

MIXED-INTEGER QUADRATIC OPTIMIZATION USING QUANTUM COMPUTING FOR PROCESS APPLICATIONS

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Abstract

Quantum computing (QC) promises a transformational leap in computing speed that may allow solving large-scale complex optimization problems that were previously unattainable. While QC efficiently solves quadratic unconstrained binary optimization (QUBO) problems, solving problems with continuous variables is still challenging. To tackle this, we have devised a framework to solve mixed-integer quadratically constrained quadratic programming (MIQCQP) optimization problems involving both integer and continuous decision variables. In our framework, we denote the continuous and integer variables via unary and binary encodings and use them to transform a MIQCQP into QUBO. In doing so, we eliminate the need for any hybrid classical-quantum scheme that requires solving subproblems using classical computing. We then solve the QUBO using quantum annealing technique. We demonstrate the utility of our framework by solving a few test problems.

Keywords

Quantum computing, Quantum optimization, MIQCQP, Binary encoding, QUBO, Quantum annealing.

Introduction

Process optimization deals with obtaining good or optimal solutions to optimization problems whose mathematical models may constitute highly nonlinear and nonconvex terms or involve thousands of variables and constraints (Monjur et al. (2022); Iftakher et al. (2022)). In spite of the remarkable development in the field of global optimization, large-scale discrete-continuous problems may still require hours or days to obtain a feasible solution with an acceptable optimality gap (Ajagekar et al. (2020)). Many design problems in chemical process systems are mixed-integer quadratically constrained quadratic programs (MIQCQP) with both continuous and integer decision variables, which are difficult optimization problems to solve (Demirel et al. (2017); Tian et al. (2018)). Many process intensification problems of real importance are also formulated as MIQCQP. In such formulations, multi-scale decisions are integrated into a single optimization model that introduces convergence issues and increased modeling complexity which makes it difficult to solve using state-of-the-art deterministic optimization solvers (e.g., BARON (Sahinidis (1996)), ANTIGONE (Misener and Floudas (2014))). Also, the solution of such mixed-integer programs may not be guaranteed within polynomial time due to them being NP-hard in nature (Zhao et al.

(2022)). Heuristic or stochastic approaches (e.g., simulated annealing, tabu search, ant colony optimization, etc.) aim to provide a good solution within a reasonable time. However, the solution quality and convergence are not always guaranteed.

To that end, quantum computing (QC) shows promise to revolutionize the way we perform computing in science, engineering, biology, finance, and many other domains. Specifically, QC shows great promise to solve many combinatorially complex optimization problems that appear in process systems engineering (PSE) applications towards sustainable, energy-efficient, and cost-effective chemical processes (Andersson et al. (2022); Ajagekar and You (2019)). As of now, a specific type of problem i.e., quadratic unconstrained binary optimization (QUBO) of the form $\min_{x \in \{0,1\}} x^T Q x$ can be solved in quantum computers. A rich class of problems has natural QUBO formulations and applications (Glover et al. (2022)). For example, any integer linear program can be converted to QUBO problems while constraints can be reformulated to QUBO by introducing a quadratic penalty to the objective function with a suitable penalty parameter. In this way, many important problems have equivalent QUBO formulations (Kochenberger et al. (2014); Anthony et al. (2017)).

Once a QUBO is formed, it is mapped onto the physical quantum device consisting of quantum bits (qubits). All the binary variables are mapped onto the qubits as nodes in a graph, while the coefficients of the linear and quadratic terms

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represent the node weights and edge strengths between two adjacent qubits, respectively. QUBO models are particularly popular as these models can easily be translated to an Ising Hamiltonian which can be minimized using quantum annealers (Glover et al. (2022)). Essentially, this results in the recasting of the QUBO model as an energy minimization problem. At the end of the annealing process, the ground state of the Hamiltonian is represented as a binary string which corresponds to the solution of the original optimization problem (Grant and Humble (2020)).

Quantum architecture is yet to be robust enough to reliably solve large-scale discrete-continuous optimization problems. This has prompted researchers to employ hybrid classical-quantum optimization techniques for solving Mixed-Integer problems. In this approach, the original model is decomposed into subproblems where the master problem involves only the integer decisions. The solution to the master problem is returned to the subproblem which is solved in the continuous domain. In this way, both the classical and quantum computers communicate and the solutions iteratively improve. Recent applications of such hybrid techniques include solving large-scale production scheduling problems (Ajagekar et al. (2022)), and theoretical advances such as hybrid quantum benders' decomposition technique (Zhao et al. (2022)).

While there exist hybrid approaches to solve mixed-integer problems that require both classical computing and QC, currently no tractable method exists to solve MIQCQP using QC alone. This is problematic because hybrid approaches (e.g., Zhao et al. (2022); Chang et al. (2020)) often fail to harness the true potential of QC in significantly reducing the computation required to solve these problems. To that, we propose a new approach to transform MIQCQP into QUBO and then solve QUBO using QC platforms alone. The transformation relies upon unary and binary encoding of the continuous variables to binary variables. We test the framework by solving a few relevant problems using D-Wave's quantum annealing simulator and compare the results against deterministic solvers. The results demonstrate the validity of our framework in solving discrete-continuous MIQCQP using QC alone. We hope that as the quantum hardware and the number of qubits scale up and algorithmic advances are made in quantum computing, the proposed method will prove to be an effective strategy for solving many process synthesis problems using QC alone, thereby evading classical computational and algorithmic resource constraints.

Problem definition

We consider solving Mixed-integer Quadratically Constrained Quadratic Program (MIQCQP) using quantum computers. The MIQCQP has the following form:

$$\begin{aligned} \min_x \quad & x^\top \mathbf{H}x + c^\top x \\ \text{s.t.} \quad & x^\top \mathbf{C}_k x + \mathbf{a}_k^\top x \leq b_k \quad k = 1, \dots, u \\ & x \in \mathbb{R}^n \times \mathbb{Z}^p, \end{aligned} \quad (1)$$

where x is an $n + p$ dimensional vector of decision variables whose first n elements are continuous variables, and the remaining p elements are integer variables, $\mathbf{H} \in \mathbb{Q}^{(n+p) \times (n+p)}$ and is symmetric, $c \in \mathbb{Q}^{(n+p)}$, $\mathbf{C}_k \in \mathbb{Q}^{(n+p) \times (n+p)}$, $\mathbf{a}_k \in \mathbb{Q}^{(n+p)}$, and $b_k \in \mathbb{R}$.

If $p = 0$, then the MIQCQP turns into a Quadratic Program (QP). On the other hand, if $\mathbf{H} = [\mathbf{0}]^{(n+p) \times (n+p)}$ and $\mathbf{C}_k = [\mathbf{0}]^{(n+p) \times (n+p)}$, then Equation (1) turns into a Linear Program (LP). If there exists only equalities, then Equation (1) becomes equality constrained MIQP. Another special case is the Integer Quadratic Program (IBP), by setting $n = 0$.

QUBO set up

The decision variables of the MIQCQP concern both the continuous and integer variables. The central idea is to represent all the variables in terms of binary variables via unary and binary encoding.

Encoding

Let $x_m \in \mathbb{R}$, with $x_m^L \leq x_m \leq x_m^U$ which can be scaled to $\tilde{x}_m \in \mathbb{R}$ such that $0 \leq \tilde{x}_m \leq 1$. Then, using unary encoding, the scaled continuous variable \tilde{x}_m can be represented by the binary variables as follows:

$$\tilde{x}_m = \sum_{j=1}^{\infty} \sum_{i=1}^{I=9} 10^{-j} z_{ijm} + 10^{-J} z_m, \quad (2)$$

where $z_{ijm} \in \{0, 1\}$. The precision for \tilde{x}_m can be approximated upto J decimal places as follows:

$$\tilde{x}_m \approx \sum_{j=1}^J \sum_{i=1}^{I=9} 10^{-j} z_{ijm} + 10^{-J} z_m. \quad (3)$$

To illustrate let $\tilde{x}_m = 0.342$, and set $J = 3$, then $\tilde{x}_m = 10^{-1}(z_{11m} + \dots + z_{91m}) + 10^{-2}(z_{12m} + \dots + z_{92m}) + 10^{-3}(z_{13m} + \dots + z_{93m})$, where any 3, 4, and 2 binary variables of the $\{z_{i1m}\}_{i=1}^9$, $\{z_{i2m}\}_{i=1}^9$, $\{z_{i3m}\}_{i=1}^9$ sequences, respectively are 1 and the remaining binary variables are 0.

One can reduce the number of binary variables by observing that the value of \tilde{x}_m at the j th decimal place (\tilde{x}_m^j) can not exceed 9. Hence, one can also employ a specific binary encoding (SBE) and reduce the number of binary variables by $5 \cdot J$ as follows:

$$\tilde{x}_m \approx \sum_{j=1}^J 10^{-j} (z_{1jm} + 2z_{2jm} + 3z_{3jm} + 3z_{4jm}) + 10^{-J} z_m, \quad (4)$$

On the other hand, if $x_m \in \mathbb{Z}$, then let I be the least positive integer such that $2^I \geq |x_m|$. Then using binary encoding, $|x_m| = \sum_{i=1}^I 2^i z_{im}$, where $z_{im} \in \{0, 1\}$.

MIQP to QUBO

To illustrate the transformation into a QUBO, let us first consider an MIQP by setting $\mathbf{C}_k = [\mathbf{0}]^{(n+p) \times (n+p)}$. Then

Equation (1) can be written as:

$$\begin{aligned} \min_x & x^T \mathbf{H}x + c^T x \\ \text{s.t.} & \mathbf{A}x \leq \mathbf{b} \\ & x \in \mathbb{R}^n \times \mathbb{Z}^p, \end{aligned} \quad (5)$$

where $\mathbf{A} \in \mathbb{Q}^{u \times (n+p)}$ and $\mathbf{b} \in \mathbb{R}^u$. To achieve QUBO, we first make the MIQP (Equation (5)) unconstrained. To do so, we first convert all inequality constraints into equalities by adding slack variables to each constraint (s), and then we add a quadratic penalty for each constraint by introducing Lagrange multipliers (λ). This can be shown in a vector notation as follows:

$$\min x^T \mathbf{H}x + c^T x + \lambda^T (\mathbf{A}x - \mathbf{b} + s)^T (\mathbf{A}x - \mathbf{b} + s) \quad (6)$$

where $\lambda \in \mathbb{Q}^{u \times u}$, and $s \in \mathbb{Q}^{u \times u}$. We scale the continuous variables $\{x_m\}_{m=1}^n$ and $\{s_v\}_{v=1}^u$ to $\{\tilde{x}_m\}_{m=1}^n$ and $\{\tilde{s}_v\}_{v=1}^u$, respectively with $0 \leq \tilde{x}_m, \tilde{s}_v \leq 1$ as follows:

$$\begin{aligned} x_m &= x_m^L + (x_m^U - x_m^L)\tilde{x}_m \\ s_v &= s_v^L + (s_v^U - s_v^L)\tilde{s}_v, \end{aligned} \quad (7)$$

where $s_v^L = 0, \forall v \in u$, and s_v^U can be calculated as follows:

$$s_v^U = \begin{cases} e_v - x_m^L A_{vm}, & \text{if } A_{vm} \geq 0 \\ e_v - x_m^U A_{vm}, & \text{otherwise} \end{cases} \quad (8)$$

After scaling, Equation (6) can be expressed in terms of scaled variables as follows:

$$\min \tilde{x}^T \tilde{\mathbf{H}}\tilde{x} + \tilde{c}^T \tilde{x}, \quad (9)$$

where $\tilde{\mathbf{H}} \in \mathbb{Q}^{(n+p+u) \times (n+p+u)}$, $\tilde{c} \in \mathbb{Q}^{(n+p+u)}$, and $\tilde{x} = \begin{bmatrix} \underbrace{[\tilde{x}_1 \dots \tilde{x}_n]}_{\text{continuous}} & \underbrace{[\tilde{x}_{n+1} \dots \tilde{x}_{n+p}]}_{\text{integer}} & \underbrace{[\tilde{s}_1 \dots \tilde{s}_u]}_{\text{slack}} \end{bmatrix}$, with $\tilde{x} \in \mathbb{Q}^{(n+p+u)}$.

After that, all the scaled variables are represented as binary variables via unary encoding or SBE. In this process, the continuous and integer variables in the standard MIQP formulation (Equation (5)), upon scaling and representation by the binary variables, can be recast as a QUBO problem as follows:

$$\begin{aligned} \min_z & z^T Qz \\ \text{s.t.} & z = \{0, 1\}^\beta, \end{aligned} \quad (10)$$

where $Q \in \mathbb{Q}^{\beta \times \beta}$ and $\beta = (n+u)(9J+1) + p$ and $(n+u)(4J+1) + p$ for unary encoding and SBE, respectively. Thus the original $n+p$ dimensional MIQP (see Equation 5) is transformed into a β dimensional QUBO.

MIQCQP to QUBO

Similar to the procedure for MIQP to QUBO transformation, we first make Equation (1) unconstrained as follows:

$$\begin{aligned} \min x^T \mathbf{H}x + c^T x + \sum_k \lambda_k (x^T \mathbf{C}_k x + \mathbf{a}_k^T x - b_k + s_k)^2 \\ = x^T \mathbf{H}x + c^T x + \underbrace{\sum_k \lambda_k (\mathbf{a}_k^T x - b_k + s_k)^2}_{\text{MIQP}} - 2x^T \mathbf{C}_k x b_k \\ + \underbrace{\sum_k \lambda_k (x^T \mathbf{C}_k x)^2}_{\text{quadrilinear}} + 2 \underbrace{\sum_k \lambda_k (x^T \mathbf{C}_k x) (\mathbf{a}_k^T x + s_k)}_{\text{trilinear}} \end{aligned} \quad (11)$$

Note that the terms that form MIQP in Equation (11) can be transformed into QUBO using the technique discussed in the previous section. Below we show the transformation for the quadrilinear and the trilinear terms.

Quadrilinear term:

$$\sum_k \lambda_k (x^T \mathbf{C}_k x)^2 = w^T \tilde{\mathbf{C}} w, \quad (12)$$

where $\tilde{\mathbf{C}} \in \mathbb{Q}^{\zeta \times \zeta}$ with $\zeta = n^2 \cdot J^2 \cdot (n+p)$, and $w \in \{0, 1\}^\zeta$. w is a vector of binary variables, whose elements are defined as: $w_{i,j,i',j',m,m'} = z_{i,j,m} \cdot z_{i',j',m'}$.

Trilinear term:

$$\begin{aligned} 2 \sum_k \lambda_k (x^T \mathbf{C}_k x) (\mathbf{a}_k^T x) + 2 \sum_k \lambda_k (x^T \mathbf{C}_k x) s_k \\ = w^T \hat{\mathbf{Q}}_1 \hat{z} + w^T \hat{\mathbf{Q}}_2 \hat{z}, \end{aligned} \quad (13)$$

where $\hat{z} \in \{0, 1\}^{I \cdot J \cdot n + n + p}$, $\hat{\mathbf{Q}}_1 \in \mathbb{Q}^{\zeta \times (I \cdot J \cdot n + n + p)}$, $\hat{z} \in \{0, 1\}^{I \cdot J \cdot u + u}$, and $\hat{\mathbf{Q}}_2 \in \mathbb{Q}^{\zeta \times (I \cdot J \cdot u + u)}$. We relate w with z using McCormick relaxation as follows:

$$\begin{aligned} w_{i,j,i',j',m,m'} &\leq z_{i,j,m} \\ w_{i,j,i',j',m,m'} &\leq z_{i',j',m'} \\ w_{i,j,i',j',m,m'} &\geq z_{i,j,m} + z_{i',j',m'} - 1 \\ w_{i,j,i',j',m,m'} &\geq 0 \end{aligned} \quad (14)$$

Since both w and z are binary variables, the relaxation is exact. Therefore, Equation (11) upon transformation can be expressed as follows:

$$\begin{aligned} \min z^T Qz + w^T \tilde{\mathbf{C}} w + w^T \hat{\mathbf{Q}}_1 \hat{z} + w^T \hat{\mathbf{Q}}_2 \hat{z} \\ \text{s.t.} \quad \tilde{\mathbf{A}} w + \tilde{\mathbf{B}} z \leq \hat{\mathbf{b}} \end{aligned} \quad (15)$$

Finally, we notice that Equation (15) is a binary quadratic program, and can be transformed to QUBO following a similar approach as the MIQP to QUBO transformation as discussed in the previous section.

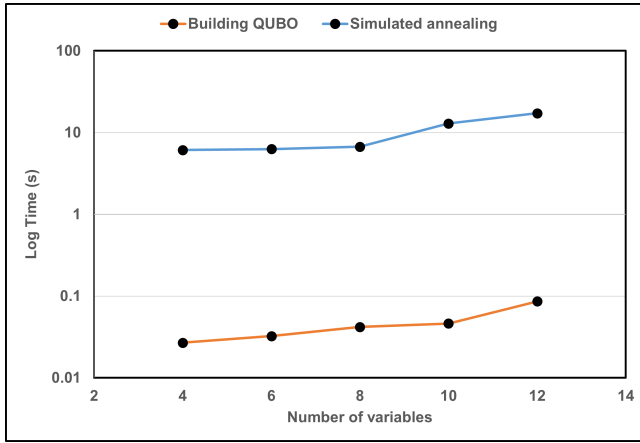


Figure 1: Relationship between the number of variables and time required to build QUBO and solve it via simulated annealing.

Computational results

The overall solution time to a MIQP or MIQCQP problem is the summation of the time taken to build the QUBO model, and the time taken to solve the problem. At first, we analyze the solution time by varying the number of variables (hence, varying the QUBO model size). We then demonstrate two case studies that involve both the integer and continuous decision variables. All the quantum computation is performed on D-Wave's quantum annealing simulator, and the results are compared to that of a deterministic solver (BARON) run on a Dell Windows system with Intel(R) Core(TM) i7-8750 2.20 GHz CPU and 8 GB of installed memory.

Solution time

To analyze the solution time, we consider solving the below unconstrained problem:

$$\begin{aligned} \min_x \quad & x^T \mathbf{H}_1 x + y^T \mathbf{H}_2 y + x^T \mathbf{H}_3 y \\ \text{s.t.} \quad & x \in \mathbb{R}^n, y \in \{0, 1\}^p, \end{aligned} \quad (16)$$

where the diagonal elements of \mathbf{H}_1 , \mathbf{H}_2 , and \mathbf{H}_3 are 1 and the non-diagonal elements are -1 . We gradually increase the size of n and p , build the QUBO using SBE and solve it in D-Wave's quantum annealing simulator by setting the following parameters: chain strength = 1000, number of reads = 10000. For all cases, Lagrange multiplier, λ is chosen to be 100, and the decimal place precision, J is fixed to 3. Table 1 and Figure 1 illustrate the time taken to form the QUBO matrix, as well as the time taken to solve it in D-Wave's quantum annealing simulator. As can be seen from these results, the time required to build QUBO is insignificant compared to the solution time.

Case study 1

We solve a non-convex MIQP with linear inequality constraints. The problem description is given below:

Table 1: Solution time using SBE

n	p	build QUBO (s)	Sim anneal (s)	Matrix dim
2	2	0.027	6.122	28×28
3	3	0.032	6.281	42×42
4	4	0.041	6.730	56×56
5	5	0.046	12.944	70×70
6	6	0.086	17.229	84×84

$$\begin{aligned} \min_{x_1, x_2, y_1, y_2} \quad & -2x_1^2 + 10x_1x_2 - x_2^2 + y_1^2 - 2y_1y_2 + x_1y_1 \\ & -2x_1y_2 - 2x_2y_1 - x_2y_2 + 2.4x_1 - 1.2x_2 \\ & + 3y_1 + 4y_2 \\ \text{s.t.} \quad & x_1 + 2x_2 - 2y_1 + y_2 \leq -1 \\ & 3x_1 + 4x_2 + y_1 - y_2 \leq -2 \\ & x \in \mathbb{R}^2, -2 \leq x_1, x_2 \leq 3, y = \{0, 1\}^2 \end{aligned} \quad (17)$$

This can be written in a vector form as follows:

$$\begin{aligned} \min_{x, y} \quad & x^T \begin{bmatrix} -2 & 5 \\ 5 & -1 \end{bmatrix} x + y^T \begin{bmatrix} 1 & -1 \\ -1 & 0 \end{bmatrix} y \\ & + x^T \begin{bmatrix} 1 & -2 \\ -2 & -1 \end{bmatrix} y + \begin{bmatrix} 2.4 \\ -1.2 \end{bmatrix}^T x + \begin{bmatrix} 3 \\ 4 \end{bmatrix}^T y \\ \text{s.t.} \quad & \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} x + \begin{bmatrix} -2 & 1 \\ 1 & -1 \end{bmatrix} y \leq \begin{bmatrix} -1 \\ -2 \end{bmatrix} \\ & x \in \mathbb{R}^2, -2 \leq x_1, x_2 \leq 3, y = \{0, 1\}^2 \end{aligned} \quad (18)$$

We solve the unconstrained form of this test problem by choosing $\lambda = 10$. The optimal solution for the choice of $\lambda = 10$ is obtained from deterministic solver (BARON) as follows:

$$x_1^* = 2.44693878, x_2^* = -2, y_1^* = 0, y_2^* = 1, f^* = -52.375918$$

We then transform this test problem to QUBO. For the consistent comparison, we set the same value for λ . Additionally, for the simulated annealing in D-Wave's quantum annealing simulator, we set the following parameter values: chain strength = 1000, number of reads = 10000. The quantum annealing simulator results for both the unary encoding and SBE are shown in Tables 2 and 3, respectively. Note that for unary encoding, when $J = 4$ the dimension of \mathbf{Q} matrix is 150×150 , while for $J = 6$, it is 222×222 . For SBE, the matrix dimension reduces significantly, i.e., when $J = 4$, the dimension of the \mathbf{Q} matrix is 70×70 , and for $J = 6$, it is 102×102 . It is evident from both of these tables that the proposed QUBO formulation and the corresponding quantum annealing simulation leads to a correct solution.

We also show the probability distribution of the quantum annealing simulator results for SBE for both $J = 4$ (see Figure 2) and $J = 6$ (see Figure 3). Note that in both of these figures, the Ising Hamiltonian is minimized 10000 times, and each bar in the plot corresponds to a solution to the energy minimization problem. We pick the minimized Ising Hamiltonian that occurs the maximum time. In other words, we

all the problem information of the constrained problem are embedded onto a single matrix in the QUBO formulation, a large choice of the λ parameter increases the condition number of the Q matrix which may require more sampling to attain the desired solution. ii) The parameters of the simulated annealing were not optimized, which could impact the solution quality.

Conclusions

We provide a framework for solving Mixed-integer quadratic programs using QC. Our framework transforms both the continuous and integer decision variables to binary variables via unary encoding and SBE which allows us to construct an equivalent QUBO formulation of a given constrained problem. We then use the framework and solve two test problems. The results demonstrate the validity of the QUBO formulation strategy. The time required to build the QUBO is insignificant compared to the solution time. Also, the solution quality is comparable to that of deterministic solvers. QUBO models being very general, allow embedding onto the quantum hardware, thereby providing an opportunity to harness the true potential of QC. However, the matrix dimension of the QUBO model is required to be tractable. Also, it is not possible to differentiate between hard and soft constraints in the QUBO formulation. As we have observed, the solutions from both the deterministic and the quantum annealing simulator exhibit constraint violation for the sub-optimal choice of Lagrange multipliers. The effect of the penalty parameter on the solution quality is, therefore, an interesting area for further investigation. In spite of the near-term quantum hardware limitations, we anticipate that as the number of qubits scales up, and algorithmic advances are made in minimizing intrinsic control error, our proposed strategy will provide a foundation for solving complex mixed-integer quadratic problems using QC alone.

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