Canonical Number and NutCracker: Heuristic Algorithms for the Graph Isomorphism Problem using Free Energy

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Abstract. This paper develops two heuristic algorithms to solve graph isomorphism, using free energy encoding. The first algorithm uses four types of encoding refinement techniques such that every graph can be distinguished by a canonical number computed by the algorithm. The second algorithm injects energy into the graph to conduct individualization such that the correspondence relation between a pair of isomorphic graphs can be found. The core principle behind the two algorithms is encoding discrete structures as real numbers. A large set of experiments demonstrated the effectiveness of our algorithms.

1 Introduction

Finding an efficient algorithmic solution to the graph isomorphism (GI) problem has been an open problem for more than four decades, where much research effort has been spent and in the 1970s, there was even a trend called “Graph Isomorphism Disease” [15] surrounding the problem. Why is this problem so fascinating and attractive to researchers? The reasons are its obvious importance in both theory and practice.

In theory, the exact complexity class of GI is still unknown. Obviously, it is in NP, but it is unknown whether it is NP-complete. Many people believe that it is in P, however, no known polynomial time algorithms exist to solve GI in general, though, for some special types of graphs, polynomial time algorithms has been shown. To list a few, trees [1], interval graphs and planar graphs [4], graphs with bounded genus [8], graphs with bounded degrees [11] and graphs with bounded tree-width [3], do have polynomial time algorithms for isomorphism. In practice, graphs are almost the universal data structure in Computer Science. In applications such as bioinformatics and graph mining, efficient graph matching algorithms are needed. For example, when biologists and chemists try to query a newly found protein with unknown biological functionalities in a protein data bank (like RCSB) where each protein in the bank is annotated with its identified functionalities, a protein molecule’s spatial structure can be used. An efficient GI algorithm can be used to design an engine to resolve this query. In many application areas, algorithms for the subgraph isomorphism are also
needed, where a solution to the GI may provide a hint of inspiration to the widely considered more difficult subgraph isomorphism (which is known to be NP-complete).

In the past 40 years, there has been some very influential research work on the GI problem. To list a few, Brendan McKay combined degree-based refinement strategies, graph automorphisms and search tree to design one of the most useful tools, Nauty in [13] and in [14] (with Piperno). László Babai introduced group theory to solve GI in 1970s. His last year’s seminal result has shown that the complexity of the GI problem is quasi-polynomial [2]. There also exist several important exact match (instead of heuristic) graph isomorphism algorithms. Ullmann algorithm [23] uses a backtrack algorithm with some pruning metrics to solve graph isomorphisms and subgraph isomorphisms. Schmidt and Druffel [19], in the same year, invented another backtracking algorithm using distance matrices. The VF2 algorithm, invented by Cordella et. al. [5], is also a backtracking algorithm that uses state space representation to reduce space complexity.

In this paper, we propose efficient and heuristic algorithms to attack the GI problem in a novel perspective from physics: thermodynamic formalism. Thermodynamic formalism provides a mathematical structure to rigorously deduce a macroscopic characteristic [16,17,25] of a many-particle system (e.g., gas) from microscopic behavior. Originally, thermodynamic formalism is mainly used to analyze physical systems and their mathematical abstractions–dynamic topological systems. Our recent research [7] introduces thermodynamic formalism to finite automata, formal languages, and programs. In this paper, we use thermodynamics formalism to encode a discrete structure (a graph optionally with weight) into a real number (called potential or energy in physics, and called weight in this paper). The theoretical underpinning of our approaches is that, when a gas molecule “walks” on the graph representing its energy changes along the time, the local potential or weight assigned on the nodes or edges will be eventually reflected in its long-term characteristic (such as equilibrium at infinitely, i.e. the far future). The main ideas in our approaches are three-fold: (1) local structure such as neighbourhood information can be encoded as a real number; (2) the real number generated from neighbourhood information can be assigned as node weights or edge weights; and (3) global information, such as shortest distance, can also be encoded as edge weights. Then, we translate a simple graph (i.e., without weights) into a weighted graph. In this way, spectrum of the weighted graph can be used (heuristically) to tell whether graphs are isomorphic. Stationary distributions can help us to find the correspondence between two isomorphic graphs.

Refinement and individualization is a well known and classic technique to solve graph isomorphism problem (see [21] or for an excellent introduction). In order to make our algorithms easy to understand, avoiding too many tedious mathematical and physical details, we try to fit our algorithms into the classic refinement and individualization framework. Hence, our readers can follow the traditional way to understand our algorithms and also make it easy to compare them to previous algorithms.
2 The philosophy behind our methods: encoding discrete structures as real numbers

Although the main mathematical tool used in this paper is thermodynamic formalism, our path to attack GI problem starts from spectral graph theory, a charming branch of graph theory. In this paper, we mainly focus on undirected graphs, though the approaches can be straightforwardly generalized to directed graphs. A graph $G$ is specified by $(V, E)$ where $V$ is the set of nodes and $E$ is the set of (undirected) edges (where each edge is an unordered pair of nodes). Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, they are isomorphic if there is a one-to-one correspondence mapping $T$ between $V_1$ and $V_2$ such that, for all $u, v \in V_1$, $(u, v) \in E_1$ iff $(T(u), T(v)) \in E_2$. A basic data structure of a graph is its adjacency matrix $A$. Spectral graph theory mainly investigates properties of graphs by their spectrum properties, e.g., their eigenvalues and eigenvectors (of its adjacency matrix). The theory provides an excellent tool set to the GI problem. For instance, the largest eigenvalue (which is called the spectral radius, or the Perron number) remains unchanged when a one-to-one permutation is applied on its nodes. Using this theory, many apparently similar graphs can be easily distinguished by their spectra, especially by their largest eigenvalues.

One of the theoretical underpinnings of using the spectral graph theory for the GI problem is roughly as follows. Let $X$ be a “most random” Markov walk on a graph $G$ with its adjacency matrix $A$. The largest eigenvalue of $A$ can tell the entropy rate (which equals the logarithm of the eigenvalue) of the Markov chain while the second largest eigenvalue of $A$ can tell the convergence rate to the entropy rate [6]. Both entropy rate and convergence rate are the long term properties of a Markov chain. In contrast to this, an edge (or a local structure) of the graph resembles one-step of the walk and hence is a short term property of the Markov chain.

For some nonisomorphic but highly symmetric graphs, it is still difficult to distinguish their spectra only using the adjacency matrices. A more powerful and well-known tool in the spectral graph theory, Laplacian matrix [22], is introduced. Roughly speaking, Laplacian matrix is another matrix representation of a simple graph $G$, in the form of $L = D - A$, where $D$ is degree matrix of $G$ and $A$ is the adjacency matrix of $G$. The degree matrix $D$ of $G$ is defined as a diagonal matrix, where the $i$-th element of diagonal is the number of nodes to which $v_i$ is connected. Analyzing the spectrum of Laplacian matrix $L$ of $G$, many graphs, which are not distinguishable under the spectrum of the adjacency matrix $A$, are now distinguishable.

The improvement made by the Laplacian matrix [22] over the adjacency matrix is essentially due to the additional information brought into the Markov chain’s short term behaviors: the degree information on each node. In the long term, this information is eventually reflected in the spectrum of the graph.

However, the Laplacian matrix approach fails on many extremely symmetric graphs, such as strongly regular graphs. Following the above thread of thinking from adjacency matrix to Laplacian matrix, we need a more “information rich” matrix representation of a graph to further improve the Laplacian matrix ap-
proach, by encoding more local structure information to its matrix form. But, it
seems difficult to achieve this goal at first because it is not straightforward how
to numerically encode a discrete structure into a real number with a mathemati-
cal meaning in the matrix. Fortunately, using thermodynamic formalism, we can
extract a node’s local structure as a subgraph. Then we compute the free energy
of the subgraph, a positive real number, as a weight on the edge. As a result,
the graph’s matrix representation is a matrix where each entry indicates local
structure information. The largest eigenvalue of the weighted matrix denotes the
free energy of the weighted matrix.

In the rest of this section, we briefly introduce the free energy of a graph. In
the next two sections we present our two heuristic algorithms for deciding graph
isomorphism and finding correspondence.

Let \( G \) be a graph while \( X \) is a Markov chain on \( G \) that defines a measure \( \mu \)
on the set of infinite walks of \( G \) (each walk is a sequence of nodes). The \( \mu \)
can be defined from the cylinder sets of the walks (we omit the details here; see [10,18]). We assume that \( G \) is connected (i.e., every node can reach every
other node). Each infinite walk \( \alpha = vv'v'' \cdots \) carries an energy defined by a
function \( \psi(\alpha) \). In a simplest setting, we define \( \psi \) on the first step of the walk;
i.e., \( \psi(\alpha) = \psi(v, v') \) and hence the potential function or the energy function \( \psi \)
assigns an energy called weight to each edge of \( G \). The free energy of \( G \), for
the given \( \psi \), is defined as \( \sup_\mu \{ h_\mu + \int \psi d\mu \} \), where \( h_\mu \) is the Kolmogorov-Sinai
entropy. It can be computed using the Gurevich matrix \( M \) where each entry \( M_{ij} \)
of the matrix is \( e^{\psi(v_i, v_j)} \) and the natural logarithm of the Perron number of this
nonnegative matrix is exactly the free energy defined earlier. In particular, the
unique \( \mu^* \), as well as the stationary distribution, called Parry measure, \( \eta \cdot \xi \) of the
Markov chain defined with the \( \mu^* \), that achieves the supreme can be computed
using the left eigenvector \( \eta \) and the right eigenvector \( \xi \), after normalization, of
the Perron number of the matrix [10].

In the sequel, for convenience, we directly treat \( e^{\psi(v_i, v_j)} \) as the energy or the
weight on an edge and treat the Perron number, that is the largest eigenvalue
(which is a positive real from the Perron-Frobenius theorem), as the free energy
of the graph.

3 **Canonical Number**: a refinement framework using
numerical encoding of various discrete structures

Notably in the previous research on GI, McKay’s color labelling refinement ap-
proaches and Schmidt and Druffel’s shortest distance matrix are both widely
used heuristic metrics to reduce the size of a search tree for backtracking al-
gorithms. McKay’s color-labelling refinement only depends on local structures,
while the shortest distance matrix approach needs a global structure. Intuitively,
if we can encode both local and global structure information into the refinement
procedure, it would be possible to distinguish or assign unique labels to more
nodes. However, this encoding strategy has a fundamental difficulty. Our answer
uses thermodynamic formalism [16] mentioned earlier, by numerically encoding
a discrete structure as a real number. Now, we need to exploit which structure information is important for GI problem and how to numerically encode it on the graph.

3.1 Shortest distance encoding

Shortest distance matrix actually is a well known metric for GI problem. This metric shows a global constraint on the nodes’ relations in a graph. The theoretical underpinning of this method is the well-known fact that the shortest distance matrix decides the graph that it represents. To fit the useful metric in our context, we make a small modification to it. For a connected graph, the shortest distance matrix is straightforward. For a graph that is not connected, when there is no path between two given nodes, the distance is defined as infinity (which is set to be a large number that only needs to be larger than the diameter of the graph). Then, we use the reciprocal of the shortest distance between nodes \( i \) and \( j \) as the weight on the edge between \( i \) and \( j \). At first, the “reciprocal”-representation of the shortest distances may seem counter-intuitive. The reason we modify it this way is that after doing so, every graph becomes connected, which is necessary in thermodynamics formalism (i.e., in this way, the Gurevich matrix is now irreducible for any graph).

3.2 Neighbourhood graph encoding

It is known that neighbourhood is an important local structure that can distinguish many similar graphs. For example, in the class of strongly regular graphs \((16,6,2,2)\), there exist two non-isomorphic graphs. The core difference between the two non-isomorphic graphs is that the neighbourhood in one graph is of two triangles while the neighbourhood in the other graph is a 6-cycle graph. Thus, if we can encode this type of structural differences, many types of graphs can be easily distinguished.

First, we need to define what is a neighbourhood graph. Given a graph \( G = (V, E) \), for a node \( v_i \) in the node set \( V \), we say \( G_i^{nh} = (V_i^{nh}, E_i^{nh}) \) is the neighbourhood graph of \( v_i \) if every node in \( V_i^{nh} \) is a node connected (with an edge) to \( v_i \) in \( G \) and any two nodes \( v_x \) and \( v_y \) in \( V_i^{nh} \) in \( G_i^{nh} \) is connected iff \( v_x \) and \( v_y \) are connected in \( G \).

To encode the neighbourhood graph as a real number we need to overcome two challenges:

- The subgraph is not necessarily connected. How can we compute the energy of an disconnected graph?
- After computing the energy of the neighbourhood graph, where can we assign the energy?

To solve the first challenge, we compute its standard shortest distance matrix first. Following the modification for shortest distance matrix in the previous subsection, now, we have an irreducible matrix and then we compute the Perron
number as the free energy of the neighbourhood graph. For the second challenge, after we compute the free energy of the neighbourhood graph, we add the energy to the existing weight (which now is the reciprocal shortest distance) of every edge between \( v_i \) and other nodes (including \( v_i \) itself).

### 3.3 Shared neighbours subgraph encoding

In strongly regular graphs, the third parameter such as in \((16,6,2,2)\) tells us the number of shared neighbours between two adjacent nodes while the fourth parameter indicates the number of shared neighbours between two adjacent graph. Hence, the shared neighbour is a useful metric to demonstrate the local structure of different nodes pairs.

Now, we need to define the shared neighbours graph. Given a graph \( G = (V, E) \), for a node \( v_i \) and \( v_j \) in the node set \( V \), we say \( G_{ij}^{sn} = (V_{ij}^{sn}, E_{ij}^{sn}) \) is the shared neighbours graph of \( v_i \) and \( v_j \) if every node in \( V_{ij}^{sn} \) is a node connected (with an edge) to both \( v_i \) and \( v_j \) in \( G \) and any two nodes \( v_x \) and \( v_y \) in \( V_{ij}^{sn} \) in \( G_{ij}^{sn} \) is connected iff \( v_x \) and \( v_y \) are connected in \( G \).

Given a pair node of \( v_i \) and \( v_j \), the encoding procedure is in the following:

- Obtain the shared neighbours graph for the node pair \( v_i \) and \( v_j \), \( G_{ij}^{sn} \).
- Compute the free energy of \( G_{ij}^{sn} \) and add the free energy to the weight on the edge between \( v_i \) and \( v_j \) on \( G \).

### 3.4 Union neighbours subgraph encoding

Shared neighbours graph is a powerful metric to inspect graph’s characteristics. But, the metric has some fundamental limitations. For example, given a bipartite graph \( G \), all nodes of \( G \) can be divided into two blocks \( V_{left} \) and \( V_{right} \). Following the definition of bipartite graph, obviously, any node in \( V_{left} \) shares zero neighbour with any node in \( V_{right} \). Hence, shared neighbours graph encoding is not enough. Our solution is union neighbours, which is also quite natural from the view of Venn diagrams. We assume that the neighbourhood of node \( i \) is \( A \) and the neighbourhood of node \( j \) is \( B \), the shared neighbour can be understood as the intersection of \( A \) and \( B \). Hence, if we use intersection operation on sets, naturally, it follows naturally that we also need a union operation on sets, i.e., the union of \( A \) and \( B \), to complete a Venn diagram.

Now, we need to define union neighbours graph. Given a graph \( G = (V, E) \), for a node \( v_i \) and \( v_j \) in the node set \( V \), we say \( G_{ij}^{un} = (V_{ij}^{un}, E_{ij}^{un}) \) is the union neighbours graph of \( v_i \) and \( v_j \) if every node in \( V_{ij}^{un} \) is a node connected to either \( v_i \) or \( v_j \) in \( G \) and any two nodes \( v_x \) and \( v_y \) in \( V_{ij}^{un} \) in \( G_{ij}^{un} \) is connected iff \( v_x \) and \( v_y \) are connected in \( G \).

Given a pair node of \( v_i \) and \( v_j \), the encoding procedure is in the following:

- Obtain the union neighbours graph for the node pair \( v_i \) and \( v_j \), \( G_{ij}^{un} \).
- Compute the free energy of \( G_{ij}^{un} \) and add the free energy to the weight on the edge between \( v_i \) and \( v_j \) on \( G \).
Algorithm 1 Canonical Number: Graph Isomorphism Testing Algorithm

**Require:** A, which is the adjacency matrix of G and the dimension of A is n.

1: function Perron(M)
2: Compute the Perron number (i.e. the largest eigenvalue) of a matrix M, λ.
3: return λ
4: end function

5: function CanonicalNumber(A)
6: n ← the dimension of A.
7: Build an n × n matrix W = \{W_{ij}\} with initial values zero.
8: Compute the shortest distance matrix \{\text{shortest distance}_{ij}\}.
9: for i, j in \{W_{ij}\} do
10: \[ W_{ij} \leftarrow \frac{1}{\text{shortest distance}_{ij}} \]
11: end for
12: Construct 1 × n matrix NHTable with zero as initial values.
13: Construct two n × n matrices SNTable and UNTable with zero as initial values.
14: for i, j in \{W_{ij}\} do
15: Obtain the shared neighbours graph of node pair (i, j): G_{ij}^{sn}
16: Compute the Perron number of the graph G_{ij}^{sn}: SNTable_{ij} ← Perron(G_{ij}^{sn})
17: Obtain the union neighbours graph of node pair (i, j): G_{ij}^{un}
18: Compute the Perron number of the graph G_{ij}^{un}: UNTable_{ij} ← Perron(G_{ij}^{un})
19: if i == j then
20: Obtain the neighbourhood graph of node i: G_{i}^{nh}
21: Compute the Perron number of graph G_{i}^{nh}: NHTable_{i} ← Perron(G_{i}^{nh})
22: end if
23: end for
24: for i, j in \{W_{ij}\} do
25: \[ W_{ij} \leftarrow W_{ij} + \text{NHTable}_{i} + \text{NHTable}_{j} + \text{SNTable}_{ij} + \text{UNTable}_{ij} \]
26: end for
27: Use the weight matrix W as the matrix representation of G
28: Compute the Perron number of graph G: canonical number = Perron(W)
29: return canonical number.
30: end function

31: CanonicalNumber(A).

7
3.5 The Algorithm **Canonical Number**

The pseudocode of our algorithm is listed in Algorithm 1. Inspired by the canonical labelling method of previous GI research, we name our algorithm the **Canonical Number** algorithm. For a given graph $G$, there exists a canonical labeled graph $G_C$ such that any graph $G'$ that is isomorphic to $G$ shares the same canonical labeled graph $G_C$. Our experiments presented in the latter section show that for all the graphs that we run our algorithm upon, any two nonisomorphic graphs have different numbers and any isomorphic graphs share the same number. This characteristics is similar to canonical labelling, hence we call the number, the free energy of the graph returned from the algorithm, the canonical number of the graph.

**Correctness** To prove the correctness of our algorithm, we need to show two parts:

- For any isomorphic graphs, they share the same canonical number.
- For any two nonisomorphic graphs, they have different canonical numbers.

The first part is obvious because the encoding process does not depend on the naming of any node. For now, we cannot mathematically prove the second part. So we call our algorithms a heuristic algorithms. However, we have the following conjecture:

**Conjecture 1** There exists at lease one encoding method that assign weights on graphs such that all isomorphic graphs share the same canonical number and any nonisomorphic graphs have different canonical numbers.

We also conjecture that our current encoding method is one of these encoding methods (and hence we conjecture that GI is in P).

**Explanation of the algorithm** We present a brief explanation to Algorithm 1. In lines 1-4, the function Perron is used the compute Perron number, i.e., the largest eigenvalue, of a given matrix. In line 5-30, the function CANONICAL-NUMBER is designed to compute the canonical number of a given graph $G$. In lines 6-11, we implement the shortest distance encoding described in Subsection 3.1. In lines 12-13, we initialize three tables to store values for neighbourhood, shared neighbours and union neighbours encoding. In lines 14-23, we iterate ev- ery edge in the graph to conduct various encoding approaches. In lines 15-16, shared neighbours encoding, described in Subsection 3.3, is implemented for the edge between node $v_i$ and $v_j$. In lines 17-18, union neighbours encoding, described in Subsection 3.4, is implemented for the edge between node $v_i$ and $v_j$. In lines 19-22, neighbourhood encoding, described in Subsection 3.2, is implemented for node $v_i$. In lines 24-26, we use previous encoding tables to update the matrix $E$, such that $E$ is a matrix representation of $G$. In lines 27-28, we compute the free energy of $E$ and return it as the canonical number of $G.$
The time complexity analysis of our algorithm Algorithm 1 includes several basic algorithms. The time complexity of computing shortest distance \[O(n^3)\] is \[O(n^3)\]; The time complexity of computing eigenvalues of a matrix with dimension \(n\) is as same as the matrix multiplication. For the ease of discussion, we use \(O(n^3)\) as its complexity although it is may a litter lower than this. In Algorithm 1, the dominating part of the time complexity is the loop in lines 13-22. In the for-loop, the complexity of one iteration depends on obtaining a subgraph and computing the subgraph’s Perron number, i.e., \(O(n^2 + n^3) = O(n^3)\). The complexity of the for loop itself is \(O(n^2)\). Hence, the time complexity of this algorithm is \(O(n^5)\).

4 NutCracker: a free energy based refinement-and-individualization for finding correspondence

In the previous section, we proposed an heuristic approach to do refinement. Then the canonical number of the refined matrix was used to identify different graphs. Can we just use the refinement procedure to find the correspondence relation between a pair of isomorphic graphs? To achieve this goal, the refinement procedure needs to be powerful enough such that every node has a unique label. For some non-symmetric graphs, this is possible. However, for many very symmetric graphs, it is almost impossible. For example, given a pentagon graph \(G\), if we conduct the previous refinement methods, we still cannot assign unique labels for every node.

Fig. 1. Nuts and singles in the NutCracker algorithm
It is true for many graphs that many nodes cannot have a unique label after refinement. In past GI research, there are two well-known methods (see [22] for a clear introduction) to solve this issue. First, one builds a search tree to search every possible case with some additional heuristics. Second, one tries to find a distinguishing set such that if all nodes in the distinguishing set are labeled first, then all the other nodes can get their unique labels through refinement. The second method is called *individualization*. Both of the methods may lead to exponential complexity.

Individualization is absolutely necessary to break the symmetry of the graph. However, do individualization methods always require a distinguishing set? Our approach and experiments show that this may not be required. In order to obtain a polynomial time individualization method, we try to design a step-by-step individualization approach where in every step only one node is individualized. This approach implicitly assumes (this assumption is actually true for all the experiments we have done) at every step, we can always choose the correct node and never need to backtrack. As a result, assuming $G$ has $n$ nodes, we need, at most, $n$ steps to finish the individualization procedure.

Now, we present the general idea of our algorithm as follows. First, we need to use the refinement procedure in the previous section and obtain a weight matrix $W$. Second, we need to compute aforementioned Parry measure of $W$. Notice that from [23], given an irreducible $W$, the Parry measure is unique. Then, we use its stationary distribution (on nodes) to distinguish different nodes. See Figure 1. After computing the Parry measure, we call a node *single* if the node has unique stationary probability and call a set of nodes *nut* if every node in the set shares the exactly same stationary probability. In Fig. 1 node 1, 3 and 5 in $G_1$ and node 2, 8 and 6 are singles; nodes 7 and 9 in $G_1$ form a nut while node 4 and 1 in $G_2$ form a nut.

For every single in $G_1$ and $G_2$, it is easy to use its stationary probability to build the correspondence. The obstacle is how to build the correspondence between nodes in the nuts. Since $G_1$ and $G_2$ are isomorphic, every correspondent nut should share exactly the same size and stationary probability. Then, it is easy to find a pair of such nuts, say $nut_{1}^{G_1}$ and $nut_{1}^{G_2}$, where $nut_{1}^{G_1}$ is in $G_1$ and $nut_{1}^{G_2}$ is in $G_2$. In $nut_{1}^{G_1}$, we randomly choose a node $v_1$ while a node $v_2$ is also randomly chosen from $nut_{1}^{G_2}$ such that if we assign a unique integer number to both $v_1$ and $v_2$ as node weight, the canonical numbers of $G_1$ and $G_2$ are still same. (In fact, $v_1$ and $v_2$ are not randomly chosen, see the following pseudo-code step 11 of the Algorithm 2.) Hence, we assign the unique integer number to $v_1$ and $v_2$. The node weight of a node $v$ can be assigned to each edge between node $v$ and all other nodes. Why did we do it in this way? Here we use a node as a cracker in a nut to crack the whole graph. The assigned node weight can be understood as an energy cracker. The energy cracker injects a small amount of energy into this node. Then the amount of energy we just injected will spread to all other nodes in the entire graph. After a moment, the dynamic system represented by the graph will enter a new equilibrium state. At this step, we check every node’s new stationary distribution. Obviously, any previous single
node is still single, and at least one node in nuts may become single. Then, we check if any nuts still exist. If so, we repeat the energy injection procedure; otherwise, every node has becomes single, i.e. every nodes has a unique label. Obtaining all unique labeled nodes, it is easy to use the unique labels to build the correspondence relation between nodes in two graphs.

4.1 Correctness and time complexity

Correctness Similar to Algorithm 1, we cannot mathematically prove the correctness of this NutCracker algorithm (otherwise, GI is polynomial). Hence, we call this algorithm an heuristic algorithm. The correspondence found by the algorithm can be easily verified whether it is indeed an isomorphic correspondence. For the graphs that we run our experiments, the algorithm is indeed correct.

Time complexity For the NutCracker in Algorithm 2, the denominating part is in Line 11. From the section, it is known that CanonicalNumber algorithm is $O(n^5)$. In line 11, the canonical number algorithm is called in a nested loop. The worse case, we may need to loop $O(n^2)$ times. So, the line 11 is $O(n^7)$. Also, Algorithm 2 is a recursive algorithm, in the worst, case, we may call it $n$ times. Thus, the worst time complexity is $O(n^8)$. Note that, this algorithm seems to be a backtrack algorithm. But, we assume at every step, we can find the correct choice; we never backtrack. If we make the wrong choice, the algorithm fails, rather than backtrack.

5 Experiments

In this subsection, we present a large set of experiments to demonstrate the effectiveness of our heuristic algorithms in practice.

5.1 Experimental subjects

In order to demonstrate the effectiveness of our algorithms, it is ideal that we carry out experiments on all available public datasets. However, it is impossible for us to do so due to limited resources (time and available high performance computers). So, we choose to run our algorithms on both “easy” graphs where other heuristic algorithms may also succeed and “challenging” graphs where other heuristic algorithms may fail. The number of graphs that we run on must also be large enough to have a practical meaning. Finally, we decide to choose the following datasets for the experiments:

- The dataset of all connected graphs with exactly 10 vertices that is maintained by McKay[12] and generated by his famous program Nauty. The dataset contains roughly 11,000,000 non-isomorphic graphs;
- Strongly regular graphs are known to be notoriously difficult for all GI algorithms. Spence [20] maintains a dataset that includes all strongly regular graph with the number of vertices less than or equal to 64. The dataset contains roughly 40,000 non-isomorphic graphs.
Algorithm 2 NutCracker algorithm

Require: $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are a pair of isomorphic graphs

1: Initialize an array $nodeweight_1$ (resp. $nodeweight_2$) for $G_1$ (resp. $G_2$) with zero as initial values.
2: Using $nodeweight_1$ (resp. $nodeweight_2$), assign node weights to every node in $G_1$ (resp. $G_2$).
3: For every node $v$ in $G_1$ (resp. $G_2$), we spread $v$’s node weights to edges between $v$ and all nodes (including $v$). (Notice that, after this step, $G_1$ and $G_2$ are weighted graphs.)
4: Using the weighted matrix representation $W_1$ (resp. $W_2$) of $G_1$ (resp. $G_2$), compute Parry measure for $G_1$ (resp. $G_2$).
5: Through Parry measure, we can easily obtain the stationary distribution $P_1$ (resp. $P_2$) of $G_1$ (resp. $G_2$).
6: Perform partition on $V_1$ (resp. $V_2$) by its values in $P_1$ (resp. $P_2$).
   - If a node in $G_1$ (resp. $G_2$) has a unique stationary probability, we add it to $singlesList_1$ (resp. $singleList_2$). Then, $singlesList_1$ (resp. $singleList_2$) is obtained.
   - If several nodes in $G_1$ (resp. $G_2$) share the same probability, we combine these nodes to form a nut and add the nut to the $nutList_1$ (resp. $nutList_2$). Hence, $nutList_1$ (resp. $nutsList_2$) is obtained.
7: If all nodes are singles, we are successful; otherwise, continue.
8: Sort the $singleList_1$ (resp. $singleList_2$) by stationary probability. Sort $nutList_1$ (resp. $nutList_2$) by the size of nut. (After this step, $singleList_1$ and $singleList_2$ should be aligned, i.e., the entry in $singleList_1$ and $singleList_2$ in the same position should have same stationary probability.)
9: Create an empty array $newNodeweigh_1$ (resp. $newNodeweigh_2$) for $G_1$ (resp. $G_2$).
10: From the starting position to the end position of both singlesLists ($singleList_1$ and $singleList_2$), we pick the nodes in the same position from two lists, position by position. We assign a unique weight to both nodes. Herein, The weight is unique to the position, rather than two lists. ($newNodeweigh_1$ and $newNodeweigh_2$ are updated).
11: For the first nut in $G_1$, $nut^{G_1}_1$, and the first nut in $G_2$, $nut^{G_2}_1$, we pick a node $v_1$ in $nut^{G_1}_1$ and a node $v_2$ in $nut^{G_2}_1$ such that, if we assign an unique weight to $v_1$ and $v_2$, the updated weighted graph $G_1$ and $G_2$ share the exactly same canonical number.
12: If we cannot find $v_1$ and $v_2$, the algorithm fails.
13: We update the $nodeweigh_1$ and $nodeweigh_2$: $nodeweigh_1 \leftarrow newNodeweigh_1$, $nodeweigh_2 \leftarrow newNodeweigh_2$
14: Go to Line 2, repeat the procedure.
5.2 Experimental Setup

Our experiments are designed to validate the following two questions.

– **Question 1.** In our graph isomorphism testing algorithm, we claimed that every graph obtains a unique canonical number generated by our algorithm. Is our algorithm effective for all graphs in the datasets?

– **Question 2.** Can our NutCracker algorithm find the correspondence between two isomorphic graphs?

We design our first experiment to answer Question 1 as follows. First, we run our canonical number algorithm on all datasets and generate an entry for each graph in the format of index number and the canonical number. Second, for all graphs with the same vertices, we sort them by the canonical numbers and find the most similar pairs where the similarity is the difference between its canonical numbers. For a pair of graphs, the less the distance is, the more similar they are.

We design our second experiment to answer Question 2. First, for every graph in our datasets, we generate a random permutation and apply the permutation to the original graph to generate an isomorphic graph. A pair of isomorphic graphs are then obtained. Second, we run our NutCracker algorithm on every isomorphic graph pair. If we find the correspondence, we verify that the correspondence is indeed an isomorphic correspondence between the two isomorphic graphs in the pair. However, if the correspondence found by the algorithm fails the verification, an error is output.

Our two programs are written in Java, with roughly 1,500 lines of code each. We carry out all our experiments on a single node of Washington State University’s high performance computing cluster. The node is an IBM dx360 computer which consists of six cores with 2.67GHz and 24 GB physical memory.

5.3 Results

**Canonical Number algorithm** For strongly regular graphs, every graph in this dataset obtained a unique canonical number from our algorithm. The program implementing the algorithm took \( \approx 12 \) hours to compute the entire dataset of the 40,000 strongly regular graphs.

For the dataset of 11,000,000 connected graphs of ten nodes, every graph also obtained a unique canonical number from our algorithm. The program took \( \approx 26 \) hours to compute the entire dataset. But, canonical numbers of a small number of graphs had an extremely small difference. For these graphs, it is better to use a multi-precision version of our program to re-verify them (N.b. Java does not have a multi-precision matrix library). We re-implemented the algorithm in MATLAB and used its high-precision symbolic package to verify that, for these graphs, the canonical numbers were indeed canonical (hence our algorithm is correct for the dataset).
**NutCracker algorithm** For strongly regular graphs, every graph in this dataset can find the isomorphic correspondence successfully, using the Java program implementing our algorithm. It took $\approx 12$ hours to compute the entire dataset of 40,000 strongly regular graphs. For the dataset of 11,000,000 connected graphs of ten nodes, under the Java double number precision using 8 digits of scientific representation, the program can find the isomorphic correspondence successfully for every pair of the graph in the dataset and its randomly permuted version, except for two graphs in the dataset. Applying 9 digits of precision, the algorithm finds the correspondence of the two graphs successfully. The algorithm took $\approx 26$ hours to compute through the entire dataset of 11,000,000 graphs.

### 5.4 Discussions

In the above experiments, our algorithms are correct for all the datasets. But, it is still possible that there exists some graphs where our heuristic algorithms may fail. The readers are welcome to use our algorithms to identify a counter example to help us more deeply understand the GI problem.

In our algorithms we use the free energy, which is a real number, to distinguish between all non-isomorphic graphs. It is known that most programming languages, such as Java, only provide double float numbers to conduct computation on real numbers. The eigen-decomposition uses complicated numerical algorithms. In the process, the precision error may be propagated from one stage to another. We spent some efforts to minimize such precision errors. But, fundamentally, Java needs a higher-precision matrix library to avoid such errors.

### 6 Applications and Future work

#### 6.1 Graph mining

As the popularity of social networks and fast development of knowledge graphs grows, graph mining will become an emerging research focus of data mining. In graph mining, there are at least two important research topics. One problem is mining frequent or common subgraphs and the other is graph clustering. For mining frequent or common subgraphs, it is possible that there exists a type of weight assignment encoding such that, after applying the encoding technique, the number of frequent subgraphs contained in a graph can be indicated by the free energy.

For graph clustering, one of the most widely used algorithm is the Markov clustering algorithm, which depends on flow simulation [23]. Applying our canonical number algorithms to graph clustering problem, the clustering problem become the simplest clustering problem—one-dimensional clustering. Also, we need to point out that the weight assignment methods are not unique and can be adapted to real world requirements.
6.2 Cheminformatics and Bioinformatics

In cheminformatics, it is an important topic that, given the spatial structure of a compound, it is efficient to find the compound in a database that only stores spatial structures. In bioinformatics, we only need to replace the compound with a protein. Our algorithms in this paper can be used to implement a tool to resolve such queries.

6.3 Future work

Our future work consists of several parts. First, we need to mathematically prove the correctness of our algorithms or find the limitation (i.e. a counter example) of our algorithms. Second, we will try to find simpler and more efficient free energy encoding strategies. Third, we will apply our theory to solve real world problems in graph mining, cheminformatics, and bioinformatics.

Acknowledgements

We would like to thank William J. Hutton III for discussions. We also would like to thank WSU High Performance Computing for providing resource to carry out our experiments.

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