Decomposed Quadratization:
Efficient QUBO Formulation for Learning Bayesian Network

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Abstract
Algorithms and hardware for solving quadratic unconstrained binary optimization (QUBO) problems have made significant recent progress. This advancement has focused attention on formulating combinatorial optimization problems as quadratic polynomials. To improve the performance of solving large QUBO problems, it is essential to minimize the number of binary variables used in the objective function. In this paper, we propose a QUBO formulation that offers a bit capacity advantage over conventional quadratization techniques. As a key application, this formulation significantly reduces the number of binary variables required for score-based Bayesian network structure learning. Experimental results on 16 instances, ranging from 37 to 223 variables, demonstrate that our approach requires fewer binary variables than quadratization by orders of magnitude. Moreover, an annealing machine that implement our formulation have outperformed existing algorithms in score maximization.

1 Introduction
A Bayesian network is a probabilistic graphical model that represents a joint probability distribution among random variables in a directed acyclic graph (DAG) (Pearl 1988). One class of associated computational problems is learning the graph structure of a Bayesian network from data. There are two principal approaches to Bayesian network structure learning: constraint-based and score-based (Kitson et al. 2023). Constraint-based algorithms construct graphs through conditional independence tests. Score-based approaches aim to find a DAG with the highest possible score. In this study, we focus on score-based approaches.

Bayesian network structure learning is NP-hard (Chickering, Heckerman, and Meek 2003). Many approaches have been proposed to improve accuracy and reduce execution time. For a small number of variables, some algorithms such as (Cussens 2011) are capable of identifying a DAG with the maximum score. For high-dimensional data, the standard methodology involves the use of approximate approaches. The hill climbing search method over the space of DAGs (Bouckaert 1994) remains competitive despite its simplicity. Approximate searches over the space of topological ordering (Teyssier and Koller 2005) are also well known as competitive algorithms.

Quadratic unconstrained binary optimization (QUBO) is capable of modeling a wide range of combinatorial optimization problems, including image synthesis in the field of computer vision (Kolmogorov and Rother 2007) and various machine learning tasks such as neural networks (Sadselli and Chin 2021) and decision trees (Yawata et al. 2022). QUBO can also be applied to score-based Bayesian network structure learning (O’Gorman et al. 2014). Note that constraint-based algorithms do not appear to be suitable for QUBO formulation. Recent developments in annealing machines have garnered significant attention for QUBO formulation. An annealing machine is a specialized hardware architecture designed to heuristically solve QUBOs (Yamamoto 2020). In particular, annealing machines based on semiconductor technology derived from simulated annealing have reportedly outperformed existing solvers in maximum cut problems (Matsubara et al. 2020).

The challenge of setting up a QUBO lies in reformulating the objective function into a quadratic polynomial using fewer binary variables. The greater the number of binary variables in a QUBO, the more difficult it generally becomes to solve. More practically, encoding a large number of binary variables onto the hardware circuit of an annealing machine is often infeasible. Quadratization is the common method of QUBO formulation (Heck 2018; Anthony et al. 2016; Boros, Crama, and Heck 2019). Algorithms have been developed to minimize the number of auxiliary variables for quadratization (Verma and Lewis 2020). However, quadratization still requires too many auxiliary variables for certain tasks, including Bayesian network structure learning. Consequently, there is a potential demand for a more efficient QUBO formulation method as an alternative to conventional quadratization.

In this study, we propose a QUBO formulation specifically designed to use fewer binary variables than quadratization. We demonstrate that this formulation offers significant advantages for learning Bayesian networks in terms of bit capacity. Figure 1 illustrates the overview of our approach. Experimental results on 16 instances, ranging from 37 to 223 variables, show that our formulation dramatically reduces the number of binary variables compared to (O’Gorman et al. 2014). These instances can be encoded on the circuit of
the Fujitsu Digital Annealer, a fully-coupled annealing machine with 100K bit capacity (Nakayama et al. 2021). The scores achieved by the Digital Annealer using our formulation were greater than those of existing approaches.

2 Preliminary

We describe a QUBO formulation for learning Bayesian networks, incorporating candidate parent sets into the approach of (O’Gorman et al. 2014). For indexed symbols, we assign the zero index to the empty set and ensure no overlap (e.g., \( W_{10} = \emptyset \) and \( \{W_{ij}\}_{i=0}^{\lambda_i} \) includes \( \lambda_i + 1 \) elements). Appendix A provides the list of symbols.

2.1 Bayesian Network Structure Learning

A Bayesian network, which is a graphical model composed of a DAG and its parameters, represents a joint probability distribution. Each vertex of the DAG corresponds to a random variable. Edges and parameters characterize conditional probability distributions. Let \( \mathcal{X} \equiv \{X_i\}_{i=1}^{n} \) denote the set of vertices, and \( \Pi_i \) denote the set of vertices with edges directed towards \( X_i \). A topological ordering of a graph exists if and only if the graph is a DAG (Cormen et al. 1990).

Definition 2.1. A topological ordering \( \prec \) is a binary relation between any two of vertices such that

\[ \begin{align*}
X_i \prec X_j \text{ and } X_j \prec X_k \Rightarrow X_i \prec X_k, \\
X_i \prec X_j \Rightarrow X_i \notin \Pi_j.
\end{align*} \]

The goal of score-based Bayesian network structure learning is to find a DAG with the maximum score. A score is the sum of local scores which only rely on the parent set of each vertex. Given complete data, the parent sets \( \Pi_1, \cdots, \Pi_n \) are optimized to maximize the score under the constraint that the graph \( \mathcal{G} \) corresponding to them is a DAG. This optimization is formulated as

\[
\text{maximize } \sum_{1 \leq i \leq n} \log S_i(\Pi_i) \text{ subject to } \mathcal{G} \text{ is a DAG},
\]

where \( S_i : 2^{\mathcal{X}\setminus\{X_i\}} \to \mathbb{R} \). For simplicity, we take \( S_i(W) = S_i(\emptyset) \) when \( |W| \) is greater than the maximum parent set size \( m \). The identification of candidate parent sets facilitates narrowing the search space by the relation between parent sets and local scores (de Campos and Ji 2010).

Definition 2.2. The candidate parent sets of \( X_i \) are defined as \( \{W \subseteq \mathcal{X} \setminus \{X_i\} \mid \forall W' \subseteq W \Rightarrow S_i(W') < S_i(W)\} \).

Let \( \{W_{ij}\}_{i=0}^{\lambda_i} \) denote the candidate parent sets of \( X_i \), and \( \mathcal{X}_i \) denote the union of them. Using the candidate parent sets, we can ignore the topological ordering of certain edges that do not produce cycles. Let \( \mathcal{E} \) denote the set of edges on possible cycles.

2.2 QUBO Formulation

QUBO is a mathematical optimization problem of minimizing a quadratic polynomial with binary variables. A pseudo-Boolean function maps binary-valued inputs to a real value. Every pseudo-Boolean function can be uniquely represented as a multilinear polynomial given by

\[
f(p) \equiv \sum_{V \in \mathcal{F}} \pi(V) \prod_{i \in V} p_i,
\]

where \( p \equiv (p_i)_{i=1}^{J} \in \{0,1\}^{J} \), \( \pi : 2^{\{1,\cdots,J\}} \to \mathbb{R} \setminus \{0\} \), \( \mathcal{F} \subseteq 2^{\{1,\cdots,J\} \setminus \{0\}} \), and we ignore the constant term. Quadratization is a major technique to convert a higher degree pseudo-Boolean function into a quadratic one using auxiliary variables \( q \equiv (q_i)_{i=1}^{J} \in \{0,1\}^{J} \).

Definition 2.3. The quadratization of \( f \) is a quadratic polynomial function \( g : \{0,1\}^{J} \times \{0,1\}^{J} \to \mathbb{R} \) such that

\[
f(p) = \min_{q \in \{0,1\}^{J}} g(p, q).
\]

Rosenberg 1975 has proven that every pseudo-Boolean function can be transformed into a quadratic polynomial through the substitution of the product of two variables with an auxiliary variable and the addition of a penalty term.

2.3 QUBO Formulation for Structure Learning

Bayesian network learning can be uniquely represented by a multilinear polynomial over the state of edges and topological ordering. The state of \( d \equiv ((d_{ij})_{i=1}^{n})_{i=1}^{n} \) is mapped
one-to-one to the set of edges, where \( d_{ij} = 1 \) if \( X_j \) is a parent of \( X_i \); otherwise, \( d_{ij} = 0 \). The score component is
\[
O(d) = \sum_{1 \leq i \leq n} \sum_{W_i \subseteq X_i} \pi_i(W) \prod_{1 \leq i \leq n, X_j \in W} d_{ij},
\]
where \( \pi_i(W) = \sum_{W' \subseteq W} (-1)^{|W'|-|W|} \log S_i(W') \). The higher-degree terms in the score component can be transformed into quadratic terms through quadratization. The state of \( r \equiv (r_{ij})_{i,j} \in \mathcal{E} \) corresponds to the topological ordering, where \( r_{ij} = 0 \) if the order of \( X_j \) is higher than \( X_i \); otherwise, \( r_{ij} = 1 \). The linear ordering of vertices and the consistency of edges in definition 2.1 are captured by
\[
C(d, r) = \sum_{(i,j), (j,k), (i,k) \in \mathcal{E}} \delta_1 R(r_{ij}, r_{jk}, r_{ik}) + \sum_{(i,j) \in \mathcal{E}} \delta_2 (d_{ij} r_{ij} + d_{ji} (1 - r_{ij}))
\]
where \( \delta_1, \delta_2 \in (0, \infty) \) and \( R(r_{ij}, r_{jk}, r_{ik}) \equiv r_{ik} + r_{ij} r_{jk} - r_{ij} r_{ik} - r_{jk} r_{ik} \). There exist \( \delta_1, \delta_2 \) such that \( C(d, r) = 0 \) when the objective function \( O(d) + C(d, r) \) is minimized. Additionally, the graph corresponding to the state of \( d \) is a DAG if \( C(d, r) = 0 \). Consequently, this QUBO formulation is equivalent to learning Bayesian networks.

3 Decomposed Quadratization

Searching over candidate parent sets is a key technique in Bayesian network structure learning. To deal with candidate parent sets in a QUBO formulation, we use auxiliary variables corresponding to the sets of primary variables. The auxiliary variables capture the score component and identify the state of primary variables. We decompose a quadratization into the optimization of auxiliary variables and the transformation that maps them to primary variables. This decomposition of quadratization is defined as

**Definition 3.1.** The decomposed quadratization of \( f \) is the pair of a function \( g_1 : \{0, 1\}^J \rightarrow \{0, 1\}^J \) and a quadratic polynomial function \( g_2 : \{0, 1\}^J \rightarrow \mathbb{R} \) such that
\[
f(p) = \min_{q \in \{0, 1\}^J : p = g_1(q)} g_2(q).
\]

**Example 3.2.** Let \( g_1(q_1, q_2) = (q_1, q_2, q_2) \) and \( g_2(q_1, q_2) = -q_1 - 3q_2 + 2q_1 q_2 \). Then \( g_1(q_1, q_2) \) is a decomposed quadratization of \( f(p_1, p_2, p_3) = -p_1 - 3p_2 + 2p_1 p_2 p_3 \).

Here we describe the behavior of decomposed quadratization. Considering the case where each \( p_i \) corresponds to \( q_i \), the concept of decomposed quadratization encompasses quadratization. To capture the subsets of the terms in \( F \), we make a set \( Q_i \subseteq \{1, \cdots, J\} \) correspond to a binary variable \( q_i \in \{0, 1\} \) one-to-one. Let \( \bar{g}_1, \bar{g}_2 \) denote
\[
\bar{g}_1(q) = \left( \min \left\{ 1, \sum_{1 \leq j \leq n} q_j \right\} \right)_{i=1}^J, \quad \bar{g}_2(q) = \sum_{1 \leq i \leq n, X_i \in X} \pi_i(Q_i, Q_j) q_i q_j + h(q),
\]
where \( \pi : 2^{[1, \cdots, J]} \times 2^{[1, \cdots, J]} \rightarrow \mathbb{R} \) and \( h : \{0, 1\}^J \rightarrow [0, \infty) \) is a quadratic polynomial. To discuss the behavior of \( \bar{g}_1, \bar{g}_2 \), we introduce theorem 3.5. Assumption 3.3 ensures the comprehensiveness of the terms in \( F \). Assumption 3.4 presents the inclusion relations among \( \{Q_i\}_{i=1} \).

**Assumption 3.3.** \( F \subseteq \bigcup_{1 \leq i \leq J} \{Q_i \cup Q_j\} \).

**Assumption 3.4.** If there exists a pair of an index \( 1 \leq i \leq J \) and a set \( W \subseteq \{1, \cdots, J\} \setminus \{i\} \) with \( |W| \geq 2 \) such that
\[
Q_i \subseteq \bigcup_{j \in W} Q_j \quad \text{and} \quad Q_i \not\subseteq \bigcup_{j \in W} Q_j \quad \text{for any} \quad W' \subseteq W,
\]
then \( Q_i = Q_j \cup Q_k \) for some \( j, k \in \{1, \cdots, J\} \setminus \{i\} \).

**Theorem 3.5.** Suppose that assumption 3.3 and assumption 3.4 hold. Then there exists \( (\bar{\pi}, h) \) such that \( \bar{g}_1, \bar{g}_2 \) is a decomposed quadratization of \( f \).

**Proof.** See appendix B.1.

To capture the inclusion relations, we consider designing a penalty function \( h \) that induces
\[
Q_i \subseteq \bigcup_{j \in W} Q_j \Rightarrow (1 - q_i) \prod_{j \in W} q_j = 0.
\]

According to lemma 3.6, one element cannot be directly covered by more than three others. This prevents the direct incorporation of eq. (10) into a penalty. Assumption 3.4 indirectly addresses it by covering one element with two others. Lemma 3.7 restricts the formulation of penalties to capture this assumption.

**Lemma 3.6.** For \( K \in \{3, 4, \cdots\} \), no quadratic polynomial function \( \phi : \{0, 1\}^{K+1} \rightarrow \mathbb{R} \) satisfies
\[
\phi(q_1, \cdots, q_K, 0) = 0 \iff \prod_{1 \leq i \leq K} q_i = 0.
\]

**Proof.** See appendix B.2.

**Lemma 3.7.** Suppose that a quadratic polynomial function \( \phi : \{0, 1\}^J \rightarrow \mathbb{R} \) satisfies eq. (11). Then the following holds:
\[
\phi(0, 0, 1) + \phi(1, 1, 1) \neq \phi(1, 0, 1) + \phi(0, 1, 1).
\]

**Proof.** See appendix B.3.

Quadratization is a specific form of decomposed quadratization that requires assumption 3.8 in addition to assumption 3.3 and assumption 3.4. This additional assumption of quadratization is disadvantageous for reducing the number of auxiliary variables in certain tasks such as example 3.9.

**Assumption 3.8.** \( \{q_i\}_{i=1} \) for all \( 1 \leq i \leq I \).

**Example 3.9.** Let \( F = \{1, 2, 3, 4\} \). A decomposed quadratization requires 3 auxiliary variables: \( Q_1 = \{1, 2, 3\} \), \( Q_2 = \{4\} \), and \( Q_3 = \{3\} \). A quadratization requires 6 auxiliary variables: \( Q_1 = \{1\} \), \( Q_2 = \{2\} \), \( Q_3 = \{3\} \), \( Q_4 = \{4\} \), \( Q_5 = \{1, 2\} \), and \( Q_6 = \{3, 4\} \). Considering the biases and variable couplers in a QUBO, the auxiliary variables satisfy \( J \geq \left\lceil -\frac{1}{4} + \frac{1}{2} \sqrt{1 + 8|F|} \right\rceil \). We minimize the number of auxiliary variables to capture assumption 3.3 and assumption 3.4. An optimal solution of \( \{Q_i\}_{i=1} \) is a subset of \( \bigcup_{V \in F} 2^V \setminus \{\emptyset\} \). Let \( V_{close}, V_{open} \subseteq
If there is only one way to represent be the terms that still cannot be ignored. We provide algo-
Row 4: If V is not a subset of any element in V_{open}, then it is not included in an optimal solution.
Row 3: We can ignore elements in V_{open} represented by pairs of elements in V_{close}.
Row 2: If there is only one way to represent W, then V is included in an optimal solution.

Proposition 4.2. \( F_i \equiv \{ W_{ij} \}_{j=1}^{\lambda_i} \subseteq \bigcup_{1 \leq j \leq k \leq n} \{ U_{ij} \cup U_{ik} \} \subseteq 2^V \setminus \{ \emptyset \} \) for all \( 1 \leq i \leq n \).

The main distinction of our approach from section 2.3 is that the objective function is represented not by edges among vertices but by candidate parent subsets. To enforce exactly one parent set per vertex (i.e., \( \sum_{1 \leq j \leq \mu_i} u_{ij} \leq 2 \)), we use the constraint characterized by a penalty coefficient \( \xi \in (0, \infty) \) and auxiliary variables \( z = (z_i)_{i=1}^{\mu_i} \in \{0, 1\}^n \).

Then the score component is
\[
\bar{O}(u, z) \equiv \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq \mu_i} \pi_i(u_{ij}, u_{ik}) u_{ij} u_{ik} + \sum_{1 \leq i \leq n} \xi(z_i - z_i) \sum_{1 \leq j \leq \mu_i} u_{ij} + \sum_{1 \leq j < k \leq \mu_i} u_{ij} u_{ik},
\]
(15)

where \( \pi_i(U, U') \equiv (-1)^{1+|\{U \cup U'\}|} (\log S_i(U \cup U') - \log S_i(U) - \log S_i(U') + \log S_i(\emptyset)) \).

Using proposition 4.2, our formulation requires equal to or fewer binary variables than the quadratization of \( O \). For candidate parent subsets in quadratization, it is essential to capture the relation between them and the edges as follows:
\[
(1 - u_{ij}) \prod_{1 \leq k \leq n; X_k \in U_{ij}} d_{ik} = 0.
\]

Lemma 3.6 demonstrates that such relation cannot be captured by a quadratic polynomial when a candidate parent subset includes more than three elements. Consequently, we benefit from the use of decomposed quadratization with candidate parent subsets. The following lemma provides a lower bound for the penalty coefficient \( \xi \).

Lemma 4.3. Let \( \xi_0 \) be defined as
\[
\xi_0 \equiv -3 \min_{1 \leq i \leq n} \min_{0 \leq j \leq \mu_i} \pi_i(U_{ij}, U_{ik}).
\]

Suppose that \( \xi > \xi_0 \) holds and the state of \( d \) aligns with candidate parent sets. Then \( (D, O) \) is a decomposed quadratization of \( O \).

Proof. See appendix B.4. \( \square \)

The constraint for definition 2.1 is also captured by candidate parent subsets. Let \( C(u, r) \) denote the right side of eq. (5) where \( d_{ij} \) is replaced by
\[
\sum_{1 \leq k \leq n; X_k \in U_{ij}} u_{ik},
\]
(18)

where this substitution does not use additional auxiliary variables, but may increase the number of terms. The objective function in our approach is \( H(u, r, z) \equiv \bar{O}(u, z) + \bar{C}(u, r) \). Figure 2 illustrates this formulation. The following theorem guarantees that optimal networks can be obtained using our QUBO formulation.

Theorem 4.4. Let \( \delta_0 \) be defined as
\[
\delta_0 \equiv \max_{1 \leq i \leq n, 0 \leq \lambda_i} (\log S_i(W_{ij}) - \log S_i(\emptyset)).
\]

Suppose that \( \xi > \xi_0 \) and \( \delta_2 > (n - 2) \delta_1 > (n - 2) \delta_0 \) hold. Then \( \bar{C}(u, r) = 0 \) holds when \( H(u, r, z) \) is minimized.
QUBO Formulation

Optimal Parent Subsets

Bayesian Network

Figure 2: Example of the QUBO formulation with candidate parent subsets. An undirected edge between two binary variables represents that the objective function contains their product term. Gray signifies that the state of a binary variable is 0 and white is 1. Each color corresponds to the edge in the DAG. Let $n = 3, m = 2, \lambda_1 = 3, \lambda_2 = 1, \lambda_3 = 1, \Pi_1 = \{X_2\}, \Pi_2 = \emptyset, \Pi_3 = \{X_1, X_2\}, W_{11} = \{X_2\}, W_{12} = \{X_3\}, W_{13} = \{X_2, X_3\}, W_{21} = \{X_1, X_3\}, W_{31} = \{X_1, X_2\}, \mu_1 = 2, \mu_2 = 1, \mu_3 = 1, U_{11} = \{X_2\}, U_{12} = \{X_3\}, U_{21} = \{X_1, X_3\}, \text{and } U_{31} = \{X_1, X_2\}.$

We also demonstrate the score maximization using some solvers with our QUBO formulation. Version 9.1.2 of the Gurobi Optimizer $^1$ was used to solve the integer linear programming problems. The fourth-generation Fujitsu Digital Annealer was employed for score maximization. All experiments, except for those using the Digital Annealer, were conducted on a 64-bit Windows machine with an Intel Xeon W-2265 @ 3.50 GHz and 128 GB of RAM. The code was implemented in the Julia programming language 1.5.3 version. As benchmarks, we adopted 3 simulated datasets from each of the 8 discrete networks: alarm ($n = 37$), barley ($n = 48$), bailfinder ($n = 56$), hepar2 ($n = 70$), win95pts ($n = 76$), pathfinder ($n = 109$), mnn ($n = 186$), and andes ($n = 223$) from the Bayesian network repository $^2$. In addition, we used 5 times non-recoverable extracted datasets from each of the 3 datasets: chess ($n = 75$), mushroom ($n = 117$), and connect ($n = 129$) from the Frequent Item Set Mining Dataset Repository $^3$. The sample size of each dataset is 1000.

5.1 QUBO Formulation

We show that our formulation reduces the number of binary variables required in a QUBO.

Settings. The objective function was $\tilde{H}(u, r, z)$. The score function was the BDeu score (Buntine 1991), where the equivalent sample size was set to 1. See appendix D.1. The identification of candidate parent sets was performed exactly. Candidate parent sets were identified by simply enumerating all the elements in $\{W \subseteq \mathcal{X} \setminus \{X_1\} \mid |W| \leq m\}$ and comparing their local scores when the inclusion relations between them were in place. The maximum parent set size $m$ for each instance with more than 75 variables was set to the largest value that allowed the identification process to be completed within 48 h. The number of candidate parent

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$^1$https://www.gurobi.com/

$^2$https://www.bnlearn.com/bnrepository/

$^3$http://fimi.uantwerpen.be/data/
sets and the execution time for their identification are found in appendix D.2. The integer linear programming problem to find optimal candidate parent subsets was formulated as appendix C.1. The time limit for each variable was 60 [s]. The execution time for the QUBO formulation includes that of algorithm 2, setting up the integer linear programming problem, solving it, and incorporating the solution into the objective function.

**Baselines.** We compare our formulation with the approach proposed by (O’Gorman et al. 2014). Each vertex requires \( \frac{1}{4}(|X_i| - 1)^2 + 2 \) auxiliary variables when \( m_i = 3 \), and \( \frac{1}{2}|X_i||X_i| - 1 + 3 \) when \( m_i = 4 \), where \( m_i \equiv \max_{S \subseteq \Omega \subseteq \{\omega_i\}} |W_{ij}| \). To investigate the merit of algorithm 2, we found candidate parent subsets using the integer linear programming problem with \( W_{open} = F_i, V_{open} = \bigcup_{V \in \mathcal{E}} 2^V \setminus \emptyset \), and \( V_{close} = \emptyset \). We refer to this as “IP only” and our approach with algorithm 2 as “IP + algorithm 2”. The candidate parent sets to formulate these baselines were the same as those in the previously described setting. The execution time for each baseline does not include the time spent on identifying candidate parent sets.

**Evaluation.** The comparison between IP + algorithm 2 and IP only in table 1 demonstrates that optimizing candidate parent subsets with algorithm 2 is advantageous in terms of both the number of binary variables and execution time when the parent set size is larger. The quadricization for some instances with \( m = 3 \) required binary variables over the 100K bit capacity of the Digital Annealer. The decomposed quadricization in our approach significantly reduced the required number of binary variables compared to the quadricization approach. The execution time of our formulation was disadvantageous for most larger networks, primarily due to the increasing number of terms. Table 2 shows that incorporating the candidate parent subsets into the QUBO introduced a significant bottleneck.

### 5.2 Score Maximization

We demonstrate score maximization using the QUBO formulation by IP + algorithm 2.

**Settings.** The time limit for each trial was set to 3600 [s]. The coefficients in the penalty terms were \( \delta_1 = 1.1 \delta_0, \delta_2 = 1.1(n - 2) \delta_1 \), and \( \xi = 1.1 \xi_0 \). We used two heuristic solvers and one exact method: the Digital Annealer (DAQ), classical simulated annealing (SAQ), and the Gurobi Optimizer (GOQ). The inequality constraint is placed outside the objective function in both DAQ and GOQ. This formulation is strictly categorized as binary quadratic programming. See appendix D.4. The parameters for DAQ and GOQ were set to their default values. The annealing schedule of SAQ was geometric, starting with \( T_0 = 100 \). See appendix D.3. Additional bits for a minor embedding (Choi 2008, 2010; Eppstein 2009) were not required because the Digital Annealer is a fully-coupled type. Note that the short description of minor embedding can be found in appendix D.6.

**Baselines.** The baseline algorithms are only score-based. We adopted three approximate approaches and one exact algorithm: the hill climbing search method (HCS), the simulated annealing over ordering space (SAO), the acyclic selection ordering-based search (ASO), and the GObNILP software 4 (GÖB). The HCS and SAO are approximate approaches described in (Scutari, Graaffland, and Gutiérrez 2019). The ASO and GOB are known as competitive algorithms. The tabu list length in HCS was set to 10, and the state of 10 randomly selected possible edges was changed

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4https://www.cs.york.ac.uk/aig/sw/gobnilp/
Table 2: Execution time for IP + algorithm 2. The execution time for each of the following three steps is displayed. Left: algorithm 2 and preparation of the integer linear programming problem. Middle: finding candidate parent subsets by solving the problem. Right: incorporating the candidate parent subsets into the objective function of the QUBO. Note that the execution time for IP only is shown in appendix D.5.

| Instance  | m | Time [s] |
|-----------|---|----------|
| alarm     | 4 | $1 \pm 0.3 \pm 1.10 \pm 1$ |
| barley    | 4 | $0 \pm 0.0 \pm 0.11 \pm 2$ |
| hailfinder| 4 | $0 \pm 0.0 \pm 0.4 \pm 1$ |
| hepar2    | 4 | $0 \pm 0.0 \pm 0.2 \pm 0$ |
| chess     | 2 | $2 \pm 0.0 \pm 0.100 \pm 4$ |
| chess     | 3 | $406 \pm 49, 2554 \pm 199, 2608 \pm 195$ |
| win95pts  | 2 | $1 \pm 0.0 \pm 0.36 \pm 4$ |
| win95pts  | 3 | $45 \pm 5, 398 \pm 82, 446 \pm 54$ |
| pathfinder| 2 | $3 \pm 0.0 \pm 0.281 \pm 19$ |
| pathfinder| 3 | $1407 \pm 272, 1679 \pm 184, 18278 \pm 3349$ |
| mushroom  | 2 | $23 \pm 1.0 \pm 0.490 \pm 22$ |
| connect   | 2 | $5 \pm 0.0 \pm 0.235 \pm 12$ |
| connect   | 3 | $2472 \pm 436, 4129 \pm 148, 13505 \pm 2114$ |
| munin1    | 2 | $12 \pm 1.0 \pm 0.1067 \pm 67$ |
| andes     | 2 | $1 \pm 0.0 \pm 0.249 \pm 35$ |
| andes     | 3 | $6 \pm 1.2 \pm 1, 209 \pm 8$ |

upon termination of the greedy search. The annealing schedule of SAO was same as that of SAQ. The ASO was the version proposed in (Scanagatta et al. 2015). The version of GOB was the pygobnilp1.0 that relies on the Gurobi Optimizer. We used common candidate parent sets in our formulation, except for HCS. To ensure a fair comparison, the time limit for each of SAO, ASO, and GOB was set at 3600 [s] plus the execution time required for the QUBO formulation by IP + algorithm 2. The time limit for HCS was further extended by the time needed to identify candidate parent sets. We ignored the time to transfer the encoding information online to the Digital Annealer environment. The HCS and ASO were restarted repeatedly during the time limit.

Evaluation. Table 3 displays the results of score maximization. The number of trials achieving the highest score is displayed. The highest score refers to the shortest execution time when the scores are the same. For the four instances above the line, the GOB identified optimal networks within a few seconds. While the GOQ identified an optimal network in only one trial of the barley instance, the execution time was longer than the GOB. The solutions for the win95pts with $m = 2$ and the connect with $m = 3$ were not proven to be optimal. The SAQ and ASO never won in any of the trials. The bold values show the greatest number of wins among all solvers.

| Instance  | m | DAQ | GOQ | HCS | SAO | GOB |
|-----------|---|-----|-----|-----|-----|-----|
| alarm     | 4 | 0   | 0   | 0   | 0   | 5   |
| barley    | 4 | 0   | 0   | 0   | 0   | 5   |
| hailfinder| 4 | 0   | 0   | 0   | 0   | 5   |
| hepar2    | 4 | 0   | 0   | 0   | 0   | 5   |

Table 3: Results of score maximization. The number of trials achieving the highest score is displayed. The highest score refers to the shortest execution time when the scores are the same. For the four instances above the line, the GOB identified optimal networks within a few seconds. While the GOQ identified an optimal network in only one trial of the barley instance, the execution time was longer than the GOB. The solutions for the win95pts with $m = 2$ and the connect with $m = 3$ were not proven to be optimal. The SAQ and ASO never won in any of the trials. The bold values show the greatest number of wins among all solvers.

Future Works. Along with further investigation addressing the above limitations, we will explore the application of decomposed quadratization to tasks beyond Bayesian network structure learning. Decomposed quadratization can serve as a promising alternative to conventional quadratization for a wide range of tasks involving multilinear polynomials with higher-degree terms.

6 Conclusion

We proposed a QUBO formulation tailored to score-based Bayesian network structure learning. The essence of this approach lies in reducing the number of required binary variables through decomposed quadratization with candidate parent subsets. We also provided an algorithm to efficiently find optimal candidate parent subsets. Experimental results demonstrated that our approach significantly reduced the number of binary variables compared to the previous work based on quadratization. Additionally, our formulation using the Digital Annealer achieved improved BDeu scores over existing methods for medium-sized instances. We expect that our approach can be more effectively applied to larger-scale structure learning problems in the future development of annealing processors.

Limitations. We have identified three limitations in our approach. First, the execution time to incorporate the candidate parent subsets into the objective function is a potential drawback for larger-scale problems. Secondly, capturing a parent set with two bits may be disadvantageous for a 1-bit inversion search, as transitioning from one candidate parent set to another necessitates an inversion of up to four bits. Lastly, our formulation could potentially have a negative impact by increasing the number of terms in a QUBO. In particular, a minor embedding requires additional bits as the number of terms increases.
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## A Notations

| Notation | Description |
|----------|-------------|
| $n$      | the number of vertices |
| $m$      | the maximum parent set size |
| $\mathcal{X}$ | the set of vertices $\{X_i\}_{i=1}^n$ |
| $d$      | $d \equiv \left(\left(d_{ij}\right)_{i,j=1}^n\right)$ with $d_{ij} \in \{0, 1\}$ corresponds to the set of edges |
| $r$      | $r \equiv \left(r_{ij}\right)_{(i,j) \in E}$ with $r_{ij} \in \{0, 1\}$ corresponds to the topological ordering |
| $p$      | $p \equiv \left(p_i\right)_{i=1}^n$ with $p_i \in \{0, 1\}$ is the set of primary variables |
| $q$      | $q \equiv \left(q_i\right)_{i=1}^n$ with $q_i \in \{0, 1\}$ is the set of auxiliary variables |
| $u$      | $u \equiv \left(u_{ij}\right)_{i,j=1}^n$ with $u_{ij} \in \{0, 1\}$ is the set of candidate parent subsets |
| $v$      | $v \equiv \left(v_i\right)_{i=1}^n$ with $v_i \in \{0, 1\}$ captures the search space of auxiliary variables |
| $z$      | $z \equiv \left(z_i\right)_{i=1}^n$ with $z_i \in \{0, 1\}$ is used to ensure that each vertex has exactly one parent set |
| $\pi$    | $\pi : 2^{\{1,\ldots, I\}} \rightarrow \mathbb{R} \setminus \{0\}$ returns the coefficients in a multilinear polynomial |
| $\bar{\pi}$ | $\bar{\pi} : 2^{\{1,\ldots, I\}} \times 2^{\{1,\ldots, I\}} \rightarrow \mathbb{R}$ returns the coefficients in a decomposed quadratization |
| $\mathcal{F}$ | $\mathcal{F} \subseteq 2^{\{1,\ldots, I\}} \setminus \{\emptyset\}$ is the terms in a multilinear polynomial |
| $\mathcal{E}$ | the set of edges on possible cycles given candidate parent sets |
| $Q_i$    | a subset of $2^{\{1,\ldots, I\}} \setminus \{\emptyset\}$ |
| $W_{ij}$ | a candidate parent set of $X_i$ |
| $U_{ij}$ | a candidate parent subset of $X_i$ |
| $\mathcal{F}_i$ | candidate parent sets of $X_i$ except for the empty set |
| $\mathcal{X}_i$ | the union of the candidate parent sets of $X_i$ |
| $m_i$    | the maximum parent set size of $X_i$ |
| $S_i$    | $S_i : 2^{X_i \setminus \{X_i\}} \rightarrow \mathbb{R}$ represents the local score function for a parent set of $X_i$ |
| $\Pi_i$  | the set of vertices that have edges directed towards $X_i$ |
| $\pi_i$  | $\pi_i(W) \equiv \sum_{i \leq j \leq W} (-1)^{i+j} \log S_i(W)$ |
| $\bar{\pi}_i$ | $\bar{\pi}_i(U, U') \equiv (-1)^{1+(U \cup U')} \left[ \log S_i(U \cup U') - \log S_i(U) - \log S_i(U') + \log S_i(\emptyset) \right]$ |
| $h$      | $h : \{0, 1\}^J \rightarrow [0, \infty)$ is a quadratic polynomial function |
| $R$      | $R(r_{ij}, r_{jk}, r_{ik}) \equiv r_{ik} + r_{ij}r_{jk} - r_{ij}r_{ik} - r_{jk}r_{ik}$ |
| $C$      | $C(d, r) \equiv \sum_{i \leq j \leq \infty} \delta_1(R(r_{ij}, r_{jk}, r_{ik})) + \sum_{i \leq j \leq \infty} \delta_2(d_{ij}r_{ij} + d_{ij}(1 - r_{ij}))$ |
| $\bar{C}$ | $\bar{C}(u, r)$ is defined as $C(d, r)$ where $d_{ij}$ is replaced by $\sum_{1 \leq |k| \leq m_i : \exists x_j \in U_{ik}} u_{ij}$ |
| $D$      | $D(u) \equiv \left(\min_{1 \leq |k| \leq m_i : \exists x_j \in U_{ik}} u_{ij}\right)_{i=1}^n$ |
| $H$      | $H(u, r, z) = \bar{C}(u, r) + \bar{C}(u, r)$ |
| $g_1$    | $g_1(q) \equiv \left(\min_{1 \leq |k| \leq m_i : \exists x_j \in U_{ik}} q_{ij}\right)_{i=1}^n$ |
| $g_2$    | $g_2(q) \equiv \sum_{1 \leq |k| \leq m_i} \bar{\pi}(Q_i, Q_j) q_{ij} + h(q)$ |
| $\xi_0$  | $\xi_0 \equiv -3 \min_{1 \leq |k| \leq m_i : \exists x_j \in U_{ik}} \bar{\pi}(Q_i, Q_j)$ |
| $\delta_0$ | $\delta_0 \equiv \max_{1 \leq |k| \leq m_i : \exists x_j \in U_{ik}} \left(\log S_i(W_{ij}) - \log S_i(\emptyset)\right)$ |
| $V_{\text{close}}$ | a subset of an optimal solution |
| $V_{\text{open}}$ | $V_{\text{close}} \cup V_{\text{open}}$ contains an optimal solution |
| $W_{\text{open}}$ | the terms that still cannot be ignored in $\mathcal{F}$ |
B Proof

B.1 Proof of Theorem 3.5
Initially, we introduce the following lemmas.

Lemma B.1. Let \( h_0 \) be defined as
\[
\begin{align*}
    h_0(q) = \sum_{1 \leq i \leq J} \sum_{\emptyset \subseteq W \subseteq \{1, \ldots, J\} \setminus \{i\} \text{ and } Q_i \subseteq \bigcup_{j \in W} Q_j} \prod_{j \in W} q_j.
\end{align*}
\]

Suppose that \( p = \bar{g}_1(q) \) holds. Then we have
\[
    h_0(q) = 0 \Rightarrow q = \left( \prod_{1 \leq i \leq J} p_i \right)_{j=1}^{J} \text{ for any } q \in \{0, 1\}^J.
\]

Proof. From \( p = g_1(q) \), if \( p_i = 1 \), then there exists an index \( j \) such that \( i \in Q_j \) and \( q_j = 1 \). Therefore, if \( h_0(q) = 0 \), then \( Q_j \subseteq \bigcup_{1 \leq i \leq J; p_i = 1} \{i\} \Rightarrow q_j = 1 \). Additionally, if \( p_i = 0 \), then \( i \in Q_j \Rightarrow q_j = 0 \). Consequently, this lemma holds.

Lemma B.2. Let \( h \) be defined as
\[
    h(q) = \kappa \left( \sum_{1 \leq i \leq J} \sum_{l \notin \{j \}, k \notin \{q_i\} \cup Q_i} (q_i q_k - 2q_i q_l - 2q_k q_l + 3q_l) + \sum_{i, j \in \{1, \ldots, J\} \setminus Q_i \subseteq Q_j} (1 - q_i) q_j \right),
\]
where \( \kappa \in (0, \infty) \). Suppose that assumption 3.4 holds. Then we have
\[
    h(q) = 0 \Rightarrow h_0(q) = 0 \text{ for any } q \in \{0, 1\}^J.
\]

Proof. We prove \( h_0(q) \neq 0 \Rightarrow h(q) \neq 0 \) for any \( q \in \{0, 1\}^J \). If \( h_0(q) \neq 0 \), there exists at least one pair of an index \( i \) and a set \( W \) such that \( q_i = 0 \) and \( \prod_{j \in W} q_j = 1 \) in \( h_0(q) \). For \( |W| = 1 \), the second term of \( h(q) \) is positive. Consider the case where \( |W| \geq 2 \). From assumption 3.4, there exists \( (a, b) \) such that \( Q_a \cup Q_b = Q_i \) and \( i \notin \{a, b\} \). By repeating this split, we reach \( Q_c \subseteq Q_j \) for some \( j \in W \). Therefore, either the first or the second term of \( h(q) \) is positive. Consequently, this lemma holds.

Let \( \pi \) satisfy
\[
    \sum_{1 \leq i \leq j \leq J, Q_i \cup Q_j = V} \pi(Q_i, Q_j) = \begin{cases} \pi(V) & (V \in \mathcal{F}) \\ 0 & (V \notin \mathcal{F}) \end{cases}.
\]

From lemma B.1 and lemma B.2, the following holds:
\[
    h(q) = 0 \Rightarrow q = \left( \prod_{1 \leq i \leq J; q_i = 0} p_i \right)_{j=1}^{J} \text{ for any } q \in \{0, 1\}^J.
\]

To induce \( h(q) = 0 \), we demonstrate a simple bound. Let \( \kappa_0 \) denote
\[
    \kappa_0 \equiv \max_{q \in \{0, 1\}^J} \sum_{1 \leq i \leq J} \pi(Q_i, Q_j) q_i q_j - \min_{q \in \{0, 1\}^J} \sum_{1 \leq i \leq J} \pi(Q_i, Q_j) q_i q_j.
\]

Suppose that \( \kappa > \kappa_0 \) holds. Then the following holds:
\[
    f(p) = \min_{q \in \{0, 1\}^J} \bar{g}_2(q).
\]

Hence, under assumption 3.3 and assumption 3.4, \((\bar{g}_1, \bar{g}_2)\) is a decomposed quadratization of \( f \).

B.2 Proof of Lemma 3.6
Considering \( \phi(1, \ldots, 0) \neq 0 \) and \( K C_2 + K C_1 + K C_0 < 2^K \), no quadratic polynomial function \( \phi : \{0, 1\}^{K+1} \rightarrow \mathbb{R} \) satisfies eq. (11) for \( K \in \{3, 4, \ldots\} \).
B.3 Proof of Lemma 3.7

Let \( \phi \) be

\[
\phi(q_1, q_2, q_3) = b_1q_1 + b_2q_2 + b_3q_3 + b_{12}q_1q_2 + b_{13}q_1q_3 + b_{23}q_2q_3. 
\]

From eq. (11), \( b_1 = b_2 = 0 \) and \( b_{12} = \phi(1, 1, 0) \neq 0 \). For \( q_3 = 1 \), the following holds:

\[
\begin{align*}
\phi(0, 0, 1) &= b_3, \\
\phi(1, 0, 1) &= b_1 + b_3 + b_{13}, \\
\phi(0, 1, 1) &= b_2 + b_3 + b_{23}, \\
\phi(1, 1, 1) &= b_1 + b_2 + b_3 + b_{12} + b_{13} + b_{23} = \phi(1, 1, 0) + b_3 + b_{13} + b_{23}.
\end{align*}
\]

Consequently, we have

\[
\phi(0, 0, 1) + \phi(1, 1, 1) - \phi(1, 0, 1) - \phi(0, 1, 1) = \phi(1, 1, 0) \neq 0.
\]

B.4 Proof of Lemma 4.3

For \( u_{ab} = 1 \) and \( \sum_{1 \leq j \leq \mu_a} u_{aj} > 2 \), the following holds:

\[
\min_{z \in \{0, 1\}^n} \bar{O}(u, z) - \min_{z \in \{0, 1\}^n} \bar{O}(u^{ab}, z) \geq (-2 + \sum_{1 \leq j \leq \mu_a} u_{aj})\xi + \sum_{1 \leq j \leq \mu_a} \pi_a(u^{ab}, u_{aj}u_{aj}),
\]

where \( u^{ab} \equiv (u_{ij}^{ab})_{ij=1}^n \) with \( u_{ij}^{ab} = 0 \) if \( (i, j) = (a, b) \); \( u_{ij}^{ab} = u_{ij} \) otherwise. If \( \xi > \xi_0 \), then we have

\[
\min_{z \in \{0, 1\}^n} \bar{O}(u, z) > \min_{z \in \{0, 1\}^n} \bar{O}(u^{ab}, z).
\]

This inequality implies that \( \sum_{1 \leq j \leq \mu_a} u_{ij} \leq 2 \) holds for all \( 1 \leq i \leq n \). Consequently, if \( \xi > \xi_0 \) holds and the state of \( d \) aligns with candidate parent sets, then \( (D, \mathcal{O}) \) is a decomposed quadratization of \( O \).

B.5 Proof of Theorem 4.4

At first, we introduce the following lemmas.

**Lemma B.3**. Let \( T \) be defined as

\[
T(r) \equiv \sum_{(i,j),(j,k),(i,k) \in \mathcal{E}} R(r_{ij}, r_{jk}, r_{ik}).
\]

Suppose that \( T(r) > 0 \) holds. Then there exists at least one integer pair \( (a, b) \) such that \( T(r) > T(r^{ab}) \), where \( r^{ab} \equiv (r_{ij}^{ab})_{ij \in \mathcal{E}} \) with \( r_{ij}^{ab} = 1 - r_{ij} \) if \( (i, j) = (a, b) \); \( r_{ij}^{ab} = r_{ij} \) otherwise.

**Proof**. Assume \( R(r_{ij}, r_{jk}, r_{ik}) > 0 \). For all \( l \) satisfying \( k < l \leq n \), the following holds:

\[
\begin{align*}
R(r_{ij}, r_{jl}, r_{il}) &= (1 - r_{ij} + r_{ij}r_{il} - r_{ij}r_{jl}) - (r_{jl} + r_{ij}r_{il} - r_{ij}r_{jl} - r_{jl}r_{il}) \nonumber \\
&= 2r_{il}(1 - r_{ij} - r_{il}) + 2r_{jl}(1 - r_{ij} - r_{jl}) + 2r_{kl}(1 - r_{ik} - r_{ikl}) \\
&= 0,
\end{align*}
\]

where \( (r_{ij}, r_{jk}, r_{ik}) \) is \( (1, 1, 0) \) or \( (0, 0, 1) \). For all \( l \) satisfying \( j < l < k \), the following holds:

\[
\begin{align*}
R(r_{ij}, r_{jk}, r_{il}) &= (1 - r_{ij} + r_{ij}r_{il} - r_{ij}r_{jk}) - (r_{il} + r_{ij}r_{il} - r_{ij}r_{jk} - r_{ij}r_{il}) \nonumber \\
&= 2r_{il}(1 - r_{ik} - r_{ij}) + 2r_{jk}(1 - r_{ik} - r_{jk}) + 2r_{jl}(1 - r_{ik} - r_{jk}) + 2(r_{ik} + r_{jk} - 1) \\
&= 0.
\end{align*}
\]
For all $l$ satisfying $i < l < j$, the following holds:

\begin{align*}
R(r_{li}, r_{ij}, r_{ij}) - R(r_{li}, 1 - r_{ij}, r_{ij}) + R(r_{ij}, 1 - r_{ik}, r_{ik}) - R(r_{il}, r_{ik}, r_{ik}) - R(r_{il}, 1 - r_{ik}, r_{ik}) \\
= (r_{ij} + r_{il}r_{ij} - r_{il}r_{ij} - r_{ij}r_{ij}) - (1 - r_{il} - r_{ij} + r_{il}r_{ij} + r_{il}r_{ij} + r_{il}r_{ij}) \\
+ (r_{ik} + r_{ij}r_{jk} - r_{ij}r_{ik} - r_{jk}r_{ik}) - (r_{ij} + r_{jk}r_{ik} - r_{ij}r_{jk} - r_{jk}r_{ik}) \\
+ (r_{ik} + r_{ir}r_{ik} - r_{ir}r_{ik} - r_{ir}r_{ik}) - (1 - r_{ik} - r_{il} - r_{ik} + r_{il}r_{ik} + r_{il}r_{ik} + r_{il}r_{ik}) \\
= 2r_{il}(1 - r_{ik} - r_{ij}) + 2r_{ik}(1 - r_{ik} - r_{jk}) + 2(r_{ij} + r_{ik} - 1) \\
= 0.
\end{align*}

For all $l$ satisfying $1 \leq l < i$, the following holds:

\begin{align*}
R(r_{li}, r_{ij}, r_{ij}) - R(r_{li}, 1 - r_{ij}, r_{ij}) + R(r_{ij}, 1 - r_{jk}, r_{ik}) - R(r_{il}, r_{ik}, r_{ik}) - R(r_{il}, 1 - r_{ik}, r_{ik}) \\
= (r_{ij} + r_{il}r_{ij} - r_{il}r_{ij} - r_{ij}r_{ij}) - (1 - r_{il} - r_{ij} + r_{il}r_{ij} + r_{il}r_{ij} + r_{il}r_{ij}) \\
+ (r_{ik} + r_{ij}r_{jk} - r_{ij}r_{ik} - r_{jk}r_{ik}) - (r_{ij} + r_{jk}r_{ik} - r_{ij}r_{jk} - r_{jk}r_{ik}) \\
+ (r_{ik} + r_{ir}r_{ik} - r_{ir}r_{ik} - r_{ir}r_{ik}) - (1 - r_{ik} - r_{il} - r_{ik} + r_{il}r_{ik} + r_{il}r_{ik} + r_{il}r_{ik}) \\
= 2r_{il}(1 - r_{ik} - r_{ij}) + 2r_{ik}(1 - r_{ik} - r_{jk}) + 2(r_{ij} + r_{ik} - 1) \\
= 0.
\end{align*}

From $R(r_{ij}, r_{jk}, r_{ik}) > 0$, the following holds:

\begin{align*}
R(r_{ij}, r_{jk}, r_{ik}) - R(1 - r_{ij}, r_{jk}, r_{ik}) + R(r_{ij}, 1 - r_{jk}, r_{ik}) - R(r_{ij}, 1 - r_{jk}, r_{ik}) + R(r_{ij}, 1 - r_{jk}, r_{ik}) - R(r_{ij}, 1 - r_{jk}, r_{ik}) = 3.
\end{align*}

Using these results, we have

\[ T(r) - T(r^{ij}) + T(r) - T(r^{ik}) + T(r) - T(r^{jk}) = 3 > 0. \]

Consequently, $T(r) > T(r^{ab})$ holds for at least one index pair $(a, b) \in \{(i, j), (j, k), (i, k)\}$. \hfill \Box

Let $u^{aef} = ((u^{aef}_{ij})_{i=1}^{n})_{j=1}^{n}$ satisfy

\[ u^{aef}_{ac} = u^{aef}_{ca} = 1, \quad u^{aef}_{aj} = 0 \quad \text{for} \quad j \notin \{e, f\}, \quad \text{and} \quad u^{aef}_{ij} = u_{ij} \quad \text{for} \quad i \neq a. \]

Assume the following conditions:

\[ u_{a0} \in \{0, 1\}, \quad (a, b) \in \mathcal{E}, \quad 0 \leq c < d \leq \mu_a, \quad 0 \leq e < f \leq \mu_a, \quad u_{ac} = u_{ad} = 1, \]
\[ u_{a0} + \cdots + u_{a\mu_a} = 2, \quad X_b \in (U_{ac} \cup U_{ad}) \setminus (U_{ac} \cup U_{af}), \quad (U_{ac} \cup U_{af}) \subset (U_{ac} \cup U_{ad}). \]

We find the range of penalty coefficients so that the difference in the return value of the objective function is negative when the input state changes to the desired state. From the discussion in appendix B.4, we consider the case where $\sum_{1 \leq l \leq \mu_a} u_{ij} \leq 2$ for all $1 \leq i \leq n$. For $\sum_{1 \leq j \leq \mu_b} X_{a} \in U_{b} \ u_{bj} \geq 1$, the following holds:

\[ \min_{z \in \{0, 1\}^n} \bar{H}(u, r, z) - \min_{z \in \{0, 1\}^n} \bar{H}(u^{aef}, r, z) \geq \delta_2 - \log S_a(U_{ac} \cup U_{ad}) + \log S_a(U_{ac} \cup U_{af}). \]

For $\sum_{1 \leq j \leq \mu_b} X_{a} \in U_{b} \ u_{bj} = 0$ and $r_{ab} = 1$, the following holds:

\[ \min_{z \in \{0, 1\}^n} \bar{H}(u, r, z) - \min_{z \in \{0, 1\}^n} \bar{H}(u^{ab}, r, z) \geq \delta_2 - (n - 2)\delta_1. \]

From lemma B.3, we could repeat reversing one element from $r$ with decreasing $T(r)$ until $T(r) = 0$. For $T(r) > T(r^{ab})$, $r_{ab} = 0$, and $\sum_{1 \leq j \leq \mu_b} X_{a} \in U_{b} \ u_{bj} = 0$, the following holds:

\[ \min_{z \in \{0, 1\}^n} \bar{H}(u, r, z) - \min_{z \in \{0, 1\}^n} \bar{H}(u^{ab}, r, z) \geq \delta_1 - \log S_a(U_{ac} \cup U_{ad}) + \log S_a(U_{ac} \cup U_{af}). \]

Here the following holds:

\[ \delta_0 \geq \max_{1 \leq a \leq n} \max_{1 \leq b \leq \mu_a} \max_{0 \leq c < d \leq \mu_a} \min_{X_e \in (U_{ac} \cup U_{ad}) \setminus (U_{ac} \cup U_{af})} \log \frac{S_a(U_{ac} \cup U_{ad})}{S_a(U_{ac} \cup U_{af})}. \]

From the above discussion, if $\xi > \xi_0$ and $\delta_2 > (n - 2)\delta_1 > (n - 2)\delta_0$ hold, then the following holds:

\[ C(u_a, r_a) = 0 \quad \text{for any} \quad \bar{H}(u_a, r_a, z_a) = \min_{u, r, z} \bar{H}(u, r, z). \]
C Integer Linear Programming for QUBO Formulation

C.1 Formulation for Reducing Binary Variables

For any $1 \leq i \leq \nu$, define

$$W_i \equiv \{ W \subseteq V_{\text{close}} \cup V_{\text{open}} \mid |W| \geq 2, V_i \subseteq \bigcup_{V \in W} V_i \text{ and } V_i \not\subseteq \bigcup_{V \in W'} V \text{ for any } W' \subset W \}.$$  

The search for an optimal solution can be formulated as an integer linear programming problem to minimize $\sum_{1 \leq i \leq \nu} v_i$ under the following constraints:

$$\sum_{1 \leq j \leq \nu} v_i + \sum_{W \notin \{ V_i \cup V_j \mid V_j \subseteq W \}} v_i v_j \geq 1 \text{ for all } W \in W_{\text{open}},$$

$$v_i \prod_{1 \leq j \leq \nu, V_j \not\subseteq W} v_j \leq \sum_{V_i \cup V_j \subseteq W} 1 + \sum_{j \in \{ 1, \ldots, \nu \} \setminus \{ i \}} v_j + \sum_{1 \leq \nu, i \not\subseteq \nu} v_j v_k,$$

for all $1 \leq i \leq \nu$ and $W \in W_i$.

Replacing $v_i v_j$ with $\rho_{ij} \in \{0, 1\}$, we transform a higher degree terms into a linear as

$$\sum_{W \in \bigcup_{V_i \subseteq \{ V_i \} \cup V_j \subseteq W} \{ V_i \} \cup V_j} v_i + \sum_{W \not\in \{ V_i \cup V_j \mid V_j \subseteq W \}} \rho_{ij} \geq 1 \text{ for all } W \in W_{\text{open}},$$

$$-|W \setminus V_{\text{close}}| + v_i + \sum_{1 \leq j \leq \nu} v_j \leq \sum_{V_i \cup V_j \subseteq W} 1 + \sum_{j \in \{ 1, \ldots, \nu \} \setminus \{ i \}} v_j + \sum_{1 \leq \nu, \nu < \nu} \rho_{jk},$$

for all $1 \leq i \leq \nu$ and $W \in W_i$,

$$2\rho_{ij} \leq v_i + v_j \leq 1 + \rho_{ij} \text{ for all } 1 \leq i < j \leq \nu.$$

To find optimal candidate parent subsets, we ignore the latter constraint.

C.2 Formulation for Term Reduction

Consider the formulation shown in appendix B.1. Let $\eta_{ij} \in \{0, 1\}$ represent the existence of a term $v_i v_j$. The number of terms is reduced by solving an integer programming problem that minimizes $\sum_{1 \leq i \leq \nu + \nu'} \eta_{ij}$ subject to the following constraints:

$$\eta_{ij} \leq v_i v_j \text{ for all } 1 \leq i \leq \nu + \nu',$$

$$v_i = 1 \text{ for all } \nu + 1 \leq i \leq \nu + \nu' \text{ and } V_i \cup V_j \subseteq F,$$

$$v_i v_j \leq \frac{1}{2} (\eta_{ij} + \eta_{\min(i,j) \max(i,j)}) \text{ for all } i, j \in \{ 1, \cdots, \nu + \nu' \} \text{ and } V_i \subseteq V_j,$$

$$-2 + v_i + v_j + v_k \leq \frac{1}{4} (\eta_{ii} + \eta_{\min(i,j) \max(i,j)} + \eta_{\min(i,k) \max(i,k)} + \eta_{jk}) \text{ for all } 1 \leq i \leq \nu + \nu', 1 \leq j < k \leq \nu + \nu', i \not\subseteq \{ j, k \}, \text{ and } V_j \cup V_k = V_i,$$

$$\sum_{1 \leq i \leq \nu + \nu'} \eta_{ij} \geq 1 \text{ for all } W \subseteq F,$$

$$-|W| + v_i + \sum_{1 \leq i \leq \nu + \nu'} v_j \leq \sum_{i \not\subseteq \nu, j \subseteq \nu'} v_j v_k \text{ for all } 1 \leq i \leq \nu \text{ and } W \in W_i,$$

where $(v_i)_{i=1}^{\nu + \nu'} \in \{0, 1\}^{\nu + \nu'}$ and $\{ V_i \}_{i=1}^{\nu + \nu'} \equiv V_{\text{close}}$. As described in appendix C.1, we transform quadratic terms into linear ones by replacing $v_i v_j$ with $\rho_{ij}$. 
D Experiment

D.1 Bayesian Dirichlet Equivalence Uniform Score

For the Bayesian Dirichlet equivalence uniform (BDeu) score, define

\[ S_i(\Pi) \equiv \prod_{1 \leq j \leq \beta_i} \frac{\Gamma(\alpha_{ij})}{\Gamma(N_{ij} + \alpha_{ij})} \prod_{1 \leq k \leq \gamma_i} \frac{\Gamma(N_{ijk} + \alpha_{ijk})}{\Gamma(\alpha_{ijk})} \]

for any \( 1 \leq i \leq n \) and \(|\Pi| \leq m_i\),

where \( N_{ij} \equiv \sum_{1 \leq k \leq \gamma_i} N_{ijk} \), \( N_{ijk} \) is the number of cases of \( \Pi \) in its \( j \)-th state and \( X_i \) in its \( k \)-th state, \( \alpha_{ij} \equiv \sum_{1 \leq k \leq \gamma_i} \alpha_{ijk} \), \( \alpha_{ijk} = \frac{\alpha}{\beta_i \gamma_i} \), \( \beta_i \) is the number of joint states of \( \Pi \), \( \gamma_i \) is the number of states of \( X_i \), and \( \alpha \in (0, \infty) \) is the equivalent sample size.

D.2 Identification of Candidate Parent Sets

Table 4: Number of candidate parent sets and execution time for their identification. The mean and standard deviation of 5 trials are presented. Empty sets were excluded from the candidate parent sets.

| Instance   | Number | Time [s] |
|------------|--------|----------|
| alarm      | 4      | 2291 ± 210 | 1700 ± 11 |
| barley     | 4      | 355 ± 12  | 235015 ± 95243 |
| hailfinder | 4      | 692 ± 16  | 90247 ± 3334 |
| hepar2     | 4      | 689 ± 59  | 40216 ± 534  |
| chess      | 2      | 32570 ± 1686 | 59 ± 0     |
| chess      | 3      | 236285 ± 15636 | 5463 ± 284 |
| win95pts   | 2      | 9231 ± 665 | 2404 ± 51   |
| win95pts   | 3      | 43657 ± 3850| 320 ± 5     |
| pathfinder | 2      | 50962 ± 3254| 44991 ± 3426|
| pathfinder | 3      | 398131 ± 47889| 83361 ± 6624|
| mushroom   | 2      | 273526 ± 12647| 689 ± 26   |
| connect    | 2      | 76996 ± 4381| 331 ± 7     |
| connect    | 3      | 710684 ± 73964| 83631 ± 6024|
| munin1     | 2      | 135570 ± 6765| 2466 ± 29  |
| andes      | 2      | 7424 ± 219 | 852 ± 52    |
| andes      | 3      | 14195 ± 556| 104683 ± 3855|

D.3 Classical Simulated Annealing

Algorithm 3: Classical Simulated Annealing

1: while the current time is within the time limit, do
2: \( \Delta \leftarrow \) the incremental return value of \( H \) when flipping a bit randomly.
3: if a random number between 0 and 1 is less than \( \exp(-\Delta/T_0 \text{current time/time limit}) \), then
4: accept the bit flip.
5: end if
6: end while

D.4 Binary Quadratic Programming

The binary quadratic programming problem for learning a Bayesian network can be defined by

\[ \text{minimize} \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq k \leq \mu_i} \pi_i(U_{ij}, U_{ik})u_{ij}u_{jk} + C(u, r) \quad \text{subject to} \sum_{1 \leq j \leq \mu_i} u_{ij} \leq 2 \text{ for all } 1 \leq i \leq n. \]

Note that we can express the DAG constraint using linear inequalities. The linear ordering of vertices is

\[ 0 \leq r_{ij} + r_{jk} - r_{ik} \leq 1 \text{ for all } (i, j), (j, k), (i, k) \in E. \]

The consistency of edges and ordering is

\[ \sum_{1 \leq k \leq \mu_i} u_{ik} \leq 2 - 2r_{ij} \text{ and } \sum_{X_j \in U_k} u_{jk} \leq 2r_{ij} \text{ for all } (i, j) \in E. \]
D.5 Identification of Candidate Parent Subsets

Table 5: Execution time for IP only. Displays are the same as table 2.

| Instance | m  | Time [s]                  |
|----------|----|---------------------------|
| alarm    | 4  | $1 \pm 0, 50 \pm 28, 10 \pm 1$ |
| barley   | 4  | $0 \pm 0, 1 \pm 0, 10 \pm 2$ |
| hailfinder | 4 | $0 \pm 0, 0 \pm 4 \pm 1$ |
| hepar2   | 4  | $0 \pm 0, 0 \pm 2 \pm 0$ |
| chess    | 2  | $6 \pm 0, 0 \pm 83 \pm 3$ |
| chess    | 3  | $639 \pm 58, 3150 \pm 167, 3480 \pm 315$ |
| win95pts | 2  | $2 \pm 2, 0 \pm 1 \pm 1$ |
| win95pts | 3  | $49 \pm 8, 530 \pm 73, 457 \pm 66$ |
| pathfinder | 2 | $18 \pm 2, 0 \pm 241 \pm 29$ |
| pathfinder | 3 | $3844 \pm 750, 2132 \pm 129, 24731 \pm 3458$ |
| mushroom | 2  | $277 \pm 19, 1 \pm 0, 403 \pm 14$ |
| connect  | 2  | $26 \pm 3, 0 \pm 203 \pm 15$ |
| connect  | 3  | $6219 \pm 1396, 4568 \pm 177, 19595 \pm 2743$ |
| munin1   | 2  | $78 \pm 6, 0 \pm 875 \pm 71$ |
| andes    | 2  | $1 \pm 0, 0 \pm 247 \pm 37$ |
| andes    | 3  | $4 \pm 0, 7 \pm 1, 493 \pm 131$ |

D.6 Minor Embedding

Annealing machines are classified into two types: nearest-neighbor and fully-coupled. A fully-coupled annealing machine allows coupling between arbitrary vertices, whereas coupling in a nearest-neighbor annealing machine is limited to adjacent vertices only. Nearest-neighbor annealing machines require additional bits to embed a highly dense logical topology into a physical one (Choi 2008, 2010). The number of additional bits for the embedding depends on the design of the hardware graphs, and embedding problems are NP-hard (Eppstein 2009).