Mapping Induced Subgraph Isomorphism Problems to Ising Models and Its Evaluations by an Ising Machine

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SUMMARY Ising machines have attracted attention as they are expected to solve combinatorial optimization problems at high speed with Ising models corresponding to those problems. An induced subgraph isomorphism problem is one of the decision problems, which determines whether a specific graph structure is included in a whole graph or not. The problem can be represented by equality constraints in the words of combinatorial optimization problem. By using the penalty functions corresponding to the equality constraints, we can utilize an Ising machine to the induced subgraph isomorphism problem. The induced subgraph isomorphism problem can be seen in many practical problems, for example, finding a particular malicious circuit in a device or particular network structure of chemical bonds in a compound. However, due to the limitation of the number of spin variables in the current Ising machines, reducing the number of spin variables is a major concern. Here, we propose an efficient Ising model mapping method to solve the induced subgraph isomorphism problem by Ising machines. Our proposed method theoretically solves the induced subgraph isomorphism problem. Furthermore, the number of spin variables in the Ising model generated by our proposed method is theoretically smaller than that of the conventional method. Experimental results demonstrate that our proposed method can successfully solve the induced subgraph isomorphism problem by using the Ising-model based simulated annealing and a real Ising machine.

key words: induced subgraph, isomorphism problem, Ising machines, Ising model, annealing machine, quadratic unconstraint binary optimization

1. Introduction

1.1 Ising Machines

Ising machines, which are also referred to as Ising model-based computers or annealing machines, have attracted attention as they are expected to solve combinatorial optimization problems at high speed with Ising models corresponding to those problems\([1]–[6]\). These combinatorial optimization problems are to search for the optimal combination of decision variables that maximizes or minimizes the objective function among a given set of decision variables under the given constraints.

As increasing the number of given decision variables in these combinatorial optimization problems, it has become more difficult to obtain an optimal or a sub-optimal solution in a practical time with conventional von Neumann type computers. Ising machines are expected to solve these problems at high speed and obtain a nearly optimal solution by mapping these problems to Ising model, which imitates natural phenomena\([7]–[12]\).

1.2 Induced Subgraph Isomorphism Problem

The induced subgraph isomorphism problem is a decision problem, which determines whether a specific graph structure is included in a whole graph or not\([13]\). If the specific graph structure is included in a whole graph, the specific graph is called an induced subgraph. The problem can be represented by equality constraints in the words of combinatorial optimization problem. By using the penalty functions correspond to the equality constraints, we can utilize an Ising machine to solve the induced subgraph isomorphism problem. The problems appear in many practical scenes, for example, finding a particular malicious circuit in a device or particular network structure of chemical bonds in a compound. In general, an induced subgraph isomorphism problem is known as an NP-complete problem, because it includes a maximum clique problem\([14], [15]\).

The Ising model mapping method to solve an induced subgraph isomorphism problem has been proposed in\([16]\). Let \(n\) and \(m\) be the number of vertices in the induced subgraph and the number of vertices in the whole graph, respectively. Here, we assume \(n < m\). The conventional mapping method\([16]\) maps the induced subgraph isomorphism problem into the Ising model with \(nm + m\) spin variables. However, due to the limitation of the number of spin variables in the current Ising machines, reducing the number of spin variables is a major concern.

1.3 Our Proposal

In this paper, we propose an efficient Ising model mapping method which maps an induced subgraph isomorphism problem into the Ising model with \(nm\) spin variables, when
an induced subgraph with \( n \) vertices and a whole graph with \( m \) vertices are given.\(^1\) Firstly, we propose a model to utilize Ising machine for the induced subgraph isomorphism problem. The model includes the constraint terms and penalty terms, which minimizes the energy function or Hamiltonian of the Ising model, only when satisfying the equality constraints in the induced subgraph isomorphism problem. Secondly, we show that the Ising model generated by our proposed method uses the smaller number of spin variables than the Ising model by the conventional method [16]. Lastly, we demonstrate the experimental results to solve induced subgraph isomorphism problems by our proposed method.

### Contributions

The contributions of this paper are summarized as follows:

1. We consider an induced subgraph isomorphism problem, where an induced subgraph with \( n \) vertices and a whole graph with \( m \) vertices are given. The conventional method [16] maps the problem into an Ising model which requires \( nm + m \) spin variables. On the other hand, our proposed method maps the problem into an Ising model which requires only \( nm \) spin variables.

   Our proposed method can contribute to reducing the number of spin variables, which is a major concern because there is a limitation of the number of spin variables of the Ising machines. Reducing the number of spin variables could also reduce the computation time as in Sect. 4.1.

2. Our proposed method can successfully obtain the solution to the induced subgraph isomorphism problem using the Ising-model based simulated annealing and a real Ising machine. In addition, our proposed method outperforms the conventional method [16].

### Problem Formulation

The induced subgraph isomorphism problem is a decision problem, which determines whether a specific graph structure is included in a whole graph. This problem is formulated as follows: Let \( G = (V, E) \) be an undirected graph, where \( V \) and \( E \) are the set of vertices and the set of edges, respectively. If there is an edge between two vertices \( u, v \in V \), the edge is expressed by \((u, v) \in E\). We define an adjacency matrix \( A \), which represents the edges between vertices on the graph \( G = (V, E) \), as follows:

\[
A = \begin{bmatrix}
a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\
a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\
a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n}
\end{bmatrix},
\]

(1)

\(^1\)The preliminary version of this paper appeared in [17]. Particularly, Sects. 4 and 5 are fully extended so that the effectiveness of the proposed method is confirmed.

where

\[
a_{i,j} = \begin{cases} 
1 & \text{(vertex } i \text{ and vertex } j \text{ are connected)} \\
0 & \text{(vertex } i \text{ and vertex } j \text{ are unconnected)} 
\end{cases}
\]

(2)

We consider two graphs \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \), where \( |V_2| = m > |V_1| = n \geq 2 \). Here, \( |V_1| \) means the number of vertices in \( V_1 \), and then \( |V_1| = n \) means that the graph \( G_1 \) has \( n \) vertices. Let \( A_1 \) and \( A_2 \) be the adjacency matrix of \( G_1 \) and the adjacency matrix of \( G_2 \), respectively. Let \( X \) be an \( n \times m \) permutation matrix, which maps \( G_1 \)'s vertices to \( G_2 \)'s vertices, as follows:

\[
X = \begin{bmatrix}
x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,m} \\
x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,m} \\
x_{3,1} & x_{3,2} & x_{3,3} & \cdots & x_{3,m} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
x_{n,1} & x_{n,2} & x_{n,3} & \cdots & x_{n,m}
\end{bmatrix}.
\]

(3)

where

\[
x_{i,j} = \begin{cases} 
1 & \text{(} i \in V_1 \text{ is mapped to } v \in V_2 \text{)} \\
0 & \text{(otherwise)}
\end{cases}
\]

The permutation matrix \( X \) corresponds to the injection function from a vertex in \( G_1 \) to a vertex in \( G_2 \).

The induced subgraph isomorphism problem is defined as follows: [14], [15]

**Definition 1:** Given two graphs, \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \), where \( |V_2| = m > |V_1| = n \geq 2 \), and their graph’s adjacency matrices \( A_1 \) and \( A_2 \), the induced subgraph isomorphism problem is to determine whether a permutation matrix \( X \) satisfying \( XA_2X^T = A_1 \) exists or not.

**Example 1:** We consider the graph \( G_1 = (V_1, E_1) \) with four vertices and the graph \( G_2 = (V_2, E_2) \) with nine vertices as shown in Fig. 1. The adjacency matrices \( A_1 \) and \( A_2 \) are expressed as follows:

\[
A_1 = \begin{bmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 \\
0 & 1 & 0 & 0
\end{bmatrix}
\]

(4)

\[
A_2 = \begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0
\end{bmatrix}
\]

(5)

When the permutation matrix \( X \) is given by the form shown in Fig. 1, \( XA_2X^T = A_1 \) is satisfied. In this example, \( G_1 \) is an induced subgraph of \( G_2 \). In other words, \( G_2 \) includes
G1 as an induced subgraph inside. In Fig. 1, the vertices corresponding to G1 in G2 are depicted in blue.

3. Ising Model Mapping of Induced Subgraph Isomorphism Problem

3.1 Ising Model and QUBO

The Ising model is one of basic models in statistical mechanics to investigate the cooperative phenomena of many-body systems [10]. The Ising model is defined on an undirected graph $G_1 = (V_1, E_1)$ as shown in Fig. 2, where $V_1$ is a set of vertices and $E_1$ is a set of connecting edges between vertices. In the Ising model, a spin exists on each vertex. Every spin has a value of either +1 or −1. Let $h_i$ be the external magnetic field acting on the spin $\sigma_i$. Let $J_{ij}$ be the interaction coefficient between the two spins $\sigma_i$ and $\sigma_j$. Here, $h_i$ and $J_{ij}$ are real values. By using these variables, the energy function $\mathcal{H}$, called as Hamiltonian, of the Ising model is defined by

$$\mathcal{H} = - \sum_{i \in V_1} h_i \sigma_i - \sum_{(i,j) \in E_1} J_{ij} \sigma_i \sigma_j. \quad (6)$$

According to the principle in physics, the lowest energy state called the ground state is the most stable state. Ising machines behave stochastically to search the ground state of the Ising model.

For convenience, let us introduce a binary variable $n_i$ taking either 1 or 0 instead of using the spin $\sigma_i$. The energy function in the form of using binary variables is called Quadratic Unconstrained Binary Optimization (QUBO). The binary variable $n_i$ and the spin variable $\sigma_i$ are transformed by

$$n_i = \frac{\sigma_i + 1}{2}. \quad (7)$$

In addition, by substituting Eq. (7) into Eq. (6), the energy function $\mathcal{H}$ of QUBO is obtained by

$$\mathcal{H} = - \sum_{i \in V_1} c_i n_i - \sum_{(i,j) \in E_1} q_{ij} n_i n_j - \text{const}, \quad (8)$$

where $c_i$ is the coefficient of linear term acting on the variables $n_i$, $q_{ij}$ is the interaction coefficient between the two binary variables $n_i$ and $n_j$, and const represents a constant which does not depend on the values of binary variables. Thus, the Ising model can be considered to be equivalent to QUBO, and this paper discusses Ising model mapping of the induced subgraph isomorphism problem using QUBO.

3.2 Ising Model Mapping of Induced Subgraph Isomorphism Problem

In this Subsection, we propose a method to map the induced subgraph isomorphism problem into the Ising model using QUBO. As explained in Sect. 2, every variable $x_{ij}$ in a permutation matrix $X$ takes either 1 or 0, where $1 \leq i \leq n$ and $1 \leq j \leq v \leq m$. We construct the energy function $\mathcal{H}$ in the QUBO form, so that there exists a permutation matrix $X$ obtained by the binary variables in the ground state of $\mathcal{H}$ if and only if a query graph $G_1$ is an induced subgraph in the whole graph $G_2$.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be an induced subgraph and a whole graph, respectively, where $|V_2| = m > |V_1| = n \geq 2$. Let $A_1$ and $A_2$ be adjacency matrices of $G_1$ and $G_2$, respectively. Let $X$ be the permutation matrix for mapping from $G_1$ to $G_2$. The energy function $\mathcal{H}$ generated by our proposed method consists of four terms $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C$, and $\mathcal{H}_D$.

3.2.1 Step 1. Induced Subgraph’s Vertex Assignment Constraint $\mathcal{H}_A$

This constraint determines the injective correspondence from the vertex of $G_1$ to the vertex of $G_2$. Since the number of vertices in $G_1$ is less than the number of vertices in $G_2$, i.e., $n < m$, each vertex on $G_1$ must correspond to one vertex on $G_2$ without duplication. Therefore, only one “1” must appear in each row of the permutation matrix $X$. The constraint that only one “1” appears in each row of the permutation matrix $X$ can be expressed as follows:

$$\sum_{i=1}^{m} x_{i,v} = 1 \quad (1 \leq i \leq n). \quad (9)$$
As shown in Fig. 1(b), only one “1” appears in each row of the permutation matrix \( X \). To represent the constraint using QUBO, we introduce the term as follows:

\[
\left( 1 - \sum_{i=1}^{n} x_{i,v} \right)^2 \quad (1 \leq i \leq n). \tag{10}
\]

This term takes the minimum value of 0 if and only if Eq. (9) is satisfied. Since Eq. (10) must be minimized for all the rows of the permutation matrix \( X \), we introduce the energy function \( \mathcal{H}_A \) as follows:

\[
\mathcal{H}_A = \sum_{i=1}^{n} \left( 1 - \sum_{v=1}^{m} x_{i,v} \right)^2. \tag{11}
\]

**Example 2:** Considering the example of Fig. 1, the induced subgraph’s vertex assignment constraint \( \mathcal{H}_A \) is given by

\[
\mathcal{H}_A = \sum_{i=1}^{4} \left( 1 - \sum_{v=1}^{9} x_{i,v} \right)^2 = \sum_{i=1}^{4} \left( 1 - 2 \sum_{v=1}^{9} x_{i,v} + \sum_{v=1}^{9} \sum_{u=1}^{9} x_{i,u} x_{i,v} \right) = 4 - 2 \sum_{i=1}^{4} \sum_{v=1}^{9} x_{i,v} + \sum_{i=1}^{4} \sum_{v=1}^{9} \sum_{u=1}^{9} x_{i,u} x_{i,v}. \tag{12}
\]

Figure 3 depicts the Ising model given by Eq. (12).

### 3.2.2 Step 2. Graph’s Vertex Assignment Constraint \( \mathcal{H}_B \)

This constraint determines the correspondence from the vertex of \( G_2 \) to the vertex of \( G_1 \). Since the number of vertices in \( G_2 \) is more than the number of vertices in \( G_1 \), i.e., \( m > n \), not every vertex on \( G_2 \) has to correspond to one vertex on \( G_1 \) without duplication. Therefore, this constraint differs from the induced subgraph’s vertex assignment constraint, which is introduced before. In summary, each column of the permutation matrix \( X \) takes only one “1” or all “0”s. This constraint can be expressed as follows:

\[
\sum_{i=1}^{n} x_{i,v} \in \{0, 1\} \quad (1 \leq v \leq m). \tag{13}
\]

For example, as shown in Fig. 1(b), only one “1” appears in the second column of the permutation matrix \( X \), whereas all the values in the third column are “0”.

To represent the constraint using QUBO, we introduce the term as follows:

\[
\left( \frac{1}{2} - \sum_{i=1}^{n} x_{i,v} \right)^2 \quad (1 \leq v \leq m). \tag{14}
\]

This term takes the minimum value of 1/4, if and only if Eq. (13) is satisfied. Since Eq. (14) must be minimized for all the columns of the permutation matrix \( X \), we introduce the energy function \( \mathcal{H}_B \) as follows:

\[
\mathcal{H}_B = \sum_{i=1}^{m} \left( \frac{1}{2} - \sum_{i=1}^{n} x_{i,v} \right)^2. \tag{15}
\]

### 3.2.3 Step 3. Connection Increase Prohibition Constraint \( \mathcal{H}_C \)

Consider that the graph \( G_1 \) is mapped to the graph \( G_2 \) using the permutation matrix \( X \). In this case, if there is no connection between two vertices in \( G_1 \), there must also be no connection between the two mapped vertices in \( G_2 \). We define this constraint as the connection increase prohibition constraint.

To represent the constraint using QUBO, we introduce a penalty term which can be minimized if and only if the constraint is satisfied. Let us consider two vertices \( u \) and \( v \) in \( G_2 \) which are mapped from \( i \) and \( j \) in \( G_1 \), respectively. Assume that the edge \((i, j)\) does not exist in \( G_1 \) but the edge \((u, v)\) exists in \( G_2 \). If \( G_1 \) is an induced subgraph of \( G_2 \), such a case is prohibited, i.e., this case does not satisfy the connection increase prohibition constraint.

To validate the constant, we introduce the energy function \( \mathcal{H}_C \), which is minimized and takes 0 when the constraint is satisfied, as follows:

\[
\mathcal{H}_C = \sum_{(i,j) \notin E_1} \sum_{(a,b) \in E_2} x_{i,a} x_{j,b}. \tag{16}
\]

### 3.2.4 Step 4. Connection Decrease Prohibition Constraint \( \mathcal{H}_D \)

Consider that the graph \( G_1 \) is mapped to the graph \( G_2 \) using the permutation matrix \( X \). In this case, if there is a connection between two vertices in \( G_1 \), there must also be a connection between the two mapped vertices in \( G_2 \). We define this constraint as the connection decrease prohibition constraint.

This constraint term can be introduced in the same way as the discussion of \( \mathcal{H}_C \). We introduce the energy function \( \mathcal{H}_D \), which is minimized and takes 0 when the constraint is satisfied, as follows:

\[
\mathcal{H}_D = \sum_{(i,j) \in E_1} \sum_{(a,b) \notin E_2} x_{i,a} x_{j,b}. \tag{17}
\]
3.2.5  Step 5. Total Energy Function

The total energy function is given by the weighted sum of the energy functions in Eqs. (11), (15), (16), and (17) as follows:

\[ H = \alpha H_A + \beta H_B + \gamma H_C + \delta H_D, \quad (18) \]

where \( \alpha, \beta, \gamma, \) and \( \delta \) are positive-valued hyperparameters.

The total energy function is given by the weighted sum of the energy functions in Eq. (18) in the ground state becomes \( \beta m/4 \).

\[ H_A = 0, \quad (19) \]
\[ H_B = \frac{m}{4}, \quad (20) \]
\[ H_C = 0, \quad (21) \]
\[ H_D = 0. \quad (22) \]

The total energy function is given by the weighted sum of the energy functions in Eq. (18). Therefore, the minimum value is obtained by:

\[ H = \alpha H_A + \beta H_B + \gamma H_C + \delta H_D \]
\[ = \frac{\beta m}{4}. \quad (23) \]

Lemma 1: If \( G_1 \) is an induced subgraph of \( G_2 \), the energy function \( H \) given by Eq. (18) in the ground state becomes \( \beta m/4 \).

Proof: According to Sects. 3.2.1 to 3.2.4, when the permutation matrix \( X \) in the given induced subgraph isomorphism problem exists, Eqs. (11), (15), (16), and (17) are minimized in the ground state. If this is the case, the minimum values of Eqs. (11), (15), (16), and (17) are calculated as follows:

\[ H_A = 0, \quad (19) \]
\[ H_B = \frac{m}{4}, \quad (20) \]
\[ H_C = 0, \quad (21) \]
\[ H_D = 0. \quad (22) \]

The total energy function is given by the weighted sum of the energy functions in Eq. (18). Therefore, the minimum value is obtained by:

\[ H = \alpha H_A + \beta H_B + \gamma H_C + \delta H_D \]
\[ = \frac{\beta m}{4}. \quad (23) \]

Lemma 2: If the energy function \( H \) given by Eq. (18) becomes \( \beta m/4 \), \( G_1 \) is an induced subgraph of \( G_2 \).

Proof: We prove this lemma by proving the contraposition that, if the solution of the induced subgraph isomorphism is false, the energy function \( H \) must not become \( \beta m/4 \).

We assume that \( G_1 \) is not an induced subgraph of \( G_2 \). Since there does not exist any permutation matrix \( X \) satisfying all of four constraints discussed in Sects. 3.2.1 to 3.2.4, at least either one of these four constraint terms (Eqs. (11), (15), (16), and (17)) does not take the minimum value. In other words, at least either one of \( H_A > 0, H_B > m/4, H_C > 0, \) or \( H_D > 0 \) holds true. Hence \( H > \beta m/4 \) is satisfied.

Based on the lemmas 1 and 2 above, we can lead the following theorem:

**Theorem 1:** When the induced subgraph isomorphism problem is mapped to Eq. (18), \( G_1 \) is an induced subgraph of \( G_2 \) if and only if Eq. (18) takes the minimum value of \( \beta m/4 \).

**Proof:** The lemmas 1 and 2 clearly lead to the theorem. □

We can further obtain the following theorem:

**Theorem 2:** When the induced subgraph isomorphism problem is mapped to Eq. (18), the number of required binary variables is just \( nm \).

**Proof:** As discussed in Sects. 3.2.1 to 3.2.4, we just use the binary variables corresponding to the permutation matrix \( X \). Hence, we require \( nm \) binary variables in Eq. (18). □

As described in Sect. 1, the conventional mapping method [16] requires \( nm + m \) variables and thus our proposed method can reduce them to \( nm \) binary variables.

4. Experiments

In this Section, we perform two experiments by using different machines. In the first experiment, we compare the performance of our method with that of the method proposed in the previous study [16] for small-scaled problems by using the Ising-model based simulated annealing (SA) [18]. Herein, we refer to the Ising-model based SA as QUBO-based SA since we consider the QUBO form given by Eq. (18). As will be explained later, we find that our method outperforms the method proposed in the previous study. In the second experiment, we examine the performance of our method for large-scaled problems by using a real Ising machine [5].

4.1 Small-Scaled Problems by Using the QUBO-Based Simulated Annealing

4.1.1 Preparation of Problems

First, we randomly generate several graph pairs, where one of the graphs in each pair is an induced subgraph of the other graph. We set the density of edges of the graphs to be 1/2. In each graph pair, a smaller graph has 5 to 10 vertices and a larger graph has 10 to 100 vertices. We map every induced subgraph isomorphism problem given by each graph pair to QUBO using our method (Eq. (18)). The QUBOs have binary variables of the range from 50 to 1000. All of Eqs. (11), (15), (16), and (17) are constraint terms. We set the hyperparameters as \( \alpha = 1, \beta = 1, \gamma = 1, \) and \( \delta = 1 \).

For comparison, we also implement the same induced subgraph isomorphism problems to QUBO by using the conventional method [16] (see the discussion below in detail). The QUBOs have binary variables of the range from 60 to 1100. Note that the number of binary variables of our
method is smaller than that of the method proposed in the previous study [16].

4.1.2 Method

In this experiment, we use a QUBO-based SA to obtain the ground state. The QUBO-based SA consists of four steps as follows:

(1) Set the initial values of binary variables randomly. The initial temperature $T_0$ is set to be a larger value than the values in the Hamiltonian.

(2) Pick up one binary variable randomly. Let $\Delta E$ be the energy difference defined by $\Delta E = E_{\text{trial}} - E_{\text{current}}$, where $E_{\text{trial}}$ is the energy after flipping the binary variable and $E_{\text{current}}$ is the energy of the current state. If $\Delta E < 0$, we flip the binary variable. If $\Delta E \geq 0$, we flip the binary variable with the probability given by $p = \exp(-\Delta E / T_k)$, where $T_k$ is the temperature at $k$-th outer iteration. This method is called the Metropolis method.

(3) Repeat (2), “Inner loop” times. Update the temperature $T_{k+1} = rT_k$, where $k$ is the number of outer iterations and $r$ is the cooling rate.

(4) Repeat (2) and (3), “Outer loop” times.

In this experiment, we attempt 100 trials for each induced subgraph isomorphism problem and count how many times we obtain the ground state. We set the parameters as shown in Table 1. The reason of the choice of parameters is as follows. The initial temperature is large enough to permit the transition between arbitrary states in the beginning of the SA process. The cooling rate, inner loop, and outer loop are set so that the final temperature is small enough compared to the parameters in QUBO. This setting is expected to increase the probability of obtaining the ground state.

The QUBO-based SA is implemented in C++ running on CentOS 7.6.1810 on 2.10GHz Intel Xeon Gold 6130 with 755GB of memory.

4.1.3 Results

Table 2 summarizes the experimental results using the QUBO-based SA. Each column is as follows:

- $N_{H_{\text{min}}}$: The number of the ground states obtained using the QUBO-based SA. Here $H_{\text{min}}$ is the energy value of the ground state.
- Time: Time to attempt 100 trials and obtain each answer.
- TTS: Time to solution (TTS), where $p = 0.99$. The definition of TTS will be shown just below.

We calculate the time to solution (TTS). TTS is defined by

$$TTS(p) = \frac{\ln(1 - p)}{\ln(1 - P_0)},$$

where $\tau$ is the time per one annealing trial, $p$ is a predetermined precision to attain the ground state and $P_0$ is the probability for attaining the ground state. TTS is often used as an indicator of the optimization performance in the community of Ising machines [5], [19]. We calculate TTS(0.99) of our proposal method and the conventional method [16] in Table 2 in order to compare the performance of both methods. In the successful cases with $P_0 = 1$, we write the actual computational time instead of the TTS(0.99) in Table 2.

Figure 4 shows the relation between the number of spin variables and computation time of the experimental results shown in Table 2. Because the computation time is almost proportional to the number of spin variables as shown in Fig. 4 using the QUBO-based SA, reducing the variables could also reduce the computation time. Note that, the large increase in computation time after 1000 spin variables is due to the computational environment, such as the data structure of the variable-length data array used in our implemented C++ code and the capacity of the CPU’s cache memory. Note also that, although Table 2 and Fig. 4 show the results using the QUBO-based SA on the conventional computer, the probability of obtaining the ground states decreases as the system size, i.e., the number of spin variables, increases according to [20]. Overall, we can conclude that reducing the spin variables can contribute to improving the Ising machine performance.

In Table 2, TTSs do not simply increase and decrease at the same rate as the number of spin variables, because TTSs are calculated by using trial times and the number of the ground states obtained as defined by Eq. (25). The computation time is almost proportional to the number of spin variables as shown in Fig. 4. On the other hand, the probability of obtaining the ground states decreases as the system size increases according to [20]. Further, the probability of obtaining the ground states depends not only on the system size, but also on the individual problem instances. Hence, in
Table 2 The QUBO-based SA experimental results.

| #vertices $(n, m)$ | #spins | $N_{H_{\text{min}}}$ | Time [s] | TTS [s] |
|-------------------|--------|----------------------|---------|--------|
| Proposed method:  |
| (5,10)            | 50     | 96                   | 1392    | 2.0 x 10^4 |
| (5,20)            | 100    | 100                  | 2528    | 2.5 x 10^4 |
| (5,50)            | 250    | 100                  | 5961    | 6.0 x 10^4 |
| (10,25)           | 250    | 3                    | 5970    | 9.0 x 10^3 |
| (10,40)           | 400    | 23                   | 9550    | 1.7 x 10^4 |
| (10,50)           | 500    | 53                   | 11717   | 7.1 x 10^2 |
| (10,60)           | 600    | 68                   | 14128   | 5.7 x 10^2 |
| (10,70)           | 700    | 81                   | 16653   | 4.6 x 10^2 |
| (10,80)           | 800    | 98                   | 19257   | 2.3 x 10^2 |
| (10,100)          | 1000   | 100                  | 46268   | 4.6 x 10^2 |

Method [16]:
| (5,10)            | 60     | 90                   | 1617    | 3.2 x 10^4 |
| (5,20)            | 120    | 98                   | 2984    | 3.5 x 10^4 |
| (5,50)            | 300    | 96                   | 7133    | 1.0 x 10^2 |
| (10,25)           | 275    | 2                    | 6560    | 1.5 x 10^4 |
| (10,40)           | 440    | 7                    | 10360   | 6.6 x 10^3 |
| (10,50)           | 550    | 14                   | 12919   | 3.9 x 10^3 |
| (10,60)           | 660    | 14                   | 15186   | 4.8 x 10^3 |
| (10,70)           | 770    | 28                   | 18569   | 2.6 x 10^3 |
| (10,80)           | 880    | 44                   | 20634   | 1.6 x 10^3 |
| (10,100)          | 1100   | 74                   | 49339   | 1.7 x 10^3 |

$N_{H_{\text{min}}}$: The number of the ground states obtained using the QUBO-based SA among 100 trials.
Time: Time to attempt 100 trials and obtain each answer.
TTS: Time to solution, where $p = 0.99$ (see Eq. (25)). * indicates the actual computation time instead of TTS.

Table 2, we can observe the following two points:

1. For any of the problems selected in this experiment, the proposed method could obtain higher probability of obtaining the ground states than the conventional method [16].
2. For any of the problems selected in this experiment, the proposed method could obtain the answers at faster speed than the conventional method [16].

In this experiment, the maximum number of vertices in the graph $G_1$ is 10 and that of the graph $G_2$ is 100. In this case, our proposal method requires 1000 spin variables. On the other hand, the conventional method [16] requires 1100 spin variables.

4.2 Large-Scaled Problems by Using a Real Ising Machine

4.2.1 Preparation of Problems

We prepare some problems in a similar way as in the previous Subsection. First, we randomly generate several graph pairs, where one of the graphs in each pair is an induced subgraph of the other graph. We set the density of edges of the graphs to be 1/2. In each graph pair, a smaller graph has 10 to 40 vertices and a larger graph has 100 to 400 vertices. We map every induced subgraph isomorphism problem given by a graph pair to QUBO using Eq. (18) based on our proposed mapping method. The QUBOs have binary variables of the range from 1000 to 8000. Difference in preparation of problems from the previous Subsection is as follows. Here, we prepare different ten problems on each same input-graph size in order to eliminate the dependence of particular problem’s condition. We attempt 100 trials for each induced subgraph isomorphism problem and count how many times we obtain the ground state and then average it.

Here we set the hyperparameters in Eq. (18) are the same, i.e., $\alpha = \beta = \gamma = \delta = 1$.

4.2.2 A Real Ising Machine

We utilize a real Ising machine to solve the induced subgraph isomorphism problems. The Ising machine used in this experiment has 8192 spins on the complete graph as a maximum for the Ising model [5]. Setting parameters in the Ising machine are as follows: the number of replicas is equal to 100, is large enough to the state exchange. In addition, in our preliminary experiments, when the number of iterations is set to $10^9$, the ground state cannot be obtained. Thus, we set the number of iterations is $10^9$ which is the upper limit of the number of iterations of the Ising machine.

Here, the number of iterations, $10^9$, is the Ising machine’s upper limit of annealing iterations and the upper limit of problem scale of the Ising machine is 8192 spin variables.

4.2.3 Results

Table 3 summarizes the experimental results using the real Ising machine. Each column is as follows:

- $N_{H_{\text{min}}}$ [%]: The ratio of the ground states obtained using the Ising machine over $10 \times 100$ trials for each input-
graph size.

- Average time: Average time to attempt 100 trials and obtain each answer.
- TTS: Time to solution, where \( p = 0.99 \). The definition of TTS is given by Eq. (25).

The results show that our proposed method can successfully solve the induced subgraph isomorphism problems by using a real Ising machine. In other words, we can solve the induced subgraph isomorphism problem by using real Ising machines. Since our proposed method given by Eq. (18) is not limited to a specific Ising machine, it is expected that the induced subgraph isomorphism problem can be solved with other various Ising machines as well. We also calculate the TTS defined by Eq. (25), where \( p = 0.99 \). As well as in the previous Subsection, we write the actual computation time instead of TTS.

The Ising machine experimental results.

| #vertices \((n, m)\) | #spins | \(N_{\text{Max}}\) [%] | Average time [ms] | TTS [ms] |
|-------------------|--------|----------------|------------------|----------|
| (10, 100)         | 1000   | 100           | 202584           | 2.03 \times 10^4^* |
| (10, 200)         | 2000   | 100           | 204506.6         | 2.05 \times 10^3 |
| (20, 100)         | 2000   | 95.5          | 204558           | 3.04 \times 10^3 |
| (15, 200)         | 3000   | 97.3          | 215832.8         | 2.75 \times 10^3 |
| (30, 100)         | 3000   | 99.9          | 215400.9         | 1.44 \times 10^3 |
| (10, 400)         | 4000   | 100           | 216823.9         | 2.17 \times 10^3 |
| (40, 100)         | 4000   | 66            | 215417.3         | 9.20 \times 10^3 |
| (10, 500)         | 5000   | 100           | 222599           | 2.23 \times 10^3 |
| (10, 800)         | 8000   | 100           | 225021.8         | 2.25 \times 10^3 |
| (40, 200)         | 8000   | 11.1          | 225602.6         | 8.83 \times 10^4 |

\(N_{\text{Max}}\): The average probability of the ground states obtained using the real Ising machine.

Average time: Average time to attempt 100 trials and obtain each answer.

TTS: Time to solution, where \( p = 0.99 \). The definition of TTS is given by Eq. (25).

5. Conclusions

In this paper, we proposed an efficient Ising model mapping method to solve the induced subgraph isomorphism problem by Ising machines. The number of spin variables in the Ising model generated by our proposed method is theoretically smaller than that of the conventional method. Experimental results demonstrate that our proposed method can successfully solve the induced subgraph isomorphism problems using the QUBO-based simulated annealing and the real Ising machine. Our proposed method can solve the induced subgraph isomorphism problems with higher probability of obtaining the ground state, and faster than the previous study [16]. We can expect that we can solve a larger induced subgraph isomorphism problem by using more spin variables.

In the future, we will investigate the reason why we have poor performance in the cases of our experiment. In addition, we will consider the meaning of the states close to the ground state from a viewpoint of the given graphs.

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