IMA Journal of Numerical Analysis (2021) **41**, 2488–2515
https://doi.org/10.1093/imanum/draa031
Advance Access publication on 17 August 2020

Positive semidefinite penalty method for quadratically constrained quadratic programming

Ran Gu* and Qiang Du
Department of Applied Physics and Applied Mathematics, Fu Foundation School of Engineering and Applied Sciences, and Data Science Institute, Columbia University, New York, NY 10027, USA
*Corresponding author: rg3142@columbia.edu qd2125@columbia.edu

and

Ya-xiang Yuan
State Key Laboratory of Scientific and Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China
yyx@lsec.cc.ac.cn

[Received on 16 May 2019; revised on 1 April 2020]

Quadratically constrained quadratic programming (QCQP) appears widely in engineering applications such as wireless communications and networking and multiuser detection with examples like the MAXCUT problem and boolean optimization. A general QCQP problem is NP-hard. We propose a penalty formulation for the QCQP problem based on semidefinite relaxation. Under suitable assumptions we show that the optimal solutions of the penalty problem are the same as those of the original QCQP problem if the penalty parameter is sufficiently large. Then, to solve the penalty problem, we present a proximal point algorithm and an update rule for the penalty parameter. Numerically, we test our algorithm on two well-studied QCQP problems. The results show that our proposed algorithm is very effective in finding high-quality solutions.

Keywords: quadratically constrained quadratic programming; semidefinite programming; semidefinite relaxation; penalty function.

1. Introduction

In this paper we consider the following quadratically constrained quadratic programming (QCQP) problem:

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & x^{\mathrm{T}}Q_0x + 2g_0^{\mathrm{T}}x \\ \text{s.t.} \quad & x^{\mathrm{T}}Q_ix + 2g_i^{\mathrm{T}}x + c_i = 0, \quad i = 1,\dots,m_e, \\ & x^{\mathrm{T}}Q_ix + 2g_i^{\mathrm{T}}x + c_i \geqslant 0, \quad i = m_e+1,\dots,m, \end{aligned} \tag{1.1}$$

where m is the number of constraints, $Q_0 \in \mathbb{S}^{n\times n}$ and $Q_i \in \mathbb{S}^{n\times n}$ $(i = 1,\dots,m)$ are real constant n by n symmetric matrices, $g_0 \in \mathbb{R}^n$ and $g_i \in \mathbb{R}^n$ $(i = 1,\dots,m)$ are n dimensional real vectors and $c_i \in \mathbb{R}$ $(i = 1,\dots,m)$ are real scalars.

Concerning (1.1) Vavasis (1990) proved that the general QCQP is NP-hard. Bar-On & Grasse (1994) derived optimality conditions for QCQP. Peng & Yuan (1997) further analyze the conditions when the number of constraints is two. Wang & Xia (2015) focused on the case that quadratic terms are uniform.

Some special instances possess hidden convexity (see Ben-Tal & Teboulle, 1996; Ye & Zhang, 2003; Beck & Eldar, 2006; Wu *et al.*, 2007; Ai & Zhang, 2009).

Intuitively, the difficulty of solving (1.1) lies not only in the nonconvexity of the objective but also in that of the constraints. The feasible region may be nonconvex or even disconnected in some problems. For example, the boolean quadratic programming (BQP) problem is given by Luo *et al.* (2010):

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & x^{\mathrm{T}}Q_0x \\ \text{s.t.} \quad & x_i^2 = 1, \quad i = 1,\dots,n. \end{aligned} \tag{1.2}$$

The constraint $x_i^2 = 1$ implies that $x_i \in \{1, -1\}$. In this case the feasible region consists of 2^n isolated points. On the other hand the problem of finding a feasible point of (1.1) may be NP-hard itself. An example of the latter is the sensor location problem: with $V_s = \{1,\dots,n\}$ and $V_a = \{n+1,\dots,n+m\}$ denoting the positions of sensors and anchors, respectively, E_{ss} representing the edges between pairs of sensors and E_{sa} representing the edges between sensors and anchors, let the positions of all the anchors and the Euclidean distances in E_{ss} and E_{sa} be specified; then the aim is to find the positions of all the sensors. The sensor location problem can be written as

$$\begin{aligned} \text{find} \quad & x_1,\dots,x_n \in \mathbb{R}^2 \\ \text{s.t.} \quad & \|x_i - x_k\|^2 = d_{ik}^2, \quad (i,k) \in E_{ss}, \\ & \|a_i - x_k\|^2 = \bar{d}_{ik}^2, \quad (i,k) \in E_{sa}, \end{aligned} \tag{1.3}$$

that is, a problem of finding a feasible point with quadratic constraints, which has been shown to be NP-hard (Saxe, 1979).

1.1 *Related works*

Algorithms for solving QCQP can in general be divided into two categories, namely, exact and approximate. In this paper, since we are interested in methods that can quickly find approximate solutions, we do not discuss exact methods. Readers can find studies on the latter, such as different branch and bound methods (Bar-On & Grasse, 1994; Dinh & Le Thi, 1998; Raber, 1998; Cartis *et al.*, 2015) and Lasserre's method (Lasserre, 2001).

To overcome the nonconvexity of the feasible region of QCQP, relaxation techniques have been used in the literature. The reconstruction-linearization technique (RLT) (Sherali, 2007) is for QCQP with bounded constraints. Without loss of generality we assume that the lower bound of each component of the variable is 0 and the upper bound is 1. The key point of RLT is to add a matrix variable $X \in \mathbb{S}^{n\times n}$ to represent xx^T. Using the fact that $x \geqslant 0$ and $e - x \geqslant 0$ we have

$$\begin{aligned} & X_{ij} \geqslant 0, && i,j = 1,\dots,n, \\ & X_{ij} - x_j - x_i \geqslant -1, && i,j = 1,\dots,n, \\ & X_{ij} - x_i \leqslant 0, && i,j = 1,\dots,n. \end{aligned}$$

RLT transforms all the quadratic constraints into linear ones and adds all the above constraints. Then one can obtain a relaxed problem as follows:

$$
\begin{array}{cll}
\min\limits_{x\in\mathbb{R}^n, X\in\mathbb{S}^n} & Q_0 \cdot X + 2g_0^{\mathrm{T}}x & \\
\text{s.t.} & Q_i \cdot X + 2g_i^{\mathrm{T}}x + c_i = 0, & i = 1, \ldots, m_e, \\
& Q_i \cdot X + 2g_i^{\mathrm{T}}x + c_i \geqslant 0, & i = m_e + 1, \ldots, m, \\
& X \geqslant 0, & \\
& ee^{\mathrm{T}} - ex^{\mathrm{T}} - xe^{\mathrm{T}} + X \geqslant 0, & \\
& xe^{\mathrm{T}} - X \geqslant 0, &
\end{array}
$$

where '$\cdot$' is the Frobenius inner product and e is the vector with all elements equal to 1. This relaxed problem is a linear programming problem, which can be solved in various ways.

Positive semidefinite relaxation (SDR) (Fujie & Kojima, 1997) uses the same approach to relax QCQP to a convex problem in matrix space. More specifically, SDR relaxes the constraint $X = xx^T$ to $X - xx^{\mathrm{T}} \succeq 0$, where '$\succeq 0$' means positive semidefinite. Then QCQP is relaxed to a semidefinite programming problem (SDP)

$$
\begin{array}{cll}
\min\limits_{x\in\mathbb{R}^n, X\in\mathbb{S}^n} & Q_0 \cdot X + 2g_0^{\mathrm{T}}x & \\
\text{s.t.} & Q_i \cdot X + 2g_i^{\mathrm{T}}x + c_i = 0, & i = 1, \ldots, m_e, \\
& Q_i \cdot X + 2g_i^{\mathrm{T}}x + c_i \geqslant 0, & i = m_e + 1, \ldots, m, \\
& X \succeq xx^{\mathrm{T}}, &
\end{array}
\tag{1.4}
$$

where $X \succeq xx^{\mathrm{T}}$ can be regarded as $\begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & X \end{pmatrix} \succeq 0$. SDR has been widely used in practice (Luo *et al.*, 2010). For some special QCQP the approximation ratio, a standard measure of the quality of the approximation, has been analyze (Ma *et al.*, 2002; Steingrimsson *et al.*, 2003). In particular for BQP in (1.2), when $Q_0 \geqslant 0$ the ratio is 1, which means that the solution of the relaxed problem is that of the original problem (Luo *et al.*, 2010).

More extended SDR-type relaxations are discussed by Bao *et al.* (2011). Comparison between RLT and SDR can be found in Anstreicher (2009). One can also find more studies on approximation methods in Beck *et al.* (2010) and Lu *et al.* (2011).

1.2 *Our contribution*

In this paper we take a different angle to interpret the SDR. To be more precise we regard SDR as a penalty function method with the penalty term being zero. By showing that the penalty function is exact for sufficiently large penalty parameters we argue that it is reasonable to study approaches based on the penalty formulation with a nonzero penalty term. Accordingly, we propose an algorithm to solve the penalty problem, together with an update rule for the penalty parameter. Numerical tests are presented to demonstrate that the proposed algorithm achieves our main target in improving the quality of solutions, in comparison with SDR, at the expense of possibly longer computational time. Moreover, in a majority of the testing cases as quantified in the reported data, our algorithm is able to find the global solutions of the prescribed problems.

1.3 *Organization*

This paper is organized as follows: in Section 2 we propose our new penalty problem and prove that the penalty is exact. In Section 3 we give our algorithm to solve the penalty problem. In Section 4 we use numerical tests to illustrate the performance of our proposed algorithm. Finally, Section 5 contains a summary of the main contributions of the paper and a perspective on some outstanding challenges.

2. Penalty problem

The QCQP problem (1.1) can be transformed into the following equivalent problem:

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} \end{pmatrix} \cdot \begin{pmatrix} 0 & g_0^{\mathrm{T}} \\ g_0 & Q_0 \end{pmatrix} \\ \text{s.t.} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\ & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e + 1, \ldots, m. \end{aligned} \tag{2.1}$$

We can add a matrix variable Z to the above problem with an additional constraint $Z = 0$; then the QCQP problem (1.1) is equivalent to

$$\begin{aligned} \min_{x\in\mathbb{R}^n, Z\in\mathbb{S}^n} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} 0 & g_0^{\mathrm{T}} \\ g_0 & Q_0 \end{pmatrix} \\ \text{s.t.} \quad & \begin{pmatrix} 1 & x^{T} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\ & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e + 1, \ldots, m, \\ & Z = 0. \end{aligned}$$

Here, Z can be regarded as $X - xx^{\mathrm{T}}$ in Section 1.

Notice that the constraint $Z = 0$ can be reformulated as two constraints, $Z \succeq 0$ and $Z \preceq 0$; then the above problem is equivalent to

$$\begin{aligned} \min_{x\in\mathbb{R}^n, Z\in\mathbb{S}^n} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} 0 & g^{\mathrm{T}} \\ g & Q \end{pmatrix} \\ \text{s.t.} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = 1, \ldots, m, \\ & Z \succeq 0, \\ & Z \preceq 0. \end{aligned} \tag{2.2}$$

The positive semidefiniteness of Z and of $\begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix}$ are equivalent, as shown in the following lemma.

LEMMA 2.1 For any real vector $x \in \mathbb{R}^n$ and real symmetric matrix $Z \in \mathbb{S}^n$, $Z \succeq 0$ is equivalent to $\begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^T+Z \end{pmatrix} \succeq 0$.

Proof. The matrix $\begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^T+Z \end{pmatrix}$ becomes $\begin{pmatrix} 1 & 0 \\ 0 & Z \end{pmatrix}$ under a congruence transformation. Then by Sylvester's law of inertia we have that $\begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \succeq 0$ if and only if $Z \succeq 0$. □

Now using Lemma 2.1, SDR (1.4) can be viewed as a relaxation of (2.2) by dropping the constraint $Z \preceq 0$. We would like to add a penalty term $P \cdot Z$ to the objective function. Here P is a positive definite matrix to be properly chosen so that the effect of $P \cdot Z$ is to control the sizes of the positive eigenvalues of Z, if any. For more discussion on the choices of P we refer to Section 3. Thus, the new penalty formulation of the original problem is given as

$$\begin{aligned}
\min_{x\in\mathbb{R}^n, Z\in\mathbb{S}^n} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} 0 & g_0^{\mathrm{T}} \\ g_0 & Q_0 \end{pmatrix} + P \cdot Z \\
\text{s.t.} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\
& \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e+1, \ldots, m, \\
& Z \succeq 0.
\end{aligned} \tag{2.3}$$

In the special case where $P = 0$, problem 2.3 becomes SDR.

2.1 *Notation*

Before we analyze the properties of the penalty problem (2.3) we first define some notation to simplify the description of the problem.

Let

$$\begin{aligned}
f(x) &:= x^{\mathrm{T}} Q_0 x + 2 g_0^{\mathrm{T}} x, \\
F &:= \Bigg\{ x \,\Bigg|\, \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = 1, \ldots, m_e, \\
&\qquad \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e+1, \ldots, m \Bigg\}, \\
G &:= \Bigg\{ (x, Z) \,\Bigg|\, Z \succeq 0, \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\
&\qquad \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e+1, \ldots, m \Bigg\}, \\
\mathscr{L}(x, Z, P) &:= f(x) + Q_0 \cdot Z + P \cdot Z.
\end{aligned}$$

Then, F and G are related by

$$F = \{x \mid (x, 0) \in G\}. \tag{2.4}$$

Using the above notation we rewrite the QCQP problem (1.1) as

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & x \in F. \end{aligned} \tag{2.5}$$

We also rewrite the penalty problem (2.3) as

$$\min_{(x,Z)\in G} \mathscr{L}(x, Z, P). \tag{2.6}$$

One can view $\mathscr{L}$ as the Lagrangian function corresponding to the constraint $Z \preceq 0$, with P being the dual variable.

2.2 *Exact penalty*

In this subsection, we prove that the penalty problem (2.6) is exact, which means that its optimal solution is also an optimal solution of QCQP problem (2.5), when all the eigenvalues of P are larger than a certain constant. These results can be found in Theorems 2.4 and 2.5.

First, we give the following lemma on the relationship between problem (2.6) and P, which reveals a monotone dependence.

LEMMA 2.2 $\min_{(x,Z)\in G} \mathscr{L}(x, Z, P_1) \leqslant \min_{(x,Z)\in G} \mathscr{L}(x, Z, P_2) \leqslant \min_{x\in F} f(x) \; \forall \, P_1 \preceq P_2$.

Proof. Due to (2.4), for any P we have

$$\min_{(x,Z)\in G} \mathscr{L}(x, Z, P) \leqslant \min_{(x,0)\in G} \mathscr{L}(x, 0, P) = \min_{x\in F} f(x).$$

For any $P_1 \preceq P_2$ we have $P_2 - P_1 \succeq 0$, which implies $(P_2 - P_1) \cdot Z \geqslant 0$ for all $Z \succeq 0$. Consequently, $P_2 \cdot Z \geqslant P_1 \cdot Z$. Thus we have

$$\mathscr{L}(x, Z, P_1) \leqslant \mathscr{L}(x, Z, P_2) \quad \forall \; Z \succeq 0.$$

Then

$$\min_{(x,Z)\in G} \mathscr{L}(x, Z, P_1) \leqslant \min_{(x,Z)\in G} \mathscr{L}(x, Z, P_2),$$

which completes our proof. □

Suppose that $x^\star$ is a local minimizer of problem (2.5). For simplification we denote each of the constraints of problem (2.5) by

$$\begin{aligned} c_i(x) &:= x^{\mathrm{T}} Q_i x + 2g_i^{\mathrm{T}} x + c_i = 0, \quad i = 1, \ldots, m_e, \\ c_i(x) &:= x^{\mathrm{T}} Q_i x + 2g_i^{\mathrm{T}} x + c_i \geqslant 0, \quad i = m_e + 1, \ldots, m. \end{aligned}$$

In the following we demonstrate the exact penalty via Karush–Kuhn–Tucker (KKT) conditions. In order for a minimum point to satisfy KKT conditions the problem should satisfy some regularity constraint qualifications. Peterson (1973) reviewed various constraint qualifications and stated their relationships. We choose the Abadie constraint qualification (ACQ) described below for our use (Abadie, 1966), which is considered to be pretty mild.

Let the set of sequence feasible directions be defined by (see Sun & Yuan, 2006)

$$\mathrm{SFD}(x) = \left\{ d | \ \exists \{d^k\} \to d, \{t_k\} \downarrow 0 : x + t_k d^k \in F \ \forall k \right\}$$

and the set of linearization feasible directions be defined by

$$\begin{aligned} \mathrm{LFD}(x) = \Big\{ & d | \nabla c_i(x)^{\mathrm{T}} d = 0, \ i = 1, \ldots, m_e, \\ & \nabla c_j(x)^{\mathrm{T}} d \geqslant 0, \ c_j(x) = 0, \ j = m_e + 1, \ldots, m \Big\}. \end{aligned}$$

The following assumption ensures that a minimum point satisfies KKT conditions.

Assumption 2.3 (ACQ) $x^\star$ is a local minimizer of problem (2.5), that is,

$$\mathrm{SFD}(x^\star) = \mathrm{LFD}(x^\star).$$

We then state our theorems.

Theorem 2.4 Suppose that $x^\star$ is a local minimizer of QCQP problem (2.5) and satisfies Assumption 2.3 and the second-order sufficient condition, which means that for any direction $d \in C := \mathrm{SFD}(x^\star)$,

$$d^T \left(Q_0 - \sum_{i=1}^{m} \alpha_i^\star Q_i \right) d > 0, \tag{2.7}$$

where $\alpha^\star$ is the multiplier corresponding to $x^\star$. Then there exists $P^\star \succeq 0$ such that $(x^\star, 0)$ is a strict local minimizer of (2.6) for all $P \succ P^\star$.

Proof. Since $x^\star$ is the local minimizer of problem (2.5), under Assumption 2.3, $(x^\star, \alpha^\star)$ satisfies the following first-order necessary conditions:

$$\begin{aligned} & \nabla f(x^\star) - \textstyle\sum_{i=1}^{m} \alpha_i^\star \nabla c_i(x^\star) = 0, \\ & c_i(x^\star) = 0, \quad i = 1, \ldots, m_e, \\ & c_i(x^\star) \geqslant 0, \quad \alpha_i^\star \geqslant 0, \quad i = m_e + 1, \ldots, m, \\ & \textstyle\sum_{i=m_e+1}^{m} \alpha_i c_i(x^\star) = 0. \end{aligned}$$

Let $M = Q_0 - \sum_{i=1}^{m} \alpha_i^\star Q_i$. The second-order sufficient condition (2.7) implies that there is a constant $\delta > 0$, which makes the following inequality satisfied for all $d \in C$:

$$d^{\mathrm{T}} M d \geqslant \delta \|d\|^2. \tag{2.8}$$

Otherwise, there exists a sequence $\{d_k\}$ such that $d_k^{\mathrm{T}} M d_k / \|d_k\|^2 \to 0$. Let $\hat{d}_k = d_k/\|d_k\|$; then $\hat{d}_k^{\mathrm{T}} M \hat{d}_k \to 0$ and $\|\hat{d}_k\| = 1$. Since C is a closed set there exists a $\bar{d} \in C$ such that $\|\bar{d}\| = 1$ and $\bar{d}_k^{\mathrm{T}} M \bar{d}_k = 0$. This is in contradiction with (2.7).

With regard to the QCQP in matrix form (2.2), its primal and dual solution (x, Z, α, S_1, S) at $x = x^\star, Z = Z^\star = 0$ satisfies

$$Q_0 - \sum \alpha_i^\star Q_i - S_1^\star + S^\star = 0, \quad S_1^\star \succeq 0, \quad S^\star \succeq 0,$$

where $S_1^\star$ is the multiplier corresponding to $Z \succeq 0$ and $S^\star$ is the multiplier corresponding to $Z \preceq 0$.

We consider the following problem:

$$\begin{aligned} \min_{x,Z} \ & f(x) + Q_0 \cdot Z + S^\star \cdot Z + \tfrac{\sigma_1}{2}\|Z\|_F^2 \\ \text{s.t.} \ & c_i(x) + Q_i \cdot Z = 0, \quad i = 1, \ldots, m_e, \\ & c_i(x) + Q_i \cdot Z \geqslant 0, \quad i = m_e + 1, \ldots, m, \\ & Z \succeq 0. \end{aligned} \tag{2.9}$$

Here we introduce problem (2.9) as the intermediate tool of this proof. We will prove that $(x^\star, 0)$ is its strict local minimum by assigning a large number to the coefficient of the quadratic term. Then we will prove that $(x^\star, 0)$ is a strict local minimum of problem (2.6) by using the fact that the square of the Frobenius norm is smaller than the linear function in the neighbourhood of 0.

First we need to prove that when σ_1 is greater than some constant, $(x^\star, 0)$ is a local strictly minimal point of problem (2.9).

The Lagrangian function of problem (2.9) is

$$\bar{\mathscr{L}}(x, Z, \alpha, S_1) := f(x) + Q_0 \cdot Z + S^\star \cdot Z + \frac{\sigma_1}{2}\|Z\|_F^2 - \sum_{i=1}^{m} \alpha_i (c_i(x) + Q_i \cdot Z) - S_1 \cdot Z.$$

Moreover, its KKT conditions are given by

$$\begin{aligned} & \nabla f(x) - \textstyle\sum_{i=1}^m \alpha_i \nabla c_i(x) = 0, \\ & Q_0 + S^\star + \sigma_1 Z - \textstyle\sum_{i=1}^m \alpha_i Q_i - S_1 = 0, \\ & c_i(x) + Q_i \cdot Z = 0, \quad i = 1, \ldots, m_e, \\ & c_i(x) + Q_i \cdot Z \geqslant 0, \quad \alpha_i \geqslant 0, \quad i = m_e + 1, \ldots, m, \\ & \textstyle\sum_{i=m_e+1}^m \alpha_i (c_i(x) + Q_i \cdot Z) = 0, \\ & Z \succeq 0, \quad S_1 \succeq 0, \quad Z \cdot S_1 = 0. \end{aligned}$$

If we set $x = x^\star$, $Z = 0$, $\alpha = \alpha^\star$, $S_1 = S_1^\star$, the above conditions are satisfied.

The second derivatives of $\bar{\mathscr{L}}(x, Z, \alpha, S_1)$ corresponding to primal variables are

$$\begin{aligned}\nabla^2_{xx}\bar{\mathscr{L}} &= Q_0 - \sum \alpha_i Q_i,\\ \nabla^2_{x\ \mathrm{vec}(Z)}\bar{\mathscr{L}} &= 0,\\ \nabla^2_{\mathrm{vec}(Z)\ \mathrm{vec}(Z)}\bar{\mathscr{L}} &= \sigma_1 I,\end{aligned}$$

where I is the identity matrix and $vec(Z)$ represents the matrix Z in vector form. Then for any feasible direction $(d, \mathrm{vec}(D))$ at $(x^\star, 0)$ in problem (2.9) we have

$$(d, \mathrm{vec}(D))^{\mathrm{T}} \left(\nabla^2_{(x,\mathrm{vec}(Z))(x,\mathrm{vec}(Z))}\bar{\mathscr{L}}\right)(d, \mathrm{vec}(D)) = d^{\mathrm{T}} M d + \sigma_1 \|D\|_F^2.$$

By the definition of distance and projection from Rockafellar (2015), the distance between d and C and the projection from d to C are defined as

$$\begin{aligned}\mathrm{dist}(d, C) &= \min_{y\in C} \|d - y\|,\\ P_C(d) &= \left\{d_1 \in C \mid \mathrm{dist}(d, C) = \|d - d_1\|\right\}.\end{aligned}$$

Here we fix any $d_1 \in P_C(d)$, and let $d_2 = d - d_1$.

If $d \notin C$ then by Assumption 2.3 there exists some $i \in \{1, \dots, m_e\}$ satisfying $\nabla c_i(x^\star)^{\mathrm{T}} d \neq 0$ or some $i \in \{m_e + 1, \dots, m\}$ satisfying $c_i(x^\star) = 0$ and $\nabla c_i(x^\star)^{\mathrm{T}} d < 0$. Let us denote

$$I = \{i \in \{m_e + 1, \dots, m\} \mid c_i(x^\star) = 0, \nabla c_i(x^\star)^{\mathrm{T}} d < 0\}.$$

From the error bounds of Hoffman (2003) there exists $\tilde{d} \in C$ and a constant $a_1 > 0$ such that

$$\max\left\{\max_{i\in\{1,\dots,m_e\}} |\nabla c_i(x^\star)^{\mathrm{T}} d|, \max_{i\in I} -\nabla c_i(x^\star)^{\mathrm{T}} d\right\} \geqslant a_1 \|d - \tilde{d}\| \geqslant a_1 \|d_2\|,$$

and a_1 is independent of d. Notice that (d, D) is a feasible direction; then for the above i we have

$$\|Q_i\| \|D\| \geqslant Q_i \cdot D \geqslant -\nabla c_i(x^\star)^{\mathrm{T}} d \geqslant a_1 \|d_2\|.$$

Since there are only finitely many different sets I there is a constant $a_2 > 0$ depending only on $x^\star$ and satisfying

$$\|d_2\| \leqslant a_2 \|D\|. \tag{2.10}$$

The case for $d \in C$ is also correct because $d_2 = 0$.

Then

$$\begin{aligned} d^TMd+\sigma_1\|D\|_F^2 &= d_1^{\mathrm{T}}Md_1+2d_1^{\mathrm{T}}Md_2+d_2^{\mathrm{T}}Md_2+\sigma_1\|D\|_F^2 \\ &\geqslant d_1^{\mathrm{T}}Md_1-\left(\tfrac{\delta}{2}\|d_1\|^2+2\delta^{-1}d_2^{\mathrm{T}}M^2d_2\right)+d_2^{\mathrm{T}}Md_2+\sigma_1\|D\|_F^2 \\ &= \left(d_1^{\mathrm{T}}Md_1-\tfrac{\delta}{2}\|d_1\|^2\right)+d_2^{\mathrm{T}}(M-2\delta^{-1}M^2)d_2+\sigma_1\|D\|_F^2 \\ &> 0 \end{aligned}$$

if we choose $\sigma_1 > a_2^2\|M-2\delta^{-1}M^2\|_F$. From (2.8) and (2.10) we know that $d^TMd+\sigma_1\|D\|_F^2 \geqslant 0$ and the equality holds if and only if $d=0, D=0$. Hence we obtain that $(x^\star,0)$ is a strict local minimizer of problem (2.9). Then there exists a constant $\delta_1 > 0$ such that when $\max\{\|x-x^\star\|,\|Z\|_F\} \leqslant \delta_1$ and $(x,Z)\in G$ we have

$$f(x)+Q_0\cdot Z+S^\star\cdot Z+\frac{\sigma_1}{2}\|Z\|_F^2 \geqslant f(x^\star),$$

where the equality holds if and only if $x=x^\star$ and $Z=0$.

When $P-S^\star \succ 0$ there is a constant $\delta_2 > 0$ such that for any Z satisfying $\|Z\|_F \leqslant \delta_2$,

$$\frac{\sigma_1}{2}\|Z\|_F^2 \leqslant (P-S^\star)\cdot Z.$$

So far, only δ_2 depends on P. One can take

$$\delta_2 \leqslant 2\lambda/\sigma_1, \tag{2.11}$$

where λ is the smallest eigenvalue of $P-S^\star$, because

$$\|Z\|_F^2 \leqslant \|Z\|_F\mathrm{tr}(Z) \leqslant \delta_2\mathrm{tr}(Z) \leqslant (2\lambda/\sigma_1)\mathrm{tr}(Z) \leqslant (2/\sigma_1)(P-S^\star)\cdot Z.$$

This statement is used in the proof of the next theorem.

Therefore, when $\max\{\|x-x^\star\|,\|Z\|_F\} \leqslant \min\{\delta_1,\delta_2\}$ and $(x,Z)\in G$,

$$\begin{aligned} f(x)+Q_0\cdot Z+P\cdot Z &= f(x)+Q_0\cdot Z+S^\star\cdot Z+(P-S^\star)\cdot Z \\ &\geqslant f(x)+Q_0\cdot Z+S^\star\cdot Z+\tfrac{\sigma_1}{2}\|Z\|_F^2 \\ &\geqslant f(x^\star), \end{aligned}$$

where the equality holds if and only if $x=x^\star$ and $Z=0$. This is to say that $(x^\star,0)$ is a strict local minimizer of problem (2.6) when $P \succ S^\star$. □

We note that Theorem 2.4 is focused on local minimizers. Next we discuss the global minimizer in the following theorem.

THEOREM 2.5 Suppose that $x^\star$ is a strict global minimizer of the QCQP problem (2.5) and satisfies Assumption 2.3 and the second-order sufficient condition. Assume that

$$\mathrm{LS} := \left\{x\middle| f(x) \leqslant \min_{x\in F} f(x), (x,Z)\in G\right\}$$

is bounded. Then there exists a $\bar{P} \succeq 0$ such that $(x^\star,0)$ is a strict global minimizer of (2.6) for all $P \succ \bar{P}$.

Proof. If there exists a $\bar{P}$ such that $(\bar{x}, 0)$ is a global minimizer of

$$\min_{(x,Z)\in G} \mathscr{L}(x, Z, \bar{P}),$$

then for any $P \succeq \bar{P}$ we obtain the following relationship from Lemma 2.2:

$$\mathscr{L}(\bar{x}, 0, \bar{P}) \leqslant \min_{(x,Z)\in G} \mathscr{L}(x, Z, P) \leqslant \mathscr{L}(\bar{x}, 0, P) = \mathscr{L}(\bar{x}, 0, \bar{P}).$$

Thus

$$\min_{(x,Z)\in G} \mathscr{L}(x, Z, P) = \mathscr{L}(\bar{x}, 0, P).$$

Hence $(\bar{x}, 0)$ is a global minimizer of problem (2.6). Since $x^\star$ is a strict global minimizer of problem (2.5) we have $\bar{x} = x^\star$.

If there does not exist any P such that $Z = 0$ is part of a global minimizer of problem (2.6) then there are two cases:

1. For any $\hat{P} \succeq S^\star + (\rho(Q_0) + \epsilon)I$, the global minimizer $(\hat{x}, \hat{Z})$ of problem (2.6) satisfies $\|\hat{Z}\|_F \geqslant \delta > 0$, where $\rho(Q_0)$ is the spectral radius of Q_0, ϵ is an arbitrary positive constant scalar and I is the identity matrix.
   Since $\hat{x} \in LS$, $\hat{x}$ and $f(\hat{x})$ are bounded, by letting $\hat{P} = \lambda I$ and $\lambda \to +\infty$, we get

$$\mathscr{L}(\hat{x}, \hat{Z}, \hat{P}) = f(\hat{x}) + (\hat{P} + Q_0) \cdot \hat{Z} \to +\infty.$$

   This is in contradiction with Lemma 2.2.

2. There exists a sequence $\{P^k\} \succeq S^\star + (\rho(Q_0) + \epsilon)I$, such that $Z^k \to 0$, but $Z^k \neq 0$, where (x^k, Z^k) is a global minimizer of $\min_{(x,Z)\in G} \mathscr{L}(x, Z, P^k)$.
   Since $x^k \in LS$, $\{x^k\}$ are bounded, there exists a cluster point of $\{x^k\}$, denoted by $\bar{x}$. Suppose that $x^{i_k} \to \bar{x}$. Due to the fact that $Z^{i_k} \to 0$ and the closeness of the set of solutions we have $(\bar{x}, 0) \in G$, i.e. $\bar{x} \in F$. It is known from Lemma 2.2 that

$$f(x^{i_k}) + (Q_0 + P^{i_k}) \cdot Z^{i_k} \leqslant \min_{x\in F} f(x). \tag{2.12}$$

   Since $(Q_0 + P^{i_k}) \cdot Z^{i_k} > 0$ we have

$$f(x^{i_k}) < \min_{x\in F} f(x).$$

   Taking the limit $i_k \to +\infty$ on both sides we have $f(\bar{x}) \leqslant \min_{x\in F} f(x)$. On the other hand, $\bar{x} \in F$, thus $f(\bar{x}) \geqslant \min_{x\in F} f(x)$. Therefore, $f(\bar{x}) = \min_{x\in F} f(x)$, which implies that $\bar{x}$ is a global minimizer of (2.5); then $\bar{x} = x^\star$. According to Theorem 2.4, for all $P \succeq S^\star + (\rho(Q_0) + \epsilon)I$, $(x^\star, 0)$ is a strict local minimizer of problem (2.6). Moreover, as mentioned in the proof of Theorem 2.4, that is (2.11), we take $\delta_2 = (2\epsilon/\sigma_1)$ to ensure that when $\max\{\|x - x^\star\|, \|Z\|_F\} \leqslant \min\{\delta_1, \delta_2\}$ and

$(x, Z) \in G$, we have

$$f(x) + Q_0 \cdot Z + P \cdot Z \geqslant f(x^\star),$$

where the equality holds if and only if $x = x^\star$ and $Z = 0$. This is in contradiction with $(x^{i_k}, Z^{i_k}) \to (x^\star, 0)$ and (2.12).

In summary, there exists a $\bar{P}$ such that $(x^\star, 0)$ is a global minimizer of problem (2.6) when $P \succ \bar{P}$. □

3. Algorithm

Compared with the feasible region of QCQP problem (2.5), which may be nonconvex or discontinuous, the feasible region of our penalty formulation (2.6) is a semipositive definite convex cone, which is easier to apply to classical optimization algorithms, such as the projection gradient method. However, an essential difficulty of the problem still remains. Indeed, problem (2.6) remains a nonconvex quadratic semidefinite programming, which is NP-hard as well.

As discussed in Section 2 the penalty factor P is a positive semidefinite matrix. The choice of P will be discussed later. When P is given, problem (2.6) can be viewed as a difference of convex (DC) functions because it can be written as

$$\begin{aligned}
\min_{x\in\mathbb{R}^n, Z\in\mathbb{S}^n} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^T + Z \end{pmatrix} \cdot \begin{pmatrix} 0 & g_0^{\mathrm{T}} \\ g_0 & Q_0 + P \end{pmatrix} - x^{\mathrm{T}} P x \\
\text{s.t.} \quad & \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^T + Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\
& \begin{pmatrix} 1 & x^{\mathrm{T}} \\ x & xx^{\mathrm{T}} + Z \end{pmatrix} \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e + 1, \ldots, m, \\
& Z \succeq 0,
\end{aligned}$$

and by Lemma 2.1 it is equivalent to

$$\begin{aligned}
\min_{x\in\mathbb{R}^n, W\in\mathbb{S}^{n+1}} \quad & W \cdot \begin{pmatrix} 0 & g_0^{\mathrm{T}} \\ g_0 & Q_0 + P \end{pmatrix} - x^T P x \\
\text{s.t.} \quad & W \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} = 0, \quad i = 1, \ldots, m_e, \\
& W \cdot \begin{pmatrix} c_i & g_i^{\mathrm{T}} \\ g_i & Q_i \end{pmatrix} \geqslant 0, \quad i = m_e + 1, \ldots, m, \\
& W_{11} = 1, \\
& W_{\{2,\ldots,n+1\}\ 1} = x, \\
& W \succeq 0.
\end{aligned}$$

As far as the authors know, there is no mature algorithm to solve a nonconvex quadratic positive semidefinite programming problem. One can use one of the methods for solving DC problems to solve problem (2.6). There have been many studies devoted to the theory of DC functions in the literature (see, for example, Hiriart-Urruty, 1985, 1989). For DC algorithms (DCA) one can find references that use the regularization approach (Fernández Cara & Moreno, 1988), the dual approach (Auchmuty, 1989), the subgradient method (Dinh & Souad, 1986) and the proximal point algorithm (Sun *et al.*, 2003). Le Thi & Dinh (2018) offered a nice survey on the 30 years of developments of these theoretical and algorithmic tools and provide more relevant information about DC and DCA.

Due to the NP-hardness we try to design an algorithm to find solutions satisfying the first-order optimality conditions:

$$
\begin{aligned}
& Q_0 x + g_0 - \sum_{i=1}^{m} \alpha_i (Q_i x + g_i) = 0, \\
& x^{\mathrm{T}} Q_i x + 2 g_i^{\mathrm{T}} x + c_i + Q_i \cdot Z = 0, \quad i = 1, \ldots, m_e, \\
& x^{\mathrm{T}} Q_i x + 2 g_i^{\mathrm{T}} x + c_i + Q_i \cdot Z \geqslant 0, \quad i = m_e + 1, \ldots, m, \\
& \alpha_i \geqslant 0, \quad i = m_e + 1, \ldots, m, \\
& \alpha_i \left(x^{\mathrm{T}} Q_i x + 2 g_i^{T} x + c_i + Q_i \cdot Z \right) = 0, \quad i = m_e + 1, \ldots, m, \\
& \left(Q_0 + P - \sum_{i=1}^{m} \alpha_i Q_i \right) \cdot Z = 0, \\
& Z \succeq 0, \\
& \left(Q_0 + P - \sum_{i=1}^{m} \alpha_i Q_i \right) \succeq 0.
\end{aligned}
\tag{3.1}
$$

We propose the entire algorithmic framework in this section, including an algorithm for problems with the penalty function and an algorithm on the update rules of P.

3.1 *Proximal point algorithm*

We choose the proximal point algorithm (PPA) proposed by Rockafellar (1976) to solve the penalty problem (2.6). Sun *et al.* (2003) extended PPA to solve general DC. The basic properties of PPA and applications of PPA in machine learning, statistics, data analysis, signal and image processing, computational economics and finance, engineering design, scheduling and resource allocation and other areas have been discussed by Parikh & Boyd (2014).

For our problem, to be more specific, we solve the following subproblem in the kth iteration:

$$
\begin{aligned}
(d^k, Z^{k+1}) = \ & \underset{d \in \mathbb{R}^n, Z \in \mathbb{S}^n}{\arg\min} \quad \mathscr{L}(x^k + d, Z, P) + d^{\mathrm{T}} P d \\
& \quad \text{s.t.} \qquad (x^k + d, Z) \in G,
\end{aligned}
\tag{3.2}
$$

where $d^{\mathrm{T}}Pd$ is the proximal term. Then we update

$$x^{k+1} = x^k + d^k.$$

In fact, problem (3.2) is a standard positive semidefinite programming problem, which can be written as

$$\begin{aligned}
\min_{d\in\mathbb{R}^n, Z\in\mathbb{S}^n} \quad & \begin{pmatrix} 1 & d^{\mathrm{T}} \\ d & dd^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} 0 & (Q_0x^k+g_0)^{\mathrm{T}} \\ Q_0x^k+g_0 & Q_0+P \end{pmatrix} \\
\text{s.t.} \quad & \begin{pmatrix} 1 & d^{\mathrm{T}} \\ d & dd^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i+2g_ix^k+{x^k}^{\mathrm{T}}Q_ix^k & (Q_ix^k+g_i)^{\mathrm{T}} \\ Q_ix^k+g_i & Q_i \end{pmatrix} = 0, \qquad i=1,\dots,m_e, \\
& \begin{pmatrix} 1 & d^{v} \\ d & dd^{\mathrm{T}}+Z \end{pmatrix} \cdot \begin{pmatrix} c_i+2g_ix^k+{x^k}^{\mathrm{T}}Q_ix^k & (Q_ix^k+g_i)^{\mathrm{T}} \\ Q_ix^k+g_i & Q_i \end{pmatrix} \geqslant 0, \qquad i=m_e+1,\dots,m, \\
& Z \succeq 0
\end{aligned} \tag{3.3}$$

or

$$\begin{aligned}
\min_{d\in\mathbb{R}^n, W\in\mathbb{S}^{n+1}} \quad & W \cdot \begin{pmatrix} 0 & (Q_0x^k+g_0)^{\mathrm{T}} \\ Q_0x^k+g & Q_0+P \end{pmatrix} \\
\text{s.t.} \quad & W \cdot \begin{pmatrix} c_i+2g_ix^k+{x^k}^{\mathrm{T}}Q_ix^k & (Q_ix^k+g_i)^{\mathrm{T}} \\ Q_ix^k+g_i & Q_i \end{pmatrix} = 0, \qquad i=1,\dots,m_e, \\
& W \cdot \begin{pmatrix} c_i+2g_ix^k+{x^k}^{\mathrm{T}}Q_ix^k & (Q_ix^k+g_i)^{\mathrm{T}} \\ Q_ix^k+g_i & Q_i \end{pmatrix} \geqslant 0, \qquad i=m_e+1,\dots,m, \\
& W_{11} = 1, \\
& W_{\{2,\dots,n+1\}\,1} = x^k, \\
& W \succeq 0,
\end{aligned}$$

for easy understanding.

The above problem can be solved in polynomial time by various methods including off-the-shelf software (for example, SDPT3, Toh *et al.*, 2009, and SDPNAL+, Yang *et al.*, 2015). Its solution

(d, Z, α, S) satisfies the first-order conditions as follows:

$$
\begin{aligned}
& Q_0(x^k+d)+g_0-\sum_{i=1}^{m}\alpha_i\left(Q_i(x^k+d)+g_i\right)+Pd=0,\\
& (x^k+d)^{\mathrm{T}}Q_i(x^k+d)+2g_i^{\mathrm{T}}(x^k+d)+c_i+Q_i\cdot Z=0, \quad i=1,\ldots,m_e\\
& (x^k+d)^{\mathrm{T}}Q_i(x^k+d)+2g_i^{\mathrm{T}}(x^k+d)+c_i+Q_i\cdot Z\geqslant 0, \quad i=m_e+1,\ldots,m\\
& \alpha_i\geqslant 0, \quad i=m_e+1,\ldots,m,\\
& \alpha_i\left((x^k+d)^{\mathrm{T}}Q_i(x^k+d)+2g_i^{\mathrm{T}}(x^k+d)+c_i+Q_i\cdot Z\right)=0, \quad i=m_e+1,\ldots,m,\\
& \left(Q_0+P-\sum_{i=1}^{m}\alpha_iQ_i\right)\cdot Z=0,\\
& Z\succeq 0,\\
& \left(Q_0+P-\sum_{i=1}^{m}\alpha_iQ_i\right)\succeq 0.
\end{aligned}
\tag{3.4}
$$

Here, we present one ingredient in our algorithmic framework, which is an algorithm for solving the penalty problem (2.6). The monotone descent property and convergence analysis of the algorithm are given in Lemma 3.1 and Theorem 3.2.

Algorithm 3.1 Proximal point algorithm for penalty problem

Step 0: give the initial point x^0.

Step 1: solve problem (3.3) to obtain d^k.

Step 2: $x^{k+1} := x^k + d^k$.

Step 3: if the termination criteria is satisfied, stop.
Otherwise, $k := k + 1$, go to Step 1.

LEMMA 3.1 Suppose that $\{x^k\}$ and $\{Z^k\}$ are generated by Algorithm 3.1; then

$$\mathscr{L}(x^{k+1}, Z^{k+1}, P) \leqslant \mathscr{L}(x^k, Z^k, P) - {d^k}^{\mathrm{T}} P d^k. \tag{3.5}$$

Proof. Since for all k we have $(x^k, Z^k) \in G$, thus

$$
\begin{aligned}
\mathscr{L}(x^{k+1}, Z^{k+1}, P) &= \left(\mathscr{L}(x^k+d^k, Z^{k+1}, P)+(d^k)^{\mathrm{T}}Pd^k\right)-(d^k)^{\mathrm{T}}Pd^k\\
&\leqslant \mathscr{L}(x^k, Z^k, P)-(d^k)^{\mathrm{T}}Pd^k.
\end{aligned}
$$

Here, the inequality holds due to (3.2). □

THEOREM 3.2 Suppose that $\{d^k\}$, $\{x^k\}$ and $\{Z^k\}$ are generated by Algorithm 3.1. If the primal and dual solutions $\{x^k\}, \{Z^k\}, \{\alpha^k\}, \{S^k\}$ of (3.3) are bounded, where $S^k = Q_0 + P - \sum_{i=1}^{m} \alpha_i^k Q_i$, then $\{d^k\}$ converges to 0 and any cluster point of $\{(x^k, Z^k, \alpha^k, S^k)\}$ is a first-order stationary point of (2.6).

Proof. From (3.5) we know that

$$\mathscr{L}(x^{k+1}, Z^{k+1}, P) \leqslant \mathscr{L}(x^0, Z^0, P) - \sum_{i=1}^{k} {d^i}^{\mathrm{T}} P d^i. \tag{3.6}$$

Due to the boundness assumption we have

$$\sum_{i=1}^{\infty} {d^i}^{\mathrm{T}} P d^i < +\infty. \tag{3.7}$$

Since $P \succ 0$ thus $d^i \to 0$.

Our boundedness assumptions imply that $\{(x^k, Z^k, \alpha^k, S^k)\}$ has at least one cluster point. Let $(\bar{x}, \bar{Z}, \bar{\alpha}, \bar{S})$ be any one of the cluster points, and subsequence $\{(x^{i_k}, Z^{i_k}, \alpha^{i_k}, S^{i_k})\} \to (\bar{x}, \bar{Z}, \bar{\alpha}, \bar{S})$. Taking $i_k \to \infty$ in (3.4) we find that $(\bar{x}, \bar{Z}, \bar{\alpha}, \bar{S})$ satisfies (3.1). □

3.2 *Update of penalty*

When solving the problem $\min_{(x,Z)\in G} \mathscr{L}(x, Z, P)$ we hope that the solution satisfies $Z = 0$. By putting $Z = 0$ in the first-order conditions (3.1) we obtain

$$\begin{aligned}
&Q_0 x + g_0 - \sum_{i=1}^{m} \alpha_i (Q_i x + g_i) = 0,\\
&x^{\mathrm{T}} Q_i x + 2 g_i^{\mathrm{T}} x + c_i = 0, \quad i = 1, \ldots, m_e,\\
&x^{\mathrm{T}} Q_i x + 2 g_i^{\mathrm{T}} x + c_i \geqslant 0, \quad i = m_e + 1, \ldots, m,\\
&\alpha_i \geqslant 0, \quad i = m_e + 1, \ldots, m,\\
&\alpha_i \left(x^{\mathrm{T}} Q_i x + 2 g_i^{\mathrm{T}} x + c_i\right) = 0, \quad i = m_e + 1, \ldots, m,\\
&\left(Q_0 + P - \sum_{i=1}^{m} \alpha_i Q_i\right) \succeq 0.
\end{aligned} \tag{3.8}$$

In fact, only the final equation of the above conditions contains P. This means that with any given feasible x and α, (3.8) can be satisfied if P is sufficiently large. We consider a simple example, that is,

$$\begin{aligned}
\min \quad & x^{\mathrm{T}} \begin{pmatrix} 6 & -3 \\ -3 & 1 \end{pmatrix}^{\mathrm{T}} x\\
\text{s.t.} \quad & x^{\mathrm{T}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} x - \begin{pmatrix} 1 & 0 \end{pmatrix} x = 0,\\
& x^{\mathrm{T}} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} x - \begin{pmatrix} 0 & 1 \end{pmatrix} x = 0.
\end{aligned}$$

There are four solutions satisfying the first five conditions of (3.8), which are

$$\begin{aligned}
x^{(1)} &= \begin{pmatrix} 0 & 0 \end{pmatrix}^{\mathrm{T}}, \ \alpha_1^{(1)} = 0, \quad \alpha_2^{(1)} = 0,\\
x^{(2)} &= \begin{pmatrix} 1 & 1 \end{pmatrix}^{\mathrm{T}}, \ \alpha_1^{(4)} = 6, \quad \alpha_2^{(4)} = -4,\\
x^{(3)} &= \begin{pmatrix} 0 & 1 \end{pmatrix}^{\mathrm{T}}, \ \alpha_1^{(3)} = 6, \quad \alpha_2^{(3)} = 2,\\
x^{(4)} &= \begin{pmatrix} 1 & 0 \end{pmatrix}^{\mathrm{T}}, \ \alpha_1^{(2)} = 12, \ \alpha_2^{(2)} = 6.
\end{aligned}$$

The global minimum is $x^{(1)}$. One may note that if $P = 0$, then none of the four solutions satisfy the last condition of (3.8). The last condition of (3.8) is satisfied only by the first solution $x^{(1)}$, $\alpha_1^{(1)}$ and $\alpha_2^{(1)}$ if $P = I$. If $P = 2I$ the last condition of (3.8) is satisfied by the first two solutions. If $P = 4I$ then the last condition of (3.8) is satisfied by the first three solutions. Moreover, if $P = 9I$ then all four solutions satisfy (3.8).

We thus can see that, if $P = 0$, there is no solution satisfying the KKT condition. On the other hand, if the initially selected P is too large (in the sense of $P \succ\succ 0$), Algorithm 3.1 might stop, with a high probability, at a solution that is not the global minimizer. Therefore, we propose to update P iteratively, rather than directly assigning a fixed and large P initially.

Notice that the penalty problem (2.6) is based on the Lagrangian function of problem (2.2) corresponding to $Z \preceq 0$, where P is its dual variable. The update of P can be obtained from the update criteria in the Lagrange relaxation method (Guignard, 2003).

We regard the optimal objective value of the penalty problem as a function of P:

$$z(P) := \min_{(x,Z)\in G} \mathscr{L}(x, Z, P). \tag{3.9}$$

Let (x^k, Z^k) be the optimal solution of $z(P^k)$. In fact, Z^k is the subgradient of $z(P)$ at P^k.

Hence, we can increase P^{k+1} along the Z^k direction, that is,

$$P^{k+1} = P^k + \mu Z^k. \tag{3.10}$$

We would like to achieve $\mathscr{L}(x^{k+1}, Z^{k+1}, P^{k+1}) = \min_{x\in F} f(x)$, though x^{k+1}, Z^{k+1} is unknown. Nevertheless, we may use x^k, Z^k as an approximation. By the formula of approximation

$$\mathscr{L}(x^k, Z^k, P^{k+1}) = \min_{x\in F} f(x),$$

we have

$$\mu = \left(\min_{x\in F} f(x) - \mathscr{L}(x^k, Z^k, P^k)\right) / \|Z^k\|_F^2.$$

Here, because $\min_{x\in F} f(x)$ is unknown, we thus use its upper bound in the computation. For example, we can generate a feasible solution $\bar{x}^k \in F$ from x^k and take the upper bound to be $f(\bar{x}^k)$. For simple constraints such as $x_i^2 = 1$, when $x_i^k \geqslant 0$, we let $\bar{x}_i^k = 1$, and when $x_i^k < 0$, we let $\bar{x}_i^k = -1$.

For more complicated constraints, if a feasible solution can not be generated from x^k, a good strategy is to add μZ^k with a constant μ as shown in (3.10) or a fixed scalar multiple of the identity δI to P each time.

In practice, adding μZ^k to P^k as in (3.10) usually offers better performance than adding a scalar multiple of the identity matrix. Moreover, the combination $\mu Z^k + \delta I$ is also a possible choice. We can design different choices of the scalar for different problems.

We now present the framework of the positive semidefinite penalty method (PSDP) in Algorithm 3.2.

Algorithm 3.2 PSDP

Step 0: let $P^0 = 0$.

Step 1: compute $(x^k, Z^k) = \underset{(x,Z)\in G}{\arg\min}\ \mathscr{L}(x, Z, P^k)$ by Algorithm 3.1.

Step 2: if the termination criteria are satisfied, stop. Otherwise, update P^{k+1} by (3.10), $k := k+1$, go to Step 1.

When performing Step 1 one can use (x^{k-1}, Z^{k-1}) as an initial point if $k \geqslant 1$. Notice that when $P^0 = 0$, $\min_{(x,Z)\in G} \mathscr{L}(x, Z, P^0)$ is SDR. Consequently, Algorithm 3.1 converges in one step from any initial point, which can be derived from KKT (3.4). Therefore, x^0 in PSDP is the solution of SDR.

We note that $Z^k = 0$ is one of the termination criteria, which means that Algorithm 3.2 finds a feasible solution and does not find a better solution in the subsequent penalty updates. Another criterion is $\mathscr{L}(x^k, Z^k, P^k) - \min_{x\in F} f(x) > 0$ because it implies that Algorithm 3.1 obtains a bad solution due to Lemma 2.2, and there is no need to implement more updates. In practice, $\min_{x\in F} f(x)$ can be approximated via generated $\{x^k\}$. The maximum number of penalty updates can also be a criterion as efficiency of the algorithm is very much affected by the number of updates taken. These termination criteria are used in our numerical tests. Interestingly, we can see that the number of updates required for a good solution is often small so that the added computational cost can be under control.

4. Numerical tests

In this section we report numerical results to demonstrate the performance of our proposed Algorithm 3.2 PSDP in terms of our proposed algorithm PSDP in terms of the quality of solutions. We solve two kinds of problems, which are binary quadratic programming and binary quadratic equations. In these tests PSDP is compared with the classic SDR.

4.1 *Binary quadratic programming*

We consider a binary quadratic programming given by

$$\begin{aligned} \min_{x\in\mathbb{R}^n}\ & x^{\mathrm{T}}Qx + 2g^{\mathrm{T}}x \\ \text{s.t.}\ & x_i^2 - x_i = 0, \quad i = 1, \ldots, n. \end{aligned}$$

The constraint $x_i^2 - x_i = 0$ implies $x_i \in \{0, 1\}$. The problem is known to be NP-hard (Garey & Johnson, 1979). It has many applications such as capital budgeting and financial analysis problems (Laughunn, 1970; McBride & Yormark, 1980), CAD problems (Krarup & Pruzan, 1978), traffic message management problems (Gallo *et al.*, 1980), machine scheduling (Alidaee *et al.*, 1994) and molecular conformation (Phillips & Rosen, 1994).

In our test Q is a random real symmetric matrix. All the entries of Q are independent identically distributed with expectation 0 and variance 1. For any x^k generated in Algorithm 3.2 we obtain the feasible solution by a binary thresholding (rounding off to 0 or 1); that is to say that we set

$$\bar{x}_i^k = \begin{cases} 1 & \text{if } x_i^k \geqslant 0.5, \\ 0 & \text{if } x_i^k < 0.5. \end{cases} \tag{4.1}$$

The operation given in (4.1) of getting $\bar{x}^k$ from x^k is referred to as the feasibilization or rounding off. Let

$$f_{\min}^k = \min_{i \leqslant k}\{f(\bar{x}^i)\}.$$

Then we update P by

$$P^{k+1} = P^k + \min\left\{\frac{f_{\min}^k - \mathscr{L}(x^k, Z^k, P^k)}{\|Z^k\|_F^2}, \frac{1}{\|Z^k\|_F}\right\} Z^k.$$

We set up $\mathscr{L}(x^k, Z^k, P^k) - f_{\min}^k > 0$ and $x^k \in F$ as the termination criteria. By Lemma 2.2 the global solution $(x_\star^k, Z_\star^k)$ satisfies $\mathscr{L}(x_\star^k, Z_\star^k, P^k) - f_{\min}^k \leqslant 0$, thus the first criterion means that the current penalty problem is badly solved, and the second implies that $(x^k, 0)$ is also the solution when $P = P^{k+1}$. If any one of them happens the algorithm stops.

We first consider a 10-dimensional example, whose g equals 0 and Q equals

$$\begin{pmatrix}
-0.9651 & 1.5216 & 3.7664 & 1.9520 & -2.0755 & -2.3319 & 2.2988 & 2.5061 & 1.9154 & 0.0699 \\
1.5216 & -0.6166 & -2.2228 & 0.6558 & 0.3684 & -1.8922 & 0.2258 & 0.6925 & 0.2724 & 1.1700 \\
3.7664 & -2.2228 & 5.3272 & 0.6296 & 2.3014 & -2.5600 & 0.9490 & -0.5105 & 1.1118 & 1.3399 \\
1.9520 & 0.6558 & 0.6296 & -3.6934 & -0.7679 & -0.5153 & 0.7695 & 1.1351 & -0.2931 & 0.6919 \\
-2.0755 & 0.3684 & 2.3014 & -0.7679 & 2.3713 & 1.0242 & 0.5173 & -2.2794 & 0.3133 & 1.2249 \\
-2.3319 & -1.8922 & -2.5600 & -0.5153 & 1.0242 & -2.0113 & 1.7500 & 1.2132 & -1.1134 & -0.9645 \\
2.2988 & 0.2258 & 0.9490 & 0.7695 & 0.5173 & 1.7500 & 0.2394 & 0.8993 & 0.0229 & -0.4947 \\
2.5061 & 0.6925 & -0.5105 & 1.1351 & -2.2794 & 1.2132 & 0.8993 & -1.4934 & 0.1274 & -1.9524 \\
1.9154 & 0.2724 & 1.1118 & -0.2931 & 0.3133 & -1.1134 & 0.0229 & 0.1274 & 4.8513 & 1.4164 \\
0.0699 & 1.1700 & 1.3399 & 0.6919 & 1.2249 & -0.9645 & -0.4947 & -1.9524 & 1.4164 & -1.3388
\end{pmatrix}.$$

The optimal solution $x^\star$ is

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}^{\mathrm{T}}.$$

The solution of SDR is given below, with only four decimal places shown to save space, by

$$\begin{pmatrix} 0.2504 & 0.7005 & 0.3709 & 0.7968 & 0.1731 & 0.9559 & 0.0002 & 0.2462 & 0.0474 & 0.4757 \end{pmatrix}^{\mathrm{T}}.$$

With the feasibilization given by (4.1) the above is transformed into

$$\begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}^{\mathrm{T}},$$

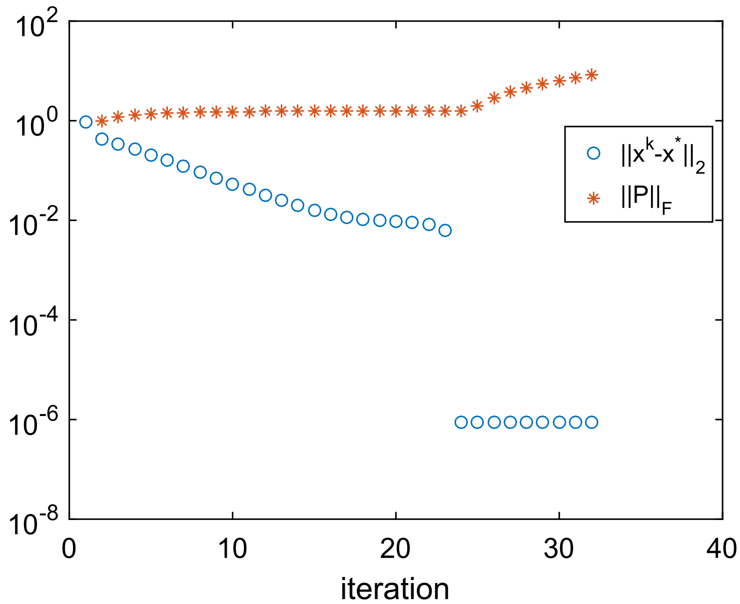

FIG. 1. Convergence of a BQP instance.

which is not the global solution. In PSDP the solution of SDR corresponds to the first solution when $P^0 = 0$. Then we update P^1 and obtain $x^1 =$

$$\begin{pmatrix} 0.1065 & 0.9441 & 0.6733 & 0.9696 & 0.0552 & 0.9945 & 0.0008 & 0.0299 & 0.0005 & 0.0056 \end{pmatrix}^{\mathrm{T}},$$

which is again shown with only four decimal places. With feasibilization, the round-off solution $\bar{x}^1$ is

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}^{\mathrm{T}},$$

which is the optimal solution $x^\star$. When we focus only on the sequence $\{x^k\}$ but not the solutions obtained by feasibilization (i.e. rounding off via (4.1)), we find that in the subsequent iterations, the difference between x^k and $x^\star$ drops gradually, then jumps to 1e$-$6 at the 24th iteration and remains almost unchanged for the rest of the iterations as shown in Fig. 1. The error tolerance 1e$-$6 is also used here to measure the accuracy of solving SDP subproblems. We regard x^k as a feasible solution if $\|x^k - \bar{x}^k\| \leqslant$ 1e$-$6. Moreover, the jump in $\|x^k - \bar{x}^k\|$ gives an indication of the exact penalty.

This example illustrates that, rather than directly rounding off an SDR solution, our Algorithm 3.2 can offer a more systematic and effective way to make the solution feasible and get closer to a global solution.

As additional examples we choose three different n ($n = 10, 15, 20$) and generate 50 random examples for each n. For these 150 examples, Fig. 2 reports the numbers of examples in which PSDP gets terminated within a suitable number of penalty updates. From Fig. 2 we see that PSDP satisfies the stopping criteria within 51 updates of the penalty parameter for all the examples. In fact, the number of penalty updates in PSDP can be further reduced if feasibilization is adopted. As shown in the example stated earlier, the number of penalty updates is 24, but just 1 update is enough for us to obtain the global solution when we consider rounding off the solutions via (4.1).

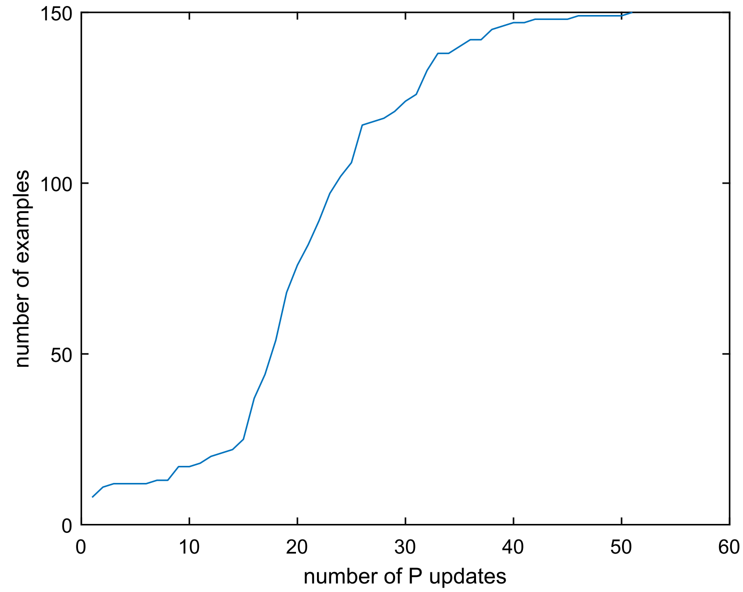

FIG. 2. Number of penalty updates of PSDP for BQP.

TABLE 1 *BQP: PSDP vs. SDR*

n	$f = f^{OPT}$			$f > f^{OPT}$		
	$f < f^{SDR}$	$f = f^{SDR}$	Total	$f < f^{SDR}$	$f = f^{SDR}$	Total
10	12	32	44	2	4	6
15	19	26	45	2	3	5
20	24	18	42	6	2	8

The comparison between PSDP and SDP in the tests is shown in Table 1. Here we consider only the objective values of their solutions due to rounding off, where f represents the objective value of the solution generated by PSDP, f^{SDR} represents the objective value of the solution generated by SDR and f^{OPT} represents the optimal objective value. Since we use their solutions obtained by rounding off we have $f^{OPT} \leqslant f^{SDR}$ and $f^{OPT} \leqslant f$. Moreover, SDR is the first step in PSDP; thus, we always have $f \leqslant f^{SDR}$. In this table we list the numbers of examples associated with the different cases. For instance, when $n = 20$, of all the 50 examples, SDR gets 18 optimal solutions, while PSDP solves 42, which is 24 more than SDR. For the remaining 8 examples that PSDP is not able to globally solve, PSDP improves in 6 of these examples on the basis of SDR and retains the same solutions as SDR in the other 2 cases. We see from the Table 1 that, with the gradual increase of n, PSDP maintains the ability to find global solutions.

In QPLIB (Furini *et al.*, 2019) we find a total of 23 BQP instances. For each of the instances, we show the first 11 rounding-off solutions of PSDP in Table 2. The first solution of PSDP is the same as SDR, and the other 10 are from 10 penalty updates. In the table, instance numbers are the same as those in QPLIB. ‘Vars’ is the number of variables and ‘Opt’ stands for the optimal objective value. The last 11 columns are the objective values of the solutions after rounding off. Since the 23 instances are all maximization problems, the larger the objective value that one gets, the better the solution is.

Table 2 shows that PSDP can improve the SDR solution with only one or two penalty updates. Moreover, with only a few updates, the quality of the solution can be greatly improved, and even optimal solution can be achieved. Therefore, it can be claimed that the number of P updates can be set to a small number to reduce the calculation cost, yet a good solution can still be obtained.

4.2 *Binary quadratic equations*

We consider the following equations:

$$\begin{aligned} &x^{\mathrm{T}} Q_i x + c_i = 0, \quad i = 1, \ldots, m, \\ &x_i^2 - x_i = 0, \qquad\; i = 1, \ldots, n. \end{aligned} \tag{4.2}$$

Similar to BQP this is also a problem of binary variables. It does not have an objective function but with more general quadratic constraints. Again, it is NP-hard to find feasible solutions (Chermakani, 2012).

The binary quadratic equation (BQE) problem has applications, for example, in the unassigned distance geometry problem. Determining the atomic positions in a nano-structure is one of the great challenges in material science and engineering (Gu *et al.*, 2019; Billinge & Levin, 2007). Unlike the assigned distance geometry problem (1.3), the assignment of each distance is not given, such as in the atomic pair distribution function data (Warren, 1969; Egami & Billinge, 2012). Here, we are concerned with a two-dimensional periodic structure reconstruction problem. Suppose that the whole structure is generated by repeating a unit cell which is a rectangle with a given size. Moreover, in the unit cell, all the atoms appear at its integral lattice points. The defects of materials will make minor changes to regular patterns, such as the disappearance of existing atoms or the production of new atoms. Our goal is to determine the existence of an atom on each integer lattice point in the unit cell based on a given distance list. Since distance is invariant under orthogonal transformation, this problem has infinitely many solutions. Here we aim to find one of the solutions.

We take an example of a unit cell with size 3 by 3. We label the positions in this cell from 1 to 9 as

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}.$$

The corresponding distance matrix D is

$$\begin{pmatrix}
3 & 1 & 1 & 1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} \\
1 & 3 & 1 & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} \\
1 & 1 & 3 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 \\
1 & \sqrt{2} & \sqrt{2} & 3 & 1 & 1 & 1 & \sqrt{2} & \sqrt{2} \\
\sqrt{2} & 1 & \sqrt{2} & 1 & 3 & 1 & \sqrt{2} & 1 & \sqrt{2} \\
\sqrt{2} & \sqrt{2} & 1 & 1 & 1 & 3 & \sqrt{2} & \sqrt{2} & 1 \\
1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 3 & 1 & 1 \\
\sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & 1 & 3 & 1 \\
\sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 & 1 & 1 & 3
\end{pmatrix},$$

where D_{ij} represents the distance between the two atoms at the ith and jth positions with consideration of periodicity. Based on the elements of D we decompose $D = A_1 + \sqrt{2}A_2 + 3A_3$, where every element of A_1, A_2, A_3 is either 0 or 1. Actually, what we observe are the total numbers of their different distances.

TABLE 2 *BQP tests on QPLIB*

Instance	Vars	Opt	SDR	1 P-up	2 P-up	3 P-up	4 P-up	5 P-up	6 P-up	7 P-up	8 P-up	9 P-up	10 P-up
3506	496	478	426	456	474	468	472	472	**476**	476	476	472	472
3565	276	282	258	268	**278**	278	278	278	278	278	272	276	276
3642	1035	1034	944	990	990	998	1000	**1016**	1000	1010	1012	1012	1016
3650	946	920	874	874	892	910	908	908	912	902	**914**	908	914
3693	1128	1148	1056	1106	1104	1114	1126	1114	1130	1128	**1132**	1130	1132
3705	378	384	346	368	380	372	380	380	378	382	380	382	**384**
3706	703	682	642	644	650	650	660	662	672	672	668	**676**	676
3738	435	422	402	408	406	406	406	**414**	410	414	414	412	412
3745	325	334	316	318	328	328	328	324	326	328	328	330	**332**
3822	861	850	798	802	824	822	822	838	**840**	838	838	834	836
3832	561	554	516	524	528	534	536	540	**544**	536	542	538	542
3838	780	746	682	700	704	708	714	714	**724**	724	724	722	722
3850	1225	1190	1110	1122	1130	1146	1160	1156	1158	1164	**1172**	1172	1166
3852	231	234	214	216	232	228	232	232	**234**	234	232	232	234
3877	630	602	558	582	594	590	590	590	590	594	592	594	**596**
5721	300	8571649	8491060	8411149	8510079	8481170	8384463	**8557031**	8494488	8530403	8496614	8551192	8510385
5725	343	33611981	29882851	32242648	32313010	32803550	32314568	32651972	32861107	31794370	**33156417**	32638390	32857871
5755	400	24838942	22086190	22179058	24163311	23956592	23954551	23917143	24079231	23920544	23906267	**24390145**	24253858
5875	200	43757	42444	42752	42920	42670	43229	42619	43272	43403	**43561**	43311	43499
5881	120	13067	12611	12799	12661	12861	12811	12978	**13017**	13001	13017	13017	12945
5882	150	25388	24631	24665	24640	24982	25022	25075	25102	**25356**	24967	25343	25299
5909	250	35726	33624	34252	34568	34702	34382	34597	35354	34816	**35560**	35524	34844
5922	500	128339	125874	126433	126485	126793	126753	127303	**127379**	126514	126911	127156	127320

If a distance exists, the atoms at both of its two ends must exist. Using this fact we regard x as a 0–1 vector, so the equations can be written as

$$\begin{aligned} x^{\mathrm{T}}A_1x &= b_1, \\ x^{\mathrm{T}}A_2x &= b_2, \\ x^{\mathrm{T}}A_3x &= b_3, \\ x_i^2 - x_i &= 0, \quad i = 1, \ldots, 9. \end{aligned} \tag{4.3}$$

Due to the equality of all positions we can assume that $x_1 = 1$ when there exists at least one distance. This reduces the number of variables.

We consider the unit cell

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

This leads to $b_1 = 16$, $b_2 = 14$, $b_3 = 6$ in (4.3). Since there is no prescribed objective function in this problem we take the minimization of $x^T Ex$ as the objective in SDR, where E is a matrix of all 1s. The solution of SDR is

$$\begin{pmatrix} 1.0000 & 0.6271 & 0.6271 & 0.6271 & 0.6229 & 0.6229 & 0.6271 & 0.6229 & 0.6229 \end{pmatrix}^{\mathrm{T}}.$$

One may do the rounding off to get

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}^{\mathrm{T}},$$

which is not the solution of (4.3). In our Algorithm 3.2 we update P by

$$P^{k+1} = P^k + Z^k.$$

Then we have $x^1 =$

$$\begin{pmatrix} 1.00 & 1.00 & 1.00 & 1.00 & 0.25 & 0.25 & 1.00 & 0.25 & 0.25 \end{pmatrix}^{\mathrm{T}}$$

and $x^2 =$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}^{\mathrm{T}},$$

where x^2 is the solution of (4.3).

We have tested more problems of sizes 3 by 3, 4 by 4 and 5 by 5. In the 4 by 4 case, besides 0–1 constraints, there are 6 quadratic equations. The same is true also in the 5 by 5 case. In Table 3 we use 'tolnum' to represent the total number of runs, 'PSDP' the number of cases solved by PSDP and 'SDR' the number of cases solved by SDR. We can see that SDR is not able to solve this kind of BQE problem in general. PSDP can solve all 3 by 3 problems within 3 penalty updates and 4 by 4 problems within 7 penalty updates. For 5 by 5 examples it can solve 12056 cases within 201 penalty updates. The ratio of success is 94%. Figure 3 reports the numbers of examples that PSDP can successfully solve within a prescribed number of penalty updates. It shows that PSDP can solve 10897 examples within 40 penalty updates, which represents 85% of all examples.

TABLE 3 *BQE: PSDP vs. SDR*

Size	tolnum	PSDP	SDR
3 by 3	11	11	2
4 by 4	306	306	1
5 by 5	12807	12056	3

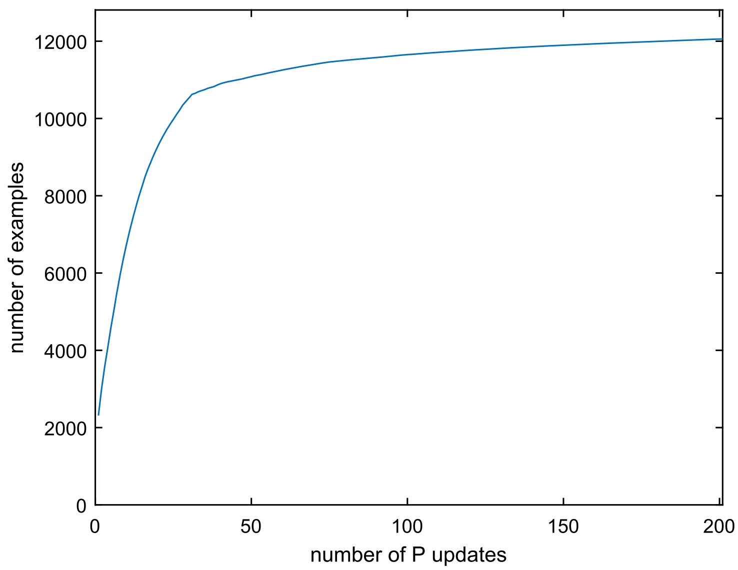

FIG. 3. Number of penalty updates of PSDP for BQE with size of 5 by 5.

5. Conclusions

In this paper we considered the problem of solving QCQP. We proposed a penalty formulation for QCQP. We studied theoretical exactness of the proposed penalty problem and its equivalence to QCQP. For this penalty formulation, we proposed a proximal point algorithm and combined it with a Lagrangian relaxation-type penalty update. Our numerical test contained two kinds of QCQP, such as BQP and BQE, both of which are popular examples. It showed the effectiveness of the proposed PSDP algorithm in finding global solutions.

We also viewed the SDR from a different angle, which is that SDR can be regarded as a penalty function method with the penalty term being zero. Therefore, our penalty function method provides a way to improve infeasible solutions from SDR. As we can see from our numerical tests, after several penalty updates, PSDP can obtain a global solution. Moreover, one can sometimes get a better solution than SDR through only one update.

Meanwhile, let us note that algorithms for solving the penalty problem deserve further investigation. Due to the difficulty of solving a nonconvex SDP, the computational cost of our algorithm is still high. It is thus desirable to develop robust and efficient algorithms for the penalty problem. Incorporating penalty updates into the inner iteration may also be interesting to explore as well.

Acknowledgements

This manuscript is largely based on Chapter 4 of the Ph.D. Thesis (Gu, 2017) of the first author.

Funding

Chinese Academy of Sciences (to R.G.); National Science Foundation (DMR 1534910 and CCF-1704833); National Natural Science Foundation of China (11331012 and 11688101 to Y.X.Y.).

References

ABADIE, J. (1966) On the Kuhn–Tucker theorem. *Technical Report*. Berkeley: Operations Research Center, University of California.

AI, W. & ZHANG, S. (2009) Strong duality for the CDT subproblem: a necessary and sufficient condition. *SIAM J. Optim.*, **19**, 1735–1756.

ALIDAEE, B., KOCHENBERGER, G. A. & AHMADIAN, A. (1994) 0-1 quadratic programming approach for optimum solutions of two scheduling problems. *Internat. J. Systems Sci.*, **25**, 401–408.

ANSTREICHER, K. M. (2009) Semidefinite programming versus the reformulation-linearization technique for nonconvex quadratically constrained quadratic programming. *J. Global Optim.*, **43**, 471–484.

AUCHMUTY, G. (1989) Duality algorithms for nonconvex variational principles. *Numer. Funct. Anal. Optim.*, **10**, 211–264.

BAO, X., SAHINIDIS, N. V. & TAWARMALANI, M. (2011) Semidefinite relaxations for quadratically constrained quadratic programming: a review and comparisons. *Math. Program.*, **129**, 129.

BAR-ON, J. & GRASSE, K. (1994) Global optimization of a quadratic functional with quadratic equality constraints. *J. Optim. Theory Appl.*, **82**, 379–386.

BECK, A., BEN-TAL, A. & TETRUASHVILI, L. (2010) A sequential parametric convex approximation method with applications to nonconvex truss topology design problems. *J. Global Optim.*, **47**, 29–51.

BECK, A. & ELDAR, Y. C. (2006) Strong duality in nonconvex quadratic optimization with two quadratic constraints. *SIAM J. Optim.*, **17**, 844–860.

BEN-TAL, A. & TEBOULLE, M. (1996) Hidden convexity in some nonconvex quadratically constrained quadratic programming. *Math. Programming*, **72**, 51–63.

BILLINGE, S. J. & LEVIN, I. (2007) The problem with determining atomic structure at the nanoscale. *Science*, **316**, 561–565.

CARTIS, C., FOWKES, J. M. & GOULD, N. I. (2015) Branching and bounding improvements for global optimization algorithms with Lipschitz continuity properties. *J. Global Optim.*, **61**, 429–457.

CHERMAKANI, D. P. (2012) NP-completeness of deciding the feasibility of linear equations over binary-variables with coefficients and constants that are 0, 1, or –1 (in press). arXiv:1210.4120.

DINH, T. P. & LE THI, H. (1998) A branch and bound method via DC optimization algorithms and ellipsoidal technique for box constrained nonconvex quadratic problems. *J. Global Optim.*, **13**, 171–206.

DINH, T. P. & SOUAD, E. B. (1986) Algorithms for solving a class of nonconvex optimization problems. Methods of subgradients. *Fermat Days 85: Mathematics for Optimization*. North-Holland Mathematics Studies, vol. 129. Amsterdam, Netherlands: Elsevier, pp. 249–271.

EGAMI, T. & BILLINGE, S. J. (2012) *Underneath the Bragg Peaks: Structural Analysis of Complex Materials*, London: Pergamon Materials Series, vol. 16. Newnes.

FERNÁNDEZ CARA, E. & MORENO, C. (1988) Critical point approximation through exact regularization. *Math. Comp.*, **50**, 139–153.

FUJIE, T. & KOJIMA, M. (1997) Semidefinite programming relaxation for nonconvex quadratic programs. *J. Global Optim.*, **10**, 367–380.

FURINI, F., TRAVERSI, E., BELOTTI, P., FRANGIONI, A., GLEIXNER, A., GOULD, N., LIBERTI, L., LODI, A., MISENER, R., MITTELMANN, H., SAHINIDIS, N. V., VIGERSKE, S. & WIEGELE, A. (2019) QPLIB: a library of quadratic programming instances. *Math. Program. Comput.*, **11**, 237–265.

Gallo, G., Hammer, P. L. & Simeone, B. New York: (1980) Quadratic knapsack problems. *Combinatorial Optimization*. Springer, pp. 132–149.

Garey, M. R. & Johnson, D. S. (1979) *Computers and Intractability: A Guide to NP-Completeness*. San Francisco: WH Freeman.

Gu, R. (2017) Research on theory and algorithm of some optimization problems. *Ph.D. Thesis*, Academy of Mathematics and Systems Science, Chinese Academy of Sciences.

Gu, R., Banerjee, S., Du, Q. & Billinge, S. J. L. (2019) Algorithm for distance list extraction from pair distribution functions. *Acta Crystallogr. A*, **75**, 658–668.

Guignard, M. (2003) Lagrangean relaxation. *Top*, **11**, 151–200.

Hiriart-Urruty, J.-B. (1985) Generalized differentiability/duality and optimization for problems dealing with differences of convex functions. *Convexity and Duality in Optimization*. New York: Springer, pp. 37–70.

Hiriart-Urruty, J.-B. (1989) From convex optimization to nonconvex optimization. Necessary and sufficient conditions for global optimality. *Nonsmooth Optimization and Related Topics*. New York: Springer, pp. 219–239.

Hoffman, A. J. (2003) On approximate solutions of systems of linear inequalities. *Selected Papers of Alan J Hoffman: With Commentary*. Singapore: World Scientific, pp. 174–176.

Krarup, J. & Pruzan, P. M. (1978) Computer-aided layout design. *Mathematical Programming in Use*. New York: Springer, pp. 75–94.

Lasserre, J. B. (2001) Global optimization with polynomials and the problem of moments. *SIAM J. Optim.*, **11**, 796–817.

Laughunn, D. (1970) Quadratic binary programming. *Oper. Res.*, **14**, 454–461.

Le Thi, H. A. & Dinh, T. P. (2018) DC programming and DCA: thirty years of developments. *Math. Program.*, **169**, 1–64.

Lu, C., Fang, S.-C., Jin, Q., Wang, Z. & Xing, W. (2011) KKT solution and conic relaxation for solving quadratically constrained quadratic programming problems. *SIAM J. Optim.*, **21**, 1475–1490.

Luo, Z.-Q., Ma, W.-K., So, A. M.-C., Ye, Y. & Zhang, S. (2010) Semidefinite relaxation of quadratic optimization problems. *IEEE Signal Process. Mag.*, **27**, 20–34.

Ma, W.-K., Davidson, T. N., Wong, K. M., Luo, Z.-Q. & Ching, P.-C. (2002) Quasi-maximum-likelihood multiuser detection using semi-definite relaxation with application to synchronous CDMA. *IEEE Trans. Signal Process.*, **50**, 912–922.

McBride, R. & Yormark, J. (1980) An implicit enumeration algorithm for quadratic integer programming. *Manage. Sci.*, **26**, 282–296.

Parikh, N. & Boyd, S. (2014) Proximal algorithms. *Found. Trends Optim.*, **1**, 127–239.

Peng, J.-M. & Yuan, Y.-X. (1997) Optimality conditions for the minimization of a quadratic with two quadratic constraints. *SIAM J. Optim.*, **7**, 579–594.

Peterson, D. W. (1973) A review of constraint qualifications in finite-dimensional spaces. *SIAM Rev.*, **15**, 639–654.

Phillips, A. T. & Rosen, J. B. (1994) A quadratic assignment formulation of the molecular conformation problem. *J. Global Optim.*, **4**, 229–241.

Raber, U. (1998) A simplicial branch-and-bound method for solving nonconvex all-quadratic programs. *J. Global Optim.*, **13**, 417–432.

Rockafellar, R. T. (1976) Monotone operators and the proximal point algorithm. *SIAM J. Control Optim.*, **14**, 877–898.

Rockafellar, R. T. (2015) *Convex Analysis*. Princeton, New Jersey: Princeton University Press.

Saxe, J. B. (1979) Embeddability of weighted graphs in k-space is strongly np-hard. *Proceedings of 17th Allerton Conference in Communications, Control and Computing, Monticello, IL*, pp. 480–489.

Sherali, H. D. (2007) RLT: a unified approach for discrete and continuous nonconvex optimization. *Ann. Oper. Res.*, **149**, 185–193.

Steingrimsson, B., Luo, Z.-Q. & Wong, K. M. (2003) Soft quasi-maximum-likelihood detection for multiple-antenna wireless channels. *IEEE Trans. Signal Process.*, **51**, 2710–2719.

Sun, W., Sampaio, R. J. & Candido, M. (2003) Proximal point algorithm for minimization of DC function. *J. Comput. Math.*, **21**, 451–462.

Sun, W. & Yuan, Y.-X. (2006) *Optimization Theory and Methods: Nonlinear Programming*. New York: Springer.
Toh, K.-C., Todd, M. J. & Tütüncü, R. (2009) *SDPT3 Version 4.0 (Beta)—A Matlab Software for Semidefinite-Quadratic-Linear Programming* [online]. Available at https://blog.nus.edu.sg/mattohkc/softwares/sdpt3/.
Vavasis, S. A. (1990) Quadratic programming is in NP. *Inform. Process. Lett.*, **36**, 73–77.
Wang, S. & Xia, Y. (2015) Uniform quadratic optimization and extensions (in press). arXiv:1508.01000.
Warren, B. E. (1969) *X-Ray Diffraction*. Mineola, New York: Courier Corporation.
Wu, Z.-Y., Li, D., Zhang, L.-S. & Yang, X. (2007) Peeling off a nonconvex cover of an actual convex problem: hidden convexity. *SIAM J. Optim.*, **18**, 507–536.
Yang, L., Sun, D. & Toh, K. (2015) SDPNAL+: a majorized semismooth Newton-CG augmented Lagrangian method for semidefinite programming with nonnegative constraints. *Math. Prog. Comp.*, **7**, 331–366.
Ye, Y. & Zhang, S. (2003) New results on quadratic minimization. *SIAM J. Optim.*, **14**, 245–267.