



Solving Constrained Quadratic Binary Problems via Quantum Adiabatic Evolution

Pooya Ronagh, Brad Woods, Ehsan Iranmanesh

Abstract

Quantum adiabatic evolution is perceived as useful for binary quadratic programming problems that are a priori unconstrained. For constrained problems, it is a common practice to relax linear equality constraints as penalty terms in the objective function. However, there has not yet been proposed a method for efficiently dealing with inequality constraints using the quantum adiabatic approach. In this paper, we give a method for solving the Lagrangian dual of a binary quadratic programming (BQP) problem in the presence of inequality constraints and employ this procedure within a branch-and-bound framework for constrained BQP (CBQP) problems.

Keywords: Adiabatic quantum computation, Constrained integer programming, Branch and bound, Lagrangian duality

1 Introduction

The unconstrained binary quadratic programming (UBQP) problem is defined by

$$\begin{aligned} & \text{Minimize} && x^T Q x \\ & \text{subject to} && x \in \{0, 1\}^n, \end{aligned}$$

where, without loss of generality, $Q \in \mathbb{Z}^{n \times n}$. Recent advancements in quantum computing technology [6, 20, 22] have raised hopes of the production of computing systems that are capable of solving UBQP problems, showing quantum speedup. The stochastic nature of such systems, together with all sources of noise and error, are challenges yet to be overcome in achieving scalable quantum computing systems of this type. This paper is regardless motivated by the assumption of the existence of systems that can solve UBQP problems efficiently and to optimality, or at least in conjunction with a framework of noise analysis of the suboptimal results. We call such a computing system a UBQP oracle.

Many NP-hard combinatorial optimization problems arise naturally or can easily be reformulated as UBQP problems, such as the quadratic assignment problem, the maximum cut problem, the maximum clique problem, the set packing problem, and the graph colouring problem (see, for instance, Boros and Prékopa [9], Boros and Hammer [8], Bourjolly et al. [10], Du and Pardalos [14], Pardalos and Rodgers [27, 28], Pardalos and Xue [29], and Kochenberger et al. [23]).

Numerous interesting applications that are expressed naturally in the form of UBQP problems appear in the literature. Barahona et al. [4, 13] formulate and solve the problem of finding exact ground states of spin glasses with magnetic fields. Alidaee et al. [2] study the problem of scheduling n jobs non-preemptively on two parallel identical processors to minimize weighted mean flow time as a UBQP problem. Bomze et al. [7] give a comprehensive discussion of the maximum clique (MC) problem. Included is the UBQP representation of the MC problem and a variety of applications from different domains. UBQP has been used in the prediction of epileptic seizures [19]. Alidaee et al. [1] discuss a number partitioning problem, formulating a special case as a UBQP problem.

In the literature, problems which naturally occur as constrained binary quadratic programming (CBQP) problems are commonly reformulated as UBQP problems by including quadratic penalties in the objective function as an alternative to explicitly imposing constraints. Although this method has been used very successfully on classical hardware, it is not a viable approach when using quantum adiabatic hardware, as the reformulation dramatically increases the density, range of coefficients, and dimension of the problem.

In this paper, we consider the CBQP problem with linear constraints, stated formally as

$$\begin{aligned} \text{(P)} \quad & \text{Minimize} && x^T Q x \\ & \text{subject to} && Ax \leq b, \\ & && x \in \{0, 1\}^n, \end{aligned}$$

where $Q \in \mathbb{Z}^{n \times n}$ and $A \in \mathbb{Z}^{m \times n}$. We present a branch-and-bound approach which uses Lagrangian duality to solve (P) and show that a UBQP oracle can be used to solve the Lagrangian dual (LD) problem with successive applications of linear programming (LP). We introduce the notion of *quantum annealing leniency*, which represents the maximum threshold of the annealing time allowed for our approach to outperform the Gurobi Optimizer.

The remainder of this paper is organized as follows. Section 2 gives an overview of the quantum adiabatic approach to computation and the relationship of the approach to UBQP. Section 3 presents lower-bounding procedures for CBQP. Section 4 presents a local search heuristic for CBQP. Branching strategies are described in Section 5. Test instances and results of our computational experiments are presented in Section 6. In Section 7 we provide practical remarks for application of our method to the D-Wave systems, and in Section 8 we mention how our method can more generally be used to solve constrained binary programming problems with higher-order objective and constraint polynomials.

2 Preliminaries

2.1 Overview of quantum computing using adiabatic evolution

Recent advancements in quantum hardware have increased the motivation to study forms of computation that differ in computational complexity from the limitations of Turing machines. The quantum gate model is a means of achieving powerful quantum algorithms such as Shor's well known quantum algorithms for factoring and discrete logarithms [32]. Aside from the quantum gate model, there are several other paradigms of quantum information technology, each of which would open a new world of possible algorithm designs for the realization of a corresponding practical quantum processor.

Farhi et al. [15, 16] propose quantum adiabatic evolution as a novel paradigm for the design of quantum algorithms. The physicist's interpretation of this quantum phenomenon is a "quantum" analogue to what an optimization theorist would view as simulated annealing. In particular, quantum adiabatic evolution can be viewed as a quantum local search that converges to a best known solution as a parameter t varies from an initial time 0 to a final time T . Just as in the case of a simulated annealing algorithm, the challenge is to show that the process converges to the best solution with nonzero probability if T is a polynomial in the size of the problem.

Van Dam et al. [33] give an example of an adiabatic quantum algorithm for searching that matches the optimal quadratic speedup obtained by Grover's search algorithm. This example demonstrates that the "quantum local search", which is implicit in the adiabatic evolution, is truly non-classical in nature from a computational perspective. In the same reference [33], Theorem 4.1 explains how the continuous-time evolution of $t \in [0, T]$ can be approximated by a quantum circuit consisting of a sequence of $\text{poly}(nT)$ unitary transformations.

All of the above considerations motivate the main assumption of this paper: practical quantum hardware can result in a significant quantum speedup in certain forms of integer programming. Our goal is to design and suggest optimization algorithms that work in conjunction with such integer programming oracles.

In the rest of this section, following [33], we review more details of the quantum adiabatic evolution and explain the quantum adiabatic approach to UBQP.

2.2 The quantum adiabatic theorem

A time-dependent quantum mechanical system is described by the Schrödinger equation

$$i\hbar \frac{d}{ds} |\psi(s)\rangle = H(s) |\psi(s)\rangle.$$

Here \hbar is Planck's constant. s is a reparametrization of time ranging in $[0, 1]$. $|\psi(s)\rangle$ is a vector in a high-dimensional Hilbert space and represents the state of the system. $H(s)$ is the *Hamiltonian* of the system, a Hermitian operator on the Hilbert space such that its eigenvectors form the set of all possible states of the system, also known as *eigenstates*. The eigenvalue spectrum of $H(s)$ refer to the different *energies* of the eigenstates. The state (eigenvector) with the lowest energy (eigenvalue) is called the *ground state* of the system.

In most scenarios the Schrödinger equation is a complicated differential equation to tackle. The main challenge in quantum physics is approximating and understanding the properties of the solution of this equation. The quantum adiabatic theorem is an example of such investigation.

The theorem states that a physical system that is initially in its ground state tends to stay in that state, provided that the Hamiltonian of the system is changed slowly enough [26]. For instance, if we add a constant *delay factor* T to the

Schrödinger equation,

$$i\hbar \frac{d}{ds} |\psi(s)\rangle = TH(s) |\psi(s)\rangle,$$

the evolution is slow enough in the sense of the adiabatic theorem, provided that T satisfies

$$T \gg \frac{\|\frac{d}{ds} H(s)\|_2}{g(s)^2}, \quad \text{for all } s \in [0, 1].$$

Here $g(s)$ is the difference between the smallest two eigenvalues of $H(s)$ and is often referred to as the *gap* at time s . Finding g as a function of s is a difficult problem of interest in condensed matter physics. However, to give a constant delay factor we need only to find a lower bound for it. We may therefore simply consider the *minimum gap* $g_{\min} := \min_s g(s)$ and also $\Delta_{\max} := \max_s \|\frac{d}{ds} H(s)\|_2$. We can then verify that a constant delay factor $T \in O(\frac{\Delta_{\max}}{g_{\min}^2})$ is sufficient for the adiabatic evolution.

2.3 Adiabatic quantum computation

Let $f : \{0, 1\}^n \rightarrow \mathbb{R}$ be a function on the binary domain that is computable in polynomial time and bounded in values by a polynomial in the size of its input argument (for example, f is a polynomial). In adiabatic quantum computation as proposed by Farhi et al. [15], we associate a physical system to f such that its Hamiltonian H_f takes the same eigenvalue spectrum as f . Hence H_f can be explicitly written as

$$H_f := \sum_{z \in \{0,1\}^n} f(z) \cdot |z\rangle\langle z|$$

in the basis of its eigenstates, also encoded as the domain $\{0, 1\}^n$.

We consider another Hamiltonian H_0 whose eigenstates are easy to compute but is not diagonal in the z -basis. An explicit suggestion for H_0 is as follows. Given

$$|\hat{0}\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad \text{and} \quad |\hat{1}\rangle := \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$

we consider the "Hadamard basis" as consisting of all states $|\hat{z}\rangle$ which would be written as $|z\rangle$ in this basis as z ranges over all binary strings $z \in \{0, 1\}^n$. Then H_0 may be defined as

$$H_0 := \sum_{z \in \{0,1\}^n} h(z) \cdot |\hat{z}\rangle\langle \hat{z}|,$$

with $h(0^n) = 0$ and $h(z) \geq 1$ for all other $z \neq 0^n$. Thus the ground state of H_0 is $|\hat{0} \cdots \hat{0}\rangle$, which is a uniform superposition of all of the states in the z -basis,

$$|\hat{0} \cdots \hat{0}\rangle = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle.$$

For any practical implementation it is necessary that the hardware can be easily set to this ground state.

The quantum adiabatic computation is defined as the time-dependent Hamiltonian

$$H(t) := \left(1 - \frac{t}{T}\right) H_0 + \frac{t}{T} H_f,$$

with $0 \leq t \leq T$ when the system is set to the ground state of H_0 at time $t = 0$:

$$|\psi(0)\rangle = |\hat{0}^n\rangle.$$

Here $T > 0$ is the delay factor of the evolution and by the adiabatic theorem this system will evolve $|\psi(0)\rangle$ to the global minimum of the function f , provided that $T \in O(\frac{\Delta_{\max}}{g_{\min}^2})$.

In what follows we work under the assumption of the existence of a *UBQP oracle*, an oracle for solving UBQP problems. This is specifically motivated by current progress of quantum adiabatic technology pioneered by D-Wave Systems, in which the connectivities of the quantum bits are only in the form of couplings between pairs of quantum bits [20]. However, we will observe that our suggested methods are easily generalizable to take advantage of systems with higher-degree interactions of quantum bits if such systems are implemented in the future (see Section 8).

3 Lower-bounding procedures

3.1 Linearization relaxation

A standard linearization of (P) involves relaxing the integrality constraint on variables x_i , ($i = 1, \dots, n$) and defining continuous variables y_{ij} for every pair $x_i x_j$ in the objective function with $i < j$, yielding the following linearized problem.

$$\begin{aligned}
 (\text{P}_{\text{LP}}) \quad & \text{Minimize} && \sum_{1 \leq i < j \leq n} 2q_{ij}y_{ij} + \sum_{i=1}^n q_{ii}x_i \\
 & \text{subject to} && Ax \leq b, \\
 & && y_{ij} \geq x_i + x_j - 1 \quad (\forall i, j \text{ such that } i < j \text{ and } q_{ij} > 0), \\
 & && y_{ij} \leq x_i \quad (\forall i, j \text{ such that } i < j \text{ and } q_{ij} < 0), \\
 & && y_{ij} \leq x_j \quad (\forall i, j \text{ such that } i < j \text{ and } q_{ij} < 0), \\
 & && 0 \leq x_i \leq 1 \quad (i = 1, \dots, n), \\
 & && y \geq 0.
 \end{aligned}$$

A lower bound to (P) can now be obtained by solving (P_{LP}) using linear programming. We employed this linearization in our computational experiments (see Section 6). We recall that there are several methods for linearization of (P) to LP problems, many of which have been mentioned in the survey [17] by Floudas and Gounaris, and depending on the specific application at hand, may be better choices. We will ignore this variety of choices, and call (P_{LP}) *the* LP relaxation of (P).

3.2 Lagrangian dual

We can give a lower bound for (P) by the LD problem

$$(\text{L}) \quad \max_{\lambda \in \mathbb{R}_+^m} d(\lambda),$$

where $d(\lambda)$ is evaluated via the *Lagrangian relaxation*

$$(\text{L}_\lambda) : \quad d(\lambda) = \min_{x \in \{0,1\}^n} L(x, \lambda) = x^T Qx + \lambda^T (Ax - b).$$

The function $d(\lambda)$ is the minimum of a finite set of linear functions of λ and hence it is concave and piecewise linear.

A number of techniques to solve (L) exist in the literature; however, finding this bound is computationally expensive, so looser bounds (for example, the LP relaxation) are typically used. We note that the problem yields a natural solution using the UBQP oracle via the outer Lagrangian linearization method. The book by Li and Sun [25] provides background and several details of this approach.

We recall that (L) can be rewritten as an LP problem:

$$\begin{aligned}
 (\text{L}_{\text{LP}}) \quad & \text{Maximize} && \mu \\
 & \text{subject to} && \mu \leq x^T Qx + \lambda^T (Ax - b) \quad (\forall x \in \{0, 1\}^n), \\
 & && \lambda \geq 0.
 \end{aligned}$$

This formulation is difficult to solve directly, as there are an exponential number of constraints. In particular, there is one linear constraint (cutting plane) for every binary point $x \in \{0, 1\}^n$. However, the restriction of the constraints to a much smaller nonempty subset $T \subseteq \{0, 1\}^n$ of binary vectors is a tractable LP problem:

$$\begin{aligned}
 (\text{L}_{\text{LP}-T}) \quad & \text{Maximize} && \mu \\
 & \text{subject to} && \mu \leq x^T Qx + \lambda^T (Ax - b) \quad (\forall x \in T), \\
 & && \lambda \geq 0.
 \end{aligned}$$

This LP problem is bounded provided that T contains at least one feasible solution. In several applications finding at least one feasible solution is easy but sometimes very difficult. In the latter cases we impose an upper bound on the vector of Lagrange multipliers, substituting the constraint $\lambda \geq 0$ by $0 \leq \lambda \leq u$. The vector u of upper bounds, may depend on an estimation of the solution to (L). In practical situations, it should also depend on the specifics of the UBQP oracle (for example, the noise and precision of the oracle). Let (μ^*, λ^*) be an optimal solution to (L_{LP-T}). It is clear that (L_{λ*}) is a UBQP problem that can be solved using the UBQP oracle. By successively adding the solutions returned by the UBQP oracle as cutting planes, and a successive application of the simplex method, we are able to solve (L_{LP}) in a similar fashion to [25, Procedure 3.2].

4 A local search heuristic

In order to prune a branch-and-bound tree effectively, it is important to quickly obtain a good upper bound. We employ an adaptation of the local search algorithm presented by Bertsimas et al. [5]. The main idea is as follows: beginning with a feasible solution x , we iteratively improve the solution by considering solutions in the 1-flip neighbourhood of x (defined as the set of solutions that can be obtained by flipping a single element of x) which are feasible, together with "interesting" solutions, until it cannot be improved further. The algorithm takes a parameter ρ which explicitly controls the trade-off between complexity and performance by increasing the size of the neighbourhood. A neighbouring solution y is considered "interesting" if it satisfies the following conditions: (i) no constraint is violated by more than one unit, and (ii) the number of violated constraints in y plus the number of loose constraints which differ from the loose constraints in the current best solution is at most ρ .

Algorithm 1 Local search heuristic

Require: matrix A, Q ; vector b ; feasible solution z_0 ; scalar parameter $\rho > 0$

Ensure: Feasible solution z such that $z^T Q z \leq z_0^T Q z_0$

```
1:  $z := z_0; S := \{z\}$ 
2: while  $S \neq \emptyset$  do
3:   get a new solution  $x$  from  $S$ 
4:   for all  $y$  adjacent to  $x$  do
5:     if  $y$  is feasible and  $y^T Q y < z^T Q z$  then
6:        $z \leftarrow y$ 
7:        $S \leftarrow y$ 
8:       goto Step 3
9:     else if  $y$  is interesting then
10:       $S \leftarrow S \cup \{y\}$ 
11:     end if
12:   end for
13: end while
```

We note that the algorithm moves to a better solution as soon as it finds a feasible one, and only when none are found does it consider moving to "interesting" solutions.

5 Branching strategies

In any branch-and-bound scheme, the performance of the algorithm is largely dependent on the number of nodes that are visited in the search tree. As such, it is important to make effective branching decisions, reducing the size of the search tree. Branching heuristics are usually classified as either static variable-ordering (SVO) heuristics or dynamic variable-ordering (DVO) heuristics. All branching heuristics used in this paper are DVO heuristics, as they are generally considered more effective because they allow information obtained during a search to be utilized to guide the search.

It is often quite difficult to find an assignment of values to variables that satisfies all constraints. This has motivated the study of a variety of approaches that attempt to exploit the interplay between variable-value assignments and constraints. Examples include the impact-based heuristics proposed by Refalo [31], the conflict-driven variable ordering heuristic proposed by Boussemart et al. [11], and the approximated counting-based heuristics proposed by Kask et al. [21], Hsu et al. [18], Bras et al. [24], and Pesant et al. [30].

5.1 Counting the solution density

One branching heuristic used in this paper is a modified implementation of the *maxSD* heuristic introduced by Pesant et al. [30]. We recall two definitions.

Definition 5.1 Given a constraint $c(x_1, \dots, x_n)$ and respective finite domains D_i ($1 \leq i \leq n$), let $\#c(x_1, \dots, x_n)$ denote the number of n -tuples in the corresponding relation.

Definition 5.2 Given a constraint $c(x_1, \dots, x_n)$, respective finite domains D_i ($1 \leq i \leq n$), a variable x_i in the scope of c , and a value $d \in D_i$, the solution density of a pair (x_i, d) in c is given by

$$\sigma(x_i, d, c) = \frac{\#c(x_1, \dots, x_{i-1}, d, x_{i+1}, \dots, x_n)}{\#c(x_1, \dots, x_n)}.$$

The solution density measures how frequently a certain assignment of a value in a variable's domain belongs to a solution that satisfies constraint c .

The heuristic maxSD simply iterates over all of the variable-value pairs and chooses the pair that has the highest solution density. If the (approximate) $\sigma(x_i, d, c)$ are precomputed, the complexity of the modified algorithm is $O(mq)$, where m is the number of constraints, and q is the sum of the number of variables that appear in each constraint. Pesant et al. [30] detail good approximations of the solution densities for knapsack constraints, which can be computed efficiently. They also provide an in-depth experimental analysis that shows that this heuristic is state of the art among counting-based heuristics.

5.2 Constraint satisfaction via an LD solution

In each node u of the branch-and-bound tree, a lower bound is computed by solving the LD problem, (L), and the primal-dual pair (x^u, λ^u) is obtained. In the standard way, we define the slack of constraint i at a point x to be $s_i = b_i - a_i^T x$, where a_i is the i th row of A . Then the set of violated constraints at x is the set $V = \{i : s_i < 0\}$. If x^u is infeasible for the original problem, it must violate one or more constraints. Additionally, we define the change in slack for constraint i resulting from flipping variable j in x^u to be

$$\delta_{ij} = a_{ij}(2x_j^u - 1).$$

We present three branching strategies which use this information at x^u to guide variable and value selection towards feasibility.

The first branching method we propose is to select the variable that maximizes the reduction in violation of the most violated constraint. That is, we select $j = \arg \max_{j \in 1, \dots, n} \delta_{ij}$ and value $1 - x_j^u$ (see Algorithm 2).

Algorithm 2 Most violated constraint satisfaction branching scheme

Require: x^u is the optimal solution to (L) at the current node.

- 1: **for all** constraints i **do**
 - 2: compute $s_i = b_i - a_i^T x^u$
 - 3: **end for**
 - 4: $i = \arg \min_{i \in 1, \dots, m} s_i$
 - 5: **if** $s_i > 0$ **then**
 - 6: LD optimal is feasible; abort violation branching
 - 7: **end if**
 - 8: **for all** variables j **do**
 - 9: compute $\delta_{ij} = a_{ij}(2x_j^u - 1)$
 - 10: **end for**
 - 11: **return** the index $j = \arg \max_{j \in 1, \dots, n} \delta_{ij}$ and value $1 - x_j^u$
-

The next branching method we discuss is more general: instead of looking only at the most violated constraint, we consider all of the violated constraints and select the variable which, when flipped in the LD solution, gives the maximum decrease in the left-hand side of all violated constraints (see Algorithm 3).

Algorithm 3 All violated constraints satisfaction branching scheme

Require: x^u is the optimal solution to (L) at the current node.

- 1: **for all** constraints i **do**
 - 2: compute $s_i = b_i - a_i^T x^u$
 - 3: **end for**
 - 4: $V := \{i : s_i < 0\}$ defines the set of violated constraints.
 - 5: **if** $V = \emptyset$ **then**
 - 6: LD optimal is feasible; abort violation branching
 - 7: **end if**
 - 8: **for all** variables j **do**
 - 9: compute $\delta_{ij} = a_{ij}(2x_j^u - 1)$
 - 10: **end for**
 - 11: **return** the index $j = \arg \max_{j \in \{1, \dots, n\}} (\sum_{i \in V} \delta_{ij})$ and value $1 - x_j^u$
-

This can be generalized to the entire constraint matrix such that we are looking for a variable which, when flipped in the LD solution, has the minimum increase in the left-hand side of the non-violated constraints and the maximum decrease in the left-hand side of the violated constraints (see Algorithm 4).

Algorithm 4 All constraints satisfaction branching scheme

Require: x^u is the optimal solution to (L) at the current node.

- 1: **for all** constraints i **do**
 - 2: compute $s_i = b_i - a_i^T x^u$
 - 3: **end for**
 - 4: **for all** constraints i **do**
 - 5: **for all** variables j **do**
 - 6: compute $\delta_{ij} = a_{ij}(2x_j^u - 1)$
 - 7: **end for**
 - 8: **end for**
 - 9: **return** the index $j = \arg \max_{j \in \{1, \dots, n\}} \left(\sum_{i=1}^m \delta_{ij} \right)$ and value $1 - x_j^u$
-

5.3 LP-based branching

Introduced in CPLEX 7.5 [3], the idea of *strong branching* is to test which fractional variable gives the best bound before branching. The test is done by temporarily fixing each fractional variable to 0 or 1 and solving the LP relaxation by the dual simplex method. Since the cost of solving several LP subproblems is high, only a fixed number of iterations of the dual simplex algorithm are performed. The variable that provides the strongest bound is chosen as the branching variable.

If the number of fractional variables is large, this process is very time consuming. There are several possible methods to overcome this difficulty. First, we can perform this test on only a subset of fractional variables (finding a proper subset is another issue; one possible way is to look only for variables with values close to 0.5). Another approach, the *k-look-ahead* branching strategy, requires an integer parameter k and a score assignment on the fractional variables (or variable-value pairs). The variables (or variable-value pairs) are then sorted according to their scores, and the above test is performed. If no better bound is found for k successive variables, the test process is stopped.

We note that the lower-bound computation performed by the UBQP oracle is fully parallelizable with strong branching or the *k-look-ahead* strategy performed on a digital processor, affording the computational time required to utilize this type of branching without significantly increasing the total running time of the algorithm.

5.4 Frequency-based branching

Motivated by the notion of *persistencies* as described by Boros and Hammer [8], and observing that the outer Lagrangian linearization method yields a number of high-quality solutions, one can perform *k-look-ahead* branching, selecting

variable-value pairs based on their *frequency*. Here, given a set $S \subseteq \{0, 1\}^n$ of binary vectors, an index $i \in \{1, \dots, n\}$, and a binary value $s \in \{0, 1\}$, the frequency of the pair (x_i, s) in S is defined as the number of elements in S with their i th entry equal to s . Moreover, when using a UBQP oracle that performs quantum annealing, the oracle returns a spectrum of solutions and all solutions can be used in the frequency calculation. This branching strategy has not, to our knowledge, previously appeared in the literature.

6 Computational experiments

6.1 Generation of test instances

In this paper we use randomly generated test instances with inequality constraints. For a desired test instance, we let n denote the number of variables and m be the number of inequality constraints. To generate the cost matrix, we construct an $n \times n$ random symmetric matrix Q of a given density d . An $m \times n$ constraint matrix is generated in a similar manner, ensuring that the CBQP problem has at least one feasible solution. For our test instances, the numbers of constraints were chosen as half the numbers of variables, and densities 0.3 and 0.5 were used for the objective functions and the constraints matrices, respectively.

6.2 Computational results

We now present the details of our computational experiments. The algorithms were programmed in C++ and compiled using GNU GCC on a machine with a 2.5 GHz Intel Core i5-3210M processor and 16 GB of RAM. Linear programming and UBQP problems were solved by the Gurobi Optimizer 6.0. We used the Gurobi Optimizer in place of a UBQP oracle and replaced the computational time with 0 milliseconds per solver call. The algorithm was coded to utilize 4 cores and to allow us to accurately report times. All other processes were paused during the solution of the UBQP problems.

In Tables 1 and 2 we report computational experiments performed on the group of test instances, evaluating each of the different branching strategies. In these tables the columns `mostviol`, `allviol`, and `allcst` respectively correspond to Algorithms 2, 3, and 4. `lp4` and `lp8` correspond respectively to the LP-based 4-look-ahead and 8-look-ahead strategies, and `freq4` and `freq8` correspond respectively to the frequency-based 4-look-ahead and 8-look-ahead strategies. Table 1 gives the number of nodes that the branch and bound requires when using each of the branching strategies. The final column reports the number of nodes that the Gurobi Optimizer used when solving the problem directly. In terms of the number of nodes explored in the branch-and-bound tree, the most violated (Algorithm 2) and all violated (Algorithm 3) constraints satisfaction branching schemes are clear winners.

Table 2 reports the time taken, in seconds, for each of the branching strategies and the Gurobi Optimizer to solve the problem to optimality, each using 4 cores. The number of queries to the UBQP oracle is given, as well as the quantum annealing leniency (QAL). The QAL column is computed by taking the difference between the time taken by the best branching strategy and the Gurobi Optimizer, and dividing by the number of queries. This column can be viewed as the maximum threshold of the average time, in milliseconds, to perform each quantum annealing process in order to solve the original problem faster than the Gurobi Optimizer. We note that the frequency-based branching heuristics terminate in the least amount of computational time.

In Figure 1, we graph the values from the QAL column of Table 2 versus problem size. The dotted line plots the mean values. In Figure 2, we graph the values from the QAL column of Table 2 versus problem size using a logarithmic scale. These graphs suggest an exponential growth in QAL with respect to the problem size. We interpret this as an indication that the difference between the computational time required for our CBQP approach (in conjunction with a scalable UBQP oracle) and the Gurobi Optimizer grows exponentially with the size of the problem.

7 Discussion

In this section we consider the specifics of the D-Wave systems as a physical invention of a UBQP oracle. We imagine any implementation of quantum adiabatic computing would have similar limitations, so we expect our algorithms to be beneficial in overcoming them.

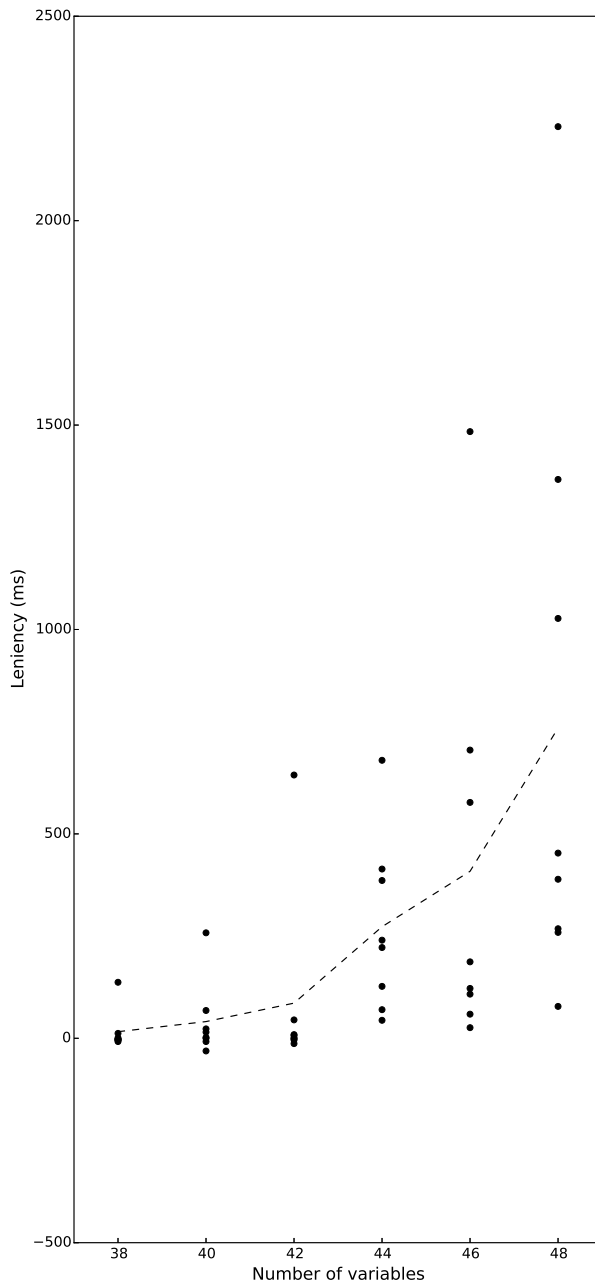


Figure 1: Quantum Annealing Leniency versus Problem Size

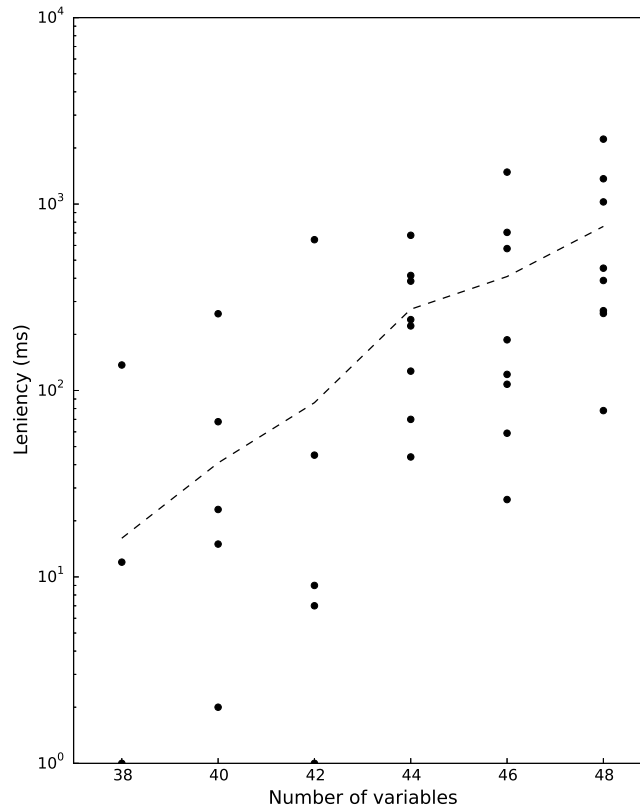


Figure 2: Quantum Annealing Leniency versus Problem Size (log scale)

Quantum adiabatic devices have not thus far allowed for fully connected systems of quantum bits. Due to this sparsity in the manufactured chips, the use of such quantum computers requires solving a *minor-embedding* problem, described in the following section, prior to programming the chip according to appropriate couplings and local fields [12].

7.1 Efficient embedding

Given a UBQP instance defined by a matrix Q , we define the underlying graph H as follows: for each variable x_i , we associate a vertex $v_i \in V(H)$; and for each nonzero entry $q_{ij} \neq 0$ of Q with $i \neq j$, we let v_i and v_j be adjacent in H . The minor-embedding problem that must be solved is to find a function $\phi : V(H) \rightarrow 2^{V(G)}$, where G is the graph defined by the quantum chip (that is, vertices correspond to the quantum bits and edges correspond to the couplings between them) such that

- (i) for each $x \in V(H)$, the subgraph induced by $\phi(x)$ in G is connected;
- (ii) $\phi(x)$ and $\phi(y)$ are disjoint for all $x \neq y$ in $V(H)$; and
- (iii) if x and y are adjacent in H , then there is at least one edge between $\phi(x)$ and $\phi(y)$ in G .

We note that for any induced subgraph of H , a minor embedding can be found simply by restricting ϕ to the subgraph. In our CBQP approach, the constraints contribute only to linear terms in the Lagrangian relaxation of the problem, and hence the embedding of a UBQP problem at any node in the branch-and-bound tree can be found from the parent node by restriction. That is, our method requires solving the minor-embedding problem only once, at the root node of the branch-and-bound tree.

7.2 Efficient programming of the quantum chips

In every node of the branch-and-bound tree, all Lagrangian relaxations generated have identical quadratic terms and only differ from each other in linear terms. This suggests that if reprogramming the quantum chip can allow for fast

updates of previous setups, then the runtime of UBQP oracle queries can also be minimized.

7.3 Post-processing and error analysis

Currently used quantum bits have significant noise. For arbitrary choices of initial and final Hamiltonians, the eigenvalues in the energy spectrum of the evolving Hamiltonian of the system may experience gap closures. Furthermore, the measurement process of the solutions of the quantum adiabatic evolution has a stochastic nature. Each of these indicate that the solutions read from the quantum system are often very noisy and even after several repetitions of the process there is no guarantee of optimality for the corresponding UBQP problem. In order to make our method practical, with a proof (or at least certainty) of optimality, it is necessary to develop a framework for error analysis for the quantum annealer. We note that for our purposes the solution errors can only propagate to final answers in the branch-and-bound tree if the proposed lower bound ℓ obtained at a node is greater than the actual lower bound $\ell - \epsilon$ and the best known upper bound u satisfies $u < \ell$. If this situation occurs, then the proposed method incorrectly prunes the subtree rooted at this node.

The quantum computing community often considers post-processing to be a procedure of descending from the best solution provided by the UBQP oracle to a better solution. However, for our purposes, the post-processing needed is only in the value of the optimal solution (that is, given some level of required certainty, finding an estimate of ϵ in the notation above).

8 Extension to quadratically constrained problems

It is straightforward to generalize the method proposed here to quadratically constrained quadratic programming (QCQP) problems in binary variables. In fact, the Lagrangian relaxations of QCQP problems are also UBQP problems. The minor-embedding problem to be solved at the root node takes the underlying graph H as follows: for each variable x_i , we associate a vertex $v_i \in V(H)$; and for any pair of distinct indices $i \neq j$, we let $(v_i, v_j) \in E(H)$ if and only if the term $x_i x_j$ appears with a nonzero coefficient in the objective function or in any of the quadratic constraints.

Assuming future quantum annealing hardware will allow higher-degree interactions between quantum bits, more general polynomially constrained binary programming problems could also be solved using a similar approach via Lagrangian duality.

9 Conclusions

Motivated by recent advancements in quantum computing technology, we have provided a method to tackle constrained binary programming problems using these technologies. Our method is a branch-and-bound algorithm where the lower bounds are computed using Lagrangian duality and queries to an oracle that solves unconstrained binary programming problems.

The conventional branching heuristics for integer programming problems rely on fractional solutions of continuous relaxations of the subproblems at the nodes of the branch-and-bound tree. Our lower-bounding methods are not based on continuous relaxations of the binary variables. In particular, the optimal solutions of the dual problems solved at the nodes of the branch-and-bound tree are not fractional. We have therefore proposed several branching strategies that rely on integer solutions and compared their performance both in time and number of nodes visited, to each other and to the conventional branching strategies that rely on fractional solutions.

To understand how powerful quantum computing hardware needs to be (in terms of the time taken for each query), we introduced the notion of quantum annealing leniency. This is, roughly speaking, the average time a query to the UBQP oracle would be able to spend so as to remain as fast as a classical algorithm for solving CBQP problems. In our computational experiments this classical algorithm is that of the Gurobi Optimizer.

Finally, although we focused on quadratic objective functions and linear inequality constraints, in Section 8 we discuss

how this method can be generalized to higher-order binary polynomial programming problems.

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Table 1: Branch-and-bound nodes needed to solve each instance

size	mostviol	allviol	allcst	lp4	lp8	freq4	freq8	gurobi
38	9	9	95	115	79	55	33	14232
	19	19	193	87	35	63	55	2823
	29	33	57	93	77	267	141	7020
	9	9	69	23	21	15	15	14405
	105	33	259	87	77	63	25	4423
	91	49	505	193	125	167	127	22916
	43	29	95	67	63	57	7	77254
40	49	75	319	115	103	191	109	49143
	27	27	159	89	87	71	45	90282
	5	5	33	37	23	25	21	8413
	55	79	705	69	65	817	361	6355
	163	167	483	277	219	191	209	39085
	5	5	7	13	11	5	5	75880
	41	41	249	165	117	35	31	38894
42	3	3	89	71	51	15	7	23092
	273	187	703	209	143	337	141	38733
	3	3	39	83	13	15	5	155591
	31	31	87	297	69	79	85	27015
	39	35	477	67	221	251	259	17179
	85	85	477	175	97	231	181	43292
	15	33	689	259	251	123	119	44184
44	11	9	273	151	79	121	27	18039
	77	75	709	271	143	299	227	31753
	27	21	211	99	147	77	35	314516
	7	7	671	239	161	147	33	296542
	5	5	297	73	47	5	5	88731
	59	59	273	83	87	123	73	156877
	67	41	683	79	267	255	89	161405
46	43	39	395	303	173	37	53	481254
	7	13	237	235	121	105	17	572913
	11	11	125	29	149	191	159	115119
	5	5	267	105	107	125	23	126330
	49	29	991	447	317	159	147	140593
	25	17	167	137	105	9	17	45621
	55	51	431	137	93	127	59	467641
48	51	55	731	31	13	147	89	361410
	13	9	175	115	147	15	21	848229
	33	33	123	91	97	39	17	193586
	33	29	351	187	173	45	31	102096
	5	5	273	89	33	41	25	737685
	23	23	67	93	63	41	11	1151380
	109	65	181	207	181	65	39	869929
48	11	11	27	47	59	55	15	1640100
	5	5	25	129	21	29	29	256597
	47	29	389	269	117	183	31	925482
	19	19	115	67	67	11	23	264846
	31	35	689	405	227	147	99	550320
	15	15	253	65	43	91	67	769463
mean	23	22	205	110	83	71	42	92978
wins	21	25	0	0	1	5	8	0

Table 2: Time required to solve each instance

size	mostviol	allviol	allcst	lp4	lp8	freq4	freq8	gurobi	queries	QAL	
38	0.955	0.939	1.063	1.96	2.537	1.627	1.2	0.849	37	-2	
	1.881	1.823	1.721	1.574	0.799	1.034	1.46	0.181	81	-8	
	2.833	2.987	0.762	1.919	2.272	2.432	1.852	0.362	78	-5	
	0.56	0.458	0.728	0.388	0.456	0.299	0.458	0.761	40	12	
	2.182	0.909	3.078	1.18	1.451	1.72	1.321	0.264	186	-3	
	3.513	2.529	6.891	2.934	3.267	3.415	4.343	1.68	271	-3	
	2.262	1.658	0.898	1.192	1.728	1.075	0.342	3.496	23	137	
	3.108	4.313	4.055	2.143	2.704	2.369	2.896	2.573	319	1	
	1.747	1.72	2.305	1.581	3.478	2.205	2.609	6.381	322	15	
	1.082	1.099	0.462	0.786	0.786	0.475	0.606	0.53	44	2	
40	2.895	3.108	7.949	3.032	3.106	11.263	5.38	0.465	79	-31	
	9.201	12.972	7.575	5.459	5.87	5.331	6.912	2.452	370	-8	
	0.982	1.088	0.115	0.12	0.116	0.166	0.209	3.991	15	258	
	2.487	2.534	3.449	2.332	1.889	0.821	0.982	2.413	68	23	
	0.556	0.57	1.144	1.714	1.626	0.584	0.927	1.444	13	68	
	5.398	3.613	15.422	4.691	3.236	7.188	5.167	3.055	1121	-0	
	0.716	0.682	0.39	0.989	0.399	0.881	0.323	11.271	17	644	
	4.602	3.565	3.322	10.625	2.315	1.393	2.127	2.123	104	7	
	5.464	5.693	13.078	2.092	8.149	4.903	4.339	1.516	147	-4	
	7.196	7.144	12.966	4.138	3.683	3.428	4.195	3.102	275	-1	
42	2.78	5.195	10.686	7.254	9.431	3.734	4.188	2.852	57	1	
	4.248	1.115	2.981	2.692	2.19	1.649	1.68	1.444	36	9	
	4.948	5.213	9.818	5.82	5.182	5.295	4.964	1.998	231	-13	
	3.57	2.296	3.93	2.276	3.989	2.701	2.576	19.461	386	45	
	44	2.63	2.525	9.813	5.021	3.768	3.611	1.99	20.968	79	240
		1.423	1.387	4.59	1.919	1.607	0.214	0.275	7.166	18	386
		3.246	3.178	6.486	1.467	2.295	2.487	1.273	9.517	117	70
		3.756	3.037	22.551	2.546	5.31	5.413	5.486	12.428	223	44
		5.699	5.428	5.237	6.491	5.841	1.545	3.787	34.576	149	222
		1.89	2.113	3.566	3.161	2.728	2.066	1.654	39.706	56	680
1.906		1.934	4.101	0.789	5.77	3.657	3.338	8.019	57	127	
1.591		1.568	4.824	2.296	3.413	2.25	2.047	10.254	21	414	
5.281		3.116	26.239	12.163	8.115	3.593	8.537	13.92	182	59	
3.341		2.543	3.244	3.006	4.047	0.404	0.991	4.293	36	108	
46	6.037	5.757	4.988	3.342	2.689	2.102	2.844	33.412	257	122	
	7.495	7.725	10.645	0.497	0.195	5.247	2.955	30.772	53	577	
	1.708	1.855	2.402	3.173	3.353	0.614	1.409	70.359	47	1484	
	3.653	3.668	1.944	1.99	2.373	1.113	1.143	13.246	65	187	
	5.767	4.422	5.828	4.132	4.435	2.199	2.359	10.551	324	26	
	1.741	1.781	3.203	1.902	0.783	1.878	1.653	52.928	74	705	
	48	3.317	3.286	1.291	3.149	1.045	2.698	0.969	81.257	36	2230
		14.462	10.672	9.82	6.138	9.82	7.238	5.852	84.355	293	268
		2.464	2.45	0.551	0.999	1.638	1.604	1.019	108.53	79	1367
		1.771	1.944	0.48	5.574	1.414	1.52	1.232	19.495	42	453
10.927		4.585	11.684	10.371	3.837	14.762	5.156	96.16	1187	78	
4.197		4.24	1.202	1.841	2.871	0.56	1.337	22.136	21	1027	
6.55		4.952	20.775	18.857	12.067	8.16	8.582	46.879	162	259	
2.835		2.758	3.807	1.065	1.376	2.738	2.77	48.871	123	389	
mean		2.601	2.617	3.403	2.437	2.392	1.968	1.927	6.605	-	-
wins		2	4	4	6	3	11	7	11	-	-

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