A BLIND PERMUTATION SIMILARITY ALGORITHM

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Abstract. This paper introduces a polynomial blind algorithm that determines when two square matrices, \( A \) and \( B \), are permutation similar. The shifted and translated matrices \( (A + \beta I + \gamma J) \) and \( (B + \beta I + \gamma J) \) are used to color the vertices of two square, edge weighted, rook’s graphs. Then the orbits are found by repeated symbolic squaring of the vertex colored and edge weighted adjacency matrices. Multisets of the diagonal symbols from non-permutation similar matrices are distinct within a few iterations, typically four or less.

1. Introduction

This paper introduces a polynomial blind algorithm for permutation similarity. Specht’s Theorem gives an infinite set of necessary and sufficient conditions for two square matrices to be unitarily similar [7, pg. 97]. Specht’s Theorem compares the traces of certain matrix products. If the traces ever fail to match, then the matrices are not unitarily similar. Subsequent work reduced the number of traces required to a finite number [7, pg. 98]. The permutation similarity algorithm is somewhat analogous, an infinite set of matrix products are checked to see if the multisets (not traces) of the diagonal elements match. If they ever fail to match, the two matrices are not permutation similar.

Permutation similarity plays a large role in the graph isomorphism problem where two graphs are isomorphic iff their adjacency matrices are permutation similar. The best theoretical results for graph isomorphism are by Babai, showing graph isomorphism is quasipolynomial [4]. The typical graph isomorphism algorithm uses equitable partitions and vertex individualization with judicious pruning of the search tree to generate canonical orderings that are compared to determine if two graphs are isomorphic [10]. However, Neuen and Schweitzer suggest that all vertex individualization based refinement algorithms have an exponential lower bound [13]. The permutation similarity algorithm does not perform vertex individualization nor does it try to construct a canonical ordering.

The overall process is as follows. Square (real or complex) matrices \( A \) and \( B \) are converted into positive integer matrices whose diagonal entries are distinct from the off-diagonal entries, \( (A + \beta I + \gamma J) \) and \( (B + \beta I + \gamma J) \). The shifted and translated matrices are used to color the vertices of edge weighted rook’s graphs. The edge weights are ‘1’ for a column edge and ‘2’ for a row edge. The resultant graphs are called permutation constraint graphs (PCGs), see Figure 2.1. The purpose of a PCG is to add symmetric permutation constraints to the original matrix. Then the vertex colored and edged weighted adjacency matrices of the PCGs are constructed. Such an adjacency matrix is called a permutation constraint matrix (PCM). It will be shown that \( A \) and \( B \) are permutation similar iff their associated PCMs are permutation similar. Next, the PCMs are repeatedly squared using symbolic matrix multiplication. Symbolic squaring generates a canonical string for each inner product. Symbols are substituted

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for the strings in a consistent fashion. After the symbol substitution, the multisets of diagonal symbols are compared. If they every differ, the matrices are not permutation similar. Symbolic squaring monotonically refines the partitions until a stable partition is reached.

Experimentally, a stable partition is reached in six iterations or less and non permutation similar matrices are separated in four iterations or less. The canonical inner product strings generated by symbolic squaring separate the orbits imposed by the automorphism group acting on the set of \((i, j)\) locations.

The necessity of the blind algorithm is proven in Section 2. Sufficiency is argued in Section 3. Section 4 provides a polynomial algorithm that uses the blind algorithm to find a permutation between permutation similar matrices. Section 5 provides some additional material that readers may find interesting. Section 6 is a summary.

2. Blind P-similarity Algorithm

Algorithm 1 contains pseudocode for the blind permutation similarity algorithm. This section is organized so the background for each function is discussed in order. The discussion will make it clear that the algorithm tests necessary conditions for two matrices to be permutation similar. A conservative complexity bound for Algorithm 1 is presented in Section 2.12. Sufficiency arguments are given in Section 3.

2.1. Permutation Similarity. Real or complex square \(m \times m\) matrices \(A\) and \(B\) are permutation similar iff there exists a permutation matrix \(P\) such that \(PAP^T = B\) [7, pg. 58]. The notation \(A \sim_P B\) is used to indicate that \(A\) and \(B\) are permutation similar. Permutation similarity will be abbreviated as p-similarity in the text.

2.2. Symmetric Permutation and Mixes. The process of applying a permutation matrix \(P\) from the left and right as \(PAP^T\) is called a symmetric permutation [6, pg. 147]. Symmetric permutations have four main characteristics:

1. Elements of a matrix are moved around by symmetric permutation but not changed, so the multiset of elements in a matrix before and after a symmetric permutation are identical. Let the multiset of all elements in a matrix be called the mix, i.e., \(\text{mix}(A) = \{\{A_{i,j}\}\}\). Then \(\text{mix}(A) = \text{mix}(PAP^T)\).
2. Elements of a row are moved together, so the multiset of elements from a row before and after being moved by a symmetric permutation are identical. Let the multiset of row multisets be called the row mix, i.e., \(\text{rowMix}(A) = \{\{\{A_{1,:}\}\}, \cdots, \{\{A_{m,:}\}\}\}\). Then \(\text{rowMix}(A) = \text{rowMix}(PAP^T)\).
3. Elements of a column are moved together, so the multiset of elements from a column before and after being moved by a symmetric permutation are identical. Let the multiset of column multisets be called the column mix, i.e., \(\text{colMix}(A) = \{\{\{A_{:,1}\}\}, \cdots, \{\{A_{:,m}\}\}\}\). Then \(\text{colMix}(A) = \text{colMix}(PAP^T)\).
4. Elements on the diagonal remain on the diagonal, so the multiset of elements on the diagonal is the same before and after a symmetric permutation. Let the multiset of diagonal elements be called the diagonal mix, i.e., \(\text{diagMix}(A) = \{\{A_{j,j}\}\}\). Then \(\text{diagMix}(A) = \text{diagMix}(PAP^T)\).

2.3. Triplet Notation for a Matrix. Because symmetric permutations move values around without changing them, the values can be replaced with a different set of symbols without changing the action. It is useful to view a \(m \times m\) matrix as a triplet consisting of i) \(\Pi\): a partition of the \((i, j)\) locations, ii)
Algorithm 1 Blind p-similarity algorithm pseudocode

01 function psim = BPSAY(M1,M2)
02 % Blind Permutation Similarity Algorithm, Yes?
03 % Inputs:
04 % M1 – m×m square matrix (real or complex)
05 % M2 – m×m square matrix (real or complex)
06 % Outputs:
07 % psim – boolean (TRUE if M1 & M2 are p–similar)
08 09 psim = FALSE; % initialize psim to FALSE
10 11 [A,B] = SymbolSubstitution(M1, M2);
12 13 S = PCM(ShiftAndTranslate(A, beta=m^2, gamma=2));
14 T = PCM(ShiftAndTranslate(B, beta=m^2, gamma=2));
15 16 repeat
17     [Ssqr ,Tsqr] = SymbolSubstitution(SymSqr(S), SymSqr(T));
18     if (~CompareDiagMultisets(Ssqr, Tsqr)), break; end if % not p–sim
19 20 converged = ComparePatterns(S, Ssqr) & ComparePatterns(T, Tsqr);
21     if (converged), psim = TRUE; end if % p–sim
22 23 S = Ssqr; T = Tsqr;
24 until (converged)
25 26 return(psim);
27 end

Σ: a set of distinct symbols, and iii) g: a bijective mapping between symbols and cells of the partition. Each cell of the partition is associated with a single symbol/value.

For example, let M be a m×m matrix. Define L as the set of all (i,j) locations,

$L = \{(i,j) | 1 \leq i \leq m, 1 \leq j \leq m\}.$

Then the triplet notation for M is

$M = (\Pi, \Sigma, g)$

where Π is a partition of L where each cell contains all of the locations associated with the same symbol, Σ is the set of distinct symbols in M, and g is a bijective mapping of symbols in Σ to cells in Π.

Often Π and Σ are assumed to be ordered. Π is ordered by first applying lexicographic ordering within each cell to order the locations in the cell. The first location in each ordered cell is designated the representative location for that cell. Next, the representative locations are collected and lexicographically ordered to order the cells themselves. The set of symbols Σ is ordered such that the first symbol is associated with the first cell of Π and the second symbol with the second cell, and so on. So the
mapping \( g \) from \( \Sigma \) to \( \Pi \) is simply the identity mapping. If the notation \( M = (\Pi, \Sigma) \) appears, it means that \( \Pi \) and \( \Sigma \) are ordered and \( g \) is the identity mapping.

To compare two partitions, \( \Pi_1 \) and \( \Pi_2 \), the representative location for each cell is assigned to all locations within the cell, essentially using the representative locations as the symbol set. Then the partition difference, \( \Pi_1 - \Pi_2 \), is defined as

\[
(\Pi_1 - \Pi_2)_{i,j} = \begin{cases} 0 & \text{if the representative locations at } (i,j) \text{ match} \\ 1 & \text{if the representative locations at } (i,j) \text{ do not match.} \\
\end{cases}
\]

The partition \( \Pi \) will be referred to as a pattern to evoke a two dimensional image. \( \Pi (A) \) is a refinement of \( \Pi (B) \), \( \Pi (A) \leq \Pi (B) \), if each cell of \( \Pi (A) \) is a subset of a cell of \( \Pi (B) \).\[\square\]

2.4. Symbol Substitution: Lines 11 & 17. A consequence of symmetric permutations moving values/symbols around without changing them is that the symbols can be replaced without changing the p-similarity relation.

**Theorem 1.** Given square matrices \( A \) and \( B \). \( A \sim B \iff A_{\Sigma} \sim B_{\Sigma} \) where \( A = (\Pi_A, \Sigma, g_A) \), \( B = (\Pi_B, \Sigma, g_B) \), \( A_{\Sigma} = (\Pi_A, \Sigma, g_A) \), \( B_{\Sigma} = (\Pi_B, \Sigma, g_B) \) and \( |\Sigma| = |\Sigma| \).

**Proof.** Assume \( A \sim B \) so there exists a permutation matrix \( P \) such that \( PAP^T = B \). Further assume that the symmetric permutation moves the symbol at location \((i,j)\) of \( A \) to location \((r,s)\) in \( B \). So \( A_{i,j} = B_{r,s} = \sigma_k \) where \( \sigma_k \in \Sigma \) is the \( k \)th symbol of \( \Sigma \). Everywhere \( \sigma_k \) appears in \( A \) and \( B \) will be replaced by \( \bar{\sigma}_k \), the \( k \)th symbol of \( \Sigma \) in \( A_{\Sigma} \) and \( B_{\Sigma} \). Similarly for each of the other symbols in \( \Sigma \). Therefore, \( PA_{\Sigma}P^T = B_{\Sigma} \) so \( A_{\Sigma} \sim B_{\Sigma} \).

For the other direction, reverse the roles of \( \Sigma \) and \( \bar{\Sigma} \).\[\square\]

A consequence of Theorem 1 is that the p-similarity problem for real or complex matrices reduces to solving p-similarity for positive integer matrices.

The symbol substitution function, \textit{SymbolSubstitution} ( ), appears on lines 11 and 17 in Algorithm 1. The function takes two square arrays of values (real or complex numbers in line 11, and strings in line 17) and outputs two square, positive integer matrices. The substitutions are performed so that distinct input values are assigned distinct output symbols and identical input values are assigned identical output symbols.

Given \( m \times m \) arrays as input, a complexity bound on symbol substitution is based on assumption that it is performed similar to the Sieve of Eratosthenes. Arrays are searched in column major order. When a previously unseen input value is encountered, a new output symbol is assigned to that input value and \( O(m^2) \) comparisons are performed on each input array to find all locations containing that input value. Once all matching input values have been replaced with the output symbol, the next unseen input value is located and the process repeats. Since there are at most \( 2m^2 \) distinct input values, there are \( O(m^2) \) comparisons. So a symbol substitution using this approach requires \( O(m^2) \) comparison operations times the cost to do a comparison operation.

The sufficiency argument in Section 3 uses a second symbol substitution function \textit{SymSub} ( ) which takes a single square array of values and output a positive integer matrix. For reproducibility, symbol assignments are performed in a permutation independent fashion. Assume there are \( n \) distinct symbols where there are \( n_1 \) distinct off-diagonal symbols and \( n_2 \) distinct diagonal symbols, with \( n = n_1 + n_2 \). The set of \( n_1 \) distinct off-diagonal strings are lexicographically ordered and then 1 is assigned to the first string in the ordered list and so on until \( n_1 \) is assigned to the last string in the ordered list. Similarly, the list of \( n_2 \) distinct diagonal strings are ordered prior to assigning \((n_1 + 1)\) to \( n \) to them. This guarantees
that any symmetric permutation applied to the array of canonical inner product strings will assign the same integer to the same string.

2.5. **Shifting and Translating: Lines 13 & 14.** The next theorem shows up in spectral graph literature with integer coefficients for $\beta$ and $\gamma$. It is presented here in the more general form where the coefficients are real numbers.

**Theorem 2.** Given square matrices $A$ and $B$. $A \sim_P B \iff (\alpha A + \beta I + \gamma J) \sim_P (\alpha B + \beta I + \gamma J)$ where $I$ is the identity matrix, $J$ is the matrix of all ones and $\alpha, \beta, \gamma \in \mathbb{R}$ with $\alpha \neq 0$.

**Proof.** By noting that $PIP^T = I$ and $PJ^TP^T = J$ for all permutation matrices $P$ so

$$
PA^TP^T = B,
\alpha PA^TP^T + \beta I + \gamma J = \alpha B + \beta I + \gamma J,
P(\alpha A + \beta I + \gamma J)P^T = \alpha B + \beta I + \gamma J.
$$

□

There is overlap in the capability to replace symbols between Theorem 1 and Theorem 2. However, if a symbol appears as a diagonal entry and as an off-diagonal entry, Theorem 2 can make the diagonal entry distinct from the off-diagonal entry by shifting the spectrum, changing the number of occurrences of that symbol. Theorem 1 cannot change the number occurrences of a symbol, it can only replace a symbol with a new symbol without changing the the number of occurrences.

The shift and translate function, $\text{ShiftAndTranslate}(\cdot)$ appears in lines 13 and 14 of Algorithm 1.

The function takes a square, positive integer matrix $M$ and positive integer values for $\beta$ and $\gamma$ as input and generates the square, positive integer matrix $(M + \beta I + \gamma J)$ as output.

2.6. **Color Matrix: Lines 11, 13 & 14.** Given $m \times m$ matrices $A$ and $B$, define their *color matrices* as the result of performing a consistent symbol substitution followed by shifting and translating so that all symbols are positive integers greater than or equal to three and the symbols on the diagonal are distinct from all off-diagonal symbols. In particular, assume $A = (\Pi_A, \Sigma, g_A)$ and $B = (\Pi_B, \Sigma, g_B)$ where $|\Sigma| = k$ is less than or equal to $m^2$. Perform a consistent symbol substitution using $\Sigma = \{1, 2, \ldots, k\}$ to get $A_{\Sigma}$ and $B_{\Sigma}$ followed by shifting and translating using $\beta = m^2$ and $\gamma = 2$ to get color matrices $A_C = (A_{\Sigma} + m^2 I + 2J)$ and $B_C = (B_{\Sigma} + m^2 I + 2J)$.

The smallest integer in $\Sigma$ is one and the largest is $k$, so shifting the spectrum of $A_{\Sigma}$ and $B_{\Sigma}$ by $m^2 I$ guarantees that the diagonal symbols are distinct from off-diagonal symbols. Then adding $2J$ guarantees the smallest symbol is greater than or equal to three.

**Theorem 3.** Given square matrices $A$ and $B$ and their associated color matrices $A_C$ and $B_C$. $A \sim_P B \iff A_C \sim_P B_C$.

**Proof.** Result follows from applying Theorem 1 to the symbol substitution followed by Theorem 2 for the shifting and translating. □

Color matrices are formed in Algorithm 1 as a two step process. Given square input matrices $A$ and $B$, the symbol substitutions are performed on line 11, followed by the shift and translations on lines 13 and 14 for $A_C$ and $B_C$ respectively.
2.7. Permutation Constraint Graph. Given a $m \times m$ matrix $M$. The permutation constraint graph (PCG) associated with $M$ is the $m \times m$ rook’s graph with distinct column and row edge weights and vertex colors matching $M_C$, $M$’s color matrix. It is called a permutation constraint graph because the weighted edges of the rook’s graph along with the vertex coloring add symmetric permutation constraints to $M$. The rationale behind PCGs is discussed in Section 5.1.

It is well known that rows and columns of rook’s graphs can be permuted independently and that the rows and columns of a square rook’s graph can be exchanged, so the total number of automorphisms is $2 \times (m!)$ [2]. The automorphism group for a PCG is a subgroup of the rook’s graph automorphism group since all of the edges are rook’s graph edges. PCGs break the symmetry that allows rows to be exchanged with columns by adding edge weights. A PCG has a column edge weight of ‘1’ and a row edge weight of ‘2’ as shown in Figure 2.1b.

To see that a PCG implements all symmetric permutation constraints, note that rook’s graph automorphisms keep rows together and columns together, similar to symmetric permutations. Symmetric permutation also requires diagonal elements to remain on the diagonal. PCGs accomplish this by having the diagonal colors be distinct from off-diagonal colors as shown in Figure 2.1b. A PCG automorphism must permute a diagonal entry to another diagonal entry as required by symmetric permutation. This forces the row permutation and the column permutation to match, leading to the following theorem.

**Theorem 4.** Given square matrices $A$ and $B$. Their respective PCGs $\Gamma_A$ and $\Gamma_B$ are isomorphic iff $A \sim_P B$.

**Proof.** Theorem 3 establishes that $A \sim B$ iff $A_C \sim_P B_C$ so if $A \sim B$ then $\Gamma_A$ and $\Gamma_B$ are isomorphic since their vertex colors are $A_C$ and $B_C$ are $p$-similar. In the other direction, assume PCGs $\Gamma_A$ and $\Gamma_B$ are isomorphic. The first step is to show that the re-labeling of vertices takes the form of a symmetric permutation. $\Gamma_A$ and $\Gamma_B$ have identical off-diagonal structure. So any re-labeling must act as an automorphism for that structure, implying the set of possible re-labelings is a subset of the rook’s graph automorphisms that do not exchange the rows and columns. Further, since the diagonal colors of $\Gamma_A$ and $\Gamma_B$ are distinct from off-diagonal colors, the set of possible re-labelings is further restricted to only
include re-labeling that apply the same permutation to rows and columns. Therefore, any re-labeling between $\Gamma_A$ and $\Gamma_B$ is applied as a symmetric permutation. Otherwise the off-diagonal structure is not maintained or diagonal vertices of $\Gamma_A$ are not mapped to diagonal vertices of $\Gamma_B$. By hypothesis, $\Gamma_A$ and $\Gamma_B$ are isomorphic, so there exists a symmetric permutation mapping vertices of $\Gamma_A$ to vertices of $\Gamma_B$ implying the color matrices $A_C$ and $B_C$ are p-similar. Then by Theorem 3 $A$ and $B$ are p-similar. □

Permutation constraint graphs are not explicitly formed in Algorithm 1. However, they provide the link to the permutation constraint matrices described in the next section.

2.8. Permutation Constraint Matrix: Lines 13 & 14. The vertex colored adjacency matrix associated with a PCG is called a permutation constraint matrix (PCM). Column major ordering is used to bijectively map the vertices of the PCG to the diagonal of the PCM. Let $M_C$ be the $m \times m$ color matrix of the PCG. Then the diagonal of the PCM is given by

\begin{equation}
D = \text{diag} \left( \text{reshape} \left( M_C, m^2, 1 \right) \right)
\end{equation}

where $\text{reshape} \left( M_C, m^2, 1 \right)$ uses column major ordering to reshape the $m \times m$ color matrix into a $m^2 \times 1$ vector and $\text{diag} \left()$ converts the $m^2 \times 1$ vector into a $m^2 \times m^2$ diagonal matrix. Applying column major ordering to the vertices of the PCG creates a regular off-diagonal structure in the PCM. Let $R$ be the $m^2 \times m^2$ matrix representing the off-diagonal structure of a PCM. $R$ is given by

\begin{equation}
R = I_m \otimes (1 \ast (J_{m \times m} - I_m)) + (J_{m \times m} - I_m) \otimes (2 \ast I_m)
\end{equation}

where $I \otimes (1 \ast (J - I))$ are the column edges, $(J - I) \otimes (2 \ast I)$ are the row edges, and $\otimes$ is the Kronecker product. So the PCM of a $m \times m$ color matrix $M_C$ is written as

\begin{equation}
\text{PCM} \left( M_C \right) = D + R.
\end{equation}

Note that all $m^2 \times m^2$ PCMs have identical off-diagonal structure. The only difference between two $m^2 \times m^2$ PCMs is the diagonal.

For example, let $M = J_{3 \times 3}$, the $3 \times 3$ matrix of all ones. The associated color matrix is $M_C = (J + 9I + 2J)$ and the PCG looks exactly like Figure 2.1b, where the white diagonal vertices are associated with ‘12’ and the off-diagonal vertices with ‘3’. The PCM generated using column major ordering is

\begin{equation}
\text{PCM} \left( J + 9I + 2J \right) =
\begin{bmatrix}
12 & 1 & 1 & 2 & 2 \\
1 & 3 & 1 & 2 & 2 \\
1 & 1 & 3 & 2 & 2 \\
2 & 3 & 1 & 2 & 2 \\
2 & 2 & 1 & 2 & 2 \\
2 & 2 & 2 & 1 & 12 \\
2 & 2 & 1 & 2 & 12 \\
2 & 2 & 1 & 1 & 12
\end{bmatrix}
\end{equation}

where column edges have a weight of ‘1’, row edges a weight of ‘2’, and the blank areas are filled with zeros. The horizontal and vertical lines in (2.4) are there to emphasize the block structure.

**Theorem 5.** Given $m \times m$ matrices $A$ and $B$ and their associated $m^2 \times m^2$ PCMs, $S = \text{PCM}(A_C)$ and $T = \text{PCM}(B_C)$, then $A \sim P B \iff S \sim P T$.

**Proof.** Using Theorem 4 and the fact that column major ordering is a bijective mapping from the $m \times m$ arrays of vertices of the PCGs to the diagonals of the $m^2 \times m^2$ PCMs. □
If PCMs $S$ and $T$ are p-similar, then the permutation symmetrically permuting $S$ to $T$ has the form $P \otimes P$. To see this, note that the adjacency matrix of an edge weighted rook's graph with a column edge weight of '1' and a row edge weight of '2' is given by $R$ in (2.2). Since rows and columns of $R$ can be permuted independently, but rows cannot be exchanged with columns, the automorphism group of $R$ is

$$\text{Aut} (R) = \{ P_c \otimes P_r \}$$

where $P_c$ and $P_r$ are $m \times m$ permutation matrices applied to the columns and rows respectively. Since the off diagonal structure of every $m^2 \times m^2$ PCM is identical to $R$, any permutation between $S$ and $T$ must have the form $P_c \otimes P_r$. However, the vertex coloring on the diagonal of the PCG, when mapped to the diagonal of the PCM, restrict the possible permutations to those of the form $P \otimes P$.

Construction of the PCMs from the color matrices occurs in lines 13 and 14 of Algorithm 1. The function $\text{PCM}()$ takes a $m \times m$ color matrix $M_C$ as input and returns the associated $m^2 \times m^2$ PCM defined by equations (2.1), (2.2), and (2.3) as output.

To recap, given (real or complex) square matrices $A$ and $B$, a symbol substitution is performed to convert all values/symbols to be positive integers. Next the color matrices $A_C$ and $B_C$ are constructed by shifting and translating the positive integer matrices so the diagonal symbols differ from the off-diagonal symbols and the smallest value is greater than or equal to three. The color matrices are used to color the vertices of edge weighted rook’s graphs where column edges have weight one and row edges weight two creating PCGs. Then PCMs $S$ and $T$ are constructed by using column major ordering to map the PCG vertices to the diagonals. Theorem 5 shows that $S$ and $T$ are p-similar iff $A$ and $B$ are p-similar.

2.9. Symbolic Matrix Multiplication.

2.9.1. Eigenspace Projector Patterns. PCMs are real symmetric matrices. Therefore they have a unique spectral decomposition in terms of the distinct eigenvalues and their associated spectral projectors

$$(2.5) \quad A = \sum \lambda_i E_i \text{ and } I = \sum E_i$$

where $\lambda_i$ is an eigenvalue and $E_i$ is its associated spectral projector [14] pg. 9]. Assume there are $k$ distinct eigenvalues. Rearrange (2.5) as

$$(2.6) \quad A_{1 \times m \times m} = [\lambda_1, \cdots, \lambda_k] \times \begin{bmatrix} E_1 \\ \vdots \\ E_k \end{bmatrix}_{k \times m \times m}$$

where the spectral projectors are stacked like a pages in a book lying on a desk and $A$ is a sheet of paper lying on the desk. Any symmetric permutation applied to $A$ on the lhs is also applied to each of the spectral projectors on the rhs. Therefore we can construct a string from each $(i, j)$ column by concatenating the values. Then substituting distinct symbols for distinct strings yields a pattern. We call this pattern the eigenspace projector pattern.

To find the eigenspace projector pattern you need to compute the eigenvalues and eigenvectors. This is an iterative process and may be susceptible to floating point arithmetic errors. Alternatively, the eigenspace projector pattern can be generated from a stack of powers of $A$ by taking advantage of
Wilkinson’s observation [18, pg. 13] that the transpose of the Vandermonde matrix
\[ V^T = \begin{bmatrix} 1 & \cdots & 1 \\ \lambda_1 & \cdots & \lambda_k \\ \vdots & \cdots & \vdots \\ \lambda_1^{k-1} & \cdots & \lambda_k^{k-1} \end{bmatrix}, \]
is non-singular. Powers of \( A \) can be stacked on the lhs as
\[
(2.7) \quad \begin{bmatrix} I \\ A \\ \vdots \\ A^{k-1} \end{bmatrix}_{k \times m \times m} = \begin{bmatrix} 1 & \cdots & 1 \\ \lambda_1 & \cdots & \lambda_k \\ \vdots & \cdots & \vdots \\ \lambda_1^{k-1} & \cdots & \lambda_k^{k-1} \end{bmatrix}_{k \times m \times m} \times \begin{bmatrix} E_1 \\ \vdots \\ E_k \end{bmatrix}_{k \times m \times m}.
\]
Examining (2.7), one sees that strings constructed on the lhs of (2.7) yield a pattern identical to the eigenspace projector pattern since \( V^T \) is non-singular. PCMs are symmetric integer matrices so integer arithmetic can be used to construct the eigenspace projector pattern. However, overflow errors may occur.

The eigenspace projector pattern is a refinement of the individual spectral projectors. So given a real symmetric matrix, the eigenspace projector pattern is the most refined pattern one would expect for that matrix. In graph isomorphism terms, the eigenspace projector pattern is like the coarsest equitable partition [9] achievable using naive color refinement. For two real symmetric matrices to be p-similar, their eigenspace projector patterns must be p-similar.

2.9.2. Computing Eigenspace Projector Patterns for SPD Matrices. For symmetric positive definite (SPD) matrices, one doesn’t need strings constructed from the stack of powers of \( A \), lhs of (2.7), to determine the eigenspace projector pattern. For a high enough power, say \( n \), the pattern \( \Pi(A^n) \) is identical to the eigenspace projector pattern.

**Theorem 6.** For real, symmetric positive definite matrix \( A \), there exists a finite integer \( n \) such that the pattern in \( A^n \) is identical to the eigenspace projector pattern, and all higher powers, \( A^{n+l}, l = 1, \ldots \), have the same pattern.

**Proof.** Assume symmetric positive definite matrix \( A \) has \( k \) distinct eigenvalues and they are ordered \( 0 < \lambda_1 < \lambda_2 < \cdots < \lambda_k \). We only need to focus on a subset of locations from the lhs and rhs of (2.7), one for each distinct string. Let \((i,j)\) and \((r,s)\) be two off-diagonal locations with distinct strings. Let \( eij = E(:,i,j) \) and \( ers = E(:,r,s) \) be the column vectors associated with the strings on the rhs of (2.7) and \( aij \) and \( ars \) be the column vectors associated with the strings on the lhs of (2.7). Note that
\[
\begin{bmatrix} 1 & \cdots & 1 \end{bmatrix} \times eij = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix} \times ers = 0
\]
from (2.5) since \((i,j)\) and \((r,s)\) are off-diagonal locations.

Let \( \delta = eij - ers \), then \( \delta \neq 0 \) since the strings differ but
\[
(2.8) \quad \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix} \times \delta = 0.
\]
Equation (2.8) also applies to differences between distinct strings on the diagonal since
\[
\begin{bmatrix} 1 & \cdots & 1 \end{bmatrix} \times eii = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix} \times ejj = 1.
\]
Comparisons between diagonal and off-diagonals strings are ignored since they can never match.
Given that $e_{ij} \neq e_{rs}$, then $a_{ij} \neq a_{rs}$ and there is at least one power $t$, $1 \leq t \leq k - 1$, such that $A_{ij}^t \neq A_{rs}^t$. The question remains, is there a finite integer $n$ such that $A_{ij}^n \neq A_{rs}^n$ and $A_{ij}^{n+l} \neq A_{rs}^{n+l}$ for all $l = 1, \ldots$.

Assume for every sequence of consecutive powers $t$ where $A_{ij}^t - A_{rs}^t \neq 0$, there is a maximum integer $n$ such that $A_{ij}^n - A_{rs}^n \neq 0$ but $A_{ij}^{n+1} - A_{rs}^{n+1} = 0$. Now write $A_{ij}^{n+1} - A_{rs}^{n+1} = 0$ as

$$A_{ij}^{n+1} - A_{rs}^{n+1} = [\lambda_1^{n+1}, \ldots, \lambda_k^{n+1}] \times \delta = [1 \cdots 1] \times \begin{bmatrix} \lambda_1^{n+1} \delta_1 \\ \vdots \\ \lambda_{k-1}^{n+1} \delta_{k-1} \\ \lambda_k^{n+1} \delta_k \end{bmatrix} = 0.$$  

(2.9)

Without loss of generality, assume that $\delta_k \neq 0$, and make the following substitution

$$\begin{bmatrix} \lambda_1^{n+1} \delta_1 \\ \vdots \\ \lambda_{k-1}^{n+1} \delta_{k-1} \\ \lambda_k^{n+1} \delta_k \end{bmatrix} = \begin{bmatrix} \lambda_1^{n+1} \delta_1 \\ \vdots \\ \lambda_{k-1}^{n+1} \delta_{k-1} \\ - (\lambda_k^{n+1} \delta_1 + \cdots + \lambda_{k-1}^{n+1} \delta_{k-1}) \end{bmatrix},$$

where the right hand vector uses (2.9) to substitute for $\lambda_k^{n+1} \delta_k$. Equating the last terms of (2.10) yields

$$\lambda_k^{n+1} \delta_k = - (\lambda_1^{n+1} \delta_1 + \cdots + \lambda_{k-1}^{n+1} \delta_{k-1}),$$

or

$$\lambda_k^{n+1} = \frac{- (\lambda_1^{n+1} \delta_1 + \cdots + \lambda_{k-1}^{n+1} \delta_{k-1})}{\delta_k}.$$

Without loss of generality, assume $\delta_{k-1} \neq 0$, and factor $\lambda_k^{n+1}$ out of the numerator

$$\lambda_k^{n+1} = \lambda_{k-1}^{n+1} \left( \frac{- (\lambda_1 \lambda_{k-1}^{-1})^{n+1} \delta_1 + \cdots + 1 \delta_{k-1}}{\delta_k} \right),$$

and rearrange to get

$$\left( \frac{\lambda_k}{\lambda_{k-1}} \right)^{n+1} = \frac{- (\lambda_1 \lambda_{k-1}^{-1})^{n+1} \delta_1 + \cdots + 1 \delta_{k-1}}{\delta_k}.$$  

(2.11)

Taking the limit of both sides of (2.11) results in

$$\lim_{n \to \infty} \left( \frac{\lambda_k}{\lambda_{k-1}} \right)^{n+1} = +\infty \quad \text{while} \quad \lim_{n \to \infty} \left( \frac{- (\lambda_1 \lambda_{k-1}^{-1})^{n+1} \delta_1 + \cdots + 1 \delta_{k-1}}{\delta_k} \right) = - \frac{\delta_{k-1}}{\delta_k},$$

creating a contradiction. Therefore, there must be some finite integer $n$ such that $A_{ij}^n \neq A_{rs}^n$ and $A_{ij}^{n+l} \neq A_{rs}^{n+l}$ for all $l = 1, \ldots$.

Applying the same argument pairwise to all distinct off-diagonal strings shows that there exists for each distinct pair of strings. Taking the maximum over all of the $n$’s yields the desired result. □
Theorem 6 does not guarantee that \( n \) is less than or equal to \( k - 1 \), or that the value for \( k \) is known. It states that mathematically the pattern in powers of a real SPD matrix converges to the eigenspace projector pattern. In practice, computer arithmetic is finite precision. So if \( n \) is large, the emergent pattern will only reflect the eigenspace projector(s) associated with the dominant eigenvalue(s).

2.9.3. Why Symbolic Matrix Multiplication. Theorem 6 says the eigenspace projector patterns of integer SPD matrices can be computed using integer arithmetic. However, it is not known when the eigenspace projector pattern will be reached, and the computation is susceptible to overflow. When the author attempted to find eigenspace projector patterns using recursive squaring, overflow would occur after a few iterations. To avoid overflow, a symbol substitution is performed to reduce the magnitude of the integers. The process repeated alternating between recursive squaring and symbol substitution until either the pattern converged or the number of symbols was so large that symbol substitution could not reduce the magnitudes enough to prevent overflow.

**Key observation:** There exist cases where the symbol substitution resulted in a matrix whose eigenspace projector pattern is a strict refinement of the original eigenspace projector pattern. These “new” matrices have the same p-similarity relationship as the original matrices but a more refined eigenspace projector pattern.

An example is the first graph of case 10 from the website http://funkybee.narod.ru/graphs.htm. The graph has 11 vertices and its adjacency matrix is given in Figure 2.2. Its eigenspace projector pattern has 29 cells but recursive squaring with symbol substitution resulted in a pattern with 30 cells. An exhaustive search revealed four automorphisms. Applying the automorphisms yielded 30 orbits. The orbits are identical to the pattern generated by the recursive squaring with symbol substitution. Comparing the orbits with the eigenspace projector pattern shows that the cell associated with symbol ‘6’ in the eigenspace projector pattern contains two orbits, see Figure 2.3.

The question is how to find these more refined eigenspace projector patterns without resorting to random symbol substitutions. This led to examining symbolic matrix multiplication as a possible method for simultaneously checking all possible symbol substitutions while avoiding overflow.

2.9.4. Canonical Inner Product Strings. It turns out symbolic matrix multiplication also has an advantage over regular matrix multiplication in separating orbits. Assume \( A \sim P B \) then there exists a \( P \) such
that $PAP^T = B$. If $P : i \rightarrow r$ and $j \rightarrow s$ then $A_{i,j} = B_{r,s}$. Also,

$$PAP^T \times PAP^T = B \times B$$

$$P (AP^T \times PA)^T P^T = B \times B$$

implying

$$[AP^T \times PA]_{i,j} = [B \times B]_{r,s}$$

where

$$A_{i,j} P^T \times PA_{i,j} = B_{r,s} \times B_{r,s}.$$  

Since symmetric application of $P$ moves row $i$ of $A$ to become row $r$ of $B$ (with the values permuted) and column $j$ of $A$ becomes column $s$ of $B$ (with the values permuted in the same way) the multiset of terms in the inner products are identical. Further, the order of the factors within a term are also identical. To see why this is interesting, assume the inner products from two locations are given by

$$\begin{bmatrix} \alpha \beta \\ \beta \alpha \end{bmatrix}\times \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \alpha \beta + \beta \alpha = \gamma$$

and

$$\begin{bmatrix} \alpha \alpha \\ \beta \beta \end{bmatrix}\times \begin{bmatrix} \beta \\ \beta \end{bmatrix} = \alpha \beta + \alpha \beta = \gamma.$$  

Using regular matrix multiplication, both inner products appear to be identical, evaluating to $\gamma$. However, symbolically the strings formed from the vector of terms

$$\begin{bmatrix} \alpha \beta \\ \beta \alpha \end{bmatrix}$$

and

$$\begin{bmatrix} \alpha \beta \\ \alpha \beta \end{bmatrix}$$

are different, implying the two locations are not in the same orbit. So symbolic inner products can separate orbits that appear to be the same to regular matrix multiplication.

**Definition 7.** Define the **canonical inner product string** of $u^T \times v$ as the ordered multiset of inner product terms where the first factor in each term is from the row vector $u^T$ and the second from the column vector $v$

$$\text{canonicalString} (u^T \times v) = \text{order} (\{(u_k, v_k)\}).$$

To create the canonical inner product string, the multiset of terms is split into two parts: terms involving diagonal symbols and terms involving two off-diagonal symbols. For terms involving diagonal symbols,
they are ordered such that the row vector diagonal symbol comes first, followed by the term involving the column diagonal symbol. For terms involving two off-diagonal symbols, they are lexicographically ordered. Then the ordered parts are concatenated, diagonal terms followed by off-diagonal terms, to construct the canonical inner product string.

2.9.5. SymSqr: Line 17. A PCM is a symmetric positive integer matrix whose diagonal symbols are distinct from off-diagonal symbols. Therefore the output of symbolically squaring a PCM has a pattern that is symmetric and the diagonal canonical inner product strings are distinct from off-diagonal canonical inner product strings. The canonical inner product strings are constructed as described in Section 2.9.4.

**Definition 8.** SymSqr() is a function that takes a symmetric matrix whose diagonal symbols are distinct from off-diagonal symbols as input and generates an array of canonical inner product strings as output. Since the canonical inner product strings at \((i,j)\) and \((j,i)\) likely differ, the output array is made symmetric by choosing the lesser of the canonical inner product strings at \((i,j)\) and \((j,i)\) to represent both locations.

Using a Jordan product to construct matching canonical strings for \((i,j)\) and \((j,i)\) was considered. If a single string is constructed from the combined terms of the inner products at \((i,j)\) and \((j,i)\), it is possible that other locations \((r,s)\) and \((s,r)\), with distinct canonical inner product strings, will generate the same string if their terms are mixed together. This would hide the fact that the locations are actually in different orbits. However, if the Jordan product is interpreted as lexicographically ordering the pair of canonical strings from \((i,j)\) and \((j,i)\) and concatenating them into a single string, the final strings will be distinct and equivalent to choosing the lesser string.

**Theorem 9.** Locations in the same orbit have identical canonical inner product strings.

*Proof.* By the arguments used in Section 2.9.4 to derive and construct the canonical inner product strings.

The contrapositive of Theorem 9 causes patterns to be refined. If two locations in the same cell of \(\Pi(M)\) have distinct canonical strings when \(M\) is symbolically squared, they cannot be in the same orbit and will be assigned to different cells in the new pattern \(\Pi(SymSqr(M))\).

**Theorem 10.** Locations whose canonical inner product strings differ are not in the same orbit.

*Proof.* Contrapositive of Theorem 9.

**Theorem 11.** If \(M\) is a square matrix whose diagonal symbols are distinct from off-diagonal symbols, then the cells of \(\Pi(SymSqr(M))\) represent disjoint sets of orbits.

*Proof.* This is a direct consequence of Theorem 9. Canonical inner product strings for locations in the same orbit are identical. Therefore locations in the same orbit are assigned to the same cell.

Theorem 11 does not guarantee there is one orbit per cell. Only that locations in an orbit will not be split across multiple cells.

The symbolic squaring function, \(SymSqr()\), appears twice on line 17 of Algorithm 1. Each input is a \(m^2 \times m^2\) symmetric, positive integer matrix whose diagonal symbols are distinct from the off-diagonal symbols. The outputs are \(m^2 \times m^2\) square arrays of canonical inner product strings, where each string is composed of \(m^2\) terms.
2.9.6. Monotonic Refinement. Let $M$ be a square matrix whose diagonal symbols are distinct from the off-diagonal symbols. The next theorem addresses repeated symbolic squaring of $M$. Theorem 12 shows that symbolic squaring monotonically refines the pattern since elements of two different cells will never be assigned to the same cell.

**Theorem 12.** Repeated symbolic squaring of a square matrix whose diagonal symbols are distinct from off-diagonal symbols monotonically refines the pattern until a stable pattern is reached.

**Proof.** Let $M$ be a square matrix whose diagonal symbols are distinct from the off-diagonal symbols. To show that refinement is monotonic, it is enough to show that two locations with distinct symbols can never have identical canonical inner product strings. To see this, let $(i, j)$ and $(r, s)$ be two off-diagonal locations where $M_{i,j} \neq M_{r,s}$. Without loss of generality assume that $i < j$ and $r < s$. Let $D$ be the diagonal of $M$. Then the inner products $[M \times M]_{i,j}$ and $[M \times M]_{r,s}$ look like

$$[M \times M]_{i,j} = \begin{bmatrix} \cdots & D_{i,i} & \cdots & M_{i,j} & \cdots \\ \vdots & & & \vdots & \\ D_{j,j} & & & \vdots & \\ \vdots & & & \vdots & \end{bmatrix} \times \begin{bmatrix} \cdots \\ M_{i,j} \\ \vdots \\ D_{j,j} \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdots \\ 1 \cdots 1 \\ \vdots \end{bmatrix} \times \begin{bmatrix} \cdots \\ D_{i,i}M_{i,j} \\ \vdots \\ M_{i,j}D_{j,j} \\ \vdots \end{bmatrix}$$

and

$$[M \times M]_{r,s} = \begin{bmatrix} \cdots & D_{r,r} & \cdots & M_{r,s} & \cdots \\ \vdots & & & \vdots & \\ M_{r,s} & & & \vdots & \\ \vdots & & & \vdots & \\ D_{s,s} & & & \vdots & \end{bmatrix} \times \begin{bmatrix} \cdots \\ \vdots \\ M_{r,s} \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdots \\ 1 \cdots 1 \\ \vdots \end{bmatrix} \times \begin{bmatrix} \cdots \\ D_{r,r}M_{r,s} \\ \vdots \\ M_{r,s}D_{s,s} \\ \vdots \end{bmatrix}.$$ 

The canonical inner product string for $[M \times M]_{i,j}$ includes terms $\{(D_{i,i}, M_{i,j}), (M_{i,j}, D_{j,j})\}$ and the canonical string for $[M \times M]_{r,s}$ includes terms $\{(D_{r,r}, M_{r,s}), (M_{r,s}, D_{s,s})\}$. Since $M_{i,j} \neq M_{r,s}$ the strings do not match, and they will be assigned distinct symbols.

A similar argument holds for diagonal inner product strings where $M_{i,i} \neq M_{r,r}$. Their canonical inner product strings have terms $\{(D_{i,i}, D_{i,i})\}$ and $\{(D_{r,r}, D_{r,r})\}$ respectively that do not match. Diagonal locations and off-diagonal locations have a different structure to their canonical inner product strings. Diagonal locations have a single term involving diagonal symbols, whereas off-diagonal locations have two terms involving diagonal symbols. Therefore, symbolic squaring either strictly refines the pattern or has reached a stable pattern. $\square$

**Theorem 13.** If $M$ is a symmetric $m \times m$ matrix whose diagonal symbols are distinct from off-diagonal symbols, then symbolic squaring followed by symbol substitution converges to a stable pattern within $m$ iterations.

**Proof.** Given $M$, a symmetric $m \times m$ matrix whose diagonal symbols are distinct from off-diagonal symbols. Recall that Theorems 1 and 2 imply that any pattern that is symmetric and has diagonal values distinct from off-diagonal values can be replaced by a SPD matrix with positive integer values. So, $M$ and the output of symbolically squaring $M$ can always be made to be SPD matrices with positive integer values.
Now consider equation (2.7). The eigenspace projector pattern on the rhs of (2.7) can be generated from the stack of \( k - 1 \) powers of \( M \) on the lhs, where \( k \) is the number of distinct eigenvalues. A \( m \times m \) matrix has at most \( m \) distinct eigenvalues. So at most \( m - 1 \) powers of \( M \) are needed on the lhs of (2.7) to construct the eigenspace projector pattern.

Next consider replacing successive powers of \( M \) by symbolic squaring with symbol substitution. At most \( m - 2 \) symbolic squarings are needed to fill the stack since \( I \) and \( M \) are the first two layers. Theorem 12 guarantees that repeated symbolic squaring monotonically refinements the pattern. Therefore, each successive layer is a refinement of all prior layers.

Theorem 6 states that the powers of a SPD matrix converge to the eigenspace projector pattern. The bottom layer of the stack constructed from repeated symbolic squaring is a refinement of all prior layers. Therefore the bottom layer is at least as refined as the eigenspace projector pattern of \( M \).

So symbolic squaring converges to a stable pattern within \( m \) iterations.

Symbolic squaring followed by symbol substitution occurs on line 17 of Algorithm 1.

**Definition 14.** Let \( M \) be a square matrix whose diagonal symbols differ from off-diagonal symbols. Define \( \Pi (M^*) \) as the stable pattern reached by repeated symbolic squaring and symbol substitution.

One might wonder why symbolic squaring does not converge in a single iteration. The answer appears to be related to the number of initial symbols and the off-diagonal structure of a PCM. For the first iteration, a PCM has at least five distinct symbols and the off-diagonal is highly structured. For the five symbol case, see (2.4), it can be shown that after the first iteration, there are 9 distinct symbols. A second symbolic squaring results in 11 distinct symbols and is the stable pattern. For another example, the PCM of a Petersen graph has six symbols. The stable pattern has 65 symbols and is reached on the third symbolic squaring. So the structure and limited number of initial symbols typically causes symbolic squaring to take several iterations to converge. In the authors experience, no case has taken more than six iterations to converge and the number of distinct symbols can be in the 10's of millions.

2.10. **Comparing Multisets:** Line 18. Theorem 9 shows that matching canonical inner product strings is a necessary condition for two locations to be in the same orbit. This implies the multiset of canonical inner product strings for \( SymSqr (A) \) and \( SymSqr (B) \) must match for \( A \) and \( B \) to be p-similar, \( \text{mix}(\text{SymSqr}(A)) = \text{mix}(\text{SymSqr}(B)) \). Conversely, if the mixes do not match, then \( A \) and \( B \) cannot be p-similar. However it is possible to detect when the mixes do not match by looking at a smaller multiset. If the mixes do not match, \( \text{mix}(\text{SymSqr}(A)) \neq \text{mix}(\text{SymSqr}(B)) \), then the column mixes do not match, \( \text{colMix}(\text{SymSqr}(A)) \neq \text{colMix}(\text{SymSqr}(B)) \), which in turn implies the diagonal mixes will not match, \( \text{diagMix}(\text{SymSqr}(A)) \neq \text{diagMix}(\text{SymSqr}(B)) \). Column mixes may differ one iteration before the diagonal mixes if the differences are in off-diagonal symbols. However, after the next iteration, the off-diagonal differences are reflected in the diagonal symbols causing the diagonal mixes to differ. Comparing diagonal mixes is performed on line 18 in Algorithm 1.

Comparing diagonal mixes to determine when two matrices are not p-similar is consistent with Specht’s Theorem [7] pp. 97-98. Specht’s Theorem gives necessary and sufficient conditions for showing when two matrices are unitarily similar. Specht’s Theorem works by comparing the traces of sequences of matrix products of various lengths. For p-similarity it is not enough to show that the traces match, the diagonal mixes must match. So, matching diagonal mixes, after every round of symbolic squaring, is a necessary condition for \( A \) and \( B \) to be p-similar. This implies differing diagonal mixes is a sufficient condition for \( A \) and \( B \) to be p-similar. Therefore, each successive layer is a refinement of all prior layers.

Symbolic squaring followed by symbol substitution occurs on line 17 of Algorithm 1.

**Definition 14.** Let \( M \) be a square matrix whose diagonal symbols differ from off-diagonal symbols. Define \( \Pi (M^*) \) as the stable pattern reached by repeated symbolic squaring and symbol substitution.

One might wonder why symbolic squaring does not converge in a single iteration. The answer appears to be related to the number of initial symbols and the off-diagonal structure of a PCM. For the first iteration, a PCM has at least five distinct symbols and the off-diagonal is highly structured. For the five symbol case, see (2.4), it can be shown that after the first iteration, there are 9 distinct symbols. A second symbolic squaring results in 11 distinct symbols and is the stable pattern. For another example, the PCM of a Petersen graph has six symbols. The stable pattern has 65 symbols and is reached on the third symbolic squaring. So the structure and limited number of initial symbols typically causes symbolic squaring to take several iterations to converge. In the authors experience, no case has taken more than six iterations to converge and the number of distinct symbols can be in the 10's of millions.

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condition for declaring two matrices non p-similar. Note that symbolic squaring with symbol substitution means the diagonal mixes of an uncountably infinite number of matrix pairs are compared each iteration.

2.11. Comparing Patterns, Line 20. The last function in Algorithm 1 compares two patterns and returns TRUE if the patterns are identical. If the pattern before, $\Pi(M)$, and after symbolic squaring, $\Pi(SymSqr(M))$, match then the stable pattern $\Pi(M^*)$ has been reached for that matrix. Necessary conditions for $A$ and $B$ to be p-similar are that the diagonal mixes match and they reach stable patterns on the same iteration. The first condition is checked on line 18 and the second on line 20 of Algorithm 1.

Note that the case where diagonal mixes match and one PCM has reached a stable pattern but the other has not, will be detected as non p-similar. The non stable pattern is refined by the symbolic squaring in the next iteration, changing the column mixes. This in turn implies the diagonal symbols will change, causing the diagonal mixes to differ. Ultimately resulting in the PCMs being declared non p-similar.

2.12. Algorithm Complexity. The overall complexity of Algorithm 1 for comparing two $m \times m$ matrices is $O(m^{12})$. The bound is conservative and computed using simple, unoptimized approaches. In particular, symbol substitutions are assumed to use the method described in Section 2.4.

Below are complexity bounds on individual functions of Algorithm 1 given two $m \times m$ matrices as input:

- **Line 11, SymbolSubstitution:** $O(m^4)$ since there are $2m^2$ locations containing values and $O(m^2)$ comparison operations per substitution with a constant cost per comparison operation.

- **Lines 13&14, ShiftAndTranslate:** $O(m^2)$ since there are $2m^2$ locations to update.

- **Lines 13&14, PCM:** $O(m^4)$ since there are $2m^4$ locations to initialize.

- **Line 17, SymSqr:** $O(m^8)$ reasoned as follows:
  - Construct terms from factors: $O(m^6)$ since there are $2m^4$ canonical strings and each string has $m^2$ terms and a constant cost to construct a term from its factors.
  - Construct canonical inner product strings from the terms: $O(m^8)$ since there are $2m^4$ strings and it takes a maximum of $O(m^4)$ comparison operations to order the $m^2$ terms of a string at a constant cost per comparison operation.
  - Select lessor string for $(i,j)$ and $(j,i)$ locations: $O(m^6)$ since there are $2m^4$ locations and comparing two strings takes $O(m^2)$ comparison operations at a constant cost per comparison operation.

- **Line 17, SymbolSubstitution:** $O(m^{10})$ since there are $2m^4$ locations and $O(m^4)$ string comparison operations per substitution at a cost of $O(m^2)$ to compare two strings.

- **Line 18, CompareDiagMultisets:** $O(m^4)$ since it takes a maximum of $O(m^4)$ comparison operations to sort a multiset with $m^2$ values at a constant cost per comparison operation. Comparing the sorted multisets takes at most $O(m^2)$ comparison operations.

- **Line 20, ComparePatterns:** $O(m^8)$ since the comparison is performed by replacing values with their representative locations and then comparing the results. To replace values with representative locations involves $2m^4$ locations and $O(m^4)$ comparison operations per substitution at a constant cost per comparison operation. This is followed by at most $O(m^4)$ comparison operations to compare the two patterns.

- **Lines 16-24, Repeat Until Iterations:** $O(m^2)$ by Theorem 13 applied to a $m^2 \times m^2$ SPD matrix.
Overall Complexity: \( O \left( m^{12} \right) \) derived from iterating the repeat until loop a maximum of \( O \left( m^2 \right) \) times, and a \( O \left( m^{10} \right) \) cost to substitute symbols for canonical inner product strings each iteration.

As mentioned previously, in the author’s experience, no case has taken more the six iterations to converge. The greatest reduction in overall complexity will come from optimizing the symbolic substitution applied to canonical inner product strings. Even better would be to find a way to avoid symbolic matrix multiplication altogether, see Section 5.2. In terms of space, Algorithm 1 requires \( O \left( m^6 \right) \) locations to hold the \( 2m^4 \) canonical inner product strings, where a location is large enough to hold a term.

3. Sufficiency Argument

In Section 2, Algorithm 1 is shown to test necessary conditions for two PCMs to be p-similar and that differing diagonal mixes are sufficient to determine that two matrices are not p-similar. The last theoretical hole is to determine whether the patterns of non p-similar PCMs can stabilize on the same iteration with matching diagonal mixes. The purpose of this section is to argue that it is not possible, implying Algorithm 1 is necessary and sufficient for determining when two matrices are p-similar.

An outline of the argument goes as follows:

1. Given a \( m^2 \times m^2 \) PCM and its automorphism group, the set of all symmetric positive definite matrices with the same automorphism group is constructed.
2. The set is shown to be convex.
3. Repeated symbolic squaring with symbol substitution is shown to act as a descent method on the convex set, implying the orbits are found within \( m^2 \) steps.
4. Having the orbits does not guarantee the symbol to orbit assignments are consistent across matrices.
5. Using properties of PCMs, it is shown that an Oracle either matches all of the columns \( S^* \) and \( T^* \), or none of the columns. This differs from cases where an Oracle is able to partially match non p-similar matrices, Section 5.1.
6. Next, the PCM of the color matrix for the direct sum of the initial pair of matrices, \( M = PCM \left( (A \oplus B)_C \right) \), is constructed and symbolically squared until its orbits, \( \Pi(M^*) \), are found. PCMs \( S \) and \( T \) are embedded within PCM \( M \).
7. The patterns at locations associated with \( S \) and \( T \) in \( \Pi(M^*) \) must match \( \Pi(S^*) \) and \( \Pi(T^*) \) since they are the orbits imposed by \( Aut(S) \) and \( Aut(T) \), respectively.
8. Since \( S \) and \( T \) are not p-similar, the Oracle guarantees no column of \( S^* \) can be matched with any column of \( T^* \). So orbits associated with locations of \( S^* \) in \( M^* \) are distinct from orbits associated with locations of \( T^* \) in \( M^* \).
9. So the diagonal symbols in \( M^* \) associated with locations of \( S^* \) and \( T^* \) are distinct.
10. Therefore, the diagonal symbols of \( S^* \) and \( T^* \) are distinct as long as consistent symbol substitution is performed each symbolic squaring.
11. This implies comparing diagonal mixes of \( S^* \) and \( T^* \) is sufficient for detecting non p-similar matrices.

3.1. Crux of the Argument. Showing that repeated symbolic squaring of a PCM converges to the orbits is the crux of the argument. Given that it is true, a simplified argument constructs \( M = PCM \left( (A \oplus B)_C \right) \) and then either the multisets of diagonal locations associated with \( A_C \) and \( B_C \) in \( M^* \) match or they differ, implying one or more of the orbits are distinct. This would work as a blind permutation similarity algorithm. This follows the graph isomorphism argument that two graphs are isomorphic iff there exists an automorphism of their direct sum that exchanges the graphs.
Repeated symbolic squaring of the direct sum \((A \oplus B)\), without constructing the PCM of the direct sum, is not guaranteed to separate non p-similar matrices. For example, the non p-similar adjacency matrices ‘had-sw-32-1’ and ‘had-sw-32-2’ from the Bliss graph collection \(\blacksquare\) do not have their orbits separated by repeated squaring of the direct sum. However, their associated PCM’s \(S\) and \(T\) have distinct diagonal mixes after the third symbolic squaring.

Algorithm \(\blacksquare\) uses \(S\) and \(T\) instead of the PCM of the direct sum \(M\) because \(S\) and \(T\) are four times smaller. This makes working with \(S\) and \(T\) more practical than working with \(M\).

3.2. WLOG Symbolic Squaring Generates SPD Matrices. As pointed out in Section 2.9.5, inputs to the symbolic squaring function \(\text{SymSqr}(\cdot)\) are symmetric, positive integer matrices whose diagonal symbols are distinct from off-diagonal symbols. The output is a symmetric array of canonical inner product strings whose diagonal strings are distinct from off-diagonal strings. This is immediately followed by a symbol substitution where the canonical inner product strings are replaced by positive integers resulting in an output that is a symmetric, positive integer matrix whose diagonal symbols are distinct from off-diagonal symbols. So, one is free to choose the symbol set, as long as they are positive integers.

In particular, assume there are \(n\) distinct canonical inner product strings, of which there are \(n_1\) distinct off-diagonal strings and \(n_2\) distinct diagonal strings, with \(n_1 + n_2 = n\). Choose the consecutive integers 1 to \(n_1\) as the set of symbols to replace off-diagonal strings and consecutive integers \((m^2n_1 + 1)\) to \((m^2n_1 + n_2)\) as the set of symbols to replace diagonal strings. Then the resulting matrix will be symmetric and diagonally dominant by construction, and so symmetric positive definite (SPD). Therefore in the sufficiency arguments below, symbolic squaring followed by symbol substitution generates SPD matrices unless otherwise noted.

3.3. SymSub. Algorithm \(\blacksquare\) uses \(\text{SymbolSubstitution}\) to perform a consistent symbol substitution on two arrays of canonical inner product strings. In this section, symbol substitution is often performed on a single array of canonical inner product strings using a function called \(\text{SymSub}\). The substitutions are performed in a permutation independent fashion. The set of \(n_1\) distinct off-diagonal strings are lexicographically ordered and then 1 is assigned to the first string in the ordered list and so on until \(n_1\) is assigned to the last string in the ordered list. Similarly, the list of \(n_2\) distinct diagonal strings are ordered prior to assigning \((m^2n_1 + 1)\) to \((m^2n_1 + n_2)\) to them. This guarantees that any symmetric permutation applied to the array of canonical inner product strings will assign the same integer to the same string and that the result is SPD.

3.4. A Convex Set. Theorem 5 shows that determining p-similarity between two square matrices is equivalent to determining the p-similarity between two PCMs. PCMs are symmetric matrices whose diagonal symbols differ from off-diagonal symbols. Since the spectrum can be shifted without affecting the p-similarity relationship, there exist SPD PCMs with the same pattern. One way to generate a SPD PCM is to re-define the color matrix to use \(\gamma = 2m^2\) instead of \(\gamma = 2\). Using \(\gamma = 2m^2\) guarantees the PCM is SPD since it is symmetric and diagonally dominant by construction.

**Definition 15.** Given a \(m^2 \times m^2\) SPD PCM \(M\), let \(\mathbb{M} = \{N \in \text{SPD} \mid \text{Aut}(N) = \text{Aut}(M)\}\) be the set of all real SPD matrices whose automorphism group is \(\text{Aut}(M)\).

**Theorem 16.** \(\mathbb{M}\) is a convex set. That is for all \(M_1, M_2 \in \mathbb{M}\), the linear combination \(\alpha M_1 + (1 - \alpha) M_2\) is also in \(\mathbb{M}\) for \(0 \leq \alpha \leq 1\).

**Proof.** Let \(M_1\) and \(M_2\) be two matrices in \(\mathbb{M}\). It is well known that the set of real SPD matrices is convex, so the focus of the proof is on showing that \(\text{Aut}(\alpha M_1 + (1 - \alpha) M_2) = \text{Aut}(M)\) for \(0 \leq \alpha \leq 1\).
⇒ For all $P \in \text{Aut}(M)$, $PM1P^T = M1$ and $PM2P^T = M2$ since $M1$ and $M2$ are in $\mathbb{M}$. So we have

$$\alpha PM1P^T + (1 - \alpha) PM2P^T = \alpha M1 + (1 - \alpha) M2$$

$$P(\alpha M1 + (1 - \alpha) M2)^T = \alpha M1 + (1 - \alpha) M2$$

showing that $\text{Aut}(M) \leq \text{Aut}(\alpha M1 + (1 - \alpha) M2)$.

⇐ For all $P \in \text{Aut}(\alpha M1 + (1 - \alpha) M2)$, we have

$$P(\alpha M1 + (1 - \alpha) M2)^T = \alpha M1 + (1 - \alpha) M2$$

for $0 \leq \alpha \leq 1$.

\[ \text{(3.1)} \]

Case 1. For $\alpha = 0$, (3.1) equals $PM2P^T = M2$ so $\text{Aut}(\alpha M1 + (1 - \alpha) M2) \leq \text{Aut}(M)$ for $\alpha = 0$.

Case 2. For $0 < \alpha \leq 1$, (3.1) can be rewritten as

$$PM1P^T + \gamma PM2P^T = M1 + \gamma M2$$

where $\gamma = \frac{(1-\alpha)}{\alpha} \geq 0$. Rearrange to get

$$PM1P^T - M1 = \gamma \left(M2 - PM2P^T\right).$$

Now the matrix differences on the lhs and rhs of (3.2) are fixed for a given $P$ and yet (3.2) holds for all $\gamma \geq 0$. This creates a contradiction unless $(PM1P^T - M1)$ and $(M2 - PM2P^T)$ are zero matrices, implying $PM1P^T = M1$ and $PM2P^T = M2$. So $\text{Aut}(\alpha M1 + (1 - \alpha) M2) \leq \text{Aut}(M)$ for $0 < \alpha \leq 1$.

Therefore $\text{Aut}(\alpha M1 + (1 - \alpha) M2) = \text{Aut}(M)$ for $0 \leq \alpha \leq 1$ so each $\alpha M1 + (1 - \alpha) M2$ is in $\mathbb{M}$ implying $\mathbb{M}$ is a convex set.

$\mathbb{M}$ is not closed under matrix multiplication. For any $N \in \mathbb{M}$, its inverse $N^{-1}$ is also in $\mathbb{M}$, but the automorphism group of $N \times N^{-1} = I$ is $S_m$, the symmetric group, which is not a subgroup of $\{P \otimes P\}$. However, the powers of a matrix in $\mathbb{M}$ are in $\mathbb{M}$.

3.5. $M_{\text{Aut}}$ and $M^*$ are in $\mathbb{M}$. Matrices in $\mathbb{M}$ can be separated into equivalence classes by their patterns (partitions). Elements of a class differ from each other by a symbol substitution.

**Definition 17.** Let $M$ be a SPD PCM. Define $M_{\text{Aut}}$ as a SPD matrix representing the orbits imposed by $\text{Aut}(M)$ on $L$, the set of $(i, j)$ locations, see Section 2.3. Locations in the same orbit are assigned the same symbol and locations in distinct orbits have distinct symbols. Symbols on the diagonal of $M_{\text{Aut}}$ are distinct from its off-diagonal symbols since the orbits of diagonal elements are distinct from the orbits of off-diagonal elements. $M_{\text{Aut}}$ is symmetric since $M$ is symmetric and the diagonal symbols are chosen so that $M_{\text{Aut}}$ is SPD.

$M_{\text{Aut}}$ is in $\mathbb{M}$ since it is SPD and $\text{Aut}(M_{\text{Aut}}) = \text{Aut}(M)$ by the definition of $M_{\text{Aut}}$.

**Definition 18.** Let $M$ be a SPD PCM. Let $M^{(i)} = \text{SymSub} \left( \text{SymSqr} \left( M^{(i-1)} \right) \right)$ be the result of the $i^{th}$ symbolic squaring and symbol substitution, where $M^{(0)} = M$. Let $s$ be the iteration where the stable pattern is reached, then $\Pi \left( M^{(s+j)} \right) = \Pi \left( M^{(s)} \right)$ for $j = 1, 2, \ldots$. Define $M^*$ as a SPD matrix whose pattern matches $M^{(s)}$, $\Pi \left( M^* \right) = \Pi \left( M^{(s)} \right)$. Each $M^{(i)}$, $i = 1, \ldots$, is SPD by Section 3.2.

The next theorem shows that the $M^{(i)}$ and $M^*$ are in $\mathbb{M}$.

**Theorem 19.** Given SPD PCM $M$ and $\mathbb{M}$. If $M^{(i)} = \text{SymSub} \left( \text{SymSqr} \left( M^{(i-1)} \right) \right)$ where $M^{(0)} = M$ and $M^*$ is a SPD matrix representing the stable pattern resulting from repeated symbolic squaring. Then the $M^{(i)}$, for $i = 1, \ldots$, and $M^*$ are in $\mathbb{M}$. 
Proof. Given PCM SPD $M$ and $\mathbb{M}$, the set of all SPD matrices whose automorphism group is $Aut(M)$, to show that $M^{(i)}$ and $M^*$ are in $\mathbb{M}$ we need to show that they are SPD and their automorphism groups match $Aut(M)$. Since $M^{(i)}$ and $M^*$ are SPD by Definition 18, the focus is on showing that their automorphism groups match $Aut(M)$.

Let $M^{(i)} = SymSub(SymSqr(M^{(i-1)}))$ where $M^{(0)} = M$.

For $i = 1$: $M^{(1)} = SymSub(SymSqr(M^{(0)}))$. To see that $Aut(M^{(1)}) = Aut(M)$, first note that Theorem 12 guarantees that

\[ \Pi(M^{(1)}) = \Pi(SymSub(SymSqr(M^{(0)}))) \leq \Pi(M^{(0)}) = \Pi(M) . \]

$\Rightarrow$ For each $P \in Aut(M^{(1)})$, if $P$ symmetrically permutes $(i,j)$ to $(r,s)$ then $M_{i,j}^{(1)} = M_{r,s}^{(1)}$ and $M_{i,j} = M_{r,s}$ since $\Pi(M^{(1)}) \leq \Pi(M)$. So $P M P^T = M$ implying $P \in Aut(M)$ and $Aut(M^{(1)}) \leq Aut(M)$.

$\Leftarrow$ For each $P \in Aut(M)$, if $P$ symmetrically permutes $(i,j)$ to $(r,s)$ then $(i,j)$ and $(r,s)$ are in the same orbit and Theorem 9 guarantees both locations have identical canonical inner product strings. Symbol substitution assigns the same symbol to identical canonical inner product strings resulting in $M_{i,j}^{(1)} = M_{r,s}^{(1)}$, so $PM^{(1)}P^T = M^{(1)}$ and $P \in Aut(M^{(1)})$ implying $Aut(M) \leq Aut(M^{(1)})$.

Therefore $Aut(M^{(1)}) = Aut(M)$.

By induction, the automorphism group of $M^{(i)}$ is $Aut(M)$ for $i = 2, \ldots$. For $M^*$, let $M^* = M^{(s)}$ where $s$ is the iteration a stable pattern is reached, i.e., $\Pi(M^{(s+1)}) = \Pi(M^{(s)})$. Then $M^*$ is in $\mathbb{M}$ since $M^{(s)}$ is in $\mathbb{M}$.

Therefore all of the intermediate $M^{(i)}, i = 1, \ldots$, and $M^*$ are in $\mathbb{M}$. \qed

3.6. Lattice and Chain. The patterns (partitions) of the matrices in $\mathbb{M}$ form equivalence classes that can be partially ordered by refinement. Let $M_{sup}$ be a PCM in $\mathbb{M}$ with the fewest distinct symbols/cells. Then the partial ordering forms a complete lattice with $\Pi(M_{sup})$ is the supremum and $\Pi(M_{Aut})$ as the infimum \[8, pg. 436\].

The subset of patterns $\{\Pi(M), \Pi(M^{(1)}), \cdots, \Pi(M^*)\}$, where

\[ \Pi(M^*) < \cdots < \Pi(M^{(1)}) < \Pi(M) \]

is a totally ordered set, called a chain, between $\Pi(M)$ and $\Pi(M^*)$ \[8\].

Both $\Pi(M^*)$ and $\Pi(M_{Aut})$ are fixed point patterns (stable partitions) of symbolic squaring,

\[ \Pi(SymSqr(M^*)) = \Pi(M^*) \]

and

\[ \Pi(SymSqr(M_{Aut})) = \Pi(M_{Aut}) . \]

Tarski’s Lattice-Theoretical Fixed Point Theorem \[15\] guarantees that the set of fixed points of symbolic squaring is not empty, and that the fixed points form a complete lattice partially ordered by refinement. Unfortunately it does not say that $\Pi(M^*)$ equals $\Pi(M_{Aut})$. If they are identical, then the process of symbolic squaring PCMs finds the orbits.

3.7. Symbolic Squaring as a Descent Method. Symbolic squaring with symbol substitution monotonically refines a PCM $M$ until a stable pattern, $\Pi(M^*)$, is reached. Cells of $\Pi(M^{(i)})$ represent disjoint sets of orbits, Theorem 11 $\mathbb{M}$ is a convex set composed of all SPD matrices whose automorphism group matches $Aut(M)$. Symbolic squaring creates a chain of strictly refined patterns from $\Pi(M)$ to $\Pi(M^*)$. The question is whether $\Pi(M^*)$ is equal to $\Pi(M_{Aut})$. 

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The process of refinement can be viewed as a descent method. Given $M$ and $\mathcal{M}$, for all $P \in \text{Aut}(M)$ one can write
\begin{equation}
M \times M - P \left( MP^T \times PM \right) P^T = 0.
\end{equation}
Equation (3.3) can be converted to a pattern difference that is symbol independent as
\begin{equation}
\|\Pi(M \times M) - \Pi\left(P \left( MP^T \times PM \right) P^T\right)\|_F^2 = 0
\end{equation}
where $\| \cdot \|_F^2$ is the square of the Frobenius norm and the pattern difference assigns zero to locations with matching representative locations and one to locations where the representative locations do not match, see Section 2.3. Convert (3.4) to using symbolic squaring with symbol substitution as
\begin{equation}
\|\Pi(\text{SymSub}(\text{SymSqr}(M))) - \Pi\left(P \left( \text{SymSub}(\text{SymSqr}(M)) \right) P^T\right)\|_F^2 = 0
\end{equation}
where the function $\text{SymSub}()$ performs symbol substitution on a single matrix using a permutation independent mapping from symbol to canonical inner product string, as described in Section 3.3.

Let $M_{\text{Aut}}$ be a SPD matrix representing the orbits imposed by $\text{Aut}(M)$, as defined in Definition 17. Let $M^{(i)} = \text{SymSub}(\text{SymSqr}(M^{(i-1)}))$ where $\Pi(M^{(0)}) = \Pi(M)$ and $M^{(i)} \in \mathcal{M}$. Then the objective is to minimize the cost function
\begin{equation}
\left\|\Pi(\text{SymSub}(\text{SymSqr}(M_{\text{Aut}}))) - \Pi\left(P \left( \text{SymSub}(\text{SymSqr}(M^{(i-1)})) \right) P^T\right)\right\|_F^2 = \text{SSE}
\end{equation}
for $i = 1, \ldots, \ast$ where SSE is the sum square error. Since $\Pi(M_{\text{Aut}})$ is a stable pattern, and each $M^{(i)}$ is in $\mathcal{M}$, (3.5) can be rewritten as
\begin{equation}
\left\|\Pi(M_{\text{Aut}}) - \Pi(M^{(i)})\right\|_F^2 = \text{SSE}.
\end{equation}
The SSE in (3.6) decreases monotonically. Each cell of $\Pi(M^{(i)})$ that contains multiple orbits, has only one orbit with the correct representative location, the remaining orbits in the cell have the wrong representative location. As symbolic squaring refines a cell, at least one additional orbit will have the correct representative location. So the SSE of the pattern difference decreases every iteration until the stable pattern $\Pi(M^\ast)$ is reached.

Although we don’t know $\Pi(M_{\text{Aut}})$ the monotonic refinement of symbolic squaring along with the convexity of $\mathcal{M}$ drives the iterations towards $\Pi(M_{\text{Aut}})$. So an iterative method given by
\begin{equation}
M^{(i)} = \text{SymSub}(\text{SymSqr}(M^{(i-1)}))
\end{equation}
that halts when
\begin{equation}
\left\|\Pi(M^{(i)}) - \Pi(M^{(i-1)})\right\|_F^2 = 0
\end{equation}
causes the successive patterns $\Pi(M^{(i)})$ to approach $\Pi(M_{\text{Aut}})$. Algorithm 1 uses a variant of (3.8), namely testing $\Pi(M^{(i)})$ and $\Pi(M^{(i-1)})$ for equality, to detect when the process has reached a stable pattern, line 20 of Algorithm 1.

In summary, repeated symbolic squaring with symbol substitution finds the most refined pattern. The refinement is monotonic and converges to a stable pattern where locations in an orbit are in the same cell. By the convexity of $\mathcal{M}$, $\Pi(M^\ast)$ equals $\Pi(M_{\text{Aut}})$.

Given that symbolic squaring finds the orbits, one can construct $\text{PCM} M = \text{PCM}((A \oplus B)_C)$ from the color matrix for the direct sum of the input matrices and check whether locations on the diagonal of $M^\ast$ associated with $A$ and $B$ are in the same orbits. If not, $A$ and $B$ are not $p$-similar. The sufficiency argument would end here. However, the author chooses to continue the sufficiency argument because a)
it will be shown that not only do the orbits differ for non p-similar matrices but no orbits match, and b) comparing multisets of diagonal elements to determine p-similarity fits nicely with Specht’s Theorem comparing traces to determine unitary similarity.

Although the process of symbolic squaring a PCM finds its orbits, it says nothing about the association of symbol to orbit. Two PCMs, $A$ and $B$, if processed separately can have the same automorphism group $\text{Aut}(A) = \text{Aut}(B)$ and partitions $\Pi(A) = \Pi(B)$ so the orbits match $M_{\text{Aut}(A)} = M_{\text{Aut}(B)}$. But if they have different symbol sets, $\Sigma_A \neq \Sigma_B$ or the same symbol set with different mappings of symbol to cell $g_A \neq g_B$, then the matrices are not p-similar. This issue is addressed in the following sections.

3.8. SymMult. Before addressing the issue of symbols to orbits, there is one more symbolic matrix multiplication function that is useful. It is called $\text{SymMult()}$ and takes two diagonal matrices and a square matrix as input. The first diagonal matrix is applied to the square matrix from the left and the second from the right, $\text{SymMult}(D_1, M, D_2)$. For example, if

$$D_1 = \begin{bmatrix} \delta_1 & 0 \\ 0 & \delta_2 \end{bmatrix}, \; M = \begin{bmatrix} M_{1,1} & M_{1,2} \\ M_{2,1} & M_{2,2} \end{bmatrix}, \text{ and } D_2 = \begin{bmatrix} \overline{\delta}_1 & 0 \\ 0 & \overline{\delta}_2 \end{bmatrix}$$

then $\text{SymMult}(D_1, M, D_2)$ is the canonical inner product string array

$$(3.9) \quad \text{SymMult}(D, M, D) = \begin{bmatrix} \delta_1 M_{1,1} \overline{\delta}_1 & \delta_1 M_{1,2} \overline{\delta}_2 \\ \delta_2 M_{2,1} \overline{\delta}_1 & \delta_2 M_{2,2} \overline{\delta}_2 \end{bmatrix}. $$

**Theorem 20.** Given square matrices $A$ and $B$ whose diagonal symbols are distinct from off-diagonal symbol. If there exists a permutation matrix $P$ such that $PAP^T = B$ and pairs of column vectors $(u, v)$ and $(x, y)$ such that $Pu = v$ and $Px = y$. Then

$$P(\text{SymMult}(D_u, A, D_x)) P^T = \text{SymMult}(D_v, B, D_y)$$

where $D_u = \text{diag}(u)$, $D_v = \text{diag}(v)$, $D_x = \text{diag}(x)$, and $D_y = \text{diag}(y)$ are diagonal matrices. Further,$$
\Pi(\text{SymMult}(D_u, A, D_x)) \preceq \Pi(A) \text{ and } \Pi(\text{SymMult}(D_v, B, D_y)) \preceq \Pi(B).$$

**Proof.** Assume $PAP^T = B$ and $(u, v)$ and $(x, y)$ are column vector pairs such that $Pu = v$ and $Px = y$. Then $PD_u P^T = D_v$ and $PD_x P^T = D_y$ where $D_u = \text{diag}(u)$, $D_v = \text{diag}(v)$, $D_x = \text{diag}(x)$, and $D_y = \text{diag}(y)$ are diagonal matrices.

Using regular matrix multiplication, multiplying $PAP^T = B$ on the left and right yields

$$(3.10) \quad PAP^T = B$$

$$(3.11) \quad (PD_u P^T) PAP^T (PD_x P^T) = D_v BD_y$$

$$(3.12) \quad P(D_u AD_x) P^T = D_v BD_y$$

so $P(D_u AD_x) P^T = D_v BD_y$.

From (3.11), the output arrays of canonical inner product strings of

$$\text{SymMult}((PD_u P^T), (PAP^T), (PD_x P^T)) \text{ and } \text{SymMult}(D_v, B, D_y)$$

are identical. To go from (3.11) to (3.12) requires

$$P(\text{SymMult}(D_u, A, D_x)) P^T = \text{SymMult}((PD_u P^T), (PAP^T), (PD_x P^T)).$$

This is true since symmetric permutations move values around without changing them. So a symmetric permutation can move strings as easily as real or complex numbers. Therefore,

$$P(\text{SymMult}(D_u, A, D_x)) P^T = \text{SymMult}(D_v, B, D_y).$$
It is easy to see from (3.9) that \( \Pi (\text{SymMult} (D_u, A, D_x)) \leq \Pi (A) \). Let \( \alpha \) be the symbol associated with one cell of \( A \). Locations within that cell are the only locations that will have \( \alpha \) as the middle symbol on the lhs of (3.9). Therefore, \( \Pi (\text{SymMult} (D_u, A, D_x)) \) is a refinement of \( \Pi (A) \). A similar argument holds for \( \Pi (\text{SymMult} (D_u, B, D_y)) \) and \( \Pi (B) \). Therefore \( \Pi (\text{SymMult} (D_u, A, D_x)) \leq \Pi (A) \) and \( \Pi (\text{SymMult} (D_v, B, D_y)) \leq \Pi (B) \) as desired.

For PCMs it can be shown that the pattern from the first symbolic squaring is the same as symbolically applying the diagonal from the left and right.

**Theorem 21.** Given \( m^2 \times m^2 \) PCM \( M = D + R \) where \( D \) is the diagonal and \( R = I \otimes (1 * (J - I)) + (J - I) \otimes (2 * I) \) are the off-diagonal values. Then

\[
\Pi (\text{SymMult} (D, M, D)) = \Pi (\text{SymSqr} (M)).
\]

**Proof.** The result is by careful consideration of the canonical inner product strings for each \((i,j)\) location.

First convert the off-diagonal values of \( R \) into symbols. The off-diagonal values of \( R \) are ‘1’, ‘2’, and ‘0’. The locations associated with ‘0’ are not explicitly called out in the equation for \( R \). Rewrite \( R \) to include those locations,

\[
R = I \otimes (1 * (J - I)) + (J - I) \otimes (2 * I) + 0 * (J - I)).
\]

Now substitute symbols in place of ‘1’, ‘2’, and ‘0’ to get

\[
\overline{R} = I \otimes (\sigma_1 * (J - I)) + (J - I) \otimes (\sigma_2 * I + \sigma_3 * (J - I)).
\]

\( \overline{R} \) has numeric zeros on its diagonal because the splitting \( M = D + R \) places the diagonal terms of \( M \) in \( D \).

Let \( \overline{D} \) be a diagonal matrix where symbols have been substituted for values on the diagonal. All off-diagonal locations of \( \overline{D} \) are a numeric zeros, due to the splitting. The \( i^{th} \) diagonal symbols is denoted as \( \delta_i \), i.e., \( D_{ii} = \delta_i \).

Let \( \overline{M} = \overline{D} + \overline{R} \). Symbolically squaring \( M \) can be written as

\[
\text{SymSqr} (M) = \overline{M} \times \overline{M} = (\overline{D} + \overline{R}) \times (\overline{D} + \overline{R}) = \overline{DD} + \overline{DR} + \overline{RD} + \overline{RR}
\]

where the rhs abuses notation by using regular matrix notation applied to arrays of symbols. Terms in the canonical inner product strings involving one or more diagonal symbols come from \( \overline{DD} + \overline{DR} + \overline{RD} \). Terms in the canonical inner product strings involving two off-diagonal symbols come from \( \overline{RR} \).

Table [[Table#Table_1]] shows all of the terms making up the canonical inner product strings from symbolically squaring \( \overline{M} \). The first column in Table [[Table#Table_1]] shows the symbol associated with an \((i,j)\) location in \( \overline{M} \). The second column shows the term(s) involving a diagonal symbol, coming from \( \overline{DD} + \overline{DR} + \overline{RD} \). The third columns shows all of the terms involving two off-diagonal symbols, coming from \( \overline{RR} \).

To use Table [[Table#Table_1]] to construct the canonical inner product string at \((i,j)\), first find the row matching the symbol at \( \overline{M}_{i,j} \) in the first column. Then using that row, concatenate the term(s) in the second column followed those in the third column after lexicographically ordering the terms in the third column. Note that the term(s) in the second column are already in the order specified for terms involving diagonal symbols.

Examining the third column of Table [[Table#Table_1]] one notes that the terms come in matching sets. For example, using the row with \( \sigma_2 \) in the first column, the third column has \((m - 1)\) copies of \( \sigma_1 \sigma_3 \) and \((m - 1)\) copies of \( \sigma_3 \sigma_1 \). In all cases if a row in column three contains \( k \) copies of \( \alpha \beta \) then it also contains \( k \).
\[ M_{i,j} = DD + DR + RD \]

| \( M_{i,j} \) | \( DD + DR + RD \) | \( RR \) |
|---------------|------------------|--------|
| \( \delta_i \) | \( \delta_i \delta_i \) | \( \sigma_1 \sigma_1 (m-1) + \sigma_2 \sigma_2 (m-1) + \sigma_3 \sigma_3 (m-1)^2 \) |
| \( \sigma_1 \) | \( \delta_i \sigma_1 + \sigma_1 \delta_j \) | \( \sigma_1 \sigma_1 (m-2) + \sigma_2 \sigma_3 (m-1) + \sigma_3 \sigma_2 (m-1) + \sigma_3 \sigma_3 (m-1)(m-2) \) |
| \( \sigma_2 \) | \( \delta_i \sigma_2 + \sigma_2 \delta_j \) | \( \sigma_1 \sigma_1 (m-1) + \sigma_3 \sigma_1 (m-1) + \sigma_2 \sigma_2 (m-2) + \sigma_3 \sigma_3 (m-1)(m-2) \) |
| \( \sigma_3 \) | \( \delta_i \sigma_3 + \sigma_3 \delta_j \) | \( \sigma_1 \sigma_3 (m-1) + \sigma_3 \sigma_1 (m-1) + \sigma_2 \sigma_3 (m-2) + \sigma_3 \sigma_3 (m-2)^2 \) |

Table 1. Canonical inner product string terms from symbolically squaring a PCM.

copies of \( \beta \alpha \). So the contribution to the canonical inner product strings at \( (i,j) \) and \( (j,i) \) from \( (RR)_{i,j} \) is identical to the contribution from \( (RR)_{j,i} \), implying \( RR \) is symmetric. Further, one sees from Table 1 that each off-diagonal symbol of \( R \) (the \( \sigma_i \) in column one) is associated with a distinct multiset of terms in \( RR \) (column three of Table 1). The diagonal of \( RR \) is associated with a fourth multiset of terms that is distinct from the three off-diagonal multisets. So, \( (\sigma_4 I + R) \) and \( RR \) have identical patterns,

\[ \Pi (\sigma_4 I + R) = \Pi (RR), \]

where the symbol \( \sigma_4 \) is chosen to be distinct from all other symbols in \( M \).

Now focus on the second column of Table 1. Assume that \( M_{i,j} = \sigma_1 \) and \( M_{r,s} = \sigma_1 \) where \( (i,j) \neq (r,s) \). Then the only difference in the canonical inner product strings are the terms involving diagonal symbols, \( \delta_i \sigma_1 + \sigma_1 \delta_j \) and \( \delta_i \sigma_1 + \sigma_1 \delta_s \) respectively. Further, note that the row associated with an off-diagonal symbol use the same off-diagonal symbol in column two. So if column one has off-diagonal symbol \( \delta_k \), \( k \in \{1,2,3\} \), then column two has the terms \( \delta_i \sigma_k + \sigma_k \delta_j \). Each two factor pair of terms \( \delta_i \sigma_k + \sigma_k \delta_j \) could be replaced by a single three factor term \( \delta_i \sigma_k \delta_j \) without changing its ability to distinguish canonical inner product strings. Further, \( \delta_i \delta_i \) can be replaced by \( \delta_i \sigma_4 \delta_i \) without changing its ability to distinguish canonical inner product strings. Performing these substitutions allows column two to be expressed as \( D (\sigma_4 I + R) D \). Now comparing the pattern of \( D (\sigma_4 I + R) D \) to the pattern of \( (DD + DR + RD) \), one sees that they are equal,

\[ \Pi (D (\sigma_4 I + R) D) = \Pi (DD + DR + RD), \]

Note that \( \Pi (D (\sigma_4 I + R) D) \preceq \Pi (\sigma_4 I + R) \) and

\[ \Pi (D (\sigma_4 I + R) D) = \Pi (D (R) D) = \Pi (DRD) \]

since \( \Pi (DDD) = \Pi (D (\sigma_4 I) D) \). Therefore,

\[ \Pi (SymMult (D, M, D)) = \Pi (SymSqr (M)) \]

for PCM \( M \) as was to be shown. \( \square \)

Theorem 21 only applies to the first symbolic squaring of a PCM. Attempting subsequent symbolic squaring by symbolically multiplying on the left and right by the new diagonal \( D^3 \) does not refine the pattern since it has the same pattern as \( D, \Pi (D^3) = \Pi (D) \).

3.9. PCMs and Oracles. In Algorithm 21 a PCM is constructed for each input matrix, \( A \) and \( B \). Let \( S = PCM(A_C) \) and \( T = PCM(B_C) \). Then symbolic squaring is applied to \( S \) and \( T \) simultaneously and the canonical inner product strings compared across products. This section examines how many columns an Oracle can match between \( S^* \) and \( T^* \) when restricted to permutations of the form \( P \otimes P \).
Theorem 22. Given $m^2 \times m^2$ PCMs $S$ and $T$ and their refined patterns $\Pi(S^*)$ and $\Pi(T^*)$ respectively. An Oracle asked to match columns of $S^*$ and $T^*$ using permutations of the form $P \otimes P$ will either match all of the columns or none of the columns.

Proof. Proof by contradiction. Assume $S \not\sim_T T$ and the Oracle matches $k$, $1 \leq k < m^2$, columns of $S^*$ and $T^*$ using a permutation $P_O \in \{P \otimes P\}$. Then $k$ columns of $P_O S^* P_O^T$ and $T^*$ match. Symmetrically permute the matched columns to the lhs using $P_{lhs}$ to get

$$P_{lhs} P_O S^* P_O^T P_{lhs}^T = \begin{bmatrix} C1 \\ C2 \\ \end{bmatrix} \begin{bmatrix} C2^T \\ S2^* \\ \end{bmatrix}$$

and

$$P_{lhs} T^* P_{lhs}^T = \begin{bmatrix} C1 \\ C2 \\ \end{bmatrix} \begin{bmatrix} C2^T \\ T2^* \\ \end{bmatrix}$$

where

$$\begin{bmatrix} C1 \\ C2 \\ \end{bmatrix}$$

are the matched columns. Both $P_{lhs} P_O S^* P_O^T P_{lhs}^T$ and $P_{lhs} T^* P_{lhs}^T$ are stable patterns, so symbolic squaring does not change the pattern.

Now apply the permutations to $S$ and $T$ to get

$$S^{(0)} = P_{lhs} P_O S^* P_O^T P_{lhs}^T$$

and

$$T^{(0)} = P_{lhs} T^* P_{lhs}^T$$

which have a conforming block structure

$$S^{(0)} = \begin{bmatrix} C1^{(0)} \\ C2^{(0)} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ S2^{(0)} \\ \end{bmatrix}$$

and

$$T^{(0)} = \begin{bmatrix} C1^{(0)} \\ C2^{(0)} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ T2^{(0)} \\ \end{bmatrix}$$

$S^{(0)}$ and $T^{(0)}$ have identical off-diagonal structure. The application of $P_O$ does not change the off-diagonal structure because $P_O \in \{P \otimes P\}$ is an automorphism of $R$. Then $P_{lhs}$ is applied to $P_O S^* P_O^T$ and $T^*$, so the off-diagonal structure changes the same way for both. The diagonal of $C1^{(0)}$ for $S^{(0)}$ and $T^{(0)}$ must match. If the diagonals in $C1^{(0)}$ differ, they will also differ in $C1$ of $P_{lhs} P_O S^* P_O^T P_{lhs}^T$ and $P_{lhs} T^* P_{lhs}^T$ creating a contradiction.

Now consider the first symbolic squaring. From Theorem 21 the pattern from the first symbolic squaring matches the pattern from $SymMult(D, M, D)$. This still holds after symmetrically permuting columns to the lhs. So $SymSqr(S^{(0)})$ and $SymSqr(T^{(0)})$ have patterns matching the patterns from $SymMult(D_{S^{(0)}}, S^{(0)}, D_{S^{(0)}})$ and $SymMult(D_{T^{(0)}}, T^{(0)}, D_{T^{(0)}})$ respectively. In block form that is

$$D^{(0)} S^{(0)} D_{S^{(0)}} = \begin{bmatrix} D_{C1^{(0)}} \\ D_{C2^{(0)}} \\ \end{bmatrix} \begin{bmatrix} C1^{(0)} \\ C2^{(0)} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ S2^{(0)} \\ \end{bmatrix} = \begin{bmatrix} D_{C1^{(0)}} \\ D_{C2^{(0)}} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ S2^{(0)} \\ \end{bmatrix}$$

and

$$D^{(0)} T^{(0)} D_{T^{(0)}} = \begin{bmatrix} D_{C1^{(0)}} \\ D_{C2^{(0)}} \\ \end{bmatrix} \begin{bmatrix} C1^{(0)} \\ C2^{(0)} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ T2^{(0)} \\ \end{bmatrix} = \begin{bmatrix} D_{C1^{(0)}} \\ D_{C2^{(0)}} \\ \end{bmatrix} \begin{bmatrix} (C2^{(0)})^T \\ T2^{(0)} \\ \end{bmatrix}.$$
There is no partial matching of \( S^* \) and \( T^* \) using a permutation of the form \( P \otimes P \). Either \( S^* \) and \( T^* \) are p-similar and the columns can be matched or \( S^* \) and \( T^* \) are not p-similar and no columns can be matched using a permutation of the form \( P \otimes P \). This is independent of comparing multisets of diagonal symbols for \( S^* \) and \( T^* \).

3.10. **Symbolic Squaring of PCM** \( ((A \oplus B)_C) \). Theorem 22 showed that given two matrices \( A \) and \( B \) and their PCMs \( S \) and \( T \), where \( S = PCM (A_C) \) and \( T = PCM (B_C) \), that either \( S^* \) is p-similar to \( T^* \) or none of the columns can be matched using an admissible permutation of the form \( P \otimes P \). However, it does not say anything about diagonal symbols.

Given non p-similar \( m \times m \) matrices \( A \) and \( B \), construct the PCM of the direct sum, \( M = PCM ((A \oplus B)_C) \). Also construct the PCMs \( S = PCM (A_C) \) and \( T = PCM (B_C) \). The color matrix of the direct sum \( (A \oplus B) \) is given by

\[
(A \oplus B)_C = \begin{bmatrix} A_C & 3J \\ 3J & B_C \end{bmatrix}.
\]

Applying column major ordering to construct the diagonal of \( M \) results in \( 2m \times 2m \) diagonal blocks where the \( k^{th} \) diagonal block in the upper left quadrant of \( M \) is given by

\[
\begin{bmatrix}
\text{diag} (A_C(:,k)) + (J-I) \\
J
\end{bmatrix}
\begin{bmatrix}
J \\
(J+2I)
\end{bmatrix}_{2m \times 2m}
\]

and the \( (m+k)^{th} \) diagonal block in the lower right quadrant of \( M \) is given by

\[
\begin{bmatrix}
J \\
\text{diag} (B_C(:,k)) + (J-I)
\end{bmatrix}
\begin{bmatrix}
(J+2I) \\
J
\end{bmatrix}_{2m \times 2m}
\]

where \( J \) is the \( m \times m \) matrix of all ones and \( I \) is the conforming identity matrix. Off-diagonal blocks of \( M \) are given by \( 2I_{2m \times 2m} \).

So, all of the entries in \( S \) and \( T \) are embedded in \( M \). The \( k^{th} \) \( m \times m \) diagonal block of \( S \), \( \text{diag} (A_C(:,k)) + (J-I) \), is the upper left portion of each \( 2m \times 2m \) diagonal block in the upper left quadrant of \( M \), see (3.13). The \( m \times m \) off-diagonal blocks of \( S \) are the upper left portion of each \( 2m \times 2m \) off-diagonal blocks in the upper left quadrant of \( M \). A similar case holds for \( T \) except the blocks occupy the lower right portion of each \( 2m \times 2m \) block in the lower right quadrant of \( M \).

Perform symbolic squaring on \( M \) until the stable pattern \( \Pi (M^*) \) is reached. By the argument in Section 3.7, \( \Pi (M^*) = \Pi (M_{Aut}) \) so each cell of \( M^* \) represents an individual orbit. The patterns associated with locations of \( S \) and \( T \) in \( M^* \) are identical to \( \Pi (S^*) \) and \( \Pi (T^*) \) since \( \Pi (S^*) \) and \( \Pi (T^*) \) are the orbits of \( S \) and \( T \) respectively. Therefore, Theorem 22 applies to the columns of \( M^* \) associated with \( S \) and \( T \).

Since \( A \) and \( B \) are non p-similar, none of the columns in \( M^* \) associated with \( S \) and \( T \) can be matched. Therefore the multisets of diagonal symbols corresponding to locations associated with \( S \) and \( T \) in \( M^* \) are distinct. Then since the patterns in \( M^* \) associated with \( S \) and \( T \) are identical to \( \Pi (S^*) \) and \( \Pi (T^*) \), the diagonal mixes from \( S^* \) and \( T^* \) are different as long as consistent symbol substitution is performed each symbolic squaring.

This is the final piece showing that comparing the multisets of diagonal symbols from \( S^* \) and \( T^* \) is necessary and sufficient to determine whether \( A \) and \( B \) are p-similar.
4. Finding $P$ using the Blind Algorithm

Given that Algorithm 1 is a polynomial blind permutation similarity algorithm, it can be used as part of a second polynomial algorithm to find a permutation between $p$-similar matrices. Such an algorithm is presented in Algorithm 2. The remainder of this section describes the concepts behind Algorithm 2.

4.1. Overall Concept. Algorithm 2 uses the blind permutation similarity algorithm, Algorithm 1, to find a permutation vector $p$, such that $M_1(p,p) = M_2$ when $M_1$ and $M_2$ are $p$-similar. If $M_1$ and $M_2$ are not $p$-similar, then $psim = FALSE$ and $p = [1 : m]^T$, the identity permutation vector, are returned as output.

The main loop in Algorithm 2, lines 23-43, looks for the column to use as $p(c)$, where $c$ is the iteration variable. The preconditions for each iteration are that i) $A$ and $B$ are $p$-similar, ii) their diagonal symbols are distinct from the off-diagonal symbols, and iii) the first $(c-1)$ locations of $p$, $p(1 : (c-1))$, are correct.

Upon entering the loop for the first time with $c = 1$, the preconditions are satisfied since:

1. $A$ and $B$ are $p$-similar by the call to Algorithm 1 on line 13 of Algorithm 2.
2. The transformations applied in lines 16-18 are similar to those constructing color matrices from the input matrices. So the diagonal symbols of $A$ and $B$ are distinct from off-diagonal symbols.
3. $(c-1) = 0$ columns have been matched correctly, satisfying the third precondition.

For each iteration, $A$ and $B$ are the remaining trailing principal submatrices to be matched. Only columns of $A$ with a diagonal symbol $A_{j,j} = B_{1,1}$ are potential matches for the first column of $B$. The nested loop, lines 25-41 searches down the diagonal of $A$ for columns where $A_{j,j} = B_{1,1}$. When it finds such a column, it is symmetrically permuted to become the first column of $AJ_1$. In Algorithm 2, the exchange happens on line 28. The exchange can be expressed as

$$AJ_1 = P_{i,j}AP_{i,j}^T$$

where permutation matrix $P_{i,j}$ exchanges rows and columns 1 and $j$. Assuming the first column of $AJ_1$ is a correct match for the first column of $B$. Then there exists a complementary permutation $P_c$ such that

$$P_c(AJ_1)P_c^T = B$$

where the structure of $P_c$ is given by

$$P_c = \begin{bmatrix} 1 & \phantom{P^{22}} \\ \hline P^{22} \end{bmatrix} .$$

Then

$$\begin{bmatrix} 1 & \phantom{P^{22}} \\ \hline P^{22} \end{bmatrix} \times \begin{bmatrix} AJ_{1,1,1} & AJ_{1,2,n} \\ AJ_{1,2,n,1} & AJ_{1,2,n,2:n} \end{bmatrix} \times \begin{bmatrix} 1 & \phantom{P^{22}} \\ \hline P^{22} \end{bmatrix}^T = \begin{bmatrix} B_{1,1} & B_{1,2,n} \\ B_{2:n,1} & B_{2:n,2:n} \end{bmatrix}$$

where

$$P^{22} \times AJ_{1,2:n,1} = B_{2:n,1}$$

$$AJ_{1,2:n} \times P^{22T} = B_{1,2:n}$$

and

$$P^{22} \times AJ_{1,2:n,2:n} \times P^{22T} = B_{2:n,2:n} .$$

Although $P^{22}$ is unknown, Algorithm 1 can be used to determine if $AJ_{1,2:n,2:n}$ and $B_{2:n,2:n}$ in (4.4) are $p$-similar. However, just testing the $(2 : n, 2 : n)$ trailing principal submatrices for $p$-similarity may give a false result. It may be that the only permutation(s), that match the trailing principal submatrices,
Algorithm 2 Pseudocode for finding the permutation using BPSAY, Algorithm 1

01 function \([\text{psim}, p] = \text{FindPUsingBPSAY}(M1, M2)\)
02 \% Find P Using BPSAY
03 \% Inputs:
04 \% \(M1\) – square (real or complex) matrix
05 \% \(M2\) – square (real or complex) matrix
06 \% Outputs:
07 \% \(\text{psim}\) – boolean (TRUE if \(M1 \& M2\) are p–similar)
08 \% \(p\) – permutation vector such that \(M1(p, p) == M2\)
09
10 \(m = \text{size}(M1, 1)\);
11 \(p = [1:m]'\); \% initialize permutation vector
12
13 \(\text{psim} = \text{BPSAY}(M1, M2)\); \% check p–similarity
14 if (~\(\text{psim}\)) , return(\(\text{psim}, p\)); end if \% not p–similar
15
16 \([A, B] = \text{SymbolSubstitution}(M1, M2)\); \% positive integer matrices
17 \(A = \text{ShiftAndTranslate}(A, \beta=m^2, \gamma=0)\); \% make diag symbols distinct
18 \(B = \text{ShiftAndTranslate}(B, \beta=m^2, \gamma=0)\); \% make diag symbols distinct
19
20 \% ASSERT: \(A\) and \(B\) are p–similar w/diag symbols distinct from off–diag symbols
21
22 \(n = m\); \% size of trailing principal submatrix
23 for \(c = 1:(m-1)\) \% search trailing principal submatrix for \(p(c)\)
24 \(\text{DBD} = \text{SymMult}(\text{diag}(B(:,1)), B, \text{diag}(B(1,:)))\);
25 for \(j = 1:n\)
26 \(\text{if } (A(j,j) \neq B(1,1)), \text{continue; end if}\)
27
28 \(\text{AJ1} = \text{ExchangeIJ}(A, 1, j)\); \% exchange rows/cols 1 \(<\rightarrow j\)
29 \(\text{DAJ1D} = \text{SymMult}(\text{diag}(\text{AJ1}( :,1)), \text{AJ1}, \text{diag}(\text{AJ1}(1,:)))\);
30 \([S, T] = \text{SymbolSubstitution}(\text{DAJ1D}, \text{DBD})\);
31
32 \% trailing principal submatrices
33 \(S22 = S(2:n,2:n)\); \(T22 = T(2:n,2:n)\);
34
35 \(\text{psim} = \text{BPSAY}(S22, T22)\); \% check p–similarity
36 \(\text{if } (\text{psim})\) \% column \(p(c+j-1)\) is amenable
37 \(p([c \ (c+j-1)]) = p([(c+j-1) \ c]); \% p(c) \(<\rightarrow p(c+j-1)\)
38 \(A = S22; \ B = T22\); \% new \(A\) and \(B\) are p–similar
39 \(\text{break; }\) \% move to next column
40 \end if
41 end
42 \(n = n - 1\); \% update size of trailing principal submatrices
43 end
44
45 return(\(\text{psim}, p\));
46 end
violate (4.2) and (4.3). To eliminate this possibility, the first column and first row of AJ1 and B are used to refine the \((2 : n, 2 : n)\) trailing principal submatrices prior to checking if they are p-similar. For AJ1, this is done by constructing diagonal matrices from the first column and first row of AJ1, \(\text{diag}(AJ1)\) and \(\text{diag}(AJ1)\) respectively, and symbolically applying them from the left and the right to AJ1, line 29. The \((2 : n, 2 : n)\) trailing principal submatrix of B is similarly refined using the first column and first row of B, line 24. Theorem 20 guarantees that the symbolic multiplication will refine the \((2 : n, 2 : n)\) trailing principal submatrices while preserving the p-similarity relationship between AJ1 and B. The left and right diagonal matrices are constructed from the first column and first row respectively because A and B might not be symmetric.

Algorithm 1 is applied to S22 and T22, the refined \((2 : n, 2 : n)\) trailing principal submatrices of \(DAJ1D\) and \(DBD\) respectively, to test for p-similarity without the possibility of a false response, line 35. If S22 and T22 are p-similar, then the amenable permutation also satisfies (4.2) and (4.3). After finding a S22 and T22 that are p-similar, the global index of the column permuted into the first column of AJ1 is saved as \(p(c)\), line 37, and A and B are set to S22 and T22 respectively, line 38. The size of the trailing principal submatrix is decremented in preparation for searching for the next column, line 42.

P-similar S22 and T22 are guaranteed to exist because the precondition for entering the loop is that A and B are p-similar.

For the next iteration \(c = 2\), again the preconditions are met. A and B are p-similar, tested on line 35, their diagonal symbols are distinct from off-diagonal symbols since the inputs to the symbol substitution, line 30, have distinct diagonal symbols, and the first \((c - 1)\) locations in \(p, p(1)\), are correct.

Therefore, for p-similar input matrices M1 and M2, Algorithm 2 finds a permutation vector \(p\) such that \(M1(p, p) = M2\) in \(O(m^2)\) iterations.

4.2. Algorithm 2 Complexity. Given \(m \times m\) input matrices, the nested loops in Algorithm 2 make \(O(m^2)\) calls to BPSAY, Algorithm 1. So the overall complexity of Algorithm 2 is \(O(m^{14})\) using symbolic squaring. If widely space primes matrices are used, Section 5.2, the overall complexity drops to \(O(m^{12})\). Therefore finding the permutation between two p-similar matrices is polynomial.

5. Discussion

In practice, it does not appear to be necessary to add edge weights to the PCG. The edge weights are added to eliminate the possibility of exchanging the rows with the columns. Edge weights simplified the arguments by avoiding the need to carry the transpose based permutations through the proofs. If rook’s graphs are compact then color refinement works on PCMs with equal edge weights. Although rook’s graphs have many of the characteristics of compact graphs, the author has not been able to show that rook’s graphs are compact.

5.1. Origin of PCGs. For a period of time the author tried to develop a graph isomorphism algorithm. For every algorithm, non isomorphic graphs were found that were not discriminated. Eventually the investigation turned to looking at why color refinement fails.

Given two non-isomorphic graphs, iterative color refinement can be applied to the adjacency matrices until they converged to a stable partition. It is well known that strongly regular graphs cannot be separated using naive color refinement. However, one could ask an Oracle to maximally column match the matrices. The result would look like

\[
A = \begin{bmatrix}
C1 & C2^T \\
C2 & A2
\end{bmatrix}
\quad \text{and} \quad
B = \begin{bmatrix}
C1 & C2^T \\
C2 & B2
\end{bmatrix}
\]
after symmetrically permuting the matched columns to the lhs. Differences are confined to the lower right blocks, where \( A_2 \neq B_2 \). We can assume the column multisets match (otherwise \( A \) and \( B \) are known to be non-isomorphic). Next consider ordering \( C_2 \) into groups of identical rows. The permutation to do this can be applied symmetrically to both \( A \) and \( B \). Now the matrices look something like

\[
A = \begin{bmatrix}
C_1 & r_1^T & r_2^T & r_3^T & r_4^T \\
\alpha & \delta & \gamma & \alpha & \beta \\
\gamma & \delta & \beta & \alpha & \gamma \\
\beta & \alpha & \gamma & \delta & \gamma \\
\end{bmatrix}
\]

and

\[
B = \begin{bmatrix}
C_1 & r_1^T & r_2^T & r_3^T & r_4^T \\
\alpha & \beta & \delta & \alpha & \gamma \\
\beta & \alpha & \delta & \beta & \gamma \\
\gamma & \delta & \beta & \gamma & \delta \\
\end{bmatrix}
\]

where \( \alpha \neq \beta \) and each \( r_j \) is a pairwise distinct row vector. Consider the first column of the unmatched region. Notice that \( A \) has \( \alpha \) at the intersection of \( r_3 \) and \( r_1^T \) whereas \( B \) has a \( \beta \) at that location and the reverse at the intersection of \( r_4 \) and \( r_1^T \). By hypothesis, \( r_1 \neq r_3 \), \( r_3 \neq r_4 \), and \( r_4 \neq r_1 \), so the author looked for ways to take advantage of this situation by constructing invariants such as all of the four-cycles. Four-cycles are permutation independent. The process always broke down when trying to compare results using multisets. The multisets either maintained row constraints and relaxed column constraints or maintained column constraints and relaxed row constraints. This happens for any comparison method based on multisets such as those described in [10, 3].

This led to asking the question: “Can symmetric permutation constraints be added to the original graphs?” If so, the symmetric permutation constraints would be part of the original problem and using multisets for comparison should not experience the same difficulty. PCGs were the result. PCGs also changed the focus from graph isomorphism to permutation similarity.

5.2. **Refinement using Regular Matrix Multiplication.** It is not clear that the sequence of refinements generated by symbolic squaring can be replicated using regular matrix multiplication. If the sequence cannot be replicated, it makes arguments using the existing machinery for SPD matrices more difficult to accept. It turns out there are two different ways the sequence of refinements can be replicated using regular matrix multiplication. They both use matrices constructed from widely-spaced prime numbers.

**Definition 23.** A **widely-spaced primes matrix** \( W \), where \( W = wspm (M) \) is constructed from a symmetric matrix \( M \), whose diagonal symbols are distinct from off-diagonal symbols. The construction uses the following method:

1. Let \( M = (\Pi, \Sigma, g) \) be a \( m \times m \) symmetric matrix whose diagonal symbols are distinct from the off-diagonal symbols.
2. Assume \( M \) has \( n = |\Sigma| \) distinct symbols where there are \( n_1 \) off-diagonal symbols and \( n_2 \) diagonal symbols with \( n_1 + n_2 = n \).
3. Let \( \Pi (W) = \Pi (M) \).
4. Choose \( n \) prime numbers, \( p_i \), to be the symbols of \( W \) using the following recurrence.
   a. Let \( p_1 > mk^2 \) be the first prime number, where \( k \in \mathbb{N}^+ \) (typically \( k = 1 \)).
   b. For \( i = 2, \ldots, n \), chose \( p_i > m + p_{i-1}^2 \).
5. Use the first \( n_1 \) primes, \( p_1, \ldots, p_{n_1} \), as off-diagonal symbols of \( W \) and use the remaining \( n_2 \) primes, \( p_{n_1+1}, \ldots, p_n \), as diagonal symbols of \( W \).

**Remark 24.** A widely-spaced primes matrix \( W \) is SPD since it is symmetric and strictly diagonally dominant by construction.
Consider squaring a \( m \times m \) widely-spaced primes matrix \( W \). Let \( W = D + O \) where \( O \) is the matrix of off-diagonal symbols and \( D \) is the diagonal. Recall that widely-spaced primes matrix has diagonal symbols that are distinct from off-diagonal symbols. Using regular matrix multiplication, the value at \((i, j)\) is given by

\[
[W \times W]_{i,j} = \begin{cases} 
D_{i,i}O_{i,j} + O_{i,j}D_{j,j} + \sum_{k \neq i} O_{i,k}O_{k,j} & \text{if } i \neq j \\
D_{i,i}D_{j,j} + \sum_{k \neq i} O_{i,k}O_{k,i} & \text{if } i = j
\end{cases}
\]

(5.2)

where terms involving diagonal symbols come first, followed by terms with two off-diagonal symbols. This is similar to the order used for canonical inner product strings.

**Remark 25.** Each term in the inner product \([W \times W]_{i,j}\) is the product of two primes.

**Remark 26.** Let \( \Sigma = \{p_1, \ldots, p_n\} \) be the set of widely-spaced primes in \( W \). Then the set of all possible distinct terms,

\[
\{p_1p_1, p_1p_2, p_2p_2, p_1p_3, p_2p_3, p_3p_3, \ldots, p_1p_n, \ldots, p_np_n\}
\]

is totally ordered by less than

\[
p_1p_1 < p_1p_2 < p_2p_2 < p_1p_3 < p_2p_3 < p_3p_3 < \cdots < p_1p_n < \cdots < p_np_n
\]

and the ratio between two adjacent terms is greater than \( mp_1 \),

\[
\frac{p_{i+1}p_i}{p_ip_{i+1}} > mp_1 \text{ for } j > i \text{ and } \frac{p_{j+1}p_j}{p_jp_{j+1}} > mp_1 \text{ for } i = j.
\]

**Lemma 27.** The inner product \([W \times W]_{i,j}\) is unique to a set of distinct terms and their multiplicities.

**Proof.** Let \( W \) be a \( m \times m \) widely-spaced primes matrix. Then each inner product \([W \times W]_{i,j}\) has \( m \) terms and can be written as

\[
[W \times W]_{i,j} = \sum m_k t_k
\]

where each \( t_k \) is a distinct term in the inner product with multiplicity \( m_k \) and \( \sum m_k = m \).

Proof is by contradiction. Assume \([W \times W]_{i,j} = [W \times W]_{r,s}\) where

\[
[W \times W]_{r,s} = \sum \bar{m}_l \bar{t}_l
\]

and \( \sum m_k = \sum \bar{m}_l = m \) but the sets of distinct terms \( \{t_k\} \) and \( \{\bar{t}_l\} \) do not match, \( \{t_k\} \neq \{\bar{t}_l\} \). Subtract terms appearing in both \([W \times W]_{i,j}\) and \([W \times W]_{r,s}\) from \( \sum m_k t_k \) and \( \sum \bar{m}_l \bar{t}_l \). Let the resultant sums be \( \sigma_{ij} \) and \( \sigma_{rs} \) respectively. Now \( \sigma_{ij} = \sigma_{rs} > 0 \) but they have no common terms. WLOG assume that \( \sigma_{ij} \) contains the largest distinct term between \( \sigma_{ij} \) and \( \sigma_{rs} \). Let \( p_{k_1}p_{k_2} \) be that largest term in \( \sigma_{ij} \) and \( p_{l_1}p_{l_2} \) be the largest term in \( \sigma_{rs} \). So \( p_{k_1}p_{k_2} > p_{l_1}p_{l_2} \). All of the terms in \( \sigma_{rs} \) are less than or equal to \( p_{l_1}p_{l_2} \). Therefore the largest \( \sigma_{rs} \) can be is \( mp_{l_1}p_{l_2} \). But by construction, the next largest distinct term greater than \( p_{l_1}p_{l_2} \) is strictly greater than \( mp_{l_1}p_{l_2} \), see Remark 26. Therefore \( \sigma_{ij} \) cannot equal \( \sigma_{rs} \), contradicting the assumption that two inner products of \( W \times W \) that are equal can be constructed from different sets of distinct terms with different multiplicities. \( \square \)

A consequence of Lemma 27 is that the inner product \([W \times W]_{i,j}\) is decomposable using modulo arithmetic by starting with the largest prime and working downward, recursively applying modulo arithmetic to both the integer multiple of the prime and the remainder.
Lemma 28. The multiplicity \( m_k \) of a distinct term, \( t_k = p_ip_r = p_ip_l \), in the inner product \([W \times W]_{ij}\) is equal to the sum of the multiplicities \( n_1 \) of \((p_i, p_r)\) and \( n_2 \) of \((p_l, p_r)\) in the canonical inner product string \( \text{SymSqr}(W)_{ij} \), \( m_k = n_1 + n_2 \).

Proof. Consequence of Lemma 27. The inner product is uniquely determined by the set of distinct terms in the inner product and their multiplicities. A distinct term, \( t_k \), is the product of a unique pair of primes, \( t_k = p_ip_r = p_ip_l \). Canonical inner product strings distinguishes between the ordered pairs \((p_i, p_r)\) and \((p_l, p_r)\) whereas the inner product does not. The result follows. \( \square \)

The next theorem shows that the square of a widely-spaced primes matrix is a refinement of the widely-spaced primes matrix.

Theorem 29. Given a real \( m \times m \) symmetric matrix \( M \) whose diagonal symbols are distinct from off-diagonal symbols, there exists a widely-spaced primes matrix \( W = \text{wspm}(M) \) such that \( \Pi(W) = \Pi(M) \)

and \( \Pi(W \times W) \leq \Pi(W) \).

Proof. Let \( M \) be a real \( m \times m \) symmetric matrix whose diagonal symbols are distinct from off-diagonal symbols. Let \( W = \text{wspm}(M) \) be a widely-spaced primes matrix. Then \( \Pi(W) = \Pi(M) \) by Definition 23.

Let \( W = D + O \) where \( O \) is the matrix of off-diagonal symbols and \( D \) is the diagonal. To see that \( \Pi(W \times W) \leq \Pi(W) \), it is enough to show that entries that differ in \( W \) also differ in \( W \times W \). Consider two off-diagonal locations \((i, j)\) and \((r, s)\) such that \( W_{i,j} \neq W_{r,s} \), i.e., \( O_{i,j} \neq O_{r,s} \). Without loss of generality, assume \( i < j \) and \( r < s \). Then using the first row of (5.2)

\[
[W \times W]_{i,j} = D_{i,i}O_{i,j} + O_{i,j}D_{j,j} + \sum_{k \neq i} O_{i,k}O_{k,j}
\]

and

\[
[W \times W]_{r,s} = D_{r,r}O_{r,s} + O_{r,s}D_{s,s} + \sum_{k \neq r} O_{r,k}O_{k,s}
\]

where the terms involving two off-diagonal symbols sum to less than the smallest diagonal symbol \( p_{n_1+1} \).

So if

\[
O_{i,j} (D_{i,i} + D_{j,j}) \text{ is distinct from } O_{r,s} (D_{r,r} + D_{s,s})
\]

then \([W \times W]_{ij}\) is guaranteed to be distinct from \([W \times W]_{rs}\). To see that the two sides of (5.5) are distinct when \( O_{i,j} \neq O_{r,s} \), consider the following cases:

Case 1. \((D_{i,i} + D_{j,j}) = (D_{r,r} + D_{s,s})\): Then \( O_{i,j} (D_{i,i} + D_{j,j}) \neq O_{r,s} (D_{r,r} + D_{s,s}) \) since \( O_{i,j} \neq O_{r,s} \).

Case 2. \((D_{i,i} + D_{j,j}) \neq (D_{r,r} + D_{s,s})\): Without loss of generality, assume that \((D_{i,i} + D_{j,j}) < (D_{r,r} + D_{s,s})\).

Further, assume that \( D_{s,s} \) is maximal among the diagonal symbols under consideration, \( D_{s,s} = \max(D_{i,i}, D_{j,j}, D_{r,r}, D_{s,s}) \), and that \( D_{s,s} = p_l \), the \( l \)th prime number.

Case i. \((D_{i,i} + D_{j,j} < D_{s,s})\) and \((D_{r,r} \leq D_{s,s})\): Substitute into (5.5) to get \( O_{i,j} (D_{i,i} + D_{j,j}) \leq 2p_{n_1}p_{n_1} < D_{s,s} \) and \( O_{r,s} (D_{r,r} + D_{s,s}) > D_{s,s} \). Therefore \( O_{i,j} (D_{i,i} + D_{j,j}) \neq O_{r,s} (D_{r,r} + D_{s,s}) \).

Case ii. \((D_{i,i} < D_{r,r} \& D_{j,j} = D_{s,s})\) and \((D_{r,r} < D_{s,s})\): Substitute into (5.5) and rearrange to get \( O_{i,j} (D_{i,i} - O_{r,s} D_{r,r}) \) versus \((O_{r,s} - O_{i,j}) D_{s,s} \). Now \(|O_{i,j} (D_{i,i} - O_{r,s} D_{r,r})| <
Theorem 30. For a widely-spaced primes matrix $\text{SymSqr}(W)$, products that symbolic squaring distinguishes that regular matrix multiplication does not. However, if those locations will also differ in separation between primes guarantees they cannot be equal. Therefore if two locations of locations only have one term involving the square of a diagonal symbol, as shown in (5.2). Again, the locations have two terms involving a diagonal symbol and an off-diagonal symbol whereas diagonal symbols $p_D$, $A$ similar argument holds when diagonal symbols $W_{i,i}$ and $W_{r,r}$ differ. In this case, only the $D_{i,i}^2$ and $D_{r,r}^2$ terms need to be considered since the remaining terms sum to less than the smallest diagonal symbol $p_{n+1}$. Inner products for diagonal and off-diagonal locations differ in $W \times W$. Off-diagonal locations have two terms involving a diagonal symbol and an off-diagonal symbol whereas diagonal locations only have one term involving the square of a diagonal symbol, as shown in (5.2). Again, the separation between primes guarantees they cannot be equal. Therefore if two locations of $W$ differ, those locations will also differ in $W \times W$ implying $\Pi(W \times W) \leq \Pi(W)$ as desired.

Theorem [29] does not say that $\Pi(W \times W) = \Pi(\text{SymSqr}(M))$. There may be some inner products that symbolic squaring distinguishes that regular matrix multiplication does not. However, if $\text{SymSqr}(W)$ refines the diagonal, then $W \times W$ also refines the diagonal.

Theorem 30. For a widely-space primes matrix $W$, if $\text{SymSqr}(W)$ strictly refines the diagonal,

$$\Pi(\text{diag}(\text{SymSqr}(W))) \prec \Pi(\text{diag}(W)),$$

then $W \times W$ also strictly refines the diagonal,

$$\Pi(\text{diag}(W \times W)) \prec \Pi(\text{diag}(W))$$

and $\Pi(\text{diag}(W \times W)) = \Pi(\text{diag}(\text{SymSqr}(W)))$.

Proof. The inner product for a diagonal symbol has the same symbol for both factors of a term, see the second row of (5.2). Therefore, the factor order doesn’t matter for the canonical inner product strings of diagonal symbols and Lemma [27] says the inner product is unique to the set of distinct terms and their multiplicities. So, if $\text{SymSqr}(W)$ refines the diagonal, $\Pi(\text{diag}(\text{SymSqr}(W))) \prec \Pi(\text{diag}(W))$, then $W \times W$ refines the diagonal, $\Pi(\text{diag}(W \times W)) \prec \Pi(\text{diag}(W))$ and

$$\Pi(\text{diag}(W \times W)) = \Pi(\text{diag}(\text{SymSqr}(W)))$$

For off-diagonal locations, there may be cases where $\text{SymSqr}(W)$ refines an off-diagonal location but $W \times W$ does not. However, if a widely-spaced primes matrix $W$ is generated from $\text{PCM}(M)$, $M = \text{PCM}(A_C)$ and $W = \text{wspm}(M)$, then for the first squaring, $\Pi(W \times W) = \Pi(\text{SymSqr}(M))$. This can be seen by looking at Table II and noting that each canonical inner product string with $(m-1)\alpha\beta$’s also has $(m-1)\beta\alpha$’s, so each distinct canonical inner product string in $\text{SymSqr}(M)$ is associated with a distinct numeric inner product of $W \times W$. Recall that symbolic squaring uses the lexicographically lessor to represent locations $(i, j)$ and $(j, i)$ so switching the roles of $\delta_i$ and $\delta_j$ in column 2 of Table II don’t matter.

Next is to take a look at how close squaring a widely-space primes matrix comes to matching a canonical inner product string for off-diagonal locations after the first symbolic squaring. Start by looking at off-diagonal locations that are not refined by symbolic squaring.

Lemma 31. Let $W$ be a $m \times m$ widely-spaced primes matrix. If $\text{SymSqr}(W)_{i,j} = \text{SymSqr}(W)_{r,s}$, then $(W \times W)_{i,j} = (W \times W)_{r,s}$. 

Proof. Given $SymSqr(W)_{i,j} = SymSqr(W)_{r,s}$, then the canonical inner product strings at $(i,j)$ and $(r,s)$ match, so the multisets of terms match. Therefore, the inner products $(W \times W)_{i,j}$ and $(W \times W)_{r,s}$ match since they are summing over the same multiset of terms.

Next is to look at off-diagonal locations that do get refined by symbolic squaring. This is the more complex case. Before addressing the general case, the instance where column mixes of the inner product vectors match but the results from symbolic squaring differ is examined.

**Theorem 32.** Let $W$ be a $m \times m$ widely-spaced primes matrix. Let $(i,j)$ and $(r,s)$ be two distinct off-diagonal locations. If $colMix([W_i,W_j]) = colMix([W_r,W_s])$ and $SymSqr(W)_{i,j} \neq SymSqr(W)_{r,s}$, then $(W \times W)_{i,j} \neq (W \times W)_{r,s}$.

**Proof.** Assume $W$ is a $m \times m$ widely-spaced primes matrix constructed as described in Definition 23 and $(i,j)$ and $(r,s)$ are two distinct off-diagonal locations such that $colMix([W_i,W_j]) = colMix([W_r,W_s])$ and $SymSqr(W)_{i,j} \neq SymSqr(W)_{r,s}$. WLOG assume that $colMix(W_i) = colMix(W_r)$ and $colMix(W_j) = colMix(W_s)$.

Proof by contradiction. Assume that $(W \times W)_{i,j} = (W \times W)_{r,s}$. Let $A = P_{ij} WP_{ij}^T$ where $P_{ij}$ symmetrically permutes columns $i$ and $j$ to be columns $1$ and $2$ of $A$ respectively. Similarly, let $B = P_{rs} WP_{rs}^T$ where $P_{rs}$ symmetrically permutes columns $r$ and $s$ to be columns $1$ and $2$ of $B$ respectively.

Note that $A$ and $B$ are symmetric and $colMix(A_1) = colMix(B_1)$ and $colMix(A_2) = colMix(B_2)$. So there exists a permutation $P_A$ that when symmetrically applied to $A$, sorts rows $3 : m$ of $A_1$ into the same contiguous groups of distinct symbols. Similarly there exists a permutation $P_B$ that sorts rows $3 : m$ of $B_1$ into the same contiguous groups of distinct symbols. Let

$$A \leftarrow P_A A P_A^T$$

and

$$B \leftarrow P_B B P_B^T.$$ 

Now $A_1 = B_1$ and $A$ and $B$ have the form shown in (5.1) where the row signatures are the groups of distinct symbols in rows $3 : m$ of $A_1$ and $B_1$. Note that $colMix(A_{3:m,2}) = colMix(B_{3:m,2})$ because $colMix(A_2) = colMix(B_2)$ and $A$ and $B$ are symmetric, so the first two elements of $A_2$ and $B_2$ are identical.

By hypothesis $SymSqr(W)_{i,j} \neq SymSqr(W)_{r,s}$ so $SymSqr(A)_{1,2} \neq SymSqr(B)_{1,2}$ but $A_1^T A_2 = B_1^T B_2$. Consider the terms in the canonical inner product strings of $SymSqr(A)_{1,2}$ and $SymSqr(B)_{1,2}$. The first two terms involving diagonal symbols match, so the differences must be in the terms from rows $3 : m$,

$$\begin{align*}
\left\{ \begin{array}{c}
(A_{3,1}, A_{3,2}) \\
\vdots \\
(A_{m,1}, A_{m,2})
\end{array} \right\} & \neq \left\{ \begin{array}{c}
(B_{3,1}, B_{3,2}) \\
\vdots \\
(B_{m,1}, B_{m,2})
\end{array} \right\}
\end{align*}$$

where the symmetry of $A$ and $B$ is used to write the left factors as entries from column 1. Since $A_1 = B_1$, rewrite (5.6) as

$$\begin{align*}
\left\{ \begin{array}{c}
(B_{3,1}, A_{3,2}) \\
\vdots \\
(B_{m,1}, A_{m,2})
\end{array} \right\} & \neq \left\{ \begin{array}{c}
(B_{3,1}, B_{3,2}) \\
\vdots \\
(B_{m,1}, B_{m,2})
\end{array} \right\}.
\end{align*}$$

Now the left hand factors on both sides of (5.7) match. Also the column mixes match, $colMix(A_{3:m,2}) = colMix(B_{3:m,2})$, and the inner products match but the multisets of terms differ. Comparing the lhs and rhs of (5.7), one sees that $A_{3:m,2}$, when compared to $B_{3:m,2}$, must have distinct symbols exchanged across the row signature boundaries established in $B_1$. The symbol exchange(s) act similar to the roles of $\alpha$ and
Let $\beta$ in (5.1). This is the only way for the multisets of terms to differ while $colMix (A_2)$ equals $colMix (B_2)$. By Lemma 27, the inner product is unique to the set of distinct terms and their multiplicities. The exchange of distinct symbols across the row signature boundaries change the multiplicities of distinct terms and possibly the set of distinct terms. So, the inner products associated with the two sides of (5.7) cannot be equal, contradicting the hypothesis that $(W \times W)_{i,j} = (W \times W)_{r,s}$.

Therefore, if $colMix ([W_i, W_j]) = colMix ([W_r, W_s])$ and $SymSqr (W)_{i,j} \neq SymSqr (W)_{r,s}$, then $(W \times W)_{i,j} \neq (W \times W)_{r,s}$ as was to be shown. 

 Widely-spaced primes matrices and regular matrix multiplication can generate a sequence of refinement that is at least as refined as the one generating $\Pi (M^*)$, it just might take twice as many iterations.

**Theorem 33.** For a widely-spaced primes matrix $W$, let $\bar{W} = wspm (W \times W)$ be a widely-spaced primes matrix generated from the result of squaring $W$. Then the pattern from squaring $\bar{W}$ is a refinement of the pattern from symbolically squaring $W$,

$$\Pi (W \times W) \preceq \Pi (SymSqr (W)).$$

**Proof.** Let $W$ be a widely-spaced primes matrix and $\bar{W} = wspm (W \times W)$ be a widely-spaced primes matrix generated from the result of squaring $W$.

From Theorem 30 and Theorem 29 one gets that,

$$\Pi (diag (W \times W)) \preceq \Pi (diag (W \times W)) = \Pi (diag (SymSqr (W))).$$

So diagonal cells of $(\bar{W} \times \bar{W})$ are a refinement of the diagonal cells of $SymSqr (W)$. The remaining question is whether the off-diagonal cells of $(\bar{W} \times \bar{W})$ are a refinement of the off-diagonal cells of $SymSqr (W)$.

Assume $W_{i,j}$ and $W_{r,s}$ are in the same off-diagonal cell so $W_{i,j} = W_{r,s}$ with $(i, j) \neq (r, s)$.

**Case 1.** If $SymSqr (W)_{i,j} \neq SymSqr (W)_{r,s}$ and $(W \times W)_{i,j} \neq (W \times W)_{r,s}$, then done since $(W \times W)_{i,j} \neq (W \times W)_{r,s}$ by Theorem 29.

**Case 2.** If $SymSqr (W)_{i,j} \neq SymSqr (W)_{r,s}$ and $(W \times W)_{i,j} = (W \times W)_{r,s}$ then consider the column mixes of $W_i$, $W_j$, $W_r$, and $W_s$.

**Case i.** Assume $colMix ([W_i, W_j]) \neq colMix ([W_r, W_s])$. Theorem 30 says $W \times W$ and $SymSqr (W)$ refine the diagonal the same way, so the multisets of diagonal symbols are not equal $\{((W \times W)_{i,i}, (W \times W)_{j,j})\} \neq \{((W \times W)_{r,r}, (W \times W)_{s,s})\}$.

Then the second squaring results in $(W \times W)_{i,j} \neq (W \times W)_{r,s}$ since the diagonal terms $\{(W_{i,i}, W_{j,j})\}$ and $\{(W_{r,r}, W_{s,s})\}$ differ in (5.3) and (5.4).

**Case ii.** Assume $colMix ([W_i, W_j]) = colMix ([W_r, W_s])$. Theorem 32 says the condition where $colMix ([W_i, W_j]) = colMix ([W_r, W_s])$ and $SymSqr (W)_{i,j} \neq SymSqr (W)_{r,s}$ means $(W \times W)_{i,j} \neq (W \times W)_{r,s}$. This contradicts the hypothesis that $(W \times W)_{i,j} = (W \times W)_{r,s}$. So this is not a valid case.

Therefore, $\Pi (\bar{W} \times \bar{W}) \preceq SymSqr (W)$ as was to be shown. 

Theorem 33 implies a sequence of constructing and squaring widely-spaced matrices will converge to a fixed point that is a refinement of $M^*$ in at most twice as many iterations as symbolic squaring.

A second method generates a sequence of refinement identical to the symbolic squaring sequence of refinement. However, instead of squaring a widely-spaced primes matrix, it multiplies two different widely-space matrices.
Theorem 34. Given a real \( m \times m \) symmetric matrix \( M \) whose diagonal symbols are distinct from off-diagonal symbols, there exist widely-spaced primes matrices \( W_1 \) and \( W_2 \) such that \( \Pi(W_1) = \Pi(W_2) = \Pi(M) \) and

\[
\Pi\left( \min\left( (W_1 \times W_2), (W_1 \times W_2)^T \right) \right) = \Pi(\text{SymSqr}(M))
\]

where \( \min() \) is the element-wise matrix minimum.

Proof. Similar to the proof of Theorem 29 widely-spaced primes are used as symbols. Assume \( M \) has \( n \) distinct symbols and \( n_1 \) are off-diagonal symbols and \( n_2 \) are diagonal symbols with \( n_1 + n_2 = n \). Let \( W_1 = \text{wspm}(M) \) be a widely-space primes matrix as described in Definition 23 where the primes are \( \{p_1, \ldots, p_n\} \), starting with \( p_1 > m \). Then let \( W_2 = \text{wspm}(M) \) be a second widely-spaced primes matrix where the primes are \( \{\pi_1, \ldots, \pi_n\} \), starting with \( \pi_1 > mp_n^2 \).

Use the first \( n_1 \) primes of \( \{p_1, \ldots, p_n\} \), \( p_1, \ldots, p_{n_1} \), as off-diagonal symbols of \( W_1 \) and the next \( n_2 \) primes, \( p_{n_1}, \ldots, p_n \), as the diagonal symbols of \( W_1 \). Then use the first \( n_1 \) primes of \( \{\pi_1, \ldots, \pi_n\} \), \( \pi_1, \ldots, \pi_{n_1} \), as off-diagonal symbols of \( W_2 \) and the last \( n_2 \) primes, \( \pi_{n_1}, \ldots, \pi_n \), as diagonal symbols of \( W_2 \). \( W_1 \) and \( W_2 \) are SPD by construction.

Now consider the matrix product \( W_1 \times W_2 \). For each \((i, j)\) location, the inner product is constructed from a row vector of \( W_1 \) and a column vector from \( W_2 \). Since the symbol sets for \( W_1 \) and \( W_2 \) are distinct, the factors of each term can be considered to be ordered. To see this, consider the canonical string at \((i, j)\) from \( W_1 \times W_2 \). Each term in an inner product is given by a \( p_c \pi_c \) where \( p_c \in \{p_1, \ldots, p_n\} \) and \( \pi_c \in \{\pi_1, \ldots, \pi_n\} \). Without loss of generality, assume that \( p_\alpha \pi_\beta \) is the largest term in the inner product inner product string. Then the inner product is less than or equal to \( mp_\alpha \pi_\beta \). But the next larger distinct factor after \( p_\alpha \pi_\beta \) is greater than \( mp_\alpha \pi_\beta \). So the inner product can be decomposed using modulo arithmetic starting with the largest prime and working downward to determine the exact number of times each term appears. This implies distinct canonical inner product strings in \( \text{SymSqr}(M) \) have distinct inner products in \( W_1 \times W_2 \).

The remaining part is to note that \( \text{SymSqr}(M) \) selects the lessor of the canonical strings at \((i, j)\) and \((j, i)\) to represent both locations for symmetric matrices. For \( W_1 \times W_2 \), this is accomplished by using the minimum of \( [W_1 \times W_2]_{i,j} \) and \( [W_1 \times W_2]_{j,i} \) to represent both locations. Recall that the product of two real symmetric matrices is not symmetric unless they have the same eigenvectors. So

\[
\Pi\left( \min\left( (W_1 \times W_2), (W_1 \times W_2)^T \right) \right) = \Pi(\text{SymSqr}(M))
\]

as desired. \qed

So the refinement sequence generated by symbolic squaring can be reproduced using regular matrix multiplication. However, it involves multiplying widely-spaced primes matrices.

One consequence of replacing symbolic squaring with regular matrix multiplication on widely-spaced primes matrices is that the bounds for Algorithm 1 reduces from \( O(m^8) \) for symbolic squaring to \( O(m^8) \) for matrix multiplication of widely-spaced primes matrices and from \( O(m^{10}) \) for symbol substitution of canonical inner product string arrays to \( O(m^8) \) for symbol substitution of positive integer matrices. Dropping the overall complexity of the algorithm from \( O(m^{12}) \) to \( O(m^{10}) \).

5.3. Symbolic “Walks”. Two vertices that are not neighbors in a rook’s graph are part of a unique four-cycle [11]. This is also true of PCGs since the connectivity, ignoring edge weights, is identical to a rook’s graph. From Theorem 21 the first symbolic squaring has a pattern identical to the pattern from symbolically multiplying \( DMD \) where the \( m^2 \times m^2 \) matrix \( M = R + D \) is a PCM. Consider the value of \( DMD \) at \((i, j)\). It is given by
\[[\text{DMD}]_{i,j} = \begin{cases} D_{ii}R_{ij}D_{jj} & \text{if } i \neq j \\ D_{ii}^3 & \text{if } i = j \end{cases}\]

which, for \( i \neq j \), may be interpreted as the relationship between the pair of vertices \( D_{ii} \) and \( D_{jj} \).

Now symbolically square \( \text{DMD} \) for the second symbolic squaring. We have

\[
(D\text{MD})(D\text{MD}) = (D(R + D)D) \times (D(R + D)D)
\]

\[
= DRD^2RD + DRD^4 + D^4RD + D^6.
\]

Focus on the \( DRD^2RD \) term, symbolically,

\[
\Pi(\text{SymMult}(D,R,D^2,R,D)) \preceq \Pi(DRD^4 + D^4RD + D^6)
\]

if the zeros on the diagonal of \( R \) are treated as symbols. Implying that

\[
\Pi(\text{SumMult}(D,R,D^2,R,D)) = \Pi(\text{SymSqr}(D\text{MD})).
\]

One sees that its value at \((i,j), i \neq j\), is equal to

\[
[DRD^2RD]_{ij} = \sum_{k=1}^{m^2} D_{ii}R_{kk}D_{kk}^2R_{kj}D_{jj}
\]

where each term is a “walk” of length two, with segments from vertex \( D_{ii} \) to vertex \( D_{kk} \) and then from \( D_{kk} \) to vertex \( D_{jj} \). Each “walk” is a term in the canonical inner product. “Walk” is in quotes since a walk normally implies an edge connecting the vertices. Here “walk” is being used more generally to represent a string of relationships between vertices.

For the third symbolic squaring, \((D\text{MD})^3\) has a term \( DRD^2RD^2RD^2RD \) whose symbolic inner product terms for \((i,j), i \neq j\), are given by

\[
(5.8) \quad [DRD^2RD^2RD^2RD]_{ij} = \sum_{k_1=1}^{m^2} \sum_{k_2=1}^{m^2} \sum_{k_3=1}^{m^2} D_{ii}R_{ik_1}D_{k_1k_1}^2R_{k_1k_2}D_{k_2k_2}^2R_{k_2k_3}D_{k_3k_3}^2R_{k_3j}D_{jj}.
\]

Now let \( i \) equal to \( j \). \((5.8)\) contains all of the four-cycles as well as other “walks” of length four. For the \( n \)th symbolic squaring, there are \( m^{2n} \) “walks” of length \( 2^{(n-1)} \) at each \((i,j)\) location.

Section \ref{3.1} described an unsuccessful attempt to just use the four-cycles to separate graphs. However, it is also pointed out that there must be unique row and column signatures that can be used to pin down the value at a location. As symbolic squaring continues, the “walks” will incorporate the row and column signatures as well as the value at the intersection.

5.4. Practical Considerations. From a practical point of view, Algorithm 1 is extremely slow and requires a large amount of memory. A \( m \times m \) matrix has a \( m^2 \times m^2 \) PCM which is symbolically dense. Testing used adjacency matrices of graphs from the Bliss graph collection \cite{1} and the Neuen-Schweitzer graph database \cite{12}. Only matrices up to 180 \( \times \) 180 were tested since their PCMs are 32400 \( \times \) 32400 and take up about 8GB of memory per PCM when using 64-bit values. To make the execution time tractable, double precision matrix multiplication with prime numbers as the symbols is used instead of symbolic matrix multiplication. Symbol substitutions are performed every iteration. When there are more than 10K symbols the symbol substitution algorithm switches to using the integers 1, \ldots, k as the symbols to reduce magnitudes. IEEE 754 double precision format has a 52 bit mantissa which can represent integers up to 15 digits long. So the process is halted if an inner product goes over \( 2^{52} \).

Lastly the heuristic compares column mixes instead of diagonal mixes since column mixes often detect non p-similar cases an iteration before the diagonal mixes as discussed in Section \ref{2.10}.
6. Summary

Permutation similarity between two (real or complex) square matrices reduces to asking whether their associated PCGs are isomorphic. PCGs add symmetric permutation constraints to matrices so multisets can be used for comparisons. Usually, multisets maintain either row or column constraints while giving up the other constraint. PCGs make row and column constraints an integral part of the problem. Then the associated PCMs are repeatedly symbolically squared and symbols substituted until stable partitions are reached or the diagonal mixes differ. If the diagonal mixes do not match, the matrices are not p-similar. The case where stable partitions are reached with matching diagonal mixes are p-similar. The necessity and sufficiency of the algorithm is shown. A second algorithm using the blind algorithm to find the permutation between two p-similar matrices is also given. Therefore permutation similarity and graph isomorphism are in P.

References

[1] Bliss collection of benchmark graphs. http://www.tcs.hut.fi/Software/bliss/
[2] Rook’s graph. https://en.wikipedia.org/wiki/Rook%27s_graph
[3] V. Arvind, Johannes Köbler, Gaurav Rattan, and Oleg Verbitsky. Graph isomorphism, color refinement, and compactness. Computational Complexity, 26(3):627–685, 2017.
[4] L. Babai. Graph isomorphism in quasipolynomial time. arXiv:1512.03547, 2015.
[5] Richard A. Brualdi. Some application of doubly stochastic matrices. Linear Algebra and its Applications, 107:77–100, 1988.
[6] Gene H. Golub and Charles F. Van Loan. Matrix Computations. John Hopkins University Press, Baltimore, 2nd edition, 1989.
[7] Roger A. Horn and Charles R. Johnson. Matrix Analysis. Cambridge University Press, New York, NY, 2nd edition, 2013.
[8] Nathan Jacobson. Basic Algebra I. W. H. Freeman and Company, San Francisco, CA, 1974.
[9] Brendan D. McKay. Practical graph isomorphism. Congr. Numer., 30:45–87, 1980.
[10] Brendan D. McKay and Adolfo Piperno. Practical graph isomorphism, ii. Journal of Symbolic Computation, 60:94–112, January 2014.
[11] J. W. Moon. On the line-graph of the complete bigraph. Annals of Mathematical Statistics, 34(2):664–667, 1964.
[12] Daniel Neuen and Pascal Schweitzer. Benchmark graphs for practical graph isomorphism. arXiv:1705.3686v1, May 2017.
[13] Daniel Neuen and Pascal Schweitzer. An exponential lower bound for individualization-refinement algorithms for graph isomorphism. arXiv:1705.03283v1, May 2017.
[14] Beresford N. Parlett. The Symmetric Eigenvalue Problem. SIAM, Philadelphia, PA, 1998.
[15] Alfred Tarski. A lattice-theoretical fixpoint theorem and its applications. Pacific J. Math., 5(2):285–309, 1955.
[16] G. Tinhofer. Graph isomorphism and theorems of birkhoff type. Computing, 36:285–300, 1986.
[17] G. Tinhofer. A note on compact graphs. Discrete Applied Mathematics, 30:253–264, 1991.
[18] J. H. Wilkinson. The Algebraic Eigenvalue Problem. Oxford University Press, 1965.