

On the application of matrix congruence to QUBO formulations for systems of linear equations

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Abstract—Recent studies on quantum computing algorithms focus on excavating features of quantum computers which have potential for contributing to computational model enhancements. Among various approaches, quantum annealing methods effectively parallelize quadratic unconstrained binary optimization (QUBO) formulations of systems of linear equations. In this paper, we simplify these formulations by exploiting congruence of real symmetric matrices to diagonal matrices. We further exhibit computational merits of the proposed QUBO models, which can outperform classical algorithms such as QR and SVD decomposition.

Index Terms—Quantum Annealing, QUBO, Matrix congruence, Systems of linear equations

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I. INTRODUCTION

Quantum computing methods have been gaining attention as a potential candidate for effectively enhancing pre-existent classical algorithms. As one of such computing techniques, quantum annealing method focuses on returning solutions which minimize energy level functions associated to optimization problems [1], [2]. The problem of finding a solution to a system of linear equations can be reformulated as an optimization problem. Borle and Lomonaco proposed a quadratic unconstrained binary optimization (QUBO) formulation of solving systems of linear equations [3]. Using the binary expansions of real numbers, quantum annealing

processors effectively parallelize the process of evaluating the minimum energy level of the QUBO model. As a result, quantum annealing based QUBO model is computationally cost efficient compared to classical algorithms such as QR and SVD. However, physical conditions arising from using quantum processors, such as the required number of qubits for the model, may negatively affect the accuracy of such models [3], [4]. It is thus a natural question to ask what additional measures can further enhance the accuracy of quantum annealing based QUBO models.

In this paper, we propose a new simplified QUBO formulation of systems of linear equations which utilizes a classical result that real symmetric matrices are congruent to real diagonal matrices [5]. We show that, under mild conditions, such a transformation substantially reduces the number of non-trivial relations among qubits used in formulating the QUBO model. Furthermore, we demonstrate with an example that utilizing the classical result greatly enhances the accuracy of quantum annealing based QUBO models.

II. METHOD

A. Background

Let $A := (a_{i,j})_{i,j=1}^n \in \mathbb{R}^{n \times n}$ be an $n \times n$ matrix, and $b := (b_i)_{i=1}^n \in \mathbb{R}^n$ an arbitrary column vector of dimension n . Denote by $x := (x_i)_{i=1}^n \in \mathbb{R}^n$ the column vector of n variables which satisfies

$$Ax = b. \quad (1)$$

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The solution to the systems of linear equations specified in (1) is the l^2 -norm minimizing solution of

$$\|Ax - b\|^2 = x^T A^T A x - 2b^T A x + b^T b. \quad (2)$$

Because $A^T A$ is a positive semidefinite symmetric matrix over \mathbb{R} , it is congruent to a diagonal matrix $D \in \mathbb{R}^{n \times n}$ [5]. In particular, there exists a non-singular matrix $R := (r_{i,j})_{i,j=1}^n \in \mathbb{R}^{n \times n}$ such that $R^T (A^T A) R$ is a diagonal matrix. Denote by $D := (d_{i,j})_{i,j=1}^n \in \mathbb{R}^{n \times n}$ the diagonal matrix $R^T (A^T A) R$.

We can hence write the l^2 -norm of $Ax - b$ as:

$$\|Ax - b\|^2 = (R^{-1}x)^T R^T A^T A R (R^{-1}x) - 2b^T A R (R^{-1}x) + b^T b \quad (3)$$

Because R is invertible, there exists a column vector $y \in \mathbb{R}^n$ such that $y = R^{-1}x$. Substituting y to (3) gives:

$$\|Ax - b\|^2 = y^T D y - 2(b^T A R) y + b^T b. \quad (4)$$

Up to linear change of variables, the solution to (1) is the l^2 -norm minimizing solution of (4).

$$\|Ax - b\|^2 = \sum_{i=1}^n d_{i,i} y_i^2 - 2 \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n b_k a_{k,j} r_{j,i} y_i + \sum_{i=1}^n b_i^2 \quad (5)$$

In the spirit of quantum annealing approach [2]–[4], [6] to formulating systems of linear equations, the l^2 -norm minimizing solution of (4) can be approximately represented by a combination of qubits $q_{i,j} \in \{0, 1\}$. Throughout this paper, we assume that the variables are approximated by the radix 2 representation:

$$y_i \approx \sum_{l=-m}^m 2^l q_{i,l}^+ - \sum_{l=-m}^m 2^l q_{i,l}^-. \quad (6)$$

We denote by m the upper bound on the number of digits or fractional digits used to represent y_i . That is, we allow l , a digit or a fractional digit of y_i , to take values between $-m$ and m . Note that the qubits $q_{i,l}^{\pm}$ can be chosen such that for any digits $-m \leq l_1, l_2 \leq m$, $q_{i,l_1}^+ q_{i,l_2}^- = 0$ [6].

B. Example

We demonstrate with an example to show how using matrix congruence relation significantly simplifies the QUBO model associated to the system of linear equations. Consider the following system of linear equations $Ax = b$ [4]:

$$\begin{pmatrix} 3 & 1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 5 \end{pmatrix}. \quad (7)$$

Suppose that the matrices D and R associated to $A^T A$ are given.

$$D = \begin{pmatrix} \frac{8}{5} & 0 \\ 0 & \frac{98}{125} \end{pmatrix}, \quad R = \begin{pmatrix} \frac{2}{5} & -\frac{1}{2^5} \\ 0 & \frac{2}{5} \end{pmatrix}. \quad (8)$$

We use the radix 2 representation of the column vector $y = R^{-1}x$:

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} q_{11} + 2q_{12} + 4q_{13} - q_{14} - 2q_{15} - 4q_{16} \\ q_{21} + 2q_{22} + 4q_{23} - q_{24} - 2q_{25} - 4q_{26} \end{pmatrix} \quad (9)$$

Define the cost function for solving the system of linear equations as

$$f(y) := \sum_{i=1}^2 d_{i,i} y_i^2 - 2 \sum_{i=1}^2 \sum_{j=1}^2 \sum_{k=1}^2 b_k a_{k,j} r_{j,i} y_i, \quad (10)$$

where our objective is to find a column vector $y \in \mathbb{R}^n$ such that $f(y) = -b^T b = -26$. Observe that (10) is the expansion of the first two terms of (5). We recall the following conditions for $i \in \{1, 2\}$ and $j \in \{1, 2, \dots, 6\}$:

$$\begin{cases} q_{i,1} q_{i,4} = q_{i,2} q_{i,4} = q_{i,3} q_{i,4} = 0 \\ q_{i,1} q_{i,5} = q_{i,2} q_{i,5} = q_{i,3} q_{i,5} = 0 \\ q_{i,1} q_{i,6} = q_{i,2} q_{i,6} = q_{i,3} q_{i,6} = 0 \\ q_{i,j}^2 = q_{i,j} \end{cases} \quad (11)$$

The first three conditions use the fact that for any digits $0 \leq l_1, l_2 \leq 2$, $q_{i,l_1}^+ q_{i,l_2}^- = 0$. The last condition holds because each qubit takes values of either 0 or 1.

Substituting (9) to (10) under the aforementioned conditions from (11) yields:

$$\begin{aligned} f(y) = & 8q_{11} + \frac{32}{5}q_{11}q_{12} + \frac{64}{5}q_{11}q_{13} + \frac{96}{5}q_{12} + \frac{128}{5}q_{12}q_{13} \\ & + \frac{256}{5}q_{13} - \frac{24}{5}q_{14} + \frac{32}{5}q_{14}q_{15} + \frac{64}{5}q_{14}q_{16} - \frac{32}{5}q_{15} \\ & + \frac{128}{5}q_{15}q_{16} - \frac{882}{125}q_{21} + \frac{392}{125}q_{21}q_{22} - \frac{1568}{125}q_{22} \\ & + \frac{784}{125}q_{21}q_{23} + \frac{1568}{125}q_{22}q_{23} - \frac{2352}{125}q_{23} + \frac{1078}{125}q_{24} \\ & + \frac{392}{125}q_{24}q_{25} + \frac{2352}{125}q_{25} + \frac{784}{125}q_{24}q_{26} + \frac{1568}{125}q_{25}q_{26} \\ & + \frac{5488}{125}q_{26}. \end{aligned} \quad (12)$$

Let \hat{Q} be the matrix defined as in (13). Denote by $q_y := [q_{11}, q_{12}, \dots, q_{26}]^T$ the column vector of qubits used in the radix 2 representations of y_1 and y_2 . Then the energy function $f(y)$ satisfies

$$f(y) = q_y^T \hat{Q} q_y = y^T D y - 2b^T A R y, \quad (15)$$

up to the equivalence relation $q_{i,j}^2 = q_{i,j}$. We note that the matrix \hat{Q} characterizes the inherent relations among the qubits used in representing the variables y_i . Solving the system of linear equations $Ax = b$ is thus equivalent to finding the column vector q_y such that $q_y^T \hat{Q} q_y = b^T b = -26$.

Suppose, on the other hand, we use the radix 2 representation of the column vector x from (2) [4]. As before, denote by $q_x := [q_{11}, q_{12}, \dots, q_{26}]^T$ the column vector of qubits used in the radix 2 representations of x_1 and x_2 . Let \hat{Q}' be the matrix defined as in (14). Then, up to the equivalence relation $q_{i,j}^2 = q_{i,j}$, we have

$$q_x^T \hat{Q}' q_x = x^T A^T A x - 2b^T A x \quad (16)$$

The matrix \hat{Q}' characterizes the inherent relations among the qubits used in representing the variables x_i . One can solve $Ax = b$ by finding q_x that satisfies $q_x^T \hat{Q}' q_x = -26$.

$$\hat{Q} := \begin{pmatrix} 8 & 6.4 & 12.8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 19.2 & 25.6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 51.2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -4.8 & 6.4 & 12.8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -6.4 & 25.6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -7.056 & 3.136 & 6.272 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -12.544 & 12.544 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -18.816 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.624 & 3.136 & 6.272 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 18.816 & 12.544 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 43.904 \end{pmatrix}, \quad (13)$$

$$\hat{Q}' := \begin{pmatrix} 26 & 40 & 80 & -20 & -40 & -80 & 2 & 4 & 8 & -2 & -4 & -8 \\ 0 & 72 & 160 & -40 & -80 & -160 & 4 & 8 & 16 & -4 & -8 & -16 \\ 0 & 0 & 224 & -80 & -160 & -320 & 8 & 16 & 32 & -8 & -16 & -32 \\ 0 & 0 & 0 & -6 & 40 & 80 & -2 & -4 & -8 & 2 & 4 & 8 \\ 0 & 0 & 0 & 0 & 8 & 160 & -4 & -8 & -16 & 4 & 8 & 16 \\ 0 & 0 & 0 & 0 & 0 & 96 & -8 & -16 & -32 & 8 & 16 & 32 \\ 0 & 0 & 0 & 0 & 0 & 0 & -13 & 20 & 40 & -10 & -20 & -40 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -16 & 80 & -20 & -40 & -80 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & -40 & -80 & -160 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 23 & 20 & 40 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 56 & 80 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 152 \end{pmatrix}, \quad (14)$$

III. IMPLEMENTATION

We implement the aforementioned example (7) on D-Wave 2000Q quantum annealer. Both QUBO models obtained from (15) and (16) are performed for 3 trials with 10,000 anneals.

A. Vanilla QUBO model

Without using matrix congruence, the solution to the 2-dimensional linear systems of equation is given by $x_1 = -1$ and $x_2 = 2$. The vanilla QUBO model (16) aims to search for possible combinations of qubits q_x . We list all possible combinations of qubits for $x_i = q_{i1} + 2q_{i2} + 4q_{i3} - q_{i4} - 2q_{i5} - 4q_{i6}$ in (17). There are 7 possible combinations for $x_1 = -1$, and 6 possible combinations for $x_2 = 2$.

$$\begin{aligned} (q_{11}, q_{12}, q_{13}, q_{14}, q_{15}, q_{16}) &\in \{(0, 0, 0, 1, 0, 0), (0, 1, 0, 1, 1, 0), \\ &\quad (0, 0, 1, 1, 0, 1), (0, 1, 1, 1, 1, 1), \\ &\quad (1, 0, 0, 0, 1, 0), (1, 0, 1, 0, 1, 1), \\ &\quad (1, 1, 0, 0, 0, 1)\} \\ (q_{21}, q_{22}, q_{23}, q_{24}, q_{25}, q_{26}) &\in \{(0, 0, 1, 0, 1, 0), (0, 1, 0, 0, 0, 0), \\ &\quad (0, 1, 1, 0, 0, 1), (1, 0, 1, 1, 1, 0), \\ &\quad (1, 1, 0, 1, 0, 0), (1, 1, 1, 1, 0, 1)\} \end{aligned} \quad (17)$$

Table I lists the results of performing the vanilla QUBO model for 3 trials on the D-Wave quantum annealer with 10,000 anneals. Here, we abbreviated the 6 possible combinations of qubits for $x_2 = 2$. Each row lists the number of occurrences with the lowest energy with the given combination of qubits $q_{11}, q_{12}, \dots, q_{16}$ for $x_1 = -1$. Out of 3 trials, the D-Wave quantum annealer finds 887, 1181, and 1065 occurrences with the lowest energy out of 10,000 anneals.

B. New QUBO model using matrix congruences

Using matrix congruence, the solution to (7) is given by $y_1 = -2$ and $y_2 = 5$. Because we further simplified the QUBO model using the equivalence relation, as shown in (11), the new QUBO model (15) searches for the following unique combination of qubits $y_i = q_{i1} + 2q_{i2} + 4q_{i3} - q_{i4} - 2q_{i5} - 4q_{i6}$:

$$\begin{aligned} (q_{11}, q_{12}, q_{13}, q_{14}, q_{15}, q_{16}) &= (0, 0, 0, 0, 1, 0) \\ (q_{21}, q_{22}, q_{23}, q_{24}, q_{25}, q_{26}) &= (1, 0, 1, 0, 0, 0) \end{aligned} \quad (18)$$

To check whether specifying the zero terms of the matrix \hat{Q} from (13) to the D-Wave system affects the performance of the linear system solver algorithm, we implement the new QUBO model under two different conditions. The first method specifies the zero terms of the upper triangular portion of \hat{Q} in the D-Wave systems code, whereas the second method omits these zero terms from the code. Table II displays the number of occurrences of the unique combination of qubits out of 10,000 anneals. The former method finds 1526, 2495, and 2063 occurrences out of three runs, whereas the latter method finds 2103, 4441, and 1727 occurrences.

IV. DISCUSSION

The new QUBO model (15), regardless of whether the zero terms of \hat{Q} are specified in the D-Wave code, clearly outperforms the vanilla QUBO model (16). A summary of the number of occurrences with the lowest energy levels using three QUBO model implementations is demonstrated in Table III.

On average, the probability that the new QUBO model solves (7) ranges between 20.28% and 27.58%. Compare this to 10.44%, the average probability obtained from the vanilla QUBO model. This is roughly half of the probability obtained

q_{11}	q_{12}	q_{13}	q_{14}	q_{15}	q_{16}	q_{21}	q_{22}	q_{23}	q_{24}	q_{25}	q_{26}	Energy	# Occurrences		
													Run 1	Run 2	Run 3
0	0	0	1	0	0	All 6 combinations						-26.0	203	66	50
0	1	0	1	1	0	All 6 combinations						-26.0	77	49	531
0	0	1	1	0	1	All 6 combinations						-26.0	131	147	251
0	1	1	1	1	1	All 6 combinations						-26.0	71	116	51
1	0	0	0	1	0	All 6 combinations						-26.0	75	43	74
1	0	1	0	1	1	All 6 combinations						-26.0	71	83	62
1	1	0	0	0	1	All 6 combinations						-26.0	259	677	46
												Total	887	1181	1065

TABLE I
NUMBER OF OCCURRENCES WITH THE LOWEST ENERGY LEVELS USING THE QUBO MODEL FROM (14)

q_{11}	q_{12}	q_{13}	q_{14}	q_{15}	q_{16}	q_{21}	q_{22}	q_{23}	q_{24}	q_{25}	q_{26}	Energy	Zero Terms	# Occurrences		
														Run 1	Run 2	Run 3
0	0	0	0	1	0	1	0	1	0	0	0	-26.0	Yes	1526	2495	2063
0	0	0	0	1	0	1	0	1	0	0	0	-26.0	No	2103	4441	1727

TABLE II
NUMBER OF OCCURRENCES WITH THE LOWEST ENERGY LEVELS USING THE QUBO MODEL FROM (13). THE FIRST ROW SHOWS THE CASE WHERE THE ZERO TERMS ARE SPECIFIED IN THE D-WAVE CODE. THE SECOND ROW DISPLAYS THE CASE WHERE THE ZERO TERMS ARE OMITTED FROM THE CODE.

# Trial	Vanilla QUBO model (Table I)	New QUBO model (Table II, row 1)	New QUBO model (Table II, row 2)
Run 1	887	1526	2103
Run 2	1181	2495	4441
Run 3	1065	2063	1727
Average # Occurrences	1044	2028	2758
Average Probability	10.44%	20.28 %	27.58 %

TABLE III
A SUMMARY OF THE NUMBER OF OCCURRENCES WITH THE LOWEST ENERGY LEVELS FOR EACH QUBO MODEL

from the proposed model. We also observe that omitting the zero entries from the implementation further enhances the performance of the new QUBO model.

The outperformance of the new QUBO model can be traced from the block diagonalization of the matrix Q characterizing the relations among qubits used in the model, as constructed in (13),(15),(14), and (16). The example (7) is a system of 2 linear equations with 2 variables. As shown in (9), the two unknown variables are approximated by the radix 2 representation with 3 digits, using a total of 12 qubits. The two matrices \hat{Q} and \hat{Q}' , both characterizing the respective QUBO models, are 12×12 matrices containing the relations among 12 qubits. Consider the matrix \hat{Q}' which characterizes the vanilla QUBO model (16). It is an upper triangular matrix, all of whose entries are non-zero. The number of non-zero entries of \hat{Q}' is at most

$$\#\text{non-zero entries of } \hat{Q}' \leq \frac{12 \times (12 + 1)}{2} = 78. \quad (19)$$

The matrix congruence relation reduces \hat{Q}' to a block diagonal matrix \hat{Q} from (13), comprised of 4 upper triangular block matrices of dimension 3×3 . The number of non-zero entries of the matrix \hat{Q} characterizing the new QUBO model, as in

(15), is at most

$$\#\text{non-zero entries of } \hat{Q} \leq 4 \times \frac{3 \times (3 + 1)}{2} = 24. \quad (20)$$

Indeed, \hat{Q} , as a block diagonal matrix comprised of 4 upper triangular matrices of size 3×3 , has all but one non-zero entries. The matrix congruence relation cuts down the number of non-zero entries of the characterizing matrix of the QUBO model by more than a factor of $\frac{1}{3}$:

$$\frac{\#\text{non-zero entries of } \hat{Q}}{\#\text{non-zero entries of } \hat{Q}'} \leq \frac{24}{78} < \frac{1}{3}. \quad (21)$$

The results thus verify that exploiting congruence relation between symmetric and diagonal matrices substantially simplifies and enhances the QUBO model for solving systems of linear equations. As for determining the matrices D and R from (5), there is room for improvement on solving systems of linear equations cost-efficiently by utilizing advantages quantum computing methods possess that classical algorithms do not. For example, some classical implementations such as QR or SVD decomposition are not effectively parallelizable or computationally expensive. Meanwhile, distinctive features of quantum computing methods, such as computational bases [7] or synthesis of quantum circuits [8], can contribute to computationally cost-efficient QR decomposition algorithms.

We shall thus expect to achieve polynomial speedup in solving systems of linear equations by combining quantum annealing approaches.

DECLARATION OF INTERESTS

The authors have no competing interests which may have influenced the work shown in this manuscript.

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