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Seeded Graph Matching for Correlated Erdős-Rényi Graphs

Vince Lyzinski VLYZINS1@JHU.EDU
Human Language Technology Center of Excellence
Johns Hopkins University
Baltimore, MD, 21218, USA

Donniell E. Fishkind DEF@JHU.EDU
Carey E. Priebe CEP@JHU.EDU
Department of Applied Mathematics and Statistics
Johns Hopkins University
Baltimore, MD, 21218, USA

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Abstract

Graph matching is an important problem in machine learning and pattern recognition. Herein, we present theoretical and practical results on the consistency of graph matching for estimating a latent alignment function between the vertex sets of two graphs, as well as subsequent algorithmic implications when the latent alignment is partially observed. In the correlated Erdős-Rényi graph setting, we prove that graph matching provides a strongly consistent estimate of the latent alignment in the presence of even modest correlation. We then investigate a tractable, restricted-focus version of graph matching, which is only concerned with adjacency involving vertices in a partial observation of the latent alignment; we prove that a logarithmic number of vertices whose alignment is known is sufficient for this restricted-focus version of graph matching to yield a strongly consistent estimate of the latent alignment of the remaining vertices. We show how Frank-Wolfe methodology for approximate graph matching, when there is a partially observed latent alignment, inherently incorporates this restricted-focus graph matching. Lastly, we illustrate the relationship between seeded graph matching and restricted-focus graph matching by means of an illuminating example from human connectomics.

Keywords: graph matching, Erdős-Rényi graph, consistency, estimation, seeded vertices, Frank-Wolfe, assignment problem

1. Background and Overview

The graph matching problem (GMP)—i.e., finding the alignment between the vertices of two graphs which best preserves the structure of the graphs—has a rich and active place in the literature. Graph matching has applications in a wide variety of disciplines, including machine learning (Cour et al., 2007; Liu and Qiao, 2012; Fiori et al., 2013), computer vision (Cho et al., 2009; Cho and Lee, 2012; Zhou and De la Torre, 2012), pattern recognition (Berg et al., 2005; Caelli and Kosinov, 2004), manifold and embedded graph alignment (Robles-Kelly and Hancock, 2007; Xiao et al., 2009), shape matching and object recognition (Huet et al., 1999), and MAP inference (Leordeanu et al., 2009), to name a few.

There are no efficient algorithms known for solving graph matching exactly. Even the easier problem of just deciding if two graphs are isomorphic is notoriously of unknown complexity (Garey and Johnson, 1979; Read and Corneil, 1977). Indeed, graph matching is a special case of the NP-hard quadratic assignment problem and, if the graphs are allowed to be directed, loopy, and weighted, then graph matching is actually equivalent to the quadratic assignment problem. Because of its practical applicability, there is a vast amount of literature devoted to approximate graph matching algorithms; for an interesting survey of the literature, see e.g., "Thirty Years of Graph Matching in Pattern Recognition" by Conte et al. (2004).

In the presence of a latent alignment function between the vertex sets of two graphs, it is natural to ask how well graph matching would mirror this underlying alignment. In Section 2.2 we describe the correlated Erdős-Rényi random graph, which provides us with a useful and natural setting to explore this question. The correlated Erdős-Rényi random graph consists of two Erdős-Rényi random graphs which share a common vertex set and a common Bernoulli-trial probability parameter; for each pair of vertices, there is a given correlation between the two vertices' adjacency in one graph and the two vertices' adjacency in the other graph. In this manner, there is a natural latent alignment between the two graphs, and we can then explore whether or not graph matching the two graphs will consistently estimate this alignment.

If $\Phi : V(G_1) \mapsto V(G_2)$ is the latent alignment function between the vertex sets of two graphs, we define a vertex $v \in V(G_1)$ to be *mismatched* by graph matching if there exists a solution ψ to the graph matching problem such that $\Phi(v) \neq \psi(v)$. The graph matching problem provides a *consistent* estimate of Φ if the number of mismatched vertices goes to zero in probability as $|V(G_1)|$ tends to infinity, and provides a *strongly consistent* estimate of Φ if the number of mismatched vertices converges to zero almost surely as $|V(G_1)|$ tends to infinity.

The first of our main results is Theorem 1, stated in Section 2.2 and proven in Appendix A. For correlated Erdős-Rényi random graphs, under mild assumptions, Theorem 1.i establishes that even very modest correlation is sufficient for graph matching to yield a strongly consistent estimate of the latent alignment; this expands and strengthens the important results in Pedarsani and Grossglauser (2011). Theorem 1.ii provides a partial converse; for very weakly correlated graphs, we prove that the expected number of permutations that align the graph more effectively (i.e., with fewer induced edge disagreements) than the latent alignment goes to infinity as the number of vertices tends to infinity. Unfortunately, since there is no known efficient algorithm for graph matching, Theorem 1.i doesn't in-of-itself provide a means of efficient graph alignment. However, it does suggest that efficient approximate graph matching algorithms may be successful in graph alignment when there is correlation between the graphs above the threshold given in Theorem 1.i.

Next, in Section 2.3, we discuss the seeded graph matching problem. This is a graph matching problem for which part of the bijection between the two graphs' vertices is prespecified and fixed, and we seek to complete the bijection so as to minimize the number of edge disagreements between the graphs; in our correlated Erdős-Rényi graph setting, the seeds are taken from the existing latent alignment. Also in Section 2.3, we describe a restricted-focus version of the graph matching problem in the context of seeding; this is a problem wherein we seek the bijection between the two seeded graphs' vertices that mini-

mizes *only the number of seeded vertex to nonseeded vertex edge disagreements* between the two seeded graphs. Restricting the focus of graph matching in this particular fashion enables this restricted-focus graph matching problem to be efficiently solved as a linear assignment problem, in contrast to the algorithmic difficulty of (unrestricted) graph matching.

Our second main result is Theorem 2, which we state in Section 2.4 and prove in Appendix A. For correlated Erdős-Rényi graphs, under mild assumptions, Theorem 2.i asserts that a logarithmic number of seeds is sufficient for restricted-focus graph matching to yield a strongly consistent estimate of the latent alignment function. Theorem 2.ii again provides a partial converse; for very weakly correlated graphs, we prove that the expected number of permutations that align the unseeded vertices more effectively (i.e., with fewer induced seeded vertex to nonseeded vertex edge disagreements) than the latent alignment goes to infinity as the number of vertices tends to infinity. Now, what should we do if we want to perform graph alignment and there are seeds, but the number of seeds is below this logarithmic threshold? The remainder of this paper deals with that situation.

Back in the setting where there are no seeds, an important class of approximate graph matching algorithms utilize a Frank-Wolfe approach; the idea is more formally described later in Section 3. To briefly describe here, such methods relax an integer programming formulation of graph matching to obtain a continuous problem, then perform an iterative procedure in which a linearization about the current iterate is optimized, and the next iterate comes from a line search between the current iterate and the linearization optimum. At the conclusion of the iterative procedure, the final iterate is projected to the nearest integer-valued point which is feasible as a graph match, and this is taken as the approximate graph matching solution. It turns out that the linear optimization done in each iteration can be formulated as a linear assignment problem, which can be solved efficiently, and this makes the Frank-Wolfe approach an appealing method in terms of speed. The Frank-Wolfe approach can also be a very accurate method for approximate graph matching as well; see Brixius and Anstreicher (2001); Vogelstein et al. (2011); Zaslavskiy et al. (2009) for Frank-Wolfe methodology and variants.

As done in Fishkind et al. (2012), we describe in Section 3.2 how this Frank-Wolfe methodology for approximate graph matching is naturally and seamlessly extended to the setting of seeded graph matching so as to perform approximate seeded graph matching. In analyzing Frank-Wolfe methodology for approximate seeded graph matching, we observe in Section 3.3 that each Frank-Wolfe iteration involves optimizing a sum of two terms. Restricting this optimization to just the first of these two terms turns out to be precisely solving the aforementioned restricted-focus graph matching problem, and restricting this optimization to just the second of these two terms turns out to be precisely the Frank-Wolfe methodology step if the seeds are completely ignored.

We conclude this paper with simulations and a real-data example from human connectomics. These simulations and experiments illuminate the relationship between seeded graph matching via Frank-Wolfe and restricted-focus graph matching via the Hungarian algorithm. We demonstrate that Frank-Wolfe methodology is often superior to restricted-focus graph matching, an unsurprising result as the Frank-Wolfe methodology merges restricted-focus graph matching with seedless Frank-Wolfe methodology. Perhaps more surprising, we also demonstrate the capacity for restricted-focus graph matching to outper-

form the full Frank-Wolfe methodology; in these cases, the noise in the unseeded adjacency can actually degrade overall performance!

2. Graph Matching, Random Graph Setting, Main Results

In this paper, all graphs will be simple graphs; in particular, edges are undirected, there are no edges with a common vertex for both endpoints, and there are no multiple edges between any pair of vertices. We will define $\mathcal{G}_n$ to be the set of simple graphs on n vertices. If $G \in \mathcal{G}_n$, we will denote the vertex set of G as $V(G)$ and the edge set of G via $E(G)$. For any $v, v' \in V(G)$, if v and v' are adjacent in G then this will be denoted $\{v, v'\} \in E(G)$, and if v and v' are not adjacent in G then this will be denoted $\{v, v'\} \notin E(G)$. For any finite set V, the symbol $\binom{V}{2}$ will denote all of the $\binom{n}{2}$ unordered pairs of distinct elements from V.

2.1 The Graph Matching Problem

We now describe the graph matching problem. Suppose G_1 and G_2 are graphs with the same number of vertices. Let $\mathit{\Pi}$ denote the set of bijections $V(G_1) \to V(G_2)$. For any $\psi \in \mathit{\Pi}$, the *number of adjacency disagreements induced by* ψ, which will be denoted $\Delta(\psi)$, is the number of vertex pairs $\{v, v'\} \in \binom{V(G_1)}{2}$ such that $[\{v, v'\} \in E(G_1)$ and $\{\psi(v), \psi(v')\} \notin E(G_2)]$ or $[\{v, v'\} \notin E(G_1)$ and $\{\psi(v), \psi(v')\} \in E(G_2)]$. The *graph matching problem* is to find a bijection in $\mathit{\Pi}$ that minimizes the number of induced edge disagreements; we will denote the set of solutions $\Psi := \arg\min_{\psi \in \mathit{\Pi}} \Delta(\psi)$. Equivalently stated, if $n := |V(G_1)| = |V(G_2)|$, and if $A, B \in \{0,1\}^{n \times n}$ are the respectively the adjacency matrices for G_1 and G_2, then the graph matching problem is to minimize $\|A - PBP^T\|_F$ over all n-by-n permutation matrices P, where $\|\cdot\|_F$ is the Frobenius matrix norm.

There are no efficient algorithms known for graph matching. Even the easier problem of just deciding if G_1 is isomorphic to G_2 (i.e., deciding if there is a bijection $V(G_1) \to V(G_2)$ which does not induce any edge disagreements) is of unknown complexity (Garey and Johnson, 1979; Read and Corneil, 1977), and is a candidate for being in an intermediate class strictly between P and NP-complete (if P$\neq$NP). Also, the problem of minimizing $\|A - PBP^T\|_F$ over all n-by-n permutation matrices P, where A and B are any real-valued matrices, is equivalent to the NP-hard quadratic assignment problem. There are numerous approximate graph matching algorithms in the literature; in Section 3 we will discuss Frank-Wolfe methodology.

2.2 Correlated Erdős-Rényi Random Graphs

Presently, we describe the correlated Erdős-Rényi random graph; this will provide a theoretical framework within which we will prove our main theorems, Theorem 1 and Theorem 2.

The parameters are a positive integer n, a real number p in the interval $(0, 1)$, and a real number ϱ in the interval $[0, 1]$; these parameters completely specify the distribution. There is an underlying vertex set V of cardinality n which is common to two graphs; call these graphs G_1 and G_2. For each $i = 1, 2$ and each pair of vertices $\{v, v'\} \in \binom{V}{2}$, let $\mathbb{1}\{\{v, v'\} \in E(G_i)\}$ denote the indicator random variable for the event $\{v, v'\} \in E(G_i)$. For each $i = 1, 2$ and each pair of vertices $\{v, v'\} \in \binom{V}{2}$, the random variable $\mathbb{1}\{\{v, v'\} \in E(G_i)\}$

is Bernoulli(p) distributed, and they are all collectively independent except that, for each pair of vertices $\{v, v'\} \in \binom{V}{2}$, the variables $\mathbb{1}\{\{v, v'\} \in E(G_1)\}$ and $\mathbb{1}\{\{v, v'\} \in E(G_2)\}$ have Pearson product-moment correlation coefficient ϱ. At one extreme, if ϱ is 1, then G_1 and G_2 are equal, almost surely, and at the other extreme, if ϱ is 0, then G_1 and G_2 are independent. After G_1 and G_2 are thus realized, their vertices are (separately) arbitrarily relabeled, so that we don't directly observe the *latent alignment function (bijection)* $\Phi : V(G_1) \to V(G_2)$ wherein, for all $v \in V(G_1)$, the vertices v and $\Phi(v)$ were corresponding vertices across the graphs before the relabeling (i.e., the same element of V).

If G_1 is graph matched to G_2, to what extent will the graph match provide a consistent estimate of the latent alignment function? The following Theorem is our first main result. We will be considering a sequence of random correlated Erdős-Rényi graphs with $n = 1$, then $n = 2$, then $n = 3 \ldots$, and the parameters p and ϱ are each functions of n; i.e., $p := p(n)$ and $\varrho := \varrho(n)$. In this paper, when we say a sequence of events holds *almost always*, we mean that, with probability 1, all but a finite number of the events hold.

Theorem 1 *Suppose there exists a fixed real number $\xi_1 < 1$ such that $p \leq \xi_1$. Then there exists fixed positive real numbers c_1, c_2, c_3, c_4 (depending only on the value of ξ_1) such that:*
i) If $\varrho \geq c_1\sqrt{\frac{\log n}{np}}$ and $p \geq c_2\frac{\log n}{n}$ then almost always $\Psi = \{\Phi\}$, and
ii) If $\varrho \leq c_3\sqrt{\frac{\log n}{n}}$ and $p \geq c_4\frac{\log n}{n}$ then $\lim_{n\to\infty} \mathbb{E}|\{\psi \in \Pi : \Delta(\psi) < \Delta(\Phi)\}| = \infty$.

For proof of Theorem 1, see Appendix A.

Note that Theorem 1.i establishes the strong consistency of the graph matching estimate of the latent alignment function in the presence of even modest correlation between G_1 and G_2. This theorem is a strengthening and an extension of the pioneering work on de-anonymizing networks in Pedarsani and Grossglauser (2011), wherein the authors proved a weaker version of Theorem 1.i in a sparse setting (in particular they require both p and ϱ to converge to 0 at rate $p\varrho^3 = O(log(n)/n)$). Note that range of values of p for which Theorem 1.i applies includes both the sparse and the dense regimes.

Because there is no known efficient algorithm for graph matching, Theorem 1.i does not directly provide a practical means of computing the latent alignment function. But it does hold out the hope that a good graph matching heuristic might be effective in approximating the latent alignment function for various classes of graphs.

When proving Theorems 1 and 2, it will be useful for us to observe an equivalent way to formulate correlated Erdős-Rényi graphs. For all pairs of vertices $\{v, v'\} \in \binom{V}{2}$, the indicator random variables $\mathbb{1}\{\{v, v'\} \in E(G_1)\}$ are independently distributed Bernoulli(p) and then (independently for the different pairs v, v'), conditioning on $\mathbb{1}\{\{v, v'\} \in E(G_1)\} = 1$, we let $\mathbb{1}\{\{v, v'\} \in E(G_2)\}$ be distributed Bernoulli($p + \varrho(1 - p)$) and, conditioning on $\mathbb{1}\{\{v, v'\} \in E(G_1)\} = 0$, we let $\mathbb{1}\{\{v, v'\} \in E(G_2)\}$ be distributed Bernoulli($p(1 - \varrho)$). It is an easy exercise to verify that as such, for each $\{v, v'\} \in \binom{V}{2}$, it holds that $\mathbb{1}\{\{v, v'\} \in E(G_2)\}$ is distributed Bernoulli(p), and that the correlation of $\mathbb{1}\{\{v, v'\} \in E(G_1)\}$ and $\mathbb{1}\{\{v, v'\} \in E(G_2)\}$ is ϱ, as desired.

2.3 Seeded Graph Matching, Restricted-focus Graph Matching

Continuing with the setting from Section 2.1, suppose that we are also given a subset $U_1 \subseteq V(G_1)$ of *seeds* and an injective *seeding function* $\phi : U_1 \to V(G_2)$, say that $U_2 \subseteq V(G_2)$ is the image of ϕ. Let Π_ϕ denote the set of bijections $\psi : V(G_1) \to V(G_2)$ such that for all $u \in U_1$ it holds that $\psi(u) = \phi(u)$. As before, for any bijection $\psi \in \Pi_\phi$, the *number of adjacency disagreements induced by* ψ, which will be denoted $\Delta(\psi)$, is the number of vertex pairs $\{v, v'\} \in \binom{V(G_1)}{2}$ such that $[\{v, v'\} \in E(G_1)$ and $\{\psi(v), \psi(v')\} \notin E(G_2)]$ or $[\{v, v'\} \notin E(G_1)$ and $\{\psi(v), \psi(v')\} \in E(G_2)]$. The *seeded graph matching problem* is to find a bijection in Π_ϕ that minimizes the number of induced edge disagreements; as before, we will denote the set of solutions $\Psi := \arg\min_{\psi \in \Pi_\phi} \Delta(\psi)$. Equivalently stated, suppose without loss of generality that $U_1 = U_2 = \{v_1, v_2, \ldots, v_s\}$, and that for all $j = 1, 2, \ldots, s$, $\phi(v_j) = v_j$; with A and B denoting the adjacency matrices for G_1 and G_2 respectively, the seeded graph matching problem is to minimize $\|A - (I \oplus P)B(I \oplus P)^T\|_F$ over all m-by-m permutation matrices P, where $m := |V(G_1)| - s$, and $\oplus$ is the direct sum, and I is the s-by-s identity matrix.

Like graph matching, there are no efficient algorithms known for seeded graph matching; in fact, seeded graph matching is at least as difficult as graph matching. In Section 3.2 we discuss how Frank-Wolfe methodology extends to provide efficient approximate seeded graph matching.

We now present a restricted version of seeded graph matching which is efficiently solvable, in contrast to graph matching and seeded graph matching. Let $W_1 := V(G_1) \backslash U_1$ denote the nonseeds in $V(G_1)$. For any $\psi \in \Pi_\phi$, let $\Delta_R(\psi)$ denote the number of pairs $(w, u) \in W_1 \times U_1$ such that $[\{w, u\} \in E(G_1)$ and $\{\psi(w), \psi(u)\} \notin E(G_2)]$ or $[\{w, u\} \notin E(G_1)$ and $\{\psi(w), \psi(u)\} \in E(G_2)]$. The *restricted-focus seeded graph matching problem* (RGM) is to find a bijection in Π_ϕ which minimizes such seed-nonseed adjacency disagreements; denote the set of solutions $\Psi_R := \arg\min_{\psi \in \Pi_\phi} \Delta_R(\psi)$. Equivalently stated, if the adjacency matrices for G_1 and G_2 are respectively partitioned as

$$A = \begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix}, \text{ and } B = \begin{pmatrix} B_{11} & B_{21}^T \\ B_{21} & B_{22} \end{pmatrix}$$

where $A_{21}, B_{21} \in \mathbb{R}^{|W_1| \times |U_1|}$ each represent the adjacencies between the nonseed vertices and the seed vertices (and the seed vertices are ordered in A_{11} conformally to B_{11}), then finding a member of Ψ_R is accomplished by minimizing $\|A_{21} - PB_{21}\|_F$ over all $|W_1| \times |W_1|$ permutation matrices P. Expanding,

$$\begin{aligned} \|A_{21} - PB_{21}\|_F^2 &= \text{trace}(A_{21} - PB_{21})^T(A_{21} - PB_{21}) \\ &= \text{trace}A_{21}^T A_{21} - \text{trace}A_{21}^T PB_{21} - \text{trace}B_{21}^T P^T A_{21} + \text{trace}B_{21}^T P^T PB_{21} \\ &= \|A_{21}\|_F^2 + \|B_{21}\|_F^2 - 2 \cdot \text{trace}\left(P^T(A_{21}B_{21}^T)\right) \quad , \end{aligned} \tag{1}$$

thus finding a member of Ψ_R is accomplished by maximizing $\text{trace}P^T A_{21}B_{21}^T$ over all $|W_1| \times |W_1|$ permutation matrices P. This is a linear assignment problem and can be exactly solved in $O(|W_1|^3)$ time with the Hungarian Algorithm (Edmonds and Karp, 1972; Kuhn, 2006). So, whereas finding a member of Ψ is intractable, finding a member of Ψ_R

can done efficiently. An important question is how well Ψ_R approximates Ψ. Slightly abusing notation, we shall refer to both the restricted-focus graph matching problem and the associated algorithm for exactly solving it by RGM.

2.4 Seeded, Correlated Erdős-Rényi Graphs

Seeded, correlated Erdős-Rényi graphs are correlated Erdős-Rényi graphs G_1 and G_2 where part of the latent alignment function is observed; specifically, there is a subset of seeds $U_1 \subseteq V(G_1)$ such that Φ is known on U_1. If we take ϕ to be the restriction of Φ to U_1 and we run RGM, we may hope that $\Psi_R = \{\Phi\}$; if this hope is true then we are provided an efficient means of computing the latent alignment function.

The next theorem is another of our main results. We will be considering a sequence of random correlated Erdős-Rényi graphs where the number of nonseed vertices is $m = 1$, then $m = 2$, then $m = 3 \ldots$, and the number of seeds s is a function of m.

Theorem 2 *Suppose there exists a fixed real number $\xi_2 > 0$ such that $\xi_2 \leq p \leq 1 - \xi_2$ and $\xi_2 \leq \varrho \leq 1 - \xi_2$. Then there exists fixed real numbers $c_5, c_6 > 0$ (depending only on ξ_2) such that:*
i) If $s \geq c_5 \log m$ then almost always $\Psi_R = \{\Phi\}$, and
ii) If $s \leq c_6 \log m$ then $\lim_{m\to\infty} \mathbb{E}|\{\psi \in \Pi_\phi : \Delta_R(\psi) < \Delta_R(\Phi)\}| = \infty$.

For proof of Theorem 2, see Appendix A.

Note that Theorem 2.i establishes that RGM provides a strongly consistent estimate of the latent alignment in the presence of a logarithmic number of seeds. As noted, a member of Ψ_R is efficiently computable, and thus Theorem 2 (unlike Theorem 1) directly provides a means to efficiently recover the latent alignment bijection Φ, if there are enough seeds.

3. The SGM Algorithm: Extending Frank-Wolfe Methodology for Approximate Graph Matching to Include Seeds

In the setting with no seeds, there are numerous approximate graph matching algorithms in the literature. One such algorithm is the FAQ algorithm of Vogelstein et al. (2011), which is an efficient, state-of-the-art approximate graph matching algorithm based on Frank-Wolfe methodology. The algorithm's performance is empirically shown to be state-of-the-art on many benchmark problems, and when a fixed constant number of Frank-Wolfe iterations are performed, the running time of FAQ is $O(n^3)$, where n is the number of vertices to be matched. Moreover, if $100 \leq |V(G_1)|$ and G_1 is selected with a discrete-uniform distribution (i.e., all possible graphs on $V(G_1)$ are equally likely) and G_2 is an isomorphic copy of G_1 with $V(G_2)$ being a discrete-uniform random permutation of $V(G_1)$, then the probability that FAQ (with, say, 20 Frank-Wolfe iterations allowed) yields the correct isomorphism is empirically observed to be very nearly 1. We choose to focus on the FAQ algorithm here because of its amenability to seeding and because it is the simplest algorithm utilizing the Frank-Wolfe methodology while also achieving excellent performance on many of the QAP benchmark problems; see Vogelstein et al. (2011).

In Section 3.2, we describe the SGM algorithm from Fishkind et al. (2012), which extends the Frank-Wolfe methodology to incorporate utilization of seeds in approximate

seeded graph matching. In Section 3.3 we point out that each Frank-Wolfe iteration in SGM involves optimizing a sum of two terms. Restricting this optimization to just the first of these two terms turns out to be precisely the optimization of RGM from Section 2.3, and restricting this optimization to just the second of these two terms turns out to be precisely the corresponding optimization step of FAQ (i.e., the seeds are completely ignored).

We conclude with simulations and real data experiments that illuminate the relationship between SGM and RGM. SGM can be superior to RGM matching, unsurprising in that SGM makes use of the unseeded adjacency information while RGM does not. Perhaps more surprisingly, we also demonstrate the capacity for RGM to outperform SGM in the presence of very informative seeds; in these case the unseeded connectivity is detrimental to overall algorithmic performance!

3.1 The Frank-Wolfe Algorithm and Frank-Wolfe Methodology

First, a brief review of the Frank-Wolfe algorithm: The general optimization problem that the Frank-Wolfe algorithm is applied to is maximize $f(x)$ such that $x \in S$, where S is a polyhedral set in a Euclidean space, and the function $f : S \to \mathbb{R}$ is continuously differentiable. The Frank-Wolfe algorithm is an iterative procedure. A starting point $x^{(1)} \in S$ is chosen in some fashion, perhaps arbitrarily. For $i = 1, 2, 3, \ldots$, a Frank-Wolfe iteration consists of maximizing the first order (i.e., linear) approximation to f about $x^{(i)}$, that is maximize $f(x^{(i)}) + \nabla f(x^{(i)})^T(x - x^{(i)})$ over $x \in S$, call the solution $y^{(i)}$ (of course, this is equivalent to maximizing $\nabla f(x^{(i)})^T x$ over $x \in S$), then $x^{(i+1)}$ is defined to be the solution to maximize $f(x)$ over x on the line segment from $x^{(i)}$ to $y^{(i)}$. Terminate the Frank-Wolfe algorithm when the the sequence of iterates $x^{(1)}, x^{(2)}, \ldots$ (or their respective objective function values) stops changing much.

Of course, the seeded graph matching problem is a combinatorial optimization problem and, as such, the Frank-Wolfe algorithm cannot be directly applied. The term *Frank-Wolfe methodology* will refer to the approach in which the integer constraints are relaxed so that the domain is a polyhedral set and the Frank-Wolfe algorithm can be directly applied to the relaxation and, at the termination of the Frank-Wolfe algorithm, the fractional solution is projected to the nearest feasible integer point. It is this projected-to point that is adopted as an approximate solution to the original combinatorial optimization problem. We next describe the SGM algorithm, which applies Frank-Wolfe methodology to the Seeded Graph Matching Problem.

3.2 The SGM Algorithm

We now describe the SGM algorithm for approximate seeded graph matching.

Suppose G_1 and G_2 are graphs, say $V(G_1) = \{v_1, v_2, \ldots, v_n\}$ and $V(G_2) = \{v'_1, v'_2, \ldots, v'_n\}$, and let A and B be the respective adjacency matrices of G_1 and G_2. Suppose without loss of generality that $U_1 = \{v_1, v_2, \ldots, v_s\}$ are seeds, and the seeding function $\phi : U_1 \to V(G_2)$ is given by $\phi(v_i) = v'_i$ for all $i = 1, 2, \ldots, s$. Denote the number of nonseed vertices $m := n - s$. Let A and B be partitioned

$$A = \begin{bmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} B = \begin{bmatrix} B_{11} & B_{21}^T \\ B_{21} & B_{22} \end{bmatrix}$$

where A_{11}, $B_{11} \in \{0,1\}^{s\times s}$, A_{22}, $B_{22} \in \{0,1\}^{m\times m}$, and $A_{21}, B_{21} \in \{0,1\}^{m\times s}$.

As mentioned in Section 2.3, the seeded graph matching problem is precisely to minimize $\|A - (I \oplus P)B(I \oplus P)^T\|_F^2 = \|A\|_F^2 + \|B\|_F^2 - 2 \cdot \text{trace}A^T(I \oplus P)B(I \oplus P)^T$ over all m-by-m permutation matrices P. Clearly, the seeded graph matching problem is equivalent to maximizing the quadratic function $\text{trace}A^T(I \oplus P)B(I \oplus P)^T$ over all m-by-m permutation matrices P.

Relax this maximization of $\text{trace}A^T(I \oplus P)B(I \oplus P)^T$ over all m-by-m permutation matrices P to the maximization of $\text{trace}A^T(I \oplus P)B(I \oplus P)^T$ over all m-by-m *doubly stochastic* matrices P (which form a polyhedral set), and then the Frank-Wolfe algorithm can be applied directly to the relaxation. Simplification yields the objective function

$$\begin{aligned} f(P) &= \text{trace}A_{11}B_{11} + \text{trace}A_{21}^T P B_{21} + \text{trace}A_{21}B_{21}^T P^T + \text{trace}A_{22}PB_{22}P^T \\ &= \text{trace}A_{11}B_{11} + 2 \cdot \text{trace}P^T A_{21}B_{21}^T + \text{trace}A_{22}PB_{22}P^T \end{aligned} \quad (2)$$

which has gradient

$$\nabla(P) = 2 \cdot A_{21}B_{21}^T + 2 \cdot A_{22}PB_{22}.$$

We start the Frank-Wolfe algorithm at an arbitrarily selected doubly stochastic m-by-m matrix $P^{(1)}$; for convenience we use the "barycenter" matrix $P^{(1)}$ with all entries equal to $\frac{1}{m}$. Then, for successive $i = 1, 2, \ldots$, the Frank-Wolfe iteration is to maximize the inner product of P with the gradient of f at $P^{(i)}$ over all m-by-m doubly stochastic matrices matrices P; this maximization problem is (ignoring a benign factor of 2) maximizing trace $P^T(A_{21}B_{21}^T + A_{22}P^{(i)}B_{22})$ over m-by-m doubly stochastic matrices. This is a linear assignment problem since the optimal P in this subproblem must be a permutation matrix (by the Birkhoff-von Neumann Theorem which states that the m-by-m doubly stochastic matrices are precisely the convex hull of the m-by-m permutation matrices), and this linear assignment problem can be solved efficiently with the Hungarian Algorithm in $O(m^3)$ time. Say the optimal value of P in this subproblem is $Y^{(i)}$; then, the function f on the line segment from $P^{(i)}$ to $Y^{(i)}$ is a quadratic that is easily maximized exactly, with $P^{(i+1)}$ defined as the doubly stochastic matrix attaining this maximum.

When the Frank-Wolfe iterates $P^{(1)}, P^{(2)}, P^{(3)}, \ldots$ stop changing much (or a constant maximum of iterations are performed—we allowed 20 iterations), then the Frank-Wolfe algorithm terminates; let the resultant approximate solution to the relaxed problem is the doubly stochastic matrix Q. The final step is to project Q to the nearest m-by-m permutation matrix. Minimizing $\|P - Q\|_F$ over permutation matrices P is again a linear assignment problem solvable in $O(m^3)$ time; indeed, minimizing

$$\|P - Q\|_F^2 = \|P\|_F^2 - 2\text{trace}P^T Q + \|Q\|_F^2$$

is equivalent to maximizing trace $P^T Q$ over permutation matrices P. This optimal permutation matrix P is adopted as the approximate solution to the seeded graph matching problem. Specifically, the algorithm output is the bijection $\psi : V(G_1) \to V(G_2)$ where, for $i = 1, 2, \ldots, s$, $\psi(v_i) = v'_i$ and, for each $i = 1, 2, \ldots, m$, $\psi(v_{s+i}) = v'_{s+j}$ for the j such that $P_{ij} = 1$. This Frank-Wolfe Methodology approach described above is called the *SGM algorithm*.

When there are no seeds, the SGM algorithm is exactly the FAQ algorithm of Vogelstein et al. (2011); the above development is a seamless extension of the Frank-Wolfe methodology for approximate graph matching when there are no seeds to Frank-Wolfe methodology for approximate seeded graph matching.

The running time for the SGM algorithm, like for the FAQ algorithm, is $O(n^3)$. This is because of the linear assignment problem formulation and the use of the Hungarian algorithm in each Frank-Wolfe iteration, and is a huge savings over using the simplex method or an interior point method for solving the linearizations in each Frank-Wolfe iteration. This trick has made Frank-Wolfe methodology a very potent weapon for efficient approximate graph matching.

3.3 Frank-Wolfe Methodology for Approximate Seeded Graph Matching Inherently Includes RGM

In each Frank-Wolfe iteration (described in Section 3.2), the linearization which is solved is maximize (trace $P^T A_{21} B_{21}^T$ +trace$P^T A_{22} P^{(i)} B_{22}$) over all m-by-m permutation matrices P. Observe that if this maximization were just over the first term trace $P^T A_{21} B_{21}^T$ then it would be precisely solving RGM from Section 2.3, as per Equation (1) there. Also observe that if the maximization were just over the second term trace$P^T A_{22} P^{(i)} B_{22}$, then it would be exactly the FAQ algorithm (ignoring all of the seeds). In this manner, the SGM algorithm can be seen as leveraging a combination of the information gleaned from the nonseed-seed relationships (the "restricted-focus term") and the nonseed-nonseed relationships (the "FAQ term").

Although performing RGM is much simpler than performing SGM, and although RGM almost always produces the correct graph alignment if there are enough seeds, nonetheless SGM may perform substantially better when there aren't enough seeds. Indeed, as noted, SGM merges RGM with FAQ, and thus utilizes the information contained in the unseeded adjacency structure. While FAQ alone is often unable to extract out this information (see Figure 1 below), the RGM term can steer the FAQ term in SGM, allowing it to extract the relevant signal in the nonseed–to–nonseed adjacency structure.

The utility of this nonseeded term depends on the amount of information captured in the seed–to–nonseed adjacency. With less informative seeds, the SGM algorithm often significantly outperforms RGM alone, as there is important signal in the unseeded adjacency which RGM discards. However, in the presence of well chosen seeds, the seed–to–nonseed adjacency structure may contain all the relevant signal about the unknown alignment, and the unseeded adjacency information can be a nuisance (see Figure 4). As the RGM algorithm is exactly and efficiently solvable, this points to the centrality of both selecting and quantifying "good" seeds. This is a direction of future research, as we do not address the problem of intelligent seed selection at present.

As we will see in Figure 1, for weakly correlated graphs, RGM can outperform SGM. Even with poorly-chosen seeds, the noise in the nonseed–to–nonseed adjacency structure can outweigh the relevant signal, and the performance of SGM is harmed by including this extra nuisance information. This further highlights the utility of RGM in real data applications, where the correlation between graphs can be low.

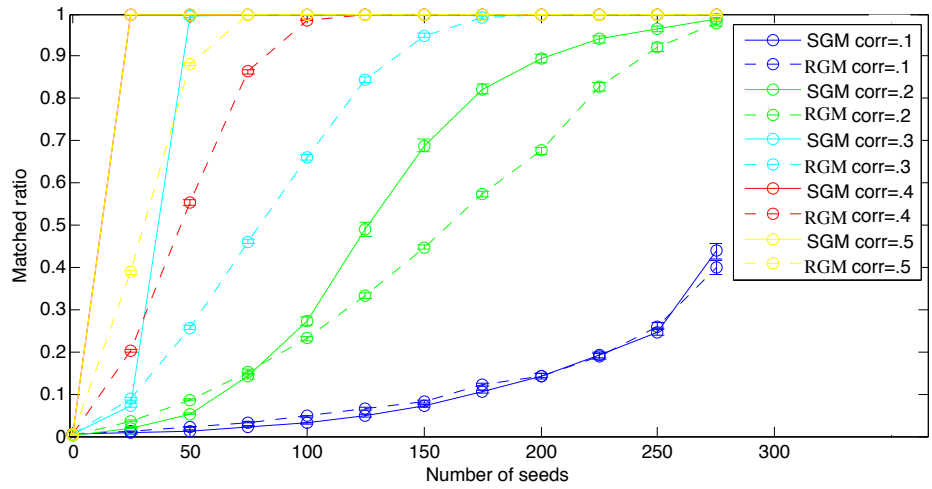
We explore the above further in Figure 1. There we compare the performance of SGM against solving RGM for correlated Erdős-Rényi graphs with $n = 300$ vertices, $p = 0.5$, seeding levels ranging from $s = 0$ to 275, and correlation ranging from $\varrho = 0.1$ to 1. For each value of ϱ and s, we ran 100 simulations and plotted the fraction of nonseeded vertices correctly matched across the graphs, with corresponding error bars of ± 2 s.e. In all cases (except $\rho = 0.1$), RGM needed more seeds to perform comparably to SGM. Indeed, with sufficiently many seeds, all available information about the unknown alignment is captured in the seed–to–nonseed connectivity, and the (exactly solvable) RGM algorithm alone is enough to properly align the graphs.

Also note the following from Figure 1. When there are no seeds, we see FAQ (which is SGM in the absence of seeds) working perfectly at capturing the latent alignment function when the two graphs are isomorphic (it bears noting that we have also observed FAQ perfectly matching when the two graphs are not isomorphic but rather *very* highly correlated), but FAQ does a surprisingly poor job (indeed, comparable to chance) when the correlation is even modestly less than one. However, with seeds, SGM quickly does a very substantially better job; indeed, the "restricted-focus" term is steering the SGM algorithm in the proper direction!

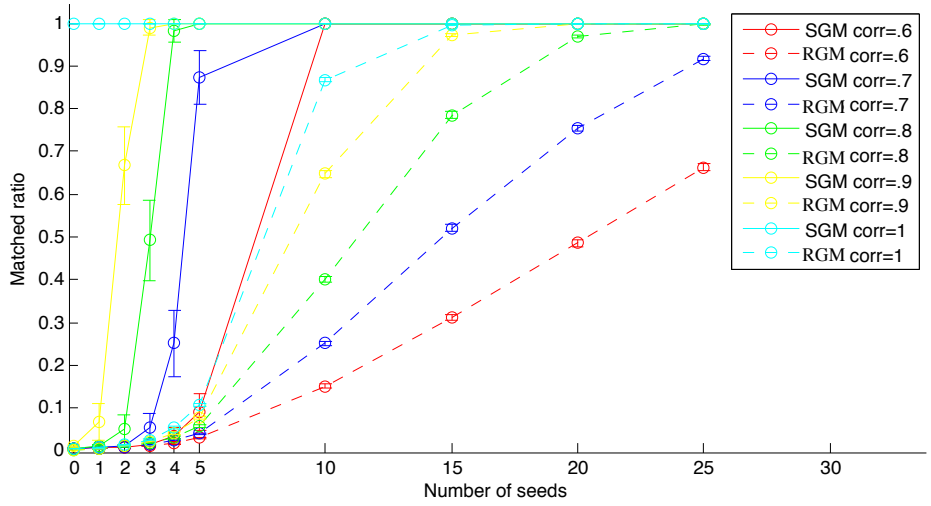
4. Matching Human Connectomes

We further illuminate the relationship between SGM and RGM through a real data experiment, which will serve to highlight both the utility of RGM and the effect of SGM's further incorporation of the unseeded adjacency information. Our data set consists of 45 graphs, each on 70 vertices, these graphs constructed respectively from diffusion tensor (DT) MRI scans of 45 distinct healthy patients. We have 21 scans from the Kennedy Krieger Institute (KKI), with raw data available at `http://www.nitrc.org/projects/multimodal/`, and 24 scans from the Nathan Kline Institute (NKI), with a description of the raw data available at `http://fcon_1000.projects.nitrc.org/indi/pro/eNKI_RS_TRT/FrontPage.html`. All raw scans were registered to a common template and identically processed with the MIGRAINE pipeline of Gray et al. (2012), each yielding a weighted, symmetric graph on 70 vertices. (All graphs can be found at `http://openconnecto.me/data/public/.MR/MIGRAINE/`). Vertices in the graphs correspond to regions in the Desikan brain atlas, with edge weights counting the number of neural fiber bundles connecting the regions (note that although the theory and algorithms presented earlier were for simple graphs, they are easily modified to handle edge weights). In addition to shedding light on the relationship between SGM and RGM, we also explore the batch effect induced by the different medical centers and demonstrate the capacity for seeding to potentially ameliorate this batch effect.

The pipeline which processes the scans into graphs first registers each of the graphs to a common template. As a result, there is a canonical alignment between the vertex sets of these graphs (vertices corresponding to respective regions in the Desikan brain atlas). How well is this alignment preserved *across* medical centers by the adjacency structure of the graphs alone? Figure 2 explores this question, and presents strong evidence for the existence of a batch effect (in both adjacency and geometric structure) induced by the different medical centers. In the figure, the heat map labeled "KKI matched to KKI" represents a 70×70 matrix, whose i, jth entry measures the relative number of times vertex



(a)



(b)

Figure 1: Fraction of vertices correctly matched for the SGM algorithm and for RGM, plotted versus the number of seeds utilized, for $n = 300$, $p = 1/2$ and correlation ϱ varying from 0.1 to 1. For each value of ϱ and s, we ran 100 simulations and plotted the fraction of nonseeded vertices correctly matched across the graphs, with corresponding error bars of ± 2 s.e.

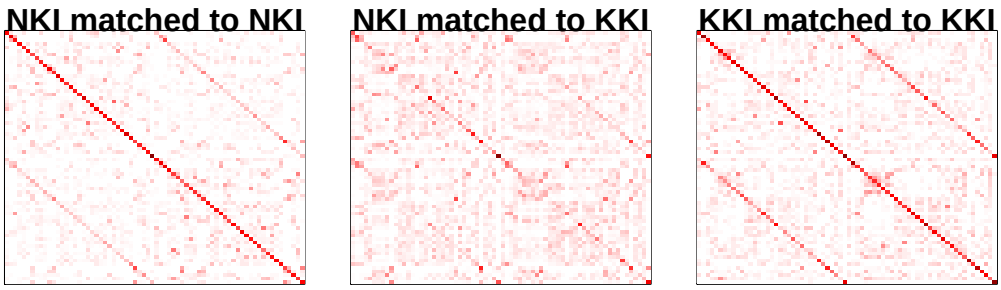


Figure 2: Left: NKI to NKI matching. Center: NKI to KKI matching. Right: KKI to KKI matching. Each plot is a 70×70 heat map with the color intensity (from white to red) representing the relative number of times vertex i was match with vertex j across the experiments (white denoting no matches, dark red denoting many matches). The dark red diagonal in the left and right heat maps (as compared to the center map), indicates presence of a substantial batch effect, i.e., the correct alignment was recovered significantly better matching within medical center versus across medical center. Vertices 1–35 and 36–70 (as ordered) correspond to the respective brain hemispheres.

i was mapped to vertex j when we ran the FAQ algorithm (i.e., no seeds) over the $\binom{21}{2}$ pairs of graphs from the KKI data set. Similarly, the "NKI to KKI" heat map counts the relative number of times vertices were matched to each other when running the FAQ algorithm over the $21 \cdot 24$ pairs of graphs, with one graph from each of the KKI and NKI data sets. The "NKI matched to NKI" heat map is defined similarly. The chromatic intensity of the pixel in the i, jth entry of each heat map represents the relative frequency in which vertex i was matched to vertex j across the experiments, with darker red implying more frequent and lighter red implying less frequent. White pixels represent vertex pairs that were never matched.

Figure 2 demonstrates the existence of significant signal in the adjacency structure alone (without the associated brain geometry and without seeding) for recovering the latent alignment in all three experiments. When matching KKI to KKI, 32.8% of the vertices are correctly matched on average; when matching NKI to NKI, 37.4% of the vertices were correctly matched on average; when matching NKI to KKI, 9.8% of the vertices were correctly matched on average (whereas chance would have matched $\approx 1.4\%$ on average). We note that the dramatic performance difference when matching within versus across medical centers is strong evidence of the presence of a batch effect induced by the different medical centers. Whether this batch effect is an artifact of experimental differences across medical centers (different MRI machines, different technicians, etc.) or the registration pipeline, it must be addressed before the data sets can be aggregated for use in further inference.

Also note that while much of the within medical center matching error was due to mismatching brain hemispheres (vertices 1–35 representing one hemisphere, and vertices 36–70 the other), the mismatch across medical centers appears significantly less structured.

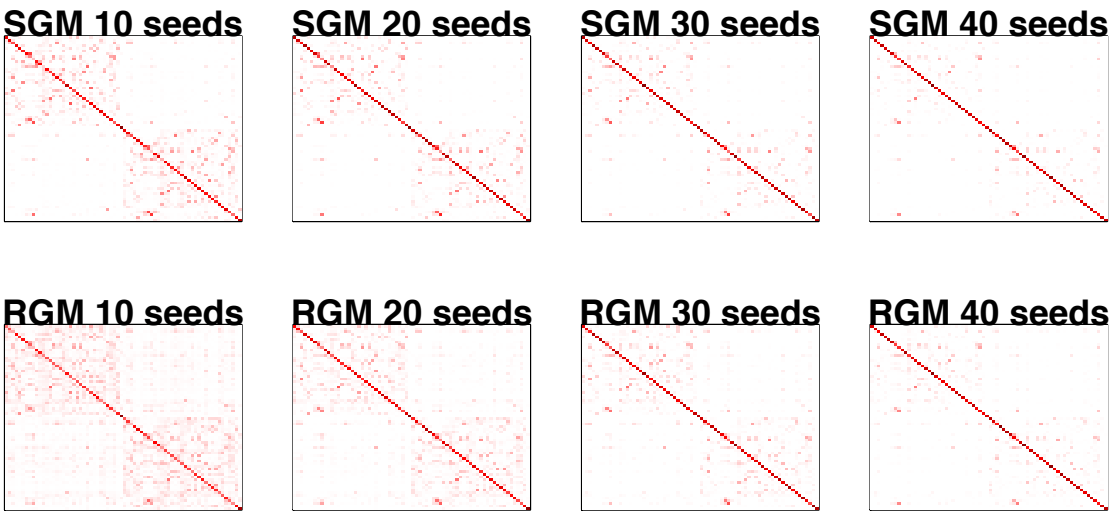


Figure 3: Clockwise from top left: SGM matching the $21 \cdot 24$ pairs of brains, one each from the NKI and KKI data sets, using 10, 20, 30, 40 seeds; RGM matching the same set of graphs using 40, 30, 20, 10 seeds. For each seed level, and each method we ran 100 paired MC replicates. Each plot is a 70×70 heat map with the color intensity (from white to red) representing the relative number of times vertex i was matched with vertex j across experiments (white denoting no matches, dark red denoting many matches). We do not count seeded vertices as being correctly matched to each other, which would have artificially inflated the diagonal.

Can we use seeding to ameliorate this batch effect? In Figure 1, we established the capacity of seeded vertices to unearth significant signal in the adjacency structure for recovering the latent alignment function, signal which was not found without seeds. Figure 3 further demonstrates this phenomenon in our present real data setting. We plot heat maps showing the $21 \cdot 24$ matchings of pairs of graphs, one each from the NKI and KKI data sets, for various seed levels. For each number of seeds$= 10, 20, 30, 40$, we ran 100 Monte Carlo replicates (for each of SGM and RGM) for each pair of matched graphs, with each seed set chosen uniformly at random from the 70 vertices. Clockwise, from the top left, we plot the performance of SGM with 10, 20, 30, and 40 seeds and then the performance of RGM with 40, 30, 20, and 10 seeds. The chromatic intensity of the pixel in the i, jth entry of each heat map represents the relative frequency in which vertex i was matched to vertex j across the experiments (seeded vertices are not counted as correctly matched here), with darker red implying more frequent and lighter red implying less frequent.

The figure conclusively demonstrates that seeding extracts statistically significant signal in the adjacency structure alone for correctly aligning graphs across medical center, signal that was effectively obfuscated in the absence of seeds. While unseeded FAQ correctly matched 9.8% of the vertices on average across medical centers, with $10, 20, 30, 40$ seeds,

SGM (RGM) correctly matches 49.9%,68.4%,78.8%, 85.1% (29.9%, 53.8%, 70.7%, 80.9%) of the unmatched vertices on average across medical centers. We also see that SGM outperforms RGM across all seed levels, with RGM requiring more seeds to achieve the same performance as SGM. This is not surprising, as RGM is not utilizing any of the adjacency information amongst the unseeded vertices.

We also see that seeding teases out additional information on the neural geometry inherent to the graphs. For instance, with only 10 seeds, 4.3% (15.1%) vertices on average are mismatched across hemispheres by SGM (RGM). In contrast, 43.8% vertices on average were mismatched across hemispheres without seeds. Interestingly, some vertex pairs are consistently mismatched across all seed levels. For example, vertex 57 is matched by SGM to vertex 47 across medical centers 23.8%, 20.8%, 23.1%, 23.5% of the time with $10, 20, 30, 40$ seeds, whereas, with no seeds, vertex 57 is matched to vertex 47 on average 10.9% of the time when matching among the NKI data set and 10% of the time when matching amongst the KKI graphs. Indeed, these persistent artifacts are indicative of substantive differences across (and within) data sets and demand further investigation.

We have noted that, on average, SGM outperformed RGM across all seed levels. How much of this performance gap is a function of the particular seeds chosen? We explore this further in Figure 4. For a pair of graphs, one each from the NKI and KKI data sets (we randomly chose graph 2 in the NKI data set and graph 7 in the KKI set—note that we see similar patterns across all tested graph pairs), we ran 200 Monte Carlo replicates of SGM and RGM seeded with the same randomly selected seeds. For each of seeds= $10, 20, 30, 40, 50$ (chosen uniformly at random from the vertices), the associated histogram plots the 200 values of the number of vertices correctly matched by SGM minus the number of vertices correctly matched by RGM.

The RGM algorithm ignores all the adjacency information amongst the unseeded vertices. If, in Figure 4, SGM performed uniformly better than RGM at each seed level, then there is consistently relevant signal in the unseeded adjacency structure, and we should never use RGM when SGM is feasibly run. However, we see that there are choices of seeds (at every level) for which RGM outperforms SGM. The unseeded adjacency information is a nuisance in these cases. As RGM is efficiently exactly solvable, this dramatically highlights the importance of intelligent seeding. Indeed, "good" seeds (and hence the RGM algorithm) have the potential to capture all of the relevant adjacency structure in the graph. While we do not pursue the question of *how* to select "good" seeds here, the figure points to the centrality of this question, and we plan on pursuing active seed selection in future work.

For higher seed levels, we note that there is significantly less difference (and less variability) in the performance of SGM and RGM. More seeds capture more information in their neighborhood structure, and the effect of the unseeded adjacency on algorithm performance is dampened. Also, at higher seed levels the particular choice of seeds is less important, as any selection of a large number of seeds will probably contain enough "good" seeds to strongly align the graphs.

5. Discussion

Estimating the latent alignment between the vertices of two graphs is an important problem in many disciplines, and our results have both theoretical and practical implications

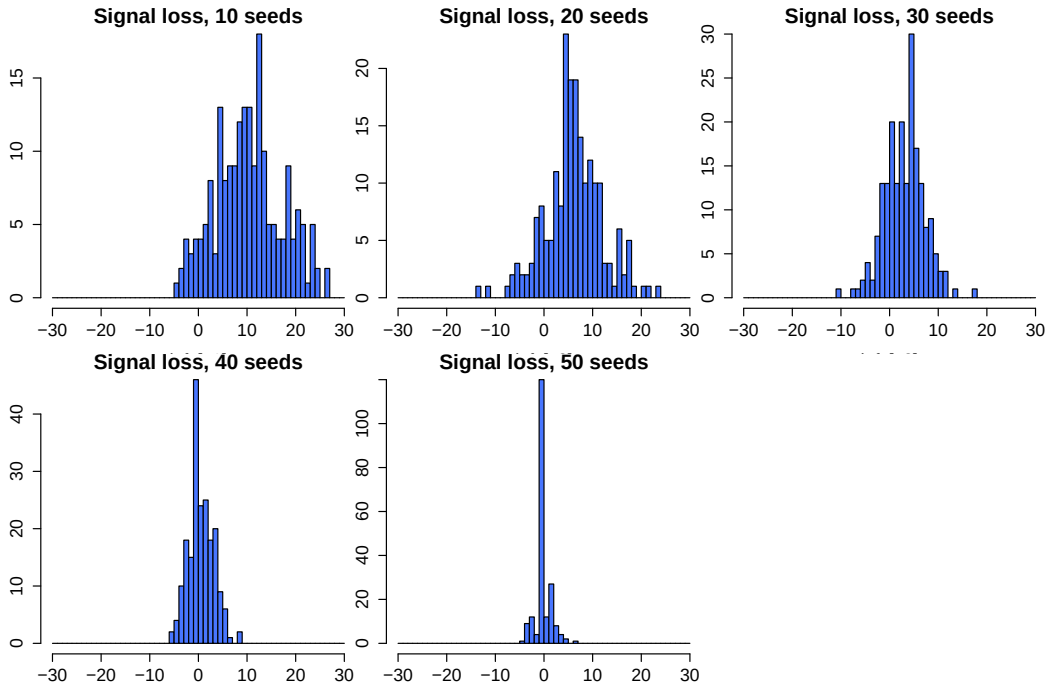


Figure 4: RGM versus SGM when matching one graph each from the NKI (graph 2) and KKI (graph 7) data sets over differing seed levels. For each of seeds= $10, 20, 30, 40, 50$ (chosen uniformly at random from the vertices), each histogram above plots 200 values of the number of vertices correctly matched by SGM minus the number of vertices correctly matched by RGM utilizing the same random seeds.

for this problem. Indeed, under mild assumptions, we proved the strong consistency of the graph matching problem—and its restricted focus subproblem—for estimating the latent alignment function between the vertex sets of two correlated Erdős-Rényi graphs. Although seeded graph matching is computationally hard, this result gives hope that efficient approximation algorithms will be effective in recovering the latent alignment across a broad array of graphs.

Embedded in the hard seeded graph matching problem is the tractable restricted-focus graph matching problem. This problem is exactly solvable and also provides a strongly consistent estimator of the latent alignment. While full seeded graph matching often out performs this restricted focus variant, we demonstrated the capacity for the restricted-focus subproblem to also outperform the full matching. The relation between the two approaches hinges on the information contained in the seeded vertices. If the seeds capture the adjacency structure of the graph, then the restricted-focus subproblem can benefit by *not* including the unseeded adjacency information, and we demonstrate this phenomenon in both real and simulation data. This points to the primacy of intelligently seeding in graph matching, and we are working on active seeding algorithms for choosing good seeded vertices.

Even when outperformed by the full matching problem, we can still use the restricted-focus problem to extract signal in the graphs that was obfuscated without seeding. In very large, complex problems, when it may be infeasible to run the full seeded graph matching algorithm, the restricted-focus approach could be run to provide a baseline matching between the graphs. We are presently investigating this further, as scalability of these approaches is an increasingly important demand of modern big-data.

Acknowledgments

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Appendix A. Proofs of Theorems 1 and 2

Theorem 1 is proved in Sections A.2, A.3, and A.4, and these three subsections are a continuation one of the other. Theorem 2 is proved in Sections A.5, A.6, and A.7 and these three subsections are a continuation one of the other. Interestingly, the underlying methodology for proving Theorem 1 is very similar (but with notable differences) to the methodology for proving Theorem 2. We begin with some results that will subsequently be used in the proof of Theorems 1 and 2.

A.1 Supporting Results

The next result, Theorem 3, is from Alon et al. (1997), in the form found in Kim et al. (2002).

Theorem 3 *Suppose random variable X is a function of η independent Bernoulli(q) random variables such that changing the value of any one of the Bernoulli random variables changes the value of X by at most 2. For any $t : 0 \leq t < \sqrt{\eta q(1-q)}$, we have* $\mathbb{P}\left[|X - \mathbb{E}X| > 4t\sqrt{\eta q(1-q)}\right] \leq 2e^{-t^2}$.

The next result, Theorem 4, is a Chernoff-Hoeffding bound which is Theorem 3.2 in Chung and Lu (2006).

Theorem 4 *Suppose X has a Binomial(η, q) distribution. Then for all $t \geq 0$ it holds that*

$$\mathbb{P}\left[X - \mathbb{E}X \geq t\right] \leq exp\left\{\frac{-t^2}{2\eta q + 2t/3}\right\}.$$

For any $r, q \in (0,1)$, define $H(r,q) := r\log\left(\frac{r}{q}\right) + (1-r)\log\left(\frac{1-r}{1-q}\right)$. This is the Kullback-Leibler divergence between binomial random variables with respective success probabilities r and q. We will later use the following rough lower bound estimate of a binomial tail probability:

Proposition 5 *Suppose X has a Binomial(η, q) distribution, and suppose that $0 < q < r < 1 - \frac{1}{\eta}$ for a real number r. Then*

$$\mathbb{P}(X \geq \eta r) \geq \frac{\sqrt{\pi}}{e^3} \cdot \sqrt{\frac{(1-r)}{r}} \eta^{-1/2} q \cdot e^{-\eta H(r,q)}.$$

Proof We compute and bound

$$\begin{aligned}
\mathbb{P}(X \geq \eta r) &\geq \mathbb{P}(X = \lceil \eta r \rceil) = \binom{\eta}{\lceil \eta r \rceil} q^{\lceil \eta r \rceil} (1-q)^{\eta - \lceil \eta r \rceil} \\
&\geq \frac{\sqrt{2\pi}}{e^2} q^{\lceil \eta r \rceil} (1-q)^{\eta - \lceil \eta r \rceil} \frac{\eta^{\eta+0.5}}{\lceil \eta r \rceil^{\lceil \eta r \rceil + 0.5} (\eta - \lceil \eta r \rceil)^{\eta - \lceil \eta r \rceil + 0.5}} \\
&= \frac{\sqrt{2\pi}}{e^2} q^{\lceil \eta r \rceil} (1-q)^{\eta - \lceil \eta r \rceil} \frac{\eta^{\eta+0.5}}{(\eta r)^{\eta r + 0.5} (\eta - \eta r)^{\eta - \eta r + 0.5}} \cdot \frac{(\eta r)^{\eta r + 0.5} (\eta - \eta r)^{\eta - \eta r + 0.5}}{\lceil \eta r \rceil^{\lceil \eta r \rceil + 0.5} (\eta - \lceil \eta r \rceil)^{\eta - \lceil \eta r \rceil + 0.5}},
\end{aligned}$$

where the inequality in the second display line follows from Stirling's formula. Now,

$$\begin{aligned}
\frac{(\eta r)^{\eta r + 0.5} (\eta - \eta r)^{\eta - \eta r + 0.5}}{\lceil \eta r \rceil^{\lceil \eta r \rceil + 0.5} (\eta - \lceil \eta r \rceil)^{\eta - \lceil \eta r \rceil + 0.5}} &= \frac{(r)^{\eta r + 0.5} (1-r)^{\eta - \eta r + 0.5}}{\left(\frac{\lceil \eta r \rceil}{\eta}\right)^{\lceil \eta r \rceil + 0.5} \left(1 - \frac{\lceil \eta r \rceil}{\eta}\right)^{\eta - \lceil \eta r \rceil + 0.5}} \\
&\geq \left(\frac{1}{\frac{\lceil \eta r \rceil}{\eta r}}\right)^{\eta r + 0.5} (1-r)^{\lceil \eta r \rceil - \eta r} \\
&\geq \left(\frac{1}{1 + \frac{1}{\eta r}}\right)^{\eta r + 0.5} (1-r) \quad \geq \quad \frac{1}{e\sqrt{2}}(1-r).
\end{aligned}$$

Combining the above, we obtain

$$\begin{aligned}
\mathbb{P}(X \geq \eta r) &\geq \frac{\sqrt{\pi}}{e^3} \cdot \frac{1-r}{r^{1/2}(1-r)^{1/2}} \eta^{-1/2} q^{\eta r + 1} (1-q)^{\eta - \eta r} \frac{\eta^{\eta}}{(\eta r)^{\eta r} (\eta - \eta r)^{\eta - \eta r}} \\
&= \frac{\sqrt{\pi}}{e^3} \cdot \sqrt{\frac{1-r}{r}} \eta^{-1/2} q \cdot e^{-\eta H(r,q)},
\end{aligned}$$

as desired. ∎

A.2 Overall Argument of the Proof for Theorem 1, Part i

It is notationally convenient to assume without loss of generality that the correlated Erdős-Rényi graphs G_1 and G_2 are on the same set of n vertices V and we do **not** relabel the

vertices. Let Π denote the set of bijections $V \to V$; here, the identity function $e \in \Pi$ is the latent alignment bijection Φ. For any $\psi \in \Pi$,

$$\Delta^+(G_1, G_2, \psi) := |\left\{ \{v, v'\} \in \binom{V}{2} \text{ s.t. } \{v, v'\} \notin E(G_1) \text{ and } \{\psi(v), \psi(v')\} \in E(G_2) \right\}|,$$

$$\Delta^-(G_1, G_2, \psi) := |\left\{ \{v, v'\} \in \binom{V}{2} \text{ s.t. } \{v, v'\} \in E(G_1) \text{ and } \{\psi(v), \psi(v')\} \notin E(G_2) \right\}|,$$

$$\Delta^{0+}(G_1, G_2, \psi) := |\left\{ \{v, v'\} \in \binom{V}{2} \text{ s.t. } \{v, v'\} \notin E(G_1),\ \{\psi(v), \psi(v')\} \in E(G_1), \right.$$
$$\left. \{\psi(v), \psi(v')\} \notin E(G_2) \right\}|,$$

$$\Delta^{0-}(G_1, G_2, \psi) := |\left\{ \{v, v'\} \in \binom{V}{2} \text{ s.t. } \{v, v'\} \in E(G_1),\ \{\psi(v), \psi(v')\} \notin E(G_1), \right.$$
$$\left. \{\psi(v), \psi(v')\} \in E(G_2) \right\}|,$$

$$\Delta(G_1, G_2, \psi) := \Delta^+(G_1, G_2, \psi) + \Delta^-(G_1, G_2, \psi).$$

First, note that

$$\Delta^+(G_1, G_1, \psi) = \Delta^-(G_1, G_1, \psi) = \frac{1}{2}\Delta(G_1, G_1, \psi) \ ; \tag{3}$$

this is because the number of edges in G_1 isn't changed when its vertices are permuted by ψ.

Next, note that

$$\Delta(G_1, G_2, \psi) - \Delta(G_1, G_2, e) = \Delta(G_1, G_1, \psi) - 2 \cdot \Delta^{0+}(G_1, G_2, \psi) - 2 \cdot \Delta^{0-}(G_1, G_2, \psi) \ ; \tag{4}$$

this is easily verified by replacing "G_2" in (4) by "G", and observing the truth of (4) as G, starting out with $G = G_1$, is changed one edge-flip at a time until $G = G_2$.

Now, consider the event, which we shall call Υ, that for all $\psi \in \Pi \backslash \{e\}$,

$$\Delta^{0+}(G_1, G_2, \psi) \ < \ \Delta^+(G_1, G_1, \psi) \cdot \left((1-p)(1-\varrho) + \frac{\varrho}{2} \right) \text{ and also} \tag{5}$$

$$\Delta^{0-}(G_1, G_2, \psi) \ < \ \Delta^-(G_1, G_1, \psi) \cdot \left(p(1-\varrho) + \frac{\varrho}{2} \right). \tag{6}$$

We will next show in Section A.3 that, under the hypotheses of the first part of Theorem 1, Υ almost always happens (in other words, with probability 1, Υ happens for all but a finite numbers of n's). Then, adding (5) to (6) and using (3), we then obtain that almost always $\Delta^{0+}(G_1, G_2, \psi) + \Delta^{0-}(G_1, G_2, \psi) < \frac{1}{2} \cdot \Delta(G_1, G_1, \psi)$ for all $\psi \in \Pi \backslash \{e\}$. Substituting this into (4) yields that almost always $\Delta(G_1, G_2, \psi) > \Delta(G_1, G_2, e)$ for all $\psi \in \Pi \backslash \{e\}$, and the first part of Theorem 1 is then proven.

A.3 Under Hypotheses of Theorem 1, Part i, Υ Occurs Almost Always

For any $k \in \{1, 2, \ldots, n\}$, let $\Pi(k)$ denote the set of bijections in Π such that the number of non-fixed-points of the bijection is exactly k; that is, $\Pi(k) := \{\psi \in \Pi : |\{v \in V : \psi(v) \neq$

$v\}| = k\}$. A simple upper bound for $|\Pi(k)|$ is $|\Pi(k)| \leq \binom{n}{k}k! = n(n-1)(n-2)\cdots(n-k+1) \leq n^k$.

Just for now, let $k \in \{1, 2, \ldots, n\}$ be chosen, and let $\psi \in \Pi(k)$ be chosen. Denoting $T(\psi) := \left\{\{v, v'\} \in \binom{V}{2} \text{ such that } v = \psi(v'),\ v' = \psi(v)\}\right\}$, we have that the random variable $\Delta(G_1, G_1, \psi)$ is a function of the $\eta := \binom{k}{2} + (n-k)k - |T(\psi)|$ independent Bernoulli(p) random variables

$$\{\mathbb{1}\{\{v, v'\} \in E(G_1)\}\}_{\{v,v'\}\in\binom{V}{2}\setminus T(\psi)\ :\ \psi(v)\neq v \text{ or } \psi(v')\neq v'}$$

and note that the hypotheses of Theorem 3 are satisfied, hence for the choice of $t = \frac{1}{20}\sqrt{\eta p(1-p)}$ in Theorem 3 we obtain that

$$\mathbb{P}\left[|\Delta(G_1, G_1, \psi) - \mathbb{E}\Delta(G_1, G_1, \psi)| > \frac{1}{5}\eta p(1-p)\right] \leq 2e^{-\eta p(1-p)/400}. \tag{7}$$

Also note that

$$\Delta(G_1, G_1, \psi) = \sum_{\substack{\{v,v'\}\in\binom{V}{2}\setminus T(\psi)\\ \text{s.t. } \psi(v)\neq v \text{ or } \psi(v')\neq v'}} \mathbb{1}\left\{\mathbb{1}\{\{v, v'\} \in E(G_1)\} \neq \mathbb{1}\{\{\psi(v), \psi(v')\} \in E(G_1)\}\right\}$$

is the sum of η Bernoulli($2p(1-p)$) random variables hence

$$\mathbb{E}\Delta(G_1, G_1, \psi) = 2\eta p(1-p). \tag{8}$$

Because $|T(\psi)| \leq \frac{k}{2}$, we have by elementary algebra that $\frac{(n-2)k}{2} \leq \eta \leq nk$. Thus, by (7) and (8) we obtain that (for large enough n; in the following our constants are very conservatively chosen)

$$\mathbb{P}\left(\frac{\Delta(G_1, G_1, \psi)}{nkp(1-p)} \notin [1/2,\ 5/2]\right) \leq 2e^{\frac{-1}{1000}nkp(1-p)} \leq 2e^{\frac{-(1-\xi_1)}{1000}nkp}. \tag{9}$$

Conditioning on G_1, random variable $\Delta^{0+}(G_1, G_2, \psi)$ has a

$$\text{Binomial}\left(\Delta^{+}(G_1, G_1, \psi), (1-p)(1-\varrho)\right)$$

distribution, and random variable $\Delta^{0-}(G_1, G_2, \psi)$ has a

$$\text{Binomial}\left(\Delta^{-}(G_1, G_1, \psi), p(1-\varrho)\right)$$

distribution. Conditioning also on the event that $\frac{\Delta(G_1,G_1,\psi)}{nkp(1-p)} \in [1/2,\ 5/2]$, we apply Theorem 4 with the value $t = \frac{\varrho}{2}\cdot\Delta^{+}(G_1, G_1, \psi)$, and we use (3) to show

$$\mathbb{P}\left[\Delta^{0+}(G_1, G_2, \psi) \geq \Delta^{+}(G_1, G_1, \psi)\cdot\left((1-p)(1-\varrho) + \frac{\varrho}{2}\right)\right] \leq e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2}, \tag{10}$$

$$\mathbb{P}\left[\Delta^{0-}(G_1, G_2, \psi) \geq \Delta^{-}(G_1, G_1, \psi)\cdot\left(p(1-\varrho) + \frac{\varrho}{2}\right)\right] \leq e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2}. \tag{11}$$

Finally, applying (9), (10) and (11), the probability of Υ^C can be bounded using sub-additivity:

$$\begin{aligned}\mathbb{P}(\Upsilon^C) &\leq \sum_{k=1}^{n}\sum_{\psi\in\Pi(k)}\left(2e^{\frac{-(1-\xi_1)}{1000}nkp}+e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2}+e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2}\right)\\ &\leq \sum_{k=1}^{n}n^k\left(2e^{\frac{-(1-\xi_1)}{1000}nkp}+2e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2}\right)\\ &\leq \sum_{k=1}^{n}\left(2e^{\frac{-(1-\xi_1)}{1000}nkp+k\log n}+2e^{\frac{-(1-\xi_1)}{40}nkp\varrho^2+k\log n}\right)\leq n\cdot\frac{4}{n^3},\end{aligned}$$

the last inequality holding if $p\geq c_2\frac{\log n}{n}$ and $\varrho\geq c_1\sqrt{\frac{\log n}{np}}$ for sufficiently large, for fixed constants c_1,c_2. Because $\sum_{n=1}^{\infty}\frac{4}{n^2}<\infty$, we have by the Borel-Cantelli Lemma that Υ almost always happens. As mentioned in Section A.2, this completes the proof of the first part of Theorem 1.

Remark 6 Note that we could tighten the constants c_1 and c_2 appearing above. Here we choose not to, instead focusing on the orders of magnitude of ϱ, and do not pursue exact constants further.

A.4 Proof of Theorem 1, Part ii

We now prove the second part of Theorem 1.

Just for now, let $\psi\in\Pi(n)$ be chosen (i.e., ψ is a derangement), and condition on $\Delta^+(G_1,G_1,\psi)=\Delta$, where $\frac{1}{4}n^2p(1-p)\leq\Delta\leq\frac{5}{4}n^2p(1-p)$. The random variables $\Delta^{0+}(G_1,G_2,\psi)$ and $\Delta^{0-}(G_1,G_2,\psi)$ are independent, and have distributions Binomial(Δ,q_1) and Binomial(Δ,q_2), respectively, where $q_1:=(1-p)(1-\varrho)$ and $q_2:=p(1-\varrho)$.

Denoting $r_1:=q_1+\frac{\varrho}{2}$ and $r_2:=q_2+\frac{\varrho}{2}$, and observing that, under the hypotheses of Theorem 2, part ii, it holds that $r_1<1-\frac{1}{\Delta}$ and $r_2<1-\frac{1}{\Delta}$ we thus have by Proposition 5 that (as $\frac{\pi}{e^6}>\frac{1}{200}$)

$$\begin{aligned}&\mathbb{P}\left(\Delta^{0+}(G_1,G_2,\psi)\geq\Delta\cdot r_1\ \text{ and }\ \Delta^{0-}(G_1,G_2,\psi)\geq\Delta\cdot r_2\right)\\ &\qquad\geq\frac{q_1q_2}{200\Delta}\sqrt{\frac{(1-r_1)(1-r_2)}{r_1r_2}}e^{-\Delta\cdot H(r_1,q_1)-\Delta\cdot H(r_2,q_2)}\end{aligned}$$

Note that we can change the inequalities "$\geq$" in the expression $\mathbb{P}(\quad)$ above into strict inequalities "$>$" with a harmless tweak. An elementary calculus argument yields that $H(x+y,y)\leq x^2/(y-y^2)$ for all $0<y<1$ and $x\geq 0$ such that $y+2x<1$. Indeed, fixing any value for y, the function value and the derivative of $H(x+y,y)$ with respect to x are both 0 at $x=0$, the function value and the derivative of $x^2/(y-y^2)$ with respect to x are both 0 at $x=0$, and the second derivative of $H(x+y,y)$ is less than the second derivative of $x^2/(y-y^2)$ for all relevant x. This, together with the fact that $1-r_1=r_2$, $1-r_2=r_1$

and assuming that ϱ is bounded away from 1 (which, indeed, will turn out to be assumed), we have that there exists a real number $c > 0$ such that

$$\begin{aligned}\mathbb{P}\Bigg(\Delta^{0+}(G_1, G_2, \psi) > \Delta \cdot r_1 \text{ and } \Delta^{0-}(G_1, G_2, \psi) > \Delta \cdot r_2\Bigg) \\ &\geq \frac{q_1 q_2}{200\Delta} e^{-\varrho^2 \Delta\left(\frac{1}{4q_1(1-q_1)} + \frac{1}{4q_2(1-q_2)}\right)} \\ &\geq \frac{c}{n^2} \cdot e^{-\varrho^2 n^2 p \cdot \left(\frac{1}{c \cdot p}\right)} \\ &= \frac{c}{n^2} \cdot e^{\frac{-\varrho^2 n^2}{c}} \quad . \end{aligned} \tag{12}$$

From (3) and (9) we have that there exists a fixed constant c_4 such that if $p \geq c_4 \frac{\log n}{n}$ then, with probability $> \frac{1}{2}$ (for n large enough) it holds that $\frac{1}{4} n^2 p(1-p) \leq \Delta^+(G_1, G_1, \psi) \leq \frac{5}{4} n^2 p(1-p)$. Thus, by (12), noting again that $r_1 + r_2 = 1$ and that $\Delta^+(G_1, G_1, \psi) = \frac{1}{2}\Delta(G_1, G_1, \psi)$, we have unconditionally

$$\mathbb{P}\left(\Delta^{0+}(G_1, G_2, \psi) + \Delta^{0-}(G_1, G_2, \psi) > \frac{1}{2} \cdot \Delta(G_1, G_1, \psi)\right) \geq \frac{c}{2n^2} \cdot e^{\frac{-\varrho^2 n^2}{c}} \tag{13}$$

Next, the number of derangements $|\Pi(n)|$ satisfies $\lim_{n\to\infty} \frac{|\Pi(n)|}{n!} = \frac{1}{e}$, thus with Stirling's formula we have that for n large enough it will hold that $|\Pi(n)| \geq \left(\frac{n}{e}\right)^n$. Thus, for n large enough, by (4) and (13),

$$\begin{aligned}\mathbb{E}\left|\left\{\psi \in \Pi : \Delta(G_1, G_2, \psi) < \Delta(G_1, G_2, e)\right\}\right| &= \sum_{\psi \in \Pi} \mathbb{P}\left(\Delta(G_1, G_2, \psi) < \Delta(G_1, G_2, e)\right) \\ &\geq \sum_{\psi \in \Pi(n)} \mathbb{P}\left(\Delta(G_1, G_2, \psi) < \Delta(G_1, G_2, e)\right) \\ &\geq \left(\frac{n}{e}\right)^n \frac{c}{2n^2} \cdot e^{\frac{-\varrho^2 n^2}{c}} \\ &= \frac{c}{2n^2} \cdot e^{\frac{-\varrho^2 n^2}{c} + n\log n - n},\end{aligned}$$

so that there exists a fixed real number $c_3 > 0$ such that if $\varrho \leq c_3 \sqrt{\frac{\log n}{n}}$ then it holds that $\mathbb{E}\left|\left\{\psi \in \Pi(n) : \Delta(G_1, G_2, \psi) < \Delta(G_1, G_2, e)\right\}\right| \to \infty$ as $n \to \infty$, and the second part of Theorem 1 is proven.

Remark 7 Note that we could tighten the constants c_3 and c_4 appearing above. Here we choose not to, instead focusing on the orders of magnitude of ϱ, and do not pursue exact constants further.

A.5 Overall Argument of the Proof for Theorem 2, part i

The proof of Theorem 2 is very similar in structure to the proof of Theorem 1. For simplicity of notation, suppose without loss of generality that the correlated Erdős-Rényi graphs G_1

and G_2 are on the same set of n vertices V, and we do **not** relabel the vertices. Let Π denote the set of bijections $V \to V$; here the identity function $e \in \Pi$ is the latent alignment bijection. Further suppose that V is partitioned into s seed vertices U, and m nonseed vertices W. Let $\phi : U \to U$ be the identity function, and let $\Pi_\phi := \{\psi \in \Pi : \forall u \in U\ \psi(u) = u\}$. For any $\psi \in \Pi_\phi$, define

$$\begin{aligned}
\Delta_R^+(G_1, G_2, \psi) &:= |\{(w,u) \in W \times U : \{w,u\} \notin E(G_1) \text{ and } \{\psi(w),u\} \in E(G_2)\}|,\\
\Delta_R^-(G_1, G_2, \psi) &:= |\{(w,u) \in W \times U : \{w,u\} \in E(G_1) \text{ and } \{\psi(w),u\} \notin E(G_2)\}|,\\
\Delta_R^{0+}(G_1, G_2, \psi) &:= \big|\{(w,u) \in W \times U : \{w,u\} \notin E(G_1),\ \{\psi(w),u\} \in E(G_1),\\
&\qquad\qquad \{\psi(w),u\} \notin E(G_2)\}\big|,\\
\Delta_R^{0-}(G_1, G_2, \psi) &:= \big|\{(w,u) \in W \times U : \{w,u\} \in E(G_1),\ \{\psi(w),u\} \notin E(G_1),\\
&\qquad\qquad \{\psi(w),u\} \in E(G_2)\}\big|,\\
\Delta_R(G_1, G_2, \psi) &:= \Delta_R^+(G_1, G_2, \psi) + \Delta_R^-(G_1, G_2, \psi).
\end{aligned}$$

First note that

$$\Delta_R^+(G_1, G_1, \psi) = \Delta_R^-(G_1, G_1, \psi) = \frac{1}{2}\Delta_R(G_1, G_1, \psi) \quad ; \tag{14}$$

this can be easily verified by considering, for each $u \in U$ and for each cycle C of the permutation ψ, the changes of status in adjacency-to-u of the vertices as the vertices of C are considered in their cyclic order. (Specifically, the number of changes along C from adjacency-to-u to nonadjacency-to-u are equal to the number of changes along C from nonadjacency-to-u to adjacency-to-u.)

Next, note that

$$\begin{aligned}
\Delta_R(G_1, G_2, \psi) - \Delta_R(G_1, G_2, e) = \Delta_R(G_1, G_1, \psi) &- 2 \cdot \Delta_R^{0+}(G_1, G_2, \psi)\\
&- 2 \cdot \Delta_R^{0-}(G_1, G_2, \psi);
\end{aligned} \tag{15}$$

this is easily verified by replacing "G_2" in (15) with "G", and observing the truth of (15) as G, starting out with $G = G_1$, is changed one edge-flip at a time until $G = G_2$.

Now, consider the event Υ_R defined as it holding that, for all $\psi \in \Pi_\phi$ besides e,

$$\Delta_R^{0+}(G_1, G_2, \psi) \;<\; \Delta_R^+(G_1, G_1, \psi) \cdot \left((1-p)(1-\varrho) + \frac{\varrho}{2}\right) \text{ and also} \tag{16}$$

$$\Delta_R^{0-}(G_1, G_2, \psi) \;<\; \Delta_R^-(G_1, G_1, \psi) \cdot \left(p(1-\varrho) + \frac{\varrho}{2}\right). \tag{17}$$

We will show in Section A.6 that, under the hypotheses of the first part of Theorem 2, Υ_R almost always happens. Then, adding (16) to (17) and using (14), we then obtain that almost always $\Delta_R^{0+}(G_1, G_2, \psi) + \Delta_R^{0-}(G_1, G_2, \psi) < \frac{1}{2} \cdot \Delta_R(G_1, G_1, \psi)$ for all $\psi \in \Pi_\phi \backslash \{e\}$. Substituting this into (15) yields that almost always $\Delta_R(G_1, G_2, \psi) > \Delta_R(G_1, G_2, e)$ for all $\psi \in \Pi_\phi \backslash \{e\}$, and the first part of Theorem 2 will then be proven.

A.6 Under Hypotheses of Theorem 2, Part i, Υ_R Occurs Almost Always

For any $k \in \{1, 2, \ldots, m\}$, denote $\Pi_\phi(k) := \{\psi \in \Pi_\phi : |\{v \in V : \psi(v) \neq v\}| = k\}$. Just for now, let $k \in \{1, 2, \ldots, m\}$ be chosen, and let $\psi \in \Pi_\phi(k)$ be chosen. The random variable

$\Delta_R(G_1, G_1, \psi)$ is a function of the $\eta' := ks$ independent Bernoulli(p) random variables

$$\{\mathbb{1}\{\{w,u\} \in E(G_1)\}\}_{(w,u)\in W\times U:\psi(w)\neq w},$$

and note that the hypotheses of Theorem 3 are satisfied, hence for the choice of $t = \frac{1}{20}\sqrt{\eta' p(1-p)}$ in Theorem 3 we obtain that

$$\mathbb{P}\left[|\Delta_R(G_1, G_1, \psi) - \mathbb{E}\Delta_R(G_1, G_1, \psi)| > \frac{1}{5}\eta' p(1-p)\right] \leq 2e^{-\eta' p(1-p)/400}. \tag{18}$$

Also note that

$$\Delta_R(G_1, G_1, \psi) = \sum_{\substack{(w,u)\in W\times U\\ \text{s.t.}\psi(w)\neq w}} \mathbb{1}\Big\{\mathbb{1}\{\{w,u\} \in E(G_1)\} \neq \mathbb{1}\{\{\psi(w),u\} \in E(G_1)\}\Big\}$$

is the sum of η' Bernoulli($2p(1-p)$) random variables hence

$$\mathbb{E}\Delta_R(G_1, G_1, \psi) = 2\eta' p(1-p). \tag{19}$$

Thus, by (18) and (19) we obtain that

$$\mathbb{P}\left(\frac{\Delta_R(G_1, G_1, \psi)}{ksp(1-p)} \notin [9/5,\ 11/5]\right) \leq 2e^{\frac{-1}{400}ksp(1-p)} \leq 2e^{\frac{-\xi_2^2}{400}ks}. \tag{20}$$

Conditioning on G_1, random variable $\Delta_R^{0+}(G_1, G_2, \psi)$ has a

$$\text{Binomial}\left(\Delta_R^{+}(G_1, G_1, \psi), (1-p)(1-\varrho)\right)$$

distribution, and random variable $\Delta_R^{0-}(G_1, G_2, \psi)$ has a

$$\text{Binomial}\left(\Delta_R^{-}(G_1, G_1, \psi), p(1-\varrho)\right)$$

distribution. Conditioning also on the event that $\frac{\Delta_R(G_1,G_1,\psi)}{ksp(1-p)} \in [9/5,\ 11/5]$, applying Theorem 4 with the value $t = \frac{\varrho}{2}\cdot\Delta_R^{+}(G_1, G_1, \psi)$, and using (14), we have that

$$\mathbb{P}\left[\Delta_R^{0+}(G_1, G_2, \psi) \geq \Delta_R^{+}(G_1, G_1, \psi)\cdot\left((1-p)(1-\varrho) + \frac{\varrho}{2}\right)\right] \leq e^{\frac{-\xi_2^4}{20}\cdot ks}, \tag{21}$$

$$\mathbb{P}\left[\Delta_R^{0-}(G_1, G_2, \psi) \geq \Delta_R^{-}(G_1, G_1, \psi)\cdot\left(p(1-\varrho) + \frac{\varrho}{2}\right)\right] \leq e^{\frac{-\xi_2^4}{20}\cdot ks}. \tag{22}$$

Finally, applying (20), (21) and (22), the probability of Υ_R^C can be bounded using subadditivity:

$$\begin{aligned}
\mathbb{P}(\Upsilon_R^C) &\leq \sum_{k=1}^{m}\sum_{\psi\in\Pi_\phi(k)}\left(2e^{\frac{-\xi_2^2}{400}ks} + e^{\frac{-\xi_2^4}{20}\cdot ks} + e^{\frac{-\xi_2^4}{20}\cdot ks}\right)\\
&\leq \sum_{k=1}^{m} m^k\left(2e^{\frac{-\xi_2^2}{400}ks} + 2e^{\frac{-\xi_2^4}{20}\cdot ks}\right)\\
&\leq \sum_{k=1}^{m}\left(2e^{\frac{-\xi_2^2}{400}ks + k\log m} + 2e^{\frac{-\xi_2^4}{20}\cdot ks + k\log m}\right) \leq m\cdot\frac{4}{m^3},
\end{aligned}$$

the last inequality holding if $s \geq c_5 \log m$ for sufficiently large, fixed constant c_5. Because $\sum_{m=1}^{\infty} \frac{4}{n^2} < \infty$ we have by the Borel-Cantelli Lemma that Υ_R almost always happens. As mentioned in Section A.5, this completes the proof of the first part of Theorem 2.

Remark 8 We do not chase the exact constant c_5 here, focusing on the order of magnitude of s instead. Also, if we allow p and ρ to vary with m, then a minor alteration of the above proof (and a tighter Chernoff-Hoeffding bound) yields the same conclusion as in Theorem 2.i if for (an arbitrary but) fixed $0 < \epsilon < 2$ and $q_1 := (1-p)(1-\varrho)$ and $q_2 := p(1-\varrho)$

$$\begin{aligned} c_5 &:= c_5(p, \varrho) \\ &> \max\left\{ \frac{2}{H(q_1 + \frac{\varrho}{2}, q_1) \cdot p(1-p)(2-\epsilon)}, \frac{2}{H(q_2 + \frac{\varrho}{2}, q_2) \cdot p(1-p)(2-\epsilon)}, \frac{16}{\epsilon^2 p(1-p)} \right\}. \end{aligned}$$

Details are left to the reader.

A.7 Proof of the Theorem 2, Part ii

We now prove the second part of Theorem 2.

Just for now, let $\psi \in \Pi(m)$ be chosen (i.e., none of the nonseeds are fixed points for ψ), and condition on $\Delta_R^+(G_1, G_1, \psi) = L$, where $\frac{9}{10} smp(1-p) \leq L \leq \frac{11}{10} smp(1-p)$. The random variables $\Delta_R^{0+}(G_1, G_2, \psi)$ and $\Delta_R^{0-}(G_1, G_2, \psi)$ are independent, and have distributions Binomial(L, q_1) and Binomial(L, q_2), respectively, where $q_1 := (1-p)(1-\varrho)$ and $q_2 := p(1-\varrho)$.

Denoting $r_1 := q_1 + \frac{\rho}{2}$ and $r_2 := q_2 + \frac{\varrho}{2}$, we have by Proposition 5 that

$$\begin{aligned} &\mathbb{P}\left(\Delta_R^{0+}(G_1, G_2, \psi) > L \cdot r_1 \text{ and } \Delta_R^{0-}(G_1, G_2, \psi) > L \cdot r_2 \right) \\ &\qquad \geq \frac{q_1 q_2}{200L} \sqrt{\frac{(1-r_1)(1-r_2)}{r_1 r_2}} e^{-L \cdot H(r_1, q_1) - L \cdot H(r_2, q_2)} \end{aligned}$$

Considering the bound on $H(x+y, y)$ described in Section A.4, we have that $H(r_1, q_1)$ and $H(r_2, q_2)$ are both bounded above by a constant. With the fact that $1 - r_1 = r_2$ and $1 - r_2 = r_1$, from the above we obtain that there is a positive real number c such that

$$\begin{aligned} \mathbb{P}\left(\Delta_R^{0+}(G_1, G_2, \psi) > L \cdot r_1 \text{ and } \Delta_R^{0-}(G_1, G_2, \psi) > L \cdot r_2 \right) &\geq \frac{c}{sm} \cdot e^{-\frac{sm}{c}} \\ &\geq \frac{c}{m \log m} \cdot e^{-\frac{sm}{c}} \end{aligned} \tag{23}$$

under the hypotheses of the second part of Theorem 2.

Next, $|\Pi_\phi(m)|$ is the number of derangements of an m element set, and it satisfies $\lim_{m\to\infty} \frac{|\Pi_\phi(m)|}{m!} = \frac{1}{e}$, thus with Stirling's formula we have that for m large enough it will

hold that $|\Pi(m)| \geq \left(\frac{m}{e}\right)^m$. Thus, for m large enough, by (15) and (23),

$$\begin{aligned}\mathbb{E}|\{\psi \in \Pi_\phi : \Delta_R(G_1, G_2, \psi) < \Delta_R(G_1, G_2, e)\}| &= \sum_{\psi \in \Pi_\phi} \mathbb{P}\Big(\Delta_R(G_1, G_2, \psi) < \Delta_R(G_1, G_2, e)\Big) \\ &\geq \sum_{\psi \in \Pi_\phi(m)} \mathbb{P}\Big(\Delta_R(G_1, G_2, \psi) < \Delta_R(G_1, G_2, e)\Big) \\ &\geq \left(\frac{m}{e}\right)^m \frac{c}{m \log m} \cdot e^{-\frac{sm}{c}} \\ &= \frac{c}{m \log m} \cdot e^{-\frac{sm}{c} + m \log m - m},\end{aligned}$$

so that there exists a fixed real number $c_6 > 0$ such that if $s \leq c_6 \log m$ then it follows that $\mathbb{E}|\{\psi \in \Pi_\phi : \Delta_R(G_1, G_2, \psi) < \Delta_R(G_1, G_2, e)\}| \to \infty$ as $m \to \infty$, and Theorem 2 part ii is proven.

Remark 9 We could tighten the constant c_6 here, but choose instead to focus on the order of magnitude of s. If we allow p and ϱ to be functions of m, then a simple alteration of the above proof yields the same results of Theorem 2.ii if

$$c_6 := c_6(p, \varrho) < \frac{1}{4\big[H(q_1 + \frac{\varrho}{2}, q_1) + H(q_2 + \frac{\varrho}{2}, q_2)\big]p(1-p)};$$

again details are left to the reader.

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