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Characterization of QUBO Reformulations for the Maximum k-Colorable Subgraph Problem

RODOLFO QUINTERO[1], DAVID BERNAL[2], TAMÁS TERLAKY[1], AND LUIS F. ZULUAGA[1]

[1]Department of Industrial and Systems Engineering, Lehigh University

[2]Department of Chemical Engineering, Carnegie Mellon University

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Rodolfo Quintero[*] David Bernal[†] Tamás Terlaky[‡] Luis F. Zuluaga[§]

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Abstract

Both adiabatic quantum computers, and algorithms for gate-based quantum computers are able to address the solution of quadratic unconstrained binary optimization (QUBO) problems. This allows the use of quantum technology to solve combinatorial optimization (COPT) problems such as the Ising model and the max-cut problem which have a natural QUBO reformulation. Moreover, quantum technology can be used to solve a wider class of constrained COPT problems thanks to the use of penalization methods to embed the COPT problem's constraints in its objective to obtain the problem's QUBO reformulation. However, the particular way in which this penalization is carried out affects the value of the penalty constants, as well as the number of additional binary variables that are needed to obtain the desired QUBO reformulation. In turn, these factors substantially affect the ability of quantum computers to efficiently solve these constrained COPT problems. This efficiency is key towards the goal of using quantum computers to solve constrained COPT problems more efficiently than with classical computers. Along these lines, we consider an important constrained COPT problem; namely, the maximum k-colorable subgraph (MkCS) problem, in which the aim is to find an induced k-colorable subgraph with maximum cardinality in a given graph. This problem arises in channel assignment in spectrum sharing networks, VLSI design, human genetic research, and cyber security. We derive two QUBO reformulations for the MkCS problem, and fully characterize the range of the penalty constants that can be used in the QUBO reformulation. Further, one of the QUBO reformulation of the MkCS problem is obtained without the need to introduce additional binary variables. To illustrate the benefits of obtaining and characterizing these QUBO reformulations, we benchmark different QUBO reformulations of the MkCS problem using an adiabatic quantum device.

1 Introduction

Quantum computing (QC) harnesses the properties of subatomic particles to perform computations in a fundamentally different way than classical computing [45]. It is

[*]Industrial and Systems Engineering, Lehigh University, USA roq219@lehigh.edu
[†]Department of Chemical Engineering, Carnegie Mellon University, USA, bernalde@cmu.edu
[‡]Department of Industrial and Systems Engineering, Lehigh University, USA, terlaky@lehigh.edu
[§]Department of Industrial and Systems Engineering, Lehigh University, USA, luis.zuluaga@lehigh.edu

widely established that QC can, in the future, revolutionize the way we perform and think about computation, and be the backbone of thrilling new technologies and products [13, 37, 45].

In particular, QC has the potential to radically transform our capability to solve extremely difficult decision-making and design optimization problems for which no traditional numerical or theoretical efficient solution algorithms are known to exist. This is particularly the case for *combinatorial optimization* (COPT) problems; that is, optimization problems that are formulated with the use of discrete (e.g., binary) decision variables [14]. A large number of COPT problems are known to be NP-Hard [see, e.g., 28]; that is, there is no known polynomial-time algorithm that can be used to solve them. A very representative problem in this class of COPT NP-Hard problems is the *Ising model* [see, e.g., 7, 12, 46]. Since its inception, the Ising model has been used to address problems arising in different physical systems (e.g., magnetism, lattice gas, spin glasses), as well as in neuroscience and socio-economics.

The Ising model belongs to the class of *quadratically unconstrained binary optimization* (QUBO) problems [see,e.g., 39]. Moreover, both adiabatic quantum computers [see, e.g., 11, 27, 35], and algorithms (such as the quantum approximate optimization algorithm (QAOA)) for gate-based quantum computers [see, e.g., 17, 54] are able to address the solution of QUBO problems. This allows the use of quantum technology to solve problems such as the Ising model and the max-cut problem which has a natural QUBO reformulation [see, e.g., 16, 29]. Moreover, quantum technology can be used to solve a wider class of constrained COPT problems that do not have a natural QUBO reformulation. This is due to the fact that penalization methods can be used to embed the COPT problem's constraints in its objective to obtain a QUBO reformulation of the problem.

For some COPT feasibility problems (i.e., without an objective) that can be formulated using linear equality constraints, the desired QUBO reformulation can be obtained using any positive penalty parameter (to penalize the constraints' violations). For example, consider the QUBO reformulations of the number partitioning problem [35, 38], the graph isomorphism problem [8], the exact cover problem [35], and some planning problems [42], to name a few. However, when the COPT problem formulation requires (or uses) nonlinear constraints and/or an objective function, the desired QUBO reformulation is only guaranteed to be obtained for values of the penalty parameter(s) that are larger than a known, and potentially large lower bound. For example, consider the QUBO reformulations for the maximum clique problem [35], the traveling salesman problem [35, 38], and the minimax matching problem [35]. Worst, in some cases, the desired QUBO reformulation is only guaranteed to be obtained for an unknown large enough value of the penalty parameter(s). For example, consider the QUBO reformulations of the job shop scheduling problem [50], the de-conflicting optimal trajectories problem [47], the traveling salesman problem with time windows [40], and some of the problems discussed in [20]. Additionally, when the COPT problem formulation requires (or uses) linear inequality constraints, a potentially large number of auxiliary (i.e., slack) binary variables need to be introduced to obtain the desired QUBO reformulation. For example, consider the maximum clique QUBO reformulation provided in [35], and the COPT problems considered in [53].

The fact that large (or unknowingly large) penalty parameters, and additional binary variables might be needed to obtain the desired QUBO reformulation can hinder the ability of quantum computers to more efficiently solve COPT problems [see, e.g., 19, 44, 53]. As the results in [22] highlight, this efficiency is key towards the goal of using *noisy intermediate scale quantum* (NISQ) devices to solve COPT problems more efficiently than with classical computers. Not surprisingly, recent articles look beyond obtaining QUBO reformulations of COPT problems such as the graph isomorphism problem as well as tree and cycle elimination problems, to look for *improved* QUBO reformulations of these problems for NISQ devices [see, e.g., 8, 19, 25, 51, 52]. That is, QUBO reformulation that are tailored to be more efficiently used in NISQ devices.

Along these lines, we consider an important COPT problem; namely, the *maximum k-colorable subgraph* (MkCS) problem [see, e.g., 31], in which the aim is to find an induced k-colorable subgraph with maximum cardinality in a given graph. This problem arises in channel assignment in spectrum sharing networks (e.g., Wi-Fi or cellular) [23, 48], VLSI design [18], human genetic research [18, 33], telecommunications [34], and cyber security [3].

We derive two QUBO reformulations of the MkCS problem. The first one is obtained from the standard formulation of the MkCS problem in which all the constraints are linear, except for the binary variable constraints. This QUBO reformulation is an improved version of the QUBO reformulation that would be obtained by using the QUBO reformulation approach of Lasserre [32] for this "linear" formulation of the MkCS. The reason for this is that we characterize the minimum penalization constants that can be used to guarantee that the desired QUBO problem, obtained by penalizing the problem's linear constraints violations, is indeed equivalent to the original problem. Furthermore, we characterize the equivalence of the QUBO reformulation not only in terms of the objective value, but also in terms of the optimal solution obtained from this QUBO reformulation. In particular, we find that when the minimal values of the penalization constants are used, the QUBO reformulation is equivalent to the MkCS in terms of the problems' objectives, but not in terms of the problems' optimal solutions. However, we show that in this case, the QUBO reformulation's optimal solution can be used, in a simple way, to obtain the MkCS problem's optimal solution. In what follows, we will refer to this QUBO reformulation of the MkCS problem as the *linear-based* QUBO reformulation.

The second QUBO reformulation of the MkCS problem is obtained from a formulation of the MkCS problem in which all the linear constrains are first formulated as nonlinear equality constraints. Analogous to the results obtained for the linear-based QUBO reformulation of the MkCS problem, we derive a *nonlinear-based* QUBO reformulation of the MkCS problem. Then, we characterize the minimum penalizations constants that can be used to guarantee that the desired nonlinear-based QUBO problem, obtained by penalizing the problem's linear constraints violations, is indeed equivalent to the original problem. Furthermore, we characterize the equivalence of the nonlinear-based QUBO reformulation not only in terms of the objective value, but also in terms of the optimal solution obtained from this nonlinear-based QUBO reformulation. In particular, we find that when the minimal values of the penalization constants are used, the nonlinear-based QUBO reformulation is equivalent to the MkCS in terms of the problems' objectives, but not in terms of the problems' optimal solutions. However, we show that in this case, the nonlinear-based QUBO reformulation's optimal solution can be used, in a simple way, to obtain the MkCS problem's optimal solution. This latter result extends the work done in characterizations of QUBO reformulations of the *stable set problem* [1, 6, 24], which is equivalent to the MkCS problem when $k = 1$. The nonlinear-based QUBO reformulation of the MkCS problem is a substantial improvement over the linear-based QUBO reformulation of the MkCS problem, in great part, because the former QUBO does not need the addition of any auxiliary (i.e., slack) binary variables beyond the ones that define the original problem's formulation.

To illustrate the benefits of obtaining and characterizing these QUBO reformulations, we benchmark different QUBO reformulations of the MkCS problem using an adiabatic quantum device, and in particular, we look at how embedding requirements and theoretical and numerical convergence rates change depending on the QUBO reformulation being used, as well as the parameters with which is used.

The rest of the article is organized as follows. In Section 2, we present some relevant discussion to motivate our work, as well as results about QUBO reformulations for COPT problems. In Section 3, we formally present the MkCS problem and two associated QUBO reformulations. The first one, in Section 3.1, is based on a "linear" (modulo the binary variable constraints) formulation of the MkCS problem. The second one, in Section 3.2, is based on a "nonlinear" (beyond the binary variable constraints) formulation of the MkCS problem. In Section 4, we benchmark these two QUBO reformulation using an adiabatic quantum device. In Section 5, we finish with some concluding remarks.

2 Preliminaries

Formally, given a set of n binary decision variables $x \in \{-1, 1\}^n$ (or $x \in \{0, 1\}^n$) when appropriate), a vector $f \in \mathbb{R}^n$, and a matrix $Q \in \mathcal{S}^n$, where $\mathcal{S}^n$ is the set of symmetric matrices in $\mathbb{R}^{n \times n}$, a *quadratically unconstrained binary optimization* (QUBO) problem is the problem of finding [see, e.g., 6, 39]:

$$z^* = \begin{array}{ll} \min & x^\intercal Q x + f^\intercal x \\ \text{s.t.} & x \in \{-1, 1\}^n. \end{array} \tag{QUBO}$$

It is well-known that the Ising model belongs to the class of QUBO problems [see, e.g., 19, 35]. Moreover, other distinguished NP-Hard COPT problems can be naturally formulated, or easily reformulated as a QUBO problem. Foremost among this type of problems is the max-cut problem [see, e.g., 21], which arises in multiple important applications in science and engineering [see, e.g. 41, Sec. 6]. Given an undirected graph $G(V, E)$, the aim in the max-cut problem is to find a subset of nodes (or cut) $S \subseteq V$, such that the cardinality of the set of edges in E between the nodes in S and $S^c := V \setminus S$ is maximized. The max-cut problem can be naturally formulated as a QUBO problem by letting $Q = A$, $f = 0$, where $A \in \mathbb{R}^{V \times V}$ is the node-to-node adjacency matrix of $G(V, E)$.

Thanks to the QUBO reformulation of the max-cut problem, the ability of quantum computing to solve the max-cut problem has been widely studied in the literature. For example, consider the use QAOA algorithms in [15, 17, 54], and of quantum adiabatic devices in [29, 30] to solve instances of the max-cut problem. Furthermore, QUBO reformulations can be obtained for a wider class of COPT problems that do not have a natural QUBO reformulation. This is done by using penalization methods to embed the COPT problem's constraints in its objective [see, e.g., 8, 19, 20, 35, 38, 42, 47, 50, 53, to name just a few]. This approach clearly broadens the class of COPT problems that can be addressed with NISQ devices. However, the efficacy of NISQ devices to solve this broader class of COPT problems can be highly affected by the way in which the corresponding QUBO reformulation is obtained. This is because the performance of NISQ devices is highly affected by the number of qubits and the constants that are required to encode a QUBO [see, e.g., 8, 19, 25].

To illustrate this fact, consider the problem of obtaining a QUBO reformulation for the *maximum clique* problem. Given a graph $G(V, E)$ the aim in the maximum clique problem is to find the set of nodes $S \subseteq V$ with the highest cardinality such that the graph induced by S is a clique; that is, a complete subgraph [see, e.g., 4]. The cardinality of the largest induced clique of G is referred as the clique number $\chi(G)$. Lucas [35, Sec. 2.3] obtains a QUBO reformulation for the maximum clique problem by first noticing that $G(V, E)$ contains a clique of size $K \in \{2, \dots, |V|\}$ (i.e., w.l.o.g. assume $|E| \geq 1$) if and only if there is $x \in \{0,1\}^{|V|}$ such that $\sum_{i=1}^{|V|} x_i = K$, and $\sum_{(i,j)\in E} x_i x_j = \frac{1}{2}K(K-1)$. Thus, the maximum clique problem can be formulated as $\chi(G) = \max\{K \in \{2, \dots, |V|\} : \sum_{i=1}^{|V|} x_i = K, \sum_{(i,j)\in E} x_i x_j = \frac{1}{2}K(K-1), x \in \{0,1\}^{|V|}\}$. Furthermore, Lucas [35, Sec. 2.3] shows that this latter problem can be reformulated as the following QUBO.

$$\begin{aligned} \chi(G) = \quad \min \quad & -\sum_{i=1}^{|V|} x_i + (\Delta+2)\left(1 - \sum_{k=2}^{\Delta} y_k\right)^2 + (\Delta+2)\left(\sum_{k=2}^{\Delta} k y_k - \sum_{i=1}^{|V|} x_i\right)^2 + \\ & \tfrac{1}{2}\left(\sum_{k=2}^{\Delta} k y_k\right)\left(-1 + \sum_{k=2}^{\Delta} k y_k\right) - \sum_{(i,j)\in E} x_i x_j \\ \text{s.t.} \quad & x \in \{0,1\}^{|V|}, y_k \in \{0,1\}, k = 2, \dots, \Delta, \end{aligned} \tag{1}$$

where Δ is the degree of $G(V, E)$, and the auxiliary variable $y_k = 1$ if $\chi(G) = k$ and $y_k = 0$ otherwise for $k = 2, \dots, \Delta$. Note that the QUBO problem (1) uses $|V| + \Delta$ logical qubits and constants that belong to the range $[-2\Delta(\Delta+2), 2\Delta^3 + 3\Delta(\Delta-1) + 4]$ (after disregarding constant terms and appropriately replacing $x_i \to x_i^2$, $i = 1, \dots, |V|$, $y_k \to y_k^2$, $k = 2, \dots, \Delta$ in the objective of (1) to make it an homogenous quadratic). The performance of NISQ devices on solving QUBO problems is negatively affected by the use of larger number of logical qubits and larger constants [see, e.g. 8, 19, 20, 25, 53]. In this context, it is natural to ask if there are *improved* [see, e.g., 8, 19, 25, 51, 52] QUBO reformulation for the maximum clique problem. For example, notice that by slightly changing the definition and number of the auxiliary variables in (1), the range of the constants used in (1) can be substantially reduced. Namely, let $y \in \{0,1\}^{\Delta}$ be defined by $\sum_{k=1}^{\Delta} y_k = K$ if $\chi(G) = K$ for $K \in \{1, \dots, \Delta\}$. Then the maximum clique problem is equivalent to:

$$\begin{aligned} \chi(G) = \quad \min \quad & -\sum_{i=1}^{|V|} x_i + (\Delta+2)\left(\sum_{k=1}^{\Delta} y_k - \sum_{i=1}^{|V|} x_i\right)^2 + \\ & \tfrac{1}{2}\left(\sum_{k=1}^{\Delta} y_k\right)\left(-1 + \sum_{k=1}^{\Delta} y_k\right) - \sum_{(i,j)\in E} x_i x_j \\ \text{s.t.} \quad & x \in \{0,1\}^{|V|}, y \in \{0,1\}^{\Delta}. \end{aligned} \tag{2}$$

Note that the QUBO problem (2) uses constants that belong to a much smaller range

$[-2(\Delta+2), 4(\Delta+2)+1]$ than the range of constants used in the QUBO problem (1) (after disregarding constant terms and appropriately replacing $x_i \to x_i^2$, $i = 1, \ldots, |V|$, $y_k \to y_k^2$, $k = 1, \ldots, \Delta$ in the objective of (1) to make it an homogenous quadratic). However, a much better QUBO formulation for the maximum clique problem can be obtained by using the fact that $\chi(G) = \alpha(G^c)$ [see, e.g. 4], where for a graph $G(V, E)$, $G^c = G(V, E^c)$ is the complement of G, and $\alpha(G)$ stands for the *stable set number* of the graph G [see, e.g., 24]; that is, the size of the largest cardinality set $S \subseteq V$, such that there are no edges between the nodes in S. This fact can be used to show that (see, e.g., [8, Thm. 6] or [4, Thm. 2.3], among others)

$$\chi(G) = \alpha(G^c) = \min\left\{-\sum_{i=1}^{|V|} x_i + 2\sum_{(i,j)\notin E} x_i x_j : x \in \{0,1\}^{|V|}\right\} \tag{3}$$

Note that the QUBO problem (3) uses $|V|$ logical qubits and constants that belong to the range $\{-1, 2\}$. Thus, in terms of number of logical qubits and range of the constants used in the QUBO reformulation, (3) improves both (2) and (1). It is worth to point out that the QUBO reformulation (3) has been stated in numerous articles [see, e.g., 1, 4, 10, 57, to name a few]. Moreover, it is well known that the range of the constants in (3) can be further reduced to $\{-1, 1\}$. Namely, it has been proved (or stated) in numerous articles [see, e.g., 1, 6, 24, 38, 39, 55] that

$$\chi(G) = \alpha(G^c) = \min\left\{-\sum_{i=1}^{|V|} x_i + \sum_{(i,j)\notin E} x_i x_j : x \in \{0,1\}^{|V|}\right\} \tag{4}$$

There is however a caveat in the QUBO reformulation (4). For any $x \in \mathbb{R}^n$, let $\operatorname{supp}(x) = \{i \in \{1, \ldots, n\} : x_i \neq 0\}$. Unlike for (1)–(3), given $x^* \in \arg\min\{(4)\}$, $\operatorname{supp}(x^*)$ might not be a clique on G (nor an independent set in G^c). That is, while the QUBO problems (1)–(3) are equivalent to the maximum clique problem in terms of both objective value and (loosely speaking) optimal solution, in general, the QUBO problem (4) is equivalent to the maximum clique problem *only* in terms of objective value. This important topic will be revisited and discussed in detail in Section 3.2.

Along these lines, in what follows we consider the problem of obtaining not only a QUBO reformulation, but improved QUBO reformulation of a keystone COPT problem; namely, the *maximum k-colorable subgraph* (MkCS) problem [see, e.g., 31].

3 The k-subgraph coloring problem

Let $k \geq 1$ colors and a graph $G = (V, E)$ on n vertices be given. A subgraph H of G is k-colorable if we can assign to each vertex of H a color such that no two adjacent vertices in H have the same color. The maximum k-colorable subgraph problem (MkCS) aims at finding a k-colorable subgraph H of G with maximum cardinality. To model this problem, notice that any k-coloring of a subgraph of G can be encoded in the following way. For any $i \in [n]$ (where for any $t \in \mathbb{N}$, $[t] := \{1, \ldots, t\}$) and $r \in [k]$, let

$$x_{ir} = \begin{cases} 1, & \text{if vertex } i \in [n] \text{ is colored with color } r \in [k], \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

Then, $x \in \{0,1\}^{n\times k}$ defines a k-coloring of a subgraph of G if and only

$$\begin{aligned} & x_{ir} + x_{jr} \leq 1, \text{ for all } (i,j) \in E, r \in [k], \\ & \sum_{r\in[k]} x_{ir} \leq 1, \text{ for all } i \in [n]. \end{aligned} \tag{6}$$

Then, the MkCS can be formulated as [see, e.g., 31]:

$$\begin{aligned} \alpha_k(G) := \quad & \max_{x\in\{0,1\}^{n\times k}} && \sum_{i\in[n], r\in[k]} x_{ir} \\ & \text{s. t.} && x_{ir} + x_{jr} \leq 1, \quad \text{for all } (i,j) \in E, r \in [k], \\ & && \sum_{r\in[k]} x_{ir} \leq 1, \quad \text{for all } i \in [n]. \end{aligned} \tag{7}$$

The MkCS problem falls into the class of NP-complete problems [56]. Moreover, even approximating this problem is known to be NP-hard [36]. For $k = 1$, the MkCS is equivalent to the maximum stable set problem (i.e., $\alpha_1(G) = \alpha(G)$) that has been widely and thoroughly studied in the literature; and in particular, in the quantum computing literature [see, e.g., 10, 38, 55]. The cases $k = 2$; which is also referred as the maximum bipartite subgraph problem, and case $k > 2$ are considered less in the literature [see 31, for details]. However, as mentioned earlier, the MkCS problem arises in channel assignment in spectrum sharing networks (e.g., Wi-Fi or cellular) [23, 48], VLSI design [18], human genetic research [18, 33], telecommunications [34], and cyber security [3]. Thus, a range of approaches have been studied in the literature to address the solution of the MkCS problem, for example, using semidefintie optimization techniques [see, e.g., 31, 49] or integer programming techniques [see, e.g., 8, 9, 26].

Next we obtain and characterize QUBO reformulations for the MkCS problem that allow to address its solution using quantum technology. Before presenting these results, let us mention some additional, very basic facts about the MkCS problem that will be relevant to the discussion next.

Notice that a MkCS H of $G(V,E)$ can be recovered from any $x^* \in \arg\max\{\alpha_k(G)\}$; that is, $H := G(V_H, E_H)$, where $V_H = \{i \in [n] : x^*_{ir} > 0 \text{ for some } r \in [k]\}$, $E_H := \{(i,j) \in E : i,j \in V_H\}$, and the coloring of the vertices is obtained by coloring vertex $i \in V_H$ with color $r \in [k]$ if and only if $x^*_{ir} = 1$. Furthermore, given $\tilde{x} \in \{0,1\}^{n\times k}$, it is very simple to obtain a feasible solution $x' \in \{0,1\}^{n\times k}$ for the MkCS problem by sequentially dropping color $r' \in [k]$ from vertex $i' \in [n]$; that is, setting $\tilde{x}_{i'r'} = 0$, if $\tilde{x}_{i'r'} = 1$ and there exists $(i',j) \in E$ such that $\tilde{x}_{i'r'} + \tilde{x}_{jr'} > 1$ or $\sum_{r\neq r'} \tilde{x}_{i'r} \geq 1$. This simple fact is formally stated in Algorithm 1, in a particular form that will be helpful in stating some of the QUBO characterization results that follow.

3.1 Linear-based QUBO reformulation

Based on the formulation (7) of the MkCS problem in which all the constraints, except for the binary variable constraints are *linear*, we can derive and characterize a *linear-based* QUBO reformulation for the MkCS problem. For that purpose, let us first introduce some notation.

Given $k \geq 1$, a graph $G = (V,E)$ on n vertices, and $x \in \{0,1\}^{n\times k}$, $s \in \{0,1\}^{|E|\times k}$, $t \in \{0,1\}^n$, let

$$H_0(x) = \sum_{i\in[n], r\in[k]} x_{ir}^2, \tag{8}$$

Algorithm 1 MkCS feasibility

Input $k \geq 1$, $G(V,E)$, $|V| = n$, $x \in \{0,1\}^{n\times k}$
for $i \in [n]$, $(i,j) \in E$, $r \in [k]$ **do**
  if $x_{ir} + x_{jr} > 1$ **then**
    $x_{ir} \to 0$
  end if
end for
for $i \in [n]$, $r \in [k]$ **do**
  if $x_{ir} = 1$ and $\sum_{p\neq r\in[k]} x_{ip} \geq 1$ **then**
    $x_{ir} \to 0$
  end if
end for
Output $x' := x$ a feasible solution for the MkSC problem

and

$$H_1^l(x,s) = \sum_{(i,j)\in E, r\in[k]} (x_{ir} + x_{jr} + s_{ijr} - 1)^2, \tag{9a}$$

$$H_2^l(x,t) = \sum_{i\in[n]} \left(\sum_{r\in[k]} x_{ir} + t_i - 1 \right)^2. \tag{9b}$$

Furthermore, we define the following simple mappings. Given $x \in \{0,1\}^{n\times k}$ and $i' \in [n], r' \in [k]$, let the mapping $\mathcal{X}_{i'r'}(x) : \{0,1\}^{n\times k} \to \{0,1\}^{n\times k}$ be defined by

$$x_{ir} \to \begin{cases} 0 & \text{if } i = i', r = r' \\ x_{ir} & \text{otherwise} \end{cases}, i \in [n], r \in [k]. \tag{10}$$

Note that $\mathcal{X}_{i'r'}(x)$ is a generalization of the mapping used on proofs regarding QUBO reformulations of the stable set number problem (i.e., M1CS) [see, e.g., 1, 6, 24, 39, 55]. Here however, to deal with the general case $k > 1$, we need an additional mapping.

Given $p = \{0,1\}$, $s \in \{0,1\}^{|E|\times k}$, $t \in \{0,1\}^n$, and $(i',j') \in E$, $r' \in [k]$, let the mapping $\mathcal{M}^p_{i'j',r'}(s,t) : \{0,1\}^{|E|\times k+n} \to \{0,1\}^{|E|\times k+n}$ be defined by

$$s_{ijr} \to \begin{cases} 1 - s_{i'jr'} & \text{if } i = i', j \neq j', r = r' \\ (1 - s_{i'jr'})p & \text{if } i = i', j = j', r = r' \\ s_{ijr} & \text{otherwise} \end{cases}, (i,j) \in E, r \in [k], \tag{11a}$$

$$t_i \to \begin{cases} 1 - p & \text{if } i = i', \\ t_i & \text{otherwise} \end{cases}, i \in [n]. \tag{11b}$$

With these definitions in hand, we can now obtain the desired linear-based QUBO reformulation of the MkCS problem. For any $c_1, c_2 > 0$ define the QUBO problem:

$$\begin{aligned} Q^l_{c_1,c_2}(k,G) := \quad & \max \quad H^l_{c_1,c_2}(x,s,t) := H_0(x) - c_1 H_1^l(x,s) - c_2 H_2^l(x,t) \\ & \text{s.t.} \quad x \in \{0,1\}^{n\times k}, s \in \{0,1\}^{|E|\times k}, t \in \{0,1\}^n. \end{aligned} \tag{12}$$

Theorem 1 (linear-based QUBO reformulation of MkCS problem)**.** *Let $k \geq 1$ and a graph $G = (V, E)$ on n vertices be given. Then, for any $c_1 > 1, c_2 > 1$, $Q^l_{c_1,c_2}(k, G) = \alpha_k(G)$, and if $\tilde{x} \in \arg\max_x\{Q^l_{c_1,c_2}(k, G)\}$ then $\tilde{x} \in \arg\max\{\alpha_k(G)\}$.*

Proof. First, notice that $\tilde{x}$ is well defined and $Q^l_{c_1,c_2}(k, G)$ is attained as (12) is defined over a compact feasible set. Also, notice that for any $c_1, c_2 > 0$ and any feasible solution $x' \in \{0, 1\}^{n\times k}$ for the MkCS problem (7) with objective value $z(x') := \sum_{i\in[n],r\in[k]} x_{ir}$, one can construct a feasible solution for (12); that is, $x = x'$, $s_{ijr} = 1 - x'_{ir} - x'_{jr}$, for all $(i, j) \in E, r \in [k]$, and $t_i = 1 - \sum_{r\in[k]} x'_{ir}$, with objective value $H^l_{c_1,c_2}(x, s, t) = z(x')$. Thus, if $c_1, c_2 > 0$, the QUBO problem (12) is a relaxation of (7), and consequently $Q^l_{c_1,c_2}(k, G) \geq \alpha_k(G)$. Thus, to prove the result, it is enough to show that when $c_1, c_2 > 1$, one has that $\tilde{x}$ is a feasible solution for (7). By contradiction, assume this is not the case and let $c_1, c_2 > 1$, $(\tilde{s}, \tilde{t}) := \arg\max_{(s,t)}\{Q^l_{c_1,c_2}(k, G)\}$. Then either: (1) there is at least an $(i', j') \in E$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} + \tilde{x}_{j'r'} > 1$; or (2) there is at least an $i' \in [n]$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} = 1$ and $\sum_{r\neq r'\in[k]} \tilde{x}_{i'r} \geq 1$.

For case (1), consider the feasible solution $(x, s^0, t^0) \in \{0, 1\}^{n\times k+|E|\times k+n}$ for (12) obtained from $(\tilde{x}, \tilde{s}, \tilde{t})$ by letting $(x, s, t) = (\mathcal{X}_{i'r'}(\tilde{x}), \mathcal{M}^0_{i'j',r'}(\tilde{s}, \tilde{t}))$ (cf., (10), (11)). It then follows from (8), (10), and the fact $\tilde{x}_{i'r'} = 1$ that

$$H_0(x) = H_0(\tilde{x}) - 1. \tag{13}$$

Also, from (9a), (10), (11a), and the fact that $\tilde{x}_{i'r'} = \tilde{x}_{j'r'} = 1$, it follows that $-H^l_1(x, s^0) = -H^l_1(\tilde{x}, \tilde{s}) + \sum_{(i',j\neq j')\in E} 4\tilde{x}_{jr'}\tilde{s}_{i'jr'} + (1 + \tilde{s}_{i'j'r'})^2$. Thus,

$$-H^l_1(x, s^0) \geq -H^l_1(\tilde{x}, \tilde{s}) + 1. \tag{14}$$

Further, from (9b), (10), (11b), and the fact that $\tilde{x}_{i'r'} = 1$, it follows that $-H^l_2(x, t^0) = -H^l_2(\tilde{x}, \tilde{t}) + 2\tilde{t}_{i'} \sum_{r\neq r'\in[k]} \tilde{x}_{i'r} + \tilde{t}^2_{i'}$. Thus,

$$-H^l_2(x, t^0) \geq -H^l_2(\tilde{x}, \tilde{t}). \tag{15}$$

Using (13), (14), (15), it follows that $H^l_{c_1,c_2}(x, s^0, t^0) \geq H^l_{c_1,c_2}(\tilde{x}, \tilde{s}, \tilde{t}) - 1 + c_1 > H^l_{c_1,c_2}(\tilde{x}, \tilde{s}, \tilde{t}) = Q^l_{c_1,c_2}(k, G)$, which contradicts the optimality of $(\tilde{x}, \tilde{s}, \tilde{t})$ for (12).

We proceed analogously for case (2). Consider the feasible solution $(x, s, t) \in \{0, 1\}^{n\times k+|E|\times k+n}$ for (12) obtained from $(\tilde{x}, \tilde{s}, \tilde{t})$ by letting $(x, s^1, t^1) = (\mathcal{X}_{i'r'}(\tilde{x}), \mathcal{M}^1_{i',r'}(\tilde{s}, \tilde{t}))$ (cf., (10), (11)). It then follows from (8), (10), and the fact that $\tilde{x}_{i'r'} = 1$ that (13) holds. Also, from (9a), (10), (11a), and the fact that $\tilde{x}_{i'r'} = 1$, it follows that $-H^l_1(x, s^1) = -H^l_1(\tilde{x}, \tilde{s}) + \sum_{(i',j)\in E} 4\tilde{x}_{jr'}\tilde{s}_{i'jr'}$. Thus,

$$-H^l_1(x, s^1) \geq -H^l_1(\tilde{x}, \tilde{s}). \tag{16}$$

Further, from (9b), (10), (11b), and the fact that $\tilde{x}_{i'r'} = 1$, $\sum_{r\neq r'\in[k]} \tilde{x}_{j'r} \geq 1$, it follows that $-H^l_2(x, t^1) = -H^l_2(\tilde{x}, \tilde{t}) + 2(\sum_{r\neq r'\in[k]} \tilde{x}_{i'r})(1 + \tilde{t}_{i'}) + \tilde{t}^2_{i'} - 1$. Thus,

$$-H^l_2(x, t^1) \geq -H^l_2(\tilde{x}, \tilde{s}) + 1. \tag{17}$$

Using (13), (16), (17), it follows that $H^l_{c_1,c_2}(x, s^1, t^1) \geq H^l_{c_1,c_2}(\tilde{x}, \tilde{s}, \tilde{t}) - 1 + c_2 > H^l_{c_1,c_2}(\tilde{x}, \tilde{s}, \tilde{t}) = Q^l_{c_1,c_2}(k, G)$, which contradicts the optimality of $(\tilde{x}, \tilde{s}, \tilde{t})$ for (12).

Therefore $\tilde{x}$ satisfies that there is no $(i', j') \in E$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} + \tilde{x}_{j'r'} > 1$, or $i' \in [n]$ and $r' \in [k]$ such that $\sum_{r\in[k]} \tilde{x}_{i'r} > 1$. Therefore $\tilde{x}$ is a feasible solution of (7), which finishes the proof. □

It is worth to mention that, loosely speaking, the general form of the QUBO reformulation (12) for the MkCS problem can be obtained by using the recent results of Lasserre [32, Thm. 2.2]. Namely, one can use this result after reformulating the MkCS problem constraints as equality constraints using the approach described in [32, Sec. 2.3]. Then, after reformulating the problem using $\{1, -1\}$ binary variables (instead of $\{0, 1\}$ binary variables), [32, Thm. 2.2] can be used to obtain a QUBO reformulation of the MkCS problem. However, this reformulation would require the use a penalty constant with a value larger than nk (cf., with the values of c_1, c_2 in Theorem 1), and require the use of more auxiliary (i.e., slack) binary variables than the ones used in Theorem 1. Thus, Theorem 1 provides an improved QUBO reformulation of the MkCS problem than the one that would be obtained using [32, Thm. 2.2].

Later, in Section 3.3, we will further characterize the QUBO reformulation (12) for the MkCS. Next, however, we derive and characterize a QUBO reformulation for the MkCS in which no auxiliary (i.e., slack) binary variables are needed.

3.2 Nonlinear QUBO reformulation

Next, we obtain an improved QUBO reformulation for the MkCS problem in terms of the number of binary decision variables required in the QUBO reformulation, when compared with the one provided and characterized in Section 3.1. For this purpose, first notice that for any $x \in \{0,1\}^{n\times k}$, the linear constraints in (6) are equivalent to the nonlinear constraints

$$\begin{aligned} &x_{ir}x_{jr} = 0, \text{ for all } (i,j) \in E, r \in [k], \\ &x_{ir}x_{ip} = 0, \text{ for all } i \in [n], (r, p \neq r) \in [k] \times [k]. \end{aligned} \tag{18}$$

Then, consistent with (18), given $k \geq 1$, a graph $G = (V,E)$ on n vertices, and $x \in \{0,1\}^{n\times k}$, let

$$H_1^n(x) = \sum_{(i,j)\in E, r\in[k]} x_{ir}x_{jr}, \tag{19a}$$

$$H_2^n(x) = \sum_{i\in[n]} \left(\sum_{r\in[k], p\neq r\in[k]} x_{ir}x_{ip} \right). \tag{19b}$$

With these definitions in hand we can now obtain the desired *nonlinear-based* QUBO reformulation of the MkCS problem. For any $c_1, c_2 > 0$ define the QUBO problem:

$$\begin{aligned} Q^n_{c_1,c_2}(k,G) := \quad \max \quad & H^n_{c_1,c_2}(x) := H_0(x) - c_1 H_1^n(x) - c_2 H_2^n(x) \\ \text{s.t.} \quad & x \in \{0,1\}^{n\times k}. \end{aligned} \tag{20}$$

Theorem 2 (nonlinear-based QUBO reformulation of MkCS problem). *Let $k \geq 1$ and a graph $G = (V,E)$ on n vertices be given. Then, for any $c_1 > 1, c_2 > 1$, $Q^n_{c_1,c_2}(k,G) = \alpha_k(G)$, and if $\tilde{x} \in \arg\max\{Q^n_{c_1,c_2}(k,G)\}$ then $\tilde{x} \in \arg\max\{\alpha_k(G)\}$.*

Proof. The proof is mostly analogous to the proof of Theorem 1. First, notice that $\tilde{x}$ is well defined and $Q^n_{c_1,c_2}(k,G)$ is attained as (20) is defined over a compact feasible set. Also, notice that for any $c_1, c_2 > 0$ and any feasible solution $x' \in \{0,1\}^{n\times k}$ for the

MkCS problem (7) with objective value $z(x') := \sum_{i\in[n],r\in[k]} x_{ir}$, one hast that x' is a feasible solution of (20) with objective value $H^n_{c_1,c_2}(x) = z(x')$ (i.e., x' satisfies (18)). Thus, if $c_1, c_2 > 0$, the QUBO problem (20) is a relaxation of (7), and consequently $Q^n_{c_1,c_2}(k, G) \geq \alpha_k(G)$. Thus, to prove the result, it is enough to show that when $c_1, c_2 > 1$, one has that $\tilde{x}$ is a feasible solution for (7). By contradiction, assume this is not the case and let $c_1, c_2 > 1$. Then either: (1) there is at least an $(i', j') \in E$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} + \tilde{x}_{j'r'} > 1$; or (2) there is at least an $i' \in [n]$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} = 1$ and $\sum_{r\neq r'\in[k]} \tilde{x}_{i'r} \geq 1$. Notice that in either case $\tilde{x}_{i'r'} = 1$. Now consider the feasible solution $x \in \{0,1\}^{n\times k}$ for (20) obtained from $\tilde{x}$ by letting $x = \mathcal{X}_{i'r'}(\tilde{x})$ (cf., (10)). Notice that from (8), (10), and the fact that $\tilde{x}_{i'r'} = 1$ one has that (13) holds. Also, from (19a), (10), and the fact that $\tilde{x}_{i'r'} = 1$, it follows that $-H^n_1(x) = -H^n_1(\tilde{x}) + \sum_{(i',j\neq j')\in E} \tilde{x}_{jr'} + \tilde{x}_{j'r'}$. Thus,

$$-H^n_1(x) \geq -H^n_1(\tilde{x}) + \tilde{x}_{j'r'}. \tag{21}$$

Further, from (19b), (10), and the fact that $\tilde{x}_{i'r'} = 1$, it follows that

$$-H^n_2(x) = -H^n_2(\tilde{x}) + \sum_{r\neq r'\in[k]} x_{i'r}. \tag{22}$$

Using (13), (21), (22), it follows that

$$H^n_{c_1,c_2}(x) \geq H^n_{c_1,c_2}(\tilde{x}) - 1 + c_1\tilde{x}_{j'r'} + c_2 \sum_{r\neq r'\in[k]} x_{i'r}. \tag{23}$$

In case (1), we have that $\tilde{x}_{j'r'} = 1$. Thus, from (23), we have that $H^n_{c_1,c_2}(x) \geq H^n_{c_1,c_2}(\tilde{x}) - 1 + c_1 > H^n_{c_1,c_2}(\tilde{x}) = Q^n_{c_1,c_2}(k, G)$, which contradicts the optimality of $\tilde{x}$ for (20). Analogously, in case (2), we have that $\sum_{r\neq r'\in[k]} \tilde{x}_{j'r} \geq 1$. Thus, from (23), we have that $H^n_{c_1,c_2}(x) \geq H^n_{c_1,c_2}(\tilde{x}) - 1 + c_2 > H^n_{c_1,c_2}(\tilde{x}) = Q^n_{c_1,c_2}(k, G)$, which contradicts the optimality of $\tilde{x}$ for (20).

Therefore $\tilde{x}$ satisfies that there is no $(i', j') \in E$ and $r' \in [k]$ such that $\tilde{x}_{i'r'} + \tilde{x}_{j'r'} > 1$, or $i' \in [n]$ and $r' \in [k]$ such that $\sum_{r\in[k]} \tilde{x}_{i'r} > 1$. Therefore $\tilde{x}$ is a feasible solution of (7), which finishes the proof. □

Next, we show that the value of the penalty constants c_1, c_2 in the definition of $Q^n_{c_1,c_2}(k, G)$ in (20) can be further reduced to the values $c_1 = c_2 = 1$, while still being able to obtain an optimal solution for the MkCS problem for $G(V, E)$ by solving the QUBO problem $Q^n_{1,1}(k, G)$. In this case, $Q^n_{1,1}(k, G)$ is equivalent to $\alpha_k(G)$ in terms of their optimal objective value, but not necessarily in terms of their optimal solutions. That is, the optimal solution $\tilde{x} := \arg\max(Q^n_{1,1}(k, G))$ might not necessarily be a feasible solution for the MkCS problem, which hinders the possibility of constructing a MkCS H for $G(V, E)$. However, as we formally show in the next corollary, the $Q^n_{1,1}(k, G)$ optimal solution $\tilde{x}$ can be simply modified to obtain an optimal solution for the MkCS problem.

Corollary 1 (unit-penalty nonlinear-based QUBO formulation of MkCS problem)**.** *Let $k \geq 1$ and a graph $G = (V, E)$ on n vertices be given, and let $\tilde{x} := \arg\max\{Q^n_{1,1}(k, G)\}$ (recall (20)). Then, $Q^n_{1,1}(k, G) = \alpha_k(G)$. Furthermore, $x' \in \arg\max\{\alpha_k(G)\}$, where $x' \in \{0,1\}^{n\times k}$ is the output obtained when k, $G(V, E)$, $|V|$, $x = \tilde{x}$ is used as input in Algorithm 1.*

Proof. The result follows from the proof of Theorem 2 and Algorithm 1. More specifically, notice that Algorithm 1(4): is equivalent to applying the mapping $\mathcal{X}_{ir}(\cdot)$ (recall (10)) to the current solution x in the Algorithm when $x_{ir} = x_{jr} = 1$ for some $(i, j) \in E$, $r \in [k]$. Thus, it follows from (23) that the value of $H^n_{1,c_2}(x)$ can only increase or stay equal after Algorithm 1(4):. Similarly, notice that Algorithm 1(9): is equivalent to applying the mapping $\mathcal{X}_{ir}(\cdot)$ (recall (10)) to the current solution x in the Algorithm when $x_{ir} = 1$, $\sum_{p\neq r\in[k]} x_{ip} \geq 1$ for some $i \in [n]$, $r \in [k]$. Thus, it follows from (23) that the value $H^n_{c_1,1}(x)$ can only increase of stay equal after Algorithm 1(9):. Thus, at the end of Algorithm 1 one obtains a feasible solution x' for the MkCS problem with objective $H^n_{1,1}(x') \geq H^n_{1,1}(\tilde{x}) = Q^n_{1,1}(k, G)$. Since $Q^n_{1,1}(k, G) \geq \alpha_k(G)$ (see beginning of proof of Theorem 2), it follows that $Q^n_{1,1}(k, G) = \alpha_k(G)$, and $x' \in \arg\max\{\alpha_k(G))\}$. □

In light of Theorem 2 and Corollary 1, it is natural to consider what happens if in the QUBO problem (20) one considers penalty values $0 < c_1, c_2 < 1$.

Proposition 1. *Let $k \geq 1$ and $c_1, c_2 > 0$ be given. If $c_1 < 1$ or $c_2 < 1$ and $k > 1$, then there exists a graph $G(V, E)$ such that $Q^n_{c_1,c_2}(k, G) > \alpha_k(G)$.*

Proof. First, consider the case in which $0 < c_1 < 1$, and let $G(V, E)$ is a clique of $k+1$ vertices. Clearly $\alpha_k(G) = k$. Now let

$$x_{ir} = \begin{cases} 1 & i = r, i \leq k \\ 1 & i = k+1, r = k \\ 0 & \text{otherwise} \end{cases}, \text{ for all } i \in [k+1], r \in [k].$$

Then, $Q^n_{c_1,c_2}(k, G) \geq H^n_{c_1,c_2}(x) = (k + 1) - c_1 > k = \alpha_k(G)$. Now, consider the case in which $0 < c_2 < 1$, and let $G(V, E)$ be the graph on $k + 1$ vertices obtained by taking a clique in $k + 1$ vertices and adding a vertex $k + 2$ and edge $(k + 1, k + 2)$. That is, $V = [k + 2]$, and $E = \{(i, j) : 1 \leq i < j \leq k + 1\} \cup \{(k + 1, k + 2)\}$. Clearly $\alpha_k(G) = k + 1$. Now let

$$x_{ir} = \begin{cases} 1 & i = r, i \leq k \\ 1 & i = k+2, r = k \\ 1 & i = k+2, r = k-1 \\ 0 & \text{otherwise} \end{cases}, \text{ for all } i \in [k+2], r \in [k].$$

Then, $Q^n_{c_1,c_2}(k, G) \geq H^n_{c_1,c_2}(x) = (k + 2) - c_2 > k + 1 = \alpha_k(G)$. □

Theorem 2 together with Corollary 1 and Proposition 1 fully characterize the QUBO problem (20) as a means to obtain a QUBO reformulation of the MkCS problem. In short, for any $c_1, c_2 \geq 1$, solving the nonlinear-based QUBO problem (20) is equivalent to solving the MkCS problem with the caveat that if either $c_1 = 1$ or $c_2 = 1$, the simple Algorithm 1 might need to be applied to the optimal solution of (20) in order to obtain an optimal solution for the MkCS problem. On the other hand, if $0 < c_1 < 1$ or $0 < c_2 < 1$, solving the nonlinear-based QUBO problem (20) is not guaranteed to provide the objective value or the solution to the MkCS problem.

As illustrated in Section 4, this full characterization gives the freedom to fine tune the QUBO reformulation of the MkCS problem to make the best use of quantum tools in addressing the solution of this problem.

In finishing this section, recall that the MkCS problem is equivalent to the stable set problem when $k = 1$. Thus the QUBO reformulation results [see, e.g., 1, 4, 6, 8, 24, 38, 39, 55] for the stable set problem of the form

$$\alpha(G) = \max \left\{ \sum_{i=1}^{n} x_i^2 - c_1 \sum_{(i,j)\in E} x_i x_j : x \in \{0,1\}^n \right\}, \tag{24}$$

for a given graph $G(V, E)$ on n vertices and $c_1 \geq 1$ follow from Theorem 2 and Corollary 1. In particular, Corollary 1 implies results in which c_1 is set to one in (24). However, Corollary 1 brings up a fact that to the best of our knowledge has been ignored in the literature; namely, that when c_1 is set to one in (24), the support of the optimal solution of (24) might not necessarily correspond to a stable set of the graph $G(V, E)$.

3.3 Linear-based QUBO reformulation revisited

After the results in Section 3.2, which provide a full characterization of the QUBO problem (20) to reformulate the MkCS problem, it is natural to consider if a similar full characterization of the QUBO problem (12) can be obtained. Indeed, it is not difficult to see that analogous results (with analogous proofs that are not included in the interest of brevity), to Corollary 1 and Proposition 1 can be obtained for the QUBO problem (12).

Corollary 2 (unit-penalty linear-based QUBO formulation of MkCS problem)**.** *Let $k \geq 1$ and a graph $G = (V, E)$ on n vertices be given, and let $\tilde{x} := \arg\max_x \{Q^l_{1,1}(k, G)\}$ (recall (12)). Then, $Q^l_{1,1}(k, G) = \alpha_k(G)$. Furthermore, $x' \in \arg\max\{\alpha_k(G)\}$, where $x' \in \{0,1\}^{n\times k}$ is the output obtained when k, $G(V, E)$, $|V|$, $x = \tilde{x}$ is used as input in Algorithm 1.*

Proposition 2. *Let $k \geq 1$ and $c_1, c_2 > 0$ be given. If $c_1 < 1$ or $c_2 < 1$ and $k > 1$, then there exists a graph $G(V, E)$ such that $Q^l_{c_1,c_2}(k, G) > \alpha_k(G)$.*

4 Benchmarking

In this section, to illustrate the benefits of this QUBO reformulation, we theoretically and experimentally benchmark it in terms of embedding requirements, and the theoretical convergence rate, when the QUBO is used to solve the MkCS problem in and adiabatic quantum device. This numerical experiments are similar in nature to those carried out in [8, 25, 51, 52] to compare different QUBO formulations of a given problem.

4.1 Minimum Gap

The *minimum gap* [see, e.g. 43] gives information about how fast would a quantum annealer converge to a solution [see, e.g., 2]. In Figure 1, we compare the minimum gap resulting when using the linear-based QUBO reformulation (NON-LINEAR Min Gap in Figure 1) and the nonlinear-based QUBO reformulations (LINEAR Min Gap in Figure 1) for the MkCS problem. In particular, we compare the minimum gaps for instances of the problem in which $k = 1$ and the graphs are randomly selected Erdös-Rénjy graphs with parameter $p = 0.25$.

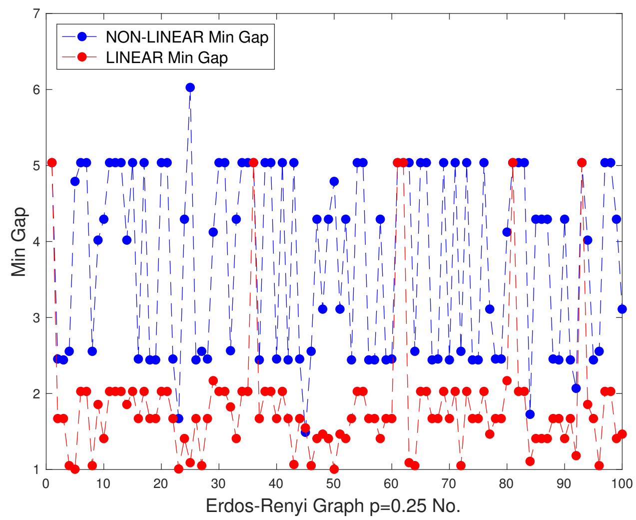

Figure 1: Minimum Gap calculation for Erdös-Rénjy $p = 0.25$ graphs

From Figure 1, it follows that the minimum gap associated to the nonlinear-based QUBO reformulation (20) in these instances is higher than the the minimum gap associated to the nonlinear-based QUBO reformulation (20) in the same instances. As a result, in theory, the nonlinear-based QUBO reformulation (20) converges faster to its solution.

4.2 Embedding

In Figure 2 and Figure 3 we compare the number of quibits that it is required to embed the QUBOs in a C16 Chimera graph [5].

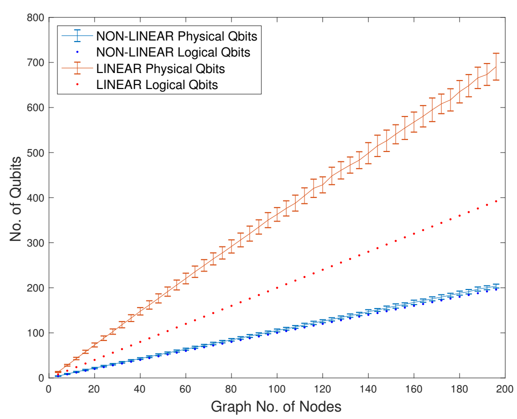

Figure 2: Cycle graphs.

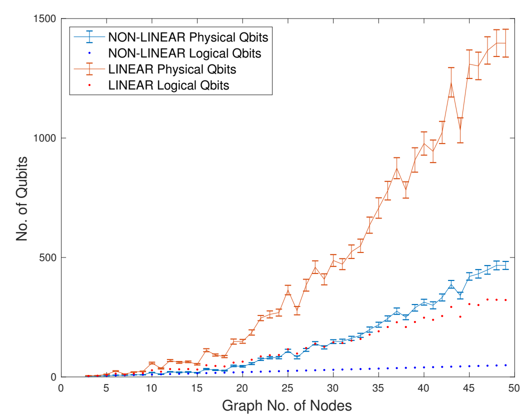

Figure 3: Erdös-Rénjy $p = 0.25$ graphs.

5 Concluding remarks

In this paper, we consider a particularly important COPT problem; namely, the maximum k-colorable subgraph problem, in which the aim is to find an induced k-colorable subgraph with maximum cardinality in a given graph. This problem arises in channel assignment in spectrum sharing networks (e.g., Wi-Fi or cellular), VLSI design, human genetic research, cyber security, cryptography, and scheduling. We show that this constrained COPT problem can be exactly reformulated as a QUBO; that is, using known and minimal penalization constants, and without the need to introduce additional logical variables. To illustrate the benefits of this QUBO reformulation, we theoretically and experimentally benchmark it in terms of embedding requirements, and theoretical and numerical convergence rate in and adiabatic quantum device.

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