Graph Automorphism partition and Canonization in Polynomial time

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Abstract

We show that the Graph Isomorphism (GI) problem can be solved in polynomial $O(n^3 + n^2m \log(n+m) + m^2n \log(n+m) + m^3 \log(n+m))$ time, on simple connected graphs with n vertices and m edges. As fundamental part of the proof, we introduce a novel method, named Symmetry Classification, which computes a canonical automorphism partition of a simple connected graph in polynomial $O(n^2 + nm \log n)$ time. The master algorithm reduces to bipartite graph isomorphism by transforming the input graph, if not bipartite, to its subdivision graph and computes the canonical form of the latter; or of the former if already bipartite. Canonical form is obtained by repeating the sequence of first applying Symmetry Classification method, then canonically selecting a vertex for individualization, and last applying the classical 1-dimensional Weisfeiler-Lehman algorithm, until a canonical discrete coloring is attained. Since both bipartite and connected graph isomorphism are isomorphism complete we conclude that GI lies in P.

Keywords: Algorithms, Graph Canonization, Graph Isomorphism, Bipartite Graph Isomorphism, Graph Automorphism Partition, Polynomial Complexity

1. Introduction

1.1. Outline

This paper is organized as follows: In current section we introduce the basic notation, definitions and tools that will be used. In section 2 we present a novel method, which we name Symmetry Classification, that computes a canonical automorphism partition of a simple connected graph. In section 3 we present the Master algorithm along with proofs of correctness and analysis of its complexity. We conclude in section 4. In appendix A we include the listings of various subroutines that are being referenced in the main algorithms of this paper. In appendix B we showcase applications of the Master algorithm in selected graphs.

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1.2. Basic definitions and tools

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For the context of this paper let G = (V, E) be a simple graph with set of vertices V_{G} and set of edges E_{G} . By simple we mean undirected with no loops or multiple edges. We assume a normalized labeling of vertices $\{0, ..., |V_G| - 1\}$. The vertices adjacent to a vertex $u \in V_{G}$ form its open neighborhood $N_{G}(u)$. Any subgraph induced by a subset of vertices $S \subset V_{G}$ is denoted as G[S]. We may omit the subscript G in cases where context is clear. Throughout this paper whenever we encounter lists of integers we assume that a sorted list obevs ascending ordering and the comparator between a pair of lists $L = [x_1, x_2, ..., x_k]$, $L^* = [x_1^*, x_2^*, ..., x_l^*]$ with cardinality k, l respectively is: $L < L^*$ when k < l, and $L \leq L^*$ if there is some $j \leq k$ such that $x_i = x_i^*$ for i < j and $x_j < x_j^*$. The comparator between a pair of lists of [list of lists] is defined in a similar manner. All algorithm listings imply zero indexed lists. Two graphs G, Hare said to be *isomorphic*, $G \cong H$, if there is a bijection $f: V_G \to V_H$ such that if $\{u, w\} \in E_{G} \iff \{f(u), f(w)\} \in E_{H}$. In this context f is an isomorphism from G to H. For a graph G any bijection $A: V_G \to V_G$ such that if $\{u, w\} \in E_{g} \iff \{A(u), A(w)\} \in E_{g}$ is called *automorphism*. Mapping each vertex to itself is the trivial automorphism. The Graph Isomorphism (GI)problem asks to determine whether two given simple graphs are isomorphic.

Definition 1.1. Given a graph G = (V, E), a set $S \subseteq V_G : |S| \ge 2$ along with its elements, is/are *symmetric*, if for any two $u, v \in S$ there is an *automorphism* $f : V_G \to V_G : f(u) = v$. A vertex w which is mapped to itself for every possible automorphism is called *asymmetric*.

Definition 1.2. Given a graph G = (V, E), vertices u, v are called *pseudo-similar* if $G[V \setminus u] \cong G[V \setminus v]$ but u, v are not symmetric.

Definition 1.3. A partition π of a set V is a set $\{V_1, ..., V_k\}$ of pairwise disjoint non-empty subsets of V, such as $\bigcup_{i=1}^k V_i = V$. The sets V_i are called *blocks* of π . A partition π is *discrete* if $|\pi| = |V|$ and *unit* if $|\pi| = 1$. Each block of size 1 is called *trivial*. Given a partition π , we write $u \sim_{\pi} v \iff \exists B \in \pi : u, v \in B$.

Definition 1.4. A partition κ of V refines a partition π of V, if $\forall u, v \in V : u \sim_{\kappa} v \Rightarrow u \sim_{\pi} v$.

Definition 1.5. Given a graph G = (V, E), a partition π of V_G is *stable* if $\forall B \in \pi, \forall u, v \in V_G : u \sim_{\pi} v \Rightarrow |N(u) \cap B| = |N(v) \cap B|$. This means that any two vertices of a non-trivial block have the same number of neighbors that reside in any block.

Proposition 1 ([1], Proposition 3). Let G = (V, E) be a graph. For every partition π of V_{c} , there is a unique coarsest stable partition τ that refines π .

Definition 1.6. Let G = (V, E) be a graph. A surjection $c: V_c \to \{1..k\}, k \leq n$ is called *k*-coloring. Given a *k*-coloring *c* of *G*, we write $C_i^c = \{u \in V_G | c(u) = i\}$ and call it color class *i*. Likewise we denote the partition $\{C_i^c, ..., C_k^c\}$ by π_c . A *k*-coloring is characterized respectively from the attributes i.e., discrete, unit, stable, of its induced partition and vice versa. For brevity we may interchange naming k-coloring with just coloring in the course of this paper.

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Definition 1.7. Given two graphs G, H with respecting k-colorings c_G , c_H , an isomorphism f from G to H is called color preserving for c_G , c_H , if $\forall u \in V_G \Rightarrow c_G(u) = c_H(f(u))$.

Definition 1.8. A coloring method is a method for obtaining a coloring c_b of a graph G, given an initial coloring c_a .

Definition 1.9. A coloring method is called *canonical*, if for any two isomorphic graphs G and H with initial colorings c_a^G resp. c_a^H and isomorphism $f: V_G \to V_H$, the following holds: if f is color preserving for c_a^G and c_a^H , then f is color preserving for the resulting colorings c_b^G and c_b^H . Resulting colorings are also called *canonical colorings* of G, H starting from c_a^G resp. c_a^H . If starting coloring is the unit one, we simply call the resulting coloring a *canonical coloring* of a graph.

Definition 1.10. Given any two graphs G, H with initial k-colorings c_{G} resp. c_{H} and an isomorphism f from G to H, we call Canonical Color Refinement (to be abbreviated as CCR) any canonical coloring method which implements 1-dimensional Weisfeiler-Leman algorithm [2], that can compute the coarsest stable partitions $\pi_{c_{G}^{*}}, \pi_{c_{H}^{*}}$ which refine $\pi_{c_{G}}, \pi_{c_{H}}$. Both resulting colorings c_{G}^{*}, c_{H}^{*} are unique 1 canonical l-colorings with $k \leq l$ starting from c_{G} resp. c_{H} .

Lemma 1.1 ([1], Theorem 9). For any graph G = (V, E) on n vertices and m edges given a k-coloring c of G, there exists a Canonical Color Refinement algorithm that halts in $O((n+m)\log n)$ time.

Definition 1.11. Given a graph G = (V, E) and a canonical stable coloring c_G of G, we call *distinguished* all vertices in trivial blocks.

Definition 1.12. Given a graph G = (V, E) and a stable non-discrete partition $\pi = \{B_1, ..., B_i\}$ of G, we call individualization of any vertex $u \in B_i : |B_i| > 1$, the process of transforming π into $\pi^u = \{B_1, ..., B_i \setminus \{u\}, ..., B_i, \{u\}\}$, or equivalently introducing a new color class q = l + 1 for $\{u\}$. By application of *CCR* on this *q*-coloring, we end up with a stable *k*-coloring c_k where $k \ge q$. We call c_k the individualized coloring of u on c_i and denote it as $Ind(u, c_i)$.

Definition 1.13. Given a simple graph G = (V, E) on n vertices, m edges and a canonical discrete coloring c_d of G, let $G(c_d)$ be an isomorphic copy of G, which is computed by relabeling the vertices of G according to their order in c_d . We call $G(c_d)$ the canonical form of G, denoted as Canon(G). The list of sorted open neighborhood label lists of each vertex of Canon(G) starting from 0 until n-1, is the certificate of G denoted as Cert(G). In case of vertices with zero degree, open neighborhood lists are empty. The routine of computing Cert(G)is described in 6.

Corollary 1.1.1. Given two simple graphs G, H, if their certificates match then they are isomorphic.

Proof. By 1.13, since their certificates match their canonical forms are the same, thus they are also isomorphic. \Box

Definition 1.14. A *bipartite* graph is a graph whose vertices can be divided into two disjoint and independent sets U_1 and U_2 , that is, every edge connects a vertex in U_1 to one in U_2 . The routine which checks whether a simple connected graph is bipartite is described in 4.

Definition 1.15. An edge subdivision is the insertion of a new vertex v_z in the middle of an existing edge $e = v_x v_y$ accompanied by the joining of the original edge endpoints with the new vertex, thus replacing edge e with two edges $e_1 = v_x v_z$ and $e_2 = v_z v_y$.

Definition 1.16. Given a simple graph G = (V, E) on n vertices, m edges, we call the subdivision graph S(G) of G, the graph obtained by sequentially applying edge subdivisions 1.15 to all edges of G. Apparently S(G) contains n + m vertices and 2m edges. The routine of computing S(G) is described in 5.

Corollary 1.1.2. Given a simple graph G = (V, E) on *n* vertices, *m* edges, its subdivision graph S(G) is a bipartite graph.

Proof. Follows from 1.14,1.16, since for S(G) the newly inserted m vertices and existing n vertices from G form two disjoint independent sets, and all newly derived edges share their endpoints between these two sets.

Definition 1.17. Given a simple connected graph G = (V, E), a surjective coloring c of G and a vertex $u \in V$, we call schema SC(u, c) of vertex u on c, the output of the routine described in 3. The output is a list of sorted color lists which represent all levels of a Breadth First Traversal of graph G (each list is one level), with vertex u as root (level 1). Each level contains the colors of its vertices stemming from coloring c.

Definition 1.18. Given a simple connected graph G = (V, E) and a surjective coloring c of G, let G[SC(u, c, l, l + 1)] be the subgraph induced by the vertices of levels l, l+1 of the schema SC(u, c) of a vertex $u \in V$. We implicitly reference the vertices of each level since schema is a Breadth First Traversal routine, but doesn't contain vertices in its structure 3.

Definition 1.19. Given two simple graphs G, H, their union will be a graph U with set of vertices $V_G \cup V_H$ and set of edges $E_G \cup E_H$.

2. Classification of symmetries

In this section we introduce a novel algorithm called *Symmetry Classification* (to be abbreviated SYM), which discovers the automorphism partition of a given simple connected graph.

2.1. Symmetry Classification Algorithm

A canonical stable coloring c_{start} of a simple connected graph G = (V, E)and a surjection from each vertex u of G to a ranked integer value of the certificate of its open neighborhood's subgraph Cert(G[N(u)]), are given as input. Ranking is based on a given comparator. Equal ranked values imply isomorphism. We assume that certificates have been generated by the same algorithm so that any comparison is relevant. Symmetry Classification 1 consists of two chained partition constructions and a final call to *Canonical Color Refinement* subroutine:

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- 1. Construct a partition $\pi_{seed} = \{B_1, ..., B_l\}$ such that for each vertex u, v $u \sim_{\pi_{seed}} v \iff c_{start}(u) = c_{start}(v) \wedge G[N(u)] \cong G[N(v)]$. Blocks of π_{seed} are ordered, based first on their color value and then on their certificate ranking (numerical ordering). The induced coloring c_{seed} is named seed coloring.
- 2. Construct a partition $\pi_{schema} = \{B_1, ..., B_k\}$ such that for each vertex u, v $u \sim_{\pi_{schema}} v \iff SC(u, c_{sed}) = SC(u, c_{sed})$. Blocks of π_{schema} are ordered, based on their schema value (list of [list of lists] comparator). The induced coloring c_{schema} is named schema coloring.
- 3. Invoke CCR subroutine with c_{schema} as input and obtain a stable coloring named symmetry coloring.

Algorithm 1 Symmetry Classification (SYM)

Inpu from	it : A simple connected Graph G on n vertices each vertex u of G to a ranked value of the c	, <i>m</i> edges, a canonical stable coloring c_S of <i>G</i> and a surjection ertificate of its open neighborhood's subgraph $Cert(G[N(u)])$.
1	put: A canonical stable coloring of G (symme	ry coloring), which represents the automorphism partition of G.
1: f	unction $SYM(G, c_S, CertMap)$	
2:	$schemaMultiMap \leftarrow MultiMap\{\}$	▷ The schema multimap
3:	$coloringMap \leftarrow Map\{\}$	▷ The color map of vertices
4:	$color \leftarrow 0$	
5:	for vertices in c _S .colorClasses do	Classify based on color from c _S
<u>6</u> :	if $vertices.size == 1$ then	▷ Trivial block
7:	$coloringMap(vertices[0]) \leftarrow color$	Trivial block inherited from input coloring
8:	$color \leftarrow color + 1$	
9:	continue	
10:	end if	
11.10	$vertices.sortwith(v_1, v_2 \rightarrow CertMa)$	$p[v_1] \ge CertMap[v_2]) > Sort by certificate ranked value$
12.	$coloring Map[vertices[0]] \leftarrow color$	
10:	for i in 1 until vertices.length do	
14:	if CertMap[vertices[i]] > CertMap[vertices[i]]	ap[vertices[i-1]] then
10:	$color \leftarrow color + 1$	▷ Different subgraph detected, new color assigned
10:	$coloringMap[vertices[i]] \leftarrow co$	lor
16	else	
10:	$coloringMap[vertices[i]] \leftarrow co$	lor
19:	end if	
20:	end for	
55:	$color \leftarrow color + 1$	N Soud coloring coloring
23.	for wantom in C wantings do	> Seed coloring calculated
$\frac{20}{24}$	ior vertex in G.vertices do	Compute Schema 5 of vertex based on seed coloring
25.	schema $O_J V$ erlex $\leftarrow SCHEMA(G, CO)$	(vertex)
20.	schema MuttiMap[schemaO] v eriex]	← vertex ▷ Add entry to multimap
20:	end for	(an hous) N Sent enhanced from multimer house
28.	sorreasenemata	(up.keys) Disort schemata from muttimap keys
20.	coloring Map.clear()	Reset coloring map for schema partition
29.	$color \leftarrow 0$	▷ Reset color pointer
00: 91.	for schema in sortedSchemata do	Construct schema partition based on schema ordering
31:	$vertices \leftarrow schemaMap[schema]$	Get all vertices with this schema value
32: 33:	for vertex in vertices do coloringMap[vertex] \leftarrow color	
34:	end for	
32	$color \leftarrow color + 1$	
30:	end for	▷ Schema coloring calculated
37:	return $CCR(G, coloringMap)$	▷ Apply CCR on schema coloring to obtain symmetry coloring
38:	end function	

Lemma 2.1. Given a simple connected graph G = (V, E) and an initial canonical stable coloring c of G, the symmetry coloring c_s induced by application of Symmetry Classification 1 on c is stable and canonical.

Proof. Seed coloring 1 is canonical, because it (potentially) refines an initial canonical coloring and every isomorphism maps vertices to vertices of the same open neighborhood subgraph. Likewise *schema coloring* 1 is also canonical because its is derived from seed coloring and by definition of *Schema* 3, as a Breadth First Traversal method, every isomorphism maps vertices to vertices of the same schema. Since *schema coloring* is canonical, application of *Canonical Color Refinement* on it, yields also a canonical stable coloring 1.10, which in this context is the *symmetry coloring*.

- **Proposition 2.** Given a simple connected graph G = (V, E) and an initial canonical stable coloring c of G, the symmetry coloring c_s induced by application of Symmetry Classification method 1 on c, classifies vertices as such:
 - 1. By the isomorphism of their open neighborhood subgraphs.
 - 2. By the number of neighbors that have the same open neighborhood subgraph.
 - 3. By their *schema* value.
 - 4. By the number of neighbors that have the same schema value.

Proof. The construction of *seed coloring* is a refinement of canonical stable coloring c, by further classifying vertices within classes of c which have the same open neighborhood subgraph. The construction of *schema coloring* classifies vertices based on their schema value on *seed coloring* so conditions (1) and (3) of the corollary are met. Subsequent invocation of *Canonical Color Refinement* with *schema coloring* as starting coloring, leads to a stable coloring 1.10, which from 1.5 satisfies all four the conditions of the corollary.



Symmetry coloring of graph \rightarrow [[0, 1, 2, 3, 4, 5], [9, 10, 11, 12, 13, 14], [8], [6], [7]]	
Schema of [0, 1, 2, 3, 4, 5] \rightarrow [[1], [1, 1, 4], [1, 1, 5], [3], [2, 2, 2, 2, 2, 2]]	
Schema of [9, 10, 11, 12, 13, 14] \rightarrow [[2], [2, 2, 3], [2, 2, 2, 5], [4], [1, 1, 1, 1, 1, 1]]	
Schema of [8] \rightarrow [[3], [2, 2, 2, 2, 2, 5], [4], [1, 1, 1, 1, 1, 1]]	
Schema of [6] \rightarrow [[4], [1, 1, 1, 1, 1, 5], [3], [2, 2, 2, 2, 2, 2]]	
Schema of $[7] \rightarrow [15] [3, 4] [1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2]$	

Figure 1: Schemata of all vertices on symmetry coloring

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Lemma 2.2. Given a simple connected graph G = (V, E) and a symmetry coloring c_s , it holds that $G[SC(u, c_s, l, l+1)]] \cong G[SC(v, c_s, l, l+1)]], \forall l \in \{1, ..., |SC(v, c_s)| - 1\}, \forall u, v$ in the same block of c_s .

Proof. Let u, v any vertices of the same block of c_s . For level 1 (root) and level 2 of $SC(u, c_s)$ and $SC(v, c_s)$, from 2 we have $G[SC(u, c_s, 1, 2)] \cong G[SC(v, c_s, 1, 2)]$ (1), because level 2 is the open neighborhood of u and v. If level count of 180 schemata is 2 then by (1) lemma holds. Let $N(t, l_1, l_2)$ denote the open neighborhood of vertex t in levels l_1, l_2 . For any vertices a, b of level 2 of same color c across both $SC(u, c_s), SC(v, c_s)$, by 2 we have $G[N(a)] \cong G[N(b)]$ (2). Let's assume that level count ≥ 3 and $G[SC(u, c_s, 2, 3)] \ncong G[SC(v, c_s, 2, 3)]$ (3). Condition (1) implies $G[N(a,1,2)] \cong G[N(b,1,2)]$ (4), because both a, b are connected to the same set of colors in level 2, thus in level 3 also. Since levels 1 and 3 have no adjacent vertices the subgraphs G[N(a, 2, 3)], G[N(b, 2, 3)] because of (4) must be isomorphic in order to satisfy (2). But because of (3) there must exist some vertices z, x of same color in level 2 of $SC(u, c_s), SC(v, c_s)$ respectively that $G[N(z,2,3)] \cong G[N(x,2,3)]$ which is contradicting. Same for all remaining pairs of levels $\{(3, 4), ...(|SC(r, c_s)| - 1, |SC(r, c_s)|)\}, r \in u, v$ of both schemata.

Theorem 2.3. Given a simple connected graph G = (V, E) and an initial canonical stable coloring c of G, the symmetry coloring c_s induced by application of Symmetry Classification method 1 on c is the automorphism partition of G.

Proof. By 2.2 for any two vertices u, v of the same block B_x we have that $G[SC(u, c_s, 1, 2)] \cong G[SC(v, c_s, 1, 2)]$ (1). If levels are 2 then by (1) the family of subgraphs $\{G[V \setminus u]\}_{u \in B_x}$ are all isomorphic. Let's assume that level count ≥ 3 and that for the union 1.19 of levels (1, 2) and (2, 3) it holds that $\bigcup_{i=1}^2 G[SC(u, c_s, l, l+1)] \ncong \bigcup_{i=1}^2 G[SC(v, c_s, l, l+1)]$ (2). Condition (2) implies that for some vertices a, b of the same color c in level 2 it is $G[N(a)] \ncong G[N(b)]$ which is contradicting because of 2. If we continue taking the union of all subsequent levels we end up again with the family of subgraphs $\{G[V \setminus u]\}_{u \in B_x}$ being all isomorphic. The last step is to prove that vertices of the same block are not pseudo-similar 1.2 which is a direct consequence from the fact that they have the same schema 2.



Figure 2: Schemata (Breadth First Traversal) of symmetrical vertices 18 and 30 (second block of symmetry coloring) of the same graph depicting the isomorphism of their neighboring levels induced subgraphs. By taking the union of all pairs of consecutive levels induced subgraphs we end up with 2 isomorphic graphs $G[V \setminus 18], G[V \setminus 30]$.

Lemma 2.4. Given a simple connected graph G = (V, E) on n vertices, m edges, Symmetry Classification Algorithm 1 takes $O(n^2 + nm \log n)$ time.

Proof. Sorting all vertices by the ranked value of the certificate of their open neighborhood subgraphs requires $O(n \log n)$ time. Constructing the seed coloring requires O(n) time. Computing schemata of all vertices requires O(n(n+m)) time. Populating the multimap with schemata for all vertices as keys requires O(nm) time, due to O(m) time for hash computation. Sorting all schemata can take up to $O(nm \log n)$ since each schema has O(m) size. Retrieving all vertices by their schema from multimap will require O(nm). Building the schema coloring takes O(n). Finally executing *Canonical Color Refinement* requires $O((n+m)\log n) + O(nm\log n) + O(nm) + O((n+m)\log n) = O(n^2 + nm\log n)$. □

²²⁰ 3. The Master Algorithm

The Master Algorithm 2 accepts a simple connected graph G = (V, E) on n vertices and m edges as input, and calculates the certificate of the subdivision graph S(G) 1.1.2, or of G if it is already bipartite. The reduction to bipartite graph isomorphism is justified by the fact that ranking of certificates of open neighborhood subgraphs in a bipartite graph is computed in O(m) time, since every subgraph consists of disconnected vertices with zero edges. Therefore their

ranked value is equal to the degree of each vertex. The construction of seed coloring in 1 for the case of reduction to bipartite could be omitted, because the degree invariant is already covered by CCR. We choose to include it for clarity, because it doesn't affect the complexity of the algorithm. Since bipartite graph isomorphism is isomorphism complete [3] the only penalty involved is an increase in the number of vertices and edges up to n + m and 2m, in case G is not already bipartite. The Master Algorithm starts by applying a CCR on the bipartite graph in order to obtain a canonical stable coloring c_k . If c_k is discrete the algorithm returns the certificate of the reduced (or not) graph and halts. In any other case it iteratively applies the sequence Symmetry Classification-Individualization-CCR until a discrete coloring is attained. The choice of which vertex to individualize is performed by selecting any vertex from the minimum ordered color class of the canonical automorphism partition derived by Symmetry Classification that either isn't trivial or that is trivial but not

²⁴⁰ by Symmetry Classification that either isn't trivial or that is trivial but not already trivial in the starting (individualized) coloring of each round.

Algorithm 2 Master Algorithm (MA)		
Inp Out	ut : A simple connected graph G on n vertice put : $Cert(S(G))$ or $Cert(G)$, if G is bipa	ces, m edges. rtite.
1:	function $MA(G)$	
2:	$q \leftarrow G$	\triangleright The graph to process. Initially set to G
3:	if $!ISBIPARTITE(G, 0)$ then	\triangleright Check if G is bipartite 4
4:	$g \leftarrow SUBDIVISION(G)$	▷ Compute subdivision graph S(G) 5
5:	end if	
6:	$certRanking \leftarrow Map\{\}$ \triangleright	vertices to ranked values of Open Neighborhood Subgraph surjection
7:	for vertex in g do	
8:	$certRanking[vertex] \leftarrow vertex.de$	gree ▷ Bipartite graph open neighborhood subgraphs are trivial
9:	end for	
10:	$c_x \leftarrow CCR(g, c_{unit})$	▷ Run CCR with unit coloring
11:	while true do	
12:	if c_x is discrete then	▷ If coloring is discrete break from loop
13:	break	
15	end if $autPartition \leftarrow SVM(a, c_{-}, cert$	Ranking) N Calculate automorphism partition on surrout solaring 1
16.	$auti utition \leftarrow 51 m(g, c_{2}, cent$	Nortex for individualization variable
17.	f	
18.	is look and a first and a firs	biorCiasses do $>$ Avoid individualizing already trivial vertex of c_x
19:	(colorClass isTrivial &	$k \left[c_{-} colorClasses\left[c_{-} (colorClass[0]) \right] is Trivial \right]$ then
20.	$u_{i} \rightarrow f_{i} = color Class[0]$	Sologi first verter from color alors
21.	bind (coror crass[0]	
$\frac{21}{22}$	oreak a :e	Dreak from loop
23:	end ii end for	
$\bar{2}4:$	$c_x \leftarrow Ind(v_{ind}, c_x)$	\triangleright Compute individualized coloring of selected vertex v_{ind}
25:	end while	
26:	return $CERTIFICATE(g, c_x)$	▷ Return certificate 6
27:	end function	

Theorem 3.1. Given a simple connected graph G = (V, E), the output obtained by applying Master Algorithm 2 on G is an invariant to test isomorphism.

Proof. Since bipartite graph isomorphism is isomorphism complete [3], an invariant for subdivision graph S(G) 1.1.2 is also valid for G. If Canonical Color Refinement, when initially invoked, induces a discrete coloring, then this is canonical 1.10. In any other case for each round we select any vertex from the minimum ordered class of symmetries that either isn't trivial (1) or is trivial but not already trivial in the current coloring (2). Symmetry Classification generates a canonical automorphism partition π_{aut} 2.1 2.3 which implies that both (1) and (2) will be deterministically derived, because π_{aut} will order all distin-

guished vertices also in a canonical way. Invoking Symmetry Classification in each round on an individualized coloring, even if its definition implies a canonical coloring of G starting from unit 1, produces the automorphism partition of a graph G_{ind} which is derived from G, by artificially making the individualized vertex u_{ind} distinct (e.g. connecting a complete graph on n vertices to u_{ind}), thus its output is valid for our canonicity context. Since in all cases we obtain a canonical discrete coloring, from 1.1.1 we conclude that Master Algorithm generates a valid invariant to test isomorphism.

Theorem 3.2. Given a simple connected graph G = (V, E) on n vertices, m edges, Master Algorithm 2 takes $O(n^3 + n^2m\log(n+m) + m^2n\log(n+m) + m^3\log(n+m))$ time.

Proof. Checking if graph is bipartite requires O(n + m) time. Computing subdivision graph S(G) requires O(n+3m) time. Since subdivision graph S(G) has n+m vertices and 2m edges we consider that all calculations are performed on S(G). Calculating ranking of open neighborhood graphs of all vertices requires at most O(n + 3m). Invoking *CCR* requires at most $O((n + 3m)\log(n + m))$ 1.1. Symmetry Classification, individualization selection and *CCR* (individualized colorings) can be invoked at most n + m - 1 times which takes $O((n + m - 1)((n + m)^2 + (n + m)2m\log(n + m)))$ 2.4 + O((n + m - 1)(n + m)) + $O((n + m - 1)(n + 3m)\log(n + m))$. Computing the certificate of discrete coloring takes O(n + 3m). So in total we have $O(n + m) + O(n + 3m) + O(n + 3m) + O((n + m - 1)(n + m)) + O((n + m - 1)((n + m)^2 + (n + m)2m\log(n + m))) = O(n^3 + n^2m\log(n + m)) + m^2n\log(n + m) + m^3\log(n + m))$. □

Theorem 3.3. Graph Isomorphism (GI) problem lies in P.

Proof. Follows from 3.1, 3.2 and because connected graph isomorphism is isomorphism complete [3]. \Box

4. Conclusion

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We have presented a new algorithm that computes an invariant to test graph isomorphism in polynomial time. The main new contribution was the introduction of *Symmetry Classification* algorithm which discovers the automorphism partition of the graph. Future work may include deeper analysis of the complexity, regarding various classes of graphs and comparison with other practical isomorphism algorithms [4]. In the same direction it is worth examining whether the structural results of this paper could provide a path for improving efficiency of Babai's Quasipolynomial Algorithm [5].

Appendices

A. Listings of subroutines used by the main algorithms

Algorithm 3 Compute Schema	a of a vertex on a surjective coloring
Input : A simple connected graph G , a surjecti Output : A list of sorted lists representing a list colors of its vertices stemming from c_x .	ve coloring c_x of G and a vertex u from a block of c_x . Breadth First Traversal of G with u as root. Each level list contains
1: function SCHEMA(G, c_x, u)	
2: $schema \leftarrow List\{\}$	\triangleright A jagged list containing the schema of the color class of u
3: $visitedVertices \leftarrow Set\{\}$	▷ Keep track of visited vertices
4: $bftQueue \leftarrow Queue\{\}$	▷ Queue to perform the Breadth First Traversal
5: $visitedVertices.add(u)$	\triangleright Initialize structures with u
6: $bftQueue.add()u)$	
7: while bftQueue.isNotEmpty do	
8: $levelSize \leftarrow bftQueue.size$	▷ Size of the current level
9: $levelColorList \leftarrow List\{\}$	▷ List that saves the current level
10: while $levelSize \neq 0$ do	
11: $vertex \leftarrow bftQueue.pop()$	
12: $levelColorList.add(c_x(vertex$	$(>))$ $(>)$ Map vertex to its color from c_x
13: for neighbor in neighborhood	!(G, vertex) do
14: if !visitedVertices.contai	ns(neighbor) then
15: bftQueue.add(neighbor	r)
16: visitedVertices.add(ne	eighbor)
17: end if	
18: end for	
20° and while	
21: schema.add(sort(levelColorList)) ▷ Sort color list and add new level
22: end while	
23: return schema	
24: end function	

Algorithm 4 Check if graph is bipartite

Input: A sin	mple connected graph G on n vertices, m edges an	d the root vertex to start.
Jutput: A	decision whether G is dipartite.	
1: functio	n ISBIPARTITE $(G, root)$	
2: edge	$eCount \leftarrow G.edges.length$	
3: ver	$texCount \leftarrow G.vertices.length$	
4: if 4	* $edgeCount > (\frac{vertexCount}{2})^2$ then	\triangleright Check edge, vertex condition if G is bipartite
5: .	return false	
<u>6</u> : end	if	
(colo	$prMap \leftarrow Map\{\}$	▷ Color map of 0-1 values
8: bft0	$Queue \leftarrow Queue\{\}$	▷ Queue to perform the Breadth First Traversal
9: bft0	Queue.add(root)	▷ Initialize structures
10: col	$orMap[root] \leftarrow 0$	
11: wh	ile bftQueue.isNotEmpty do	
12:	$vertex \leftarrow bftQueue.pop()$	
13:	$color \leftarrow color Map[vertex]$	
14:	for neighbor in neighborhood(G , vertex) do	
15:	if $color == colorMap[neighbor]$ then	▷ If colors match graph is not bipartite
16:	return false	
17:	else	
18:	$colorMap[neighbor] \leftarrow color - 1 $	▷ Assign different color
19:	bftQueue.add(neighbor)	
20:	end if	
21:	end for	
22: end	d while	
23: ret	urn true	
∠4: end fu	inction	

Algorithm 5 Compute Subdivision graph

Input : A simple connected graph G on n vertices, m edges and the root vertex to start. Output : The subdivision graph $S(G)$.		
1: fu	nction SUBDIVISION (G)	
2:	$subdivision \leftarrow SimpleGraph\{\}$	▷ The empty subdivision graph
3:	$visitedEdges \leftarrow Set\{\}$	\triangleright Keep track of visited edges of G
4:	for vertex in G.vertices do	
о: С	if !subdivision.containsVertex(vertex) then	
0: 7:	subdivision.addVertex(vertex)	
8	end if for neighbor in neighborhood(G verter) do	
g.	if subdivision containsVerter(neighbor) the	
10:	subdivision.addVertex(neighbor)	
11:	end if	
12:	if !visited.contains(Edge(vertex, neighbor)) t	hen
13:	$subdivision vertex \leftarrow Vertex\{\}$	▷ New vertex to be added in subdivision graph
14:	subdivision.addVertex (subdivisionVertex) ▷ Add new vertex
15:	subdivision. add Edge (Edge (vertex, subdivi	sionVertex)) ▷ Create two new edges
16:	subdivision.addEdge(Edge(subdivisionVertication))	tex, neighbor))
17:	visited.add(Edge(vertex, neighbor))	\triangleright Mark edge of G as visited
18:	end if	
20	end for	
$\overline{2}1$	return subdivision ▷ Ret	Irn subdivision graph on $n + m$ vertices, $2m$ edges
22: •	nd function	

Algorithm 6 Compute Certificate of Graph **Input:** A simple graph G on n vertices, m edges and a canonical discrete coloring c_d . **Output:** The certificate Cert(G). 1: function $CERTIFICATE(G, c_d)$ 2 $gCopy \leftarrow SimpleGraph\{\}$ \triangleright The empty copy of graph G $\frac{3:}{4:}$ $\begin{array}{c} \textbf{for } vertex \textbf{ in } G.vertices \textbf{ do} \\ gCopy.addVertex(c_d(vertex)) \end{array}$ \triangleright Add relabeled vertices based on c_d end for for vertex in G.vertices do for neighbor in neighborhood(G, vertex) do $gCopy.addEdge(c_d(vertex), c_d(neighbor))$ \triangleright Add relabeled edge endpoints based on c_d 9: 10: 11: end for end for $certificate \leftarrow List\{\}$ > The list of sorted open neighborhood lists 12:13:14:certificate.add(neighbors)▷ Add list to certificate end for return certificate 15: 16: \triangleright Return certificate of G 17: end function

B. Application of Master Algorithm in selected Graphs

Below we showcase the application of *Master Algorithm* for some example graphs. The comparators used for sorting operations adhere to what is described in 1.2. For brevity we omit including the computation of subdivision graphs and the ranking of certificates for open neighborhood subgraphs. We use abbreviations for *Canonical Color Refinement (CCR)* and *Symmetry Classification (SYM)* subroutines. Canonical Color Refinement subroutine is implemented as defined in [1].

B.1. Miyazaki Graphs

Miyazaki [6] graphs are regular and form special cases of Cai–Fürer–Immerman 300 construction based on Fürer gadgets[7].



Figure 3: Miyazaki M_1 graph G

Listing 1: Application of Master Algorithm on Miyazaki graph G



[81], [17], [76], [78], [18], [57], [16], [52], [5], [50, 53], [46], [34], [71, 96], [13, 35], [69, 97], [58, 70], [14, 36], [72, 91], [73, 98], [37], [77]]
[5]. Individualize 45 for next round.
Calculation completed after 5 rounds.
Discrete coloring→[165], [0], [42], [19], [58], [1], [21], [41], [84], [22], [86], [23], [87], [2], [47], [60], [20], [62], [44], [9], [63], [31, [46], [4], [12], [66], [49], [11], [66], [61], [63], [63], [61], [23], [61], [23], [61], [23], [61], [23], [61], [61], [62], [63], [63], [63], [63], [63], [61], [63], [61], [63], [61], [63], [61], [61], [62], [63], [61], [61], [63], [61], [61], [63], [61],

B.2. Strongly Regular Graphs

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A strongly regular graph G is a simple graph defined by the tuple (n, d, l, m)where n is the number of vertices, d is the number of neighbors for each $u \in V$, l is the number of common neighbors for each pair of adjacent vertices and m the number of common neighbors for each pair of non-adjacent vertices.



Figure 4: Strongly regular graph G of the family (16,6,2,2).

Listing 2: Application of Master Algorithm on Strongly regular graph G

	[0]. Subdivision of input graph computed. [0]. Ranking of open neighborhood subgraphs computed.
400	[1]. CCR→[[16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0, 41, 42, 43, 44, 45, 46, 47, 48, 49, 54, 45, 46, 51]
	[1] SYM-5[16, 17, 18, 19, 00, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63], [0,
	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]] [1]. Individualize 16 for next round.
	$ \begin{array}{c} \text{(21. CCR} \rightarrow [[17, \ 22], \ [0, \ 1], \ [16], \ [8, \ 11], \ [60, \ 61, \ 62, \ 63], \ [2, \ 3], \ [5, \ 6], \ [19, \ 20, \ 23, \ 24], \ [42, \ 43, \ 45, \ 46], \ [12, \ 13, \ 14, \ 15], \ [4, \ 7, \ 9, \ 10], \ [18, \ 21, \ 25, \ 26], \ [48, \ 49, \ 38, \ 54, \ 39, \ 55, \ 56, \ 57], \ [36, \ 40, \ 40], \ [43, \ 41], \ [51, \ 52, \ 56, \ 56], \ 57], \ [36, \ 40, \ 41], \ [52, \ 56, \ 56], \ 57], \ [36, \ 40],$
	$ \begin{array}{c} 1, \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ $

[2]. Individualize 17 for next round.
[3]. CCR→[[22], [0], [16], [8, 11], [60, 61, 62, 63], [3], [5, 6], [19, 20], [42, 43, 45, 46], [12, 13, 14, 16], [4, 9], [18, 21], [38, 54, 39, 55], [36, 41], [51, 52, 58, 59], [37, 53], [27], [32, 34], [33, 35], [17], [1], [2], [28, 30], [28, 31], [7, 10], [25, 26], [48, 48, 56, 57], [40, 44], [50, 47], [23, 24]
[3]. SYM→[[22], [0], [16], [8, 11], [60, 63], [61, 62], [3], [5, 6], [19, 20], [42, 46], [43, 45], [13, 15], [12, 14], [4, 9], [18, 211, [38, 54], [39, 55], [36, 41], [52, 52], [51, 53], [57], [53], [53], [53], [53], [53], [53], [53], [51], [11], [21], [22], [23, 24]]
[3]. Individualize 8 for next round.
Calculation completed after 3 rounds.
Discrete coloring→[[22], [0], [16], [11], [60], [3], [6], [20], [45], [12], [4], [18], [38], [36], [51], [53], [53], [53], [53], [53], [17], [11], [22], [26], [43], [40], [51], [41], [57], [44], [50], [24], [49]]
Certificate→[[20, 21], [2, 7, 11, 19, 42, 47], [1, 20], [31, 32, 33, 34, 35, 55], [9, 61], [16, 17, 18, 19, 33, 49], [7, 8, 13, 27, 29, 53], [10, 30], [10, 30], [52, 21], [54], [51], [51, [54], [54], [51], [65], [54], [56

B.3. Frucht Graph

A Frucht Graph [8] has no symmetric vertices, thus possesses only the trivial automorphism (identity or rigid graph).



Figure 5: Frucht graph G



[0]. Subdivision of input graph computed.
 [0]. Ranking of open neighborhood subgraphs computed.
 [1]. CCR→[[12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29], [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 [1]. SYN→[[19], [21], [20], [24], [26], [17], [15], [13], [12], [4], [3], [9], [8], [6], [2], [1], [0], [5], [7], [25], [23], [18], [10], [29], [27], [11], [28], [14], [22], [16]]
 [1]. Individualize 19 for next round.
 Calculation completed after 1 rounds.
 Discrete coloring→[[16], [44], [19], [11], [29], [11], [51, [21], [22], [6], [23], [7], [13], [25], [0], [14], [10], [22], [17], [15], [3], [20], [27], [18], [9], [26], [28], [8], [24], [12]]
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 Certificate→[[1, 5], [0, 2, 7], [1, 20], [4, 15, 26], [3, 16], [0, 19, 29], [7, 8, 21], [1, 6], [6, 9], [8, 10, 28], [9, 11], [10, 12, 13], [11, 14], [11, 27], [12, 15, 29], [3, 14], [4, 22, 23], [18, 19, 23], [17, 20], [5, 17], [2, 18, 21], [6, 20], [16, 24], [16, 17], [22, 26, 26], [24, 27], [3, 24], [13, 25, 28], [14, 27], [21, 16, 21], [16, 20], [16, 24], [16, 17], [22, 26, 26], [24, 27], [3, 24], [13, 25, 28], [14, 27], [2, 18, 21], [6, 20], [16, 24], [16, 17], [22, 26, 26], [24, 27], [3, 24], [13, 25, 28], [14, 27], [21, 16, 21], [16, 20], [16, 24], [16, 17], [22, 26, 26], [24, 27], [3, 24], [13, 25, 28], [14, 27], [21, 16, 21], [21, 20

B.4. Bipartite Graphs



Figure 6: Bipartite graph G

Listing 4: Application of Master Algorithm on bipartite graph G

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