

A projection algorithm based on KKT conditions for convex quadratic semidefinite programming with nonnegative constraints

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Abstract The dual form of convex quadratic semidefinite programming (CQSDP) problem, with nonnegative constraints, is a 4-block separable convex optimization problem. It is known that, the directly extended 4-block alternating direction method of multipliers (ADMM4d) is very efficient to solve the dual, but its convergence is not guaranteed. In this paper, we reformulate the dual as a 3-block convex programming by introducing an extra variable, so as to design a parallel modified 3-block ADMM with larger step size that can exceed the conventional upper bound of $(1 + \sqrt{5})/2$. We show that the proposed 3-block ADMM is equivalent to a projection algorithm with two operators projecting onto the positive semidefinite and nonnegative matrix cones respectively. The global convergence and non-ergodic convergence rate $o(1/(k + 1))$ are established by using a fixed-point argument and the non-expansion property of the projection operators. Numerical experiments on the various classes of CQSDP problems illustrate that our proposed algorithm performs better than ADMM4d with the aggressive step size of 1.618.

Keywords Quadratic semidefinite programming · Nonnegative constraints · Alternating direction method of multipliers · Projection · Convergence analysis

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1 Introduction

We consider the following convex quadratic semidefinite programming (CQSDP) with nonnegative constraints on the matrix variable:

$$\begin{aligned} \min \quad & \frac{1}{2} \langle X, \varphi(X) \rangle + \langle C, X \rangle \\ \text{s.t.} \quad & \mathcal{A}(X) = b, \\ & X \in \mathcal{S}_+^n, \quad X \in \mathcal{N}^n, \end{aligned} \tag{1}$$

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where \mathcal{S}_+^n denotes the symmetric and positive semi-definite matrices cone in the space of $n \times n$ symmetric matrices \mathcal{S}^n , endowed with the standard trace inner product $\langle \cdot, \cdot \rangle$ and its induced norm $\|\cdot\|$. $C \in \mathcal{S}^n$, $b \in \mathbb{R}^m$ are given data. \mathcal{N}^n is a closed convex set and

$$\mathcal{N}^n = \{X \in \mathcal{S}^n \mid X \geq 0\}.$$

The operator $\mathcal{A} : \mathcal{S}^n \rightarrow \mathbb{R}^m$ is linear, and its adjoint with respect to the standard inner product in \mathcal{S}^n and \mathbb{R}^m is denoted by \mathcal{A}^* . $\varphi : \mathcal{S}^n \rightarrow \mathcal{S}^n$ is a given self-adjoint positive semidefinite linear operator, for instance, $\varphi(X) = BXB^T$ for a given positive-definite matrix $B \in \mathcal{S}^n$, $\varphi(X) = B \circ X$ for $B \in \mathcal{N}^n$ (“ \circ ” denotes the Hardamard product of two matrices and $\varphi(X) = \frac{BX+XB}{2}$ for $B \in \mathcal{S}_+^n$).

Let $\mathcal{D}^n = \mathcal{S}_+^n \cap \mathcal{N}^n$, named as the doubly nonnegative cone in [1], its dual cone is $\mathcal{S}_+^n + \mathcal{N}^n$. Thus the dual of problem (1) can be formulated as in [2,3]:

$$\begin{aligned} \min \quad & \frac{1}{2} \langle W, \varphi(W) \rangle - b^T y \\ \text{s.t.} \quad & -\varphi(W) + \mathcal{A}^*(y) + Z + S = C, \\ & W \in \mathcal{S}^n, y \in \mathbb{R}^m, Z \in \mathcal{S}_+^n, S \in \mathcal{N}^n. \end{aligned} \quad (2)$$

And the Karush-Kuhn-Tuck (KKT) conditions for problem (1) and its dual (2) can be written as follows:

$$\left. \begin{aligned} \mathcal{A}(X) = b, \quad \varphi(W) = \varphi(X), \\ -\varphi(W) + \mathcal{A}^*(y) + Z + S = C, \\ X \in \mathcal{S}_+^n, Z \in \mathcal{S}_+^n, \langle X, Z \rangle = 0, \\ X \in \mathcal{N}^n, S \in \mathcal{N}^n, \langle X, S \rangle = 0. \end{aligned} \right\} \quad (3)$$

By interior-point methods scheme, Toh et al. [4,5,6] proposed inexact primal-dual path following algorithm for solving the CQSDP problems without nonnegative constraints. To handle the CQSDP problems beyond moderate scale can be a challenging task using the interior-point methods, due to the extremely high computational cost per iteration or the inherent ill-conditioning of the linear systems governing the search directions. In addition, there are many methods proposed for solving some special CQSDP problems, see [8,9,10,11,12,13]. Of these methods, ADMM-type algorithms by dealing with the dual reveal excellent numerical results.

Due to the constraints on the doubly nonnegative cone, it is difficult to solve the primal problem (1) directly. In this paper, we pay attention to the dual (2) for its separable structure, which can be expressed in the form of the following convex optimization with four separate blocks in the objective function and a coupling linear equation constraint:

$$\begin{aligned} \min \quad & \frac{1}{2} \langle W, \varphi(W) \rangle - b^T y + \delta_{\mathcal{S}_+^n}(Z) + \delta_{\mathcal{N}^n}(S) \\ \text{s.t.} \quad & -\varphi(W) + \mathcal{A}^*(y) + Z + S = C, \end{aligned} \quad (4)$$

where $\delta_{\mathcal{C}}(Y)$ is the indicator function over a given set \mathcal{C} such that $\delta_{\mathcal{C}}(Y) = 0$ if $Y \in \mathcal{C}$ and $+\infty$ otherwise.

Let $\sigma > 0$ be given. The augmented Lagrangian function for (4) reads as

$$\begin{aligned} \mathcal{L}_\sigma(W, y, Z, S, X) = & \frac{1}{2} \langle W, \varphi(W) \rangle - b^T y + \delta_{\mathcal{S}_+^n}(Z) + \delta_{\mathcal{N}^n}(S) \\ & + \langle X, -\varphi(W) + \mathcal{A}^*(y) + Z + S - C \rangle \\ & + \frac{\sigma}{2} \| -\varphi(W) + \mathcal{A}^*(y) + Z + S - C \|^2, \end{aligned} \quad (5)$$

where $(W, y, Z, S, X) \in \mathcal{S}^n \times \mathbb{R}^n \times \mathcal{S}_+^n \times \mathcal{N}^n \times \mathcal{S}^n$. For a chosen initial point, the directly extended 4-block ADMM (ADMM4d) for (4) consists of the iterations:

$$\left. \begin{aligned} W^{k+1} &= \arg \min_{W \in \mathcal{S}^n} \mathcal{L}_\sigma(W, y^k, Z^k, S^k, X^k), \\ y^{k+1} &= \arg \min_{y \in \mathbb{R}^n} \mathcal{L}_\sigma(W^{k+1}, y, Z^k, S^k, X^k), \\ Z^{k+1} &= \arg \min_{Z \in \mathcal{S}_+^n} \mathcal{L}_\sigma(W^{k+1}, y^{k+1}, Z, S^k, X^k), \\ S^{k+1} &= \arg \min_{S \in \mathcal{N}^n} \mathcal{L}_\sigma(W^{k+1}, y^{k+1}, Z^{k+1}, S, X^k), \\ X^{k+1} &= X^k + \tau \sigma(-\varphi(W^{k+1}) + \mathcal{A}^*(y^{k+1}) + Z^{k+1} + S^{k+1} - C), \end{aligned} \right\} \quad (6)$$

where $\tau > 0$, e.g., $\tau \in (0, \frac{1+\sqrt{5}}{2})$, is a constant that controls the step size in (6). If choosing $\tau > 1$, the step size of updating the Lagrange multiplier is enlarged, and it is usually beneficial to induce faster convergence.

The direct extension of the classic ADMM to the case of the multi-block convex optimization problem is not necessarily convergent from [15, 16], though it often performs very well in practice. With σ being small enough, the convergence of ADMM4d was obtained in [17] for a special 4-block problem with two objective functions being strongly convex. Furthermore, it is shown that, the convergence can not be guaranteed only requiring one strongly convex function, by giving a concrete example in [17]. Thus, even for the simplest case with $\varphi(W) = W$ (the objective function $\frac{1}{2}\langle W, W \rangle$ is strongly convex), ADMM4d (6) is not necessarily convergent to solve problem (4).

Generally, there exists two types of methods to develop ADMM's variants, aiming to guarantee convergence and preserve the numerical advantages of the directly extended ADMM. One method is to add a simple correction step, for example, a convergent alternating direction method with a Gaussian back substitution (ADM-G) proposed by He et al. in [18, 19], in which each iteration consists of a forward procedure (ADM procedure) and a backward procedure (Gaussian back substitution procedure), the correction step is completely free from step-size computing and its step size is bounded away from zero for all iterates. The other is to employ a simple proximal for solving each subproblem inexactly, which has been suggested by many researchers, see [3, 9, 21, 22, 23]. In addition, many modified ADMM-based algorithms were introduced in [24, 25, 20, 28].

More recently, by leveraging on the inexact block symmetric Gauss-Seidel (sGS) decomposition technique, Chen, Sun and Toh [21] had employed the dual approach by proposing an efficient inexact ADMM-type first-order method (the sGSimsPADMM) for solving problem (2). Furthermore, based on the inexact sGS decomposition technique and the semismooth Newton-CG algorithm, Li, Sun and Toh proposed a two-phase proximal augmented Lagrangian method for convex quadratic semidefinite programming, named QSDPNAL [2]. It extended the ideas from SDPNAL [26] and SDPNAL+ [27] for the linear SDP problems to the QSDP problems.

By making full use of the KKT conditions, Chang et al. [28] presented a modified ADMM to solve the dual of the CQSDP problem in standard form (without nonnegative constraints), which is an extension of the method proposed by Wen et al. [36]. This modified ADMM can always skip the subproblems with respect to the block-variable W , which will save both the computational cost and the memory for variable storage at each iteration. Inspired by the success of modified ADMM [28] as well as aforementioned work on the ADMM-based methods, we present a projection method by modifying 3-block ADMM to solve an equivalent of the KKT system (3). The main contributions of this paper are as follows:

- (1). By introducing an auxiliary variable, we reformulate the 4-block separable convex problem (4) as a 3-block separable convex problem, and apply the directly extended 3-block ADMM (ADMM3d) to this reformulation. Based on the iterative scheme of ADMM3d, we testify the KKT system (3) is equivalent to an equation system having two projection operators onto the positive semidefinite and nonnegative matrix cones respectively.
- (2). We propose a projection method for solving this equation system. Essentially, the proposed method can be explained as a parallel 3-block ADMM with larger step size (can be greater than $(1 + \sqrt{5})/2$), and does not have to solve the subproblem with variable W exactly. Skipping the calculation of W can save $\mathcal{O}(n^3)$ for some operators φ , while the cost is only about $\mathcal{O}(n^2)$ for computing the auxiliary variable

introduced, see Section 3.3. This confirms that at least our methods require less computation than the existing ADMM [3, 18, 32] in one iteration.

- (3). The global convergence of the proposed method as well as its non-ergodic $o(1/(k+1))$ convergence rate are established to a KKT point by using a fixed-point argument and the projection operator's non-expansion, when the condition on the penalty parameter is satisfied. The numerical experiments show that, our proposed algorithm performs better than ADM-G and ADMM4d with the aggressive step-length of 1.618.

The rest of this paper is organized as follows. Some preliminary results are provided in Section 2. We reformulate the dual (2) as a 3-block convex optimization problem, and introduce how to solve the subproblems from ADMM3d in Section 3. The projection method based on the KKT conditions (3) is presented in Subsection 4. The convergence of the proposed method is analysed in Section 5. Section 6 is devoted to the implementation and numerical experiments to solve the CQSDP problems generated randomly. Finally, the paper is summarized in Section 7.

2 Preliminaries

Most of the definitions and notations used in this paper are standard and can be found in [29]. Throughout, Ω is an arbitrary finite dimensional real Euclidean space with inner product $\langle \cdot, \cdot \rangle$ and its induced norm $\|\cdot\|$. A single-valued mapping $\mathcal{G} : \Omega \rightarrow \Omega$ is called β -cocoercive (or β -inverse-strongly monotone), for a certain constant $\beta > 0$, if $\beta\mathcal{G}$ is firmly nonexpansive, i.e.,

$$\langle \mathcal{G}(x) - \mathcal{G}(x'), x - x' \rangle \geq \beta \|\mathcal{G}(x) - \mathcal{G}(x')\|^2, \quad \forall x, x' \in \Omega.$$

Let φ be a self-adjoint non zero positive semidefinite linear operator, we use $\lambda_{\max}(\varphi)$ to denote its largest eigenvalue, then φ is $\frac{1}{\lambda_{\max}(\varphi)}$ -cocoercive.

Let $\Gamma_0(\Omega)$ be the class of proper lower semicontinuous convex functions from Ω to $(-\infty, +\infty]$. For any $f \in \Gamma_0(\Omega)$, the subdifferential mapping ∂f of f is then maximal monotone and

$$\mathcal{J}_{\sigma\partial f}(x) = (\mathcal{I} + \sigma\partial f)^{-1}(x) = \operatorname{argmin}_z \left\{ f(z) + \frac{1}{2\sigma} \|x - z\|^2 \right\}, \quad \forall x \in \Omega,$$

where $\mathcal{I} : \Omega \rightarrow \Omega$ is the identity operator.

For a given closed convex \mathcal{C} , $\delta_{\mathcal{C}}$ is closed proper convex function and $\mathcal{J}_{\sigma\partial\delta_{\mathcal{C}}}(x) = \Pi_{\mathcal{C}}(x)$, i.e. the metric projection of x onto \mathcal{C} , and

$$\partial\delta_{\mathcal{C}}(x) = \mathcal{N}_{\mathcal{C}}(x) := \{z \mid \langle z, x' - x \rangle \leq 0 \ \forall x' \in \mathcal{C}\},$$

which is a closed convex cone.

We will denote by $\operatorname{Fix} \mathcal{T}$ the set of fixed points of operator \mathcal{T} , i.e., $\operatorname{Fix} \mathcal{T} := \{x^* \in \Omega \mid x^* = \mathcal{T}(x^*)\}$.

3 Reformulation of (2) and Directly Extended 3-Block ADMM.

Firstly, we make the following assumptions.

Assumption 1 (i). For the CQSDP problem (1), there exists a feasible solution $X \in \mathcal{S}_+^n$ such that

$$\mathcal{A}(X) = b, \quad X \in \mathcal{S}_{++}^n, \quad X \in \mathcal{N}^n. \quad (7)$$

(ii). For the dual problem (2), there exists a feasible solution $(W, y, Z, S) \in \mathcal{S}^n \times \mathbb{R}^m \times \mathcal{S}_+^n \times \mathcal{N}^n$ such that

$$-\varphi(W) + \mathcal{A}^*(y) + Z + S = C, \quad Z \in \mathcal{S}_{++}^n, \quad S \in \mathcal{N}^n. \quad (8)$$

It is known from convex analysis (e.g, Corollary 5.3.6 in [33]) that under Assumption 1, the strong duality for (1) and (2) holds and the KKT conditions (3) have solutions.

Assumption 2 *The linear operator \mathcal{A} is surjective.*

Under Assumption 2, the operator $\mathcal{A}\mathcal{A}^*$ is invertible, then the solution of the subproblem with variable y can be well-defined for ADMM4d.

3.1 3-block Convex Optimization Reformulation

By introducing an auxiliary variable \tilde{X} , we can rewrite (1) equivalently as

$$\begin{aligned} \min \quad & \frac{1}{2}\langle X, \varphi(X) \rangle + \langle C, X \rangle \\ \text{s.t.} \quad & X - \tilde{X} = 0, \mathcal{A}(X) = b, \\ & X \in \mathcal{S}_+^n, \tilde{X} \in \mathcal{N}. \end{aligned} \quad (9)$$

Defining $U = \begin{pmatrix} X \\ \tilde{X} \end{pmatrix}$, (9) can be simplified as:

$$\begin{aligned} \min \quad & \theta(U) \\ \text{s.t.} \quad & \mathcal{H}(U) = \tilde{b}, \quad U \in \mathcal{S}_+^n \times \mathcal{N}^n, \end{aligned} \quad (10)$$

where $\theta(U) = \frac{1}{2}\langle X, \varphi(X) \rangle + \langle C, X \rangle$, and

$$\mathcal{H} = \begin{pmatrix} \mathcal{I} & -\mathcal{I} \\ \mathcal{A} & 0 \end{pmatrix}, \quad \tilde{b} = \begin{pmatrix} 0 \\ b \end{pmatrix}. \quad (11)$$

By setting

$$\begin{aligned} f(W) &:= \frac{1}{2} \left\langle \begin{pmatrix} \varphi(W) \\ 0 \end{pmatrix}, \begin{pmatrix} W \\ 0 \end{pmatrix} \right\rangle = \frac{1}{2} \langle W, \varphi(W) \rangle, \\ g(Z, U) &:= \delta_{\mathcal{S}_+^n}(Z) + \delta_{\mathcal{N}^n}(U), \\ h(S, y) &:= \left\langle \begin{pmatrix} 0 \\ -b \end{pmatrix}, \begin{pmatrix} S \\ y \end{pmatrix} \right\rangle = \langle 0, S \rangle - b^T y, \end{aligned}$$

and

$$\begin{aligned} \mathcal{F}^*(W) &:= \begin{pmatrix} -\varphi & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} W \\ 0 \end{pmatrix} = \begin{pmatrix} -\varphi(W) \\ 0 \end{pmatrix}, \\ \mathcal{G}^*(Z, U) &:= \begin{pmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{I} \end{pmatrix} \begin{pmatrix} Z \\ U \end{pmatrix} = \begin{pmatrix} Z \\ U \end{pmatrix}, \\ \mathcal{H}^*(S, y) &:= \begin{pmatrix} \mathcal{I} & \mathcal{A}^* \\ -\mathcal{I} & 0 \end{pmatrix} \begin{pmatrix} S \\ y \end{pmatrix} = \begin{pmatrix} S + \mathcal{A}^*(y) \\ -S \end{pmatrix}, \\ \tilde{C} &:= \begin{pmatrix} C \\ 0 \end{pmatrix}, \end{aligned}$$

then the dual of problem (10) can be reformulated as

$$\begin{aligned} \min \quad & f(W) + g(Z, U) + h(S, y) \\ \text{s.t.} \quad & \mathcal{F}^*(W) + \mathcal{G}^*(Z, U) + \mathcal{H}^*(S, y) = \tilde{C}. \end{aligned} \quad (12)$$

Actually, it is equivalent to (4).

Notice that from Assumption 2 and the definition of \mathcal{H} , we can obtain the following results easily.

Lemma 1 Under Assumption 2, then we have

- (i). $\mathcal{H}\mathcal{H}^*$ is invertible.
- (ii). the inverse of $\mathcal{H}\mathcal{H}^*$ can be computed by:

$$(\mathcal{H}\mathcal{H}^*)^{-1} = \begin{pmatrix} \frac{1}{2}\mathcal{I} + \frac{1}{2}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A} - \mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1} & \\ -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A} & 2(\mathcal{A}\mathcal{A}^*)^{-1} \end{pmatrix}. \quad (13)$$

Specially, for the operator $\mathcal{A} = \text{diag}$, we have $\mathcal{A}\mathcal{A}^* = \mathcal{I}$, and

$$(\mathcal{H}\mathcal{H}^*)^{-1} = \begin{pmatrix} \frac{1}{2}\mathcal{I} + \frac{1}{2}\mathcal{A}^*\mathcal{A} - \mathcal{A}^* & \\ -\mathcal{A} & 2\mathcal{I} \end{pmatrix}. \quad (14)$$

From Lemma 1, the solution of the subproblem with variable (S, y) can be well-defined for using ADMM3d to (12). Additionally, reformulation (12) has many advantages for designing efficiency ADMM-based algorithm, for instance, the subproblem with variable (S, y) or (Z, U) can be implemented in parallel and that with variable W can be skipped, the convergence rate of the proposed ADMM can be analysed in non-ergodic case, different with the existing multi-block ADMM, see Section 4 and 5.

3.2 ADMM3d for Solving (12)

Recall that the augmented lagrangian function of the problem (12) has the following form:

$$\begin{aligned} \widehat{\mathcal{L}}_\sigma(W, (Z, U), (S, y), \widehat{X}) &= f(W) + g(Z, U) + h(S, y) + \\ &\quad \left\langle \widehat{X}, \mathcal{F}^*(W) + \mathcal{G}^*(Z, U) + \mathcal{H}^*(S, y) - \tilde{C} \right\rangle + \\ &\quad \frac{\sigma}{2} \|\mathcal{F}^*(W) + \mathcal{G}^*(Z, U) + \mathcal{H}^*(S, y) - \tilde{C}\|^2, \end{aligned} \quad (15)$$

where $W \in \mathcal{S}^n$, $(Z, U) \in \mathcal{S}_+^n \times \mathcal{N}^n$, $(S, y) \in \mathcal{S}^n \times \mathbb{R}^n$ and $\widehat{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ ($X_1, X_2 \in \mathcal{S}^n$), $\sigma > 0$ is a penalty parameter. Then, the iterative scheme of ADMM3d for solving (12) reads as:

$$W^{k+1} = \arg \min_{W \in \mathcal{S}^n} \widehat{\mathcal{L}}_\sigma \left(W, (Z^k, U^k), (S^k, y^k), \widehat{X}^k \right), \quad (16)$$

$$(S^{k+1}, y^{k+1}) = \arg \min_{(S, y) \in \mathcal{S}^n \times \mathbb{R}^n} \widehat{\mathcal{L}}_\sigma \left(W^{k+1}, (Z^k, U^k), (S, y), \widehat{X}^k \right), \quad (17)$$

$$(Z^{k+1}, U^{k+1}) = \arg \min_{(Z, U) \in \mathcal{S}_+^n \times \mathcal{N}^n} \widehat{\mathcal{L}}_\sigma \left(W^{k+1}, (Z, U), (S^{k+1}, y^{k+1}), \widehat{X}^k \right), \quad (18)$$

$$\widehat{X}^{k+1} = \widehat{X}^k + \tau \sigma (\mathcal{F}^*(W) + \mathcal{G}^*(Z, U) + \mathcal{H}^*(S, y) - \tilde{C}), \quad (19)$$

where $\tau \in (0, \frac{1+\sqrt{5}}{2})$.

Now, we label $\widehat{\mathcal{L}}_\sigma(W, y, Z, S, X)$ as $\widehat{\mathcal{L}}_\sigma$, and solve these subproblems (17)-(18). From the first-order optimality condition of problem (17), we have

$$\nabla_{(S, y)} \widehat{\mathcal{L}}_\sigma = \mathcal{H} \begin{pmatrix} X_1 - \sigma(\varphi(W) - Z + C) \\ X_2 + \sigma U \end{pmatrix} + \sigma \mathcal{H}\mathcal{H}^* \begin{pmatrix} S \\ y \end{pmatrix} - \begin{pmatrix} 0 \\ b \end{pmatrix} = 0.$$

By Lemma 1, we have

$$\begin{pmatrix} S \\ y \end{pmatrix} = -(\mathcal{H}\mathcal{H}^*)^{-1} \mathcal{H} \begin{pmatrix} \frac{1}{\sigma} X_1 - \varphi(W) + Z - C \\ \frac{1}{\sigma} X_2 + U \end{pmatrix} + \frac{1}{\sigma} (\mathcal{H}\mathcal{H}^*)^{-1} \begin{pmatrix} 0 \\ b \end{pmatrix}, \quad (20)$$

and can compute $S^{k+1} = \phi_S(W^{k+1}, Z^k, U^k, X_1^k, X_2^k)$, where

$$\phi_S(W, Z, U, X_1, X_2) := -\frac{1}{2}\mathcal{Q}_- \left(\frac{1}{\sigma}X_1 - \varphi(W) + Z - C \right) + \frac{1}{2}\mathcal{Q}_+ \left(\frac{1}{\sigma}X_2 + U \right) - \frac{1}{\sigma}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b), \quad (21)$$

and

$$\mathcal{Q}_- = \mathcal{I} - \mathcal{M}, \quad \mathcal{Q}_+ = \mathcal{I} + \mathcal{M}, \quad \mathcal{M} = \mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}. \quad (22)$$

It is easy to check that the four operators \mathcal{A} , \mathcal{M} , \mathcal{Q}_+ and \mathcal{Q}_- satisfy the following properties:

- Lemma 2** (i). $\mathcal{M}^* = \mathcal{M}$, $\mathcal{Q}_-^* = \mathcal{Q}_-$, $\mathcal{Q}_+^* = \mathcal{Q}_+$.
(ii). $\mathcal{M}^*\mathcal{M} = \mathcal{M}$, $\mathcal{Q}_-^*\mathcal{Q}_- = \mathcal{Q}_-$, $\mathcal{Q}_+^*\mathcal{Q}_+ = \mathcal{Q}_+$.
(iii). $\mathcal{M}\mathcal{A}^* = \mathcal{A}^*$, $\mathcal{A}\mathcal{M} = \mathcal{A}$, $\mathcal{A}\mathcal{Q}_- = 0$, $\mathcal{Q}_-\mathcal{A}^* = 0$, $\mathcal{A}\mathcal{Q}_+ = 2\mathcal{A}$, $\mathcal{Q}_+\mathcal{A}^* = 2\mathcal{A}^*$.

In addition, it is from Assumption 2 that, we can obtain $y^{k+1} = \phi_y(W^{k+1}, Z^k, U^k, X_1^k, X_2^k)$, where

$$\phi_y(W, Z, U, X_1, X_2) := -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A} \left(\frac{1}{\sigma}X_1 - \varphi(W) + Z - C + \frac{1}{\sigma}X_2 + U \right) + 2\frac{1}{\sigma}(\mathcal{A}\mathcal{A}^*)^{-1}b. \quad (23)$$

Similarly, according to the first-order optimality conditions of problem (18), let

$$\phi_{V_Z}(W, S, y, X_1) := -\frac{1}{\sigma}X_1 + \varphi(W) - S - \mathcal{A}^*(y) + C, \quad (24)$$

$$\phi_{V_U}(S, X_2) := S - \frac{1}{\sigma}X_2, \quad (25)$$

compute $V_Z^{k+1} = \phi_{V_Z}(W^{k+1}, S^{k+1}, y^{k+1}, X_1^k)$ and $V_U^{k+1} = \phi_{V_U}(S^{k+1}, X_2^k)$, then we can get $U^{k+1} = \Pi_{\mathcal{N}^n}(V_U^{k+1})$ and $Z^{k+1} = \Pi_{\mathcal{S}_+^n}(V_Z^{k+1})$ in parallel. By the projection operator's properties, the following properties are easy to obtain by direct computation.

- Lemma 3** Suppose that $\{Z^{k+1}, U^{k+1}, X_1^{k+1}, X_2^{k+1}\}$ are generated by (16)-(19) with $\tau = 1$, then we have
(i). $V_Z^{k+1} = Z^{k+1} - \frac{1}{\sigma}X_1^{k+1}$, $Z^{k+1} \in \mathcal{S}_+^n$, $X_1^{k+1} \in \mathcal{S}_+^n$, $\langle Z^{k+1}, X_1^{k+1} \rangle = 0$;
(ii). $V_U^{k+1} = U^{k+1} - \frac{1}{\sigma}X_2^{k+1}$, $U^{k+1} \in \mathcal{N}^n$, $X_2^{k+1} \in \mathcal{N}^n$, $\langle U^{k+1}, X_2^{k+1} \rangle = 0$.

3.3 Solving the Subproblem (16) with Variable W .

In this section, we introduce how to solve the subproblem (16) efficiently, though it is not necessarily for designing our algorithm. The main objective is to show what our algorithm skips and how to get W^{k+1} for other ADMM-based methods in our numerical experiments.

Since the first-order optimality condition of (16) has the form

$$\nabla_W \widehat{\mathcal{L}}_\sigma = \varphi(W - X_1 + \sigma\varphi(W) - Z - S - \mathcal{A}^*(y) + C) = 0, \quad (26)$$

the structure of φ is important for computing W^{k+1} . For the simplest $\varphi(W) = W$ as used in the least squares SDP problem [11, 13], we can compute W^{k+1} with easy from

$$W^{k+1} = \frac{1}{1+\sigma}(X_1^k + \sigma(Z^k + S^k + \mathcal{A}^*(y^k) - C)), \quad (27)$$

because $\varphi(W) = 0$ if only if $W = 0$.

However, it is not the case for all the operators φ . If $\varphi(W) = \frac{BW+WB}{2}$ as used in [2], for a given matrix $B \in \mathcal{S}_+^n$, the operator φ may not be invertible, then the equation $\varphi(W) = 0$ has many solutions. Although we actually do not need W explicitly in each iterations, only $\varphi(W)$ is needed, but it is generally not easy to obtain $\varphi(W)$ from (26), which will cost $\mathcal{O}(n^3)$ flops for some operators φ . Next, we will introduce how to get $\varphi(W^{k+1})$ effectively from (26).

For the problems with $\varphi(W) = \frac{BW+WB}{2}$, we suppose that the eigenvalue decomposition is $B = PAP^T$, where $A = \text{diag}(\lambda)$ and $\lambda = (\lambda_1, \dots, \lambda_n)^T$ is the vector of eigenvalues of B . Then, we have $\varphi = \mathcal{B}^*\mathcal{B}$, where $\mathcal{B}(X) = H \circ (P^T X P)$, $\mathcal{B}^*(Y) = P(H \circ Y)P^T$ and $H_{ij} = \sqrt{\frac{\lambda_i + \lambda_j}{2}}$, which implies $\mathcal{B}\mathcal{B}^* = H \circ H \circ$. Thus we can obtain the inverse of $\mathcal{I} + \sigma\mathcal{B}\mathcal{B}^*$ by

$$(\mathcal{I} + \sigma\mathcal{B}\mathcal{B}^*)^{-1} = \widehat{H} \circ,$$

with $\widehat{H}_{ij} = \frac{1}{1 + \sigma H_{ij}^2}$. By [34, Lemma 4] and setting $\Xi = \widehat{H} \circ$, we have

$$\begin{aligned} (\mathcal{I} + \sigma\varphi)^{-1} &= (\mathcal{I} + \sigma\mathcal{B}^*\mathcal{B})^{-1} \\ &= \mathcal{I} - \sigma\mathcal{B}^*(\mathcal{I} + \sigma\mathcal{B}\mathcal{B}^*)^{-1}\mathcal{B} \\ &= \mathcal{I} - \sigma\mathcal{B}^*\Xi\mathcal{B}. \end{aligned}$$

Thus, $\varphi(W)$ can be computed efficiently by

$$\varphi(W) = (\mathcal{I} - \sigma\mathcal{B}^*\Xi\mathcal{B})\varphi(X_1 + \sigma(Z + S + \mathcal{A}^*(y) - C)). \quad (28)$$

For the problems with $\varphi(W) = BWB^T$, if the eigenvalue decomposition of B is PAP^T , where $A = \text{diag}(\lambda)$ and $\lambda = (\lambda_1, \dots, \lambda_n)^T$ is the vector of eigenvalues of B . We can still write $\varphi = \mathcal{B}^*\mathcal{B}$, where $\mathcal{B}(X) = H \circ (P^T X P)$, $\mathcal{B}^*(Y) = P(H \circ Y)P^T$ but $H_{ij} = \sqrt{\lambda_i \lambda_j}$. By using the same idea as above, $\varphi(W)$ can be computed efficiently by (28).

Suppose that the eigenvalue decomposition of $B = PAP^T$ is already computed, which is performed only once and needs $9n^3$ flops by the symmetric QR algorithm. If B is a low rank matrix, computing $\varphi(W)$ can be very cheap as the matrix H is sparse, else if B is a positive definite matrix (not an identity matrix), computing $\mathcal{B}(X) = H \circ (P^T X P)$ and $\mathcal{B}^*(Y) = P(H \circ Y)P^T$ needs at least $8n^3$ flops to get $\varphi(W)$ at each iteration.

4 Projection Method

In this section, we define following operators by the metric projection:

$$\mathcal{P}_{\mathcal{S}_+^n}(V) := \left(\Pi_{\mathcal{S}_+^n}(V), \Pi_{\mathcal{S}_+^n}(V) - V \right), \quad (29)$$

$$\mathcal{P}_{\mathcal{N}^n}(V) := \left(\Pi_{\mathcal{N}^n}(V), \Pi_{\mathcal{N}^n}(V) - V \right), \quad (30)$$

$$\mathcal{P}(V) := (\mathcal{P}_{\mathcal{S}_+^n}(V), \mathcal{P}_{\mathcal{N}^n}(V)), \quad (31)$$

for any matrix $V \in \mathcal{S}^n$. By these operators and the iterative scheme (16)-(19), we show the equivalence of the KKT system (3) to an equation system. Then, a projection method for solving the equation system is presented.

In addition, we define a set

$$\mathcal{K} = \{(W, Z, U, X_1, X_2) \mid W \in \mathcal{S}^n, Z \in \mathcal{S}_+^n, U \in \mathcal{N}^n, X_1 \in \mathcal{S}^n, X_2 \in \mathcal{S}^n\}, \quad (32)$$

which will simplify our analysis.

4.1 Properties

By Moreau decomposition [35] and two operators $\mathcal{P}_{\mathcal{S}_+^n}(\cdot)$ and $\mathcal{P}_{\mathcal{N}^n}(\cdot)$ defined above, we now present the most important conclusion on the KKT system (3) in the following theorem. Based on this conclusion, we propose the projection method to obtain a KKT point.

Theorem 1 (i) For any $(W, Z, U, X_1, X_2) \in \mathcal{K}$ satisfying the following system

$$\left. \begin{aligned} \varphi(W) = \varphi(X_1), \quad S = \phi_S(W, Z, U, X_1, X_2), \quad y = \phi_y(W, Z, U, X_1, X_2), \\ (Z, \frac{1}{\sigma}X_1) = \mathcal{P}_{\mathcal{S}_+^n} \circ \phi_{V_Z}(W, S, y, X_1), \quad (U, \frac{1}{\sigma}X_2) = \mathcal{P}_{\mathcal{N}^n} \circ \phi_{V_U}(S, X_2), \end{aligned} \right\} \quad (33)$$

where the operators ϕ_S , ϕ_y , ϕ_{V_Z} and ϕ_{V_U} are defined in (21), (23), (24) and (25), then (W, y, Z, S, X_1) is a solution of the KKT system (3), namely,

$$\left. \begin{aligned} \mathcal{A}(X_1) = b, \quad \varphi(W) = \varphi(X_1), \\ -\varphi(W) + \mathcal{A}^*(y) + Z + S = C, \\ X_1 \in \mathcal{S}_+^n, \quad Z \in \mathcal{S}_+^n, \quad \langle Z, X_1 \rangle = 0, \\ X_1 \in \mathcal{N}^n, \quad S \in \mathcal{N}^n, \quad \langle S, X_1 \rangle = 0. \end{aligned} \right\} \quad (34)$$

(ii) If the point (W, y, Z, S, X) satisfies the KKT system (3), by setting $X_1 = X_2 = X$ and $U = S$, then $(W, Z, U, X_1, X_2) \in \mathcal{K}$ is a solution of the system (33).

Proof. (i) By $(Z, \frac{1}{\sigma}X_1) = \mathcal{P}_{\mathcal{S}_+^n} \circ \phi_{V_Z}(W, S, y, X_1)$, we have

$$X_1 \in \mathcal{S}_+^n, \quad Z \in \mathcal{S}_+^n, \quad \langle Z, X_1 \rangle = 0,$$

and $\phi_{V_Z}(W, S, y, X_1) = Z - \frac{1}{\sigma}X_1$. With the definition of $\phi_{V_Z}(W, S, y, X_1)$ in (24), we obtain

$$-\varphi(W) + \mathcal{A}^*(y) + Z + S = C. \quad (35)$$

Notice that from $y = \phi_y(W, Z, U, X_1, X_2)$ and $W = X_1$, we deduce that

$$\begin{aligned} (\mathcal{A}\mathcal{A}^*)y &= -\mathcal{A} \left(\frac{1}{\sigma}X_1 - \varphi(W) + Z - C + \frac{1}{\sigma}X_2 + U \right) + 2\frac{1}{\sigma}b \\ &= -\mathcal{A} \left(\frac{1}{\sigma}X_1 - S - \mathcal{A}^*(y) + \frac{1}{\sigma}X_2 + U \right) + 2\frac{1}{\sigma}b. \end{aligned} \quad (36)$$

On the other hand, it follows from Lemma 2 and (21), we have

$$\mathcal{A}(S) = \mathcal{A} \left(\frac{1}{\sigma}X_2 + U \right) - \frac{1}{\sigma}b. \quad (37)$$

Substituting (37) into (36), we have $\mathcal{A}(X_1) = b$.

In addition, since $(U, \frac{1}{\sigma}X_2) = \mathcal{P}_{\mathcal{N}^n} \circ \phi_{V_U}(S, X_2)$ and $\phi_{V_U}(S, X_2) = S - \frac{1}{\sigma}X_2$, we have $S = U$, which implies

$$X_2 \in \mathcal{N}^n, \quad S \in \mathcal{N}^n, \quad \langle S, X_2 \rangle = 0.$$

It is follows from $S = \phi_S(W, Z, U, X_1, X_2)$ and (35), that

$$\begin{aligned} S &= -\frac{1}{2}\mathcal{Q}_- \left(\frac{1}{\sigma}X_1 - S - \mathcal{A}^*(y) \right) + \frac{1}{2}\mathcal{Q}_+ \left(\frac{1}{\sigma}X_2 + S \right) - \frac{1}{\sigma}\mathcal{M}(X_1) \\ &= -\frac{1}{2} \left(\frac{1}{\sigma}X_1 - S - \mathcal{A}^*(y) - \frac{1}{\sigma}X_2 - S \right) + \frac{1}{2}\mathcal{M} \left(\frac{1}{\sigma}X_1 - S - \mathcal{A}^*(y) + \frac{1}{\sigma}X_2 + S - 2\frac{1}{\sigma}X_1 \right) \\ &= \frac{1}{2\sigma} (X_2 - X_1) + \frac{1}{2\sigma}\mathcal{M}(X_2 - X_1) + S, \end{aligned}$$

which means $X_2 = X_1$. Thus, $X_1 \in \mathcal{N}^n$, $S \in \mathcal{N}^n$, $\langle S, X_1 \rangle = 0$. Finally, note that $\varphi(W) = \varphi(X_1)$, we obtain (34).

(ii) By (3) and $S = U$, we have

$$\begin{aligned} \phi_{V_Z}(W, S, y, X_1) &= Z - \frac{1}{\sigma}X_1, \\ \phi_{V_U}(S, X_2) &= S - \frac{1}{\sigma}X_2 = U - \frac{1}{\sigma}X_2. \end{aligned}$$

Using Moreau decomposition and $X_1 = X_2 = X$, it is not difficult to obtain $(Z, \frac{1}{\sigma}X_1) = \mathcal{P}_{S_+^n} \circ \phi_{V_Z}(W, S, y, X_1)$ and $(U, \frac{1}{\sigma}X_2) = \mathcal{P}_{N^n} \circ \phi_{V_U}(S, X_2)$. In addition, from (23) we have

$$\begin{aligned}\phi_y(W, Z, U, X_1, X_2) &= -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}\left(\frac{1}{\sigma}X_1 - \mathcal{A}^*(y) - S + \frac{1}{\sigma}X_2 + S\right) + 2\frac{1}{\sigma}(\mathcal{A}\mathcal{A}^*)^{-1}b \\ &= -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}\left(\frac{1}{\sigma}X - \mathcal{A}^*(y) + \frac{1}{\sigma}X\right) + 2\frac{1}{\sigma}(\mathcal{A}\mathcal{A}^*)^{-1}b \\ &= (\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}\mathcal{A}^*(y) - (\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}\left(\frac{2}{\sigma}X\right) + 2\frac{1}{\sigma}(\mathcal{A}\mathcal{A}^*)^{-1}b \\ &= y\end{aligned}$$

and

$$\begin{aligned}\phi_S(W, Z, U, X_1, X_2) &= -\frac{1}{2}\mathcal{Q}_-\left(\frac{1}{\sigma}X_1 - \mathcal{A}^*(y) - S\right) + \frac{1}{2}\mathcal{Q}_+\left(\frac{1}{\sigma}X_2 + S\right) - \frac{1}{\sigma}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b) \\ &= -\frac{1}{2}\mathcal{Q}_-\left(\frac{1}{\sigma}X - S\right) + \frac{1}{2}\mathcal{Q}_+\left(\frac{1}{\sigma}X + S\right) - \frac{1}{\sigma}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b) \\ &= S + \frac{1}{\sigma}\mathcal{M}(X) - \frac{1}{\sigma}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b) \\ &= S.\end{aligned}$$

This completes our proof. \square

From Theorem 1, we can deduce the following relation:

$$(W, y, Z, S, X) \text{ is a KKT point. } \xleftrightarrow[X_1=X_2=X]{U=S} (W, Z, U, X_1, X_2) \text{ satisfies the system (33),}$$

which implies that the system (33) is nonempty from Assumption 1. The most important thing is that $\varphi(W) = \varphi(X_1)$ in the system (33), which gives us a confidence to believe that, we don't have to solve the subproblem with variable W exactly, even not have to compute $\varphi(W)$, but a KKT point of problem (1) and its dual (2) can be obtained as long as we can get a solution of the system (33). Therefore, we will in the next section design a projection method for solving the system (33).

4.2 Projection Method

Now, we define the following notations to simplify our analysis,

$$w = (Z, \frac{1}{\sigma}X_1, U, \frac{1}{\sigma}X_2), \quad w^k = (Z^k, \frac{1}{\sigma}X_1^k, U^k, \frac{1}{\sigma}X_2^k), \quad w^* = (Z^*, \frac{1}{\sigma}X_1^*, U^*, \frac{1}{\sigma}X_2^*).$$

Since $\varphi(W) = \varphi(X_1)$ in the system (33), we can remove the item $\varphi(W)$, and replace $\varphi(W)$ with $\varphi(X_1)$ in the definition of ϕ_S , ϕ_y , ϕ_{V_Z} and ϕ_{V_U} , e.g.,

$$\left. \begin{aligned}\phi_S(w) &= -\frac{1}{2}\mathcal{Q}_-\left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi\right)(X_1) + Z - C\right) + \frac{1}{2}\mathcal{Q}_+\left(\frac{1}{\sigma}X_2 + U\right) - \frac{1}{\sigma}\mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b), \\ \phi_y(w) &= -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A}\left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi\right)(X_1) + Z - C + \frac{1}{\sigma}X_2 + U\right) + 2\frac{1}{\sigma}(\mathcal{A}\mathcal{A}^*)^{-1}b, \\ \phi_{V_Z}(S, y, X_1) &= -\left(\frac{1}{\sigma}\mathcal{I} - \varphi\right)(X_1) - S - \mathcal{A}^*(y) + C, \\ \phi_{V_U}(S, X_2) &= S - \frac{1}{\sigma}X_2.\end{aligned}\right\} \quad (38)$$

Accordingly, $\varphi(W) = \varphi(X_1)$ can be left out, then we can rewrite the system (33) as

$$\left. \begin{aligned}S &= \phi_S(w), \quad y = \phi_y(w), \\ (Z, \frac{1}{\sigma}X_1) &= \mathcal{P}_{S_+^n} \circ \phi_{V_Z}(S, y, X_1), \\ (U, \frac{1}{\sigma}X_2) &= \mathcal{P}_{N^n} \circ \phi_{V_U}(S, X_2).\end{aligned}\right\} \quad (39)$$

Furthermore, we will use the following notations,

$$v_Z(w) = \phi_{V_Z}(\phi_S(w), \phi_y(w), X_1), \quad v_U(w) = \phi_{V_U}(\phi_S(w), X_2), \quad v(w) = (v_Z(w), v_U(w)), \quad (40)$$

$$\mathcal{J} = \{w \mid Z \in \mathcal{S}_+^n, U \in \mathcal{N}^n, X_1 \in \mathcal{S}^n, X_2 \in \mathcal{S}^n\}. \quad (41)$$

By these notations, the system (39) can be expressed as

$$w = \mathcal{P} \circ v(w) = \left(\mathcal{P}_{\mathcal{S}_+^n} \circ v_Z(w), \mathcal{P}_{\mathcal{N}^n} \circ v_U(w) \right), \quad (42)$$

its solution set can be viewed as the set of fixed points of operator $\mathcal{P} \circ v$, i.e., $\text{Fix } \mathcal{P} \circ v := \{w^* \in \mathcal{J} \mid w^* = \mathcal{P} \circ v(w^*)\}$. From Assumption 1 and Theorem 1, we have $\text{Fix } \mathcal{P} \circ v \neq \emptyset$, so we can design our projection method as follows.

Algorithm 1 (Projection Method for solving the system (39))

Step 0. Let $\sigma \in (0, \frac{2}{\lambda_{\max}(\varphi)})$ and $\rho \in (0, 2 - \frac{\sigma \lambda_{\max}(\varphi)}{2})$ be given parameters. Choose $w^0 \in \mathcal{J}$, set $k = 0$.

Step 1. Compute

$$S^{k+1} = \phi_S(w^k), \quad y^{k+1} = \phi_y(w^k);$$

Step 2. Project

$$\tilde{w}^k = \left[\mathcal{P}_{\mathcal{S}_+^n} \circ \phi_{V_Z}(S^{k+1}, y^{k+1}, X_1^k), \mathcal{P}_{\mathcal{N}^n} \circ \phi_{V_U}(S^{k+1}, X_2^k) \right]. \quad (43)$$

Step 3. Generalize

$$w^{k+1} = (1 - \rho)w^k + \rho\tilde{w}^k.$$

Set $k = k + 1$, and go to Step 1.

Remark 1 By (42), we have $\tilde{w}^k = \mathcal{P} \circ v(w^k)$, and our projection method above is a Krasnosel'skiĭ-Mann algorithm with

$$w^{k+1} = (1 - \rho)w^k + \rho\mathcal{P} \circ v(w^k),$$

for any $\rho \in (0, 2 - \frac{\sigma \lambda_{\max}(\varphi)}{2})$. The parameter ρ is similar to the relaxation factor in the generalized Douglas-Rachford operator splitting [30]. Notice that $1 < 2 - \frac{\sigma \lambda_{\max}(\varphi)}{2} < 2$, it can numerically accelerate our projection method for $\rho > 1$.

Remark 2 From the ADMM perspective, the projection method can be explained as a modified 3-block ADMM with larger step size ρ and a correction step for correcting (Z, U) :

$$\begin{cases} W^{k+1} &= X_1^{k+1} \\ (S^{k+1}, y^{k+1}) &= \arg \min_{(S, y) \in \mathcal{S}^n \times \mathbb{R}^m} \hat{\mathcal{L}}_\sigma \left(W^{k+1}, (Z^k, U^k), (S, y), \hat{X}^k \right), \\ (\tilde{Z}^k, \tilde{U}^k) &= \arg \min_{(Z, U) \in \mathcal{S}_+^n \times \mathcal{N}^n} \hat{\mathcal{L}}_\sigma \left(W^{k+1}, (Z, U), (S^{k+1}, y^{k+1}), \hat{X}^k \right), \\ \hat{X}^{k+1} &= \hat{X}^k + \rho\sigma(\mathcal{F}^*(W^{k+1}) + \mathcal{G}^*(\tilde{Z}^k, \tilde{U}^k) + \mathcal{H}^*(S^{k+1}, y^{k+1}) - \tilde{C}), \\ \text{Correction step} & \\ (Z^{k+1}, U^{k+1}) &= (1 - \rho)(Z^k, U^k) + \rho(\tilde{Z}^k, \tilde{U}^k). \end{cases} \quad (44)$$

Remark 3 Restricting $\sigma \in (0, \frac{2}{\lambda_{\max}(\varphi)})$ is to guarantee the convergence of our projection method, which is significantly larger than the range $\sigma \in (0, \frac{2}{5\|\Phi^T\Phi\|})$ shown in [17] for ADMM3d, where $\text{vec}(\varphi(X)) = \Phi \text{vec}(X)$. For some problems with Φ having a larger eigenvalue, the restriction of σ on a small interval may hinder its effective adjustment according the progress of algorithm, and then reduce the convergence speed.

Remark 4 The projection method with $\rho = 1$ is not a classic 2-block ADMM, although its computational procedure is $(S, y) \rightarrow (Z, U) \rightarrow (X_1, X_2)$ when $\varphi(W^k)$ is set to be $\varphi(X_1^k)$. The reason is that, X_1 in our projection method plays a dual role: the Lagrangian multiplier and the variable of the first block.

Remark 5 If $\varphi = 0$, problem (1) is the SDP problem with nonnegative constraints and its dual reformulation (12) will be a 2-block convex optimization problem. In this case, our projection method is a classic 2-block ADMM but the step size can close to 2, it is convergent for any $\sigma > 0$.

5 Convergence Analysis

In this section, we explore the properties of operators v , $\mathcal{P} \circ v$ and $v \circ \mathcal{P}$, and then establish the convergence of our projection method.

Lemma 4 [36] For any $V, V^* \in \mathcal{S}_+^n$,

(i). $\|\mathcal{P}_{\mathcal{S}_+^n}(V) - \mathcal{P}_{\mathcal{S}_+^n}(V^*)\|^2 \leq \|V - V^*\|^2$, with equality holding if only if

$$\left(\Pi_{\mathcal{S}_+^n}(V)\right)^T \left(\Pi_{\mathcal{S}_+^n}(V^*) - V^*\right) = 0 \quad \text{and} \quad \left(\Pi_{\mathcal{S}_+^n}(V) - V\right)^T \Pi_{\mathcal{S}_+^n}(V^*) = 0.$$

(ii). $\|\mathcal{P}_{\mathcal{N}^n}(V) - \mathcal{P}_{\mathcal{N}^n}(V^*)\|^2 \leq \|V - V^*\|^2$, with equality holding if only if

$$\left(\Pi_{\mathcal{N}^n}(V)\right)^T \left(\Pi_{\mathcal{N}^n}(V^*) - V^*\right) = 0 \quad \text{and} \quad \left(\Pi_{\mathcal{N}^n}(V) - V\right)^T \Pi_{\mathcal{N}^n}(V^*) = 0.$$

Lemma 5 For any $w, w^* \in \mathcal{J}$, then we have

$$\begin{aligned} v_Z(w) - v_Z(w^*) &= -\frac{1}{2}\mathcal{Q}_- \left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi \right) (X_1 - X_1^*) \right) + \frac{1}{2}\mathcal{Q}_+(Z - Z^*) \\ &\quad - \frac{1}{2}\mathcal{Q}_- \left(\frac{1}{\sigma}(X_2 - X_2^*) + (U - U^*) \right), \end{aligned} \quad (45)$$

$$\begin{aligned} v_U(w) - v_U(w^*) &= -\frac{1}{2}\mathcal{Q}_- \left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi \right) (X_1 - X_1^*) \right) - \frac{1}{2}\mathcal{Q}_-(Z - Z^*) \\ &\quad - \frac{1}{2}\mathcal{Q}_- \left(\frac{1}{\sigma}(X_2 - X_2^*) \right) + \frac{1}{2}\mathcal{Q}_+(U - U^*). \end{aligned} \quad (46)$$

Proof. Using the definition of ϕ_S and ϕ_y in (38), we deduce that

$$\begin{aligned} \phi_y(w) - \phi_y(w^*) &= -(\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A} \left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi \right) (X_1 - X_1^*) + (Z - Z^*) \right) \\ &\quad + (\mathcal{A}\mathcal{A}^*)^{-1}\mathcal{A} \left(\frac{1}{\sigma}(X_2 - X_2^*) + (U - U^*) \right), \end{aligned} \quad (47)$$

$$\begin{aligned} \phi_S(w) - \phi_S(w^*) &= -\frac{1}{2}\mathcal{Q}_- \left(\left(\frac{1}{\sigma}\mathcal{I} - \varphi \right) (X_1 - X_1^*) + (Z - Z^*) \right) \\ &\quad + \frac{1}{2}\mathcal{Q}_+ \left(\frac{1}{\sigma}(X_2 - X_2^*) + (U - U^*) \right). \end{aligned} \quad (48)$$

Together with the definition of ϕ_{V_Z} and ϕ_{V_U} in (38), it is not difficult to get the results. \square

Lemma 6 Suppose that $\varphi \neq 0$, for any $\sigma > 0$ such that $\sigma < \frac{2}{\lambda_{max}(\varphi)}$, then

$$\left\| \left(\frac{1}{\sigma}\mathcal{I} - \varphi \right) (X) \right\|^2 \leq \left\| \frac{1}{\sigma}X \right\|^2, \quad (49)$$

with equality holding if and only if $\varphi(X) = 0$.

Proof. Recall that φ is a self-adjoint positive semidefinite linear operator, we have

$$\left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X) \right\|_F^2 = \left\| \frac{1}{\sigma} X \right\|_F^2 - \left\langle X, \left(\frac{2}{\sigma} \varphi - \varphi^2 \right) (X) \right\rangle.$$

It follows from $\sigma < \frac{2}{\lambda_{\max}(\varphi)}$ that $\frac{2}{\sigma} \mathcal{I} - \varphi$ is positive definite, then $\frac{2}{\sigma} \varphi - \varphi^2$ is positive semidefinite. Namely, $\langle (X), (\frac{2}{\sigma} \varphi - \varphi^2)(X) \rangle \geq 0$, so $\|(\frac{1}{\sigma} \mathcal{I} - \varphi)(X)\|_F^2 \leq \|\frac{1}{\sigma} X\|_F^2$.

If the equality in (49) holds, $\langle X, (\frac{2}{\sigma} \varphi - \varphi^2)(X) \rangle = 0$, which implies $\varphi(X) = 0$. \square

Lemma 7 For any $w, w^* \in \mathcal{J}$, we have

(i).

$$\|v(w) - v(w^*)\|_F^2 \leq \|w - w^*\|_F^2. \quad (50)$$

(ii). If the equality in (50) holds, and $w^* \in \text{Fix } \mathcal{P} \circ v$ then

$$v_Z(w) = -\frac{1}{\sigma} X_1 + Z, \quad (51)$$

$$v_U(w) = -\frac{1}{\sigma} X_2 + U. \quad (52)$$

Proof. (i). Since for any matrix A, B , $\|A\|_F^2 + \|B\|_F^2 = \frac{1}{2}(\|A + B\|_F^2 + \|A - B\|_F^2)$, by Lemma 5 we infer that

$$\begin{aligned} \|v(w) - v(w^*)\|_F^2 &= \left\| \begin{array}{c} v_Z(w) - v_Z(w^*) \\ v_U(w) - v_U(w^*) \end{array} \right\|_F^2 \\ &= \frac{1}{2} \|(v_Z(w) - v_Z(w^*)) + (v_U(w) - v_U(w^*))\|_F^2 + \frac{1}{2} \|(v_Z(w) - v_Z(w^*)) - (v_U(w) - v_U(w^*))\|_F^2 \\ &= \frac{1}{2} \left\| \mathcal{M}((Z - Z^*) + (U - U^*)) - \mathcal{Q}_- \left(\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right) \right\|_F^2 \\ &\quad + \frac{1}{2} \|(Z - Z^*) - (U - U^*)\|_F^2. \end{aligned}$$

From the definition of \mathcal{M} and \mathcal{Q}_- , the spectral radius of the operator \mathcal{M} and \mathcal{Q}_- is no more than 1 and $\mathcal{M}\mathcal{Q}_- = 0$, then

$$\begin{aligned} &\frac{1}{2} \left\| \mathcal{M}((Z - Z^*) + (U - U^*)) - \mathcal{Q}_- \left(\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right) \right\|_F^2 \\ &\leq \frac{1}{2} \|(Z - Z^*) + (U - U^*)\|_F^2 + \frac{1}{2} \left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right\|_F^2. \end{aligned} \quad (53)$$

If the equality above holds, that is,

$$(\mathcal{I} - \mathcal{M})((Z - Z^*) + (U - U^*)) = 0, \quad (54)$$

$$\mathcal{M} \left(\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right) = 0. \quad (55)$$

Thus,

$$\begin{aligned}
& \|v(w) - v(w^*)\|_F^2 \\
& \leq \frac{1}{2} \|(Z - Z^*) - (U - U^*)\|_F^2 + \frac{1}{2} \|(Z - Z^*) + (U - U^*)\|_F^2 \\
& \quad + \frac{1}{2} \left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right\|_F^2 \\
& = \|Z - Z^*\|_F^2 + \|U - U^*\|_F^2 + \frac{1}{2} \left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right\|_F^2 \\
& \leq \|Z - Z^*\|_F^2 + \|U - U^*\|_F^2 + \left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) \right\|_F^2 + \left\| \frac{1}{\sigma} (X_2 - X_2^*) \right\|_F^2.
\end{aligned} \tag{56}$$

If the equality in (56) holds, that is,

$$\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) = \frac{1}{\sigma} (X_2 - X_2^*). \tag{57}$$

For any $\sigma \in (0, \frac{2}{\lambda_{\max}(\varphi)})$, it follows from Lemma 6 that

$$\left\| \left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) \right\|_F^2 \leq \left\| \frac{1}{\sigma} (X_1 - X_1^*) \right\|_F^2 \tag{58}$$

with equality holding if and only if

$$\varphi(X_1 - X_1^*) = 0, \tag{59}$$

which implies $(\frac{1}{\sigma} \mathcal{I} - \varphi)(X_1 - X_1^*) = \frac{1}{\sigma}(X_1 - X_1^*)$. Thus, we deduce

$$\begin{aligned}
\|v(w) - v(w^*)\|_F^2 & \leq \|Z - Z^*\|_F^2 + \|U - U^*\|_F^2 + \left\| \frac{1}{\sigma} (X_2 - X_2^*) \right\|_F^2 + \left\| \frac{1}{\sigma} (X_1 - X_1^*) \right\|_F^2 \\
& = \|w - w^*\|_F^2.
\end{aligned}$$

(ii). If the equality in (50) holds, it also holds in (53), (56) and (58), so we have the conditions (54), (55), (57) and (59). Substituting these conditions into the results of Lemma 5, we have

$$\begin{aligned}
& v_Z(w) - v_Z(w^*) \\
& = -\frac{1}{2} \mathcal{Q}_- \left(\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right) + \frac{1}{2} \mathcal{Q}_+ (Z - Z^*) - \frac{1}{2} \mathcal{Q}_- (U - U^*), \\
& = -\frac{1}{2} \left(\left(\frac{1}{\sigma} \mathcal{I} - \varphi \right) (X_1 - X_1^*) + \frac{1}{\sigma} (X_2 - X_2^*) \right) + (Z - Z^*), \\
& = -\frac{1}{\sigma} (X_1 - X_1^*) + (Z - Z^*) \\
& = \left(-\frac{1}{\sigma} X_1 + Z \right) - \left(-\frac{1}{\sigma} X_1^* + Z^* \right).
\end{aligned}$$

By using $w^* \in \text{Fix } \mathcal{P} \circ v$ and the proof of Lemma 3, we get $v_Z(w^*) = -\frac{1}{\sigma} X_1^* + Z^*$. Therefore, the equality $v_Z(w) - v_Z(w^*) = (-\frac{1}{\sigma} X_1 + Z) - (-\frac{1}{\sigma} X_1^* + Z^*)$ implies $v_Z(w) = -\frac{1}{\sigma} X_1 + Z$. Similarly, we can obtain $v_U(w) = -\frac{1}{\sigma} X_2 + U$ when the equality in (50) holds. The proof is finished. \square

Theorem 2 For the sequence $\{w^k\}$ generated by Algorithm 1 with $\rho = 1$, we have

$$\|w^{k+1} - w^*\|_F^2 = \|\mathcal{P} \circ v(w^k) - \mathcal{P} \circ v(w^*)\|_F^2 \leq \|w^k - w^*\|_F^2,$$

where $w^* \in \text{Fix } \mathcal{P} \circ v$,

Proof. It follows from Remark 1 and Lemma 4 that,

$$\begin{aligned}
\|w^{k+1} - w^*\|_F^2 &= \|\mathcal{P} \circ v(w^k) - \mathcal{P} \circ v(w^*)\|_F^2 \\
&= \left\| \begin{array}{l} \mathcal{P}_{\mathcal{S}_+^n} \circ v_Z(w^k) - \mathcal{P}_{\mathcal{S}_+^n} \circ v_Z(w^*) \\ \mathcal{P}_{\mathcal{N}^n} \circ v_U(w^k) - \mathcal{P}_{\mathcal{N}^n} \circ v_U(w^*) \end{array} \right\|_F^2 \\
&\leq \left\| \begin{array}{l} v_Z(w^k) - v_Z(w^*) \\ v_U(w^k) - v_U(w^*) \end{array} \right\|_F^2 \\
&= \|v(w^k) - v(w^*)\|_F^2.
\end{aligned}$$

By Lemma 7, we can obtain the results. \square

Theorem 2 show that the operator $\mathcal{P} \circ v$ is quasinonexpansive. Next, we will further explore that the operator $\mathcal{P} \circ v$ is α -averaged with coefficient

$$\alpha := \frac{2}{4 - \sigma \lambda_{\max}(\varphi)} \in \left(\frac{1}{2}, 1\right), \quad (60)$$

for $\sigma \in (0, \frac{2}{\lambda_{\max}(\varphi)})$.

Theorem 3 For the operators v and \mathcal{P} defined in (40) and (42), we have

(i). $v \circ \mathcal{P} = \mathcal{L}^{-1} \circ \mathcal{T} \circ \mathcal{L}$ with $\mathcal{L} = -\sigma \mathcal{I}$ and

$$\mathcal{T} = \mathcal{I} - \mathcal{J}_{\sigma g} + \mathcal{J}_{\sigma \mathcal{N}_{\mathcal{K}}} \circ (2\mathcal{J}_{\sigma g} - \mathcal{I} - \sigma \nabla \theta \circ \mathcal{J}_{\sigma g}), \quad (61)$$

where $\mathcal{K} = \{U \in \mathcal{S}^n \times \mathcal{S}^n \mid \mathcal{H}(U) = \tilde{b}\}$.

(2). $\mathcal{P} \circ v$ is α -averaged.

Proof. (i). For the sequence $\{w^k\}$ generated by Algorithm 1 with $\rho = 1$, we have

$$\begin{aligned}
\mathcal{T} \circ \mathcal{L} \circ v(w^k) &= \mathcal{T} \begin{pmatrix} -\sigma v_Z(w^k) \\ -\sigma v_U(w^k) \end{pmatrix} \\
&= \begin{pmatrix} -\sigma V_Z^{k+1} + X_1^{k+1} \\ -\sigma V_U^{k+1} + X_2^{k+1} \end{pmatrix} + \Pi_{\mathcal{K}} \begin{pmatrix} 2X_1^{k+1} + \sigma V_Z^{k+1} - \sigma(\varphi(W^{k+1}) + C) \\ 2X_2^{k+1} + \sigma V_U^{k+1} \end{pmatrix} \\
&= \begin{pmatrix} -\sigma Z^{k+1} \\ -\sigma U^{k+1} \end{pmatrix} + \Pi_{\mathcal{K}} \begin{pmatrix} X_1^{k+1} - \sigma(\varphi(W^{k+1}) - Z^{k+1} + C) \\ X_2^{k+1} + \sigma U^{k+1} \end{pmatrix}.
\end{aligned}$$

Note that

$$\Pi_{\mathcal{K}}(U) = U - \mathcal{H}^*(\mathcal{H}\mathcal{H}^*)^{-1}(\mathcal{H}U - \tilde{b}), \quad \forall U \in \mathcal{S}^n \times \mathcal{S}^n,$$

then, by using (20) we can deduce

$$\begin{aligned}
\mathcal{T} \circ \mathcal{L} \circ v(w^k) &= \begin{pmatrix} -\sigma Z^{k+1} \\ -\sigma U^{k+1} \end{pmatrix} + \begin{pmatrix} X_1^{k+1} - \sigma(\varphi(W^{k+1}) - Z^{k+1} + C) + \sigma S^{k+2} + \sigma \mathcal{A}^*(y^{k+2}) \\ X_2^{k+1} + \sigma U^{k+1} - \sigma S^{k+2} \end{pmatrix} \\
&= \begin{pmatrix} X_1^{k+1} - \sigma(\varphi(W^{k+1}) + C) + \sigma S^{k+2} + \sigma \mathcal{A}^*(y^{k+2}) \\ X_2^{k+1} - \sigma S^{k+2} \end{pmatrix} \\
&= -\sigma v(w^{k+1}) \\
&= -\sigma v \circ \mathcal{P} \circ v(w^k).
\end{aligned}$$

By $\mathcal{L} = -\sigma \mathcal{I}$, we have $v \circ \mathcal{P} = \mathcal{L}^{-1} \circ \mathcal{T} \circ \mathcal{L}$.

(2). Note that $\nabla \theta$ is $\frac{1}{\lambda_{\max}(\varphi)}$ -cocoercive, it follows from [31, Proposition 2.1] that \mathcal{T} is α -averaged. Then, $v \circ \mathcal{P}$ is α -averaged from (i). Since \mathcal{P} is invertible, we have $\mathcal{P} \circ v = \mathcal{P} \circ \mathcal{L}^{-1} \circ \mathcal{T} \circ \mathcal{L} \circ \mathcal{P}^{-1}$, which implies $\mathcal{P} \circ v$ is α -averaged too. \square

It follows from [29, Proposition 5.15] and [38, Theorem 1], the convergence result for Algorithm 1 is stated in the following theorem.

Theorem 4 *Under Assumptions 1 and 2, for any $\sigma \in (0, \frac{2}{\lambda_{\max}(\varphi)})$ and $\rho \in (0, \frac{1}{\alpha})$, assume the sequence $\{w^k\}$ is generated by Algorithm 1. Then the following results hold:*

- (i). *For any $w^* \in \text{Fix } \mathcal{P} \circ v$, $\{\|w^{k+1} - w^*\|\}$ is monotonically nonincreasing.*
- (ii). *The fixed-point residual sequence $\{\|\mathcal{P} \circ v(w^k) - w^k\|\}$ is monotonically nonincreasing and converges to 0.*
- (iii). *The sequence $\{w^k\}$ converges to some point $w^* \in \text{Fix } \mathcal{P} \circ v$.*
- (iv). *$\|\mathcal{P} \circ v(w^k) - w^k\|^2 \leq \frac{\frac{\alpha^2}{\rho(\alpha-\rho)} \|w^0 - w^*\|^2}{k+1}$ and $\|\mathcal{P} \circ v(w^k) - w^k\|^2 = o(\frac{1}{k+1})$.*

Theorem 4 shows that, the sequence $\{w^k\}$ generated by Algorithm 1 is convergent to a solution w^* of the system (39). Therefore, by Theorem 1 we can obtain a KKT point $(W^*, Z^*, y^*, S^*, X^*)$ with

$$\varphi(W^*) = \varphi(X^*), \quad X^* = X_1^*, \quad S^* = U^* \quad \text{and} \quad y^* = \phi_y(w^*),$$

where ϕ_y is defined as in (38). Since the simplest choice of W is X satisfying $\varphi(W) = \varphi(X)$, so we set $W^k = X^k = X_1^k$ in the following numerical experiments.

6 Numerical experiments

In this section, we report the numerical performance of our projection method for the CQSDP problems generated randomly in MATLAB R2013B. We denote the random number generator by *seed* for generating data again in MATLAB. All experiments are performed on an Intel(R) Core(TM) i5-4590 CPU@ 3.30 GHz PC with 8GB of RAM running on 64-bit Windows operating system.

6.1 Doubly non-negative CQSDP problems

In our numerical experiments, we test two types of doubly non-negative CQSDP problems. One is that with $\varphi(X) = \frac{BX+XB}{2}$ for a given matrix $B \in \mathcal{S}_+^n$. So in this case, $\lambda_{\max}(\varphi) = \lambda_{\max}(B)$. The matrix B is a random symmetric positive semidefinite matrix, generated by `temp=randn(n,r); B=temp*temp'`; We set $r = 10$, i.e., $\text{rank}(B)=10$ as in [3]. The other is with $\varphi(X) = X$, as for least squares semidefinite programming in [13, 14], then $\lambda_{\max}(\varphi) = 1$.

In this paper, we test the problems arising from the relaxation of maximum stable set problems and a binary integer nonconvex quadratic (BIQ) programming. The instances are considered as in [3], [32], and [37]. For instance, we construct QSDP-BIQ problem sets based on the formulation in [3] as follows:

$$\begin{aligned} \min \quad & \frac{1}{2} \langle X, \varphi(X) \rangle + \langle Q, X_0 \rangle + \langle c, x \rangle \\ \text{s.t.} \quad & \text{diag}(X_0) - x = 0, \quad \alpha = 1, \\ & X = \begin{pmatrix} X_0 & x \\ x^T & \alpha \end{pmatrix} \in \mathcal{S}_+^n, \quad X \in \mathcal{C}^n. \end{aligned} \tag{62}$$

The test data for Q and c are taken from Biq Mac Library maintained by Wiegele, which is available at <http://biqmac.uni-klu.ac.at/biqmaclib.html>. In the same sprit, we construct test problems QSDP-BIQ and QSDP- θ_+ .

6.2 Numerical results

In this section, we report the numerical results obtained by our projection method, ADM-G and ADMM4d in solving various instances of the random CQSDP problems with nonnegative constraints.

In order to compare with ADM-G ($\alpha = 0.99$) and ADMM4d ($\tau = 1.618$) for solving 4-block dual (2), we measure the accuracy of the approximate optimal solution (W, y, Z, S, X) (with $W = X$) by using the following relative residual:

$$\delta := \max \{ \text{pinf}, \text{dinf}, p\delta_{S_+^n}, p\delta_{\mathcal{N}^n}, d\delta_{S_+^n}, d\delta_{\mathcal{N}^n}, \delta_{XZ}, \delta_{XS} \}, \quad (63)$$

where

$$\text{pinf} = \frac{\|\mathcal{A}(X) - b\|}{1 + \|b\|}, \quad \text{dinf} = \frac{\|C + \varphi(X) - Z - \mathcal{A}^*(y)\|}{1 + \|C\|}, \quad (64)$$

$$p\delta_{S_+^n} = \frac{\|H_{S_+^n}(-X)\|}{1 + \|X\|}, \quad p\delta_{\mathcal{N}^n} = \frac{\|H_{\mathcal{N}^n}(-X)\|}{1 + \|X\|}, \quad (65)$$

$$d\delta_{S_+^n} = \frac{\|H_{S_+^n}(-Z)\|}{1 + \|Z\|}, \quad d\delta_{\mathcal{N}^n} = \frac{\|H_{\mathcal{N}^n}(-S)\|}{1 + \|S\|}, \quad (66)$$

$$\delta_{XZ} = \frac{|\langle X, Z \rangle|}{1 + \|X\| + \|Z\|}, \quad \delta_{XS} = \frac{|\langle X, S \rangle|}{1 + \|X\| + \|S\|}. \quad (67)$$

Additionally, we compute the relative gap by

$$\delta_g = \frac{|\text{pobj} - \text{dobj}|}{1 + |\text{pobj}| + |\text{dobj}|},$$

where $\text{pobj} = \frac{1}{2}\langle X, \varphi(X) \rangle + \langle C, X \rangle$ and $\text{dobj} = -\frac{1}{2}\langle X, \varphi(X) \rangle + b^T y$.

We choose the initial point $X_1^0 = X_2^0 = \mathcal{A}^*(\mathcal{A}\mathcal{A}^*)^{-1}(b)$, and $Z^0 = U^0 = 0$. We terminate all the solvers when $\delta < 10^{-6}$ with the maximum number of iterations set at 25000.

The penalty parameter σ is dynamically adjusted according to the progress of the algorithms, but it satisfies $0 < \sigma < \frac{2}{\lambda_{\max}(\varphi)}$ for our projection method from the discussion in Section 5. Thus, we set $\sigma_{\max} = \epsilon_0 \frac{2}{\lambda_{\max}(\varphi)}$ (ϵ_0 is a constant, e.g., $\epsilon_0 = 0.999$.) and $\sigma_{\min} = 10^{-6}$ for our projection method. In our numerical experiments, we use the same adjustment strategy for our projection method, ADM-G and ADMM4d to solve all the tested problems, but $\sigma_{\max} = 10^6$ and $\sigma_{\min} = 10^{-6}$ for ADM-G and ADMM4d. The key idea for adjusting σ is to balance the progress of primal and dual feasibilities: $\eta_p = \max\{\text{pinf}, p\delta_{S_+^n}, p\delta_{\mathcal{N}^n}\}$ and $\eta_d = \max\{\text{dinf}, d\delta_{S_+^n}, d\delta_{\mathcal{N}^n}\}$. For details, see Appendix 1.

The initial σ_0 for our projection method is chosen to be $10^{-2} \times \sigma_{\max}$. For ADM-G and ADMM4d, we set $\sigma_0 = 1$. We use σ_k to denote the penalty parameter at k -th iteration, set

$$\rho_k = \eta \frac{1}{\alpha_k} \quad \text{with} \quad \alpha_k = \frac{2}{4 - \sigma_k \lambda_{\max}(\varphi)},$$

where $\eta \in (0, 1)$ since $\rho_k < \frac{1}{\alpha_k}$. Generally, the larger η can produce better results, so we set $\eta = 0.95$ in this paper. Figure 1 shows the evolutions of ρ_k with respect to iterations for the problems ‘‘theta4’’, ‘‘be100.1’’ and ‘‘gka1d’’, from the results shown we see that the step size ρ_k (and relaxation factor) is always greater than 1.85 in spite of fluctuating with respect to σ_k .

The detailed numerical results are reported in the tables 1-4. Figures 2 and 3 show the performance profiles in terms of the number of iterations and computing time for all the problems tested with $\varphi(X) = \frac{BX+XB}{2}$ and $\varphi(X) = X$, respectively.

Recall that a point (x, y) is in the performance profiles curve of a method if and only if it can solve $(100y)\%$ of all the tested problems no slower than x times of any other methods. We may observe that, our project method takes the least number of iterations and computational time for the majority of the tested

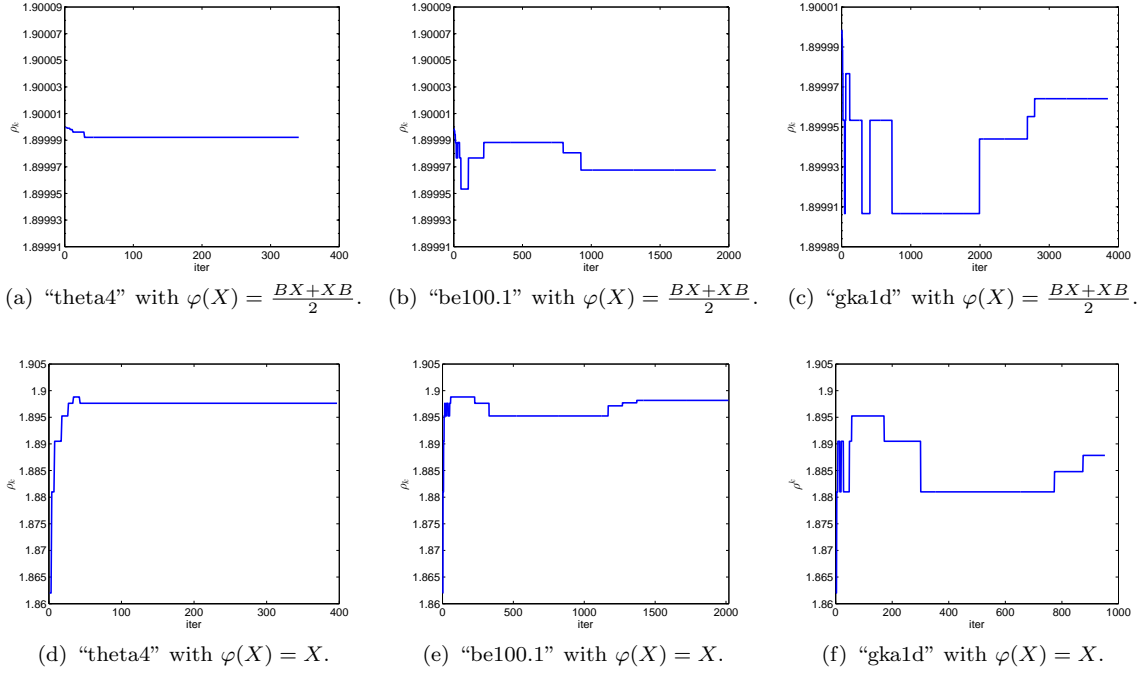


Fig. 1 Evolutions of ρ_k with respect to iterations.

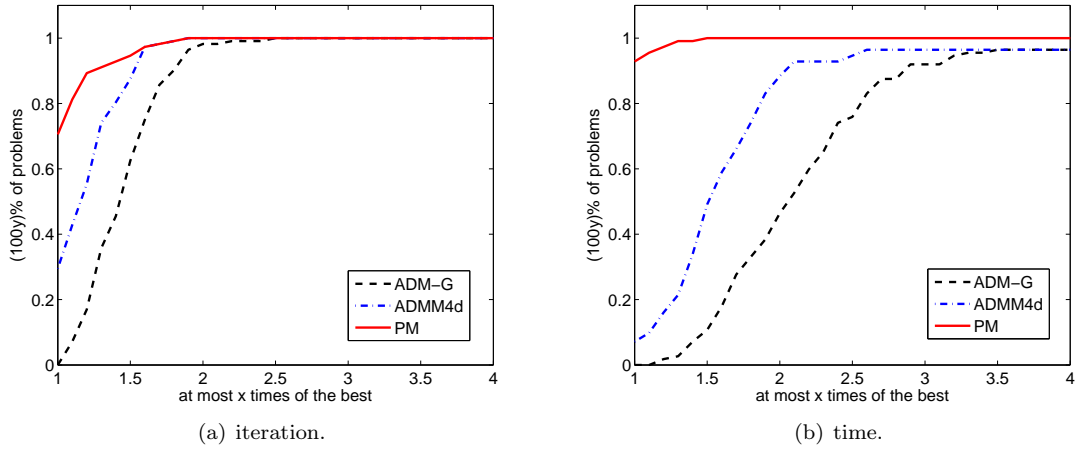


Fig. 2 Performance profiles (iteration and time) of our projection method, ADMM4d and ADM-G for the CQSDP problems with $\varphi(X) = \frac{BX+XB}{2}$ (Tables 1-2).

problems. The main reason behind the efficiency of our projection method, we think, is larger step size (can be greater than $(1 + \sqrt{5})/2$) and skipping the computation of W^{k+1} . In addition, our project method and ADMM4d outperform ADM-G in terms of iteration and computational time, even though the convergence of ADMM4d can not be guaranteed.

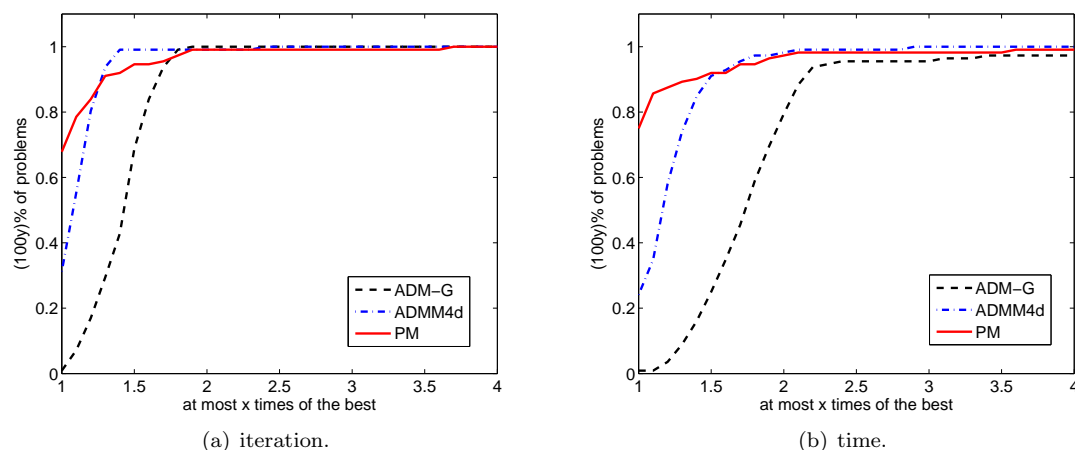


Fig. 3 Performance profiles (iteration and time) of our projection method, ADMM4d and ADM-G for the CQSDP problems with $\varphi(X) = X$ (Tables 3-4).

7 Conclusion

In this paper, we presented a projection method based on the KKT condition for solving the CQSDP problems with nonnegative constraints, and establish its global convergence and $o(\frac{1}{k+1})$ convergence rate. At each iteration, our projection method does not have to solve the subproblem with variable W , compared to the existing multi-block ADMM [3, 21] for solving (4) and (12). Numerical experiments on various large scale QSDPs have demonstrated the efficiency of our proposed ADMM in finding medium accuracy solutions.

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Appendix 1 *Details on the adjusting of σ .*

The key idea for adjusting σ is to balance the progress of primal and dual feasibilities:

$$\mathbf{eta_1} = \max\{p_{inf}, p_{S_+^n}, p_{N^n}\}, \quad \mathbf{eta_2} = \max\{d_{inf}, d_{S_+^n}, d_{N^n}\}.$$

Let

$$\mathbf{theta} = \max\{p_{inf}, d_{inf}, p\delta_{S_+^n}, p\delta_{N^n}, d\delta_{S_+^n}, d\delta_{N^n}, \delta_{XZ}, \delta_{XS}\},$$

$$\mathbf{gamma} = 0.5; \quad \mathbf{sigma_max} = \sigma_{max} \text{ and } \mathbf{sigma_min} = \sigma_{min}.$$

the adjusting of σ is expressed as following:

```

dtmp=eta_1/eta_2;
if iter<=21;      h=3;
  elseif iter<=61; h=6;
  elseif iter<=121; h=50;
  else            h=100;
end
if      theta<1e-5;  gamma=0.8;
elseif  theta<1e-3; gamma=0.6;
end

it_pinf = 0;
it_dinf = 0;
if dtmp<=0.8
  it_pinf = it_pinf+1; it_dinf = 0;
  if it_pinf>h
    sigma = min((1/gamma)*sigma, sigma_max);  it_pinf=0;
  end
else if dtmp>1.25
  it_dinf = it_dinf+1; it_pinf = 0;
  if it_dinf>h
    sigma = max(gamma*sigma, sigma_min); it_dinf = 0;
  end
end
end
end

```


Table 2 The performance of our projection method, ADMM4d and ADM-G on the CQSDP problems with $\varphi(X) = \frac{BX+XB}{2}$ ($seed = 1$). In the table, “PM” and “4d” stands for our projection method and ADMM4d, respectively.

| problem | m_E | n_S | iteration | | | δ | | | δ_g | | | time (second) | | |
|--------------|-------|-------|-----------|-------|-------|----------|---------|---------|------------|---------|---------|---------------|--------|--------|
| | | | ADM-G | 4d | PM | ADM-G | 4d | PM | ADM-G | 4d | PM | ADM-G | 4d | PM |
| theta4 | 1949 | 200 | 574 | 494 | 342 | 9.90e-7 | 9.93e-7 | 9.49e-7 | 8.88e-7 | 1.51e-6 | 1.15e-6 | 6.8 | 6.0 | 3.1 |
| theta42 | 5986 | 200 | 397 | 335 | 515 | 9.90e-7 | 9.85e-7 | 9.83e-7 | 6.68e-7 | 6.87e-7 | 3.96e-7 | 7.2 | 6.1 | 4.6 |
| theta6 | 4375 | 300 | 448 | 389 | 444 | 9.47e-7 | 9.75e-7 | 9.88e-7 | 1.41e-6 | 1.78e-6 | 2.34e-6 | 26.5 | 23.0 | 9.2 |
| theta62 | 13390 | 300 | 437 | 415 | 511 | 9.79e-7 | 9.87e-7 | 9.77e-7 | 8.63e-7 | 9.64e-7 | 6.71e-7 | 30.7 | 31.8 | 19.4 |
| theta8 | 7905 | 400 | 518 | 478 | 461 | 9.92e-7 | 9.87e-7 | 8.95e-7 | 3.82e-7 | 4.60e-7 | 8.48e-7 | 70.7 | 76.4 | 39.5 |
| theta82 | 23872 | 400 | 463 | 392 | 460 | 9.88e-7 | 9.83e-7 | 9.83e-7 | 1.26e-6 | 1.30e-6 | 1.01e-6 | 70.9 | 70.5 | 47.2 |
| theta10 | 12470 | 500 | 613 | 553 | 477 | 9.95e-7 | 9.88e-7 | 8.38e-7 | 3.75e-7 | 4.87e-7 | 7.10e-7 | 146.4 | 151.6 | 78.3 |
| theta102 | 37467 | 500 | 487 | 459 | 485 | 8.88e-7 | 9.87e-7 | 9.92e-7 | 1.01e-6 | 1.43e-6 | 1.08e-6 | 122.3 | 138.3 | 88.4 |
| theta103 | 62516 | 500 | 479 | 463 | 553 | 9.80e-7 | 9.88e-7 | 9.93e-7 | 1.85e-6 | 2.05e-6 | 1.22e-6 | 130.1 | 134.4 | 102.4 |
| theta104 | 87254 | 500 | 510 | 493 | 585 | 9.84e-7 | 9.87e-7 | 9.95e-7 | 2.50e-6 | 2.56e-6 | 2.08e-6 | 135.6 | 144.9 | 103.5 |
| MANN-a27 | 703 | 378 | 1735 | 1308 | 700 | 9.95e-7 | 9.89e-7 | 9.85e-7 | 1.41e-7 | 6.60e-7 | 4.91e-7 | 199.0 | 152.8 | 17.2 |
| san200-0.7-1 | 5971 | 200 | 2363 | 1939 | 2639 | 9.52e-7 | 9.91e-7 | 9.98e-7 | 2.45e-6 | 3.96e-6 | 2.46e-6 | 116.7 | 86.7 | 41.5 |
| sanr200-0.7 | 6033 | 200 | 376 | 321 | 513 | 9.90e-7 | 9.85e-7 | 9.89e-7 | 7.79e-7 | 8.28e-7 | 5.42e-7 | 17.9 | 15.0 | 10.7 |
| c-fat200-1 | 18367 | 200 | 989 | 801 | 644 | 9.98e-7 | 9.95e-7 | 9.91e-7 | 1.00e-6 | 1.12e-6 | 8.35e-7 | 50.6 | 36.8 | 14.6 |
| brock200-1 | 5067 | 200 | 390 | 327 | 495 | 9.82e-7 | 9.74e-7 | 9.80e-7 | 5.05e-7 | 6.17e-7 | 4.03e-7 | 18.7 | 15.6 | 12.9 |
| brock200-4 | 6812 | 200 | 392 | 373 | 471 | 9.81e-7 | 9.81e-7 | 9.94e-7 | 1.10e-6 | 1.16e-6 | 8.25e-7 | 19.3 | 18.0 | 12.1 |
| brock400-1 | 20078 | 400 | 468 | 393 | 460 | 9.89e-7 | 9.81e-7 | 9.93e-7 | 1.07e-6 | 1.15e-6 | 1.00e-6 | 75.5 | 70.6 | 38.4 |
| keller4 | 5101 | 171 | 1338 | 994 | 873 | 9.91e-7 | 9.98e-7 | 9.96e-7 | 2.14e-7 | 3.14e-7 | 2.35e-7 | 59.0 | 42.1 | 20.9 |
| p-hat300-1 | 33918 | 300 | 1207 | 980 | 1023 | 1.00e-6 | 9.98e-7 | 9.98e-7 | 1.54e-6 | 1.48e-6 | 1.18e-6 | 110.1 | 99.9 | 56.7 |
| 1dc.128 | 1472 | 128 | 1255 | 1010 | 847 | 9.98e-7 | 9.99e-7 | 9.95e-7 | 1.16e-6 | 1.28e-6 | 8.88e-7 | 36.9 | 28.2 | 15.8 |
| 1et.128 | 673 | 128 | 7141 | 5834 | 4576 | 1.00e-6 | 1.00e-6 | 1.00e-6 | 7.59e-7 | 8.46e-7 | 1.15e-6 | 216.8 | 176.7 | 96.6 |
| 1tc.128 | 513 | 128 | 5579 | 4353 | 2822 | 9.99e-7 | 1.00e-6 | 1.00e-6 | 1.05e-6 | 1.09e-6 | 1.67e-6 | 165.4 | 121.0 | 62.0 |
| 1zc.128 | 1128 | 128 | 586 | 413 | 717 | 9.99e-7 | 9.93e-7 | 9.96e-7 | 4.47e-7 | 5.85e-8 | 8.36e-7 | 16.8 | 11.2 | 14.2 |
| 1dc.256 | 3840 | 256 | 2286 | 1870 | 1510 | 1.00e-6 | 9.99e-7 | 9.99e-7 | 1.10e-6 | 1.16e-6 | 1.51e-6 | 148.4 | 135.4 | 72.7 |
| 1et.256 | 1665 | 256 | 6425 | 5133 | 4250 | 1.00e-6 | 1.00e-6 | 1.00e-6 | 4.32e-7 | 6.69e-7 | 1.77e-6 | 423.0 | 387.3 | 214.9 |
| 1tc.256 | 1313 | 256 | 7636 | 6094 | 5283 | 1.00e-6 | 1.00e-6 | 9.78e-7 | 4.05e-7 | 2.20e-7 | 8.98e-7 | 512.4 | 458.4 | 272.4 |
| 1zc.256 | 2817 | 256 | 2627 | 2008 | 1553 | 9.99e-7 | 9.99e-7 | 9.99e-7 | 1.19e-7 | 1.96e-7 | 4.05e-7 | 175.9 | 151.7 | 80.7 |
| gka1d | 101 | 101 | 4262 | 3663 | 3849 | 1.00e-6 | 9.98e-7 | 1.00e-6 | 1.04e-7 | 1.48e-7 | 8.09e-8 | 48.2 | 27.3 | 23.1 |
| gka1e | 201 | 201 | 7881 | 7158 | 7228 | 1.00e-6 | 1.00e-6 | 9.99e-7 | 5.15e-7 | 7.00e-7 | 5.54e-7 | 329.7 | 252.5 | 210.5 |
| gka1f | 501 | 501 | 12629 | 10311 | 11511 | 9.99e-7 | 1.00e-6 | 1.00e-6 | 1.23e-6 | 1.32e-6 | 6.96e-7 | 2925.4 | 2723.4 | 1897.5 |
| gka2d | 101 | 101 | 2834 | 2261 | 1939 | 9.95e-7 | 1.00e-6 | 9.99e-7 | 1.25e-6 | 1.13e-6 | 8.31e-7 | 74.7 | 45.1 | 32.6 |
| gka2e | 201 | 201 | 7167 | 5652 | 6123 | 9.99e-7 | 1.00e-6 | 9.99e-7 | 8.39e-7 | 5.96e-7 | 3.75e-7 | 322.4 | 370.7 | 196.4 |
| gka2f | 501 | 501 | 12074 | 9720 | 10596 | 9.95e-7 | 1.00e-6 | 1.00e-6 | 1.14e-6 | 7.36e-7 | 6.09e-7 | 2754.9 | 2486.0 | 1706.0 |
| gka3d | 101 | 101 | 4292 | 3456 | 2880 | 9.98e-7 | 1.00e-6 | 1.00e-6 | 7.66e-7 | 5.58e-7 | 5.95e-7 | 111.1 | 80.4 | 50.7 |
| gka3e | 201 | 201 | 5513 | 4695 | 4388 | 9.99e-7 | 9.97e-7 | 9.99e-7 | 3.48e-7 | 1.22e-6 | 5.77e-7 | 246.5 | 201.1 | 143.7 |
| gka3f | 501 | 501 | 12001 | 9996 | 9425 | 9.96e-7 | 9.99e-7 | 9.99e-7 | 1.66e-6 | 4.48e-7 | 6.13e-7 | 2793.1 | 2616.8 | 1512.5 |
| gka4d | 101 | 101 | 3463 | 3037 | 2264 | 9.95e-7 | 1.00e-6 | 9.99e-7 | 8.38e-7 | 7.32e-7 | 4.36e-7 | 97.5 | 61.9 | 41.7 |
| gka4e | 201 | 201 | 6908 | 5457 | 5692 | 9.99e-7 | 9.92e-7 | 9.99e-7 | 9.90e-7 | 8.09e-7 | 6.68e-7 | 313.2 | 258.6 | 189.1 |
| gka4f | 501 | 501 | 12679 | 9744 | 9366 | 1.00e-6 | 9.98e-7 | 9.99e-7 | 4.77e-7 | 1.45e-6 | 3.52e-7 | 2993.1 | 2669.6 | 1480.2 |
| gka5d | 101 | 101 | 4637 | 3854 | 3104 | 9.99e-7 | 9.99e-7 | 9.99e-7 | 6.91e-7 | 6.81e-7 | 1.96e-7 | 119.6 | 86.3 | 54.4 |
| gka5e | 201 | 201 | 5310 | 4385 | 4328 | 9.99e-7 | 1.00e-6 | 1.00e-6 | 6.01e-7 | 5.17e-7 | 3.45e-7 | 241.4 | 189.3 | 143.5 |
| gka5f | 501 | 501 | 9823 | 9659 | 9751 | 9.99e-7 | 9.99e-7 | 1.00e-6 | 5.99e-6 | 1.25e-6 | 3.60e-7 | 2856.3 | 2557.7 | 1569.5 |
| gka6b | 71 | 71 | 1182 | 983 | 1834 | 9.98e-7 | 9.96e-7 | 9.99e-7 | 5.99e-6 | 7.49e-6 | 1.39e-5 | 6.5 | 4.8 | 7.1 |
| gka6d | 101 | 101 | 3406 | 2619 | 2426 | 1.00e-6 | 1.00e-6 | 9.98e-7 | 7.98e-7 | 8.84e-7 | 6.07e-7 | 54.6 | 28.0 | 25.2 |
| gka7b | 81 | 81 | 425 | 389 | 522 | 9.83e-7 | 9.89e-7 | 9.93e-7 | 5.98e-6 | 5.62e-6 | 1.36e-5 | 7.8 | 5.7 | 6.0 |
| gka7d | 101 | 101 | 2829 | 2339 | 1678 | 1.00e-6 | 9.99e-7 | 9.99e-7 | 3.15e-7 | 5.08e-7 | 3.05e-7 | 63.9 | 41.3 | 25.0 |
| gka8b | 91 | 91 | 1236 | 1192 | 1762 | 9.98e-7 | 9.95e-7 | 1.00e-6 | 2.05e-5 | 2.41e-6 | 4.82e-5 | 27.2 | 23.7 | 26.9 |
| gka8d | 101 | 101 | 3082 | 2720 | 1828 | 9.98e-7 | 1.00e-6 | 9.98e-7 | 5.82e-8 | 1.47e-7 | 5.81e-9 | 76.8 | 57.0 | 32.2 |
| gka9b | 101 | 101 | 2894 | 2148 | 3476 | 9.99e-7 | 1.00e-6 | 9.99e-7 | 1.73e-5 | 1.61e-5 | 3.23e-5 | 68.9 | 50.1 | 58.1 |
| gka9d | 101 | 101 | 3280 | 2720 | 1737 | 9.98e-7 | 9.97e-7 | 9.97e-7 | 3.38e-7 | 3.47e-7 | 1.12e-7 | 82.8 | 62.7 | 31.8 |
| gka10b | 126 | 126 | 2571 | 2226 | 3279 | 1.00e-6 | 1.00e-6 | 1.00e-6 | 2.96e-5 | 2.65e-5 | 5.09e-5 | 67.8 | 61.6 | 64.9 |
| gka10d | 101 | 101 | 4059 | 3555 | 2974 | 9.99e-7 | 1.00e-6 | 1.00e-6 | 5.14e-7 | 4.28e-7 | 4.08e-7 | 104.5 | 81.2 | 54.5 |

Table 4 The performance of our projection method, ADMM4d and ADM-G on the CQSDP problems with $\varphi(X) = X$ ($seed = 1$). In the table, “PM” and “4d” stands for our projection method and ADMM4d, respectively.

| problem | m_E | n_S | iteration | | | δ | | | δ_g | | | time (second) | | |
|--------------|-------|-------|-----------|------|------|----------|---------|---------|------------|---------|---------|---------------|-------|-------|
| | | | 4d | PM | | 4d | PM | | 4d | PM | | 4d | PM | |
| theta4 | 1949 | 200 | 596 | 523 | 402 | 9.99e-7 | 9.90e-7 | 9.91e-7 | 9.72e-7 | 1.48e-6 | 1.50e-6 | 6.2 | 4.7 | 3.6 |
| theta42 | 5986 | 200 | 510 | 459 | 461 | 9.97e-7 | 9.97e-7 | 9.91e-7 | 3.41e-7 | 9.38e-7 | 5.34e-7 | 5.6 | 4.6 | 4.1 |
| theta6 | 4375 | 300 | 567 | 516 | 452 | 9.97e-7 | 9.93e-7 | 8.82e-7 | 1.25e-6 | 1.32e-6 | 8.74e-7 | 15.6 | 15.0 | 8.4 |
| theta62 | 13390 | 300 | 440 | 414 | 513 | 9.81e-7 | 9.88e-7 | 9.91e-7 | 9.38e-7 | 1.28e-6 | 8.33e-7 | 18.7 | 16.9 | 15.0 |
| theta8 | 7905 | 400 | 688 | 598 | 462 | 9.83e-7 | 1.00e-6 | 7.75e-7 | 4.28e-7 | 1.00e-6 | 4.22e-7 | 51.4 | 47.6 | 28.9 |
| theta82 | 23872 | 400 | 485 | 393 | 490 | 9.84e-7 | 9.76e-7 | 9.99e-7 | 7.84e-7 | 1.48e-6 | 1.02e-6 | 43.4 | 37.6 | 38.5 |
| theta10 | 12470 | 500 | 607 | 632 | 530 | 8.06e-7 | 9.98e-7 | 7.48e-7 | 6.05e-7 | 1.08e-6 | 5.57e-7 | 86.8 | 95.7 | 69.6 |
| theta102 | 37467 | 500 | 573 | 469 | 518 | 9.95e-7 | 9.83e-7 | 9.95e-7 | 1.53e-6 | 1.61e-6 | 9.54e-7 | 90.8 | 74.0 | 75.8 |
| theta103 | 62516 | 500 | 482 | 463 | 679 | 9.31e-7 | 9.91e-7 | 9.85e-7 | 1.79e-6 | 2.16e-6 | 2.56e-6 | 82.2 | 74.1 | 102.3 |
| theta104 | 87254 | 500 | 511 | 495 | 896 | 9.99e-7 | 9.87e-7 | 9.89e-7 | 2.57e-6 | 2.65e-6 | 3.75e-6 | 92.7 | 79.0 | 127.7 |
| MANN-a27 | 703 | 378 | 1284 | 697 | 2564 | 9.13e-7 | 9.74e-7 | 9.55e-7 | 2.41e-6 | 2.11e-6 | 1.58e-6 | 89.4 | 47.3 | 166.2 |
| san200-0.7-1 | 5971 | 200 | 2551 | 2029 | 3564 | 9.97e-7 | 8.57e-7 | 9.94e-7 | 1.97e-6 | 2.11e-6 | 6.61e-6 | 102.8 | 72.5 | 122.8 |
| sanr200-0.7 | 6033 | 200 | 478 | 440 | 509 | 9.82e-7 | 9.76e-7 | 9.86e-7 | 9.44e-7 | 9.88e-7 | 6.19e-7 | 19.2 | 15.2 | 16.7 |
| c-fat200-1 | 18367 | 200 | 1015 | 987 | 970 | 9.91e-7 | 9.91e-7 | 9.86e-7 | 2.91e-7 | 2.20e-7 | 1.63e-7 | 39.1 | 29.8 | 26.0 |
| brock200-1 | 5067 | 200 | 489 | 413 | 474 | 9.84e-7 | 9.90e-7 | 9.95e-7 | 7.96e-7 | 8.33e-7 | 3.89e-7 | 21.5 | 14.9 | 15.9 |
| brock200-4 | 6812 | 200 | 409 | 382 | 560 | 9.88e-7 | 9.94e-7 | 9.78e-7 | 1.09e-6 | 1.21e-6 | 1.08e-6 | 18.2 | 12.4 | 17.8 |
| brock400-1 | 20078 | 400 | 570 | 473 | 387 | 9.87e-7 | 9.87e-7 | 9.92e-7 | 6.55e-7 | 1.29e-6 | 6.72e-7 | 62.5 | 52.1 | 39.2 |
| keller4 | 5101 | 171 | 819 | 724 | 794 | 9.94e-7 | 9.96e-7 | 9.93e-7 | 4.66e-7 | 5.57e-7 | 5.22e-7 | 25.3 | 19.4 | 19.5 |
| p-hat300-1 | 33918 | 300 | 1184 | 946 | 1237 | 9.99e-7 | 1.00e-6 | 9.86e-7 | 1.45e-6 | 1.44e-6 | 1.66e-6 | 80.9 | 58.8 | 72.7 |
| 1dc.128 | 1472 | 128 | 1129 | 855 | 786 | 9.92e-7 | 9.92e-7 | 9.93e-7 | 3.41e-7 | 2.98e-6 | 8.59e-7 | 29.7 | 18.4 | 15.7 |
| 1et.128 | 673 | 128 | 1279 | 1239 | 997 | 9.90e-7 | 9.96e-7 | 9.99e-7 | 2.72E-10 | 1.26e-7 | 2.55e-7 | 31.9 | 26.7 | 19.0 |
| 1tc.128 | 513 | 128 | 1041 | 928 | 1161 | 9.79e-7 | 9.34e-7 | 9.98e-7 | 2.43e-6 | 4.36e-7 | 3.92e-6 | 27.1 | 20.3 | 24.5 |
| 1zc.128 | 1128 | 128 | 272 | 251 | 321 | 9.65e-7 | 8.51e-7 | 7.37e-7 | 2.46e-6 | 1.54e-6 | 4.47e-8 | 6.9 | 5.4 | 5.8 |
| 1dc.256 | 3840 | 256 | 2583 | 2331 | 1722 | 1.00e-6 | 9.98e-7 | 9.96e-7 | 3.95e-6 | 3.92e-6 | 4.26e-6 | 130.2 | 102.9 | 70.1 |
| 1et.256 | 1665 | 256 | 2781 | 3755 | 1614 | 9.99e-7 | 1.00e-6 | 9.99e-7 | 5.85e-7 | 5.02e-7 | 7.86e-7 | 133.9 | 176.1 | 61.6 |
| 1tc.256 | 1313 | 256 | 5263 | 4018 | 2997 | 1.00e-6 | 1.00e-6 | 9.99e-7 | 1.52e-6 | 1.68e-6 | 1.36e-6 | 254.1 | 171.1 | 119.7 |
| 1zc.256 | 2817 | 256 | 295 | 250 | 307 | 9.22e-7 | 9.01e-7 | 9.49e-7 | 1.73e-6 | 9.48e-7 | 9.18e-7 | 13.4 | 9.1 | 10.6 |
| gka1d | 101 | 101 | 1356 | 1074 | 953 | 9.90e-7 | 9.96e-7 | 9.98e-7 | 2.02e-7 | 3.85e-7 | 8.48e-7 | 30.9 | 6.0 | 4.7 |
| gka1e | 201 | 201 | 2565 | 1946 | 1881 | 9.97e-7 | 1.00e-6 | 1.00e-6 | 1.11e-6 | 7.63e-7 | 1.06e-6 | 91.8 | 35.8 | 27.8 |
| gka1f | 501 | 501 | 3222 | 2454 | 2177 | 1.00e-6 | 9.95e-7 | 9.99e-7 | 2.04e-7 | 1.43e-6 | 3.11e-6 | 479.5 | 299.6 | 290.6 |
| gka2d | 101 | 101 | 1339 | 953 | 855 | 9.90e-7 | 9.77e-7 | 9.96e-7 | 4.62e-7 | 5.26e-7 | 1.38e-6 | 31.6 | 15.7 | 15.3 |
| gka2e | 201 | 201 | 2328 | 1743 | 1434 | 9.98e-7 | 9.94e-7 | 9.94e-7 | 8.47e-7 | 7.39e-7 | 6.16e-7 | 91.6 | 52.0 | 45.8 |
| gka2f | 501 | 501 | 4937 | 3907 | 3063 | 9.95e-7 | 1.00e-6 | 9.99e-7 | 9.45e-7 | 2.03e-7 | 6.75e-7 | 766.3 | 532.5 | 445.3 |
| gka3d | 101 | 101 | 2339 | 1944 | 1877 | 9.77e-7 | 9.93e-7 | 9.65e-7 | 3.14e-7 | 2.90e-7 | 3.86e-7 | 55.1 | 33.6 | 33.9 |
| gka3e | 201 | 201 | 3458 | 2785 | 2477 | 9.98e-7 | 9.97e-7 | 9.99e-7 | 7.81e-7 | 9.36e-7 | 2.80e-7 | 133.2 | 88.5 | 79.0 |
| gka3f | 501 | 501 | 6603 | 5240 | 4600 | 9.99e-7 | 9.99e-7 | 9.99e-7 | 1.08e-6 | 9.29e-7 | 7.40e-7 | 1009.6 | 741.2 | 678.9 |
| gka4d | 101 | 101 | 1747 | 1200 | 1184 | 9.94e-7 | 9.95e-7 | 9.99e-7 | 7.67e-7 | 4.85e-7 | 9.53e-7 | 39.3 | 21.1 | 21.1 |
| gka4e | 201 | 201 | 2993 | 2328 | 1729 | 9.87e-7 | 9.89e-7 | 9.95e-7 | 8.91e-8 | 8.71e-7 | 1.56e-6 | 110.0 | 70.1 | 53.6 |
| gka4f | 501 | 501 | 6225 | 5246 | 4244 | 1.00e-6 | 9.99e-7 | 9.98e-7 | 8.99e-7 | 1.57e-6 | 1.85e-6 | 962.8 | 752.6 | 618.2 |
| gka5d | 101 | 101 | 1775 | 1159 | 1117 | 9.74e-7 | 9.99e-7 | 9.91e-7 | 7.41e-7 | 4.86e-9 | 1.21e-6 | 42.9 | 20.1 | 20.4 |
| gka5e | 201 | 201 | 3624 | 2781 | 2599 | 9.97e-7 | 9.99e-7 | 9.98e-7 | 7.16e-7 | 6.03e-7 | 7.11e-7 | 132.8 | 86.1 | 81.2 |
| gka5f | 501 | 501 | 6598 | 5522 | 4783 | 9.96e-7 | 1.00e-6 | 9.98e-7 | 1.02e-6 | 1.53e-6 | 1.62e-6 | 982.1 | 794.6 | 677.6 |
| gka6b | 71 | 71 | 784 | 789 | 968 | 9.95e-7 | 9.90e-7 | 9.96e-7 | 1.99e-5 | 2.29e-5 | 4.73e-5 | 15.3 | 3.5 | 14.5 |
| gka6d | 101 | 101 | 1889 | 1375 | 1156 | 9.97e-7 | 9.92e-7 | 9.97e-7 | 3.05e-7 | 6.49e-7 | 1.97e-7 | 45.0 | 10.5 | 21.0 |
| gka7b | 81 | 81 | 799 | 671 | 955 | 9.98e-7 | 9.94e-7 | 9.94e-7 | 1.23e-5 | 1.33e-5 | 2.82e-5 | 16.5 | 7.7 | 14.7 |
| gka7d | 101 | 101 | 1711 | 1273 | 1196 | 9.98e-7 | 9.95e-7 | 9.97e-7 | 5.38e-7 | 8.34e-7 | 5.01e-7 | 39.5 | 19.4 | 20.7 |
| gka8b | 91 | 91 | 922 | 795 | 1335 | 9.98e-7 | 9.95e-7 | 9.94e-7 | 2.72e-5 | 2.72e-5 | 5.46e-5 | 19.9 | 12.9 | 20.9 |
| gka8d | 101 | 101 | 1873 | 1367 | 1284 | 9.94e-7 | 9.58e-7 | 9.97e-7 | 7.97e-7 | 1.33e-6 | 5.78e-7 | 44.1 | 23.4 | 23.3 |
| gka9b | 101 | 101 | 851 | 751 | 1313 | 9.97e-7 | 9.95e-7 | 9.96e-7 | 1.54e-5 | 1.64e-5 | 2.63e-5 | 19.1 | 13.3 | 24.4 |
| gka9d | 101 | 101 | 1713 | 1293 | 1215 | 9.87e-7 | 9.72e-7 | 9.95e-7 | 5.08e-7 | 1.85e-7 | 1.06e-7 | 41.0 | 24.6 | 21.4 |
| gka10b | 126 | 126 | 3619 | 2319 | 4351 | 1.00e-6 | 1.00e-6 | 1.00e-6 | 4.62e-5 | 4.98e-5 | 1.12e-4 | 93.9 | 47.2 | 86.7 |
| gka10d | 101 | 101 | 2257 | 1697 | 1519 | 1.00e-6 | 9.97e-7 | 1.00e-6 | 7.17e-7 | 3.03e-7 | 1.01e-6 | 56.9 | 33.2 | 27.4 |