Abstract

of

CANONICAL FORMS, OVER-COLORING, AND POLYTIME GRAPH ISOMORPHISM

by

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The question of Graph Isomorphism's (GI) true time complexity classification has remained a mystery for years. It is certainly in NP but uncertain whether or not it is in P, with many suggesting it is in fact NP-Intermediate. Despite many special case polytime solvers existing, a recent breakthrough in the field has only improved the problem's time complexity to "quasi-polytime" $O(n^{log^c n})$. This thesis proposes an "over-coloring" approach to canonical label construction that is $O(n^4)$ and conjectures based on reasoning and empirical evidence that it is a bijective (1:1) map from graph symmetric groups to canonical labels. That is to say, the proposed function overColor(G) takes as input a graph G and outputs a canonical label for G: a label that is unique to only G and the set of all graphs isomorphic to G. Then, three comparison algorithms that can each be used to distinguish the labels in polytime, polytime, and factorial time respectively are provided. The first algorithm used for comparison is a valid polytime GI solver if and only if the function overColor(G) is invertible (1:1). The second allows for a naïve reconstruction of the permutation between input graphs. The third offers a true reconstruction of this permutation matrix that leverages canonical labels to prune the permutation search space. A proof for the reduction of polytime GI to the invertibility of overColor(G) is offered and future work is discussed for how this proof can be used to aid in solving polytime GI itself. Lastly, supporting experimental evidence for both random graphs and specific k-regular and Johnson graphs is offered to demonstrate overColor(G)'s robustness in these spaces that suggests it may be 1:1.

______________________________, Committee Chair
Dr. Anna Baynes

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Date

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1. Introduction.

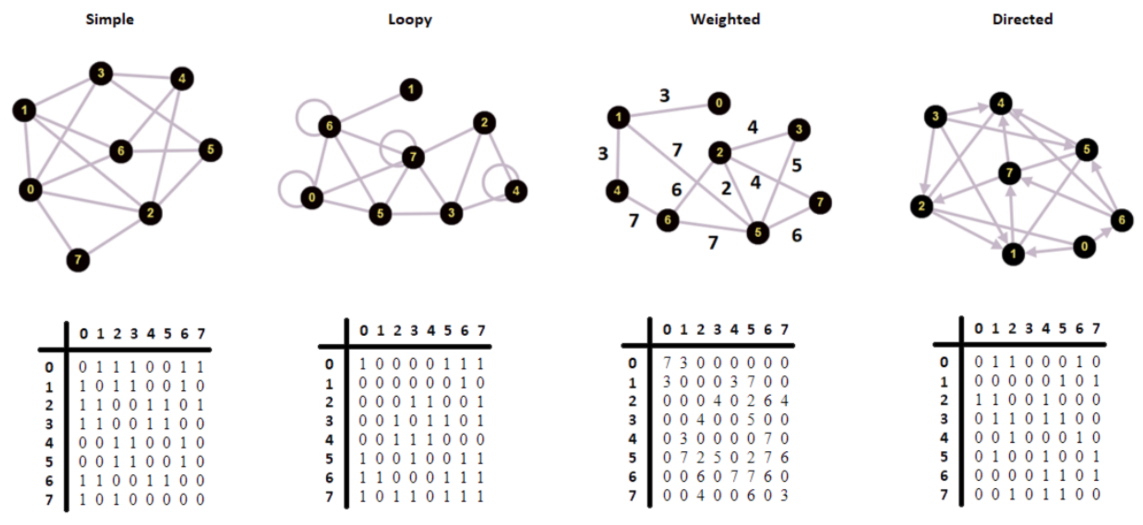
Graph isomorphism (GI), simply stated, is the test of whether two graphs are essentially the same graph. More formally, given the adjacency matrices of two graphs, $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, does there exist a permutation matrix ϕ such that $(\phi)(G_1)(\phi^T) = G_2$? From a graph theory perspective this asks if there exist a bijection ϕ between the vertex sets V_1 and V_2 such that for every edge $e(v_a, v_b) \in E_1$ there exists a bijected edge $e(\phi(v_a), \phi(v_b)) \in E_2$? GI is a well studied problem with many special case polytime solvers [4–6, 9, 15, 17] and for most practical purposes can be polytime solved by NAUTY, TRACES, and their derivatives [8]. However, no known universal polytime solver yet exists and despite $GI \in NP$, it is unknown whether or not $GI \in P$. Such problems are thought to fall into a possible NP-Intermediate (NPI) complexity class where they are members of $NP - P$ but not NP-Complete [13] . Examples of other problems suspected to be in NPI include integer factorization as evidence by the best known algorithms remaining exponential [14, 20, 22], the closely related discrete log problem [22], and minimum circuit size [12].

Some examples of special case polytime GI solvers include instances where input graphs have bounded tree width [5], bounded genus [17], bounded degree [4], or are permutation graphs [6]. There are also instances of linear time solvers such as in the case of graphs that are planer embeddable [9]. However, the fastest known general case solver for GI was introduced in 2015 and runs in quasi-polytime at $O(n^{log^c n})$ [1], beating out the previous record holder of $e^{O(\sqrt{nlogn})}$ [3] that held since 1983. Another interesting approach worth mentioning is invariant testing to solve GI that simply checks through a list of relatively easy to compute graph invariants. If enough invariants are checked with no unequal values between two graphs, they can be considered relatively isomorphic. However, this is often only used as a pre-process to more robust GI methods rather than the primary method.

This paper proposes a highly generalized $O(n^4)$ polytime near-solver for the GI problem that covers all finite connected graphs; both weighted and unweighted, directed and undirected, with or without loops, and with or without multi-edges. The algorithm works by first constructing set canonical labels (SCL) for each rooted graph embedded in the input graphs using the overColor() function described in **8. Algorithm and Discussion**. Then comparison algorithms perform set comparisons on these SCLs, attempt a naive reconstruction of the permutation matrix ϕ, or attempt a heuristic pruning of the permutation search space before using a backtracking approach to find ϕ. This paper will discuss the pseudo code for these algorithms, the theory behind them, and experimental results obtained by testing these algorithms on generated semi-random, k-regular, and Johnson subgraphs embeded graph pairs. It also offers a conjecture for polytime GI based on the invertability of overColor() as well as proof that if the conjecture were true, polytime GI is shown. Lastly, a discussion is had about the usability of an over-coloring approach to canonical label construction and how it may be applied to solving polytime GI itself. The implemented PHP code, test suite, and results repository can be found in the Appendix A as well.

2. Problem Statement. Does there exist a polytime algorithm that can compute canonical forms of simple connected graphs? If so, can this algorithm be expanded to include graph loops, edge weights, directed edges, and multi-edges? Lastly, can the SCL canonical forms of two graphs be compared in polytime?

3. Background. A graph G is made up of a vertex set V and an edge set E and a graph's creation is often denoted as $G = (V, E)$ [7]. A common representation of a graph is a two dimensional, $|V|$ x $|V|$ matrix in which each cell represents an edge/non-edge between vertices $(v_a, v_b) \in G$ and each row and column represents a vertex $v \in G$ [21]. This representation is referred to as an adjacency matrix, which we will also denote as G. In the case of simple graphs, an adjacency matrix is symmetric and each cell contains a 0 for no edge or a 1 for edge. In the case of edge weighted graphs, the 1 is replaced by the edge weight $w \in W$ (assumed to be non-zero) where W is the set of all weights in G. For directed graphs, the adjacency matrix becomes asymmetrical because some edge $e(v_1, v_2)$ does not necessarily have a partnering edge $e(v_2, v_1)$ as it would have had in the symmetric adjacency matrix of an undirected graph. A loop is a vertex that is both the origin and terminus of an edge, denoted as $e(v_1, v_1)$. A loop in an adjacency matrix is represented by an edge in a cell along the diagonal from the origin of the matrix. A multigraph is a graph that contains multi-edges. A multi-edge is a set of edges connecting the same two vertices and is represented in an adjacency matrix by an array in the cell corresponding the the vertices $(v_a, v_b) \in G$. Lastly, a sub-graph is simply a graph SG contained inside of another graph G such that $SG \subseteq G$.



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3	1	1	0	0	1	1	0	0
4	0	0	1	1	0	0	1	0
5	0	0	1	1	0	0	1	0
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	0	1	2	3	4	5	6	7
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	0	1	2	3	4	5	6	7
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4	0	0	1	0	0	0	1	0
5	0	1	0	0	1	0	0	1
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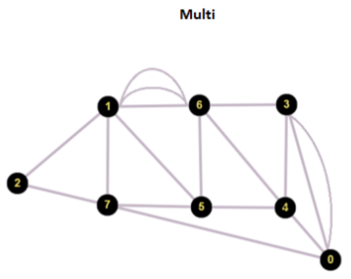
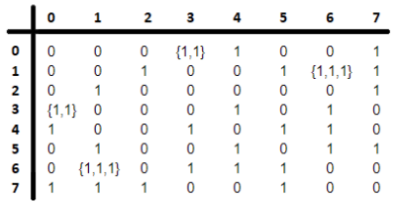
FIG. 3.1. *Graphs and their adjacency matrices*





	0	1	2	3	4	5	6	7
0	0	0	0	{1,1}	1	0	0	1
1	0	0	1	0	0	1	{1,1,1}	1
2	0	1	0	0	0	0	0	1
3	{1,1}	0	0	0	1	0	1	0
4	1	0	0	1	0	1	1	0
5	0	1	0	0	1	0	1	1
6	0	{1,1,1}	0	1	1	1	0	0
7	1	1	1	0	0	1	0	0

FIG. 3.2. *Graphs and their adjacency matrices 2*

A permutation matrix ϕ is a matrix in which for any given row or column, only one of the cells contains a 1 while all others contains 0 [2]. This is the matrix representation of the bijection ϕ between two isomorphic graphs. In order to permute a graph G_1 in to G_2 we matrix multiply such that $G_2 = (\phi)(G_1)(\phi^T)$ where ϕ^T is the transpose of ϕ. The question of two graphs being isomorphic to each other is as simple as asking does there exist a matrix ϕ for which this calculation can be performed? Although relatively straight forward, computing ϕ is often hard to do in general.

A common approach to tackling GI is to use canonical labeling schemes to give all graphs in the same symmetric group the same unique label and to ensure no other symmetric group of graphs shares that label, or a close approximation of this through refinement techniques [8]. In this way, GI can be reduced to a checking of these canonical labels. It should be noted, although refinement techniques are considered the best algorithms at present for efficient general case GI, they are still lower bounded by exponential time complexity [18]. A symmetric group in this case is the set of all graphs that can be created given one graph G transformed via $G_n = (\phi)(G)(\phi^T)$ for all possible ϕ of appropriate size [2], and a symmetric group in this case is $|V|!$ in size. As of now, no canonical labeling scheme has been created that can construct these labels in polytime in general. It should be noted, a canonical labeling approach to GI does not necessarily involve computing ϕ nor does it necessarily include ϕ as an output [8]. Instead, it assigns labels to graphs such that iff two graphs are isomorphic, they share a label (or ”if” in the case of near canonical labels).

A rooted graph is simply a graph that has a vertex designated as the root of the graph. Given an unrooted graph $G = (V, E)$, there are $|V|$ rooted sub-graphs that use the entire sets $(V, E) \in G$; one for each vertex in

G. Graph coloring is the process of assigning colors to vertices of G such that no vertex neighbors another vertex of the same color [21]. Minimum coloring is the method in which this is done using the least number of colors. N-coloring is the process of attempting to color G using at most N colors. Over-coloring is the process of continually 2-coloring vertices in the same way as standard 2-coloring but doing so until the entire graph is monochromatic. That is to say, once 2-coloring is broken by adjacent vertices having the same color, continue coloring anyways and color over vertices that already have color assigned to them, as can be seen **Figure 3.3**.

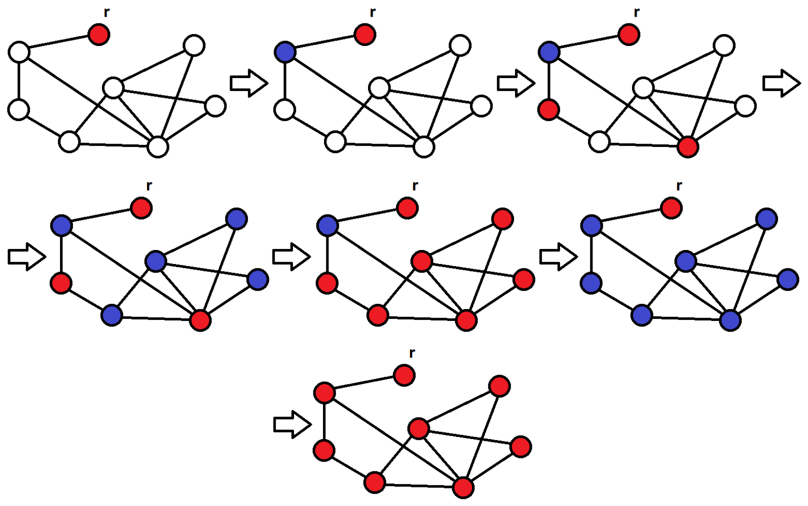


FIG. 3.3. *Visualizing the over-coloring process*

Note, over-coloring requires that an odd cycle exist in G for termination to occur per **Lemma 4.6**. Gamma matrices (Γ) are produced via the overColor() process described in the section **8. Algorithm and Discussion**. Essentially, they are codified representations of the step by step over-coloring of graphs, starting at each possible root. Note, a Γ matrix is equal to the return of overColor(G). For simplicity sake, the variable Γ is used slightly differently in the canonicalNameCompare() function as explained in **Lemma 4.5**, but in all other cases, it is as described above. Degree or neighborship of a vertex v is the number of adjacent vertices to v. Lastly, color influence (CI) is a time sensitive analogous to neighborship of vertices in the over-color process. A vertex's CI during any given round of overColor()s while loop (line 8) is the number of its neighbors who are currently colored the same as the current rounds color variable. This is simply a measure of the number of neighbors that will color v during a particular round.

A regular graph is a graph whose vertices all have the same number of neighbors [7]. A k-regular graph is a graph for which all vertices have exactly k neighbors. A graph G can be said to contain a symmetry if two vertices' adjacency lists can be swapped and the resulting graph remains isomorphic to G; also known as an automorphism [19]. Three important function types are surjective, injective, and bijective. Surjective functions map all elements of the function's range to at least one element in its domain. An injective function maps all elements of a domain to exactly one element in its range. A bijective function is one that is both injective and surjective [10]; mapping all elements of the function's domain to exactly one element in its range such that all elements in its range are accounted for. Also, bijective functions are by definition invertible which means given a function f, there exists a function f^{-1} such that $f^{-1}(f(x)) = x$.

A graph is said to be amenable if the surjective process of color refinement successfully canonically labels a graph [23]. Color refinement and the more generalized individualization refinement are common techniques used in industry for GI. [8, 18, 23]. An example set for which no graph is amenable by color refienemnt is the set of k-regular graphs [23]. That is to say, given any two non-isomorphic, k-regular graphs with an equal number of vertices, color refinement fails to successfully identify them as non-isomorphic. Another problem area for existing GI solvers that rely on individualization refinement is for graphs that contain Johnson subgraphs as a large proportion of the total graph [1]. A Johnson graph is constructed by first listing the set of all combinations of elements $\{1, 2, ..., n\}$ for an n choose k, denoted $\binom{n}{k}$. This list is the vertex set $V \in G$. Then, for each pair of vertices $(v_a, v_b) \in V$, iff the size of their intersection of elements $i = k - 1$, the elements share an edge $e(v_a, v_b) \in E$ [11]. Specifically for small k values, and especially for $k = 2$, these graphs tend to cause individualization refinement algorithms to fail or exceed their average time complexity of polytime when they are embedded in slightly larger graphs [1]. Often, mountains of heuristics are used to combat these issues while using color refinement and more generalized individualization refinement, but in general these two graph classes seem to cause issues with these most broadly applicable base algorithms.

Another common technique worth mentioning is the checking of invariant lists of input graphs. A graph invariant is a property that is unchanged regardless of how a graph is permuted; for example, a graph's vertex count. This means they are excellent for quickly ruling out trivial cases of non-isomorphic pairs of graphs. These algorithms are probabilistic in the sense that they check the input graphs for unequal invariants and if none are found, the algorithm says they are relatively isomorphic. To this date, no polynomial sized list of invarients have been found that can be computed in polytime and guarantee isomorphism if all are equal. Doing so would imply the existence of a polytime GI solver. Although this technique varies wildly in terms of accuracy and speed, it provides a framework for easily exchanging accuracy for speed and vice versa depending on the application. It also provides an easy pre-processing tool for proper GI that can rule out trivial cases.

4. Lemmas. This section will discuss the necessary prerequisites for section **5. Conjectures** and section **6. Proof**.

Lemma 4.1. If a connected simple graph G of at least 5 vertices is bipartite, its complement G^C will include an odd cycle and be connected so long as the original graph was not complete bipartite.

Proof. Suppose G is a connected simple bipartite graph. If one of its bipartitions contains at least three vertices (v_1, v_2, v_3), the vertices (v_1, v_2, v_3) form a triangle in G^C. If G is not complete bipartite, there exists at least two vertices, one in each bipartition, that are not adjacent. This means they are connected in G^C which implies G^C must be connected.

Lemma 4.2 If two simple or loopy graphs G_1 and G_2 are isomorphic, their complements G_1^C and G_2^C are also isomorphic.

Proof. Given two simple or loopy isomorphic graphs G_1 and G_2 and their bijection ϕ_a, it follows that $G_2 = (\phi_a)(G_1)(\phi_a^T)$ by the definition of isomorphism. Let us define graph complement as the function $f(G) = G'$ where each 0 in the adjacency matrix of G is set to 1, and each 1 originally in G is set to zero (assume no weights). f is obviously invertible because $f(f(G)) = G$. This implies it is bijective and that the bijection ϕ_b such that $(\phi_b)(G_1^C)(\phi_b^T) = G_2^C$ is equal to ϕ_a. Because a bijection ϕ_b exists, G_1^C and G_2^C must be isomorphic.

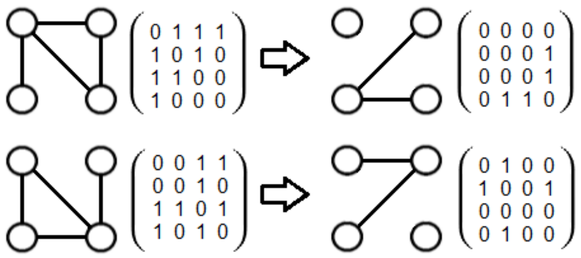


FIG. 4.1. *Graphs and their complements*

Lemma 4.3 Given two simple complete bipartite graphs G_1 and G_2 with an equal number of vertices and $|V_1| > 4$, if the size of the two bipartitions $(b_1, b_2) \in G_1 = |b_1|, |b_2|$ and the sizes of bipartitions $(b_3, b_4) \in G_2 = |b_3|, |b_4|$, then iff $|b_1|$ and $|b_2| \neq |b_3|$ nor $|b_4|$, G_1 and G_2 cannot be isomorphic.

Proof. Given a simple complete bipartite graph G_m, the number of edges can be calculated by $|E_m| = |b_x| * |b_y|$. If $|b_1|$ and $|b_2| \neq |b_3|$ nor $|b_4|$, then $|b_1| * |b_2| \neq |b_3| * |b_4|$ if $|b_1| + |b_2| = |b_3| + |b_4|$ and $|b_1| + |b_2| = |V_1| > 4$. Thus, (G_1, G_2) are isomorphic iff $|b_1| * |b_2| = |b_3| * |b_4|$ and $|b_1| + |b_2| = |b_3| + |b_4|$ for $|V_1| > 4$. This means because we know $|V_1| = |V_2|$, we know G_1 and G_2 are isomorphic if the graphs are simple complete bipartite.

Note: If the isomorphism of the simple complete bipartite graphs is established and only the edge weights can break G_1 and G_2's isomorphism, uniformly inserting edges for all non-edges in G_1 and G_2 that all share a unique edge weight outside of the domain of edge weights originally in G_1 and G_2 preserves any bijective properties G_1 and G_2 may have. This is demonstrated by lines 18 and 19 in GI() and results in the succesful classifications described in section **7. Experimental results**.

Lemma 4.4 The bijection ϕ_a between isomorphic graphs G_1 and G_2 is the same as the bijection ϕ_b between Γ_1 and Γ_2 where Γ_a = overColor(G_a). For a better understanding of overColor(), see **Lemmas 4.6, 4.7, Conjecture 5.1** and **Algorithm 8.3**.

Proof. The string contained in each cell $c(a, b) \in \Gamma_1$ corresponds to how vertex v_b was colored by overColor(G_1) when vertex v_a was selected as the root. The string contained in each cell $c(\phi(a), \phi(b)) \in \Gamma_2$ corresponds to how vertex $\phi(v_b)$ was colored by overColor(G_2) when vertex $\phi(v_a)$ was selected as the root. Because v_a and v_b are isomorphically equivalent to $\phi(v_a)$ and $\phi(v_b)$, the edge $e(v_a, v_b)$ is equivalent to $e(\phi(v_a), \phi(v_b))$. This means the edge cell $c(a, b) \in G_1$ being equivalent to the edge cell $c(\phi(a), \phi(b)) \in G_2$ implies the cell $c(a, b) \in \Gamma_1$ is equivalent to the cell $c(\phi(a), \phi(b)) \in \Gamma_2$ if overColor() is deterministic. Since overColor() is obviously deterministic due to lack of any randomization methods, this holds true.

Note: This means the set of cell values in the output matrix of overColor() is graph invariant. Evidence to

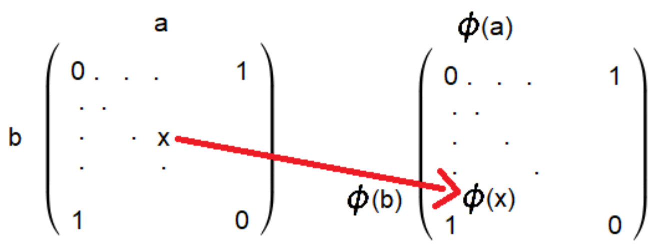


FIG. 4.2. *A mapping for edge x = (a,b) from the graph on the left to the graph on the right.*

support this can be seen in lines 7 and 8 of canonicalNameCompare() and the resulting succesful classification rate shown in section **7. Experimental results**. If $\phi_a \neq \phi_b$, this action would cause the arrays A and B in cannonicalNameCompare() to contain different elements even when G_1 is isomorphic to G_2 and $\phi_a \neq$ the identity matrix. This implies $\phi_a = \phi_b$ when G_1 and G_2 are isomorphic.

Lemma 4.5 Given a gamma matrix Γ_1 = overColor(G_1), concatenating G_1's adjacency matrix via $G_1 \oplus \Gamma_1$ preserves the canonical property of Γ_1 while including the required edge weight information needed to determine isomorphism of edge weighted graphs.

Proof. Following from **Lemma 4.4**, the bijection ϕ_a between G_1 and G_2 is the same as the bijection ϕ_b between Γ_1 and Γ_2. This implies $(\phi_a)((G_1) \oplus (\Gamma_1))(\phi_a^T) = (\phi_b)((G_1) \oplus (\Gamma_1))(\phi_b^T)$.

Note: Matrix concatenation in this case is the concatenation of each cell $M_1(a,b)$ of one matrix with the corresponding cell $M_2(a,b)$ of another.

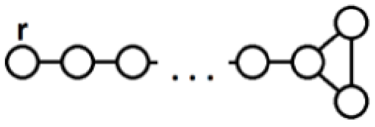
Lemma 4.6 The function overColor(G) will always terminate when given a connected, finite graph G that contains an odd cycle.

Proof. If a graph G has an odd cycle, there must exist at least two adjacent vertices (v_1, v_2) equidistant from a third vertex v_3. This implies regardless of the root $v_3 \in G$ selected, overColor(G) will eventually cause G to exist in a state where two neighboring vertices $(v_1, v_2) \in G$ have the same color given G contains an odd cycle. This monochromatic group of vertices is μ. On every cycle of overColor()'s while loop after μ is formed, all members of μ and all neighbors of vertices in μ will form the monochromatic group μ. Because G is connected finite, all vertices $v \in G$ must eventually join μ which eventually results in $|\mu| = |V|$ which implies G is monochromatic. Then overColor(G) cycles to the next starting root. Because there are a finite number of roots to select from, overColor(G) must eventually terminate.

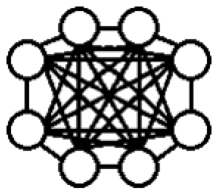
Lemma 4.7 The function overColor(G) will always terminate in $O(n^4)$ when given a connected finite graph G that contains an odd cycle and $n = |V|$.

Proof. The loose upper bound $O(n^4)$ can be obtained by combining the following worst case scenarios.

1. The first worst case is the greatest number of cycles overColor(G)'s while loop will execute before μ is formed. A depiction of this worst case input graph can be seen in graph 1 below. If n is the number of vertices in G, overColor(G)'s while loop will have $n-1$ cycles before μ is formed by the two vertices furthest distance from r. Which implies $2n$ until termination, which is $O(n)$.
2. The second worst case is when in a given cycle, every vertex in G must color its neighbors, and each of these vertices neighbors $n-1$ vertices. In this scenario, $O(n^2)$ colorings would occur in this cycle. This is the case of a complete graph, as can be seen in graph 2 below.



Graph 1



Graph 2

FIG. 4.3. *Worst case graphs*

Thus, if $O(n)$ cycles are required to achieve a monochromatic graph, and on each cycle, $O(n^2)$ coloring operations occur, then $O(n^3)$ operations will occur after all cycles are run. It should be obvious G could not be both of these cases and thus overColor(G)'s while loop could not take more than the number of operations required to terminate in this hypothetical. Now, if the above scenario is expanded such that it is run for every possible root $r \in G$, n cycles of $O(n^3)$ operations will occur. Hence, overColor(G) can be naively upper bounded by $O(n^4)$.

Lemma 4.8 In GI(), any directed graph G is equivalent to a directed graph G in which every uni-directional edge in G is complemented with a new edge in G, connected to the same vertices but pointed in the opposite direction whose weight is outside of the domain of weights for edges originally in G.

Proof. Given a graph G_1 whose edge weights form the set W, let us define the function f that takes every cell $c(a, b) \in G_1$ that contains a non-zero value and puts in the cell $c(b, a) \in G_1$ the value $x \notin W$ if $c(b, a)$ does not already contain a non-zero value. Let us then define f^{-1} as the function that looks at G_1 and for every cell $c(a, b)$ that contains the value x, replaces it with 0. Because f is invertible per $G_1 = f^{-1}(f(G_1))$ it is bijective and $\phi_a = \phi_b$ for $(\phi_a)(G_1)(\phi_a^T) = G_2$ and $(\phi_b)(f(G_1))(\phi_b^T) = f(G_2)$. Thus, for any directed graph G, transforming G such that $G = f(G)$ as a pre-process for GI() maintains any isomorphism or lack thereof for inputs of GI().

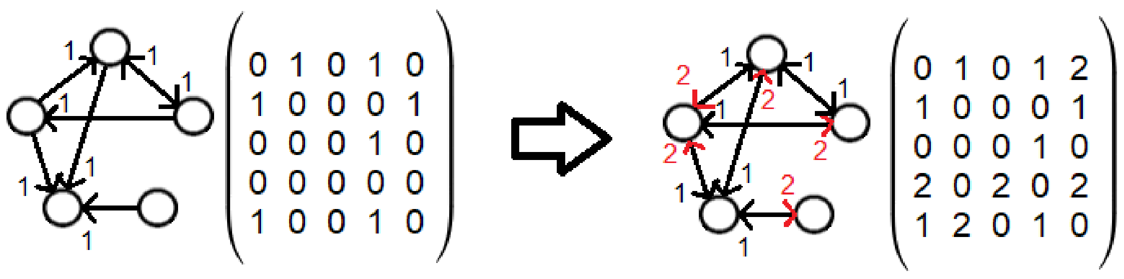


FIG. 4.4. *Directed graph to undirected weighted graph.*

Lemma 4.9 In GI(), multigraphs are equivalent to edge weighted graphs with no multi-edges.

Proof. Given a graph G_1 whose edge weights form the set W, let us define the function f that takes every cell $c(a,b) \in G_1$ that contains an array of multi-edges and replaces the array in c with a string that equals the weight-sorted ordering of the multi-edges in c, separating each weight in the string by $x \notin W$. Let us then define f^{-1} as the function that looks at G_1 and for every cell $c(a,b) \in G_1$ that contains a string with a character x, replaces it with an array of edge weights equal to that string exploded by the character x. Because f is invertible per $G_1 = f^{-1}(f(G_1))$ it is bijective and $\phi_a = \phi_b$ for $(\phi_a)(G_1)(\phi_a^T) = G_2$ and $(\phi_b)(f(G_1))(\phi_b^T) = f(G_2)$. Thus, for any directed graph G, transforming G such that $G = f(G)$ as a pre-process for GI() maintains any isomorphism or lack thereof for inputs of GI().

Lemma 4.10 The SCLs, or Γ matrices of two graphs can be compared in polytime.

Proof. Logically, a column v in a Γ matrix represents a particular vertex v selected as a root for a round of overColor() and each element u in that column is how the vertex u was colored throughout overColor() in the round in which v was the root. If **Conjecture 5.1** holds, the set of strings contained in these cells are unique to only graphs in the same symmetric group which means sorting the column does not destroy the uniqueness of the information. This means if each column of Γ is sorted, the uniqueness of the set of elements of Γ is maintained. Thus, comparing two Γ matrices can be done via an $O(n^2 logn)$ sort where each of the n columns is sorted individually. Then each column concatenates its elements into strings where each element is separated by some character $y \notin (W + x)$. These strings are then placed in arrays A and B for Γ_1 and Γ_2 respectively. Lastly, sort A and B in $O(nlogn)$. Afterwards, an O(n) loop string compares the elements of A and B for equality.

Lemma 4.11 If G is monochromatic, all edges have necessarily been traversed during overColor(G) except for edges connected to the vertices colored in the final round prior to G becoming monochromatic. If one additional round of over-coloring is performed, all edges must have been traversed at least once.

Proof. Let us say overColor()s while loop round number is d and the vertex furthest from root r is distance x from r. When $d = 1$, all edges connected to r are traversed. When $d = 2$, all edges of vertices distance 1 from r are traversed. In general, when $d = n$, all edges of vertices distance $n - 1$ from r are traversed. When $d = x$, all edges of vertices $x - 1$ are traversed. This means on round $x + 1$, all edges of vertices distance x from r are traversed.

Lemma 4.12 If G_1 and G_2 are isomorphic, leaving the arrays A and B unsorted in the last step of the process described in **Lemma 4.10** allows for the recreation of ϕ assuming G_1 and G_2 do not contain partitions of vertices that are symmetric with eachother within their respective graphs.

Proof. String 1 in A corresponding to Γ_1 matching string x in B corresponding to Γ_2 means the original permutation matrix's first row contained a 1 in position x (starting from 1). Repeating this until all strings are matched reconstructs ϕ. If G_1 is not isomorphic with G_2, A and B should not contain the same set of elements if **Conjecture 5.1** holds. However, if G_1 is isomorphic to G_2, A and B are guaranteed to contain the same set of elements due to **Lemma 4.4**'s proof of bijection preservation.

Note: If a graph G has a symmetry to it such that two of its own vertices can be swapped and the resulting graph G' is isomorphic with G, these vertices will produce the same string in G's Γ. This means even if two graphs are isomorphic, rebuilding ϕ as described above may result in an invalid permutation. To correct this, an algorithm would need to check every possible bijection of Γ_1 and Γ_2 to find the original ϕ that permutes G_1 into G_2. The naive approach as described in the above proof can be seen in **Algorithm 8.4**. A backtracking algorithm that heuristically prunes the original permutation search space using Γ and then checks all remaining possible bijections can be seen in **Algorithm 8.5, 8.6**.

Lemma 4.13 The size of the pruned ϕ space **Algorithm 8.6** searches through has a factorial growth rate that is less than or equal to $n!$ where $n = |G|$.

Proof. Given a graph G with m vertices that satisfy the condition described in **Lemma 4.12**'s note, there are $m!$ ways in which those vertices could be interchanged and thus $m!$ potential ϕ's to check. If G contains a set M of different vertex sets that all satisfy the same condition, the size of the ϕ search space $|\Phi| = \prod(M_x!)$ which implies $|\Phi| \leq n!$ where $|\Phi| \rightarrow n!$ as any $|m| \in M \rightarrow n$.

Note: The larger $|\Phi|$ becomes, the more G can be said to be symmetric, which can potentially be exploited for further heuristic reductions of the search space (See **10. Author's Notes**).

5. Conjecture. Conjecture 5.1. overColor() is a bijective function.

Firstly, the empirical evidence reported in section **7. Experimental Results** demonstrates overColor() is at least "good" at uniquely assigning SCLs to graphs according to their symmetric groups. If overColor() is in fact a proper canonical labeling function, it would mean overColor() bijectively maps symmetric groups of simple and loopy graphs into the SCL space of its outputs.

Reasoning to support this claim is as follows: Iff G_a is not isomorphic to G_b, there must exist an edge $e_1(v_a, v_b) \in G_a$ that does not have a corresponding edge $e_2(\phi(v_a), \phi(v_b)) \in G_b$ by definition of isomorphism. What overColor(G) is doing is traversing all edges in a graph G and recording for every vertex when it is pathed to by the over-coloring process starting at each root r. Like in the process described in **Lemma 4.11**, every edge must be traversed at least once for overColor()s while loop to exit. This means the existence of $e_1 \in G_1$ causes at least one path the over-coloring process takes during overColor(G_1) to be different than any path taken by overcolor(G_2) for G_2.

If our permutation matrix is the identity matrix, let us salt G_2 such that G_1 is not isomorphic to G_2. The way in which we salt is to transplant an edge from the vertex pair (v_a, v_b) to the vertex pair (v_c, v_d) such that the pairs are distinct from each other and do not result in a graph symmetry with each other. This means $e_1(v_a, v_b) \in G_1$ is no longer equivalent to $e_2(v_a, v_b) \in G_2$. As an aside, if G_1 and G_2 were still isomorphic after salting, $e_1(v_a, v_b)$ would still have a bijected edge $e_2(v_c, v_d)$. Because the over-coloring process must traverse e_1 at some point during overColor(G_1) per **Lemma 4.11**, one of the paths taken to v_a and/or v_b must be different from any path taken by the over-coloring process in overColor(G_2) for either vertex of e_2. This means the CI of at least one of the vertices of $e_1 \in G_1$ must be different at some point during overColor() from either of the vertices in e_2. This means the string contained at either $\Gamma_1[r][a]$ and/or $\Gamma_1[r][b]$ must be different than the string contained in either $\Gamma_2[r][a]$ and/or $\Gamma_2[r][b]$. This implies the set of strings contained in column r of Γ_1 must necessarily be different than the set of strings contained in any column of Γ_2, so long as the salting process broke G_2 from G_1's symmetric group. Therefor, overColor() is injective because only in the case of graphs being isomorphic can $e_1(v_a, v_b)$ have an equivalent $e_2(\phi(v_a), \phi(v_b))$. Finally, because overColor() is injective, and surjective **Lemma 4.6**, overColor() is bijective for simple and loopy graphs.

If overColor() can formally be shown to be invertible, it is automatically shown to be bijective. Conversely, showing it is not invertible proves overColor() is not a proper canonical labeling scheme and is only "good" at distinguishing symmetric groups in its labeling process.

6. Proof. Given two simple connected graphs with or without loops G_1 and G_2, either both graphs are bipartite, neither are bipartite, or one is bipartite and one is not. Given the first case, the two graphs must be inverted for overColor() to terminate per **Lemma 4.6**. We know because of **Lemma 4.1** this complement of a graph guarantees an odd cycle exists in overColor()'s input graph and that this graph complement guarantees a connected graph except when the original graph was complete bipartite. This is a valid operation in an isomorphism test because of **Lemma 4.2**. We know overColor() will produce some label for G_1 and G_2 in $O(n^4)$ time because of **Lemma 4.6** and **Lemma 4.7**. If overColor() is shown to be invertible, we also know the labeling produced will be canonical due to **Conjecture 5.1**. These two labels can then be compared in polytime to determine isomorphism of G_1 and G_2 because **Lemma 4.10**. For the second case, the graphs need not be inverted because an odd cycle already exists in both and are simply plugged into compareCanonicalNames(G_1, G_2) from GI(). The third case is trivial because one graph contains an odd cycle and the other does not. This implies they cannot be isomorphic. Lastly, in the event the original graphs were complete bipartite, have the same edge counts, and have the same vertex counts, they must be isomorphic per **Lemma 4.3**.

Assuming **Conjecture 5.1**: Given a simple graph with loops, the graph is obviously not bipartite and can therefore be covered under GI() because of **Lemma 4.6**. Given a weighted graph, concatenating the adjacency matrix and its gamma matrix provides a valid canonical labelling because of **Lemma 4.4** and **Lemma 4.5**. For directed graphs, bijectively transforming them to their equivalent weighted forms via the process described in **Lemma 4.8** provides valid canonization through the use of GI() as well, again because of **Lemma 4.4** and **Lemma 4.5**. Multigraphs can be bijectively mapped to weighted non-multigraphs because **Lemma 4.9** which implies valid canonization through GI() once again because of **Lemma 4.4** and **Lemma 4.5**. Lastly, **Lemma 4.3** simply provides justification for the weighted complete bipartite graph scenario in GI() which can be seen on lines 18 and 19 of GI(). Given the above and because **Lemma 4.7**, graph isomorphism for connected simple, loopy, weighted, directed, and/or mutligraphs is polytime solvable if **Conjecture 5.1** can be proved.

Finally, **Lemma 4.12** provides an alternative to the conjecture dependence above. If a ϕ can be found such that $(\phi)(G_1)(\phi^T) = G_2$, G_1 and G_2 are obviously isomorphic. One way it can be found is by simply finding a bijection between sets A and B from **Lemma 4.10**. Typically, only one exists and thus a ϕ is trivially construct able within polytime per **Lemma 4.12**. However, as stated in the note of **Lemma 4.12**, this is not always the case. For these instances, an algorithm must search a set of possible ϕs to find the specific ϕ that satisfies $(\phi)(G_1)(\phi^T) = G_2$. A backtracking algorithm is presented in **Algorithms 10.5, 10.6** to do just that. However, **Lemma 4.13** suggests its worst case runtime appears outside polytime. Thus, the comparison algorithm offered in **Algorithms 10.2** is polytime as shown in **Lemmas 4.6, 4.7** but is only conjectured to be a proper solver. The comparison algorithm offered in **Algorithms 10.4** is polytime, guarantees correctness if it returns true, but can potentially return a false negative if the circumstance described in **Lemma 4.12** occurs. Lastly, the comparison algorithm offered in **Algorithms 10.5, 10.6** guarantees total accuracy, but through **Lemma 4.13** and empirical testing has been found to not be within polytime.

7. Experimental Results. The procedure used in testing GI() for random graph pair cases was as follows: randomly create a graph G_1 following an Erdös-Rényi like approach to graph generation, maintaining a rough graph density of between 0.25 and 0.75. Then, permute the graph to create G_2. Afterwards, randomly chose on 50/50 odds to salt G_2 such that it is no longer isomorphic to G_1 and record which choice was made. Lastly, call GI(G_1, G_2) and compare the result to the expected outcome recorded when choosing to salt or not. Then repeat this process ad nauseam. The types of graphs generated for testing include simple, simple directed, unweighted bipartite, weighted bipartite, complete bipartite, loopy, loopy weighted, loopy weighted multi, and loopy weighted directed multigraphs. The salting patterns used include edge transplant, edge removal, and edge weight change. In the case of the edge transplant salt, transplanting would be iterated randomly anywhere from 1 to 10 times. Across roughly one million test cases for graphs varying in size from 25 to 150 vertices, zero cases were found where GI() returned an incorrect answer. Plots of the time and space complexity for these test cases can be seen below in **Fig. 7.1**. Note, the time complexity is much better than $O(n^4)$ in practice because of the naivety of the upper bound given in **Lemma 4.7**. From the data gathered during testing specifically, it can be estimated GI() is upper bounded by approximately $n^{2.5}$.

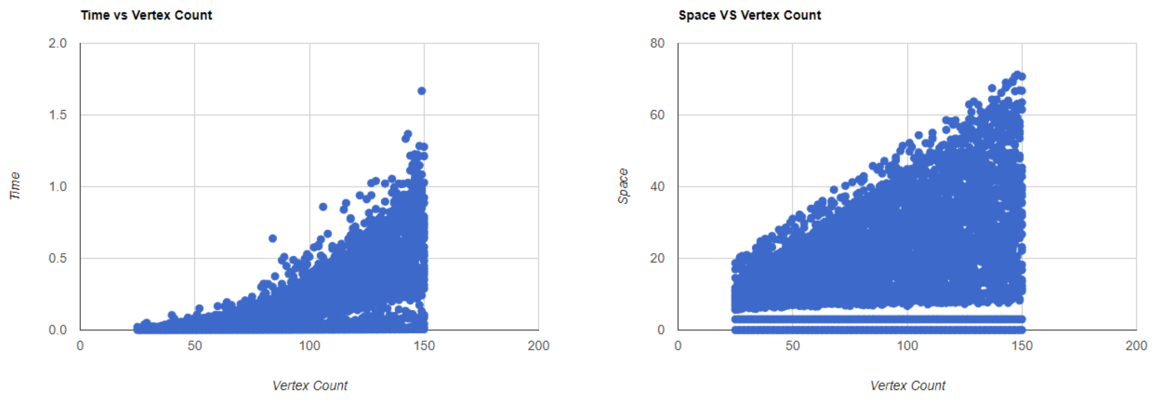
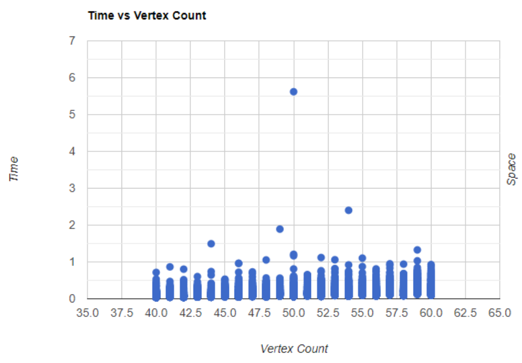


FIG. 7.1. *Time vs vertex count and Space vs vertex count for Random Graphs*

For targeted testing, two specific test cases were looked at: Johnson sub-graphs and k-regular graphs. These two were chosen because they appear to have the highest problem incidence among leading GI solvers. The following targeted tests also only test for false positives because these are the tests for which existing solvers take issue. Also, due to the deterministic nature of overColor(), it has become apparent while testing that there is no need to actually test for true positives as the algorithm is incapable of producing a false negative **Lemma 4.4, 4.5**. Lastly, the following two targeted examples were run using **Algorithm 8.2** specifically because it is the one **Conjecture 5.1** is concerned with.

In the case of k-regular graphs, the following procedure was used: generate two k-regular graphs $G_1 = K(n,k), G_2 = K(n,k)$ for $n = rand(40,60)$ and $k = rand(4,5)$. These numbers were chosen because of the computational complexity of random graph generation for k-regular graphs for large n and k values. Because G_1 and G_2 are random k-regular graphs, it is highly unlikely they are isomorphic, so for testing they were assumed to be non-isomorphic pairs while remaining k-regular with equal numbers of vertices and edges. Next, $GI(G_1, G_2)$ is called and its output recorded. Any instance in which the output returned is ”true,” it can be said the algorithm failed to properly identify the pair as not isomorphic. It should also be noted, finding any case in which the proposed algorithm successfully identifies non-isomorphic pairs of k-regular graphs of equal vertex and edge counts demonstrates its superiority to standard color refinement because it fails in every such case. However, because this set’s history of complication in GI, many random graphs within this set are tested for. A test of roughly 10,000 random k-regular graph pairs was used to test GI() and zero missed classifications were found. See **Fig. 7.2** below for time and space complexity charts.



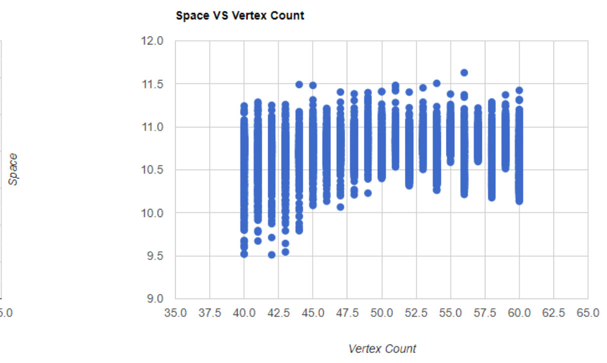
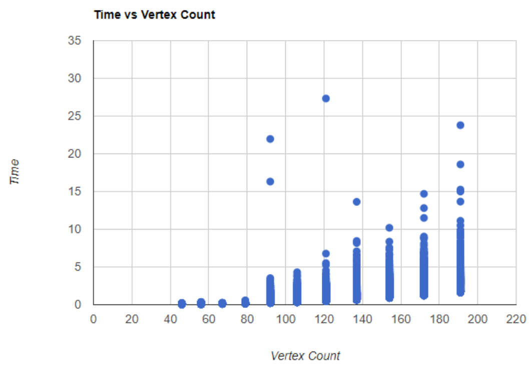


FIG. 7.2. *Time vs vertex count and Space vs vertex count for K-Regular Graphs*

In the case of Johnson graphs, the following procedure was used: generate a Johnson graph $G = J(n, k)$ for $n = rand(10, 20)$ and $k = 2$. Copy this graph to graphs G_1, G_2 and then create a random binary array B_1 of length $|G|$. Append B_1 to the adjacency matrix of G_1 by appending each row $r \in G_1$ with element $e_r \in B_1$. Then push B_1 to G_1 so that it is the new last row of G_1's adjacency matrix. Next, randomly shuffle B_1 to make B_2 such that $B_1 \neq B_2$ and perform the same process as described for G_1, B_1 with G_2, B_2. This produces two graphs G_1, G_2 that have an exceptionally small likely hood of being isomorphic while still both containing the same Johnson sub-graph that constitutes the majority of their structures. Then run a test $GI(G_1, G_2)$ and record the result. Any instance in which the output returned is "true," it can be said the algorithm failed to properly identify the pair as not isomorphic. For roughly 100,000 random Johnson graph embedded graph pairs tested for, one false positive was found; a graph with an embedded Johnson J(10, 2) subgraph. This implies overColor() as described in this paper is not truly a bijective function and thus GI() is not a proper GI solver, only a near solver. However, multiple approaches described in **10. Author's Notes** can be added to GI() which provides a proper classification for this particular case. See **Fig. 7.3** below for the time and space complexity charts.



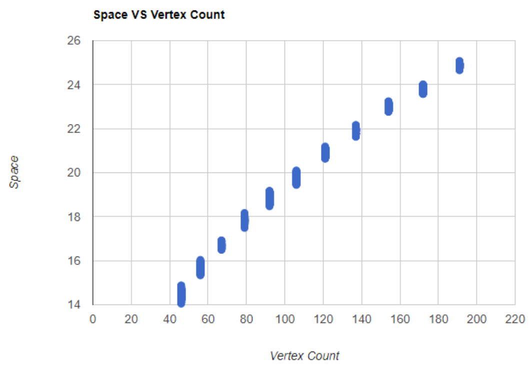


FIG. 7.3. *Time vs vertex count and Space vs vertex count for Embedded Johnson Graphs*

Over the course of testing on roughly 1,000,000 random graph pairs, 10,000 k-regular graph pairs, and 100,000 Johnson embedded graph pairs, one counter example of the invertability of overColor() as described above has been found; a false positive involving the J(10,2) subgraph. However, this specific counter example was then correctly classified as a true negative with the addition of other mechanism described in **10. Author's Notes**. Neither of these additions have been rigorously studied yet and as such are only an addendum to this paper, but they both individually provide a mechanism for properly classifying the mentioned counter example with no observed additional effects on the classifications of graph pairs that have been properly classified.

8. Algorithm and Discussion. See Appendix A for the implemented code.

The function GI(G_1, G_2) is the actual GI solver called to determine if two graphs are isomorphic. Its primary function is to pre-process the input graphs for canonicalNameCompare() to determine if they are obviously not isomorphic due to differing edge or vertex counts, if one contains an odd cycle and the other does not, and to perform the processes describe in **Lemma 4.8** and **Lemma 4.9**. It then goes through some minor tree logic to determine if the input graphs should be inverted and does further pre-processing in the case of the input graphs being complete bipartite per **Lemma 4.3** to account for edge weighting. At the end of the tree logic, it calls canonicalNameCompare($G_1, G_2, invert$).

Algorithm 8.1 GI(G_1, G_2)

```
1: set x and y $\notin W_1$ or $W_2$ such that $x \neq y$
2: if $|E_1| \neq |E_2|$ or $|V_1| \neq |V_2|$ then
3:    return false
4: else
5:    if $G_1$ and/or $G_2$ has multi edges then
6:       Perform process described in Lemma 4.9, using x as separator.
7:    end if
8:    if $G_1$ and/or $G_2$ is directed then
9:       Perform process described in Lemma 4.8, using x for weighting.
10:   end if
11:   if isNotConnected($G_1$) or isNotConnected($G_2$) then
12:      return invalid input
13:   end if
14:   if isNotBipartite($G_1$) and isNotBipartite($G_2$) then
15:      return canonicalNameCompare($G_1$, $G_2$, false)
16:   else if isBipartite($G_1$) and isBipartite($G_2$) then
17:      if isCompleteBipartite($G_1$) and isCompleteBipartite($G_2$) then
18:         Perform process described in Lemma 4.3's note, using y for weighting
19:         return canonicalNameCompare($G_1$, $G_2$, false)
20:      else
21:         canonicalNameCompare($G_1$, $G_2$, true)
22:      end if
23:   else
24:      return false
25:   end if
26: end if
```

The function canonicalNameCompare(G_1, G_2, invert), called by GI(), is responsible for calling overColor() to build the SCLs for the input graphs G_1, G_2 and then comparing their SCLs for equivalence. It inverts the input graphs in the event the boolean ”invert” is true because **Lemma 4.1**, **Lemma 4.2**, and **Lemma 4.6**. After calling $\Gamma_1 =$ overColor(G_1) and $\Gamma_2 =$ overColor(G_2), it concatenates the original input graphs to the results of overColor() because **Lemma 4.4** and **Lemma 4.5**. Lastly, because SCLs are dependent on set equivalence in which order does not matter, the Γ matrices are sorted so that string compare can be used to determine equivalence as described in **Lemma 4.10**.

Algorithm 8.2 canonicalNameCompare(G_1, G_2, *invert*)

```
$OG_1 = G_1$
$OG_2 = G_2$
if $invert$ then
    $G_1 =$ graphComplement($G_1$)
    $G_2 =$ graphComplement($G_2$)
end if
$\Gamma_1 =$ Matrix concatenate $OG_1$ and overColor($G_1$)
$\Gamma_2 =$ Matrix concatenate $OG_2$ and overColor($G_2$)
A = B = array()
Perform the process described in Lemma 4.10 using A and B as the arrays
if A == B then
    return true
else
    return false
end if
```

Lastly, overColor(G) is the process described in **Lemma 4.6**, **Lemma 4.7**, and **Conjecture 5.1**. It over-colors an input graph and records this step by step process in Γ. It then returns Γ. Note, $root$ is a vertex in G and the notation "Array[$root$]" refers to the column position of $root$ in the adjacency matrix G. $Color$ can be thought of as being either red or blue (1 or 0). The notation "$color^{-1}$" refers to swapping "color" to the opposite color of its current color; either from 1 to 0 or from 0 to 1. The notation "x .= y" means set x equal to x concatenate y. Finally, "$v.c$" means the current color of the vertex v.

Algorithm 8.3 overColor(G)

```
$\Gamma$ = 2D array()
for each vertex $root \in G$ do
    Clear all coloring from G
    $color = 1$
    $root.c = color$
    $\Gamma[root][root]$ .= $root.c$
    $lock$ = true
    while $G$ is not monochromatic or lock do
        if $G$ is monochromatic then
            $lock$ = false
        end if
        for each vertex $i \in G$ where $i.c == color$ do
            for each neighbor $n$ of $i$ do
                $n.c = color^{-1}$
                $\Gamma[root][n]$ .= $n.c$
            end for
        end for
        $color = color^{-1}$
    end while
end for
return $\Gamma$
```

The additional functions 4 and 5 offer alternatives to function 2 as described in **Lemmas 4.12, 4.13**. Function 4 is a naive polytime approach to reconstructing ϕ that relies on the non-existence of graph symmetries that produce a disordering of vertex bijections between two sets A and B. Function 5 does not rely on this assumption but sacrifices time complexity such that it is no longer polytime. Function 6 is the actual backtracking algorithm used by function 5 to reconstruct ϕ. Both functions 4 and 5 are constructed very similarly to function 2 and only differ in the criteria necessary to return true. They all still rely on function 3 to perform the most crucial part of the over all GI algorithm; over-coloring.

Algorithm 8.4 canonicalNameCompare2(G_1, G_2, $invert$)

```
1: $OG_1 = G_1$
2: $OG_2 = G_2$
3: if $invert$ then
4:     $G_1 =$ graphComplement($G_1$)
5:     $G_2 =$ graphComplement($G_2$)
6: end if
7: $\Gamma_1 =$ Matrix concatenate $OG_1$ and overColor($G_1$)
8: $\Gamma_2 =$ Matrix concatenate $OG_2$ and overColor($G_2$)
9: $A = B =$ array()
10: $tmpA = tmpB =$ array()
11: Perform process described in Lemma 4.10 using $A$ and $B$ as arrays but copy $A$, $B$ to $tmpA$,
    $tmpB$ prior to the final sort.
12: if $A == B$ then
13:     $tmpG =$ Perform process described in Lemma 4.12 using $tmpA$ and $tmpB$ as arrays, with
        output being the permuted graph $(\phi)(G_1)(\phi^T)$
14:     if $OG_2 == tmpG$ then
15:         return true
16:     else
17:         return false
18:     end if
19: else
20:     return false
21: end if
```

Algorithm 8.5 canonicalNameCompare3(G_1, G_2, *invert*)

```
1: $OG_1 = G_1$
2: $OG_2 = G_2$
3: **if** *invert* **then**
4:     $G_1$ = graphComplement($G_1$)
5:     $G_2$ = graphComplement($G_2$)
6: **end if**
7: $\Gamma_1$ = Matrix concatenate $OG_1$ and overColor($G_1$)
8: $\Gamma_2$ = Matrix concatenate $OG_2$ and overColor($G_2$)
9: $A = B =$ array()
10: $tmpA = tmpB =$ array()
11: Perform process described in **Lemma 4.10** using $A$ and $B$ as arrays but copy $A$, $B$ to $tmpA$,
    $tmpB$ prior to the final sort.
12: **if** $A == B$ **then**
13:     $used$ = 1D array of -1s with size = $|A|$
14:     $\phi$ = 2D array of 0s with size = $|OG_1|$
15:     **return** bt($tmpA$, $tmpB$, $OG_1$, $OG_2$, $\phi$, $used$, 0)
16: **else**
17:     **return** false
18: **end if**
```

Algorithm 8.6 bt(A, B, G_1, G_2, ϕ, *used*, *row*)

```
1: **if** $row == |G_1|$ **then**
2:     **if** $(\phi)(G_1)(\phi^T) = G_2$ **then**
3:         **return** true
4:     **else**
5:         **return** false
6:     **end if**
7: **else**
8:     **for** $col = 0$; $col < |B|$; $col$++ **do**
9:         **if** $used[col] == -1$ and $A[row] == B[col]$ **then**
10:            $tmp\phi = \phi$
11:            $tmpUsed = used$
12:            $tmp\phi[row][col] = 1$
13:            $tmpUsed[col] = row$
14:            **if** bt($A$, $B$, $G_1$, $G_2$, $tmp\phi$, $tmpUsed$, $row + 1$) **then**
15:                **return** true
16:            **end if**
17:        **end if**
18:    **end for**
19:    **return** false
20: **end if**
```

9. Conclusion. The question of Graph Isomorphisms time complexity being NPI or P has been around for years. Many techniques exist that allow specific cases of GI to fall into P. A common approach to tackling GI involves searching for a permutation matrix that permutes one graph into the other. However, another common approach involves canonical labeling. This technique relies on unique labels assigned to the symmetric groups of graphs so that any two graphs that are isomorphic share the same label, and no two symmetric groups share the same label. This idea was used as the premise for overColor(). This function can generate canonical labels for non-bipartite, connected simple or loopy graphs. It was also shown that in the case input graphs are bipartite, GI() can use the graph complements of input graphs for testing isomorphism. Due to the bijective nature of overColor() proposed in **Conjecture 5.1**, the pre-processed adjacency matrices of weighted graphs, directed graphs, and multigraphs where shown to be concatable to the SCL of their more simplified simple or loopy representations. It was shown that overColor() is polytime at $O(n^4)$.

Three comparison algorithms were presented that rely on overcolor() in their assessment of isomorphism. The first, 8.2, simply compares SCLs directly and is polytime. The second, 8.4, attempts a naive reconstruction of ϕ but is clearly only a near GI solver, and is also polytime. Third, functions 8.5 and 8.6, present a backtracking approach that exhaustively searches ϕ space to test for isomorphism while heuristically pruning its search by leveraging the canonical properties of overColor()'s SCLs, but sarifices speed such that only its average case is polytime while its worst case is factorial. Lastly, experimental evidence was provided to demonstrate GI() using overColor() to compare graphs for isomorphism. In doing so, it can be observed the real world performance of GI() has an average running time of roughly $n^{2.5}$ for the sample cases tested for. Also, specific test cases on sets of k-regular graphs and Johnson graphs were evaluated using the comparison algorithm 8.2 which demonstrates these common problematic graph types for GI could also be handled by the proposed algorithm. However, a counter example was found involving the Johnson subgraph J(10,2) that shows definitively overColor() as imagined in this paper is not bijective. Yet, additional techniques described in **10. Author's Notes** brings GI() back into the realm of potential bijectivity. These experimental results suggest that GI() is at worst an exceptional near GI solver. But further exploration is required in the development of over-coloring as a method for solving GI in general.

10. Author's Notes and Future Work.

1. Additional Mechanism. It should be noted the counter example mentioned in this paper was found months after the initial paper was written and during the end stages of writing this Thesis paper. Because of this, a deep exploration of the following solution has yet been explored and is not included in the main paper. However, it does solve the issue of improper classification of the particular fail case mentioned in the paper.

After having found a proper counter example to **Conjecture 5.1**, the obvious follow up was to study the counter example and find ways of filling the gap in GI() this fail case exposed. Additional graph invariants were tested for and new subroutines in overColor() were tried in order to get a proper classification from this graph pair. Eventually a rather inelegant solution was found for this specific fail case and is as follows:

Algorithm 10.1 GIwrapper($g1$,g2)

```
counter1 = counter2 = 0
for each vertex $v \in G_1$ do
  counter1++
  Remove all loops from $G_1$
  Add loop $v, v$ to $G_1$
  for each vertex $w \in G_2$ do
    Remove all loops from $G_2$
    Add loop $w, w$ to $G_2$
    if GI($G_1, G_2$) then
      counter2++
      break
    end if
  end for
  if counter1 $\neq$ counter2 then
    return false
  end if
end for
return true
```

First and foremost, this solution brings the algorithm's overall time complexity up to $O(n^6)$; not ideal but still polytime. Second, this algorithm assumes the initial input graphs do not contain loops. This is a valid assumption specifically for Johnson graphs because they are inherently devoid of loops. Also, it should be obvious this "wrapper" for GI() does not make overColor() itself bijective. There may be ways to modify overColor() itself to achieve this, but this solution does not. Instead, this wrapper is attempting to compensate for the lack of bijectivity in overColor() by using overColor() repeatedly on a set of graphs generated from the input graph, of which one may have an injective map into Γ space.

Important properties of this wrapper algorithm are: it does not change the classifications of true positive results for GI() nor does it effect false negatives nor true negatives. It does however effect false positives such as in the case of the counter example involving the J(10,2) subgraph. In plain English, this wrapper compares the results of GI() for each modified graph of G_1, G_2 where "random" vertices are assigned loops one at a time. If simple graphs G_1, G_2 are isomorphic, if a vertex in G_1 is given a loop such that isomorphism is broken, there must exist a vertex in G_2 which when given a loop becomes isomorphic with G_1 again. If G_1, G_2 are not isomorphic, there must exist a case where this loop assignment does not create two isomorphic graphs. Because GI() is a near GI solver, using it in this model may be sufficient for GIwrapper() to be a proper GI solver. I can offer no proof for this, but it does properly solve the single fail case found and its associated family without effecting any other cases tested for.

2. Line Graphs. In addition to the above wrapper function, another approach involving line graphs has been able to successfully produce a correct isomorphism determination for the counter example found in the paper. In order for two graphs to be isomorphic, their line graph representations must also be isomorphic in general. A Line graph L(G) of a graph G is constructed by considering every edge in G to be a vertex in L(G) and two vertices in L(G) share an edge iff the two vertices (edges in G) share a common vertex in G. When the counter example graph pair were converted to their line graphs and used as input to GI(), a correct result of non-isomorphic was returned. An important observation to make is the line graph of a Johnson graph is not a Johnson graph itself. This means the issues that arise from the existence of a Johnson subgraph in overColor() no longer apply. This approach relies more on established graph theory than the above approach and the time complexity becomes $O(|E|^4)$ where $|E|$ is the size of the edge set in G. This also has the advantage of being a faster solution than the one presented above because the greatest number of edges a simple graph can contain is less than n^2.

3. Johnson Graph Testing. A problem quickly discovered during testing is a density of meta false positives for small Johnson graphs. As the graphs got smaller, the more likely their appended random bit strings would produce isomorphic graph pairs. This would cause the proposed algorithm to state the graphs are isomorphic even though the test assumed they were not. A sample of these “failed” test cases were manually tested in the NAUTY command line function Dreadnaut [16] and all cases tested were found to be isomorphic except one. But manualy entering graphs into Dreadnaut made testing the proposed algorithm for small Johnson graphs untenable without additional automation to test these cases in Dreadnaut. The one failed, fail case in this test was the counter example mentioned in the paper that included an embedding of the Johnson J(10, 2) subgraph. Every other “fail” case logged during testing were for J((6,7), 2) with 6 being the lowest n value tested for.

4. Symmetry Reduction. The reason for the existence of **Algorithms 8.5 and 8.6** is to overcome potential symmetries in the input graphs resulting in non-unique column sets in Γ matrices. Theoretically, if as a pre-process to overcolor() it could be ensured no symmetries exist in the input graphs to overColor(), GI() would be a proper GI solver because **Algorithm 8.4** would be able to guarantee a reconstruction of ϕ. One way these symmetries could be removed would be to input G_1, G_2 into overColor() as normal and record the resulting Γ_1, Γ_2. Then use these outputs to partition the vertices of G_1, G_2 into their symmetric groups with respect to their graph by grouping all equal column sets (much like refinement techniques do). If G_1, G_2 are isomorphic, these sets would have bijections and if they are not isomorphic, this bijection could not exist. Random changes may be applied to a given partition and its supposed bijected partition in order to break the vertex symmetries of these given partitions. If done in a uniform manner between the two sets of partitions, the resulting graphs could be maid to contain no symmetries while still maintaining at least one of their permutations if one exists and could then be used as inputs for GI() with the polytime **Algorithm 8.2** used as the comparator. This then makes the “random changes” part the next step to develop if this method were to be explored.

5. Optimizations. The overColor() function, most of canonicalNameCompare(), and even parts of GI() can all be parallelized because of the lack of dependencies in the functions. overColor(G_1) and overColor(G_2) can be done in parallel for example. Also, each iteration of the outermost forloop of overColor() can be done in parallel. And the list goes on.

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