWP^T)_{ij}\} + \log(1 - p) \sum_{i > j} 1 \{A_{ij} = (PWP^T)_{ij}\}
\]

\[
= -\lambda_p \|A - PWP^T\|_F^2 + c_p,
\]

with \( \lambda_p = \log((1 - p)/p) \) and \( c_p = \log(1 - p)n(n - 1)/2 \). The constraint (2.4) can be used here to relate \( \Theta \) and \( W \), and the graph matching problem is

\[
(\hat{P}, \hat{\Theta}, \hat{\beta}) = \arg \max_{P, \Theta, \beta} \ell(\Theta, \beta) - \lambda_p \|A - PWP^T\|_F^2
\]

subject to

\[
W_{ij} = 1 \{\Theta_{ij} \neq 0\}, \quad i \neq j,
\]

\[
P \in \Pi_n, \quad \Theta \in \mathbb{R}^{n \times n}, \quad \beta \in \mathbb{R}^n.
\]

In this formulation, the edge perturbation probability \( p \) can be seen as a penalty parameter that controls how similar the edges of the network \( A \) and the graphical model \( W \) are. Formulations (2.11) and (2.12) are very similar, and in fact equivalent when \( p = 0 \). Next, we present methods to approximate the solution of Equation (2.11), but these can be extended to approximate the solution of formulation (2.12).

3 Solving the unipartite to bipartite matching problem

Under the graphical model for the bipartite network described before, the graph matching problem seeks to match the edges of \( A \) with the non-zero entries of the graphical model for \( B \). In principle, one can approach this matching problem by first collapsing the bipartite graph into an estimator of \( \Theta \) or the set of edges of the graphical model \( \{(i, j) : \Theta_{ij} \neq 0\} \), and then matching the vertices of this estimator—which can be represented as a (weighted) unipartite graph—with the graph \( A \). Estimating the edges of an undirected graphical model is a well studied problem, and multiple existing methods have addressed this estimation from different perspectives, both for discrete (Ravikumar et al., 2010; Yang et al., 2012; Bresler, 2015) and continuous (Meinshausen and Bühlmann, 2006; Banerjee et al., 2008; Friedman et al., 2008; Rothman et al., 2008) graphical models. Although this two step procedure can succeed in some situations, there are multiple challenges that discourage this approach. Finding an accurate estimator of the edge set of a graphical model might require a large amount of signal, and the error induced by this noisy estimate can significantly affect the matching performance. In addition, methods require conditions on the topology of the graph that do not always hold (Bento and Montanari, 2009; Loh and Wainwright,
yielding those estimators inconsistent in some circumstances. Often, there are tuning parameters involved in this estimation process, such as $\ell_1$ regularization approaches for variable selection, and choosing the right model can be a complicated task (Meinshausen and Bühlmann, 2010).

In contrast, our approach to matching the vertices of graphs $A$ and $B$ is based on finding an approximate solution to the optimization problem (2.11). This is motivated by the following theorem, which is a consequence of the consistency of the maximum likelihood estimator in Markov random fields (see for example Wainwright and Jordan (2008)).

**Theorem 1.** Let $A \in \{0,1\}^{n \times n}$ be the adjacency matrix of a simple unipartite graph, and let $B^{(m)} \in \mathbb{R}^{n \times m}$ be a random adjacency matrix with its columns distributed as i.i.d. samples from the Ising model or the Gaussian graphical model, with $\Theta^* \in \mathbb{R}^{n \times n}$ with bounded entries, $\beta^* \in \mathbb{R}^n$ and $P^* \in \Pi_n$ the parameters of the model such that Equation (2.4) holds for $W = (P^*)^T A P^*$. Let $\hat{P}_m$ be a solution of (2.11). Suppose that (i) $\ell^*(\Theta, \beta) := E[\ell(\Theta, \beta)]$ has a unique minimizer at $(\Theta^*, \beta^*)$ and (ii) $\Theta^* \not= 0$ for all $(i, j)$ with $W_{ij} = 1$. Then, as $m \rightarrow \infty$,

$$
\|\hat{P}_m^T A \hat{P}_m - (P^*)^T A P^*\|_F \overset{P}{\rightarrow} 0.
$$

If $A$ does not have non-identity automorphisms, then $\hat{P} \overset{P}{\rightarrow} P^*$ as $m \rightarrow \infty$.

**Proof.** First, let us assume that $\beta = 0$ in the model (2.5). Then, the empirical log-likelihood for a value of $m$ is given by

$$
\hat{\ell}_m(\Theta) := \frac{1}{m} \sum_{k=1}^m \left( \sum_{i \neq j} \Theta_{ij} B_{ik} B_{jk} - 2 \sum_{i=1}^n \Theta_{ii} C(B_{ik}) \right) - \log(Z(\Theta)),
$$

with $Z(\Theta)$ the partition function. Note that the log-likelihood function here is concave because the model belongs to the exponential family.

Define $\hat{\Theta}_m := \arg\max_{\Theta} \hat{\ell}(\Theta)$, and $\hat{\Theta}_{P,m} := \arg\max_{\Theta} \hat{\ell}(\Theta)$ subject to $\Theta_{ij} (1 - (P^T A)_{ij}) = 0$. To apply Theorem 5.2.2 of Bickel and Doksum (2015) in order to show consistency of $\hat{\Theta}_{P*,m}$ and $\hat{\Theta}_m$, we observe that the normalizing constant in Equation (2.5) is finite for any $\Theta \in \mathbb{R}^{n \times n}$ for both the Ising model and the multivariate Gaussian distribution, so the natural parameter space is open. In addition, the restriction in the optimization problem enforces the structure of $\hat{\Theta}_{P*,m}$, to have zero entries in the same places as $\Theta^*$, so the effective parameters are the non-zero entries of $\Theta^*$. Therefore, the estimators $\hat{\Theta}_{P*,m}$ and $\hat{\Theta}_m$ are consistent for $\Theta^*$. By the weak law of large numbers, $\frac{1}{m} \sum_{k=1}^m B_{ik} B_{jk} \rightarrow E[B_{i1} B_{j1}]$, and hence, by continuity of the function $Z(\Theta)$, $\hat{\ell}_m(\hat{\Theta}_m) \overset{P}{\rightarrow} \ell^*(\Theta^*)$ and $\hat{\ell}_m(\hat{\Theta}_{P*,m}) \overset{P}{\rightarrow} \ell^*(\Theta^*)$.

Now, suppose that there exists sequences $\{m_k\}_{k=1}^\infty \subset \mathbb{N}$ and $\{P_{mk}\}_{k=1}^\infty$ such that for each $m_k$, the solution of (2.11) for $\hat{\ell}_{m_k}$ is $P_{mk}$. Because $\Pi_n$ is finite, there exists a permutation $\bar{P}$ for which $\bar{P} = P_{mk}$ for infinitely many values of $k$. This permutation should satisfy

$$
\hat{\ell}_{m_k}(\hat{\Theta}_{mk}) \geq \hat{\ell}_{m_k}(\hat{\Theta}_{P,m_k}) \geq \hat{\ell}_{m_k}(\hat{\Theta}_{P*,m_k}).
$$

The left inequality is a consequence of the optimality of $\hat{\Theta}_{mk}$ in the unrestricted problem, while the right inequality is the assumption in the definition of $\bar{P}$. Hence, $\hat{\ell}_{m_k}(\hat{\Theta}_{P,m_k}) \overset{P}{\rightarrow} \ell^*(\Theta^*)$. The sequence of functions $\{\hat{\ell}_m\}$ and $\ell^*$ are concave (Theorem 1.6.3 of Bickel et al. 2013; Bresler, 2015), yielding those estimators inconsistent in some circumstances.
in addition to the linearity w.r.t. Θ in Equation (3.1)). This implies that for any compact set \( K \subset \mathbb{R}^{m \times n} \), \( \hat{\ell}_m \) converges uniformly in probability to \( \ell^* \) in \( K \) (Theorem II.1 of Andersen and Gill (1982)). Taking \( K_{\Theta^*} \) such that \( \Theta^* \) is in the interior of \( K_{\Theta^*} \), condition (i) implies that \( \lim P(\hat{\Theta}_{P,m} \in \text{int}(K_{\Theta^*})) = 1 \), and therefore the uniform convergence implies that \( \hat{\Theta}_{P,m} \xrightarrow{P} \Theta^* \). Since \( \hat{\Theta}_{ij}^*(1(\tilde{T}^T A \hat{P})_{ij}) = 0 \), condition (ii) guarantees that \( \hat{P}^T A \hat{P} = (P^*)^T A P^* \). This is valid for any \( P \) that appears infinitely many times on \( \{P_{m_k}\} \), which implies the result.

The last statement of the theorem trivially holds because if \( A \) does not have non-identity automorphisms then \( \tilde{P} = P^* \) is the only solution for \( P \) in \( \hat{P}^T A \hat{P} = (P^*)^T A P^* \). The proof for the case in which \( \beta \neq 0 \) follows mutatis mutandis.

The previous theorem shows that the optimal permutation \( \tilde{P} \) that solves (2.11) converges in probability to a permutation in the automorphism group of \( A \), and when this group contains a unique element then it also converges to the correct unshuffling permutation. One implication of this theorem is that regardless of the topology of the graph, this solution can guess the edges of the graphical model correctly, as opposed to the naive approach outlined before (Bento and Montanari, 2009). Unfortunately, solving this optimization problem requires searching over all elements in \( \Pi_n \), a discrete set of cardinality \( n! \), which is computationally infeasible. Nevertheless, the space of all possible undirected graphical models has a size \( 2^{n(n-1)/2} \), that is orders of magnitude larger than \( |\Pi_n| \), which suggests that graphical model estimation is a harder problem than graph matching in this context. We focus on finding an approximate solution to this problem next.

### 3.1 Profile likelihood

In light of Theorem 1, solving problem (2.11) provides a principled heuristic for aligning the vertices of \( A \) to those in \( W \). Given this, our model also offers some insights into when collapsing \( B \) onto \( W \) is justified. Recall the collapsed graph \( \tilde{B} = \frac{1}{m} BB^T \) previously defined, which counts the number of common neighbors between every pair of vertices in \( W \). Under a restricted Ising model, solving the bipartite–to–unipartite matching problem (2.11) is equivalent to a unipartite matching between \( A \) and \( \tilde{B} \), as shown next.

**Theorem 2.** Suppose that in the Ising model for the bipartite graph defined in Equation (2.5), the parameters satisfy \( \beta = 0 \) and \( \Theta_{ij} = \theta_0 \mathbf{1}\{(P^*)^T A P^*\}_{ij} = 1 \) for all \( i, j \in [n] \), \( i \neq j \), with \( \theta_0 \in \mathbb{R} \), and the graph \( A \) is non-empty. Define \( \hat{P}_{\text{MLE}} \) and \( \hat{\theta}_{\text{MLE}} \) as the maximum likelihood estimators for \( \theta_0 \) and \( P^* \). We then have that

\[
\hat{P}_{\text{MLE}} = \begin{cases} 
\arg\max_{P \in \Pi_n} \text{Tr}(P^T A \tilde{B}) = \arg\min_{P \in \Pi_n} ||A - P \tilde{B} P^T||_F^2, & \text{if } \hat{\theta}_{\text{MLE}} > 0, \\
\arg\min_{P \in \Pi_n} \text{Tr}(P^T A \tilde{B}) = \arg\max_{P \in \Pi_n} ||A - P \tilde{B} P^T||_F^2, & \text{if } \hat{\theta}_{\text{MLE}} < 0, \\
\text{any } P \in \Pi_n, & \text{if } \hat{\theta}_{\text{MLE}} = 0.
\end{cases}
\]  

**Proof.** Under the assumptions of the theorem, the expression of the log-likelihood can be
simplified via
\[
\hat{\ell}_m(\theta, P) = \frac{1}{m} \sum_{k=1}^{m} \left[ \theta \sum_{i \neq j} (P^T A P)_{ij} B_{ik} B_{ij} - \log Z(\theta) \right]
\]
\[= \theta \text{Tr} \left( P^T A \hat{B} \right) - \Psi(\theta),
\]
where \(\Psi(\theta) := Z(\theta) = \log \left( \sum_{u \in U} \exp(\theta u) \right)\) is the corresponding log-partition function with \(U = \{ y^T A y : y \in \{0, 1\}^n \}\). Observe that \(\Psi(\theta)\) does not depend on \(P\).

Define \(\hat{\theta}_P\) as the profile MLE of \(\theta\) given \(P \in \Pi_n\), i.e.,
\[
\hat{\theta}_P = \arg\max_{\theta \in \mathbb{R}} \hat{\ell}(\theta, P).
\]

By taking a derivative of the log-likelihood and equating to zero, the profile MLE satisfies
\[
\text{Tr} \left( P^T A \hat{B} \right) = \frac{d\Psi(\theta)}{d\theta} \bigg|_{\theta = \hat{\theta}_P} = \frac{\sum_{u \in U} u \exp(u \hat{\theta}_P)}{Z(\hat{\theta}_P)}.
\]

The last equation is an increasing function of \(\hat{\theta}_P\). To observe that, we show that the second derivative of \(\Psi(\theta)\) is positive. This is given by
\[
\frac{d^2\Psi(\theta)}{d\theta^2} = \frac{Z(\theta) \left[ \sum_{u \in U} u^2 \exp(u \theta) \right] - \left( \sum_{u \in U} u \exp(u \theta) \right) \left( \sum_{v \in U} v \exp(v \theta) \right)}{(Z(\theta))^2}
\]
\[= \sum_{u,v} \frac{1}{2} (u - v)^2 \left[ \exp(u \theta) \exp(v \theta) \right] \geq 0,
\]
and it is only equal to zero when \(u = v\) for all \(u, v \in U\), which implies that \(A = 0\). Hence, the second derivative of \(\Psi(\theta)\) is strictly positive.

Using Equation (3.3), the MLE for \(P\) is
\[
\hat{P}_{\text{MLE}} = \arg\max_{P \in \Pi_n} \hat{\ell}(\hat{\theta}_P, P)
\]
\[= \arg\max_{P \in \Pi_n} \left\{ \hat{\theta}_P \left. \frac{d\Psi(\theta)}{d\theta} \right|_{\theta = \hat{\theta}_P} - \Psi(\hat{\theta}_P) \right\}.
\]

Observe that the previous objective function only depends on \(\hat{\theta}_P\). Moreover, the derivative of this function with respect to \(\hat{\theta}_P\) is equal to
\[
\hat{\theta}_P \left. \frac{d^2\Psi(\theta)}{d\theta^2} \right|_{\theta = \hat{\theta}_P}.
\]
When \(\hat{\theta}_{\text{MLE}} = \hat{\theta}_{\hat{P}_{\text{MLE}}}\) is positive, this derivative is greater than 0, and \(\hat{P}_{\text{MLE}}\) is chosen via
\[
\hat{P}_{\text{MLE}} = \arg\max_{P \in \Pi_n} \text{Tr} \left( P^T A \hat{B} \right) = \arg\min_{P \in \Pi_n} \|A - P \hat{B} P^T\|_F^2.
\]
To see this, consider the existence of a $P$ such that
\[ \text{Tr} \left( P^T A \hat{B} \right) > \text{Tr} \left( \hat{P}_{\text{MLE}}^T A \hat{P}_{\text{MLE}} \hat{B} \right). \]

Then from Equation (3.3), $0 < \hat{\theta}_{\text{MLE}} < \hat{\theta}_P$ and
\[ \ell(\hat{\theta}_P, P) > \ell(\hat{\theta}_{\text{MLE}}, \hat{P}_{\text{MLE}}) \]
yielding the desired contradiction. Analogously, when $\hat{\theta}_P$ is negative, the derivative of Equation (3.4) is negative, and hence the MLE for $P$ is obtained via
\[ \hat{P}_{\text{MLE}} = \arg\min_{P \in \Pi_n} \text{Tr} \left( P^T A \hat{B} \right) = \arg\max_{P \in \Pi_n} \| A - P \hat{B} P^T \|_F^2. \]

Finally, if $\hat{\theta}_{\text{MLE}} = 0$, then $\hat{\theta}_P = 0$ for all $P$ (by considering the contradiction present for $\hat{\theta}_P \neq 0$ from Equation (3.3)). Therefore, any $P$ achieves the optimum value in Equation .

We note that the equivalence in Theorem 2 is only true under a restricted model framework, and that $\hat{B}$ and $W$ need not be related to each other, even for large $m$. This further complicates solving the optimization problem (3.1) in practice.

### 3.2 Matching via inverse covariance estimation

Computing the likelihood of the bipartite graph is challenging because the calculation of the partition function is infeasible for some distributions, including for the Ising model. For a Gaussian graphical model however, the likelihood takes a simpler form, as observed in Equation (2.9), and the MLE for $\mu$ is $\hat{\mu} = \frac{1}{m} \sum_{k=1}^m B_k$ (with $B_k$ being row $k$ of $B$), which does not depend on $P$, so the log-likelihood of the bipartite graph can be expressed only in terms of $\Theta$ as
\[ \hat{\ell}(\Theta) = \log \det \Theta - \text{Tr}(\hat{\Sigma} \Theta), \]
where $\hat{\Sigma} = \frac{1}{m} \sum_{k=1}^m (B_k - \hat{\mu})(B_k - \hat{\mu})^T$ is the sample covariance of the rows of the bipartite incidence matrix (see for example (Friedman et al., 2008)). The bipartite–to–unipartite matching problem constrains $\Theta$ to satisfy $\Theta_{ij}(1 - (P^T A)_{ij}) = 0$ for $i, j \in [n]$.

Solving the graph matching optimization problem for both $P$ and $\Theta$ is computationally infeasible due to the combinatorial constraint set. On the other hand, if some $P$ is fixed, finding the profile MLE for $\Theta$, denoted as $\hat{\Theta}_P$, is a convex optimization problem and therefore can be solved efficiently. Using this profile MLE, the fit of different permutations can be compared by evaluating $\hat{\ell}(\hat{\Theta}_P)$.

To find an approximate solution of (2.11) for both $P$ and $\Theta$, we relax the graph matching problem by replacing $P \in \Pi_n$ with a real-valued matrix $D \in \mathcal{D}_n$, where $\mathcal{D}_n$ denotes the set of $n \times n$ doubly stochastic matrices $\mathcal{D}_n = \{ D \in \mathbb{R}^{n \times n} : D 1_n = D^T 1_n = 1, D_{ij} \geq 0 \}$. This is effectively relaxing the permutation search space to its convex hull (Vogelstein et al., 2014). Additionally, the equality constraints in (2.11) are replaced with a penalty function (Nocedal and Wright, 2006) with a penalty parameter $\lambda > 0$. We choose a non-smooth penalty based on the $\ell_1$-norm to induce a sparse solution. The new optimization problem then becomes
\[ \left( \hat{D}(\lambda), \hat{\Theta}(\lambda) \right) = \arg\max_{D, \Theta} \left\{ \log \det \Theta - \text{Tr}(\hat{\Sigma} \Theta) - \lambda \sum_{i \neq j} \left| (1 - (D^T A)_{ij}) \Theta_{ij} \right| \right\} \]
subject to $D \in \mathcal{D}_n$, $\Theta \in \mathbb{R}^{n \times n}$, $\Theta \succ 0$. 

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The optimization problem above is closely related to lasso penalized problems for estimating the inverse covariance in a Gaussian graphical model (Banerjee et al., 2008; Friedman et al., 2008; Rothman et al., 2008). In particular, for a fixed \( D = \frac{1}{n}1_n1_n^T \) (so no prior information about the correct matching is given) all off-diagonal entries of \( \Theta \) are equally penalized. On the other hand, if \( D = P^* \), only the entries of \( \Theta \) for which \( \Theta_{ij}^* = 0 \) are penalized, which potentially results in better estimation of the graphical model when the matching of the vertices is performed correctly.

In order to solve (3.8), we use an alternating minimization strategy by fixing \( D \) or \( \Theta \), and solve the resulting problem to obtain a sequence of estimators \( \{ (\hat{D}(t,\lambda), \hat{\Theta}(t,\lambda)) \}_{t=1}^{T^*} \). We iterate this until a maximum number of iterations \( T^* \) is reached. The initialization value is set to \( \hat{D}(1,\lambda) = \frac{1}{n}1_n1_n^T \). Optimizing \( \Theta \) with a fixed \( \hat{D}(t,\lambda) \) requires to solve a problem analogous to the graphical lasso, given by

\[
\hat{\Theta}(t,\lambda) = \arg\max_{\Theta \succ 0} \left\{ \log \det \Theta - \text{Tr}(\hat{\Sigma}\Theta) - \lambda \sum_{i \neq j} \omega_{ij}^{(t,\lambda)}|\Theta_{ij}| \right\},
\]

with \( \omega_{ij}^{(t,\lambda)} = 1 - (\hat{D}(t,\lambda)^T A\hat{D}(t,\lambda))_{ij} \). This is a convex optimization problem that can be efficiently solved by the method presented in Friedman et al. (2008) and implemented in the \texttt{glasso} R package. Optimizing \( D \) given a fixed \( \hat{\Theta}(t,\lambda) \) results in a non-convex quadratic assignment problem

\[
\hat{D}(t,\lambda) = \arg\min_{D \in \mathcal{D}_n} \text{Tr} \left( D^T A|\hat{\Theta}(t,\lambda)| \right),
\]

with \( |\hat{\Theta}(t,\lambda)| \) the entrywise absolute value operator. We solve the problem above using the Fast Approximate Quadratic assignment problem (FAQ) algorithm (Vogelstein et al., 2014; Lyzinski et al., 2016), which uses the Frank-Wolfe methodology to obtain an approximate local minimizer of (3.10), and then projects \( \hat{D}(t,\lambda) \) onto the set of permutations \( \Pi_n \) to obtain a permutation \( \hat{P}(t,\lambda) \). This is implemented with the \texttt{iGraphMatch} package (https://github.com/dpmcsuss/iGraphMatch). The alternating minimization is repeated until the solution has converged (measured by the change in the loss function (3.7) between consecutive iterations) or \( T^* \) iterations have been reached. The parameter \( \lambda \) controls the sparsity of the solution in (3.9). To select an appropriate value, we repeat the procedure for a sequence of values \( \lambda_1, \ldots, \lambda_{S^*} \), resulting in a set of solutions \( \{ \hat{P}(t,\lambda), t \in [T^*], s \in [S^*] \} \). The optimal permutation among this set is chosen by calculating the value of the loss function \( \hat{\ell}(\hat{P}_s) \) in Equation (3.7). This process is summarized in Algorithm 1.

The method outlined above can be understood as a matching between the optimal permutation and the non-zero elements of the population inverse covariance matrix of the rows of \( B \). In a Gaussian distribution, this non-zero elements actually coincide with the edges of the undirected graphical model for \( B \). This is not necessarily the case in non-Gaussian distributions, but penalized inverse covariance estimators sometimes still produce accurate results for estimating undirected graphical models even in those cases Banerjee et al. (2008); Loh and Wainwright (2013), and thus the matching solution can potentially succeed. Alternatively, another approach based on the appropriate distribution of the data is described next.
Algorithm 1 Unipartite to bipartite matching via penalized inverse covariance estimation

Input: Adjacency matrix $A$, incidence matrix $B$.

for each $\lambda \in \{\lambda_s\}_{s=1}^{S^*}$ do
  Initialize $\hat{D}^{(1,\lambda)} = \frac{1}{n}1_n1_n^T$.
  for $t = 1, \ldots, T^*$, or until convergence do
    Update $\hat{\Theta}^{(t,\lambda)}$ by solving (3.9).
    Update $\hat{D}^{(t+1,\lambda)}$ by solving (3.10).
    Set $\hat{P}^{(t+1,\lambda)}$ as the projection of $\hat{D}^{(t,\lambda)}$ into $\Pi_n$.
  end for
end for

Choose the permutation with the smallest value of $\hat{\ell}(\hat{\Theta}\hat{P})$ among the permutations $P \in \{P^{(t,\lambda_s)}, s \in [S^*], t \in [T^*]\}$.

Output: Permutation $\hat{P}$, inverse covariance estimate $\hat{\Theta}\hat{P}$.

3.3 A pseudo-likelihood approach

Because of the intractability of the likelihood, an alternative approach is to substitute the loss function of problem (2.11) with the pseudo-likelihood. We follow a similar procedure as in the previous section to obtain an approximate solution to the pseudo-likelihood problem. The method in this section is outlined for an Ising model, but the same approach can be followed for other distributions.

The log-pseudo-likelihood of the bipartite graph for an Ising model is given by

$$\tilde{\ell}(\Theta, \beta) = \sum_{j=1}^{n} \left\{ \sum_{k=1}^{m} - \log \left( 1 + \exp \left[ -B_{jk}(\beta_j + B_k^T\Theta_j) \right] \right) \right\},$$

(3.11)

with $\Theta \in \mathbb{R}^{n \times n}$, $\text{diag}(\Theta) = 0$, $\beta \in \mathbb{R}^{n}$, $\Theta_j$ indicates the $j$-th column of $\Theta$ and $\beta_j$ indicates the $j$-th entry of $\beta$. As before, given a fixed value of $P$, the profile pseudo-likelihood estimators $\hat{\Theta}_P$ and $\hat{\beta}_P$ can be numerically obtained via convex optimization to compute $\tilde{\ell}(\hat{\Theta}_P, \hat{\beta}_P)$.

To find an approximate solution for $P$ in maximizing (3.11), we follow the same process as in the previous section, by relaxing $P$ to be a doubly stochastic matrix and replacing the constraints with a penalty term. This results in an optimization problem analogous to (3.8), with the inclusion of the variable $\beta$, and with $\Theta \in \mathbb{R}^{n \times n}$ only constrained to have zeros in the diagonal. The alternating optimization proceeds by maximizing $(\Theta, \beta)$ and $D$. Given a fixed value $\hat{D}^{(t,\lambda)}$, the resulting problem for $(\Theta, \beta)$ can be split into $n$ separate problems for $(\Theta_j, \beta_j), j \in [n]$, given by

$$(\hat{\Theta}_j^{(t,\lambda)}, \hat{\beta}_j^{(t,\lambda)}) = \arg\max_{\Theta_j \in \mathbb{R}^{n}, \beta_j \in \mathbb{R}} \left\{ -\log \left( 1 + \exp \left[ -B_{jk}(\beta_j + B_k^T\Theta_j) \right] \right) - \lambda \sum_{i=1}^{n} \omega_{ij}^{(t,\lambda)}|\Theta_{ij}| \right\},$$

(3.12)

with $\Theta_{jj} = 0$. The optimization above is a lasso penalized logistic regression (Friedman et al., 2010), and the solution is implemented using the glmnet R package (Friedman et al., 2009). Algorithm 2 summarizes the process for estimating $P$ with the pseudolikelihood loss function.
Algorithm 2 Unipartite to bipartite matching via penalized pseudolikelihood

Input: Adjacency matrix $A$, incidence matrix $B$.

for each $\lambda \in \{\lambda_s\}_{s=1}^{S^*}$ do
  Initialize $\hat{D}(1,\lambda) = \frac{1}{n}1_n1_n^T$.
  for $t = 1, \ldots, T^*$, or until convergence do
    for $j = 1, \ldots, n$ do
      Update $(\hat{\Theta}_j^{(t,\lambda)}, \hat{\beta}_j^{(t,\lambda)})$ by solving (3.12).
    end for
    Update $\hat{D}(t+1,\lambda)$ by solving (3.10).
    Set $\hat{P}(t+1,\lambda)$ as the projection of $\hat{D}(t,\lambda)$ into $\Pi_n$.
  end for
end for

Choose the permutation with the smallest value of $\tilde{\ell}(\hat{\Theta}_{\hat{P}})$ among $P \in \{P^{(t,\lambda)}, s \in [S^*], t \in [T^*]\}$.

Output: Permutation $\hat{P}$, estimated parameters $\hat{\Theta}_{\hat{P}}$ and $\hat{\beta}_{\hat{P}}$.

3.4 Seeded graph matching

In some applications, a partial alignment of the vertices is known a priori, and the goal is to match the remaining vertices. This setting is known as seeded graph matching, and vertices with a known correspondence are referred as seeds. The methods we developed can incorporate seed vertices by adapting the Frank-Wolfe methodology of FAQ to incorporate seeds as in Lyzinski et al. (2014); Fishkind et al. (2019). Without loss of generality, assume that the first $n_1 < n$ are seed vertices, and let $R \in \Pi_{n_1}$ be the corresponding permutation that unshuffles the seeded vertices. The seeded graph matching problem can then be formulated in an analogous way as problem (2.11) with the additional constraint that $P_{ij} = R_{ij}$ for $i, j \in [n_1]$, and $P_{ij} = 0$ for $i \in [n_1], j \in [n] \setminus [n_1]$ or $j \in [n_1], i \in [n] \setminus [n_1]$. These restrictions can then be used in the initialization of the algorithms 1 and 2 for $D^{(1,\lambda)}$, and in the quadratic assignment problem (3.10), which can be approximately solved via the SGM algorithm of Fishkind et al. (2019).

4 Simulations

The accuracy of the proposed methods is evaluated in synthetic data. Given a graph $A$ (with a distribution that will be specified), the columns of the bipartite graph $B$ follow the Ising model distribution (2.6). The number of common nodes in the graphs is set to $n = 100$ while varying $m$, the nodes that are only in the bipartite graph. The value of the parameters is set to $\Theta_{ij}^* = 0.4$ for all $(i, j)$ for which $A_{ij} = 1$, and $\mu_i = -1/2 \sum_{j=1}^{n} \Theta_{ij}^*$ for $i \in [n]$ to make the marginal distributions of the rows of $B$ approximately the same. The graph $A$ is generated using two different models:

* Chain graph: Given the ordering of the vertices according to the rows and columns of the adjacency matrix, each vertex is connected by an edge to its adjacent neighbor, such that $A_{ij} = A_{ji} = 1$ for $i \in [n - 1]$ and $j = i + 1$,

* Erdős-Rényi (ER) graph: The edges of $A$ are independent Bernoulli random vari-
ables with $P(A_{ij} = 1) = 0.05$ for $i > j$.

In the first scenario with a chain graph, the simple dependency structure usually facilitates the estimation of the edges in the graphical model, but the regularity of the structure makes vertex matching a hard task since only a few errors in estimating the edges of $A$ can destroy the identifiability of the vertex order. On the contrary, the long-range correlations in the ER graph make graphical model estimation a harder problem (Bento and Montanari, 2009), but vertex matching is an easier task due to the irregular structure of $A$ (Arroyo et al., 2018).

In addition to the bipartite matching methods introduced in Algorithms 1 (B-InvCov) and 2 (B-Pseudo), we measure the performance of unipartite matching between $A$ and a collapsing of $B$ to an $n \times n$ matrix. These collapsing methods include the one-mode projection $\tilde{B}$ (C-OMP), the sample covariance matrix $\hat{\Sigma}$ of the rows of $B$ (C-Cov), and estimates of the edges of the graphical model for $B$ based on the graphical lasso (C-GLasso) and the method of Meinshausen and Bühlmann (2006) (C-M&B). To implement the last two estimators, we use the R package huge (Zhao et al., 2012), and the parameter tuning is done with the default options of this package. Given a bipartite graph collapsing, graph matching between $A$ and the collapsed graph is performed with the FAQ algorithm (Vogelstein et al., 2014). In Algorithms 1 and 2, we set the maximum number of iterations $T^*$ as 20, and the grid for the tuning parameter $\lambda$ contains $S^* = 10$ values logarithmically spaced between $10^{-2.5}$ and $10^{-0.5}$.

The methods result in an estimator $\hat{P} \in \Pi_n$ of the true unshuffling permutation $I_n$. We measure the vertex matching error as $\frac{1}{n^2} \| \hat{P} - I_n \|_F^2$, which counts the percentage of vertices incorrectly matched, and the edge matching error as the percentage of incorrect edges $\frac{1}{2 |A|_F^2} \| A - \hat{P}^T A \hat{P} \|_F^2$. In addition, some methods provide an estimate $\hat{W}$ of the edges of the undirected graphical model $W = P^T A P$. For Algorithms 1 and 2 this is given by the non-zero pattern of the estimated $\hat{\Theta}_{\hat{P}}$. The accuracy of $\hat{W}$ is measured using the edge false positive and false negative rates, defined as

$$\text{FPR} = \frac{\sum_{i > j} 1(\hat{W}_{ij} = 1) 1(W_{ij} = 0)}{\sum_{i > j} 1(W_{ij} = 0)}, \quad \text{FNR} = \frac{\sum_{i > j} 1(\hat{W}_{ij} = 0) 1(W_{ij} = 1)}{\sum_{i > j} 1(W_{ij} = 1)}.$$  

These errors are measured on 30 different Monte Carlo simulations of each scenario for different values of $m$.

The average matching and estimation errors across all the Monte Carlo simulations are shown in Figures 4.1 and 4.2. In general, methods improve their performance as $m$ grows, both for matching and graphical model estimation, although collapsing methods based on covariance or one-mode projection do not show a noticeable improvement. Our bipartite methods have a superior performance in graph matching with respect to collapsed matching methods. Among those, only the methods based in graphical model estimation show a decent performance for large $m$, when the edge set of the graphical model is accurately estimated as shown in Figure 4.2. The results of this figure also suggest by the performance of our methods that the knowledge of $A$, up to some permutation, does reduce the graphical model learning error in the ER graph scenario, where this problem is harder.

5 Evaluation on real networks

We next explore the application of our methodology on two real-data network pairs.
Figure 4.1: Graph matching percentage error for different methods and unipartite graph models. Our methods show superior performance than matching the collapsed bipartite graph.
Figure 4.2: Error in estimating the graphical model of the bipartite graph. All methods show a good control of false positives, but for small sample sizes our bipartite matching algorithms present better edge discovery due to the knowledge of $A$. 
5.1 Co-authorship network and paper-authorship networks

The co-authorship and citation networks between statisticians (Ji et al., 2016) contain data from scientific papers in some of the most popular journals in statistics. We use these data to construct a co-authorship unipartite graph and a bipartite graph between authors and papers cited by them (Figure 1.1), and then evaluate the performance of our approach in matching the authors when they are anonymized across the two graphs.

The original data consists of a unipartite directed graph of the citations between \( m' = 3248 \) papers, and a bipartite graph that indicates authorship of those papers by their corresponding \( n' = 3608 \) authors. Based on these data, we constructed two graphs as follows:

- **Co-authorship graph.** For every pair of authors in the list, two authors are connected if they have published a paper together, resulting in a matrix \( A' \in \{0, 1\}^{n' \times n'} \).

- **Author-citation network.** A matrix \( B' \in \{0, 1\}^{n' \times m'} \) encodes a bipartite network between authors and papers, in which each author is connected to the papers that the author has cited.

To select a substantial subset of vertices with enough information for performing graph matching, vertices with low or high degree were removed as follows. First, the authors that have cited at least 10 papers on the list were selected. Second, in the resulting subgraph of \( A' \), authors that have degrees larger than 1 and smaller than 10 were chosen. Next, the largest connected component of the resulting subgraph of \( A' \) was chosen. Finally, vertices for which rows in \( B' \) are co-linear were discarded. After these steps, the resulting graphs \( A \) and \( B \) have \( n = 161 \) shared vertices that represent the number of authors, and \( m = 1109 \) vertices representing the papers.

The performance of different algorithms is compared in a similar way as in Section 4. We include seeded vertices (on the \( x \)-axis, we have the fraction of randomly chosen seeds), and we perform seeded graph matching, measuring the vertex and edge matching errors in the subgraph induced by the unseeded vertices. For each fraction of seeds considered, the process of selecting random vertices as seeds is repeated 10 times and results are averaged over these 10 iterates; results are summarized in Figure 5.1. Most methods perform similarly well in terms of vertex matching, and overall the performance improves as more seeds are present, which is expected. While exact vertex matching is hard due to the presence of low degree vertices, our methods show superior performance in terms of edge matching, especially when the number of seeds is not very large. Note that the C-M&B method of Meinshausen and Bühlmann (2006) usually results in a very sparse estimated graph due to the difficulty of parameter selection, which explains the poor performance.

5.2 MRI data

Functional activation patterns in the brain have been linked to the structural connectivity, which constraints co-activation patterns in different brain regions (Abdelnour et al., 2014; Meier et al., 2016). Assuming the existence of such relation, we use our matching algorithm to identify the mapping between brain regions in the structural connectivity and the functional activation time series data.

The HNU1 data (Zuo et al., 2014) contains magnetic resonance imaging (MRI) brain scans from multiple healthy subjects. A post-processed version of these data was obtained
Figure 5.1: Graph matching error in the co-authorship graph (Ji et al., 2016) as a function of the fraction of seeds. Exact vertex matching is hard due to the small degree of the vertices, but our algorithms show a superior performance in edge matching.

from https://neurodata.io/mri/, computed with NeuroData’s MR to graphs package (ndmg) (Kiar et al., 2018). The data consists of diffusion MRI (dMRI) derived brain networks of each testing subject (computed with version v0.0.048 of ndmg), and functional MRI (fMRI) time series of blood oxygenation level-dependent (BOLD) signals on each subject (computed with version v0.0.1f). We use data from the first scan of the first subject in the dataset, and employ the DS00140 parcellation, composed of $n = 139$ brain regions. Only a subset of those brain regions is present (123 for the dMRI network and 129 for the fMRI time series), and the mapping between those regions is unknown to us. The data is encoded into a $139 \times 139$ binary matrix representing the dMRI graph, and a matrix of size $139 \times 291$ representing the BOLD measurements on $m = 291$ time steps. The entries for the unobserved regions were filled with zeros, and the time series of the region were centered and standardized by brain region.

We use our graph matching method based on inverse covariance (Algorithm 1) to find the mapping between the brain regions in the dMRI graph (Figure 5.2a) and the fMRI measurements. Despite the dependency across time in the fMRI measurements, the graphical lasso is often used to infer the functional dependence between different brain regions (Narayan et al., 2015). This estimate is shown in Figure 5.2b, with the rows and columns ordered according to the estimated permutation from our algorithm. Overall, the edges with the strongest signals in the GLasso estimate correspond with edges in the dMRI network. Figure 5.2c shows the estimate of the graphical model for the fMRI measurements obtained by Algorithm 1, which enforces the graphical structure of the dMRI network after the vertex matching has been estimated. If the graph alignment has been performed correctly, and the edges of the dMRI and fMRI graphs coincide, the estimate of the inverse covariance obtained by our algorithm should be more accurate than the graphical lasso, which does
Figure 5.2: Structural connectivity graph (left) and estimates of the inverse covariance of the fMRI data (center and right) from a scan of the subject in the HNU1 dataset. Brain regions in the fMRI plots are ordered according to the matching solution obtained by Algorithm 1. Edge weights in the fMRI graphs are larger for edges in the dMRI graph.

not use the information on the dMRI network.

6 Conclusion

Network data is ubiquitous. While multiple methodologies have been developed to analyze this type of data, most of the studies have focused on the unipartite graph setting. More complex data structures often cannot be fully represented with unipartite graphs, and in practice, information is commonly discarded or collapsed in order to adapt the data to the existing methodologies. In this paper we have shown that from the graph matching perspective, collapsing the graph into a unipartite network is not always the right approach and can often fail. However, addressing the problem with methods tailored for the specific data yield significant gains in accuracy. More complex data designs, such as vertex or edge attributes, missing data, multilayer networks, among others, present new challenges in network analysis, and we are working to adapt our approach to these more complex settings.

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