Graph Similarity and Approximate Isomorphism

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Abstract

The graph similarity problem, also known as approximate graph isomorphism or graph matching problem, has been extensively studied in the machine learning community, but has not received much attention in the algorithms community: Given two graphs $G, H$ of the same order $n$ with adjacency matrices $A_G, A_H$, a well-studied measure of similarity is the Frobenius distance

$$\text{dist}(G, H) := \min_\pi \| A_G^{\pi} - A_H \|_F,$$

where $\pi$ ranges over all permutations of the vertex set of $G$, where $A_G^{\pi}$ denotes the matrix obtained from $A_G$ by permuting rows and columns according to $\pi$, and where $\|M\|_F$ is the Frobenius norm of a matrix $M$. The (weighted) graph similarity problem, denoted by GSIm (WSIm), is the problem of computing this distance for two graphs of same order. This problem is closely related to the notoriously hard quadratic assignment problem (QAP), which is known to be NP-hard even for severely restricted cases.

It is known that GSIm (WSIm) is NP-hard; we strengthen this hardness result by showing that the problem remains NP-hard even for the class of trees. Identifying the boundary of tractability for WSIm is best done in the framework of linear algebra. We show that WSIm is NP-hard as long as one of the matrices has unbounded rank or negative eigenvalues: hence, the realm of tractability is restricted to positive semi-definite matrices of bounded rank. Our main result is a polynomial time algorithm for the special case where one of the matrices has a bounded clustering number, a parameter arising from spectral graph drawing techniques.

1 Introduction

Graph isomorphism has been a central open problem in algorithmics for the last 50 years. The question of whether graph isomorphism is in polynomial time is still wide open, but at least we know that it is in quasi-polynomial time [4]. On the practical side, the problem is largely viewed as solved; there are excellent tools [9, 16, 21, 22] that efficiently decide isomorphism on all but very contrived graphs [25]. However, for many applications, notably in machine learning, we only need to know whether two graphs are “approximately isomorphic”, or more generally, how “similar” they are. The resulting graph similarity problem has been extensively studied in the machine learning literature under the name graph matching (e.g. [1, 10, 15, 29, 30]), and also in the context of the schema matching problem in database systems (e.g. [23]). Given the practical significance of the problem, surprisingly few theoretical results are known. Before we discuss these known and our new results, let us state the problem formally.

Graph similarity. It is not obvious how to define the distance between two graphs, but the distance measure that we study here seems to be the most straightforward one, and it certainly
is the one that has been studied most. For two $n$-vertex graphs $G$ and $H$ with adjacency matrices $A_G$ and $A_H$, we define the Frobenius distance between $G$ and $H$ to be

$$
\text{dist}(G, H) := \min_{\pi} \| A_G^\pi - A_H \|_F.
$$

Here $\pi$ ranges over all permutations of the vertex set of $G$, $A_G^\pi$ denotes the matrix obtained from $A_G$ by permuting rows and columns according to $\pi$, and the norm $\| M \|_F := \sqrt{\sum_{i,j} M_{ij}^2}$ is the Frobenius norm of a matrix $M = (M_{ij})$. Note that $\text{dist}(G, H)^2$ counts the number of edge mismatches in an optimal alignment of the two graphs. The graph similarity problem, denoted by $\text{GSim}$, is the problem of computing $\text{dist}(G, H)$ for graphs $G, H$ of the same order, or, depending on the context, the decision version of this problem (decide whether $\text{dist}(G, H) \leq d$ for a given $d$). We can easily extend the definitions to weighted graphs and denote the weighted graph similarity problem by $\text{WSim}$. In practice, this is often the more relevant problem. Instead of the adjacency matrices of graphs, we may also use the Laplacian matrices of the graphs to define distances. Recall that the Laplacian matrix of a graph $G$ is the matrix $L_G := D_G - A_G$, where $D_G$ is the diagonal matrix in which the entry $(D_G)_{ii}$ is the degree of the $i$th vertex, or in the weighted case, the sum of the weights of the incident edges. Let $\text{dist}_L(G, H) := \min_{\pi} \| L_G^\pi - L_H \|_F$ be the corresponding distance measure. Intuitively, in the definition of $\text{dist}_L(G, H)$ we prefer permutations that map vertices of similar degrees onto one another. Technically, $\text{dist}_L(G, H)$ is interesting, because the Laplacian matrices are positive semidefinite (if the weights are nonnegative). Both the (weighted) similarity problem and its version for the Laplacian matrices are special cases of the problem $\text{MSim}$ of computing $\min_P \| A - PBP^{-1} \|_F$ for given symmetric matrices $A, B \in \mathbb{R}^{n \times n}$. In the Laplacian case, these matrices are positive semidefinite.$^1$

The QAP. The graph similarity problem is closely related to quadratic assignment problem (QAP) [6]: given two $(n \times n)$-matrices $A, B$, the goal is to find a permutation $\pi \in S_n$ that minimizes $\sum_{i,j} A_{ij} B_{\pi(i)\pi(j)}$. The usual interpretation is that we have $n$ facilities that we want to assign to $n$ locations. The entry $A_{ij}$ is the flow from the $i$th to the $j$th facility, and the entry $B_{ij}$ is the distance from the $i$th to the $j$th location. The goal is to find an assignment of facilities to locations that minimizes the total cost, where the cost for each pair of facilities is defined as the flow times the distance between their locations. The QAP has a large number of real-world applications, as for instance hospital planning [12], typewriter keyboard design [27], ranking of archeological data [18], and scheduling parallel production lines [14]. On the theoretical side, the QAP contains well-known optimization problems as special cases, as for instance the Travelling Salesman Problem, the feedback arc set problem, the maximum clique problem, and all kinds of problems centered around graph partitioning, graph embedding, and graph packing.

In the maximization version $\text{MAX-QAP}$ of QAP the objective is to maximize $\sum_{i,j} A_{ij} B_{\pi(i)\pi(j)}$ (see [19, 24]). Both QAP and $\text{MAX-QAP}$ are notoriously hard combinatorial optimization problems, in terms of practical solvability [28] as well as in terms of theoretical hardness results even for very restricted special cases [5, 8, 7]. It is easy to see that $\text{MSim}$ is equivalent to $\text{MAX-QAP}$, because in reductions between QAP and $\text{MSim}$ the sign of one of the two matrices is flipped. Most of the known results for $\text{GSim}$ and its variants are derived from results for $\text{MAX-QAP}$.

$^1$Note that the notion of similarity that we use here has nothing to do with the standard notion of “matrix similarity” from linear algebra.
Previous Work. It seems to be folklore knowledge that GSIM is NP-complete. For example, this can be seen by a reduction from the Hamiltonian path problem: take $G$ to be the $n$-vertex input graph and $H$ a path of length $n$; then $\text{dist}(G, H) \leq \sqrt{|E(G)|} - n$ if and only if $G$ has a Hamiltonian path. By the same argument, we can actually reduce the subgraph isomorphism problem to GSIM. Arvind, Köbler, Kuhnert, and Vasudev [3] study several versions of what they call approximate graph isomorphism; their problem Min-PGI is the same as our GSIM. They prove various hardness of approximation results. Based on an earlier QAP-approximation algorithm due to Arora, Frieze, and Kaplan [2], they also obtain a quasi-polynomial time approximation algorithm for the related problem Max-PGI. Further hardness results were obtained by Makarychev, Manokaran, and Sviridenko [19] and O’Donnell, Wright, Wu, and Zhou [26], who prove an average case hardness result for a variant of GSIM problem that they call robust graph isomorphism. Keldenich [17] studied the similarity problem for a wide range matrix norms (instead of the Frobenius norm) and proved hardness for essentially all of them.

Spectral Graph Visualization. Since WSIM and MSIM are essentially linear algebraic problems, it is reasonable to hope that the spectral structure of the input (adjacency) matrices is closely related with the computational complexity of these problems. In this regard, we remark that spectral graph drawing is a well-established technique for visualizing graphs via their spectral properties. Formally, let $G$ be a $n$-vertex graph: a graph drawing is a map $\rho : V(G) \mapsto \mathbb{R}^k$, where the ambient space has dimension $k \ll n$. For spectral graph drawings, this map is typically defined as follows. We select a suitable matrix representation of the graph and select up to $k$ eigenvectors $u_1, \ldots, u_k$ of this matrix. Then, the mapping $\rho : V(G) \mapsto \mathbb{R}^k$ is defined by the rows $\{r_1, \ldots, r_n\}$ of the $n \times k$ matrix $[u_1 \cdots u_k]$. The choice of the matrix representation and the selection of eigenvectors usually depends on the problem at hand. The most useful matrix representation in the spectral drawing framework is the well-known Laplacian matrix: the eigenvectors $u_1, \ldots, u_k$ corresponding to $k$ smallest eigenvalues define the drawing $\rho$ of interest.

Observe that the graph drawing $\rho$ defined above is not injective in general. Given such a drawing $\rho$, we define the clustering number of a graph $G$ to be the cardinality of the set $\text{Image}(\rho)$. The elements of $\text{Image}(\rho)$ correspond to subsets of $V(G)$: every vertex in such a ‘cluster’ has identical adjacency.

Our results. So where does all this leave us? Well, GSIM is obviously an extremely hard optimization problem. We start our investigations by adding to the body of known hardness results: we prove that GSIM remains NP-hard even if both input graphs are trees (Theorem 3.2). Note that in strong contrast to this, the subgraph isomorphism problem becomes easy if both input graphs are trees [20]. The reduction from Hamiltonian path sketched above shows that GSIM is also hard if one input graph is a path. We prove that GSIM is tractable in the very restricted case that one of the input graphs is a path and the other one is a tree (Theorem 3.3).

As WSIM and MSIM are essentially linear algebraic problems, it makes sense to look for algebraic tractability criteria. We explore bounded rank (of the adjacency matrices) as a tractability criterion for WSIM and MSIM. Indeed, the NP-hardness reductions for GSIM involve graphs which have adjacency matrices of high rank (e.g. paths, cycles). We show that the problem GSIM (and WSIM) remains NP-hard as long as one of the matrices has unbounded rank or negative eigenvalues. (Theorems 3.4, 3.5 and 3.6). Consequently, the realm of tractability for WSIM (and MSIM) is restricted to the class of positive semi-definite matrices of bounded rank. We feel that for a problem as hard as QAP or MSIM, identifying any somewhat natural tractable special case is worthwhile. Our main result (Theorem 4.1) is a polynomial time algorithm for MSIM if both input matrices are positive semidefinite (as it is the case for the Laplacian version.
of WSIM) and have bounded-rank, and where one of the matrices has a bounded clustering number.

For the proof of Theorem 4.1, we can re-write the (squared) objective function as \( \|AP - PB\|_F^2 \), where \( P \) ranges over all permutation matrices. This is a convex function, and it would be feasible to minimize it over a convex domain. The real difficulty of the problem lies in the fact that we are optimizing over the complicated discrete space of permutation matrices. Our approach relies on a linearization of the solution space, and the key insight (Lemma 4.2) is that the optimal solution is essentially determined by polynomially many hyperplanes. To prove this, we exploit the convexity of the objective function in a peculiar way.

2 Preliminaries

2.1 Notation

We denote the set \( \{1, \ldots, n\} \) by \([n]\). Unless specified otherwise, we will always assume that the vertex set of an \( n \)-vertex graph \( G \) is \([n]\). We denote the degree of a vertex \( v \) by \( d_G(v) \).

Matrices. Given an \( m \times n \) matrix \( M \), the \( i \)th row (column) of \( M \) is denoted by \( M^i (M^i) \). The multiset \( \{M^1, \ldots, M^m\} \) is denoted by \( \text{rows}(M) \). Given \( S \subseteq [m] \), the sum \( \sum_{i \in S} M^i \) is denoted by \( M^S \). We denote the \( n \times n \) identity matrix by \( I_n \).

A real symmetric \( n \times n \) matrix \( M \) is called positive semi-definite (p.s.d), denoted by \( M \succeq 0 \), if the scalar \( z^T M z \) is non-negative for every \( z \in \mathbb{R}^n \). The following conditions are well-known to be equivalent.

1. \( M \succeq 0 \)
2. Every eigenvalue of \( M \) is non-negative.
3. \( M = W^T W \) for some \( n \times n \) matrix \( W \). In other words, there exist \( n \) vectors \( w_1, \ldots, w_n \in \mathbb{R}^n \) such that \( M_{ij} = w_i^T w_j \).

Given two vectors \( x, y \in \mathbb{R}^n \), their dot product \( \langle x, y \rangle \) is defined to be \( x^T y \). Given \( M \succeq 0 \), the inner product of \( x, y \) w.r.t. \( M \), denoted by \( \langle x, y \rangle_M \), is defined to be \( x^T M y \). The usual dot product corresponds to the case \( M = I \), the identity matrix.

Every \( n \times n \) symmetric matrix \( M \) of rank \( k \) has a spectral decomposition \( M = U \Sigma U^T \). Here, \( \Sigma \) is a \( k \times k \) diagonal matrix with the eigenvalues \( \lambda_1, \ldots, \lambda_k \in \mathbb{R} \) on the diagonal. The matrix \( U \) is a \( n \times k \) matrix with the corresponding eigenvectors \( v_1, \ldots, v_k \) as the columns \( U_1, \ldots, U_k \).

Graphs and Matrices. The Laplacian matrix of a (weighted) undirected graph \( G \), denoted by \( L_G \), is defined as follows. Let \( A \in \mathbb{R}^{n \times n} \) be the symmetric (weighted) adjacency matrix of \( G \). Let \( D \) be a \( n \times n \) diagonal matrix, such that \( D_{ii} \) is the sum of weights of the edges incident on the \( i \)th vertex. For simple undirected graphs, \( D_{ii} = d_G(v_i) \). Define the Laplacian of \( G \) as \( L(G) = D - A \). This definition allows us to express the quadratic form \( x^T L_G x = \sum_{\{i,j\} \in E(G)} a_{ij} (x_i - x_j)^2 \).

The above expression immediately implies that \( L_G \) is positive semi-definite.

Clustering Number. Recall the following definitions from Section 1. Given a \( n \)-vertex graph \( G \), a graph drawing is a map \( \rho : V(G) \rightarrow \mathbb{R}^k \), where the ambient dimension \( k \ll n \). We will use
the adjacency matrix $A$ of a graph $G$ to generate spectral graph drawings as follows. Let the rank of $A$ be $k$, and let $A = U \Lambda U^T$ be a spectral decomposition. Denote $U = [u_1 \cdots u_k]$, where $u_1, \ldots, u_k$ are the eigenvectors of $A$. The mapping of our interest $\rho : V(G) \rightarrow \mathbb{R}^k$ is defined by the rows $\{r_1, \ldots, r_n\}$ of the $n \times k$ matrix $U$. Given any two spectral decompositions $A = U \Lambda U^T$ and $A = U' \Lambda U'^T$, it holds that $U' = UO_k$ for some $k \times k$ orthogonal matrix $O_k$. Since $O_k$ is invertible, the number of distinct tuples in the set rows$(U)$ is equal to the corresponding number for the set rows$(U')$. This allows us to define the clustering number of a graph $G$: it is equal to the cardinality of the set $\text{Image}(\rho)$, where $\rho$ is defined via some spectral decomposition of $A$, as above. The above definitions generalize to weighted (undirected) graphs in an analogous manner.

**Frobenius Norm.** The trace of a matrix $M$, denoted by $\text{Tr}(M)$, is defined to be $\sum_{i \in [n]} M_{ii}$. The trace inner product of two matrices $A$ and $B$, denoted by $\text{Tr}(A, B)$, is the scalar $\text{Tr}(A^T B)$. The Frobenius norm $\|M\|_F$ of a matrix $M$ is defined in the introduction. It is easy to check that $\|M\|_F^2 = \text{Tr}(M, M)$.

Given two $n$-vertex graphs $G$ and $H$ and a permutation $\pi \in S_n$, a $\pi$-mismatch between $G$ and $H$ is a pair $\{i, j\}$ such that $\{i, j\} \in E(G)$ and $\{\pi(i), \pi(j)\} \notin E(H)$ (or vice-versa). In other words, $\pi : V(G) \rightarrow V(H)$ does not preserve adjacency for the pair $\{i, j\}$. The following claim will be useful as a combinatorial interpretation of the Frobenius norm. Let $\Delta$ denote the number of $\pi$-mismatches between $G$ and $H$.

**Claim 2.1** $\|A_G^\pi - A_H\|_F^2 = 2\Delta$.

**Proof.** The only non-zero terms in the expansion of summation $\|A_G^\pi - A_H\|_F^2$ correspond to $\pi$-mismatches. Since every mismatch $\{i, j\}$ contributes 1 and is counted twice in the summation, the claim follows. $\square$

### 2.2 Convex Optimization

A hyperplane $H$ in the Euclidean space $\mathbb{R}^k$ is a $(k - 1)$-dimensional affine subspace. The usual representation of a hyperplane is a linear equation $(c, x) = \alpha$ for some $c \in \mathbb{R}^k, \alpha \in \mathbb{R}$. The convex sets $\{x | (c, x) > \alpha\}$ and $\{x | (c, x) < \alpha\}$ are called the open half-spaces corresponding to $H$, denoted by $H^+, H^-$ respectively.

Two sets $(S, T)$ are weakly linearly separated if there exists a hyperplane $H$ such that $S \subseteq H^+ \cup H$ and $T \subseteq H^- \cup H$. In this case, we call them to be weakly linearly separated along $H$. A family of sets $S_1, \ldots, S_p$ is weakly linearly separated if for every $l, m \in [p]$, the sets $S_l, S_m$ are weakly linearly separated. Let $\Pi$ be a partition of a set $S$ into $p$ sets $S_1, \ldots, S_p$. The partition $\Pi$ is said to be mutually linearly separated if the family of sets $S_1, \ldots, S_p$ is weakly linearly separated.

A subset $S \subseteq \mathbb{R}^k$ is called convex if for every $x, y \in S$, $\alpha x + (1 - \alpha)y \in S$, $\alpha \in [0, 1]$. A function $f : \mathbb{R}^k \rightarrow \mathbb{R}$ is called convex on a convex set $S$ if for every $x, y \in S$, $f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y)$. The following theorem about linearization of convex differentiable functions is well-known and is stated without proof. The gradient of a function $f : \mathbb{R}^k \rightarrow \mathbb{R}$, denoted by $\nabla f$, is the vector-valued function $[\frac{\partial f}{\partial x_1} \cdots \frac{\partial f}{\partial x_k}]$. Given $X^* \in \mathbb{R}^k$, let $\mu^*$ denote the vector $\nabla f(X^*)$.

**Theorem 2.1** (Convex function linearization) Let $f : \mathbb{R}^k \rightarrow \mathbb{R}$ be a convex function. For all $X \in \mathbb{R}^k$, $f(X) - f(X^*) \geq \langle \mu^*, X - X^* \rangle$. 


Next, we show that the linearization of a convex function can be useful in understanding its optima over a finite domain. We prove the following lemma about convex functions, which is interesting in its own right.

**Lemma 2.1** Let \( \Omega \) be a finite subset of \( \mathbb{R}^k \times \mathbb{R}^\ell \). Let \( G : \mathbb{R}^k \to \mathbb{R} \), \( H : \mathbb{R}^\ell \to \mathbb{R} \) such that \( H \) is convex, and let \( F : \mathbb{R}^k \times \mathbb{R}^\ell \to \mathbb{R} \) be defined as \( F(X,Y) = G(X) + H(Y) \). Let \( (X^*, Y^*) \in \text{arg max}_{(X,Y)\in \Omega} F(X,Y) \).

Then there exist a \( \mu^* \in \mathbb{R}^\ell \) such that:

(i) \( (X^*, Y^*) \in \text{arg max}_{(X,Y)\in \Omega} L(X,Y) \) where \( L(X,Y) = G(X) + \langle \mu^*, Y \rangle \);

(ii) \( \text{arg max}_{(X,Y)\in \Omega} L(X,Y) \subseteq \text{arg max}_{(X,Y)\in \Omega} F(X,Y) \).

In other words, for every \( (X^*, Y^*) \) which maximizes \( F \) over \( \Omega \), there exists a partially “linearized” function \( L \) such that \( (X^*, Y^*) \) maximizes \( L \) over \( \Omega \). Moreover, every maximizer of \( L \) over \( \Omega \) is a maximizer of \( F \) over \( \Omega \). This additional condition is necessary so that this “linearization” does not create spurious optimal solutions.

**Proof.** Let \( (X^*, Y^*) \in \text{arg max}_{(X,Y)\in \Omega} F(S) \). Since \( H \) is convex, we can use Theorem 2.1 to linearize \( H \) around \( Y^* \in \mathbb{R}^\ell \). Hence, there exists a \( \mu^* \in \mathbb{R}^\ell \) such that \( H(Y) - H(Y^*) \geq \langle \mu^*, Y - Y^* \rangle \), or equivalently,

\[
H(Y) - \langle \mu^*, Y \rangle \geq H(Y^*) - \langle \mu^*, Y^* \rangle, \tag{2}
\]

for all \( Y \in \mathbb{R}^\ell \). Hence with \( L(X,Y) = G(X) + \langle \mu^*, Y \rangle \), for all \( (X,Y) \in \Omega \) we have

\[
L(X^*, Y^*) = F(X^*, Y^*) - H(Y^*) + \langle \mu^*, Y^* \rangle \geq F(X,Y) - H(Y) + \langle \mu^*, Y \rangle = L(X,Y),
\]

where the inequality holds by (2) and because \( (X^*, Y^*) \) maximizes \( F \). Hence \( (X^*, Y^*) \) maximizes \( L \) as well, which proves (i).

For (ii), consider \( (X^{**}, Y^{**}) \in \text{arg max}_{(X,Y)\in \Omega} L(X,Y) \). To prove that \( (X^{**}, Y^{**}) \in \text{arg max}_{(X,Y)\in \Omega} F(X,Y) \), it suffices to prove that \( F(X^{**}, Y^{**}) \geq F(X^*, Y^*) \). By (i), we have

\[
L(X^{**}, Y^{**}) = L(X^{**}, Y^*) + H(Y^{**}) - \langle \mu^*, Y^{**} \rangle \geq L(X^*, Y^*) + H(Y^*) - \langle \mu^*, Y^* \rangle = F(X^*, Y^*),
\]

where the inequality holds by (2) with \( (X,Y) := (X^{**}, Y^{**}) \) and as \( (X^{**}, Y^{**}) \) maximizes \( L \). \( \square \)

**Corollary 2.1** Let \( \Omega \) be a finite subset of \( \mathbb{R}^{kp} \). For all \( i \in [k] \), let \( G_i : \mathbb{R}^k \to \mathbb{R} \) be a convex function, and let \( F : \mathbb{R}^{kp} \to \mathbb{R} \) be defined by \( F(X_1, \ldots, X_k) := G_1(X_1) + \ldots + G_k(X_k) \). Let \( X^* = (X^*_1, \ldots, X^*_k) \in \text{arg max}_{X \in \Omega} F(X) \).

Then there are \( \mu^*_1, \ldots, \mu^*_k \in \mathbb{R}^p \) such that:

(i) \( X^* \in \text{arg max}_{X \in \Omega} L(X) \) where \( L(X_1, \ldots, X_k) = \sum_{i=1}^k \langle \mu^*_i, X_i \rangle \);

(ii) \( \text{arg max}_{X \in \Omega} L(X) \subseteq \text{arg max}_{X \in \Omega} F(X) \).

**Proof.** Inductively apply the lemma to the functions

\[
F^i((X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_k), X_i) = \left( \sum_{j=1}^{i-1} \langle \mu^*_j, X_j \rangle + \sum_{j=i+1}^k G_j(X_j) \right) + G_i(X_i) =: H^i(X_i).
\]

Finally, we state an important fact about the convexity of quadratic functions. Given a p.s.d. matrix \( M \in \mathbb{R}^{k \times k} \), the quadratic function \( Q_M : \mathbb{R}^k \to \mathbb{R} \) is defined as \( Q_M(x) = \langle x, x \rangle_M \).
Lemma 2.2 (Convexity of p.s.d) \( Q_M \) is convex on \( \mathbb{R}^k \).

Proof. For all \( \alpha \in [0, 1] \), \( Q_M(\alpha x + (1 - \alpha)y) = (\alpha x + (1 - \alpha)y, (\alpha x + (1 - \alpha)y))_M = \alpha^2(x, x)_M + (1 - \alpha)^2(y, y)_M + 2\alpha(1 - \alpha)(x, y)_M \). Using \( (x - y, x - y)_M \geq 0 \), we can show that \( (x, x)_M + (y, y)_M \geq 2(x, y)_M \). Combining, we have \( Q_M(\alpha x + (1 - \alpha)y) \leq \alpha^2 Q_M(x) + (1 - \alpha)^2 Q_M(y) + \alpha(1 - \alpha)(Q_M(x) + Q_M(y)) \leq \alpha Q_M(x) + (1 - \alpha)Q_M(y) \). Hence, \( Q_M \) is convex. \( \square \)

2.3 Simulation of Simplicity

In this section, we describe an elegant technique for handling degeneracy in the input data for geometrical algorithms that is due to Edelsbrunner and M"ucke [11]. We also state an important lemma which will be directly useful for our algorithmic results in Section 4.

An input set \( S \) of \( n \) points \( w_1, \ldots, w_n \in \mathbb{R}^k \) is said to be in general position, if there is no subset \( S' \subseteq S \) with \( |S'| > k \) that lies on a common hyperplane. If we are optimizing a certain function of this input on a discrete space \( \Omega \), infinitesimally small perturbations of \( w_1, \ldots, w_n \) will not change the set \( \Omega^* \subseteq \Omega \) of optimal solutions. Hence we may always assume (modulo infinitesimal perturbations) that such input sets are in general position and do not contain degenerate subsets. From the algorithmic point of view, the caveat is that these perturbations might be so small that we cannot even represent them efficiently.

In this context, Edelsbrunner and M"ucke [11] developed a useful technique to handle degeneracy in input data, called Simulation-of-Simplicity. The idea is to introduce conceptual perturbations which eliminate all degeneracies: the perturbations are never computed explicitly, and in fact, the perturbations are just certain conveniently chosen polynomials in a parameter \( \epsilon \), that brings them into general position. We select \( nk \) perturbations \( \epsilon_{ij} \) for \( i \in [k] \) and \( j \in [n] \) as follows. We perturb the \( i^{th} \) coordinate of vector \( w_j \) by adding \( \epsilon_{ij} \). In our algorithmic application, we need to consistently answer queries of the type: "Given points \( w_{i_1}, \ldots, w_{i_k} \) (with \( i_1 < \cdots < i_k \)) and a point \( w_{k+1} \), does the point \( w_{k+1} \) lie below, on, or above the hyperplane determined by \( w_{i_1}, \ldots, w_{i_k} \)?" We can implement and answer such queries in \( O(k^2) \) time as follows. The answer to the query depends on the sign of the determinant of the following \( (k + 1) \times (k + 1) \) matrix \( \tilde{M} \), which is also the signed volume of the parallelopiped defined by the vectors \( w_{i_1} - w_{i_{k+1}}, \ldots, w_{i_k} - w_{i_{k+1}} \).

\[
\begin{vmatrix}
  w_{i1} + \epsilon_{i1} & w_{i2} + \epsilon_{i2} & \cdots & w_{i_{k+1}} + \epsilon_{i_{k+1}} \\
  \vdots & \vdots & \ddots & \vdots \\
  w_{i_{k+1}} + \epsilon_{i_{k+1}} \\
  1 & \cdots & \cdots & 1 \\
  1 & 1 & \cdots & 1
\end{vmatrix}
\]

The determinant of matrix \( \tilde{M} \) is a polynomial in the \( \epsilon_{ij} \), which can be computed in \( O((k+1)!) = O(k^k) \) time by using the Leibniz expansion

\[
\text{det}(\tilde{M}) = \sum_{\sigma \in S_{k+1}} (\text{sgn}(\sigma) \prod_{i=1}^{k+1} \tilde{M}_{i,i'})
\]

It is easy to see that this polynomial is not identically zero, as every term in the Leibniz expansion yields a different polynomial. This property ensures the non-degeneracy in our conceptual perturbations. We impose a lexicographic ordering on \( \epsilon_{ij} \) as follows: \( \epsilon_{11} < \cdots < \epsilon_{1n} < \epsilon_{21} < \cdots < \epsilon_{2n} < \cdots < \epsilon_{kn} \). This induces a natural lexicographic ordering on the monomials in the
polynomial \( \det(\tilde{M}) \). The lexicographically least monomial in this ordering has either a positive or a negative coefficient: we interpret the sign of this coefficient as the relative position of \( w_{k+1} \) with respect to the hyperplane determined by \( w_{i_1}, \ldots, w_{i_k} \). We refer the reader to [11] for further details. We summarize the above discussion in the following lemma.

**Lemma 2.3** Given a set \( W = \{w_1, \ldots, w_n\} \) of \( n \) points in \( \mathbb{R}^k \),

- The lexicographic ordering of the \( \epsilon_{ij} \) yields a canonical perturbation of the points \( w_1, \ldots, w_n \) such that the resulting set is in general position.
- There exists an \( O(k^k) \) time subroutine which computes the relative position of a canonically perturbed point with respect to the hyperplane determined by \( k \) canonically perturbed points.

### 3 Hardness Results

In this section, we show several new hardness results for problems GS\( \text{Sim} \), WS\( \text{Sim} \) and MS\( \text{Sim} \). As we will observe, these problems turn out to be algorithmically intractable, even for severely restricted cases. We begin by recalling the following observation.

**Theorem 3.1 (Folklore)** GS\( \text{Sim} \) is \( \text{NP} \)-hard for the class of simple undirected graphs.

In fact, the problem turns out to be \( \text{NP} \)-hard even for very restricted graph classes. The following theorem is the main hardness result of this section.

**Theorem 3.2** GS\( \text{Sim} \) is \( \text{NP} \)-hard for the class of trees.

On the other hand, if we restrict one of the input instances to be a path, the problem can be solved in polynomial time. The following theorem provides a positive example of tractability of GS\( \text{Sim} \).

**Theorem 3.3** An input instance \((G, H)\) of GS\( \text{Sim} \), where \( G \) is a path and \( H \) is a tree, can be solved in polynomial time.

The above results exhibit the hardness of GS\( \text{Sim} \), and consequently, the hardness of the more general problems WS\( \text{Sim} \) and MS\( \text{Sim} \). Since the graphs (for instance cycles and paths) involved in the hardness reductions have adjacency matrices of high rank, it is natural to ask whether MS\( \text{Sim} \) would become tractable for matrices of low rank. Our following theorem shows that MS\( \text{Sim} \) is \( \text{NP} \)-hard even for matrices of rank at most 2. The underlying reason for hardness is the well-known problem QAP, which shares the optimization domain \( S_n \).

**Theorem 3.4** MS\( \text{Sim} \) is \( \text{NP} \)-hard for symmetric matrices of rank at most 2.

The key to the above reduction is the fact that one of the matrices has non-negative Eigenvalues while the other matrix has non-positive Eigenvalues. We show that the MS\( \text{Sim} \) is \( \text{NP} \)-hard even for positive semi-definite matrices. The main idea is to reformulate the hardness reduction in Theorem 3.1 in terms of Laplacian matrices.

**Theorem 3.5** MS\( \text{Sim} \) is \( \text{NP} \)-hard for positive semi-definite matrices.

In fact, we show that the problem remains \( \text{NP} \)-hard, even if one of the matrices is of rank 1. The proof follows by modifying the matrices in the proof of Theorem 3.4 so that they are positive semi-definite.

**Theorem 3.6** MS\( \text{Sim} \) is \( \text{NP} \)-hard for positive semi-definite matrices, even if one of the matrices has rank 1.

Therefore, the realm of tractability for MS\( \text{Sim} \) is restricted to positive definite matrices of low rank. In the next section, we prove algorithmic results in this direction.
4 Algorithmic Results

In this section, we present the main algorithmic result of this paper. As established in the previous section, the domain of tractability for MSim is restricted to p.s.d. matrices with low rank. The main theorem of this section is stated as follows. Given an instance \((A, B)\) of MSim, let \(\text{rank}(A), \text{rank}(B) \leq k\). Let \(p\) be the clustering number of \(B\).

**Theorem 4.1** There is an \(O^*(n^{O(kp^2)})\) algorithm for MSim. Here, the \(O^*\) notation hides factors polynomial in the size of input representation.

In order to prove Theorem 4.1, we define a closely related optimization problem, called the Quadratic-Vector-Partition (QVP). Let \(\mathcal{P}\) be the set of all (ordered) partitions of \([n]\) into \(p\) sets of size \(n_1, \ldots, n_p\). i.e., an element \(P \in \mathcal{P}\) is an ordered partition \(T_1 \cup \cdots \cup T_p\) of \([n]\), where \(|T_l| = n_l, l \in [p]\). Given a set \(W\) of \(n\) vectors \(\{w_1, \ldots, w_n\} \subseteq \mathbb{R}^k\), we will employ two important notations. Denote \(W[T_i]\) to be the point-set \(\{w_j \mid j \in T_i\}\) corresponding to \(T_i \subseteq [n]\). Denote \(W^T = \sum_{i \in T} w_i, T \subseteq [n]\).

The input instance to QVP is a set \(W\) of \(n\) vectors \(\{w_1, \ldots, w_n\} \subseteq \mathbb{R}^k\), along with two matrices \(K\) and \(\Lambda\). The matrix \(K\) is a p.s.d matrix of size \(p \times p\). The matrix \(\Lambda\) is a diagonal matrix with \(k\) positive entries. The objective is to search for a partition \(P \in \mathcal{P}\) which maximizes the following quadratic objective function \(F\).

\[
F(P) = \sum_{l, m \in [p]} K_{lm} \langle W^{T_l}, W^{T_m} \rangle_{\Lambda}.
\]

Informally, the goal is to ‘cluster’ the set \(W\) into \(p\) sets \(W_1, \ldots, W_p\) of cardinalities \(n_1, \ldots, n_p\) such that the quadratic function above is maximized. The connection to MSim arises due to the following observation. We can interpret a permutation \(\pi\) as a bijection \(\pi : \text{rows}(U) \rightarrow \text{rows}(V)\) where \(A = UAU^T\) and \(B = VTV^T\) are the respective spectral decompositions. Since \(\text{rank}(A), \text{rank}(B) \leq k\), we must have \(U, V \in \mathbb{R}^{n \times k}\) and consequently, \(\text{rows}(U), \text{rows}(V) \subseteq \mathbb{R}^k\).

Since the set \(\text{rows}(V)\) has only \(p\) distinct tuples (the clustering number), it sufﬁces to examine the partitions of \(\text{rows}(U)\) into \(p\) sets of certain fixed cardinalities. It remains then to show that the minimization of the objective function for MSim can be reformulated as the maximization of the objective function for QVP.

The proof of Theorem 4.1 proceeds in three steps. First, in Section 4.1, we show a reduction from MSim to QVP. In particular, the dimension \(k\) and the parameter \(p\) for the QVP instance are equal to the rank \(k\) and the clustering number \(p\) in Theorem 4.1 respectively. Second, in Section 4.2, we show that the optimal solutions for a QVP instance have a nice geometrical structure. In particular, the convex-hulls of the point-sets in the partition are mutually disjoint (upto some caveats). Third, in Section 4.3, we describe a \(O^*(n^{O(kp^2)})\) algorithm for QVP. The algorithm essentially enumerates all partitions with the optimal solution structure. This finishes the proof of Theorem 4.1.

4.1 Reduction to QVP

In this subsection, we prove the following reduction lemma. Given two matrices \(A, B \in \mathbb{R}^{n \times n}\), let \(\text{rank}(A), \text{rank}(B) \leq k\). Let \(p\) be the cluster-number of \(B\).

**Lemma 4.1** Given a MSim instance \((A, B)\), we can compute a QVP-instance \(W, K, \Lambda\) where \(W \subseteq \mathbb{R}^k\) of size \(n\) and \(K \in \mathbb{R}^{p \times p}\), \(\Lambda \in \mathbb{R}^{k \times k}\), in \(O^*(1)\) time such that the following holds. Given an optimal solution for the QVP-instance \(W \subseteq \mathbb{R}^k\), we can compute \(\min_{\pi \in S_n} \|A^\pi - B\|_F\) in \(O(1)\) time.
Therefore, it suffices to design a $O^*(n^{O(kp^2)})$ algorithm for QVP for the proof of Theorem 4.1. The proof of Lemma 4.1 is deferred to the appendix.

### 4.2 Optimal Structure of QVP

In this section, we show that the optimal solutions for a QVP instance have, in fact, a nice geometrical structure. Let $\Omega^* \subseteq \mathcal{P}$ denote the set of optimal solutions for a QVP instance $W, K, \Lambda$, where $W \subseteq \mathbb{R}^k$ of size $n$. Recall from Section 2 that a partition $W_1, \ldots, W_p$ of $W$ is mutually linearly separated if for every $i, j \in [n]$, there exists a hyperplane $H_{ij}$ which weakly linearly separates $W_i$ and $W_j$.

**Lemma 4.2** Let $P = (T_1, \ldots, T_p) \in \Omega^*$ be an optimal partition for a QVP instance $W, K, \Lambda$. The corresponding partition $W[T_1], \ldots, W[T_p]$ is mutually linearly separated.

The proof of Lemma 4.2 proceeds in three steps. Claim 4.1 shows that we can reformulate QVP as a convex programming problem in $\mathbb{R}^p$. Claim 4.2 stipulates certain necessary conditions for optimality, in this reformulated version. Using Claim 4.3, we revert back to the original QVP formulation in $\mathbb{R}^k$. This allows us to interpret the optimality conditions in Claim 4.2 as the mutually linearly separated property in Lemma 4.2.

Given a partition $T_1, \ldots, T_p$ of $W$, let $X_q$ be the vector of length $p$ corresponding to the $q^{th}$ coordinates of vectors $W^{T_1}, \ldots, W^{T_p}$. Formally, $X_q$ denotes the vector $[(W^{T_1})_q, \ldots, (W^{T_p})_q] \in \mathbb{R}^p$, $q \in [k]$. Recall that $\Lambda$ is a diagonal matrix with positive entries, say $\lambda_1, \ldots, \lambda_k$. The following claim shows that we can describe our problem as a convex programming problem in $\mathbb{R}^p$. The objective function is a sum of $k$ vector norms (squared).

**Claim 4.1** $\Omega^* = \arg\max_{P \in \mathcal{P}} \sum_{q=1}^{k} \lambda_q \langle X_q, X_q \rangle_K$.

The proof is deferred to the appendix.

The second step constitutes the key insight to the proof of Lemma 4.2. We show that an optimal solution for the convex program of Claim 4.1 must be an optimal solution for some linear program. The proof of this claim builds on the statements in Subsection 2.2 about linearization of convex objective functions. Recall that the set $\Omega^* \subseteq \mathcal{P}$ denote the set of optimal solutions for the QVP instance $W, K, \Lambda$.

**Claim 4.2** For every $P^* \in \Omega^*$, there exist vectors $\mu_1^*, \ldots, \mu_k^* \in \mathbb{R}^p$ such that $P^*$ is an optimal solution for the objective function

$$ L = \arg\max_{P \in \mathcal{P}} \sum_{q=1}^{k} \lambda_q \langle \mu_q^*, X_q \rangle_K. $$

Moreover, the set of optimal solutions of $L$ is a subset of $\Omega^*$.

The proof is deferred to the appendix.

Finally, we undo the transformation of Claim 4.1 and revert back to $\mathbb{R}^k$ in the following claim. Consequently, we can reformulate the optimality conditions of Claim 4.2 as follows.

**Claim 4.3** For every $P^* \in \Omega^*$, there exist vectors $\mu_1, \ldots, \mu_k \in \mathbb{R}^k$ such that $P^*$ is an optimal solution for the objective function

$$ L_{\mu_1, \ldots, \mu_p} = \max_{P \in \mathcal{P}} \sum_{q=1}^{p} \langle \mu_q, W^{T_q} \rangle $$
Moreover, the set of optimal solutions of $\mathcal{L}_{\mu_1,\ldots,\mu_p}$ is a subset of $\Omega^*$.

The proof is deferred to the appendix.

We finish with the proof of Lemma 4.2.

**Proof of Lemma 4.2.** Since $P = (T_1,\ldots,T_p)$ is an optimal partition for a QVP instance $W$, by Claim 4.3, there exist vectors $\mu_1,\ldots,\mu_k \in \mathbb{R}^k$ such that $P^*$ is an optimal solution for the objective function

$$\mathcal{L}_{\mu_1,\ldots,\mu_p} = \max_{P \in P} \sum_{q=1}^{p} (\mu_q, W^{T_q}).$$

Recall the notation $W[T_q] = \{w_i \mid i \in T_q\}$. Suppose there exist $q, r$ such that $W[T_q]$ and $W[T_r]$ are not (weakly) linearly separated. We claim that this is a contradiction. Indeed, we can isolate the terms $(\mu_q, W^{T_q}) + (\mu_r, W^{T_r})$ and rewrite them as $(\mu_q - \mu_r, W^{T_q}) + (\mu_r, W^{T_q} + W^{T_r})$.

Now we (weakly) linearly separate the set $W[T_q] \cup W[T_r]$ along the direction $(\mu_q - \mu_r)$, that is, we choose a partition $T'_q \cup T'_r$ of $T_q \cup T_r$ such that $T'_q = \{i \in T_q \cup T_r \mid \langle \mu_q - \mu_r, w_j \rangle \geq 0\}$. Then $(\mu_q - \mu_r, W^{T'_q}) > (\mu_q - \mu_r, W^{T'_r})$, because $T'_q$ and $T'_r$ are not (weakly) linearly separated by $\mu_q - \mu_r$, and $(\mu_r, W^{T'_q} + W^{T'_r}) = (\mu_r, W^{T_q} + W^{T_r})$, because $T'_q \cup T'_r = T_q \cup T_r$. Hence $(\mu_q, W^{T'_q}) + (\mu_r, W^{T'_r}) > (\mu_q, W^{T_q}) + (\mu_r, W^{T_r})$, which contradicts the maximality of $P^* = (T_1,\ldots,T_p)$. Therefore, it must be the case that the sets $T_q$ and $T_r$ are already (weakly) linearly separated along $(\mu_q - \mu_r)$.

\[ \square \]

### 4.3 Algorithm for QVP

In this subsection, we describe a $\mathcal{O}^*(n^{O(kp^3)})$ algorithm for QVP. Along with the reduction stated in Lemma 4.1, this finishes the proof of Theorem 4.1.

We proceed with an informal description of the algorithm. Recall that a QVP instance is $(W, K, \Lambda)$ where $W = \{w_1,\ldots,w_n\} \subset \mathbb{R}^k$. The output is an ordered partition $(T_1,\ldots,T_p)$ of $[n]$ satisfying $|T_i| = n_i$, for some fixed $n_1,\ldots,n_p$. Our strategy is simple: we enumerate all partitions $(T_1,\ldots,T_p)$ of $[n]$ such that the sets $W[T_1],W[T_2]$ are weakly linearly separated for every $i,j \in [p]$. By Lemma 4.2, this suffices to obtain an optimal partition. We briefly describe our algorithm. We first guess the $\binom{p}{2}$ separating hyperplanes $H_{ij}$, $i,j \in [p]$, where $H_{ij}$ weakly linearly separates $W[T_i]$ and $W[T_j]$. Let $\mathcal{H}$ be the set of $\binom{p}{2}$ hyperplanes defined by $k$-subsets of $W$. It is sufficient to pick $H_{ij}$ from the set $\mathcal{H}$, since a hyperplane in $\mathbb{R}^k$ can be equivalently replaced by a hyperplane in $\mathcal{H}$, without changing the underlying (weakly) linear separation. These hyperplanes partition $\mathbb{R}^k$ into convex regions. For every $w_i \in W$, we check its relative position with respect to these hyperplanes. We assign $w_i$ to one of the sets $T_1,\ldots,T_p$, depending of its relative position. We claim that every weakly linearly separated family of sets $W[T_1],\ldots,W[T_p]$ can be discovered on some branch of our computation. The choice of $p^2$ hyperplanes implies a $\binom{n}{k}^{p^2}$ branching. Therefore, the overall branching factor is $n^{O(kp^3)}$. Algorithm 4.3 gives a formal description of our algorithm.

There are two caveats. First, we also pick an orientation $\sigma_{ij} \in \{+1,-1\}$ for every hyperplane $H_{ij}$. The +1 orientation indicates that $T_i \subset H^+ \cup H, T_j \subset H^- \cup H$ (and vice-versa). Second, there may exist some points which lie on the hyperplanes, and hence, their assignments cannot be determined by their relative positions to these hyperplanes. To handle this degeneracy, we use the Simulation-of-Simplicity technique and assume general position. Therefore, there are at most $p^2 \cdot k$ such ambiguous points. Since this is a bounded number, we can brute-force try all $p$ possible sets $T_1,\ldots,T_p$ for such points. This leads to a branching factor of $p^{2k}$. The overall branching factor is still $n^{O(kp^3)}$. We now proceed to give a formal description as Algorithm 4.3.
Algorithm 4.3

Input: $W = \{w_1, \ldots, w_n\} \subset \mathbb{R}^k$, matrices $K, \Lambda$.
Output: A partition $T_1, \ldots, T_p$ of $W$ where $|T_i| = n_i$ for some fixed $n_1, \ldots, n_p$.

1. For every choice of $\binom{p}{2}$ hyperplanes $H_{ij}, i \in [p], j \in [p]$ from the set $\mathcal{H}$ with an orientation $\sigma_{ij} \in \{+1, -1\}$,
   (a) Let $W' = \emptyset$.
   (b) For every $w_i \in W$ and $q \in [p]$, check if $w_i$ belongs to the convex region $R_q$ corresponding to the intersection of open halfspaces
   $$R_q = \bigcap_{i=1, i \neq q}^p H_{qi}^{\sigma_{qi}}$$
   We use the Simulation-of-Simplicity subroutine of Section 2.3 to check the relative position of $w_i$ with respect to the hyperplanes.
   (c) If $w_i$ belongs to some region $R_q$, we assign $w_i$ to the set $T_q$. Otherwise, we add $w_i$ to the set $W'$.
   (d) For every point $w_i \in W'$, try each of the $p$ assignments to $T_1, \ldots, T_p$.
   (e) Check if the constraints $|T_i| = n_i$ are satisfied, otherwise reject this branch of computation.

2. For every partition $(T_1, \ldots, T_p)$ computed above, evaluate the QVP objective function and output an optimal solution.

Claim 4.4 Given a QVP instance, Algorithm 4.3 correctly computes an optimal solution in $O^*(n^{O(kp^2)})$ time.

Proof. We first show the correctness. By Lemma 4.2, it suffices to show that Algorithm 4.3 computes all partitions $(T_1, \ldots, T_p)$ of $[n]$ such that the family of sets $W[T_1], \ldots, W[T_p]$ is weakly linearly separated. We claim that Algorithm 4.3 discovers every such family of sets in Step 1. Indeed, for such a family $W[T_1], \ldots, W[T_p]$, there exist $p^2$ hyperplanes $H_{ij}$ which weakly linearly separate the sets $W[T_i], W[T_j]$, for $i, j \in [p]$. By S-o-S technique of Section 2.3, we can assume general position for the input set $W$. It can be shown that for every hyperplane $H_{ij}$, we can equivalently find another hyperplane $\tilde{H}_{ij}$ in $\mathcal{H}$ with the following property. If $(A, B)$ is a partition of $[n]$ such that $H_{ij}$ weakly linearly separates $W[A], W[B]$, then $\tilde{H}_{ij} \in \mathcal{H}$ also weakly linearly separates $W[A], W[B]$. (Refer to Claim A.1 in the appendix). Therefore, there exists a branch of the algorithm in Step 1 such that we discover the hyperplanes $\tilde{H}_{ij}$. Steps 1 (b)-(d) ensure that we recover the partition $W[T_1], \ldots, W[T_p]$.

The running time can be bounded as follows. The branching in Step 1 is bounded by $\binom{n}{k}^p 2^{p^2}$. In Step 1 (b), the number of calls to the Simulation of Simplicity subroutine is bounded by $n \cdot p \cdot p$, since we have $n$ points, $p$ regions and $p$ queries $(H_{q_1}, w_p), \ldots, (H_{q_p}, w_p)$. By Lemma 2.3, every call to this subroutine has a cost $O^*(k^{O(k)})$. In Step 1 (c), there is an additional branching factor of $p^{|W'|}$ for brute-force assignment of points in $W'$. These are precisely the points which
lie on some hyperplane $H_{ij}$, and hence $|W'| \leq p^2 \cdot k$. This incurs an additional $p^{2\cdot k}$ branching. The remaining steps are usual polynomial time computations. The overall running time is thus bounded by $(\binom{n}{k})^2 \cdot 2p^2 \cdot p^{2\cdot k} \cdot O^*(kO(k)) \leq O^*(n^{O(kp^k)})$.

Finally, we summarize this section with the proof of our main theorem.

**Proof of Theorem 4.1.** Lemma 4.1 and Claim 4.4 together imply the proof.

5 Conclusion

Through our results, we were able to gain insight into the tractibility of the problems GSIM and MSIM. However, there are a few open threads which remain elusive. The regime of bounded rank $k$ and unbounded clustering number $p$ is still not fully understood for MSIM, in the case of positive semi-definite matrices. It is not clear whether the problem is P-time or NP-hard in this case. Indeed, an $n^{O(k)}$ algorithm for MSIM, in the case of positive semi-definite matrices, remains a possibility. From the perspective of parameterized complexity, we can ask if MSIM is W[1]-hard, where the parameter of interest is the rank $k$. Finally, the approximability for the problems MSIM deserves further examination, especially for the case of bounded rank.

A Appendix

Proofs in Section 3

**Proof of Theorem 3.1.** The proof is done by reduction from the NP-hard Hamiltonian Cycle problem in 3-regular graphs (HAM-CYCLE); see [13]. Given a 3-regular graph $G$ on $n$ vertices as an instance of HAM-CYCLE, the reduction computes the $n$-vertex cycle $C_n$ and graph $G$ as inputs for GSIM. We recall from Section 2 that the squared Frobenius distance $\|A_{C_n}^r - A_G\|_F^2$ between these two graphs equals twice the number of $\pi$-mismatches. Since $C_n$ and $G$ have $n$ and $\frac{3n}{2}$ edges, respectively, there are at least $\frac{3n}{2} - n = \frac{n}{2}$ mismatches for any $\pi \in S_n$. We claim that $G$ has a Hamiltonian cycle if and only if there exists a $\pi$ for which the number of $\pi$-mismatches is exactly $\frac{n}{2}$. Indeed, if $G$ has a Hamiltonian cycle, the natural bijection $\pi : V(C_n) \rightarrow V(G)$ will cause exactly $\frac{n}{2}$ mismatches. Conversely, if there exists a $\pi$ for which the number of mismatches is exactly $\frac{3n}{2} - n$, it must map every edge of $C$ onto an edge of $G$. Hence, $G$ has a Hamiltonian cycle.

**Proof of Theorem 3.2.** The proof is by a reduction from the following NP-hard variant of the Three-Partition problem [13], which is defined as follows. The input consists of integers $A$ and $a_1, \ldots, a_{3m}$ in unary representation, with $\sum_{i=1}^{3m} a_i = mA$ and with $A/4 < a_i < A/2$ for $1 \leq i \leq 3m$. The question is to decide whether $a_1, \ldots, a_{3m}$ can be partitioned into $m$ triples so that the elements in each triple sum up to precisely $A$.

We first show that the restriction of GSIM to forests is NP-hard. Given an instance of THREE-PARTITION, we compute an instance of GSIM on the following two forests $F_1$ and $F_2$. Forest $F_1$ is the disjoint union of $3m$ paths with $a_1, \ldots, a_{3m}$ vertices, respectively. Forest $F_2$ is the disjoint union of $m$ paths that each consists of $A$ vertices. We claim that the THREE-PARTITION instance has answer YES, if and only if there exists a permutation $\pi$ such that there are at most $2m$ mismatches. If the desired partition exists, then for each triple we can pack the three corresponding paths in $F_1$ into one of the paths in $F_2$ with two mismatches per triple. Conversely, if there exists a permutation $\pi$ with at most $2m$ mismatches, then these
2m mismatches cut the paths in $F_2$ into $3m$ subpaths (we consider isolated vertices as paths of length 0). As each of these $3m$ subpaths must be matched with a path in $F_1$, we easily deduce from this a solution for the Three-Partition instance.

To show that $GSim$ is NP-hard for the class of trees, we modify the above forests $F_1$ and $F_2$ into trees $T_1$ and $T_2$. Formally, we add a new vertex $v_1$ to $V(F_1)$ and then connect one end-point of every path in $F_1$ to $v_1$ by an edge; note that the degree of vertex $v_1$ in the resulting tree is $3m$. Analogously, we add a new vertex $v_2$ to $V(F_2)$, connect it to all paths, and thus produce a tree in which vertex $v_2$ has degree $m$. For technical reasons, we furthermore attach $8m$ newly created leaves to every single vertex in $V(F_1)$ and $V(F_2)$. $k$ The resulting trees are denoted $T_1$ and $T_2$, respectively.

We claim that the considered Three-Partition instance has answer YES, if and only if there exists $\pi : V(T_1) \to V(T_2)$ with at most $4m$ mismatches. If the desired partition exists, the natural bijection maps every original forest edge in $T_1$ to an original forest edge in $T_2$, except for some $2m$ out of the $3m$ edges that are incident to $v_1$ in $T_1$; this yields a total number of $2m + 2m = 4m$ mismatches. Conversely, suppose that there exists a permutation $\pi$ with at most $4m$ mismatches. Then $\pi$ must map $v_1$ in $T_1$ to $v_2$ in $T_2$, since otherwise we pay a penalty of more than $4m$ mismatches alone for the edges incident to the vertex mapped into $v_2$. As the number of mismatches for edges incident to $v_1$ and $v_2$ amounts to $2m$, there remain at most $2m$ further mismatches for the remaining edges. Similarly as in our above argument for the forests, these at most $2m$ mismatches yield a solution for the Three-Partition instance. □

Proof of Theorem 3.3. If $G$ is a path and $H$ is a tree, $GSim$ boils down to the problem of finding a system of disjoint paths in the tree $H$ that contains the maximal number of edges. We root the tree $H = (V,E)$ at an arbitrary vertex, and for every $v \in V$ we let $H(v)$ denote the induced maximal sub-tree of $H$ that is rooted at $v$. For $v \in V$, we let $A(v)$ denote the maximal number of edges that can be covered by a system of disjoint paths in tree $H(v)$. Furthermore, we let $B(v)$ denote the maximal number of edges that can be covered by a system of disjoint paths in tree $H(v)$ subject to the condition that one of these paths starts in vertex $v$. For a leaf $v$ in $H$, we have $A(v) = B(v) = 0$. For non-leaves $v$ in $H$, a straightforward dynamic programming approach computes $A(v)$ and $B(v)$ in linear time from the corresponding $A$-values and $B$-values for the children of $v$. All in all, this yields a polynomial time algorithm. □

Proof of Theorem 3.4. The proof is by a reduction from the NP-hard Partition problem [13], defined as follows. Given a set $S$ of $2n$ positive integers $\{a_1, \ldots, a_{2n}\}$, where $a_1 + \cdots + a_{2n} = 2A$, decide whether there exists a subset $I \subseteq \{1, \ldots, 2n\}$ with $|I| = n$ such that $\sum_{i \in I} a_i = A$.

We construct the following $2n \times 2n$ real symmetric matrices $C$ and $B$ as our MSim instance. The matrix $C$ is defined as $C_{ij} := a_i \cdot a_j$. The matrix $B$ is defined as

$$B_{ij} := \begin{cases} -1 & i \in [1,n], \ j \in [1,n] \\ -1 & i \in [n+1,2n], \ j \in [n+1,2n] \\ 0 & \text{otherwise} \end{cases}$$

Indeed, $\|C^\pi - B\|_F^2 = \|C^\pi\|_F^2 + \|B\|_F^2 - 2\text{Tr}(C^\pi, B)$. Since $\|C^\pi\|_F^2 = \|C\|_F^2$ does not depend on
\( \pi \), it suffices to minimize the term \((-1) \text{Tr}(C^\pi, B)\). The term

\[
\text{Tr}(C^\pi, B) = \sum_{i,j \in [2n]} c_{i^\pi j^\pi} b_{ij}
\]

\[
= \sum_{i,j \in [1,n]} c_{i^\pi j^\pi} (-1) + \sum_{i,j \in [n+1,2n]} c_{i^\pi j^\pi} (-1)
\]

\[
= (-1) \left( \sum_{i,j \in [1,n]} c_{i^\pi j^\pi} + \sum_{i,j \in [n+1,2n]} c_{i^\pi j^\pi} \right)
\]

\[
= (-1) \left( \left( \sum_{i \in [1,n]} a_{i^\pi} \right)^2 + \left( \sum_{i \in [n+1,2n]} a_{i^\pi} \right)^2 \right).
\]

Let \( S_1 = \{ i^\pi \mid i \in [1,n] \} \). Let \( S_2 = \{ i^\pi \mid i \in [n+1,2n] \} \). Let \( X_1, X_2 \) be the sum of elements corresponding to the sets \( S_1, S_2 \) respectively. Clearly, \( X_2 = 2A - X_1 \). Then,

\[
(-1) \text{Tr}(C^\pi, B) = \left( \sum_{i \in S_1} a_i \right)^2 + \left( \sum_{i \in S_2} a_i \right)^2
\]

\[
= X_1^2 + (2A - X_1)^2
\]

\[
\geq 2A^2
\]

using the inequality \( \frac{x_1^2 + x_2^2}{2} \geq \left( \frac{x_1 + x_2}{2} \right)^2 \) for \( x_1, x_2 \geq 0 \). Moreover, equality is attained only for \( x_1 = x_2 \), which implies \( X_1 = 2A - X_1 \), and hence \( X_1 = X_2 = A \). Therefore, the given PARTITION instance has a partition of the desired kind if and only if there exists a \( \pi \) such that \((-1) \text{Tr}(C^\pi, B)\) attains the minimum value \(2A^2\). Hence, the problem of minimizing \((-1) \text{Tr}(C^\pi, B)\), and consequently \(\|C^\pi - B\|_F^2\), over \( \pi \in S_n \) must be NP-hard.

Finally, we show that \( C \) and \( B \) are matrices of rank 1 and rank 2 respectively. The matrix \( C \) can be expressed as a rank 1 matrix \( uu^T \), where \( u = [a_1, \ldots, a_{2n}] \) is a column vector of length \( 2n \). The corresponding Eigenvalue can be checked to be \( \|u\|^2 = (a_1^2 + \cdots + a_{2n}^2) \). In particular, \( A \) is positive semi-definite. The matrix \( B \) can be expressed as the sum of two rank-1 matrices \( B_1 + B_2 \) where (a) \( B_1 = (-1)v_1 v_1^T \), \( B_2 = (-1)v_2 v_2^T \) and (b) \( v_1 \) is a 0-1 column vector of length \( 2n \) such that the \( i \)th coordinate of \( v_1 \) is 1 iff \( 1 \leq i \leq n \). Similarly, \( v_2 \) is a 0-1 column vector of length \( 2n \) such that the \( i \)th coordinate of \( v_2 \) is 1 iff \( n+1 \leq i \leq 2n \). The corresponding Eigenvalues can be checked to be \(-\|v_1\|^2, -\|v_2\|^2\) which is the multiset \( \{-n, -n\} \).

\[ \square \]

**Proof of Theorem 3.5.** In the proof of Theorem 3.1, instead of considering the adjacency matrices of \( C_n \) and \( G \), we consider their Laplacian matrices \( L_{C_n} \) and \( L_G \). Since \( L_{C_n} = D_{C_n} - A_{C_n} \) and \( C_n \) is 2-regular, \( L_{C_n} = 2I_n - A_{C_n} \). Since \( L_G = D_G - A_G \) and \( G \) is 3-regular, \( L_G = 3I_n - A_G \). Therefore, the quantity

\[
\|L_{C_n}^\pi - L_G\|_F^2 = \| (2I_n - A_{C_n})^\pi - (3I_n - A_G) \|_F^2
\]

\[
= \|2I_n - A_{C_n}^\pi - (3I_n - A_G) \|_F^2
\]

\[
= \| - I_n - (A_{C_n}^\pi - A_G) \|_F^2
\]

\[
= \| (A_{C_n}^\pi - A_G) + I_n \|_F^2
\]

\[
= \| (A_{C_n}^\pi - A_G) \|_F^2 + \|I_n\|_F^2
\]

\[
= \| (A_{C_n}^\pi - A_G) \|_F^2 + n.
\]
The second last equality follows because $I_n$ has only diagonal entries whereas every diagonal entry of $(A_{C_n}^{*} - A_G)$ is zero. The above calculation shows that these two quantities differ by $n$ (which is independent of $\pi$). Therefore, computing the Frobenius distance between the two Laplacian matrices $L_{C_n}$ and $L_G$ is NP-hard as well.

**Proof of Theorem 3.6.** We modify the hardness proof for Theorem 3.4. We define the matrix $C$ to be the same as in the proof of Theorem 3.4. We define the matrix $B := B + nI_n$ where $B$ is the matrix from the proof of Theorem 3.4. Since the Eigenvalues were shown to be $-n$ with multiplicity 2 and 0 with multiplicity $n-2$, adding the matrix $nI_n$ to $B$ shifts the Eigenvalues by $+n$, and hence $B'$ is p.s.d. It remains to observe that the significant quantity $\text{Tr}(C', B')$ differs from the corresponding $\text{Tr}(C, B)$ by a constant independent of $\pi$. Indeed,

$$\text{Tr}(C', B') = \sum_{i,j \in [2n]} c_{\pi} b_{ij}$$

$$= \sum_{i,j \in [2n]} c_{\pi} b_{ij} + \sum_{i \in [2n]} c_{\pi} n$$

$$= \sum_{i,j \in [2n]} c_{\pi} b_{ij} + \sum_{i \in [2n]} a_i^2 n$$

$$= \text{Tr}(C, B) + n \left( \sum_{i \in [2n]} a_i^2 \right).$$

Hence, the problem of minimizing $\|C - B\|_F^2$ over $\pi \in S_n$ must be NP-hard. Recall that the matrix $C$ was shown to be positive semi-definite in the proof of Theorem 3.4. This finishes the proof of our theorem.

**Proofs in Section 4**

**Proof of Lemma 4.1.** The spectral decompositions of $A$ and $B$ are represented by $A = U \Lambda U^T$ and $B = VTV^T$. Since the cluster-number of $B$ is $p$, let $V = \{V^1, \ldots, V^p\}$ be the set of distinct vectors in the multiset rows($V$). Let $n_1, \ldots, n_p$ be the multiplicity of the elements $V^1, \ldots, V^p$ respectively. Clearly, $n_1 + \cdots + n_p = n$. Let $P$ be the natural partition arising from this clustering. In other words, $P = S_1 \cup \cdots \cup S_p$ be a partition of $[n]$ where $S_l = \{i \mid V^i = V^l\}, l \in [p]$.

Let $\Pi^*$ denote the set $\arg\min_{\pi} \|A^\pi - B\|_F$. We first restate $\Pi^*$ as follows. Observe that $\|A^\pi - B\|_F^2 = \text{Tr}(A^\pi - B, A^\pi - B) = \text{Tr}(A^\pi, A^\pi) + \text{Tr}(B, B) - 2\text{Tr}(A^\pi, B)$. Since $\text{Tr}(A^\pi, A^\pi) = \|A^\pi\|_F^2 = \|A\|_F^2 = \text{Tr}(A, A)$, we have $\|A^\pi - B\|_F^2 = \text{Tr}(A, A) + \text{Tr}(B, B) - 2\text{Tr}(A^\pi, B)$. Therefore, we can equivalently maximize $\text{Tr}(A^\pi, B)$ over $\pi \in S_n$. We have

$$\Pi^* = \arg\min_{\pi} \|A^\pi - B\|_F$$

$$= \arg\max_{\pi} \text{Tr}(A^\pi, B)$$

$$= \arg\max_{\pi} \sum_{i,j \in [n]} a_{\pi} b_{ij}$$

$$= \arg\max_{\pi} \sum_{i,j \in [n]} \langle U^\pi, U^\pi \rangle_A \cdot \langle V^i, V^j \rangle_{\Gamma}. $$
Restating $\Pi^*$ further, we get

$$\Pi^* = \arg \max_{\pi} \sum_{i,j \in [n]} \langle U^i, U^j \rangle \Lambda \cdot \langle V^i, V^j \rangle \Gamma,$$

$$= \arg \max_{\pi} \sum_{l,m \in [p]} \left( \sum_{i \in S_l, j \in S_m} \langle U^i, U^j \rangle \Lambda \cdot \langle V^i, V^j \rangle \Gamma \right),$$

$$= \arg \max_{\pi} \sum_{l,m \in [p]} \left( \sum_{i \in S_l} \sum_{j \in S_m} \langle U^i, \sum_{j \in S_m} U^j \rangle \Lambda \cdot \langle \tilde{V}^i, \tilde{V}^m \rangle \Gamma \right),$$

$$= \arg \max_{\pi} \sum_{l,m \in [p]} \langle U^{S_l}, U^{S_m} \rangle \Lambda \cdot \langle \tilde{V}^l, \tilde{V}^m \rangle \Gamma,$$

where we recall the notation $U^{S} = \sum_{i \in S} U^i$, $S \subseteq [n]$. Let $K$ be the $p \times p$ matrix defined as $K_{lm} = \langle \tilde{V}^l, \tilde{V}^m \rangle \Gamma$. Clearly, $K$ is positive semi-definite. Simplifying, we obtain

$$\Pi^* = \arg \max_{\pi \in S_n} \sum_{l,m \in [p]} K_{lm} \langle U^{S_l}, U^{S_m} \rangle \Lambda.$$

Given a permutation $\pi \in S_n$, we can bijectively associate a partition $P_{\pi} = (S_{\pi}^1 \cup \cdots \cup S_{\pi}^p) \in \mathcal{P}$. Recall that $(S_1, \ldots, S_p)$ is the partition corresponding to the clustering of rows$(V)$. Therefore, the set $\Pi^*$ is in one-to-one correspondence with the set

$$\Omega^* = \arg \max_{P \in \mathcal{P}} \sum_{l,m \in [p]} K_{lm} \langle U^{T_l}, U^{T_m} \rangle \Lambda.$$

Clearly, this is an instance of QVP with the input set rows$(U) \subseteq \mathbb{R}^k$ of size $n$, along with the corresponding matrices $K$ and $\Lambda$. This instance can be computed directly from the spectral decompositions of $A$ and $B$, which can be done in $O^*(1)$ time. Moreover, given an optimal solution for this QVP instance, we can uniquely recover an optimal permutation $\pi \in \Pi^*$ in $O(1)$ time. Hence, proved.

Proof of Claim 4.1.

$$\Omega^* = \arg \max_{P \in \mathcal{P}} \sum_{l,m \in [p]} K_{lm} \langle W^{T_l}, W^{T_m} \rangle \Lambda$$

$$= \arg \max_{P \in \mathcal{P}} \sum_{l,m \in [p]} K_{lm} \left( \sum_{q=1}^{k} \lambda_q (W^{T_l})_q (W^{T_m})_q \right)$$

$$= \arg \max_{P \in \mathcal{P}} \sum_{q=1}^{k} \lambda_q \left( \sum_{l,m \in [p]} (W^{T_l})_q \cdot K_{lm} \cdot (W^{T_m})_q \right)$$

$$= \arg \max_{P \in \mathcal{P}} \sum_{q=1}^{k} \lambda_q \langle X_q, X_q \rangle_K.$$
Proof of Claim 4.2. Let $F = \sum_{q=1}^{k} \lambda_q \langle X_q, X_q \rangle_K$ denote the objective function of Claim 4.1. Let $G_q(X)$ denote the function $\lambda_q \langle X, X \rangle_K$. Since $\lambda_i > 0$, Lemma 2.2 implies that $G_q$ is a convex function for $q \in [p]$. Applying Corollary 2.1 for $G_1, \ldots, G_k$ finishes the proof. □

Proof of Claim 4.3. 

\[
\begin{align*}
\sum_{q=1}^{k} \lambda_q \langle X_q^*, X_q \rangle_K &= \sum_{q=1}^{k} \lambda_q \left( \sum_{l,m=1}^{p} (X_q^*)_l K_{lm} (X_q)_m \right) \\
&= \sum_{l,m=1}^{p} K_{lm} \left( \sum_{q=1}^{k} \lambda_q (X_q^*)_l (X_q)_m \right) \\
&= \sum_{l,m=1}^{p} K_{lm} \langle W^{T_l^*}, W^{T_m} \rangle \Lambda \\
&= \sum_{l=1}^{p} \langle \mu_l, W^{T_m} \rangle.
\end{align*}
\]

for some vectors $\mu_1, \ldots, \mu_p \in \mathbb{R}^k$. □

Claim A.1 Let $W$ be a set of $n$ points $\{w_1, \ldots, w_n\} \subset \mathbb{R}^k$ in general position, where $n > k$. Suppose $W_1, W_2$ is a weakly linear separation of $W$ by a hyperplane $H$. Then, there exists another hyperplane $\tilde{H}$ with the following properties: (a) $\tilde{H}$ passes through exactly $k$ points of $W$, and (b) $\tilde{H}$ also weakly linearly separates $W_1, W_2$.

Proof. Let $S \subseteq W$ be the set of points in $W$ which already lie on $H$. Since $W$ is in general position, $|S| \leq k$. If $|S| = k$ already, we are done. Otherwise, $|S| = l < k$. Let $S = \{w_1, \ldots, w_l\}$. Moreover, let $H$ be represented by the linear equation $c^T x = \alpha$, where $c \in \mathbb{R}^k$ and $\alpha \in \mathbb{R}$. Since $l < k$, there exists a vector $\delta \in \mathbb{R}^k$ satisfying the system of $l$ linear equations $\delta^T w_1 = \ldots = \delta^T w_l = 0$. Let $\gamma \in \mathbb{R}$. Consider the hyperplane $H_\gamma := (c + \gamma \delta)^T x = \alpha$. Clearly, $S$ lies on $H_\gamma$. We select $\gamma$ suitably as follows. We slowly increase (or decrease) the value of $\gamma$ from zero such that the hyperplane $H_\gamma$ hits a point $w \in W \setminus S$ for the first time. Therefore, we obtain a new hyperplane $H'_\gamma$ such that the set $S \cup \{w\}$ lies on $H'$. Moreover, it is easy to check that (a) for every point $w \not\in S \cup \{w\}$, the relative position w.r.t $H_\gamma$ is same as the relative position w.r.t $H$ (in terms of the halfspaces $H^+, H^-$) and hence, (b) if $W_1, W_2$ is a weak linear separation of $W$ by $H$, it remains a weak linear separation of $H'$. Repeating this argument, we ultimately obtain a hyperplane $\tilde{H}$ which passes through a set $W'$ of size $k$, satisfying $W \supset W' \supset S$. Hence, proved. □

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