SPECTRE: Seedless Network Alignment via Spectral Centralities

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Abstract

Network alignment consists of finding a correspondence between the nodes of two networks. From aligning proteins in computational biology, to de-anonymization of social networks, to recognition tasks in computer vision, this problem has applications in many diverse areas. The current approaches to network alignment mostly focus on the case where prior information is available, either in the form of a seed set of correctly-matched nodes or attributes on the nodes and/or edges. Moreover, those approaches which assume no such prior information tend to be computationally expensive and do not scale to large-scale networks. However, many real-world networks are very large in size, and prior information can be expensive, if not impossible, to obtain.

In this paper we introduce SPECTRE, a scalable, accurate algorithm able to solve the network alignment problem with no prior information. SPECTRE makes use of spectral centrality measures and percolation techniques to robustly align nodes across networks, even if those networks exhibit only moderate correlation. Through extensive numerical experiments, we show that SPECTRE is able to recover high-accuracy alignments on both synthetic and real-world networks, and outperforms other algorithms in the seedless case.

Keywords: Network Alignment | Percolation | Spectral Graph Theory

1 Introduction

Network alignment, also known as graph matching or graph reconciliation, refers to the problem of finding a bijection between the nodes of two non-isomorphic networks in order to maximize the overlap between the sets of edges of both networks. The network alignment problem can be easily understood with the following particular example: assume we are given an arbitrary network $G$. From this network, we generate another network $G_1$ by randomly choosing a subset of edges from $G$ and shuffling the labels of nodes via a random permutation. We then repeat this procedure to generate another network $G_2$ by choosing another random subset of edges from $G$ and an independent random permutation of the nodal labels of $G_2$. As a result, we obtain from $G$ two non-isomorphic and correlated graphs, $G_1$ and $G_2$. Given these two graphs, the network alignment problem consists of finding a one-to-one correspondence between the sets of nodes of $G_1$ and $G_2$ (see Figure 1). This network alignment problem is a generalization
of the classical graph isomorphism problem, in which $G_1$ and $G_2$ are isomorphic, rendering a problem expected to be NP hard \cite{1}. In contrast, in the network alignment problem, the two graphs $G_1$ and $G_2$ need not be isomorphic and, therefore, a prescribed metric, such as the percentage of edge overlap, is maximized instead \cite{27}.

![Example of network alignment](https://example.com/fig1.png)

(a) Original graph, $G$. (b) First correlated graph, $G_1$. (c) Second correlated graph, $G_2$.  

Figure 1: Example of network alignment. First, we create an Erdős-Rényi graph $G(10, 0.42)$. We then generate two correlated graphs, $G_1$ and $G_2$, by independently dropping out edges of $G$ with probability $s = 0.2$. The ground-truth correspondence is illustrated by the position of the nodes: those in the same location across the three graphs correspond to one another.

Network alignment has applications in a wide range of disciplines. For example, in the field of social networks, it may be used to unveil the identities of anonymous individuals by aligning the structure of different online social networks, such as Facebook and Twitter \cite{30}.  

Another relevant example can be found in computational biology; in particular, in the study of protein-protein interaction (PPI) networks \cite{37, 20, 26}. The study of PPI networks provides an understanding of the system-level functions of each protein, as well as insights into how biological motifs are conserved through evolution. The problem of finding corresponding proteins across different species is instrumental in predicting their functionality. However, due to mutations, sometimes these proteins are expressed very differently \cite{39} and, thus, the alignment of PPI networks needs to rely on their structural correlation. A further application is in the field of computer vision, where graph alignment is used for tasks such as image registration, object recognition or symmetry analysis \cite{12}. In these problems, nodes represent salient points in images and edges are used to encode distances between them; thus, the network corresponding to an object can be aligned to networks built from a database in order to find images containing the same object.

In a pioneering work, Narayanan and Shmatikov \cite{30} considered the network alignment problem with partial side knowledge; in particular, they assume that apart from the graphs $G_1$ and $G_2$, the true correspondence between a subset of nodes, denoted as the seed set, is known \textit{a priori}. The authors in \cite{30} showed that by leveraging this seed set of correctly-matched nodes, it was possible to de-anonymize social networks with millions of users. Since this pioneering work was proposed, most approaches to network alignment assume the availability of side information in the form of seed sets \cite{44, 28}, or other types of side information, such as node and/or edge attributes \cite{46}. Although we find in the literature some approaches not using any form of side information \cite{21, 32}, their computational cost is of order $O(n^2)$ or higher, which quickly becomes infeasible for even moderately-sized networks. In practice, many real-world networks are very
large in size and, in many cases, prior side information is not available to solve the alignment problem. For example, in PPI networks, true correspondence information is essentially non-existent, as the proteins in the two networks to be aligned belong to different species. In such cases, retrieving useful prior information may become as hard as the alignment task itself. It is for this reason that an accurate, scalable algorithm with no prior side information is needed for alignment of large-scale networks.

In this paper, we present \textbf{SPECTRE} (Seedless PErcolation via spectral CenTRalitiEs), which is a scalable algorithm able to solve the network alignment problem with high accuracy without using prior side information. As described below, the algorithm is based on a “seed and expand” strategy: in the “seed” phase, we create a noisy seed estimate by matching nodes across networks according to spectral centrality measures. This initial seed estimate is then used in the “expand” phase, where nodes across networks are matched according to a similarity score relating to the set of correctly matched nodes \cite{19, 32}. The seed and expand phases of the SPECTRE algorithm can deal with a noisy seed set; in other words, we do not require the initial estimated seed set to be perfect.

In Section 5, we present extensive numerical results illustrating our algorithm’s performance, including comparisons to existing algorithms in social and biological networks. As we will see in Section 5 \textbf{SPECTRE} is able to align moderately correlated, large-scale networks with high accuracy. Moreover, \textbf{SPECTRE} shows a significant improvement over the state-of-the-art methods in aligning PPI networks. For example, on PPI networks of \textit{C. jejuni} and \textit{E. coli} bacteria, the best achieved performance in the literature for two popular metrics, called “edge correctness” and “induced conserved structure (ICS) score” \cite{32}, are 24% and 9%, respectively. However, by using \textbf{SPECTRE}, we obtain a 32% edge correctness and a 35% ICS score.

\textbf{Our Contributions:} Below we provide a summary of the main contributions of this paper.

- We introduce a new algorithm for network alignment called \textbf{SPECTRE}. To the best of our knowledge, this is the first scalable algorithm able to align graphs with high accuracy without prior side information.

- We propose the use of eigenvector centrality to rank nodes in order to create an initial noisy seed estimate. This initial seed estimate is then used in a “seed and expand” strategy to percolate an alignment through the networks. If necessary, our algorithm will run multiple percolation iterations in order to boost performance.

- We evaluate and analyze our algorithm on a number of real-world networks, as well as randomly generated synthetic networks. We show that \textbf{SPECTRE} exhibits excellent performance in terms of accuracy of the final matching, while being computationally scalable. Moreover, we show that the selection of the algorithm’s parameters can be done by directly examining the size of the final matching. We also compare \textbf{SPECTRE} to other algorithms in the literature, showing that it outperforms them in terms of runtime and also is able to handle dramatically larger networks.
2 Related Work

From a complexity theory standpoint, there have been recent developments in the study of the network alignment problem, as well as the closely-related graph isomorphism problem. In particular, a recent paper by Babai [1] provides an algorithm to solve this problem in quasi-polynomial time. A common benchmark to study the network alignment problem is the particular case in which $G$ is an Erdös-Rényi graph $G(n, p)$, hence, $G_1$ and $G_2$ are two correlated Erdös-Rényi graphs [33, 40]. For this particular choice, several polynomial-time algorithms for network alignment have been proposed for different sparsity regimes. In the case where the two graphs are perfectly correlated, Bollobás proposed in [5] linear time algorithms able to recover the exact matching with high probability when in the sparse regime $np = \log n + o(1)$. Moreover, Wright proved in [43] that, in the perfect correlation case, with probability $1 - o(1)$ it is information-theoretically impossible to perfectly solve the alignment problem outside of the regime $\log n + \omega(1) \leq np \leq n - \log n - \omega(1)$. A perfect recovery result as well as a converse impossibility bound were later established for correlated Erdös-Rényi graphs [10, 9]. Most notably, Mossel and Xu proposed in [29] a polynomial time algorithm able to recover the true alignment up to the theoretical threshold for Erdös-Rényi graphs. These results provide a very solid treatment of the alignment problem for the Erdös-Rényi model, but do not provide any guarantees for real-world graphs, for which more applicable heuristics have arisen.

In the case when $G_1$ and $G_2$ are two highly correlated non-isomorphic graphs, the network alignment problem can be formulated as a Quadratic Assignment Problem (QAP), see for example [13, 7]. This QAP has been shown to be difficult; even an approximation of the optimum within a factor of $2^{(\log n)^{1-\varepsilon}}$ is not solvable in polynomial time [25]. However, approximations to the QAP have been proposed, including: (1) exact search methods based on branch and bound [4] and cutting plane [3]; (2) linearizations of the problem [23, 18, 15], which tend to introduce many new variables and hinder the efficiency of mixed integer linear programming algorithms; (3) semidefinite and convex relaxations, aiming to bound the optimal value of the QAP [14]; (4) projected eigenvalue bounds [34] and matrix splittings [16], although in general these methods tend to incur a high computational cost and can only be used on small graphs.

In contrast with the theoretical efforts aiming to find rigorous quality guarantees for random graphs, we find an alternative literature focusing on the development of heuristic algorithms aiming to solve the network alignment problem for large-scale real-world networks. One of these algorithms was proposed in [30], where Narayanan and Shmatikov explored the idea of percolating correct matches starting from a given seed set. Further work has focused on deriving theoretical conditions for such percolations to be successful, both in terms of the given seed set [44] and properties of the graphs [8]. The authors of [19] expand on this idea by proposing an algorithm that is robust to incorrectly matched pairs in the given seed set. As a result, the proposed algorithm is able to increase accuracy while requiring fewer initial seeds. Another family of algorithms attempts to solve the network alignment problem by designing node-level signatures using different neighborhood statistics. For example, the GRAAL family
of algorithms uses a signature based on graphlet degree distributions and matches nodes with a range of methods ranging from seed-and-expand [22] to the Hungarian algorithm [21]. In [32] the authors propose another algorithm called GHOST, which uses a spectral signature of the 1-hop neighborhood of nodes and matches using a seed-and-expand procedure.

The aforementioned algorithms could, in principle, be used to align networks without an initial seed set, but the associated computational cost scales very poorly (worse than $O(n^2)$). The authors of [29] show that there exists a quasi-polynomial algorithm for the seedless case in Erdős-Rényi correlated networks guaranteeing a perfect alignment (with high probability) for a certain sparsity regime. However, their algorithm is based on the “beacon” method, which creates multiple seed sets by considering all possible assignments of a random set of nodes, which in practice is not feasible for large networks. In [11] we find an algorithm with a complexity of $O(n^2 \log n)$ based on matching high degree nodes, which asymptotically produces a perfect matching with high probability for correlated Erdős-Rényi graphs. This algorithm, although efficient, is only proven to work on a very narrow sparsity regime. Unfortunately these algorithms are not effective in the alignment of arbitrary networks.

On the other hand, several scalable methods have been proposed in the literature. For example, NetAlign [2] approximates an integer quadratic programming (for sparse networks) with a conditional random field which is solved using message-passing. EigenAlign [13] proposes a formulation similar to GRAAL and GHOST, building a node similarity metric using eigenvector centrality. EigenAlign then performs a bipartite matching to align the networks. This method was further adapted in [31] to build a low-rank approximation of the similarity matrix and perform a low-rank matching. The authors show that this low-rank matching sacrifices a small amount of accuracy for a dramatic improvement in runtime. In [17], the authors propose REGAL, an algorithm that jointly learns a node embedding for the two networks based on neighborhood statistics (and potentially other features). REGAL then finds a low-rank factorization that approximates a node similarity metric which is used to greedily match nodes. This algorithm significantly outperforms some other algorithms in the literature, but only for almost perfectly correlated networks (above 95% similarity). However, in most practical situations, networks will not be so highly correlated. Therefore, it is important to design algorithms able to produce accurate alignments when networks are only moderately similar.

### 3 Preliminaries

In this work we consider undirected graphs $G = (V, E)$, where $V = \{1, \ldots, n\}$ is the set of nodes and $E \subseteq V \times V$ is the set of unweighted edges. We assume $G$ is simple, i.e., it has no self-loops or multi-edges. If the edge $\{i, j\} \in E$ exists, we write $i \sim j$. We define the neighbors of node $i$ in $G$ as $N_i(G) := \{j \in V : i \sim j\}$, and the degree matrix as $D(G) = \text{diag}(|N_1(G)|, \ldots, |N_n(G)|)$. The adjacency matrix $A = A(G)$ is the matrix with entries $[A]_{ij} = 1\{i \sim j\}$. The product graph $G_{1\times 2}$ of $G_1$ and $G_2$ is the graph with vertex set $V_{1\times 2} = V_1 \times V_2$, and edge set $\{(i, j), (u, v)\} : \{i, u\} \in E_1, \{j, v\} \in E_2 \subseteq V_{1\times 2} \times V_{1\times 2}$. We refer to the eigenvalues of
a matrix \( M \in \mathbb{R}^{n \times n} \) in decreasing order of magnitude as \( \{ \lambda_1(M), \ldots, \lambda_n(M) \} \), and the largest eigenvalue as \( \lambda_{\text{max}}(M) = \lambda_1(M) \).

Formally, the problem of graph matching on two networks \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \) is to find a matching set \( M \subset V_1 \times V_2 \), so that \( (i, j) \in M \) means \( i \in V_1 \) corresponds to the same unique entity as \( j \in V_2 \), which we write as \( i \leftrightarrow j \). For example, in the context of social networks, we may imagine matching the account of an individual on Twitter to a Facebook account owned by the same individual. However, since the sets of users may be different in both networks, we may only hope to match pairs of nodes in \( V_1 \cap V_2 \). Given a matching \( M \), we will define the correspondence \( f_M : V_1 \to V_2 \) as \( f_M(i) = j \) if \( (i, j) \in M \), and undefined otherwise. Similarly, we define the set of matched nodes in \( V_2 \) as \( M(V_1) = \{ f_M(i) : i \in V_1, i \text{ matched} \} \) and the set of matched edges as \( M(E_1) = \{ (f_M(i), f_M(j)) : (i, j) \in E_1; i, j \text{ matched} \} \), which may include edges not present in \( E_2 \).

In order to measure the performance of our proposed algorithm, SPECTRE, it is necessary to have correlated networks where the true matching of nodes is available. In our numerical experiments, we create such networks from real-world data [36]. In order to symmetrically generate two networks while preserving access to the true matching information, we use the following procedure. We start with an arbitrary graph \( G = (V, E) \) and generate a random graph \( \tilde{G}_1 \) by independently subsampling each edge in \( G \) with a probability \( 1 - s \). Hence, \( \tilde{G}_1 \) has the same node set as \( G \) and an expected number of edges \( (1 - s)|E| \). We repeat this procedure, independently, to obtain a second graph \( \tilde{G}_2 \). Notice that, as a result of subsampling edges, \( \tilde{G}_1 \) and/or \( \tilde{G}_2 \) may become disconnected. To overcome this issue, we follow the iterative procedure described below. In a first step, we find the largest connected components of the two graphs, denoted by \( \tilde{C}_1 \) and \( \tilde{C}_2 \) respectively. We then look at the subgraphs of \( \tilde{G}_1 \) and \( \tilde{G}_2 \) induced by the nodes in \( \tilde{C}_1 \cap \tilde{C}_2 \). If these induced subgraphs are connected, we call them \( G_1 \) and \( G_2 \) and take them as the pair of networks to be aligned; if they are disconnected, we find their largest connected components and repeat these steps. This approach to generate correlated random graphs was introduced in [33] where the following edge similarity measure was also proposed:

\[
\text{Sim}_e(G_1, G_2) = 2 \sum_{i,j \in \tilde{V}_1} \frac{1 \{ \{i, j\} \in E_1, \{i, j\} \in E_2 \}}{|E_1| + |E_2|},
\]

although there are other ways to measure the similarity of two graphs [45].

4 Algorithms

In this section we introduce SPECTRE, a scalable algorithm to solve the network alignment problem in the absence of side information. The idea behind the algorithm is to create an initial set of seed pairs based on a naive matching of nodes with high spectral centrality, and then find new potential matchings by spreading this into the rest of the network. This spreading is done in two phases: (i) by matching a small number of pairs with high “confidence”, and (ii) subsequently performing a looser alignment on what remains. The resulting matching typically does
not fully percolate throughout the networks, and tends to have moderate accuracy. However, SPECTRE repeats this procedure multiple times by feeding the moderate-quality matching back to the algorithm in order to find a new seed set able to achieve much higher accuracy.

SPECTRE uses spectral properties of $G_1$ and $G_2$ to create a noisy initial seed set $A_0$, which will contain a number of correct pairs and many incorrect ones, as we will describe in Subsection 4.1. This initial set is not a proper matching, since the same node can be present in numerous pairs. $A_0$ is then used to build a true seed set estimate $A$, where nodes appear in at most one pair, following a procedure described in Subsection 4.3. In Subsection 4.3, we propose a mechanism to use this seed estimate to percolate a matching $M$ over the networks; if the percolation does not grow above a fraction $f$ of the networks’ size, the final matching is used as input to the algorithm again as if it were a noisy seed set, and the process is repeated. Typically we choose $f = 3/4$, but this parameter may be increased if a larger matching is desired.

Our algorithm is based on a seed-and-expand strategy for network alignment, originally proposed in [30]. This concept was further adapted in [19] to operate on a very small initial seed set through the use of “noisy pairs”, i.e., pairs that are included in the seed set but are not necessarily correct. While the adaptation in [19] dramatically reduced the reliance on the initial seed set, it still required ground-truth information in order to be effective. In Algorithm 1 below, we provide the general structure of SPECTRE, and in the following subsections we describe each subroutine in detail.

**Algorithm 1 SPECTRE.** SelectSeeds, BuildAndExpand, and Percolate are described in Subsections 4.1, 4.3, and 4.4, respectively.

**Input:** $G_1, G_2$, graphs to align; $k$, number of top seeds; $w$, size of window; $r$, token threshold

**Output:** $M$, the matching

\[ C_1, C_2 \leftarrow \text{eigenvector centralities of } G_1 \text{ and } G_2 \text{ (resp.)} \]

\[ A_0 \leftarrow \text{SelectSeeds}(k, w, C_1, C_2) \]

\[ \text{while } |M| < f \ast \min\{|V_1|, |V_2|\} \text{ do} \]

\[ A \leftarrow \text{BuildAndExpand}(r, A_0) \]

\[ M \leftarrow \text{Percolate}(A) \]

\[ A_0 \leftarrow M \]

\[ \text{end while} \]

\[ \text{return } M \]

### 4.1 SelectSeeds subroutine

SelectSeeds, the first subroutine in SPECTRE, constructs an initial noisy seed set containing some correct pairs, i.e., pairs of nodes that are correctly matched across the networks. To ensure that this occurs, nodes across networks should be matched using a procedure that is robust to perturbations in the network structure. In SPECTRE, this procedure is based on comparing the spectral centralities of nodes in different networks; an in-depth description of this choice is presented in Section 4.2. In particular, in order to create an initial noisy seed set $A_0$, we
rank the nodes of $G_1$ and $G_2$ by their centrality scores and keep the top $k$ most central nodes in each network. Then, we construct a list of potential matches across the networks by creating a bipartite graph $A_0$, where each part contains the top $k$ most central nodes in $G_1$ and $G_2$, respectively. The nodes in each part are ordered according to their relative ranking. The edges in this bipartite graph connect nodes across parts whose centralities differ by at most $w$ ranks for a given $w \in \mathbb{N}$. The rationale behind this choice of potential matches is that, for correlated graphs $G_1$ and $G_2$, nodes with high centrality in $G_1$ are likely to be aligned with nodes of high centrality in $G_2$. Furthermore, the centrality ranking of matched nodes should be similar for the most central nodes. As a result, our bipartite graph contains $(2w + 1)k - w(w + 1)$ pairs, of which no more than $k$ represent correct matches (see Example 1). While higher values of $w$ increase the probability of finding $k$ correct pairs, it also increases the number of incorrect pairs by $O(k)$, and thus we must be conservative with our choice of the parameter $k$.

**Example 1 (SelectSeeds).** Assume we wish to align the networks shown in Figure 2(a). The ground-truth matching is illustrated by labelling corresponding nodes as $\{i, i'\}$. To build the noisy seed estimate $A_0$ with $k = 3$ and $w = 1$, SelectSeeds will rank the nodes of each graph by their eigenvector centralities, and then pair the top $k = 3$ nodes with a window size of $w = 1$, i.e., each one of the 3 most central nodes from $G_1$ creates a pair with those nodes in $G_2$ whose centrality ranking differ in at most 1 with its own ranking, as shown in Figure 2(b). In this case, of the 7 noisy seed pairs created, only $(1, 1')$ and $(3, 3')$ are correct.

**Algorithm 2 SelectSeeds**

**Input:** $k$, number of top seeds; $w$, size of window; $C_1, C_2$, centrality scores

**Output:** $A_0$, noisy seed set

1. $A_0 \leftarrow \emptyset$
2. for each of top $k$ nodes $i \in V_1$ according to $C_1$ do
   1. add pairs $(i, j)$ to $A_0$ by selecting the correspondingly ranked node $j \in V_2$ according to $C_2$, as well as $w$ nodes before and after $j$ in the ranking.
3. end for

return $A_0$
4.2 Centrality

In order for SPECTRE to be successful, it is important that we are able to rank nodes using a feature representation that is robust to perturbations in network topology. In this paper, we choose several notions of centrality as our nodal feature. Node centralities are commonly used to measure the importance of nodes, and can be used to estimate the influence of individuals in social networks [42], the importance of web pages [6], or the certainty of node measurements [35]. In SPECTRE, we use two spectral centrality measures, namely the eigenvector centrality $C_{ev}$ and the PageRank centrality $C_{pr}$, which are formally defined as

$$C_{ev}(i) = [v_1]_i,$$

where $v_1$ is the eigenvector of $A(G)$ for $\lambda_{max}(A)$,

$$C_{pr}(i) = \beta + \alpha \sum_{j \in N_i} \frac{C_{pr}(j)}{|N_j|},$$

where $0 \leq \alpha < \lambda_{max}(D^{-1}A)^{-1}$ and $\beta > 0$ are constants.

These centrality measures are capable of being computed efficiently, even for large-scale networks. Indeed, modern algorithms allow the calculation of these centrality measures in $O(m)$ time and storage, where $m = |E|$, and the constants depend on $\lambda_1(A)$ and $\lambda_2(A)$ [41]. Interestingly, in practice, perturbations of the network topology do not dramatically change the ranking induced by these two centrality measures, at least for the nodes with the highest centrality. This phenomenon is illustrated in Figs. 7(c) and 8(c), where we show that even with an edge similarity of 60%, SelectSeeds is able to collect as many as 70% of the correct seed pairs. In this case 14 of the top 20 nodes, as measured by eigenvector centrality, changed no more than 3 spots in their relative rankings in both $G_1$ and $G_2$.

4.3 BuildAndExpand subroutine

The subroutine BuildAndExpand uses the initial noisy seed set $A_0$ from SelectSeeds to construct a proper seed estimate, i.e., a matching where each node is present in at most one pair (see Algorithm 3). BuildAndExpand builds a confidence score for each possible pair in $V_1 \times V_2$ by the accumulation of tokens spreading through the edges of the product graph $G_1 \times G_2$. In particular, each pair of nodes $(i, j) \in A_0$ creates and passes a token to each one of its neighboring pairs in $G_{1 \times 2}$. Notice that this set of neighboring pairs corresponds to all the pairs of nodes in $N_i(G_1) \times N_j(G_2)$. It is worth remarking that the originating pair $(i, j)$ does not accumulate the token created by itself. At the end of this spreading process, each pair of nodes in $V_1 \times V_2$ may have some number of tokens. In particular, only pairs which are neighbors (in the product graph) of pairs in the noisy seed set $A_0$ will receive any tokens.

In what follows, we sequentially grow the set of seed estimates $A$ according to the following procedure. First, we find the set of pairs in $V_1 \times V_2$ with the highest number of tokens, and pick one of these pairs at random. If the number of tokens accumulated by this chosen pair is greater than or equal to a thresholding parameter $r \in \mathbb{N}$, then we consider this pair to be a correct seed pair.

Other centrality measures were tested, including degree, betweenness, and closeness, but eigenvector and PageRank performed best empirically.
match and add it to the set $\mathcal{A}$. Based on the percolation bounds established in [44], the value of $r$ is typically chosen to be 4. Next, this chosen pair spreads new tokens to its neighboring pairs (in the product graph), increasing their scores by one. According to this updated score, we pick the pair with the highest number of tokens (breaking ties at random), excluding any pair containing an already matched node (i.e., any node contained in any pair in $\mathcal{A}$). We then add the chosen pair to $\mathcal{A}$, spread new tokens from this pair, and repeat this procedure until all remaining pairs have less than $r$ tokens. At the end of this iterative procedure, we obtain the set of seed estimates $\mathcal{A}$ representing a matching between nodes of $G_1$ and $G_2$. This matching is, in general, not perfect, since some nodes may be left unmatched.

Figure 3: Example of BuildAndExpand, with matching threshold $r = 3$. White pairs have no tokens, yellow have at least one token (with border thickness denoting total number), green are matched, and red are removed (one or both nodes already matched in another pair). Arrows describe the direction in which tokens are spread.

**Example 2 (BuildAndExpand).** To illustrate BuildAndExpand, we will continue from Example II using the product graph $G_{1\times2}$ of the networks in Figure II. Since the product graph contains 25 nodes and is cumbersome to visualize, in Figure IV we only show the subgraph of $G_{1\times2}$ induced by the neighboring pairs of $(3, 3')$. Since $(1, 1'), (3, 3')$ and $(2, 1')$ are in the initial seed set $\mathcal{A}_0$, they will be the pairs spreading tokens in the initial stage of this subroutine. After all tokens are spread, the pair with the highest number of tokens is $(2, 2')$; hence, this pair is added to $\mathcal{A}$. As a consequence, the nodes 2 ∈ $V_1$ and 2' ∈ $V_2$ are matched and we remove $(2, 1')$ and $(1, 2')$ from the set of candidate pairs. Following our algorithm, new tokens are spread from $(2, 2')$, increasing the scores of its neighboring pairs by one. We then find the new set of

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2Note that, in reality, the final seed estimate $\mathcal{A}$ obtained from the entire product graph would be slightly different.
highest-scoring pairs, randomly choose \((1, 1')\) from this set, add it to \(A\), and spread new tokens from it. After this, the only remaining pair to be matched is \((3, 3')\). Since the number of tokens accumulated by \((3, 3')\) is greater than \(r = 3\), we add this last pair to \(A\). In this example, all three pairs that are matched are correct.

**Algorithm 3 BuildAndExpand**

**Input:** \(r\), token threshold; \(A_0\), noisy seed set  
**Output:** \(A\), seed estimate  

\[
A \leftarrow \emptyset  
\]

\[
\text{for each pair } (i, j) \in A_0 \text{ do} \quad \triangleright \text{Build seed estimate}  
\]

\[
\quad \text{spread tokens to each neighboring pair of } (i, j)  
\]

\[
\text{end for}  
\]

\[
\text{while any unmatched pair has score } \geq r \text{ do} \quad \triangleright \text{Expand seed estimate}  
\]

\[
\quad \text{select } (i, j) \text{ at random from highest-scoring pairs and add to } A  
\]

\[
\quad \text{spread tokens to each neighboring pair of } (i, j)  
\]

\[
\text{end while}  
\]

\[
\text{return } A  
\]

**4.4 Percolate subroutine**

The last subroutine, **Percolate**, takes the seed estimate set \(A\) as an input and repeatedly grows a final matching (see Algorithm 4). **Percolate** starts by spreading tokens from all the pairs in \(A\). Then, we find all the pairs composed of unmatched nodes with the highest number of tokens. Among those pairs, we select the pair with the lowest difference in the centrality scores and add it to \(M\). The selected pair then spreads tokens to its neighbors in the product graph only if it has not previously spread tokens. We use this procedure to iteratively add pairs to \(M\) until no pairs composed of unmatched nodes have two or more tokens. Then, \(A\) is rebuilt from scratch by taking all unmatched neighbors of matched pairs (i.e., all unmatched pairs with exactly one token), and the process is repeated. This continues until no unmatched neighbors of matched pairs exist, and the final matching \(M\) is returned.

It is noteworthy to emphasize that the initial seed set \(A_0\), generated by **SelectSeeds**, typically contains a large fraction of incorrect pairs. However, since correct pairs spread tokens more effectively, the algorithms **BuildAndExpand** and **Percolate** are able to robustly percolate and find an accurate alignment, even in the presence of many incorrect pairs in \(A_0\). Indeed, a correct pair is much more likely to receive tokens from other correct pairs rather than wrong pairs. As a result, provided that there are a sufficient amount of correct pairs in the initial seed set, then **BuildAndExpand** and **Percolate** will be able to overcome the presence of wrong pairs and percolate over the set of all the correct pairs.

**Example 3 (Percolate).** Assume we receive a seed estimate \(A = \{(1, 1'), (2, 2'), (3, 3')\}\). We repeat the seed-and-expand procedure from **BuildAndExpand**, matching pairs with 2 or more
tokens and breaking ties in highest-scoring pairs by the difference in nodal centrality, rather than randomly. For illustration purposes we show the rebuilding step: assume only \((1, 2')\) is matched. After exhausting all pairs with 2 or more tokens, we rebuild \(A\) using all unmatched neighbors of matched pairs, as shown in Figure 3. These pairs spread tokens if they have not done so already, and the matching continues. If no such pairs remain, Percolate ends.

(a) \((1, 2')\) matched and spreads, (b) \(A = \{(1, 1'), (3, 3'), (2, 2')\}\) (c) Pairs in \(A\) spread tokens, if no other pairs have 2+ tokens. is rebuilt from scratch. they have not already.

Figure 4: Example of Percolate rebuilding. White pairs have no tokens, yellow have at least one, and green are matched. Arrows describe the direction in which tokens are spread.

**Algorithm 4 Percolate**

**Input:** \(A\), seed estimate

**Output:** \(M\), the matching

\[
M, Z \leftarrow \emptyset; Z \text{ is used pairs}
\]

while \(|A| > 0\) do

for each pair \((i, j) \in A\) do

spread tokens to each neighboring pair of \((i, j)\), add \((i, j)\) to \(Z\)

end for

while any pair of unmatched nodes has \(\geq 2\) tokens do

from highest-scoring pairs, select \((i, j)\) with lowest \(|C_1(i) - C_2(j)|\) and add it to \(M\) if \((i, j) \not\in Z\) then

spread tokens to each neighboring pair of \((i, j)\), add \((i, j)\) to \(Z\)

end if

end while

\(A \leftarrow \{(i', j') | (i', j') \text{ neighbor of } (i, j) \in M, (i', j') \not\in Z, i' \& j' \text{ unmatched}\}\)

end while

return \(M\)
5 Numerical Experiments

In order to verify the effectiveness of SPECTRE, we ran numerous experiments on a variety of networks, both from real-world data such as protein-protein interactions (PPI) \[37, 20, 26\], as well as social networks \[36, 24\]. We measure the performance of SPECTRE across five different metrics. The first is *Precision*, which measures the percentage of correct pairs in the final matching $\mathcal{M}$. The second is *Recall*, or true positive rate, which is the fraction of possible correct pairs that are identified in $\mathcal{M}$. Since our algorithm may only hope to label nodes with degree at least 2 (due to how Percolate matches pairs), we measure the fraction of these nodes which are in $\mathcal{M}$.

We will also measure the performance of SelectSeeds on finding correct pairs in the initial noisy seed estimate $\mathcal{A}_0$. The number and percent of correct pairs are simply the number (resp. percentage) of total pairs in $\mathcal{A}_0$ generated by SelectSeeds which actually correspond to one another. Lastly, we measure the runtime of SPECTRE, i.e. the total time it takes to run on the given networks (these experiments were performed on an Inter Core i7 at 2.2GHz). In summary, we can formally define the first four metrics as follows:

\[
\text{Prec}(\mathcal{M}) = \frac{|\{(i, j) \in \mathcal{M} : i \leftrightarrow j\}|}{|\mathcal{M}|},
\]

\[
\text{Recall}(\mathcal{M}) = \frac{|\{(i, j) \in \mathcal{M} : i \leftrightarrow j\}|}{|\{v \in \mathcal{V}_1 \cap \mathcal{V}_2 : |\mathcal{N}_v(\mathcal{G}_1)| \geq 2, |\mathcal{N}_v(\mathcal{G}_2)| \geq 2\}|},
\]

\[
\text{Number Correct}(\mathcal{A}_0) = |\{(i, j) \in \mathcal{A}_0 : i \leftrightarrow j\}|,
\]

\[
\text{Percent Correct}(\mathcal{A}_0) = \frac{|\{(i, j) \in \mathcal{A}_0 : i \leftrightarrow j\}|}{|\mathcal{A}_0|}.
\]

An issue with these metrics is that they require us to know the ground truth of the node correspondences. However, in most realistic scenarios, these correspondences would not be available to us. Following the approach in \[32\], we measure the quality of our alignments using the Edge Correctness (EC) and Induced Conserved Structure (ICS) score. As described below, these two scores depend solely on topological information. In particular, Edge Correctness measures the fraction of matched edges from $\mathcal{E}_1$, denoted by $\mathcal{M}(\mathcal{E}_1)$, which are present in $\mathcal{E}_2$. In other words, EC measures the fraction of edges which are correctly matched by $\mathcal{M}$. However, EC does not penalize $\mathcal{M}$ for omitting edges in $\mathcal{E}_2$ which should be present. For this reason we also measure the ICS score, which measures the fraction of matched edges present in the subgraph of $\mathcal{G}_2$ induced by the nodes which are matched, i.e., those nodes in $\mathcal{M}(\mathcal{V}_1)$. The ICS score penalizes the matching both for omitting edges that are present in $\mathcal{E}_1$ and those that are present in $\mathcal{E}_2$. Formally,

\[
\text{EC}(\mathcal{G}_1, \mathcal{G}_2, \mathcal{M}) = \frac{|\mathcal{M}(\mathcal{E}_1) \cap \mathcal{E}_2|}{|\mathcal{E}_1|},
\]

\[
\text{ICS}(\mathcal{G}_1, \mathcal{G}_2, \mathcal{M}) = \frac{|\mathcal{M}(\mathcal{E}_1) \cap \mathcal{E}_2|}{|\{(i, j) \in \mathcal{E}_2 : i, j \in \mathcal{M}(\mathcal{V}_1)\}|}.
\]
5.1 Correlated Networks

Our first numerical experiments are run on correlated networks generated by randomly sampling the edges of a given arbitrary graph $G$. In particular, we select each edge in $G$ with a probability $1 - s$, independently of other samples. Performing this sampling twice and shuffling the labels of the resulting graphs, we obtain two sparse graphs, $G_1$ and $G_2$, to be aligned. We generate these networks so that the ground-truth information about node correspondences is available to us; hence, we can measure the accuracy of the alignment SPECTRE produces. Moreover, by tuning the edge dropout probability $s$, we may test our algorithm on pairs of networks with different levels of correlation. Hence, we can measure the performance of SPECTRE as a function of the level of correlation of the networks to be aligned.

Our first set of experiments use pairs of correlated graphs generated from a real dataset called GEMSEC-Artists [36], which is a (social) network taken from the Facebook pages of artists. The nodes in this network represent artists’ pages, with an edge between a pair of artists if one liked the other’s page. The network properties of the pairs of graphs generated by the edge dropout process are shown in Table 1. Figures 5 to 9 show how SPECTRE performs on these networks based on the metrics described earlier. Notably, as shown in Figures 5 and 9, SPECTRE is able to achieve high-precision matchings in reasonable amounts of time for large-scale networks, even when the pairs of networks to be aligned exhibit low levels of correlation. This point illustrates the robustness of our approach, which is an important differentiating factor between SPECTRE and other scalable seedless algorithms, such as [17].

Table 1: Network Properties

| Orig. Network     | $Sim_\varepsilon(G_1, G_2)$ | $|V_1| = |V_2|$ | $|\mathcal{E}_1|$ | $|\mathcal{E}_2|$ | Avg. Deg. |
|------------------|----------------------------|----------------|-----------------|----------------|-----------|
| GEMSEC-Artists   | 0.90024                    | 49,914         | 737,828         | 737,147        | 14.78     |
|                  | 0.80068                    | 48,960         | 654,135         | 654,094        | 13.36     |
|                  | 0.60030                    | 48,512         | 490,365         | 489,905        | 10.10     |
|                  | 0.50506                    | 45,167         | 407,824         | 406,753        | 9.03      |

We can see the percolation behavior in Figures 5(c) and 6(c) specifically, the efficacy of repeatedly re-running BuildAndExpand and Percolate to boost the alignment performance. In these figures, we observe thresholding behavior; in particular, the matching will either succeed in percolating throughout the networks, achieving high precision and recall, or it will fail and perform poorly. This empirical result is similar to the percolation phenomenon in Erdős-Rényi graphs [44], as well as empirical studies on real-world networks [38]. The main reason for performing the boosting step in SPECTRE is to encourage the success of this percolation. By seeding BuildAndExpand with the previous matching that did not spread well, we may enable the percolation to succeed after further iterations have taken place. In practice this effect induces a much larger and more accurate network alignment. As Figure 5(c) shows, we may achieve high-quality alignments even in networks which are not very correlated.
As discussed in Section 4.1, the process of seed selection requires the parameters $k$ and $w$ to be chosen manually. We do a sweep of the parameters with $k \in \{20, 30, \ldots, 100\}$ and $w \in \{1, 2, 3\}$ to study their influence on the performance of SPECTRE. As suggested in Section 4, we fix $f = \frac{3}{4}$, $r = 4$, and use eigenvector centrality to build the initial noisy seed estimate. Since we will be running SPECTRE multiple times, we compute the eigenvector centrality once for the first set of parameters and do not include it in our runtime (this calculation takes around 45 seconds for this large network on an Intel Core i7 at 2.2GHz). Intuitively, increasing $k$ should allow for the possibility of more correct pairs to be included, and a larger $w$ increases the probability of placing correct pairs in the initial seed estimate. This intuition is supported by our empirical results, as shown in Fig. 7. However, increasing these parameters is not free since a larger proportion of incorrect (or noisy) pairs are included in the seed set, as shown in Fig. 8. In a situation with no prior or side information about the network, it is not clear how to choose the optimal $k$ and $w$. We do observe that networks which are more correlated require a smaller $w$. Indeed, when the networks are very correlated, any values of $k$ and $w$ tend to perform well, as illustrated in Figures 5(a) and 6(a). Fortunately, in all our cases, there is a strong correlation between the size of the percolation and the accuracy of the resulting matching. More precisely, if SPECTRE manages to percolate throughout a large portion of both networks, it is likely that the resulting matching will have high accuracy, as shown in Figures 5 and 6 (most clearly in 5(c) and 6(c)). In all cases, we limit the number of iterations of BuildAndExpand and Percolate to be no more than five. Hence, in a practical situation, one may try several values for the parameters $k$ and $w$ and pick the matching with the largest final size, or number of matched pairs, and with high likelihood it will be the most accurate.

Another practical consideration is that larger values of $k$ and $w$ tend to induce higher run-times, as larger noisy seed estimates takes longer to spread in the BuildAndExpand subroutine. However, the largest impact on running time is from the boosting rounds, as each additional iteration of BuildAndExpand and Percolate takes several minutes on large networks. This effect can clearly be seen in Figure 9(e) notice that the behavior is not exactly monotonic due to the randomness in the way BuildAndExpand breaks ties, which in some cases may result in poor seed estimates.

![Figure 5: Precision (y-axis) of SPECTRE on GEMSEC-Artists network.

(a) 90% Correlated  (b) 80% Correlated  (c) 60% Correlated  (d) 50% Correlated](image-url)
Figure 6: Recall (y-axis) of SPECTRE on GEMSEC-Artists network.

Figure 7: Number of correct pairs (y-axis) from SelectSeeds on GEMSEC-Artists network.

Figure 8: Percentage of correct pairs (y-axis) from SelectSeeds on GEMSEC-Artists network.

Figure 9: Runtime in minutes (y-axis) of SPECTRE on GEMSEC-Artists network.

5.2 Protein-Protein Interaction Networks

In the case of protein-protein interaction (PPI) networks, nodes correspond to proteins, and edges are placed between them if they participate in interactions together. We may not know the ground-truth matching, but we are looking for proteins that perform similar functions across species. We will consider the PPI networks of the bacteria species Campylobacter jejuni (C. jejuni) and Escherichia Coli (E. coli) from the HitPredict Database [24], which have been used as a benchmark by other algorithms such as MI-GRAAL [22] and GHOST [32]. Using SPECTRE, we achieve an Edge Correctness of 32% and ICS score of 35%, which is a significant...
increase over both GHOST and MI-GRAAL.

Figure 10 summarizes the results of running SPECTRE on the PPI networks. In these experiments, we fix $f = 3/4$, $r = 4$, use eigenvector centrality to generate the initial seed estimate, and ran a sweep of our parameters with $k \in \{20, 30, \ldots, 100\}$ and $w \in \{1, 2, 3\}$. We permitted SPECTRE to run no more than five iterations of BuildAndExpand and Percolate. Again we observe a correlation between the size of the final matching and the quality of the alignment, both as measured by Edge Correctness and ICS score. The runtime of SPECTRE is lowest for $w = 1$ and, interestingly, the best alignment in terms of Edge Correctness and ICS score is for $w = 1$, with $k = 90$. These results illustrate that SPECTRE is robust even when aligning large-scale real-world networks without any prior information. Moreover, it outperforms most approaches found in the literature in terms of accuracy, while being much more computationally scalable.

![Figure 10: Performance of SPECTRE on C. jejuni and E. coli PPI networks.](image)

(a) Edge Correctness  
(b) ICS score  
(c) Runtime (sec)

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