# The Graph Isomorphism Algorithm 

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#### Abstract

We present a new polynomial-time algorithm for determining whether two given graphs are isomorphic or not. We prove that the algorithm is necessary and sufficient for solving the Graph Isomorphism Problem in polynomial-time, thus showing that the Graph Isomorphism Problem is in $\mathbf{P}$. The semiotic theory for the recognition of graph structure is used to define a canonical form of the sign matrix of a graph. We prove that the canonical form of the sign matrix is uniquely identifiable in polynomial-time for isomorphic graphs. The algorithm is demonstrated by solving the Graph Isomorphism Problem for many of the hardest known examples. We implement the algorithm in $\mathrm{C}++$ and provide a demonstration program for Microsoft Windows.


Recommendation: http://www.geocities.com/dharwadker/tevet/isomorphism/

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## Selgitus

Teavik on pühendatud graafide isomorfismiprobleemile, st graafide isomorfismi tuvastamise algoritmi konstrueerimisele. See probleem võis kerkida ülesse juba siis, kui A. Cayley [1857] tegeles orgaaniliste isomeeride alaste uuringutega.

Isomorfismi tuvastamise ülesanne kujutab praegu endast graafiteooria keskset ülesannet. Klassifikaatori ,2000 Mathematics Subject Classification" (MSC2000) järgi on graafide isomorfismi tuvastamine koos taastatavuse probleemiga kombinatoorne nähtus indeksiga 05 C 60 . Isomorfismi tuvastamine seisneb vaid vastuses küsimusele, kas graaf $\boldsymbol{G}_{\boldsymbol{A}}$ on isomorfne graafiga $\boldsymbol{G}_{\boldsymbol{B}}$ ning esitada isomorfne substitutsioon.

Isomorfismi tuvastamise teoreetiline algoritm täiesti olemas - see seisneb graafi $\boldsymbol{G}_{\boldsymbol{B}}$ seosmaatriksi ridade ja nendele vastavate veergude ümberpaigutamises (permuteerimises, ümberjärjestamises, übervahetamises) niikaua, kui see ei lange kokku graafi $\boldsymbol{G}_{\boldsymbol{A}}$ seosmatriksiga. Sellel on vaid üks puudus see on väga keeruline, selle sammude arv läheneb $\boldsymbol{n}$ ! ( $\boldsymbol{n}$-faktoriaalini). Veel kümmekond aastat tagasi arvati, et 16 ! permutatsiooni arvutamine võtaks kuni 40 aastat aega. Teiste lahenduste otsimine kestab.

Soovitus: http://www.graphs.ee

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## 1. Introduction

We present a historical perspective of the Graph Isomorphism Problem and discuss the reasons why this problem has such a distinguished place in the history of mathematics and philosophy.

### 1.1. Some Historical Observations

Isomorphism (Greek word isos - same; morphe - form) constitutes a philosophical category, a one-to-one correspondence between structures of objects [1][2]. Such a one-to-one correspondence can only exist between abstract, idealized objects.

In mathematics we define isomorphism as a one-to-one mapping of one system onto another system, which preserves the structure, i.e. relations, ordering, topology etc., of the systems. For example: isomorphism of graphs (to be defined below), ordered sets, groups, vector spaces and other algebraic structures; the image of a mapping and its mathematical expression. Isomorphism is an invertible morphism, which has an opposite morphism, such that their product is the unity morphism. A topological isomorphism is called a homeomorphism.

Structure (Latin word structura - building) is also a philosophical category, that is defined as an unchangeable, constant connection, relation or organization form of the elements of a system [1][3]. In other words, structure is an abstraction of the system, its "skeleton", where its elements and relations (connections) are abstracted from their empirical meanings and what remains is only an elementary set of their organizing properties, such as connectivity, regularity, symmetry etc. Mathematical means, concepts and methods are the most appropriate "langue" for the expression of structure. With the concept of structure is due a special, but at the same time universal, relation type - composition - that can be expressed by mathematical formulas, equations, matrices, graphs etc. The differences of structural elements are expressed by their conjugacy mode - positions - in the structure. The exact definition of structure can be give by concept of the isomorphism. Since structure is a formation of related (connected) elements, it may be represented by a graph. Immanuel Kant and Georg Wilhelm Friedrich Hegel are often regarded as the originators of the structure concept.

The isomorphism problem is to design an algorithm that recognizes the isomorphism of two objects. The graph isomorphism problem first came into prominence in 1857, when Arthur Cayley reported his research on organic isomers. Subsequently, isomorphism became a central problem in graph theory. According to the "2000 Mathematics Subject Classification" (MSC2000), isomorphism recognition together with the reconstruction problem, is a combinatorial phenomenon 05 C 60 , even when graph theory itself is not yet classified as a separate subject!

Two graphs are called isomorphic, if they differ only in the labeling of their vertices. An isomorphic mapping from graph $\boldsymbol{G}_{\boldsymbol{A}}$ to graph $\boldsymbol{G}_{\boldsymbol{B}}$ is an isomorphic substitution $\varphi: \boldsymbol{V}_{\boldsymbol{A}} \rightarrow \boldsymbol{V}_{\boldsymbol{B}}$

$$
\begin{array}{cccccc}
\boldsymbol{v}_{1} & \boldsymbol{v}_{2} & \ldots & \boldsymbol{v}_{i} & \ldots & \boldsymbol{v}_{\boldsymbol{n}} \\
\varphi\left(\boldsymbol{v}_{1}\right) & \varphi\left(\boldsymbol{v}_{2}\right) & \ldots & \varphi\left(\boldsymbol{v}_{\boldsymbol{i}}\right) & \ldots & \varphi\left(\boldsymbol{v}_{\boldsymbol{n}}\right)
\end{array}
$$

Isomorphism recognition is an answer to the question, is graph $\boldsymbol{G}_{\boldsymbol{A}}$ isomorphic to graph $\boldsymbol{G}_{\boldsymbol{B}}$ ? If so, one must also provide the isomorphic substitution. On the structural aspect we can be say that graphs $\boldsymbol{G}_{\boldsymbol{A}}$ and $\boldsymbol{G}_{\boldsymbol{B}}$ are isomorphic if and only if these have one and the same structure.

A naïve algorithm for isomorphism recognition obviously exists - try all possible substitutions (permutations) of the rows and columns of the adjacency matrix of $\boldsymbol{G}_{\boldsymbol{B}}$ until it coincides with adjacency matrix of graph $\boldsymbol{G}_{\boldsymbol{A}}$. However, this is an impossible task to perform for all practical purposes, since the number of permutations that one may need to check can go up to $\boldsymbol{n}$ ! ( $\boldsymbol{n}$ factorial). For example, checking 16! permutations could take up to 40 years of time on the fastest computers presently available.

We must then begin to seek other, more useful ways for isomorphism testing. Ideally, we should try to find a polynomial-time algorithm for the graph isomorphism problem. That is, we should try to show that the graph isomorphism problem in P. During the 1970's, this was a very popular research activity. For example, S. Toida [4] presents for this purpose the concept of a "distance matrix". Non-isomorphism can be recognized by distance matrices "almost always", and isomorphism testing is possible in many cases, but not always.

Algorithms of this period were heavily criticized by R. C. Read, D. G. Corneil [5] and G. Gati [6], who called this "hobby" the "isomorphism disease". The isomorphism problem became taboo during this period. This problem is avoided in some graph textbooks to this day. For example, B. Bollobas' "Modern Graph Theory" [7] dedicates only two words for the isomorphism problem. Nevertheless, a small visual example of graph isomorphism is presented in almost all textbooks - and nothing more is said.

There are numerous monographs dedicated specially to the isomorphism problem. The aspect of group theory was treated by C. Hoffmann [8], who asserted that the "structure" of groups was quite similar to the general isomorphism problem. Unfortunately, this similarity turned out to be elusive. The isomorphism problem is treated in great depth by Netchepurenko et al [9] where they also present corresponding algorithms and computer programs that work "almost always". In the monograph by G. Köbler, H. Schönig and J. Toran [10] this problem is treated on the basis of structural complexity.

Without good algorithms, the treatment of the isomorphism problem is senseless. Some partial progress was made by L. Babai [11], who found that in certain cases a Monte-Carlo algorithm is suitable. G. Tinhofer, M. Lödeke, S. Baumann, L. Babel [12] feel convinced that isomorphism testing is solvable by Weisfeiler-Leman algorithm. Vidya Raj and M. S. Shivakumar [13], give some attributes for solving the problem under certain conditions. At the same time, some monographs of algorithmic graph theory, such as N. Chistofiedes [14], have nothing to say about isomorphism. S. Pemmaraju and S. Skiena [15] are limited to studying time complexity of the isomorphism problem.

The isomorphism problem has mostly been studied just on the complexity aspect [16]. It is not known whether this problem is NP-complete. Whereas nobody found any polynomial-time solutions in $\mathbf{P}$ before us, it has been presented as an intermediary variant, marked SPP [17].

The methods of isomorphism recognition can be divides to: a) sorting or non-sorting methods; and, b) methods with using local or global invariants.

An invariant is an attribute of an object, such as a size, form of an expression etc., which stays unchangeable in case of certain transformations, i.e. it is an invariant in relation to these
transformations. For example, local invariants can be degrees of the vertices, distances between vertices, pair signs etc. Similarly, global invariants can be a degree frequency vector, various codes, polynomials, spectrums etc. of a graph. If the observed transformation does not change some attribute of an object, then it is a complete invariant [18]. For example, a complete invariant of isomorphic graphs is their common structure that does not change in case of relabelling (remarking) and/or transposition of their vertices.

The concept of invariants has been used in mathematics since the middle of the $19^{\text {th }}$ century. Invariant theory had great importance in geometry. Invariant theory is treated classically as an algebraic theory [19]. Later, this specific concept was promoted to a philosophical category.

According to F. Harary [18], the isomorphism problem is solvable by complete system of global invariants (polynomials, spectra) of graphs. S. Locke [20] found that 3-cube-codes (super-long binary codes) are sometimes useful for isomorphism testing. From A. Zykov's point of view [21], the isomorphism problem is solvable on the basis of a system of local invariants that characterize the compactness, cycles (girths), paths etc., of a graph.

In our historical journey so far, the question remains: is the graph isomorphism problem in $\boldsymbol{P}$ ? Clearly, some essential ideas are still missing.

### 1.2. An Approach: Structure Semiotics

Semiotics is the study of sign processes, or signification and communication, signs and symbols, both individually and grouped into sign systems. It includes the study of how meaning is constructed and understood.

A sign is an entity which signifies another entity. A natural sign is an entity which bears a causal relation to the signified entity, as thunder is a sign of a storm. A conventional sign signifies by agreement, as a full stop signifies the end of a sentence. Semiotics, epistemology, logic, and philosophy of language are concerned about the nature of signs, what they are and how they signify.

As far back as 1938, H. Hermes [22] was of the view that semiotics was a discipline suitable for exploring the very foundations of mathematics. Structure semiotics or semiotics of structure [23] is a research domain at the frontiers of graph theory and semiotics, where the subject of investigation is the structure (i.e. graph) as such. It is a complex of heuristic methods for exploring structure and its attributes. From the philosophical point of view, it is an objectoriented study of semiotics.

Structure semiotics treats structural invariants (codes, vectors) on their meaning aspect, i.e. treats them as signs. The pair signs characterize the shortest paths, girths, cliques, bridges etc of a graph. Their systems in the form of a sign matrix $\boldsymbol{S}$ constitute a text of the structure of a graph. Structure can be recognized and investigated just by its sign matrix [23].

The isomorphism problem is solvable on the grounds of structure semiotics, as a complete invariant of a graph in the form of its sign matrix $\boldsymbol{S}$. The first step in our graph isomorphism algorithm, cf. procedures 2.3.1, 2.3.2 and 2.3.3, is to compute the sign matrices of the given graphs in polynomial-time.

### 1.3. The Symmetry Problem

When we compute the sign matrices of isomorphic graphs, the sets of row and column sign frequency vectors are always the same. The second step in our graph isomorphism algorithm, cf. procedure 2.3.3, is to arrange the sign frequency vectors in lexicographic order to obtain the canonical forms of the sign matrices of the given graphs. The vertices of the graphs are partitioned into equivalence classes or orbits. For isomorphic graphs, the unordered sets of orbits are always the same. These constitute important attributes of structure and are directly connected with symmetry properties of the graphs.

Symmetry (A) (Greek word symmetria) is a structural attribute that is expressed as a regular repetition (recurrence) of similar components (parts, particles) of an object in space and/or time [1].

Unfortunately, there is a commonly restricted understanding of symmetry as a "stump" of the full definition of symmetry (A):

Symmetry (B) is a property of an object, where the components that are placed at the same distance from a centre or axis are similar [3].

Both concepts are valid, and we may say that (B) is an "axle-symmetry" only.
Symmetry has the status of a philosophical category in countries of Mainland-Europe. However, in Anglo-Saxon countries, and also in Estonia, symmetry has not yet been assigned such an honour [24][25].

The general concept of symmetry (A) in mathematics is defined as the existence of the transitivity domain of authomorphisms or orbits in Aut $\boldsymbol{G}$, for example in a graph $\boldsymbol{G}$. An orbit is essentially an equivalence class. Symmetry is measurable. Its value is maximum, if there exists only one orbit and its value is 0 , if the number of orbits corresponds to the number of elements. The general concept of symmetry is used in graph theory, structure-semiotics, arts etc.

The main symmetry properties of graphs are: a) vertex symmetry, if there exist only a vertex orbit; b) edge symmetry, if there exist only an edge orbit; c) bisymmetry, if there exist only an edge orbit and only a "non-edge" orbit, i.e. an orbit of disadjacent vertex pairs,

So far, our graph isomorphism algorithm computes the canonical forms of the sign matrices of the given graphs in polynomial-time. However, it may still happen that the canonical forms of the obtained sign matrices do not coincide for isomorphic graphs. Finally, we define a polynomial-time procedure 2.3.4, that reorders the rows and columns of the sign matrices to guarantee coincidence in the case of isomorphic graphs. Hence, we can say that the canonical form of the sign matrix is uniquely identifiable in polynomial-time for isomorphic graphs.

To summarize, we prove that our graph isomorphism algorithm is necessary and sufficient for solving the graph isomorphism problem: if graphs $G_{A}$ and $G_{B}$ are isomorphic, then the algorithm finds an explicit isomorphism function; if graphs $G_{A}$ and $G_{B}$ are not isomorphic, then the algorithm determines that no isomorphism function can exist. Finally, we show that the algorithm has polynomial-time complexity. Thus, we prove that the Graph Isomorphism Problem is in $\mathbf{P}$.

## 2. THE GRAPH ISOMORPHISM PROBLEM IS IN P

We are pleased to announce the discovery of a new polynomial-time algorithm for determining whether two given graphs are isomorphic or not.

### 2.1. Introduction

One of the most fundamental problems in graph theory is the Graph Isomorphism Problem: given two graphs $G_{A}$ and $G_{B}$, are they isomorphic? Graphs $G_{A}$ and $G_{B}$ are said to be isomorphic if their vertices can be rearranged so that the corresponding edge structure is exactly the same. To show that graphs $G_{A}$ and $G_{B}$ are isomorphic, it suffices to find one such rearrangement of vertices. On the other hand, to show that $G_{A}$ and $G_{B}$ are not isomorphic, one must prove that no such rearrangement of vertices can exist. Without a good algorithm, this problem can be very difficult to solve even for relatively small graphs.


Figure 2.1.1. Are graphs $G_{A}$ and $G_{B}$ isomorphic?
We present a new polynomial-time GRAPH ISOMORPHISM ALGORITHM for determining whether two given graphs are isomorphic or not. If the given graphs are isomorphic, the algorithm finds an explicit isomorphism function in polynomial-time. In Section 2.2, we provide precise DEFINITIONS of all the terminology used and introduce the essential concept of a sign matrix according to the semiotic theory for the recognition of graph structure. In Section 2.3, we present a formal description of the ALGORITHM followed by an example to show how the algorithm works step-by-step. In Section 2.4, we prove that the algorithm is NECESSARY AND SUFFICIENT for solving the Graph Isomorphism Problem: if graphs $G_{A}$ and $G_{B}$ are isomorphic, then the algorithm finds an explicit isomorphism function; if graphs $G_{A}$ and $G_{B}$ are not isomorphic, then the algorithm determines that no isomorphism function can exist. In Section 2.5 , we show that the algorithm has polynomial-time complexity. Thus, we prove that the Graph Isomorphism Problem is in P. In Section 2.6, we provide an IMPLEMENTATION of the algorithm as a C++ program, together with demonstration software for Microsoft Windows.

### 2.2. Definitions

To begin with, we present elementary definitions of all the terminology used, following [26]. Thereafter, we introduce the essential concept of a sign matrix according to the semiotic theory for the recognition of graph structure, following [27].

A finite simple graph $G$ consists of a set of vertices $V$, with $|V|=n$, and a set of edges $E$, such that each edge is an unordered pair of distinct vertices. The definition of a simple graph $G$ forbids loops (edges joining a vertex to itself) and multiple edges (many edges joining a pair of vertices), whence the set $E$ must also be finite, with $|E|=m$. We label the vertices of $G$ with the integers $1,2, \ldots, n$. If the unordered pair of vertices $\{u, v\}$ is an edge in $G$, we say that $u$ is adjacent to $v$ and write $u v \in E$. Adjacency is a symmetric relationship: $u v \in E$ if and only if $v u$ $\in E$. The degree of a vertex $v$ is the number of vertices that are adjacent to $v$. A $(u, v)$-path $P$ in $G$ is a sequence of distinct vertices $u=v_{1}, v_{2}, \ldots, v_{k}=v$ such that $v_{i v i+1} \in E$ for $i=1,2, \ldots, k-1$. If such a $(u, v)$-path $P$ exists, then the vertices $u$ and $v$ are said to be connected by a path of length $k-1$. Given any pair of vertices $(u, v)$ in $G$, we define the distance

$$
\begin{aligned}
& d(u, v)=0, \text { if } u=v, \\
& d(u, v)=\text { the length of a shortest }(u, v) \text {-path, if } u \text { and } v \text { are connected, and } \\
& d(u, v)=\infty, \text { otherwise. }
\end{aligned}
$$

We now introduce the key ingredients of semiotic theory. For any pair of vertices $(u, v)$ in $G$, the collateral graph $G \mid u v$ is defined as follows:

- If $u v \in E$, then $G \mid u v$ is obtained by deleting the edge $u v$ from $G$ while preserving all the vertices of $G$. We use the binary sign + to distinguish the distance function in this case.
- If $u v \notin E$, then $G \mid u v=G$. We use the binary sign - to distinguish the distance function in this case.

The pair graph $G_{u v}$ for any pair of vertices $(u, v)$ in $G$ is defined as follows:

- $\quad w$ is a vertex of $G_{u v}$ if and only if $w$ belongs to a shortest $(u, v)$-path in $G \backslash u v$, and
- $w x$ is an edge of $G_{u v}$ if and only if $w x$ is also an edge of $G$.

For any pair of vertices $(u, v)$ in $G$, we write the $(u, v)$-sign, denoted by the symbol $s_{u v}$, as follows:

$$
s_{u v}= \pm d_{u v} \cdot \boldsymbol{n}_{u v} \cdot \boldsymbol{m}_{u v}
$$

where

- the leading binary sign is positive if $u v \in E$, or negative if $u v \notin E$;
- $d_{u v}$ is the distance $d(u, v)$ in the collateral graph $G \backslash u v$;
- $n_{u v}$ is the number of vertices of the pair graph $G_{u v}$
- $m_{u v}$ is the number of edges of the pair graph $G_{u v}$.

The sign matrix $S$ of the graph $G$ is written as an $n \times n$ array with the $(u, v)$-sign $s_{u v}$ as the entry in row $u$ and column $v$,

$$
S=\left[s_{u v}\right] .
$$

The adjacency matrix of $G$ is an $n \times n$ matrix with the entry in row $u$ and column $v$ equal to 1 if $u v \in E$ and equal to 0 if $u v \notin E$. Thus, the adjacency matrix of the graph $G$ can be recovered from the leading binary signs of the entries of the sign matrix $S$. Note that for a simple graph $G$, both the adjacency matrix and the sign matrix $S$ are symmetric. We shall now define a canonical form $S^{*}$ of the sign matrix by ordering the rows and columns of $S$ in a certain way. First, write the set of all distinct $(u, v)$-signs $s_{u v}$ in lexicographic order $s 1, s 2, \ldots, s r$. Then, for each row $i$ of the sign matrix, $i=1,2, \ldots, n$, compute the sign frequency vector

$$
f_{i}=\left(f_{i}^{(1)}, f_{i}^{(2)}, \ldots, f_{i}^{(r)}\right)
$$

Where $f_{i}^{(k)}$ is the number of times the sign $s k$ occurs in row $i$. Since $S$ is symmetric, the sign frequency vector for column $i$ is the same as the sign frequency vector for row $i$, for $i=1,2, \ldots$, $n$. Now, write the sign frequency vectors $f_{1}, f_{2}, \ldots, f_{n}$ in lexicographic order $f_{i_{1}}, f_{i_{2}}, \ldots, f_{i_{n}}$. Reorder the rows and columns of the sign matrix according to the permutation $i, i 2, \ldots, i_{n}$ of the vertices $1,2, \ldots, n$ of $G$ to obtain the canonical form $S^{*}$ of the sign matrix.

The vertices of $G$ are partitioned into equivalence classes consisting of vertices with the same sign frequency vectors. Thus, the canonical form $S^{*}$ of the sign matrix is uniquely defined only upto permutations of vertices within each equivalence class.

Graphs $G_{A}$ and $G_{B}$ are said to be isomorphic if there exists a bijection

$$
\varphi: V_{A} \rightarrow V_{B}
$$

from the vertices of graph $G_{A}$ to the vertices of graph $G_{B}$, such that $u v$ is an edge in graph $G_{A}$ if and only if $\varphi(u) \varphi(v)$ is an edge in graph $G_{B}$. The graph isomorphism problem is to determine whether two given graphs are isomorphic or not.

An algorithm is a problem-solving method suitable for implementation as a computer program. While designing algorithms we are typically faced with a number of different approaches. For small problems, it hardly matters which approach we use, as long as it is one that solves the problem correctly. However, there are many problems for which the only known algorithms take so long to compute the solution that they are practically useless. For instance, the naïve approach of computing all $n$ ! possible permutations of the $n$ vertices to show that a pair of graphs $G_{A}$ and $G_{B}$ are not isomorphic is impractical even for small inputs.

A polynomial-time algorithm is one whose number of computational steps is always bounded by a polynomial function of the size of the input. Thus, a polynomial-time algorithm is one that is actually useful in practice. The class of all problems that have polynomial-time algorithms is denoted by $\mathbf{P}$. If graphs $G_{A}$ and $G_{B}$ are isomorphic then they must have the same sign frequency vectors in lexicographic order ${ }_{i_{1}},{ }_{i} i_{2}, \ldots, f_{i_{n}}$ and we shall show that our algorithm obtains identical canonical forms of their sign matrices $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ in polynomial time, thus exhibiting an explicit isomorphism function $\varphi$. Conversely, we shall show that our algorithm determines in polynomial-time that the sign matrices $S_{A} *$ and $S_{B}{ }^{*}$ cannot be expressed in identical canonical forms if and only if the graphs $G_{A}$ and $G_{B}$ are not isomorphic. Thus, we have a polynomial-time algorithm for solving the graph isomorphism problem, showing that the graph isomorphism problem is in $\mathbf{P}$.

### 2.3. Algorithm

We are now ready to present a formal description of the algorithm. After that, the steps of the algorithm will be illustrated by an example. We begin by defining four procedures.
2.3.1. Procedure. This procedure is Dijkstra's algorithm [28]. Given a graph $G$ and a vertex $u$, we compute shortest $(u, v)$-paths to all vertices $v$ of $G$. Define $a(u, v)=1$ if $u v \in E$ and $a(u, v)=$ $\infty$ if $u v \notin E$. We maintain a set $V_{\text {known }}$ of vertices to which the shortest $(u, v)$-path is known and a tentative distance $d^{\prime}(u, w)$ for each vertex $w$ outside $V_{\text {known }}$.

- Initialization: Set $V_{\text {known }}=\{u\}, d(u, u)=0$ and $d^{\prime}(u, w)=a(u, w)$ for each vertex $w$ outside $V_{\text {known }}$.
- Iteration: Select a vertex $w_{\text {min }}$ outside $V_{\text {known }}$ such that $d^{\prime}\left(u, w_{\text {min }}\right)$ is a minimum. Add $w_{\text {min }}$ to $V_{\text {known }}$ and update the tentative distance $d^{\prime}(u, w)=\min \left\{d^{\prime}(u, w), d(u, w)+\right.$ $a(u, w)\}$ for each vertex $w$ outside $V_{\text {known }}$.
- Termination: Iterate until $V_{\text {known }}$ contains all the vertices of $G$ or until $d^{\prime}(u, w)=\infty$ for each vertex $w$ outside $V_{\text {known }}$. In the later case, no further vertex can be selected and the remaining vertices are not connected to the vertex $u$.
2.3.2. Procedure. Given a graph $G$ and vertices $u$ and $v$, we compute the distance $d(u, v)$ in the collateral graph $G \mid u v$ and the pair graph $G_{u v}$.
- Using Procedure 2.3.1, compute shortest $(u, x)$-paths to all vertices $x$ of $G \mid u v$.
- Using Procedure 2.3.1, compute shortest $(v, y)$-paths to all vertices $y$ of $G \mid u v$.
- In particular, the length of any shortest $(u, v)$-path in $G \backslash u v$ is the distance $d(u, v)$.
- If $u=u_{1}, u_{2}, \ldots, u_{r}$ and $v=v_{1}, v_{2}, \ldots, v_{s}$ are shortest paths found above such that $u_{r}=v_{s}$ and the sum of the lengths of the two paths is the distance $d(u, v)$ in the collateral graph $G \backslash u v$, then the union of vertices of the two paths are vertices of the pair graph $G_{u v}$. Every vertex $w$ of the pair graph $G_{u v}$ is obtained this way, because any shortest $(u, v)$-path containing $w$ is obtained by connecting some shortest ( $u, w$ )-path with some shortest ( $w$, $v$ )-path in $G \mid u v$. Thus, at least one pair of shortest paths found above must satisfy $u_{r}=v_{s}$ $=w$, for each vertex $w$ of the pair graph $G_{u v}$.
2.3.3. Procedure. Given a graph $G$, we compute the sign matrix $S$ and its canonical form $S^{*}$.
- Using Procedure 2.3.2, for every pair of vertices $u$ and $v$, we compute the distance $d(u, v)$ in the collateral graph $G \backslash u v$ and the pair graph $G_{u v}$.
- The entry in row $u$ and column $v$ of the sign matrix $S$ is $s_{u v}= \pm d_{u v} \cdot n_{u v} \cdot m_{u v}$, where the leading binary sign is positive if $u v \in E$, and negative if $u v \notin E ; d_{u v}$ is the distance $d(u$, $v$ ) in the collateral graph $G \backslash u v ; n_{u v}$ is the number of vertices of the pair graph $G_{u v}$; and $m_{u v}$ is the number of edges of the pair graph $G_{u v}$.
- Write the set of all distinct signs $s_{u v}$ in lexicographic order $s_{1}, s_{2}, \ldots, s_{r}$.
- For each row $i$ of the sign matrix $S, i=1,2, \ldots, n$, compute the sign frequency vector $f_{i}=\left(f_{i}^{(1)}, f_{i}^{(2)}, \ldots, f_{i}^{(r)}\right)$, where $f_{i}^{(k)}$ is the number of times the sign $s_{k}$ occurs in row $i$. Since $S$ is symmetric, the sign frequency vector for column $i$ is the same as the sign frequency vector for row $i$, for $i=1,2, \ldots, n$.
- Write the sign frequency vectors $f_{1}, f_{2}, \ldots, f_{n}$ in lexicographic order ${ }_{i_{1}}, f_{i_{2}}, \ldots, f_{i_{n}}$.
- Reorder the rows and columns of the sign matrix according to the permutation $i_{1}, i_{2}, \ldots, i_{n}$ of the vertices $1,2, \ldots, n$ of $G$ to obtain the canonical form $S^{*}$.
2.3.4. Procedure. Given graphs $G_{A}$ and $G_{B}$ such that the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ are the same, $\left({ }_{A} i_{1},{ }_{A} i_{2}, \ldots,{ }_{A} i_{n}\right)=\left({ }_{B} i^{\prime}{ }_{1},{ }_{B} i^{\prime}{ }_{2}, \ldots,{ }_{B} i^{\prime}{ }_{n}\right)$, we compute a reordering $i^{\prime \prime}{ }_{1}, i^{\prime \prime}{ }_{2}, \ldots, i^{\prime \prime}{ }_{n}$ of the vertices of $G_{B}$ such that either the first entry of $S_{B}{ }^{*}$ that does not match the corresponding entry of $S_{A}{ }^{*}$ occurs at the greatest possible index in row major order or $S_{A} *=S_{B}{ }^{*}$.
- $\operatorname{Set} A=S_{A}{ }^{*}$ and $B=S_{B}{ }^{*}$.
- Read the matrices $A$ and $B$ in row major order (read each row from left to right and read the rows from top to bottom). If all corresponding entries $A_{i j}$ and $B_{i j}$ of $A$ and $B$ match, then stop. Else, find the first entry $B_{i j}$ in $B$ that does not match the corresponding entry $A_{i j}$ in $A$. Find $k>i$ such that interchanging rows $(k, j)$ and columns $(k, j)$ of $B$ ensures that the first mismatch occurs later than $B_{i j}$ in row major order (or there is no mismatch at all). If no such $k$ exists, then stop. Repeat this process until the corresponding $k$ cannot be found or all corresponding entries of $A$ and $B$ match.
- We obtain a reordering $i^{\prime \prime}{ }_{1}, i^{\prime \prime}{ }_{2}, \ldots, i^{\prime \prime}{ }_{n}$ of the vertices of $G_{B}$ such that either the first entry of $B$ that does not match the corresponding entry of $A$ occurs at the greatest possible index in row major order or $A=B$.
2.3.5. Algorithm. Given graphs $G_{A}$ and $G_{B}$, we determine whether $G_{A}$ and $G_{B}$ are isomorphic or not. If $G_{A}$ and $G_{B}$ are isomorphic, we exhibit an explicit isomorphism function.
- Using Procedure 2.3.3, we compute the canonical forms of the sign matrices $S_{A} *$ and $S_{B}{ }^{*}$. If the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ are different, then $G_{A}$ and $G_{B}$ are not isomorphic and we stop.
- Else, the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ are the same, ( $\left.f_{A} i_{1},{ }_{A}{ }_{A} i_{2}, \ldots,{ }_{A} i_{n}\right)=\left({ }_{B}{ }_{B} i^{\prime},{ }_{1},{ }_{B} i^{\prime}{ }_{2}, \ldots,{ }^{f}{ }_{B} i^{\prime}{ }_{n}\right)$.
o For $k=1,2, \ldots, n$ :
- Set $A=S_{A}{ }^{*}$ and $B=S_{B}{ }^{*}$.
- Interchange rows $(1, k)$ and columns $(1, k)$ of $B$.
- Using Procedure 3.4, if $A=B$ then stop. Else, start with the next value of $k$. If $k=n$ then stop.
o If $A \neq B$, then $G_{A}$ and $G_{B}$ are not isomorphic. Else $A=B, G_{A}$ and $G_{B}$ are isomorphic and the reordering $i^{\prime \prime}, i^{\prime \prime}{ }_{2}, \ldots, i^{\prime \prime}{ }_{n}$ of the vertices of $G_{B}$ to obtain $S_{B} *=B$ provides an explicit isomorphism function $\varphi\left(i_{1}\right)=i^{\prime \prime}{ }_{1}, \varphi\left(i_{2}\right)=i^{\prime \prime}{ }_{2}, \ldots, \varphi\left(i_{n}\right)$ $=i^{\prime \prime}{ }_{n}$.
2.3.6. Example. We demonstrate the steps of the algorithm with an example. The input consists of Turán [29] graphs $G_{A}$ and $G_{B}$, with vertices labeled $V_{A}=\{1,2,3,4,5,6,7,8\}$ and $V_{B}=\{1,2$, 3, 4, 5, 6, 7, 8$\}$ as shown below in Figure 2.3.6.1.


Figure 2.3.6.1. An example to demonstrate the steps of the algorithm : input

The algorithm first computes all the pair graphs of $G_{A}$. To see how this is done, let us explicitly compute the pair graph $G_{12}$ for the pair of vertices (1, 2). First, Procedure 2.3.2 computes the shortest paths from vertex 1 in $G_{A} \mid 12$ as (1), (1, 7, 2), ( $1,7,3$ ), (1, 7), (1, 8), $(1,4),(1,5)$ and $(1,6)$. Then, Procedure 2.3.2 computes the shortest paths from vertex 2 in $G_{A} \backslash 12$ as $(2),(2,7,1),(2,7,3),(2,7),(2,8),(2,4),(2,5)$ and $(2,6)$. The distance $d(1,2)=2$ is given by the length of any shortest $(1,2)$-path found in $G_{A} \backslash 12$ so far. Now, Procedure 2.3.2 obtains the shortest $(1,2)$-paths $(1,7,2),(1,8,2),(1,4,2),(1,5,2)$ and $(1,6,2)$ whose union gives the 7 vertices of the pair graph $\{1,2,4,5,6,7,8\}$. The pair graph has 16 edges $\{1,7\}$, $\{1,8\},\{1,4\},\{1,5\},\{1,6\},\{2,7\},\{2,8\},\{2,4\},\{2,5\},\{2,6\},\{7,4\},\{7,5\},\{8,4\},\{8,5\},\{4,6\}$ and $\{5,6\}$. Since $\{1,2\}$ is not an edge in $G_{A}$, the leading binary sign is negative and Procedure 2.3.3 computes the sign $s_{12}=-2.7 .16$. Similarly, Procedure 2.3.3 computes all the signs $s_{i j}$ for $i, j$ $=1,2,3,4,5,6,7,8$. Note that for $i=j$ the sign is always -0.1 .0 . Thus, Procedure 2.3.3 computes the sign matrix $S_{A}$. Then, Procedure 2.3.3 counts the number of times each sign occurs in a column of $S_{A}$ and obtains the sign frequency vectors for each column of $S_{A}$. Finally, Procedure 2.3.3 reorders the rows and columns of $S_{A}$ according to the lexicographic order of the sign frequency vectors, to obtain the canonical form of the sign matrix $S_{A}{ }^{*}$. We use the following convention to display the sign matrix: the row and column headers show the vertex labels and the equivalence classes of vertices are distinguished by different shades of blue; the sign frequency vectors, vertex degrees and equivalence class numbers are displayed along the column footers.

| $S_{A}{ }^{*}$ | 4 | 5 | 1 | 2 | 3 | 7 | 8 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | -0.1.0 | -2.8.21 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 |
| 5 | -2.8.21 | -0.1.0 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 |
| 1 | +2.5.7 | +2.5.7 | -0.1.0 | -2.7.16 | -2.7.16 | +2.4.5 | +2.4.5 | +2.4.5 |
| 2 | +2.5.7 | +2.5.7 | -2.7.16 | -0.1.0 | -2.7.16 | +2.4.5 | +2.4.5 | +2.4.5 |
| 3 | +2.5.7 | +2.5.7 | -2.7.16 | -2.7.16 | -0.1.0 | +2.4.5 | +2.4.5 | +2.4.5 |
| 7 | +2.5.7 | +2.5.7 | +2.4.5 | +2.4.5 | +2.4.5 | -0.1.0 | -2.7.16 | -2.7.16 |
| 8 | +2.5.7 | +2.5.7 | +2.4.5 | +2.4.5 | +2.4.5 | -2.7.16 | -0.1.0 | -2.7.16 |
| 6 | +2.5.7 | +2.5.7 | +2.4.5 | +2.4.5 | +2.4.5 | -2.7.16 | -2.7.16 | -0.1.0 |
| Signs | 4 | 5 | 1 | 2 | 3 | 7 | 8 | 6 |
| -2.7.16. | 0 | 0 | 2 | 2 | 2 | 2 | 2 | 2 |
| -2.8.21. | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| -0.1.0. | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| +2.4.5. | 0 | 0 | 3 | 3 | 3 | 3 | 3 | 3 |
| +2.5.7 | 6 | 6 | 2 | 2 | 2 | 2 | 2 | 2 |
| Degrees | 6 | 6 | 5 | 5 | 5 | 5 | 5 | 5 |
| Classes | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 |

Similarly, Procedure 2.3 .3 obtains the canonical form of the sign matrix $S_{B}{ }^{*}$ :

| $S_{B}{ }^{*}$ | 1 | 8 | 7 | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | -0.1.0 | -2.8.21 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 |
| 8 | -2.8.21 | -0.1.0 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 | +2.5.7 |
| 7 | +2.5.7 | +2.5.7 | -0.1.0 | +2.4.5 | -2.7.16 | +2.4.5 | +2.4.5 | -2.7.16 |
| 2 | +2.5.7 | +2.5.7 | +2.4.5 | -0.1.0 | +2.4.5 | -2.7.16 | -2.7.16 | +2.4.5 |
| 3 | +2.5.7 | +2.5.7 | -2.7.16 | +2.4.5 | -0.1.0 | +2.4.5 | +2.4.5 | -2.7.16 |
| 4 | +2.5.7 | +2.5.7 | +2.4.5 | -2.7.16 | +2.4.5 | -0.1.0 | -2.7.16 | +2.4.5 |
| 5 | +2.5.7 | +2.5.7 | +2.4.5 | -2.7.16 | +2.4.5 | -2.7.16 | -0.1.0 | +2.4.5 |
| 6 | +2.5.7 | +2.5.7 | -2.7.16 | +2.4.5 | -2.7.16 | +2.4.5 | +2.4.5 | -0.1.0 |
| Signs | 1 | 8 | 7 | 2 | 3 | 4 | 5 | 6 |
| -2.7.16. | 0 | 0 | 2 | 2 | 2 | 2 | 2 | 2 |
| -2.8.21. | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| -0.1.0. | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| +2.4.5. | 0 | 0 | 3 | 3 | 3 | 3 | 3 | 3 |
| +2.5.7. | 6 | 6 | 2 | 2 | 2 | 2 | 2 | 2 |
| Degrees | 6 | 6 | 5 | 5 | 5 | 5 | 5 | 5 |
| Classes | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 |

Next, the algorithm checks that the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ are the same,

$$
\begin{gathered}
\left({ }_{A}^{f} 4,{ }_{A}^{f} 5,{ }_{A}^{f} 1,{ }_{A}^{f} 2,{ }_{A}^{f} 3,{ }_{A}^{f} 7,{ }_{A} 8,{ }_{A} 6\right)=\left({ }_{B}^{f} 1,{ }_{B} 8,{ }_{B}{ }_{B} 7,{ }_{B} 3,{ }_{B} 6,{ }_{B} 4,{ }_{B} 5,{ }_{B} 2\right)= \\
=(01106,01106,20132,20132,20132,20132,20132,20132) .
\end{gathered}
$$

Finally, the algorithm runs through the loop $k=1,2,3,4,5,6,7,8$ to find an explicit isomorphism if it exists. Starting with $k=1$, set $A=S_{A}{ }^{*}$ and $B=S_{B}{ }^{*}$ :

| Matrix $A$ | 4 | 5 | 1 | 2 | 3 | 7 | 8 | 6 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 4 | -0.1 .0 | -2.8 .21 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 5 | -2.8 .21 | -0.1 .0 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 1 | +2.5 .7 | +2.5 .7 | -0.1 .0 | -2.7 .16 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 2 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -0.1 .0 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 3 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -2.7 .16 | -0.1 .0 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 7 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -0.1 .0 | -2.7 .16 | -2.7 .16 |
| 8 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -0.1 .0 | -2.7 .16 |
| 6 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -2.7 .16 | -0.1 .0 |


| Matrix B | 1 | 8 | 7 | 2 | 3 | 4 | 5 | 6 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | -0.1 .0 | -2.8 .21 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 8 | -2.8 .21 | -0.1 .0 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 7 | +2.5 .7 | +2.5 .7 | -0.1 .0 | +2.4 .5 | -2.7 .16 | +2.4 .5 | +2.4 .5 | -2.7 .16 |
| 2 | +2.5 .7 | +2.5 .7 | +2.4 .5 | -0.1 .0 | +2.4 .5 | -2.7 .16 | -2.7 .16 | +2.4 .5 |
| 3 | +2.5 .7 | +2.5 .7 | -2.7 .16 | +2.4 .5 | -0.1 .0 | +2.4 .5 | +2.4 .5 | -2.7 .16 |
| 4 | +2.5 .7 | +2.5 .7 | +2.4 .5 | -2.7 .16 | +2.4 .5 | -0.1 .0 | -2.7 .16 | +2.4 .5 |
| 5 | +2.5 .7 | +2.5 .7 | +2.4 .5 | -2.7 .16 | +2.4 .5 | -2.7 .16 | -0.1 .0 | +2.4 .5 |
| 6 | +2.5 .7 | +2.5 .7 | -2.7 .16 | +2.4 .5 | -2.7 .16 | +2.4 .5 | +2.4 .5 | -0.1 .0 |

Since $k=1$, there is no initial interchange of rows and columns of $B$. Now, the algorithm uses Procedure 2.3.4. The entries of $A$ and $B$ are read in row major order. The first mismatch is found in the third row and fourth column, shown underlined. The algorithm finds that exchanging the fourth column with the fifth column (and the fourth row with the fifth row) of $B$ will push the first mismatch further along the row major order:

| Matrix B | 1 | 8 | 7 | 3 | 2 | 4 | 5 | 6 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | -0.1 .0 | -2.8 .21 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 8 | -2.8 .21 | -0.1 .0 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 7 | +2.5 .7 | +2.5 .7 | -0.1 .0 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 |
| 3 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -0.1 .0 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 |
| 2 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | -0.1 .0 | -2.7 .16 | -2.7 .16 | +2.4 .5 |
| 4 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -0.1 .0 | -2.7 .16 | +2.4 .5 |
| 5 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -2.7 .16 | -0.1 .0 | +2.4 .5 |
| 6 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -0.1 .0 |

The first mismatch is found in the third row and fifth column, shown underlined. The algorithm finds that exchanging the fifth column with the eighth column (and the fifth row with the eighth row) of $B$ will push the first mismatch further along the row major order:

| Matrix B | 1 | 8 | 7 | 3 | 6 | 4 | 5 | 2 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | -0.1 .0 | -2.8 .21 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 8 | -2.8 .21 | -0.1 .0 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 | +2.5 .7 |
| 7 | +2.5 .7 | +2.5 .7 | -0.1 .0 | -2.7 .16 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 3 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -0.1 .0 | -2.7 .16 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 6 | +2.5 .7 | +2.5 .7 | -2.7 .16 | -2.7 .16 | -0.1 .0 | +2.4 .5 | +2.4 .5 | +2.4 .5 |
| 4 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -0.1 .0 | -2.7 .16 | -2.7 .16 |
| 5 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -0.1 .0 | -2.7 .16 |
| 2 | +2.5 .7 | +2.5 .7 | +2.4 .5 | +2.4 .5 | +2.4 .5 | -2.7 .16 | -2.7 .16 | -0.1 .0 |

Now there is no mismatch, $A=B$. The algorithm exits the final loop and reports that an isomorphism has been found. The explicit isomorphism $\varphi$ is given by reading the vertex labels of $A$ and $B$ in this order:

| Graph $G_{A}$ | Graph $G_{B}$ |
| :--- | :--- |
| 4 | 1 |
| 5 | 8 |
| 1 | 7 |
| 2 | 3 |
| 3 | 6 |
| 7 | 4 |
| 8 | 5 |
| 6 | 2 |

If the graphs $G_{A}$ and $G_{B}$ are redrawn with vertices ordered in this way, the isomorphism $\varphi$ is easy to visualize.


Figure 2.3.6.2. An example to demonstrate the steps of the algorithm: output

### 2.4. Necessity and Sufficiency

Here we prove that the algorithm is necessary and sufficient for solving the Graph Isomorphism Problem:

- if graphs $G_{A}$ and $G_{B}$ are isomorphic, then the algorithm finds an explicit isomorphism function;
- if graphs $G_{A}$ and $G_{B}$ are not isomorphic, then the algorithm determines that no isomorphism function can exist.
2.4.1. Proposition. If graphs $G_{A}$ and $G_{B}$ are isomorphic, then the algorithm finds an isomorphism.

Proof. Suppose graphs $G_{A}$ and $G_{B}$ are isomorphic and let $\varphi: V_{A} \rightarrow V_{B}$ be an isomorphism from the vertices of $G_{A}$ to the vertices of $G_{B}$. Note that distances are preserved bijectively under the isomorphism,

$$
d(u, v)=d(\varphi(u), \varphi(v))
$$

for all vertices $u, v$ of $G_{A}$. Thus, all the corresponding pair graphs are isomorphic and the signs

$$
s_{u v}=s_{\varphi(u) \varphi(v)}
$$

are also preserved bijectively under the isomorphism for all vertices $u, v$ of $G_{A}$. Hence, the sign frequency vectors in lexicographic order for the canonical sign matrices $S_{A} *$ and $S_{B}{ }^{*}$ are the same,

$$
\left({ }_{A}^{f} i_{1},{ }_{A} i_{2}, \ldots,{ }_{A} i_{A} i_{n}\right)=\left({ }^{f}{ }_{B} i^{\prime} 1,{ }_{B},{ }_{B} i^{\prime}, \ldots,{ }^{\prime},{ }_{B} i^{\prime}{ }_{n}\right) .
$$

Since $\varphi$ is surjective, the algorithm finds a value of $k$ such that if vertex $v_{1}$ is the label of row 1 and column 1 of $A=S_{A} *$ then vertex $\varphi\left(v_{1}\right)$ is the label of row $k$ and column $k$ of $B=S_{B}^{*}$. Then, rows ( $1, k$ ) and columns ( $1, k$ ) of $B$ are interchanged. We now use induction on the rows of $B$ to show that Procedure 2.3.4 matches each row of $B$ with the corresponding row of $A$. For the base of the induction, consider row 1 of $B$. Since vertex $v_{1}$ is the label of row 1 of $A$ and $\varphi\left(v_{1}\right)$ is the label of row 1 of $B$, the corresponding sign frequency vectors are equal. By counting sign frequencies, as long as there is a mismatch in row 1 , it is always possible to interchange the columns of $B$ such that row 1 of $A$ and row 1 of $B$ are perfectly matched by Procedure 2.3.4. For the induction hypothesis, assume that rows $1, \ldots, t$ of $A$ and $B$ have been perfectly matched by Procedure 2.3.4 such that the vertex labels for the rows $1, \ldots, t$ of $A$ are $v_{1}, \ldots, v_{t}$ and the vertex labels for the rows $1, \ldots, t$ of $B$ are $\varphi\left(v_{1}\right)=v_{1}^{\prime}, \ldots, \varphi\left(v_{t}\right)=v_{t}^{\prime}$ respectively. Since the sign matrices are symmetric, Procedure 2.3.4 also ensures that the columns $1, \ldots, t$ of $A$ and $B$ are perfectly matched with the same vertex labels as the rows. Thus, the first entry $B_{i j}$ in $B$ that does not match the corresponding entry $A_{i j}$ in $A$ must now occur in row $i=t+1$ and column $j \geq t+1$. By the induction hypothesis, the subgraph $G_{A}{ }^{t}$ of $G_{A}$ with vertices $\left\{v_{1}, \ldots, v_{t}\right\}$ and the subgraph $G_{B}{ }^{t}$ of $G_{B}$ with vertices $\left\{\varphi\left(v_{1}\right)=v_{1}^{\prime}, \ldots, \varphi\left(v_{t}\right)=v_{t}^{\prime}\right\}$ are isomorphic under $\varphi$. Thus, there must be a vertex $v_{t+1}$ of $G_{A}$ outside the subgraph $G_{A}{ }^{t}$ such that the corresponding vertex $\varphi\left(v_{t+1}\right)$ of $G_{B}$ is outside the subgraph $G_{B}{ }^{t}$. Since there is a mismatch at the entry $B_{i j}$, the vertex $\varphi\left(v_{t+1}\right)$ must be the label for a column $j^{\prime}>j$. Hence, Procedure 2.3 .4 will always interchange rows $\left(j, j^{\prime}\right)$ and columns $\left(j, j^{\prime}\right)$ of $B$ and repeat the process until rows $i=$ $t+1$ of $A$ and $B$ are perfectly matched and the vertex label for row $t+1$ of $B$ is $\varphi\left(v_{t+1}\right)=v_{t+1}^{\prime}$. This completes the induction, showing that Procedure 2.3.4 matches each row of $B$ with the corresponding row of $A$. Thus, the algorithm finds an explicit isomorphism function $\varphi\left(v_{1}\right)=v_{1}^{\prime}$, $\ldots, \varphi\left(v_{n}\right)=v_{n}^{\prime}$.
2.4.2. Proposition. If graphs $G_{A}$ and $G_{B}$ are not isomorphic, then the algorithm determines that there cannot be an isomorphism.

Proof. Suppose graphs $G_{A}$ and $G_{B}$ are not isomorphic. The algorithm first computes the canonical forms of the sign matrices $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$. If the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}^{*}$ are different, then the algorithm concludes that $G_{A}$ and $G_{B}$ are not isomorphic. If the sign frequency vectors in lexicographic order for $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ are the same, ( $\left.{ }_{A} i_{1},{ }_{A}{ }_{A} i_{2}, \ldots,{ }_{A} i_{n}\right)=\left({ }_{B}{ }_{B} i^{\prime}{ }_{1},{ }_{B}{ }_{B} i^{\prime}{ }_{2}, \ldots,{ }_{B} i^{\prime}{ }_{n}\right)$, then the algorithm runs through the final loop for $k=1$, $2, \ldots, n$ and cannot find any isomorphism. By Proposition 2.4.1, if $G_{A}$ and $G_{B}$ were isomorphic, then the algorithm would have found an explicit isomorphism for some value of $k$. Therefore, the algorithm concludes that there cannot be an isomorphism.

From Propositions 2.4.1 and 2.4.2, we have
2.4.3. Theorem. The algorithm solves the Graph Isomorphism Problem.

### 2.5. Complexity

We shall now show that the algorithm terminates in polynomial-time, by specifying a polynomial of the larger of the two number of vertices $n$ of the input graphs, that is an upper bound on the total number of computational steps performed by the algorithm. Note that we consider

- checking whether a given pair of vertices is connected by an edge in $G_{A}$ or $G_{B}$, and
- comparing whether a given integer is less than another given integer
to be elementary computational steps. Thus, we shall show that the Graph Isomorphism Problem is in $\mathbf{P}$.
2.5.1. Proposition. Given a graph $G$ with $n$ vertices, Procedure 2.3 .1 takes at most $3 n^{2}+3 n$ steps to find shortest paths from an initial vertex $u$ to all other vertices.

Proof. Initialization takes at most $3 n$ steps. To find the minimum distance of an unknown vertex from the initial vertex $u$ takes at most $n$ steps and to update the tentative distances takes at most $n$ steps. There are at most $n$ iterations until all the vertices are known. Finally, it takes at most $n^{2}$ steps to recover the vertices of the shortest paths. Thus, Procedure 2.3.1 terminates after at most $3 n+n(n+n)+n^{2}=3 n^{2}+3 n$ steps.
2.5.2. Proposition. Given a graph $G$ with $n$ vertices, Procedure 2.3 .2 takes at most $7 n^{2}+7 n$ steps to compute the distance $d(u, v)$ in the collateral graph $G \mid u v$ and the pair graph $G_{u v}$ for a given pair of vertices $u$ and $v$.

Proof. The graph $G \mid u v$ also has $n$ vertices. By Proposition 2.5.1, Procedure 2.3.1 takes at most $3 n^{2}+3 n$ steps to find shortest paths from the initial vertex $u$ to all other vertices and at most $3 n^{2}$ $+3 n$ steps to find shortest paths from the initial vertex $v$ to all other vertices. Then it takes at most $n$ steps to determine the distance $d(u, v)$. Finally, it takes at most $n^{2}$ steps to run through pairs of shortest paths to find the vertices of the pair graph $G_{u v}$. Thus, Procedure 2.3.2 terminates after at most $3 n^{2}+3 n+3 n^{2}+3 n+n+n^{2}=7 n^{2}+7 n$ steps.
2.5.3. Proposition. Given a graph $G$ with $n$ vertices, Procedure 2.3 .3 takes at most $7 n^{4}+7 n^{3}+2 n^{2}$ steps to compute the canonical form of the sign matrix $S^{*}$.

Proof. By Proposition 2.5.2, for each pair of vertices it takes at most $7 n^{2}+7 n$ steps to compute the sign $s_{u v}$. Since there are $n^{2}$ signs, it takes at most $n^{2}\left(7 n^{2}+7 n\right)=7 n^{4}+7 n^{3}$ steps to compute the sign matrix $S$. Then it takes at most $n^{2}$ steps to compute the sign frequency vector and at most $n^{2}$ steps to sort it in lexicographic order. Thus, Procedure 2.3.3 terminates after at most $7 n^{4}$ $+7 n^{3}+n^{2}+n^{2}=7 n^{4}+7 n^{3}+2 n^{2}$ steps.
2.5.4. Proposition. Given a sign matrices $S_{A}{ }^{*}$ and $S_{B}{ }^{*}$ such that the sign frequency vectors in lexicographic order $\left({ }_{A}{ }_{A} i_{1},{ }_{A} i_{2}, \ldots,{ }_{A} i_{n}\right)=\left({ }_{B} i^{\prime} i^{\prime},{ }_{B}{ }_{B} i^{\prime}{ }_{2}, \ldots,{ }_{B} i_{B}{ }_{n}\right)$, Procedure 2.3.4 takes at most $2 n^{4}$ steps to terminate.

Proof. Since there are $n^{2}$ entries in $S_{B}{ }^{*}$, it takes at most $n^{2}$ steps to find a mismatch $(i, j)$ with the corresponding entry in $S_{A} *$ in row major order. Then, it takes at most $n^{2}$ steps along the row $i$ to find a column $j^{\prime}$ such that interchanging rows ( $j, j^{\prime}$ ) and columns $\left(j, j^{\prime}\right)$ leads to a mismatch later in the row major order. This may be repeated at most $n^{2}$ times until either the
corresponding interchange column $j^{\prime}$ cannot be found or all the entries in the sign matrices are perfectly matched. Thus, Procedure 2.3.4 terminates after at most $n^{2}\left(n^{2}+n^{2}\right)=2 n^{4}$ steps.
2.5.5. Proposition. Given graphs $G_{A}$ and $G_{B}$ with $n$ vertices, the algorithm takes at most $2 n^{5}+$ $14 n^{4}+14 n^{3}+4 n^{2}$ steps to terminate.

Proof. By Proposition 2.5.3, Procedure 2.3.3 takes at most $2\left(7 n^{4}+7 n^{3}+2 n^{2}\right)=14 n^{4}+14 n^{3}+$ $4 n^{2}$ steps to compute the canonical forms of the sign matrices $S_{A} *$ and $S_{B}{ }^{*}$. If the sign frequency vectors in lexicographic order $\left({ }_{A}{ }_{A} i_{1},{ }_{A} i_{2}, \ldots,{ }_{A} i_{n}\right)=\left({ }_{B}{ }_{B} i_{1},{ }^{f}{ }_{B} i^{\prime}{ }_{2}, \ldots,{ }_{B}{ }_{B} i_{n}{ }_{n}\right)$ are the same, then by Proposition 2.5.4 the final loop for $k=1,2, \ldots, n$ takes at most $n\left(2 n^{4}\right)=2 n^{5}$ steps. Thus, the algorithm terminates after at most $2 n^{5}+14 n^{4}+14 n^{3}+4 n^{2}$ steps.

From Theorem 2.4.3 and Proposition 2.5.5, we have
2.5.6. Theorem. The Graph Isomorphism Problem is in $\mathbf{P}$.

### 2.6. Implementation

We provide a demonstration program for the Graph Isomorphism Algorithm written in $C++$ for Microsoft Windows. The input consists of the files Graph A.txt and Graph B.txt containing the adjacency matrices of graph $G_{A}$ and graph $G_{B}$ respectively. The program computes the sign matrices $S_{A} *$ and $S_{B} *$ in canonical form and determines whether $G_{A}$ and $G_{B}$ are isomorphic or not, in polynomial-time.


Figure 2.6.1. A demonstration program for Microsoft Windows [download]

We show how to write the input for the computation performed in Example 2.3.6:


Figure 2.6.2. Input for the demonstration program
The $C++$ program is shown below:

| \#include <iostream> |
| :--- | :--- |
| \#include <fstream> |
| \#include <string> |
| \#include <vector> |
| \#include <map> |
| \#include <set> |
| \#include <algorithm> |
| using namespace std; |
| vector<vector<int\gg dijkstra(vector<vector<int\gg graph); |
| vector<vector<int\gg reindex(vector<vector<int\gg graph, vector<int> index); |
| vector<int> inv(vector<int> index); |
| vector<int> transform(map<vector<int>,vector<int\gg signmatrixA, |
| map<vector<int>,vector<int\gg signmatrixB, vector<int> vertexA, |
| vector<int> vertexB, vector<int> isoB); |
| ifstream infileA("graphA.txt"); |
| ifstream infileB("graphB.txt"); |
| ofstream outfile("result.txt"); |
| int main() |
| \{ |
| cout<<"The Graph Isomorphism Algorithm"<<endl; |
| cout<<"by Ashay Dharw adker and John-Tagore Tevet"<<endl; |
| cout<<"http://w w w.geocities.com/dharw adker/tevet/isomorphism"<<endl; |
| cout<<"Copyright (c) 2009"<<endl; |
| \& $\square$ |

Figure 2.6.3. A C++ program for the graph isomorphism algorithm [download]

The output of the program for the input in Figure 2.6.2 is shown in Example 2.3.6. The next section shows many more examples of input/output files. The download package also contains a visualizer for drawing graphs according to the output of the demonstration program.

## 3. PROCESSING RESULTS: EXAMPLES

We demonstrate the processing results of algorithm by solving the Graph Isomorphism Problem for several examples in cases of recognition the isomorphism and non-isomorphism.

### 3.1. Isomorphism Cases

We now demonstrate the Graph Isomorphism Algorithm for several examples of graphs in the hardest known cases.. The first set of examples 3.1.1-3.1.5 consists of isomorphic graphs whose vertices have been permuted randomly so that the isomorphism is well and truly hidden.
3.1.1. Example. We run the program on isomorphic Petersen [30] graphs A and B as input:

| Graph A |
| :---: |
| $\begin{array}{rlllllllll} 10 & & & & & & & \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \end{array}$ |
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The algorithm finds an explicit isomorphism, shown below.


Figure 3.1.1. The bisymmetric and strongly regular Petersen graphs are isomorphic
3.1.2. Example. We run the program on isomorphic Icosahedron [31] graphs $A$ and $B$ as input:

| Graph A |
| :---: |
| $\begin{array}{rlllllllllll} 12 & & & & & & & & & & & \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \end{array}$ |
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| Graph B |
| :---: |
| $\begin{array}{rrllllllllll} 12 & & & & & & & & & & & \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{array}$ |
|  |  |
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|  |  |

The algorithm finds an explicit isomorphism, shown below.


Figure 3.1.2. The vertex- and edge-symmetric Icosahedron graphs are isomorphic
3.1.3. Example. We run the program on isomorphic Ramsey [32] graphs $A$ and $B$ as input:

## Graph A

17
$\begin{array}{lllllllllllllllll}0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1\end{array}$

$1 \begin{array}{llllllllllllllll}1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1\end{array} 0$
$\begin{array}{lllllllllllllllll}0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1\end{array}$

$\begin{array}{llllllllllllllllll}0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0\end{array}$
$0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1110$
00000100111001101010000011
100000110011001101001000001
11100000110011100110010000
$\begin{array}{lllllllllllllllll}0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0\end{array}$
$0<01110000010011010110010$

1000001110000110111001100 $\begin{array}{lllllllllllllllll}0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1\end{array}$

11001000001100000100110

## Graph B

$$
\begin{array}{rcccccccccccccccc}
17 & & & & & & & & & & & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\
0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\
0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0
\end{array}
$$

The algorithm finds an explicit isomorphism, shown below.


Figure 3.1.3. The self-complemented, bisymmetric and strongly regular Ramsey graphs are isomorphic
3.1.4. Example. We run the program on isomorphic Dodecahedron [31] graphs A and B as input:



The algorithm finds an explicit isomorphism, shown below.


Figure 3.1.4. The vertex- and edge-symmetric Dodecahedron graphs are isomorphic
3.1.5. Example. We run the program on isomorphic Coxeter [33] graphs $A$ and $B$ as input:



The algorithm finds an explicit isomorphism, shown below.


Figure 3.1.5. The vertex- and edge-symmetric Coxeter graphs are isomorphic

### 3.2. Non-Isomorphism Cases

The second set of examples 3.2.1-3.2.4 consists of graphs that are not isomorphic and yet have a very similar structures, hence deciding that they are not isomorphic in polynomial-time demonstrates the power of the algorithm.
3.2.1. Example. We run the program on non-isomorphic Praust [34] graphs A and B as input:

```
Graph A
20
    0 1 1 1 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0
    1011 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0
    1 0 1 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0
    111000001000010000 0 0 0 0 0
    10 0 0 0 1 1 1 0 0 0 0 1 0 0 0 0 0 0 0
    1 0 0 1 0 1 1 0 0 0 0 0 1 0 0 0 0 0 0
    0}0100101001100000000011000000 0
    0}001111110000000000010000
    1000 0 0 0 0 0 1 1 1 0 0 0 0 1 0 0 0
    01000000001101110000 0 0 1 0 0
    0 0 1 0 0 0 0 0 1 1 0 1 0 0 0 0 0 0 1 0
    0}001100000111110000000000 1
    0 0 0 0 1 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0
    0}0000010000000011011111000
    0 0 0 0 0 0 1 0 0 0 0 0 1 1 0 1 0 0 0 1
    0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 0 0 0 1 0
    0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 1 1 1
    0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 1 0 1 1
    0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 0 1
    0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 1 1 1 0
```

```
Graph B
20
    1 1 1 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0
    0 1 1 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0
    10011000110000100 0 0 0 0 0 0 0 0
    11 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0
    1000 0 1 1 1 0 0 0 0 1 0 0 0 0 0 0 0
    0 1 0 0 1 0 1 1 0 0 0 0 0 0 0 0 0 0 0 1
    0 1 0 1 1 0 1 0 0 0 0 0 0 1 0 0 0 0 0
    0}001111110000000000000100
    10 0 0 0 0 0 0 0 1 1 1 0 0 0 0 1 0 0 0
    0100 0 0 0 0 0 1 0 1 1 0 1 0 0 0 0 0 0
    0}011000000001\mp@code{1 0 1 0 0 0 0 0 0 0 0 1 0
    0 0 0 1 0 0 0 0 1 1 1 0 0 0 0 1 0 0 0 0
    0 0 0 0 1 0 0 0 0 0 0 0 0 1 1 0 0 1 0 1
    0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 1 1 0 1 0
    0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 1 0 1 0 1
    0 0 0 0 0 0 0 0 0 0 0 1 0 1 1 0 1 0 1 0
    0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 1 0 1 1 0
    0 0 0 0 0 0 0 1 0 0 0 0 1 0 1 0 1 0 0 1
    0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 1 1 0 0 1
    0 0 0 0 0 1 0 0 0 0 0 0 1 0 1 0 0 1 1 0
```

Graph A and Graph B have the same sign frequency vectors in lexicographic order, so their structure is very similar. The algorithm determines that the graphs are not isomorphic, shown below.


Figure 3.2.1. The vertex-symmetric Praust graphs are not isomorphic
3.2.2. Example. We run the program on nonisomorphic Mathon [35] graphs A and B as input:

$$
\begin{aligned}
& \text { Graph A } \\
& 25 \\
& 00000000001111111000000000 \\
& 000000000011000011111000000 \\
& 000000000000010100001010000111000 \\
& 00000000001001000100010011 \\
& 000000000001100000010001011 \\
& 000000000001000100001101010 \\
& 00000000000010010101000101 \\
& 0000000000000011001010000101 \\
& 00000000000001011100101010 \\
& 00000000000000110110111000 \\
& 1111100000000000000000000000 \\
& 1100110000000000000000000 \\
& 10100101000000000000000000 \\
& 1001000110000000000000000 \\
& 1000010101000000000000000 \\
& 10000000101110000000000000000000 \\
& 01100000110000000000000000 \\
& 0101001001000000000000000 \\
& 0100100101000000000000000 \\
& 0100011010000000000000000 \\
& 00111010000100000000000000000 \\
& 0010010000011000000000000000000000 \\
& 0010011100000000000000000 \\
& 000011110001000000000000000000000 \\
& 0001101100000000000000000
\end{aligned}
$$

## Graph B

$$
\begin{aligned}
& 25 \\
& 000000000011111110000000000 \\
& 000000000000110000011111000000 \\
& 00000000001010001000011100 \\
& 000000000010010001010010011 \\
& 00000000000110000001001011 \\
& 00000000000100100001101010 \\
& 0000000000000010001010010001001 \\
& 000000000000011001010000101 \\
& 000000000000010100011111000 \\
& 0000000000000001111100001010 \\
& 111110000000000000000000000 \\
& 11000111000000000000000000000 \\
& 1010101000000000000000000 \\
& 1001000110000000000000000 \\
& 1000010100100000000000000000 \\
& 1000001011000000000000000 \\
& 01110000001010000000000000000000 \\
& 010100010010000000000000000 \\
& 01000100110000000000000000
\end{aligned}
$$

$$
\begin{aligned}
& 00110010010000000000000000 \\
& 0010100011000000000000000 \\
& 001100011 \begin{array}{llllllllllllllllll}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array} \\
& 0001110001000000000000000 \\
& 0001101100000000000000000
\end{aligned}
$$

Graph A and Graph B have the same sign frequency vectors in lexicographic order, so their structure is very similar. The algorithm determines that the graphs are not isomorphic, shown below.


Figure 3.2.2. The bipartite Mathon graphs are not isomorphic
3.2.3. Example. We run the program on nonisomorphic Weisfeiler [36] graphs $A$ and $B$ as input:

## Graph A

$$
\begin{aligned}
& 25 \\
& 011111111111111000000000000 \\
& 1001111111000000001111111100000000 \\
& 11001111100000000000001111111 \\
& 11100000111000011100001111000 \\
& 1 \begin{array}{lllllllllllllllllllllllll}
1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0
\end{array} \\
& 11100000010101010101010101 \\
& 1111000000010101001001100010011 \\
& 10011000011100010100010000111 \\
& 10010101010010001111001100
\end{aligned}
$$

$$
\begin{aligned}
& 100011001000110110011100010 \\
& 1000100100110111100100011100 \\
& 1000001100101100101110001010001 \\
& 010110001000110111000001101 \\
& 01011010001110010010010110010 \\
& 01010001100010110000111110001 \\
& 01001100110011100010100011 \\
& 010001101001100100001100111001000 \\
& 010001111101000110100001110 \\
& 00111100010010100111000110010 \\
& 00011 \begin{array}{lllllllllllllllllllllll}
0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1
\end{array} \\
& 001100010100011111000011000110 \\
& 0010011011100010100001100110001 \\
& 001001011001100010101011010001 \\
& 0010011101001101100010110
\end{aligned}
$$

```
Graph B
25
0 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0
1}0
1
```



```
1
```



```
1}111100000000000 1 0 1 1 1 0 0 0 1 0 0 1 1 1 0 0 0 1 0 0 1 1 1
```



```
10}00
100}0
```





```
0
0
```



```
0
```




```
0
0}001
0}001
0}0
```




Graph A and Graph B have common pair signs but different sign frequency vectors in lexicographic order. The algorithm determines that the graphs are not isomorphic, shown below.


Figure 3.2.3. The self-complemented and strongly regular Weisfeiler graphs are not isomorphic
3.2.4. Example. We run the program on nonisomorphic Siberian [9] graphs $A$ and $B$ as input:


| Graph A |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 40 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 0001101011 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 001000100010001010001001000000001000011011 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{array}{lllllllllllllllllllllllllllllllllllllllll} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{array}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| 100100001000000000011000001110011001001 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 0100000001010000010001000001111111000100 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 0000100000011101000011000000010100110010 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 00100100000001001100010000010000011111000 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| 1100100000001000010000010010010011010100 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 0001001100000011010100000000100001010101 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 00000001001000000111010001110000000001011 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 00000001110000100010100100101100000001100 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| 000000101011100010001010101010000010000 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| 0110010100000100010100101000010010000001 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 00110011110001000000000110000000011000010 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| 0101000000100100001101100000101000110000 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 000000000100000001101010010000110101010110 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 0011100001001000100100001000110000001100 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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Graph A and Graph B have the same sign frequency vectors in lexicographic order, so their structure is very similar. The algorithm determines that the graphs are not isomorphic, shown below.


Figure 3.2.4. The bisymmetric and strongly regular Siberian graphs are not isomorphic. It was a more complicated case for isomorphism testing.

## References

[1] Filosoofia leksikon, Tallinn, 1985.
[2] Новая философская энциклопедия, Москва, 2001.
[3] H. Schmidt, Philosophisches Wörterbuch. Stuttgard, 1991.
[4] S. Toida, Isomorphism of graphs - Proc $16^{\text {th }}$ Midwest Symp. Circuit Theory, Waterloo, 1973, XVI.5.1-5.7.
[5] R.C. Read and D. G. Corneil, The graph isomorphism disease. - J. of Graph Theory, 1 (1977), 339363.
[6] G. Gati, Further annotated bibliography on the isomorphism disease. - J. of Graph Theory, 3 (1979), 95-109.
[7] B. Bollobas, Modern Graph Theory, Springer, 1998.
[8] C. Hoffmann, Group-Theoretic Algorithms and Graph Isomorphism. Springer, 1982.
[9] M. Netchepurenko et al., Algorithms and programs for solution of problems in graphs and networks, Novosibirsk, 1990.
[10] G. Kobler, H. Schönig and J. Toran, The Graph Isomorphism Problem: Its Structural Complexity, 1993.
[11] L. Babai, http://cs.mu.oz.au/481/Author/BABAI-L.
[12] G. Tinhofer, M. Lödecke, S. Baumann, L. Babel, STABCOL, Graph Isomorphism Testing on the Weisfeiler-Leman Algorithm, 1997, $\mathrm{http}: / / \mathrm{citeseerx}$. ist.psu.edu/viewdoc/summary/dol=10.1.1.56.6704
[13] C. V. Raj and M. S. Shivakumar, 2008, http://www.informatik.uni-trier.de/ ~ley/indices/atrees/S/Shivakumar.M=_S=html
[14] N. Chistofiedes, Graph Theory: An algorithmic approach. Academic Press, 1975.
[15] S. Pemmaraju and S. Skiena, Computational Discrete Mathematics: Combinatorics and Graph Theory with Mathematica ${ }^{\circledR}$, Cambrige University Press, 2003.
[16] E. Reingold, J. Nievergelt, N. Deo, Combinatorial Algorithms: Theory and Practice, 1977.
[17] V. Arvind, P. P. Kurur, Graph isomorphism is in SPP, 2006, http://www.portal.acm.org/citation.cfm?ld=1149036
[18] F. Harary, Graph Theory, Addison-Wesley, 1969.
[19] R. Wetzenböck, Invarianten-Theorie. Gröningen, 1923.
[20] S. Locke, www.math.fau.edu/locke/isotest.
[21] A. Zykov, Основы теории графов. Москва, 1987.
[22] H. Hermes, Semiotik: eine Theorie der Zeichengestalten als Grundlage für Untersuchungen von formalisierte Sprachen. Leipzig, 1938.
[23] John-Tagore Tevet, Structure Semiotic Approach to the Graphs. S.E.R.R., Tallinn, 2006. http://ester.nlib.ee:80/record=b2367627~S1*est
[24] The Oxford Companion of Philosophy, 1995.
[25] I. Meos, Filosoofia põhiprobleemid. Tallinn, 1998.
[26] Ashay Dharwadker and Shariefuddin Pirzada, Graph Theory, Orient Longman and Universities Press of India, 2008.
[27] John-Tagore Tevet, Recognition of the Structure, Symmetry and Systems of Graphs, Baltic Horizons, No. 8 (107), Special Issue Dedicated to 270 Years of Graph Theory, 2007.
[28] E. W. Dijkstra, A note on two problems in connexion with graphs, Numerische Mathematik, 1, 1959.
[29] P. Turán, An extremal problem in graph theory, Mat. Fiz. Lapok, 1941.
[30] J. Petersen, Die Theorie der regulären Graphen, Acta Math., 1891.
[31] Plato, Timaeaus, circa 350 B.C.
[32] F.P. Ramsey, On a problem of formal logic, Proc. London Math. Soc., 1930.
[33] H.S.M. Coxeter and W.T. Tutte, The Chords of the Non-Ruled Quadratic in PG(3,3), Canad. J. Math., 1958.
[34] John-Tagore Tevet, Constructive Representation of Graphs: A Selection of Examples, S.E.R.R., Tallinn, 2008. http://ester.nlib.ee:80/record=b2161461~S1*est
[35] R. Mathon, Sample graphs for isomorphism testing, Proc. 9th S-E. Conf. Combinatorics, Graph Theory and Computing, 1980.
[36] B. Weisfeiler, On Construction and Identification of Graphs, Springer Lecture Notes Math., 558, 1976.

