Solving nuclear norm regularized and semidefinite matrix least squares problems with linear equality constraints

Kaifeng Jiang, Defeng Sun, Kim-Chuan Toh

Abstract We introduce a partial proximal point algorithm for solving nuclear norm regularized and semidefinite matrix least squares problems with linear equality constraints. For the inner subproblems, we show that the positive definiteness of the generalized Hessian of the objective function for the inner subproblems is equivalent to the constraint nondegeneracy of the corresponding primal problem, which is a key property for applying a semismooth Newton-CG method to solve the inner subproblems efficiently. Numerical experiments on large scale matrix least squares problems arising from low rank matrix approximation, as well as regularized kernel estimation and Euclidean distance matrix completion problems in molecular conformation, show that our algorithm is efficient and robust.

1 Introduction

Let $\Re^{p \times q}$ be the space of all $p \times q$ matrices equipped with the standard trace inner product $\langle X, Y \rangle = \mathrm{Tr}(X^T Y)$ and its induced Frobenius norm $\| \cdot \|$. Without loss of generality, we assume $p \leq q$ throughout this paper. For a given $X \in \Re^{p \times q}$, its nuclear norm $\|X\|_*$ is defined as the sum of all its singular values and its operator norm $\|X\|_2$ is the largest singular value. Let $\mathscr{S}^n$ be the space of all $n \times n$ symmetric matrices and

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$\mathscr{S}_+^n$ be the cone of symmetric positive semidefinite matrices. We use the notation $X \succeq 0$ to denote that X is a symmetric positive semidefinite matrix.

In this paper, we consider the following nuclear norm regularized matrix least squares problem with linear equality constraints:

$$\min_{X \in \mathfrak{R}^{p \times q}} \left\{ \frac{1}{2} \|\mathscr{A}(X) - b\|^2 + \rho \|X\|_* + \langle C, X \rangle \ : \ \mathscr{B}(X) = d \right\}, \tag{1}$$

where $\mathscr{A} : \mathfrak{R}^{p \times q} \to \mathfrak{R}^m$ and $\mathscr{B} : \mathfrak{R}^{p \times q} \to \mathfrak{R}^s$ are given linear maps, $C \in \mathfrak{R}^{p \times q}, b \in \mathfrak{R}^m, d \in \mathfrak{R}^s$, and ρ is a given positive parameter. Note that the nuclear norm has been a very popular regularizer which favors a low rank solution of (1) [4, 9, 10, 24]. The problem (1) arises in many applications when one needs to find a low rank approximation of a given matrix while preserving certain desired structures. In many data analysis problems, the collected empirical data, which are usually messy and incomplete, typically do not have the specified structure or the desired low rank. It is important to find the nearest low rank approximation of the given matrix while maintaining the underlying structure of the original system. For example, in statistics, the regression matrix for the multiple regression model with a constant term has a column of all ones, and this column should not be perturbed during the low rank approximation.

When $C = 0$ and either $\mathscr{A}$ or $\mathscr{B}$ is absent in (1), the problem (1) includes the well studied matrix completion problem if either $\mathscr{B}$ or $\mathscr{A}$ is the projection onto the set of observed matrix entries. We should mention that many specialized first-order algorithms have been designed for various variants of the matrix completion problem; see for example [3, 22, 29, 19]. But as far as we are aware of, no papers have specifically discussed the nuclear norm regularized matrix least squares problem with additional structural constraints. The problem can of course be solved by several general first-order methods such as [6, 7, 8, 12, 13]. However, our numerical experiments show that these first-order methods may not achieve a satisfactory level of accuracy within a reasonable time.

In this paper, we design a partial proximal point algorithm (PPA) proposed by Ha [16] for solving (1), in which only some of the variables appear in the quadratic proximal term. Given a sequence of parameters σ_k such that

$$0 < \sigma_k \uparrow \sigma_\infty \leq +\infty, \tag{2}$$

and an initial point $X^0 \in \mathfrak{R}^{p \times q}$, the partial PPA for solving (1) generates a sequence $\{(u^k, X^k)\} \subseteq \mathfrak{R}^m \times \mathfrak{R}^{p \times q}$ via the following scheme:

$$(u^{k+1}, X^{k+1}) \approx \arg\min \left\{ f_\rho(u, X) + \frac{1}{2\sigma_k} \|X - X^k\|^2 \ : \ \mathscr{A}(X) + u = b, \mathscr{B}(X) = d \right\}, \tag{3}$$

where $f_\rho(u, X) := \frac{1}{2} \|u\|^2 + \rho \|X\|_* + \langle C, X \rangle$. A key issue in the partial PPA which we must address is how to solve the partially regularized problem (3) efficiently. In our algorithm, we solve (3) via its dual, which is an unconstrained concave maximization problem whose objective function is continuously differentiable but not

twice continuously differentiable. Because of the latter property, standard Newton's method cannot be used to solve the inner subproblem. However, we can show that the objective function is strongly semismooth due to the strong semismoothness of the soft thresholding operator [18, Theorem 2.1]. Thus we can apply the semismooth Newton method of Qi and Sun [23] to solve the inner subproblem. Recently Zhao, Sun and Toh [32] proposed a Newton-CG augmented Lagrangian (SDPNAL) method for solving SDP problems, in which the inner subproblems are solved by using an inexact semismooth Newton-CG method. Their numerical results on a variety of large scale SDP problems demonstrated that the SDPNAL method is very efficient. This strongly motivated us to use a semismooth Newton-CG (SSNCG) method to solve the inner subproblems for achieving fast convergence. For our case, the global and fast local convergence of the SSNCG method is established under a constraint nondegeneracy condition, together with the strong semismoothness property of the soft thresholding operator.

The partial PPA which we will develop for solving (1) can easily be modified to solve the following semidefinite matrix least squares problem:

$$\min_{X \in \mathscr{S}^n} \left\{ \frac{1}{2} \|\mathscr{A}(X) - b\|^2 + \langle C, X \rangle \ : \ \mathscr{B}(X) = d, \ X \succeq 0 \right\}, \tag{4}$$

where $\mathscr{A} : \mathscr{S}^n \to \mathfrak{R}^m$ and $\mathscr{B} : \mathscr{S}^n \to \mathfrak{R}^s$ are given linear maps, $b \in \mathfrak{R}^m, d \in \mathfrak{R}^s$, and $C \in \mathscr{S}^n$. Thus in this paper, we also design a partial PPA to solve (4).

For the partial PPA (with SSNCG method for solving the inner subproblems) we have designed and implemented numerical experiments on large scale matrix least squares problems arising from low rank matrix approximation, as well as regularized kernel estimation and Euclidean distance matrix completion problems in molecular conformation, show that our algorithm is efficient and robust.

The remaining parts of this paper are organized as follows. In section 2, we present some preliminaries about semismooth functions. In section 3, we describe how to use the partial PPA to solve (1) and introduce a SSNCG method for solving the inner subproblems. The convergence analysis of our proposed algorithm is also established. In section 4, we briefly explain how the SSNCG partial PPA for solving (1) can be modified to solve (4). In section 5, we report the numerical performance of our algorithm for solving the various classes of problems mentioned in the last paragraph. We conclude the paper in section 6.

2 Preliminaries

In this section, we give a brief introduction on some basic concepts such as the B-subdifferential and Clarke's generalized Jacobian of the soft-thresholding operator. These concepts and properties will be critical for us to develop a SSNCG method for solving the inner subproblems in our partial PPA.

Let $F : \mathfrak{R}^m \longrightarrow \mathfrak{R}^l$ be a locally Lipschitz function. By Rademacher's theorem, F is Fréchet differentiable almost everywhere. Let D_F denote the set of points where

F is differentiable. The B-subdifferential of F at $x \in \mathfrak{R}^m$ is defined by

$$\partial_B F(x) := \{V : V = \lim_{k \to \infty} F'(x^k), \ x^k \longrightarrow x, \ x^k \in D_F\},$$

where $F'(x)$ denotes the Jacobian of F at $x \in D_F$. Then Clarke's [5] generalized Jacobian of F at $x \in \mathfrak{R}^m$ is defined as the convex hull of $\partial_B F(x)$, i.e., $\partial F(x) = \text{conv}\{\partial_B F(x)\}$.

Let $Y \in \mathfrak{R}^{p \times q}$ admit the following singular value decomposition (SVD):

$$Y = U[\Sigma \ 0]V^T, \tag{5}$$

where $U \in \mathfrak{R}^{p \times p}$ and $V \in \mathfrak{R}^{q \times q}$ are orthogonal matrices, $\Sigma = \text{Diag}(\sigma_1, \cdots, \sigma_p)$ is the diagonal matrix of singular values of Y, with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$. Define $g_\rho : \mathfrak{R} \to \mathfrak{R}$ by

$$g_\rho(t) := (t - \rho)_+ - (-t - \rho)_+. \tag{6}$$

For each parameter $\rho > 0$, the soft-thresholding operator $D_\rho : \mathfrak{R}^{p \times q} \to \mathfrak{R}^{p \times q}$ is defined by

$$D_\rho(Y) = U[\Sigma_\rho \ 0]V^T, \tag{7}$$

where $\Sigma_\rho = \text{Diag}(g_\rho(\sigma_1), \ldots, g_\rho(\sigma_p))$. From [18, Thorem 2.1], we know that $D_\rho(\cdot)$ is strongly semismooth everywhere in $\mathfrak{R}^{p \times q}$. Decompose $V \in \mathfrak{R}^{q \times q}$ into the form $V = [V_1 \ V_2]$, where $V_1 \in R^{q \times p}$ and $V_2 \in \mathfrak{R}^{q \times (q-p)}$. Let the orthogonal matrix $Q \in \mathfrak{R}^{(p+q) \times (p+q)}$ be defined by

$$Q := \frac{1}{\sqrt{2}} \begin{bmatrix} U & U & 0 \\ V_1 & -V_1 & \sqrt{2}V_2 \end{bmatrix}, \tag{8}$$

and $\Xi : \mathfrak{R}^{p \times q} \to \mathscr{S}^{p+q}$ be defined by

$$\Xi(Y) := \begin{bmatrix} 0 & Y \\ Y^T & 0 \end{bmatrix}, \ Y \in \mathfrak{R}^{p \times q}. \tag{9}$$

Then, by [14, Section 8.6], we know that the symmetric matrix $\Xi(Y)$ has the following spectral decomposition:

$$\Xi(Y) = Q \begin{bmatrix} \Sigma & 0 & 0 \\ 0 & -\Sigma & 0 \\ 0 & 0 & 0 \end{bmatrix} Q^T, \tag{10}$$

i.e., the eigenvalues of $\Xi(Y)$ are $\pm\sigma_i, i = 1, \ldots, p$, and 0 of multiplicity $q - p$. For any $W = P\text{Diag}(\lambda_1, \cdots, \lambda_{p+q})P^T \in \mathscr{S}^{p+q}$, define $G_\rho : \mathscr{S}^{p+q} \to \mathscr{S}^{p+q}$ by

$$G_\rho(W) := P\text{Diag}(g_\rho(\lambda_1), \cdots, g_\rho(\lambda_{p+q}))P^T = (W - \rho I)_+ - (-W - \rho I)_+,$$

where $(\cdot)_+$ denotes the projection onto the cone of positive semidefinite matrices. By direct calculations, we have

$$\Psi(Y) := G_\rho(\Xi(Y)) = Q \begin{bmatrix} \Sigma_\rho & 0 & 0 \\ 0 & -\Sigma_\rho & 0 \\ 0 & 0 & 0 \end{bmatrix} Q^T = \begin{bmatrix} 0 & D_\rho(Y) \\ D_\rho(Y)^T & 0 \end{bmatrix}. \quad (11)$$

Note that (11) provides an easy way for us to calculate the derivative (if it exists) of D_ρ at Y, as we shall see in Proposition 1. For later discussion, we define the following three index sets:

$$\alpha := \{1,\ldots,p\}, \quad \gamma := \{p+1,\ldots,2p\}, \quad \beta := \{2p+1,\ldots,p+q\}. \quad (12)$$

For any $\lambda = (\lambda_1,\ldots,\lambda_{p+q})^T \in \Re^{p+q}$ and $\lambda_i \neq \pm\rho, i = 1,\ldots,p+q$, we denote by Ω the $(p+q) \times (p+q)$ first divided difference symmetric matrix of $g_\rho(\cdot)$ at λ [2] whose (i,j)th entry is given by

$$\Omega_{ij} = \begin{cases} \dfrac{g_\rho(\lambda_i) - g_\rho(\lambda_j)}{\lambda_i - \lambda_j} & \text{if } \lambda_i \neq \lambda_j, \\ g_\rho'(\lambda_i) & \text{if } \lambda_i = \lambda_j. \end{cases}$$

Proposition 1. *Let $Y \in \Re^{p\times q}$ admit the SVD in (5). If $\sigma_i \neq \rho, i = 1,\ldots,p$, then $D_\rho(\cdot)$ is differentiable at Y, and for any $H \in \Re^{p\times q}$, we have*

$$D_\rho'(Y)H = U\left[\left(\Omega_{\alpha\alpha} \circ \left(\frac{H_1 + H_1^T}{2}\right) + \Omega_{\alpha\gamma} \circ \left(\frac{H_1 - H_1^T}{2}\right)\right)V_1^T + \left(\Omega_{\alpha\beta} \circ H_2\right)V_2^T\right], \quad (13)$$

where $H_1 = U^T H V_1$ and $H_2 = U^T H V_2$.

Proof. For any $\lambda = (\lambda_1,\ldots,\lambda_{p+q})^T \in \Re^{p+q}$, let $\lambda_i = \sigma_i$ for $i \in \alpha$, $\lambda_i = -\sigma_{i-p}$ for $i \in \gamma$, and $\lambda_i = 0$ for $i \in \beta$. Since $\sigma_i \neq \rho, i = 1,\ldots,p$, from (10) and (11) we can obtain the first divided difference matrix for $g_\rho(\cdot)$ at λ:

$$\Omega = \begin{pmatrix} \Omega_{\alpha\alpha} & \Omega_{\alpha\gamma} & \Omega_{\alpha\beta} \\ \Omega_{\alpha\gamma}^T & \Omega_{\gamma\gamma} & \Omega_{\gamma\beta} \\ \Omega_{\alpha\beta}^T & \Omega_{\gamma\beta}^T & \Omega_{\beta\beta} \end{pmatrix}. \quad (14)$$

Since $g_\rho(\cdot)$ is an odd function, we have the following results:

$$\Omega_{\gamma\gamma} = \Omega_{\alpha\alpha}, \quad \Omega_{\alpha\gamma} = \Omega_{\alpha\gamma}^T, \quad \Omega_{\gamma\beta} = \Omega_{\alpha\beta}, \quad \Omega_{\beta\beta} = 0.$$

Now, by a result of Löwner [20], we have from (11) that for any $H \in \Re^{p\times q}$,

$$\Psi'(Y)H = G_\rho'(\Xi(Y))\Xi(H) = Q\left[\Omega \circ (Q^T \Xi(H)Q)\right]Q^T.$$

Since

$$Q^T \Xi(H)Q = \frac{1}{2}\begin{bmatrix} H_1 + H_1^T & H_1^T - H_1 & \sqrt{2}H_2 \\ H_1 - H_1^T & -(H_1 + H_1^T) & \sqrt{2}H_2 \\ \sqrt{2}H_2^T & \sqrt{2}H_2^T & 0 \end{bmatrix}, \quad (15)$$

by simple algebraic calculations, we have that

$$\Psi'(Y)H = Q\big[\Omega \circ (Q^T\,\Xi(H)Q)\big]Q^T = \begin{bmatrix} 0 & M_{12} \\ M_{12}^T & 0 \end{bmatrix}, \tag{16}$$

where $M_{12} = U\Big[\Big(\Omega_{\alpha\alpha}\circ\big(\frac{H_1+H_1^T}{2}\big) + \Omega_{\alpha\gamma}\circ\big(\frac{H_1-H_1^T}{2}\big)\Big)V_1^T + \big(\Omega_{\alpha\beta}\circ H_2\big)V_2^T\Big]$. Since

$$\Psi'(Y)H \ = \ \begin{bmatrix} 0 & D_\rho'(Y)H \\ (D_\rho'(Y)H)^T & 0 \end{bmatrix},$$

we have from (16) that $D_\rho'(Y)H = M_{12}$

Next, we give a characterization of the generalized Jacobian of $D_\rho(\cdot)$, which was presented in [31, Lemma 2.3.6 and Proposition 2.3.7]. For any $\lambda = (\lambda_1, \ldots, \lambda_{p+q})^T \in \Re^{p+q}$, let $\lambda_i = \sigma_i$ for $i \in \alpha$, $\lambda_i = -\sigma_{i-p}$ for $i \in \gamma$, and $\lambda_i = 0$ for $i \in \beta$. For each threshold parameter $\rho > 0$, we decompose the index set α into the following three subindex sets:

$$\alpha_1 := \{i\,|\,\sigma_i(Y) > \rho\}, \ \alpha_2 := \{i\,|\,\sigma_i(Y) = \rho\}, \ \alpha_3 := \{i\,|\,\sigma_i(Y) < \rho\}. \tag{17}$$

Let Γ denote the following $(p+q) \times (p+q)$ symmetric matrix

$$\Gamma = \begin{pmatrix} \Gamma_{\alpha\alpha} & \Gamma_{\alpha\gamma} & \Gamma_{\alpha\beta} \\ \Gamma_{\alpha\gamma}^T & \Gamma_{\gamma\gamma} & \Gamma_{\gamma\beta} \\ \Gamma_{\alpha\beta}^T & \Gamma_{\gamma\beta}^T & \Gamma_{\beta\beta} \end{pmatrix}, \tag{18}$$

whose (i,j)th entry is given by

$$\Gamma_{ij} = \begin{cases} \dfrac{g_\rho(\lambda_i) - g_\rho(\lambda_j)}{\lambda_i - \lambda_j} & \text{if } \lambda_i \neq \lambda_j, \\ 1 & \text{if } \lambda_i = \lambda_j \text{ and } |\lambda_i| > \rho, \\ \in \partial g_\rho(\lambda_i) = [0,1] & \text{if } \lambda_i = \lambda_j \text{ and } |\lambda_i| = \rho, \\ 0 & \text{if } \lambda_i = \lambda_j \text{ and } |\lambda_i| < \rho. \end{cases} \tag{19}$$

Proposition 2. *Let $Y \in \Re^{p \times q}$ admit the SVD in (5). Then, for any $\mathscr{V} \in \partial_B\Psi(Y)$ and any $H \in \Re^{p \times q}$, we have*

$$\mathscr{V}(H) = Q(\Gamma \circ (Q^T\,\Xi(H)Q))Q^T. \tag{20}$$

Moreover, for any $\mathscr{W} \in \partial_B D_\rho(Y)$, we have

$$\mathscr{W}(H) = U\Big[\Big(\Gamma_{\alpha\alpha}\circ\big(\frac{H_1+H_1^T}{2}\big) + \Gamma_{\alpha\gamma}\circ\big(\frac{H_1-H_1^T}{2}\big)\Big)V_1^T + \big(\Gamma_{\alpha\beta}\circ H_2\big)V_2^T\Big], \tag{21}$$

where $H_1 = U^T H V_1$, $H_2 = U^T H V_2$, and

$$\Gamma_{\alpha\alpha} = \begin{pmatrix} \tau_{\alpha_1\alpha_1} & \tau_{\alpha_1\alpha_2} & \tau_{\alpha_1\alpha_3} \\ \tau_{\alpha_1\alpha_2}^T & v_{\alpha_2\alpha_2} & 0 \\ \tau_{\alpha_1\alpha_3}^T & 0 & 0 \end{pmatrix}, \quad \begin{array}{l} \tau_{ij} = 1, \text{ for } i \in \alpha_1, \, j \in \alpha_1 \cup \alpha_2, \\ \tau_{ij} = \dfrac{\sigma_i - \rho}{\sigma_i - \sigma_j}, \text{ for } i \in \alpha_1, \, j \in \alpha_3, \\ v_{ij} = v_{ji} \in [0,1], \text{ for } i, j \in \alpha_2, \end{array} \quad (22)$$

$$\Gamma_{\alpha\gamma} = \begin{pmatrix} \omega_{\alpha_1\alpha_1} & \omega_{\alpha_1\alpha_2} & \omega_{\alpha_1\alpha_3} \\ \omega_{\alpha_1\alpha_2}^T & 0 & 0 \\ \omega_{\alpha_1\alpha_3}^T & 0 & 0 \end{pmatrix}, \quad \omega_{ij} := \frac{(\sigma_i - \rho)_+ + (\sigma_j - \rho)_+}{\sigma_i + \sigma_j}, \text{ for } i \in \alpha_1, \, j \in \alpha,$$

$$(23)$$

$$\Gamma_{\alpha\beta} = \begin{pmatrix} \mu_{\alpha_1\bar\beta} \\ 0 \end{pmatrix}, \, \bar\beta = \beta - 2p = \{1, \ldots, q - p\}, \, \mu_{ij} = \frac{\sigma_i - \rho}{\sigma_i}, \text{ for } i \in \alpha_1, \, j \in \bar\beta. \quad (24)$$

Proof. See [31, Lemma 2.3.6 and Proposition 2.3.7].

Let the operator $\mathscr{W}^0 : \mathfrak{R}^{p \times q} \to \mathfrak{R}^{p \times q}$ be defined by

$$\mathscr{W}^0(H) = U \left[\left(\Gamma_{\alpha\alpha}^0 \circ \left(\frac{H_1 + H_1^T}{2} \right) + \Gamma_{\alpha\gamma} \circ \left(\frac{H_1 - H_1^T}{2} \right) \right) V_1^T + \left(\Gamma_{\alpha\beta} \circ H_2 \right) V_2^T \right],$$

$$(25)$$

where $\Gamma_{\alpha\alpha}^0$ is of the form (22) with $(\Gamma_{\alpha\alpha}^0)_{\alpha_2\alpha_2} = 0$. Then we have that $\mathscr{W}^0$ is an element in $\partial_B D_\rho(Y)$.

3 A partial proximal point algorithm for matrix least squares problems

In this section, we will show how to use the partial proximal point algorithm (PPA) to solve the problem (1).

It is easy to see that (1) can be rewritten as follows:

$$\min_{u \in \mathfrak{R}^m, X \in \mathfrak{R}^{p \times q}} \left\{ f_\rho(u, X) := \frac{1}{2} \|u\|^2 + \rho \|X\|_* + \langle C, X \rangle \, : \, \mathscr{A}(X) + u = b, \mathscr{B}(X) = d \right\}.$$

$$(26)$$

Note that the objective function $f_\rho(u, X)$ is strongly convex in u for all $X \in \mathfrak{R}^{p \times q}$. Let $l(u, X; \zeta, \xi) : \mathfrak{R}^m \times \mathfrak{R}^{p \times q} \times \mathfrak{R}^m \times \mathfrak{R}^s \to \mathfrak{R}$ be the Lagrangian function for (26):

$$l(u, X; \zeta, \xi) := f_\rho(u, X) + \langle \zeta, b - \mathscr{A}(X) - u \rangle + \langle \xi, d - \mathscr{B}(X) \rangle. \quad (27)$$

Then the essential objective function in (26) is

$$f(u, X) := \sup_{\zeta \in \mathfrak{R}^m, \, \xi \in \mathfrak{R}^s} l(u, X; \zeta, \xi) = \begin{cases} f_\rho(u, X) & \text{if } (u, X) \in \mathscr{F}_P, \\ +\infty & \text{if } (u, X) \notin \mathscr{F}_P, \end{cases} \quad (28)$$

where $\mathscr{F}_P = \{(u, X) \in \mathfrak{R}^m \times \mathfrak{R}^{p \times q} \mid \mathscr{A}(X) + u = b, \mathscr{B}(X) = d\}$ is the feasible set of (26). The dual problem of (26) is given by:

$$\max \left\{ g_\rho(\zeta, \xi) : \mathscr{A}^*(\zeta) + \mathscr{B}^*(\xi) + Z = C, \|Z\|_2 \le \rho, \ \zeta \in \Re^m, \ \xi \in \Re^s, \ Z \in \Re^{p \times q} \right\},$$
$$\tag{29}$$

where $g_\rho(\zeta, \xi) := -\frac{1}{2} \|\zeta\|^2 + \langle b, \zeta \rangle + \langle d, \xi \rangle$. Since $f(u, X)$ is strongly convex in u for all $X \in \Re^{p \times q}$, we apply the partial PPA proposed by Ha [16] to the maximal monotone operator $\mathscr{T}_f = \partial f$, in which only the variable X appears in the quadratic proximal term. Let $\Pi : \Re^m \times \Re^{p \times q} \to \Re^m \times \Re^{p \times q}$ be the orthogonal projector of $\Re^m \times \Re^{p \times q}$ onto $\{0\} \times \Re^{p \times q}$, i.e., $\Pi(u, X) = (0, X)$ and $P_\sigma := (\Pi + \sigma \mathscr{T}_f)^{-1} \Pi$ for a given positive parameter σ. From [18, Proposition 3.1], we know that the operator P_σ is single-valued. Given a starting point $(u^0, X^0) \in \Re^m \times \Re^{p \times q}$, the partial PPA for solving problem (26) can be expressed as follows:

$$(u^{k+1}, X^{k+1}) \approx P_{\sigma_k}(u^k, X^k) := \underset{u \in \Re^m, X \in \Re^{p \times q}}{\operatorname{argmin}} \left\{ f(u, X) + \frac{1}{2\sigma_k} \|X - X^k\|^2 \right\}, \quad (30)$$

where the sequence $\{\sigma_k\}$ satisfies (2). Note that for the standard PPA, the map Π in P_σ is replaced by the identity map.

Next we compute the partial quadratic regularization of f in (30), which plays a key role in the study of the partial PPA for solving (26). For a given parameter $\sigma > 0$, the partial quadratic regularization of f in (28) associated with σ is given by

$$F_\sigma(X) = \min_{u \in \Re^m, Y \in \Re^{p \times q}} \left\{ f(u, Y) + \frac{1}{2\sigma} \|Y - X\|^2 \right\}. \tag{31}$$

From [18, Section 3], we have that

$$F_\sigma(X) = \sup_{\zeta \in \Re^m, \ \xi \in \Re^s} \theta_\sigma(\zeta, \xi; X),$$

where

$$\theta_\sigma(\zeta, \xi; X) := -\frac{1}{2} \|\zeta\|^2 + \langle b, \zeta \rangle + \langle d, \xi \rangle + \frac{1}{2\sigma} \|X\|^2 - \frac{1}{2\sigma} \|D_{\rho\sigma}(W(\zeta, \xi; X))\|^2$$
$$\tag{32}$$

and $W(\zeta, \xi; X) = X - \sigma(C - \mathscr{A}^*\zeta - \mathscr{B}^*\xi)$. By the saddle point theorem [25, Theorem 28.3], we have that for any

$$(\zeta(X), \xi(X)) \in \underset{\zeta \in \Re^m, \ \xi \in \Re^s}{\operatorname{argsup}} \ \theta_\sigma(\zeta, \xi; X),$$

the point $(\zeta(X), D_{\rho\sigma}(W(\zeta(X), \xi(X); X)))$ is the unique solution to (31).

Now we formally present the partial PPA for solving (26).

Algorithm 1. Given a tolerance $\varepsilon > 0$, $(u^0, X^0) \in \mathfrak{R}^m \times \mathfrak{R}^{p \times q}$, $\sigma_0 > 0$. Set $k = 0$. Iterate:

Step 1.   Compute an approximate maximizer

$$(\zeta^{k+1}, \xi^{k+1}) \approx \underset{\zeta \in \mathfrak{R}^m, \xi \in \mathfrak{R}^s}{\mathrm{argsup}} \; \theta_{\sigma_k}(\zeta, \xi; X^k), \tag{33}$$

where $\theta_{\sigma_k}(\zeta, \xi; X^k)$ is defined in (32).
Step 2.   Compute $W^{k+1} := W(\zeta^{k+1}, \xi^{k+1}; X^k)$. Set

$$u^{k+1} = \zeta^{k+1}, \; X^{k+1} = D_{\rho\sigma_k}(W^{k+1}), \quad Z^{k+1} = \frac{1}{\sigma_k}(D_{\rho\sigma_k}(W^{k+1}) - W^{k+1}).$$

Step 3.   If $\|(X^k - X^{k+1})/\sigma_k\| \leq \varepsilon$; stop; else; update σ_k; end.

Suppose that $(\bar{\zeta}(X^k), \bar{\xi}(X^k))$ is an optimal solution of the inner subproblem (33) for each X^k. In order to terminate (33) in the above partial PPA, we introduce the following stopping criteria:

$$\sup \theta_k(\zeta, \xi) - \theta_k(\zeta^{k+1}, \xi^{k+1}) \leq \frac{\varepsilon_k^2}{4\sigma_k}, \tag{34a}$$

$$\|\zeta^{k+1} - \bar{\zeta}(X^k)\|^2 \leq \frac{1}{2}\varepsilon_k^2, \quad \varepsilon_k > 0, \; \sum_{k=0}^{\infty} \varepsilon_k < \infty, \tag{34b}$$

$$\sup \theta_k(\zeta, \xi) - \theta_k(\zeta^{k+1}, \xi^{k+1}) \leq \frac{\delta_k^2}{2\sigma_k}\|X^{k+1} - X^k\|^2, \tag{34c}$$

$$\|\zeta^{k+1} - \bar{\zeta}(X^k)\|^2 \leq \delta_k^2\|\zeta^{k+1} - \zeta^k\|^2, \quad \delta_k > 0, \; \sum_{k=0}^{\infty} \delta_k < \infty, \tag{34d}$$

$$\|\nabla\theta_k(\zeta^{k+1}, \xi^{k+1})\| \leq \frac{\delta_k'}{\sigma_k}\|X^{k+1} - X^k\|, \quad 0 \leq \delta_k' \to 0. \tag{34e}$$

In [18], it has been shown that under mild assumptions, the sequence $\{(u^k, X^k)\}$ generated by the partial PPA under criterion (34a) and (34b) converges to an optimal solution $(\bar{u}, \overline{X})$ of (26), and $\{(\zeta^k, \xi^k)\}$ is asymptotically maximizing for problem (29). If, in addition, (34c) and (34d) are also satisfied and $\mathscr{T}_f^{-1}$ is Lipschitz continuous at the origin, then $\{(u^k, X^k)\}$ locally converges to the unique optimal solution $(\bar{u}, \overline{X})$ of (26) at least at a linear rate which tends to zero as $\sigma_k \to +\infty$. For details on the convergence analysis, we refer the reader to [18, Theorem 3.1 & Theorem 3.2].

3.1 A semismooth Newton-CG method for solving unconstrained inner subproblems

In this subsection, we introduce a semismooth Newton-CG (SSNCG) method for solving the unconstrained inner subproblem (33), which is the most expensive step in each PPA iteration. For later convenience, we let

$$\widehat{\mathscr{A}} = \begin{pmatrix} \mathscr{A} \\ \mathscr{B} \end{pmatrix},\ \widehat{b} = (b;d) \in \mathfrak{R}^{m+s},\ T = \begin{bmatrix} I_m & 0 \\ 0 & 0 \end{bmatrix} \in \mathfrak{R}^{(m+s)\times(m+s)},\ y = (\zeta;\xi) \in \mathfrak{R}^{m+s}. \tag{35}$$

For the convergence analysis, we assume that the following Slater condition holds:

$$\begin{cases} \mathscr{B} : \mathfrak{R}^{p\times q} \to \mathfrak{R}^s \text{ is onto,} \\ \exists X_0 \in \mathfrak{R}^{p\times q} \text{ such that } \mathscr{B}(X_0) = d. \end{cases} \tag{36}$$

In our proposed partial PPA, for some fixed $X \in \mathfrak{R}^{p\times q}$ and $\sigma > 0$, we need to solve an inner subproblem of the following form:

$$\min_{y \in \mathfrak{R}^{m+s}} \left\{ \varphi(y) := \frac{1}{2}\langle y, Ty \rangle + \frac{1}{2\sigma}\|D_{\rho\sigma}(W(y;X))\|^2 - \langle \widehat{b}, y \rangle \right\}, \tag{37}$$

where $W(y;X) = X - \sigma(C - \widehat{\mathscr{A}}^* y)$ and $\widehat{\mathscr{A}}^* = (\mathscr{A}^*, \mathscr{B}^*)$ is the adjoint of $\widehat{\mathscr{A}}$. The optimality condition for (37) is given by

$$\nabla\varphi(y) = Ty + \widehat{\mathscr{A}}D_{\rho\sigma}(W(y;X)) - \widehat{b} = 0. \tag{38}$$

Since the soft-thresholding operator $D_{\rho\sigma}(\cdot)$ is Lipschitz continuous with modulus 1 [19, 18], the mapping $\nabla\varphi(y)$ is Lipschitz continuous on $\mathfrak{R}^{m+s}$. Thus for any $y \in \mathfrak{R}^{m+s}$, the generalized Hessian of $\varphi(y)$ is well defined and it is given by

$$\partial^2\varphi(y) := \partial(\nabla\varphi)(y), \tag{39}$$

where $\partial(\nabla\varphi)(y)$ is the Clarke's generalized Jacobian of $\nabla\varphi$ at y [5]. However, it is hard to express $\partial^2\varphi(y)$ exactly, so we define the following alternative for $\partial^2\varphi(y)$,

$$\hat{\partial}^2\varphi(y) := T + \sigma\widehat{\mathscr{A}}\partial D_{\rho\sigma}(W(y;X))\widehat{\mathscr{A}}^*. \tag{40}$$

From [5, p.75], we have for any $h \in \mathfrak{R}^{m+s}$,

$$\partial^2\varphi(y)h \subseteq \hat{\partial}^2\varphi(y)h, \tag{41}$$

which implies that if all elements in $\hat{\partial}^2\varphi(y)$ are positive definite, so are those in $\partial^2\varphi(y)$.

Since the soft-thresholding operator $D_{\rho\sigma}(\cdot)$ is strongly semismooth, $\nabla\varphi(\cdot)$ is also strongly semismooth. We can solve the nonlinear equation (38) by using a SSNCG method for which the direction r at an iterate y is computed from the following

linear system of equations:

$$\underbrace{(T + \sigma \widehat{\mathscr{A}} \mathscr{W} \widehat{\mathscr{A}^*})}_{\mathscr{V}} r = -\nabla \varphi(y), \tag{42}$$

where $\mathscr{W}$ is any element in $\partial D_{\rho\sigma}(W(y;X))$. Note that if $s = 0$, i.e., the constraint $\mathscr{B}X = d$ is absent, then $\mathscr{V}$ is always positive definite due to the fact that all the elements in $\partial D_{\rho\sigma}(\cdot)$ are positive semidefinite [18, Proposition 2.1] and $T = I_m$.

Define the operator $\mathscr{W}_y^0 : \mathfrak{R}^{p \times q} \to \mathfrak{R}^{p \times q}$ as in (25). To implement the above SS-NCG method, we need to choose an explicit element $\mathscr{W}$ in $\partial D_{\rho\sigma}(W(y;X))$, which we take to be $\mathscr{W}_y^0$. With this specific choice, then the coefficient matrix in (42) is given by

$$\mathscr{V}_y^0 = T + \sigma \widehat{\mathscr{A}} \mathscr{W}_y^0 \widehat{\mathscr{A}^*} \in \hat{\partial}^2 \varphi(y). \tag{43}$$

Next, we shall study a certain constraint nondegeneracy condition and its connection to the positive definiteness of $\mathscr{V}_y \in \hat{\partial}^2 \varphi(y)$. Suppose that the Slater condition (36) holds and $\bar{y} = (\bar{\zeta}; \bar{\xi}) \in \mathfrak{R}^{m+s}$ is the optimal solution to problem (37). Let $W(\bar{y};X) = X - \sigma(C - \widehat{\mathscr{A}^*}\bar{y})$ and $\overline{X} = D_{\rho\sigma}(W(\bar{y};X))$. Let $W(\bar{y};X)$ admit the SVD as in (5). For the given threshold value $\rho\sigma$, we decompose the index set $\alpha = \{1, \ldots, p\}$ into the following three subindex sets:

$$\alpha_1 := \{i \mid \sigma_i(W) > \rho\sigma\}, \ \alpha_2 := \{i \mid \sigma_i(W) = \rho\sigma\}, \ \alpha_3 := \{i \mid \sigma_i(W) < \rho\sigma\}.$$

The constraint nondegeneracy condition is said to hold at $\overline{X}$ [18] if

$$\mathscr{B}(\mathscr{T}(\overline{X})) = \mathfrak{R}^s, \tag{44}$$

where the subspace $\mathscr{T}(\overline{X})$ of $\mathfrak{R}^{p \times q}$ is defined as

$$\mathscr{T}(\overline{X}) := \left\{ H \in \mathfrak{R}^{p \times q} \mid [U_{\alpha_2} \ U_{\alpha_3}]^T H [V_{\alpha_2} \ V_{\alpha_3} \ V_2] = 0 \right\}, \tag{45}$$

and its orthogonal complement is given by

$$\mathscr{T}^{\perp}(\overline{X}) = \left\{ H \in \mathfrak{R}^{p \times q} \mid U_{\alpha_1}^T H = 0, \ H V_{\alpha_1} = 0 \right\}. \tag{46}$$

The following lemma will be needed to analyze the connection between the constraint nondegeneracy condition at $\overline{X}$ and the positive definiteness of the elements of $\hat{\partial}^2 \varphi(\bar{y})$.

Lemma 1. *Let $W(\bar{y};X)$ admit the SVD as in (5). For any $\mathscr{W} \in \partial D_{\rho\sigma}(W(\bar{y};X))$ and $H \in \mathfrak{R}^{p \times q}$ such that $\mathscr{W}H = 0$, it holds that*

$$H \in \mathscr{T}^{\perp}(\overline{X}). \tag{47}$$

Proof. Let $\mathscr{W} \in \partial D_{\rho\sigma}(W(\bar{y};X))$ and $H \in \mathfrak{R}^{p \times q}$ be such that $\mathscr{W}H = 0$. Then we have

$$0 = \langle H, \mathscr{W}H \rangle = \frac{1}{2}\langle \Xi(H), \Xi(\mathscr{W}H) \rangle = \frac{1}{2}\langle \Xi(H), Q(\Gamma \circ (Q^T \Xi(H)Q))Q^T \rangle$$
$$= \frac{1}{2}\langle Q^T \Xi(H)Q, \Gamma \circ (Q^T \Xi(H)Q) \rangle = \frac{1}{2}\langle \widetilde{H}, \Gamma \circ \widetilde{H} \rangle,$$

where $\Gamma \in \mathscr{S}^{p+q}$ is defined as in (18) and $\widetilde{H} = Q^T \Xi(H)Q$. Let $H_1 = U^T HV_1, H_2 = U^T HV_2, H_1^s = (H_1 + H_1^T)/2$ and $H_1^a = (H_1 - H_1^T)/2$. From (15) and (21), we have

$$0 = \frac{1}{2}\langle \widetilde{H}, \Gamma \circ \widetilde{H} \rangle = \sum_{i \in \alpha}\sum_{j \in \alpha}\Gamma_{ij}(H_1^s)_{ij}^2 + \sum_{i \in \alpha}\sum_{j \in \gamma}\Gamma_{ij}(H_1^a)_{ij}^2 + \sum_{i \in \alpha}\sum_{j \in \beta}\Gamma_{ij}(H_2)_{ij}^2.$$

Since $\Gamma_{ij} \in [0,1]$ for all $i, j = 1, \ldots, p+q$, it follows that

$$\sum_{i \in \alpha}\sum_{j \in \alpha}\Gamma_{ij}(H_1^s)_{ij}^2 = 0, \quad \sum_{i \in \alpha}\sum_{j \in \gamma}\Gamma_{ij}(H_1^a)_{ij}^2 = 0, \quad \sum_{i \in \alpha}\sum_{j \in \beta}\Gamma_{ij}(H_2)_{ij}^2 = 0.$$

Then from (22), (23) and (24), we have that

$$(H_1^s)_{\alpha_1 \alpha} = 0, \ (H_1^s)_{\alpha \alpha_1} = 0, \ (H_1^a)_{\alpha_1 \alpha} = 0, \ (H_1^a)_{\alpha \alpha_1} = 0, \ (H_2)_{\alpha_1 \bar{\beta}} = 0,$$

where $\bar{\beta} = \{1, \ldots, q-p\}$. Since $H_1 = H_1^s + H_1^a$, we have that $(H_1)_{\alpha_1 \alpha} = 0$ and $(H_1)_{\alpha \alpha_1} = 0$. From $H_1 = [U_{\alpha_1}\, U_{\alpha_2}\, U_{\alpha_3}]^T H[V_{\alpha_1}\, V_{\alpha_2}\, V_{\alpha_3}]$ and $H_2 = [U_{\alpha_1}\, U_{\alpha_2}\, U_{\alpha_3}]^T HV_2$, we obtain that

$$U_{\alpha_1}^T HV_1 = 0, \quad U_{\alpha_1}^T HV_2 = 0, \quad U^T HV_{\alpha_1} = 0.$$

Since both U and $V = [V_1\, V_2]$ are orthogonal matrices, we have $U_{\alpha_1}^T H = 0, HV_{\alpha_1} = 0$, which means that $H \in \mathscr{T}^{\perp}(\overline{X})$.

Proposition 3. *Suppose that the Slater condition (36) is satisfied. Let $\bar{y}$ be the optimal solution to problem (37), $W(\bar{y};X) = X - \sigma(C - \widehat{\mathscr{A}^*}\bar{y})$ admit the SVD as in (5), and $\overline{X} = D_{\rho\sigma}(W(\bar{y};X))$. Then the following conditions are equivalent:*

(a) The constraint nondegeneracy condition (44) holds at $\overline{X}$.
(b) Every $\mathscr{V}_{\bar{y}} \in \hat{\partial}^2\varphi(\bar{y})$ is symmetric and positive definite.
(c) $\mathscr{V}_{\bar{y}}^0 \in \hat{\partial}^2\varphi(\bar{y})$ is symmetric and positive definite.

Proof. "(a) $\Rightarrow$ (b)". Let $\mathscr{V}_{\bar{y}}$ be an arbitrary element in $\hat{\partial}^2\varphi(\bar{y})$. Then there exists an element $\mathscr{W}_{\bar{y}} \in \partial D_{\rho\sigma}(W(\bar{y};X))$ such that

$$\mathscr{V}_{\bar{y}} = T + \sigma\widehat{\mathscr{A}}\mathscr{W}_{\bar{y}}\widehat{\mathscr{A}^*} = T + \sigma\begin{bmatrix} \mathscr{A}\mathscr{W}_{\bar{y}}\mathscr{A}^* & \mathscr{A}\mathscr{W}_{\bar{y}}\mathscr{B}^* \\ \mathscr{B}\mathscr{W}_{\bar{y}}\mathscr{A}^* & \mathscr{B}\mathscr{W}_{\bar{y}}\mathscr{B}^* \end{bmatrix}. \tag{48}$$

Since $\mathscr{W}_{\bar{y}}$ is self-adjoint and positive semidefinite [18, Proposition 2.1], we have that $\mathscr{V}_{\bar{y}}$ is self-adjoint and positive semidefinite. From (48) we obtain that $\mathscr{V}_{\bar{y}}$ is positive definite if only if $\mathscr{B}\mathscr{W}_{\bar{y}}\mathscr{B}^*$ is positive definite. Hence, it it enough to show the positive definiteness of $\mathscr{B}\mathscr{W}_{\bar{y}}\mathscr{B}^*$. Let $h \in \mathfrak{R}^s$ be such that $\mathscr{B}\mathscr{W}_{\bar{y}}\mathscr{B}^*h = 0$. Then we have

$$0 = \langle h, \mathscr{B} \mathscr{W}_{\bar{y}} \mathscr{B}^* h \rangle = \langle \mathscr{B}^* h, \mathscr{W}_{\bar{y}} \mathscr{B}^* h \rangle \geq \langle \mathscr{W}_{\bar{y}} \mathscr{B}^* h, \mathscr{W}_{\bar{y}} \mathscr{B}^* h \rangle,$$

where the last inequality follows from [18, Proposition 2.1], which implies that $\mathscr{W}_{\bar{y}} (\mathscr{B}^* h) = 0$. From Lemma 1, we have $\mathscr{B}^* h \in \mathscr{T}(\overline{X})^\perp$. Since the constraint non-degeneracy condition holds at $\overline{X}$, there exists a $Y \in \mathscr{T}(\overline{X})$ such that $\mathscr{B} Y = h$. Then, we have

$$\langle h, h \rangle = \langle h, \mathscr{B} Y \rangle = \langle \mathscr{B}^* h, Y \rangle = 0.$$

Thus $h = 0$, which implies that $\mathscr{B} \mathscr{W}_{\bar{y}} \mathscr{B}^*$ is positive definite. Hence, $\mathscr{V}_{\bar{y}}$ is positive definite.

"(b) $\Rightarrow$ (c)". This is obviously true since $\mathscr{V}_{\bar{y}}^0 \in \hat{\partial}^2 \varphi(\bar{y})$.

"(c) $\Rightarrow$ (a)". Suppose that the constraint nondegeneracy condition (44) does not hold at $\overline{X}$. Then there exists a non-zero $h \in [\mathscr{B} \mathscr{T}(\overline{X})]^\perp$. And we have

$$0 = \langle h, \mathscr{B} Y \rangle = \langle H, Y \rangle \quad \forall Y \in \mathscr{T}(\overline{X}),$$

where $H = \mathscr{B}^* h$, which implies that $H \in \mathscr{T}(\overline{X})^\perp$. From (46), we have $U_{\alpha_1}^T H = 0$ and $H V_{\alpha_1} = 0$. Then it follows that

$$U_{\alpha_1}^T H V = U_{\alpha_1}^T H [V_1 \; V_2] = 0 \quad \text{and} \quad U^T H V_{\alpha_1} = 0. \tag{49}$$

Let $H_1 = U^T H V_1$ and $H_2 = U^T H V_2$. We have from (49) that

$$(H_1)_{\alpha_1 \alpha} = 0, \quad (H_1)_{\alpha \alpha_1} = 0, \quad \text{and} \; (H_2)_{\alpha_1 \bar{\beta}} = 0,$$

where $\bar{\beta} = \{1, \ldots, q - p\}$, from which we can further have that

$$(H_1^s)_{\alpha_1 \alpha} = 0, \quad (H_1^s)_{\alpha \alpha_1} = 0, \quad (H_1^a)_{\alpha_1 \alpha} = 0, \quad \text{and} \; (H_1^a)_{\alpha \alpha_1} = 0,$$

where $H_1^s = (H_1 + H_1^T)/2$ and $H_1^a = (H_1 - H_1^T)/2$. Then we have

$$\Gamma_{\alpha\alpha}^0 \circ (H_1^s) = 0, \quad \Gamma_{\alpha\gamma} \circ (H_1^a) = 0, \quad \text{and} \; \Gamma_{\alpha\beta} \circ H_2 = 0.$$

From the definition of $\mathscr{W}_{\bar{y}}^0$ in (25), it follows that $\mathscr{W}_{\bar{y}}^0 (H) = 0$, and hence

$$\langle h, \mathscr{B} \mathscr{W}_{\bar{y}}^0 \mathscr{B}^* h \rangle = \langle H, \mathscr{W}_{\bar{y}}^0 (H) \rangle = 0. \tag{50}$$

Since $\mathscr{V}_{\bar{y}}^0$ is positive definite, it follows from (48) that $\mathscr{B} \mathscr{W}_{\bar{y}}^0 \mathscr{B}^*$ is also positive definite. Then (50) implies that $h = 0$, which contradicts the assumption that $h \neq 0$. Hence, we have that (a) holds.

Now we present the steps of the SSNCG algorithm for solving (37).

Algorithm 2: A semismooth Newton-CG method

Given $y^0 \in \Re^{m+s}$, $\eta \in (0,1)$, $\tau \in (0,1]$, $\tau_1, \tau_2 \in (0,1)$, and $c \in (0,1/2)$, $\delta \in (0,1)$. Set $t = 0$. Iterate:

Step 1.   Compute $\eta_t := \min\{\eta, \|\nabla\varphi(y^t)\|^{1+\tau}\}$. Apply the CG method to find an approximation solution r^t to

$$(\mathcal{V}_t + \varepsilon_t I)\, r = -\nabla\varphi(y^t), \tag{51}$$

where $\mathcal{V}_t \in \hat{\partial}^2\varphi(y^t)$ is defined in (43) and $\varepsilon_t = \min\{\tau_2, \tau_1\|\nabla\varphi(y^t)\|\}$, so that r^t satisfies the following condition:

$$\|(\mathcal{V}_t + \varepsilon_t I)r^t + \nabla\varphi(y^t)\| \leq \eta_t. \tag{52}$$

Step 2.   Set $\alpha_t = \delta^{m_t}$, where m_t is the first nonnegative integer m for which

$$\varphi(y^t + \delta^m r^t) \ \leq\ \varphi(y^t) + c\delta^m \langle r^t, \nabla\varphi(y^t)\rangle.$$

Step 3.   Set $y^{t+1} = y^t + \alpha_t r^t$.

In Algorithm 2, since $\mathcal{V}_t$ is always positive semidefinite, the matrix $\mathcal{V}_t + \varepsilon_t I$ is positive definite as long as $\nabla\varphi(y^t) \neq 0$. From [32, Lemma 3.1], we know that the generated search direction r^t is always a descent direction.

To analyze the global convergence of Algorithm 2, we assume that $\nabla\varphi(y^t) \neq 0$ for any $t \geq 0$. The global convergence and the rate of local convergence of Algorithm 2 can be derived similarly as in [32].

Theorem 1. *Suppose that the Slater condition (36) holds. Then Algorithm 2 is well defined and any accumulation point $\bar{y}$ of $\{y^t\}$ generated by Algorithm 2 is an optimal solution to the inner subproblem (37).*

Proof. See [32, Theorem 3.4].

Theorem 2. *Suppose that the Slater condition (36) holds. Let $\bar{y}$ be an accumulation point of the infinite sequence $\{y^t\}$ generated by Algorithm 2 for solving the inner subproblem (37). Suppose also that at each step $t \geq 0$, the inexact direction r^t satisfies the accuracy condition in (52). Assume that the constraint nondegeneracy condition (44) holds at $\overline{X} := D_{\rho\sigma}(W(\bar{y};X))$. Then the whole sequence $\{y^t\}$ converges to $\bar{y}$ and*

$$\|y^{t+1} - \bar{y}\| = O(\|y^t - \bar{y}\|^{1+\tau}). \tag{53}$$

Proof. See [32, Theorem 3.5].

4 Semidefinite matrix least squares problems

In this section, we show that the partial PPA developed for solving (26) can easily be adapted for solving the semidefinite matrix least squares problem (4). It is easy to see that (4) can be rewritten as follows:

$$\min_{u\in\mathfrak{R}^m, X\in\mathscr{S}^n} \left\{ \frac{1}{2}\|u\|^2 + \langle C, X\rangle \; : \; \mathscr{A}(X)+u = b, \; \mathscr{B}(X) = d, \; X \succeq 0 \right\}. \quad (54)$$

The dual problem of (54) is given by:

$$\max_{\zeta\in\mathfrak{R}^m, \xi\in\mathfrak{R}^s, Z\in\mathscr{S}^n} \left\{ -\frac{1}{2}\|\zeta\|^2 + \langle b, \zeta\rangle + \langle d, \xi\rangle \; : \; \mathscr{A}^*(\zeta) + \mathscr{B}^*(\xi) + Z = C, \; Z \succeq 0 \right\}. \quad (55)$$

For some fixed $X \in \mathscr{S}^n$ and $\sigma > 0$, the partial quadratic regularization of problem (54) is given by:

$$\min_{u\in\mathfrak{R}^m, Y\in\mathscr{S}^n} \left\{ \frac{1}{2}\|u\|^2 + \langle C, Y\rangle + \frac{1}{2\sigma}\|Y - X\|^2 \; : \; \mathscr{A}(Y)+u = b, \; \mathscr{B}(Y) = d, \; Y \succeq 0 \right\}, \quad (56)$$

and the Lagrangian dual problem of (56) is given by

$$\max_{\zeta\in\mathfrak{R}^m, \xi\in\mathfrak{R}^s} \theta_\sigma(\zeta,\xi;X) := \inf_{u\in\mathfrak{R}^m, Y\succeq 0} L_\sigma(u, Y; \zeta, \xi, X), \quad (57)$$

where

$$L_\sigma(u, Y; \zeta, \xi, X) = \frac{1}{2}\|u\|^2 + \langle C, Y\rangle + \frac{1}{2\sigma}\|Y - X\|^2 + \langle \zeta, b - \mathscr{A}(Y) - u\rangle + \langle \xi, d - \mathscr{B}(Y)\rangle$$

$$= \frac{1}{2}\|u\|^2 - \langle \zeta, u\rangle + \langle b, \zeta\rangle + \langle d, \xi\rangle + \frac{1}{2\sigma}\|Y - W(\zeta,\xi;X)\|^2 + \frac{1}{2\sigma}(\|X\|^2 - \|W(\zeta,\xi;X)\|^2),$$

where $W(\zeta,\xi;X) = X - \sigma(C - \mathscr{A}^*\zeta - \mathscr{B}^*\xi)$. By minimizing $L_\sigma(u, Y; \zeta, \xi, X)$ over $Y \succeq 0$, we have

$$\theta_\sigma(\zeta,\xi;X) = -\frac{1}{2}\|\zeta\|^2 + \langle b, \zeta\rangle + \langle d, \xi\rangle + \frac{1}{2\sigma}\|X\|^2 - \frac{1}{2\sigma}\|\Pi_{\mathscr{S}^n_+}(W(\zeta,\xi;X))\|^2, \quad (58)$$

where $\Pi_{\mathscr{S}^n_+}(\cdot)$ is the metric projector of $\mathscr{S}^n$ onto $\mathscr{S}^n_+$. The problem (57) is an unconstrained continuously differentiable convex optimization problem, and it can be efficiently solved by the SSNCG method developed in [32]. The SSNCG method for solving (57) is analogous to Algorithm 2 where for some fixed $X \in \mathscr{S}^n$ and $\sigma > 0$, the function φ is now given by

$$\varphi(y) = \frac{1}{2}\langle y, Ty\rangle + \frac{1}{2\sigma}\|\Pi_{\mathscr{S}^n_+}(W(y;X))\|^2 - \langle \widehat{b}, y\rangle$$

and the operator $\mathscr{V}_t$ in (51) is replaced by

$$\mathscr{V}_t = T + \sigma \widehat{\mathscr{A}} \Pi'_{\mathscr{S}^n_+}(W(y^t;X)) \widehat{\mathscr{A}}^*, \tag{59}$$

where $\Pi'_{\mathscr{S}^n_+}(W(y^t;X))$ denotes an element of $\partial \Pi_{\mathscr{S}^n_+}(W(y^t;X))$.

The fast local convergence of the SSNCG method for solving (57) can be established in a similar fashion as Theorem 2 where the positive definiteness of the element $\mathscr{V}_{\bar{y}}$ defined in (59) at the optimal solution $\bar{y}$ is again equivalent to a constraint nondegeneracy condition similar to (44) at $\overline{X} := \Pi_{\mathscr{S}^n_+}(W(\bar{y};X))$.

5 Numerical Results

In this section, we report some numerical results to demonstrate the efficiency of our SSNCG partial PPA. We implemented our algorithm in MATLAB 2012a (version 7.14), and the numerical experiments are run in MATLAB under a Windows 7 64-bit system on an Intel Xeon 4 Cores 3.20GHz CPU with 12GB memory.

In our numerical implementation, we use the alternating direction method of multipliers (ADMM) [8] to generate a reasonably good starting point for our SSNCG partial PPA. The augmented Lagrangian function for (29) corresponding to the linear equality constraints is defined as:

$$L_\sigma(y,Z;X) = -\frac{1}{2}\langle y,Ty\rangle + \langle \widehat{b},y\rangle + \langle X, C - \widehat{\mathscr{A}}^*y - Z\rangle - \frac{\sigma}{2}\|C - \widehat{\mathscr{A}}^*y - Z\|^2,$$

where $X \in \mathfrak{R}^{p\times q}$ and $\sigma > 0$. Given a starting point $(X^0; y^0; Z^0)$, the ADMM generates new iterates by the following procedure:

$$y^{k+1} := \mathrm{argmax}_{y\in\mathfrak{R}^{m+s}} L_\sigma(y,Z^k;X^k), \tag{60}$$

$$Z^{k+1} := \mathrm{argmax}_{\|Z\|_2\leq\rho} L_\sigma(y^{k+1},Z;X^k) = \frac{1}{\sigma}(D_{\rho\sigma}(W^{k+1}) - W^{k+1}), \tag{61}$$

$$X^{k+1} := D_{\rho\sigma}(W^{k+1}), \tag{62}$$

where $W^{k+1} = X^k - \sigma(C - \widehat{\mathscr{A}}^*y^{k+1})$. Note that the iterate y^{k+1} in (60) can be computed by solving the following linear system of equations:

$$(T + \sigma\widehat{\mathscr{A}}\widehat{\mathscr{A}}^*)y = \widehat{b} - \widehat{\mathscr{A}}(X^k) + \sigma\widehat{\mathscr{A}}(C - Z^k).$$

We measure the infeasibilities and optimality for the primal problem (26) and the dual problem (29) as follows:

$$R_P = \frac{\|\widehat{b} - (\zeta;0) - \widehat{\mathscr{A}}(X)\|}{1+\|\widehat{b}\|}, R_D = \frac{\|C - \widehat{\mathscr{A}}^*y - Z\|}{1+\|\widehat{\mathscr{A}}^*\|}, \mathrm{relgap} = \frac{f_\rho(\zeta,X) - g_\rho(\zeta,\xi)}{1+|f_\rho(\zeta,X)|+|g_\rho(\zeta,\xi)|},$$

where $y = (\zeta;\xi), Z = (D_{\rho\sigma}(W) - W)/\sigma$ with $W = X - \sigma(C - \widehat{\mathscr{A}}^*y)$, and $f_\rho(\zeta,X)$ and $g_\rho(\zeta,\xi)$ are the objective functions of the primal and dual problems, respec-

tively. The infeasibility of the condition $\|Z\|_2 \leq \rho$ is not checked since it is satisfied up to machine precision throughout the algorithm. In our numerical experiments, we stop the partial PPA when

$$\max\{R_P, R_D\} \leq \mathtt{Tol}, \tag{63}$$

where $\mathtt{Tol}$ is a pre-specified accuracy tolerance. We choose the initial $\sigma_0 = 1$ and update it as $\sigma_{k+1} = \min(2\sigma_k, 10^8)$ if $R_D^{k+1}/R_D^k > 0.5$; otherwise $\sigma_{k+1} = \sigma_k$. Unless otherwise specified, we set the parameter ρ in (1) to be $\rho = 10^{-3}\|\mathscr{A}^*b\|_2$ and $\mathtt{Tol} = 10^{-6}$ as the default.

In solving the subproblem (37), the SSNCG algorithm is stopped when $R_P = \|\nabla\varphi(y)\|/(1+\|\widehat{b}\|) \leq 0.2R_D$ or the number of Newton iterations exceeds 50. We cap the number of CG steps for solving each Newton system of linear equations at 600 and stop the CG solver when $\|(\mathscr{V} + \varepsilon I)r + \nabla\varphi(y)\| \leq \min(0.05, 0.1\|\nabla\varphi(y)\|)$.

The reason we used the ADMM instead of other first order methods to generate a starting point is based on our belief and experience that the ADMM is perhaps the most efficient first order method for solving the problems which we are interested in. Since this belief may be challenged without strong numerical evidence to support it, as suggested by one of the referees, we also tested the primal-dual splitting method by Condat [7] for solving (1). To apply Condat's method in [7], we rewrite (1) in the following form:

$$\min_X F(X) + G(X) + H(\mathscr{B}(X)), \tag{64}$$

where $F(X) = \frac{1}{2}\|\mathscr{A}(X) - b\|^2 + \langle C, X\rangle$ with $\nabla F(X) = \mathscr{A}^*(\mathscr{A}(X) - b) + C$, $G(X) = \rho\|X\|_*$, and $H(\cdot)$ is the indicator function over the singleton set $\{d\}$. Note that the optimality condition for (64) is given by:

$$\text{find } (X, y) \text{ such that } \begin{pmatrix} 0 \\ 0 \end{pmatrix} \in \begin{pmatrix} \nabla F(X) + \partial G(X) + \mathscr{B}^*y \\ -\mathscr{B}(X) + \partial H^*(y) \end{pmatrix} \tag{65}$$

where H^* is the conjugate function of H with $H^*(y) = \langle d, y\rangle$. Let L_F be a Lipschitz constant for ∇F, which in our case can be set to $L_F = \lambda_{\max}(\mathscr{A}^*\mathscr{A})$. Given parameters $\lambda > 0, \beta > 0$ such that $\lambda^{-1} \geq L_F/2 + \beta\lambda_{\max}(\mathscr{B}\mathscr{B}^*)$, a sequence of positive numbers $\{\mu_k\}$, and a starting point $(X^0, y^0) \in \Re^{p\times q} \times \Re^s$, Condat's primal-dual splitting method generates new iterates as follows:

$$\widetilde{X}^{k+1} = \text{prox}_{\lambda G}(X^k - \lambda\nabla F(X^k) - \lambda\mathscr{B}^*(y^k)) = D_{\rho\lambda}(W^k), \tag{66}$$

$$\widetilde{y}^{k+1} = \text{prox}_{\beta H^*}(y^k + \beta\mathscr{B}(2\widetilde{X}^{k+1} - X^k)) = y^k + \beta(\mathscr{B}(2\widetilde{X}^{k+1} - X^k) - d), \tag{67}$$

$$(X^{k+1}, y^{k+1}) = \mu_k(\widetilde{X}^{k+1}, \widetilde{y}^{k+1}) + (1 - \mu_k)(X^k, y^k), \tag{68}$$

where $W^k = X^k - \lambda\nabla F(X^k) - \lambda\mathscr{B}^*(y^k)$ and $\text{prox}_{\lambda G}$ denotes the proximal point mapping associated with λG defined by $\text{prox}_{\lambda G}(X) = \text{argmin}_{Y\in\Re^{p\times q}}\lambda G(Y) + \frac{1}{2}\|Y - X\|^2$. We can estimate how close the iterate $(\widetilde{X}^{k+1}, \widetilde{y}^{k+1})$ is to optimality by noting that $\text{dist}(0, -\mathscr{B}(\widetilde{X}^{k+1}) + \partial H^*(\widetilde{y}^{k+1})) = \|d - \mathscr{B}(\widetilde{X}^{k+1})\|$, and

$$\text{dist}(0, \nabla F(\widetilde{X}^{k+1}) + \partial G(\widetilde{X}^{k+1}) + \mathscr{B}^* \tilde{y}^{k+1}) \leq \|\frac{1}{\lambda}(W^k - \widetilde{X}^{k+1}) + \mathscr{B}^* \tilde{y}^{k+1} + \nabla F(\widetilde{X}^{k+1})\|,$$

based on the fact that $W^k - \widetilde{X}^{k+1} \in \partial(\lambda G)(\widetilde{X}^{k+1})$. By letting $Z^{k+1} = \frac{1}{\lambda}(\widetilde{X}^{k+1} - W^k), u^{k+1} = \zeta^{k+1} = b - \mathscr{A}(\widetilde{X}^{k+1})$ and $\xi^{k+1} = -\tilde{y}^{k+1}$, then

$$\|[\mathscr{A}\widetilde{X}^{k+1} + u^{k+1} - b; d - \mathscr{B}(\widetilde{X}^{k+1})]\| = \|d - \mathscr{B}(\widetilde{X}^{k+1})\|$$

$$\|\frac{1}{\lambda}(W^k - \widetilde{X}^{k+1}) + \mathscr{B}^* \tilde{y}^{k+1} + \nabla F(\widetilde{X}^{k+1})\| = \|C - (\mathscr{A}^* \zeta^{k+1} + \mathscr{B}^* \xi^{k+1} + Z^{k+1})\|,$$

which correspond to the residuals of the primal and dual equality constraints in (26) and (29), respectively. Therefore, we can stop the primal-dual splitting method when (63) is satisfied. In our numerical experiments, we also stop the method when the number of iterations exceeds 2000.

5.1 Example 1

We consider the low rank matrix approximation problem in which certain specified entries of the matrix are fixed. In [15], Golub, Hoffman and Stewart derived an explicit formula for finding the nearest lower-rank approximation of the target matrix while certain specified columns of the matrix are fixed. In our numerical experiments, we assume that only partial information of the original matrix is available and the specified fixed entries can be in any random position of the original matrix. For each triplet (p, q, r), we first generate a random matrix $M \in \mathfrak{R}^{p \times q}$ by setting $M = M_1 M_2^T$ where $M_1 \in \mathfrak{R}^{p \times r}$, $M_2 \in \mathfrak{R}^{q \times r}$ have i.i.d. Gaussian entries. Then we sample a subset $\mathscr{E}$ of m entries of M uniformly at random, and generate a random matrix $N_{\mathscr{E}} \in \mathfrak{R}^{p \times q}$ with sparsity pattern $\mathscr{E}$ and i.i.d Gaussian entries. Then we assume that the observed data is given by $\widetilde{M}_{\mathscr{E}} = M_{\mathscr{E}} + \tau N_{\mathscr{E}} \|M_{\mathscr{E}}\| / \|N_{\mathscr{E}}\|$, where τ is the noise factor. The minimization problem which we solve can be stated as follows:

$$\min_{X \in \mathfrak{R}^{p \times q}} \left\{ \frac{1}{2} \|X_{\mathscr{E}} - \widetilde{M}_{\mathscr{E}}\|_F^2 + \rho \|X\|_* : X_{i_t, j_t} = M_{i_t, j_t}, 1 \leq t \leq k \right\}, \tag{69}$$

where $(i_1, j_1), \dots, (i_k, j_k)$ are distinct pairs. In our numerical experiments, we set $k = \lceil 10^{-3} pq \rceil$, which is the number of prescribed entries selected uniformly at random, and the noise level $\tau = 0, 0.1$.

For each triplet $(p, q, r), m$ and τ, we generate 5 random instances. In Table 1, we report the average number of the following quantities: number of sampled entries (m); number of outer iterations (it); total number of inner iterations (itsub); number of CG steps taken to solve each linear system in (51) (cg); infeasibilities (R_p, R_D); relative duality gap (relgap); relative mean square error MSE $:= \|X - M\| / \|M\|$; numerical rank of X (#sv); and the CPU time taken. Here we report the numerical rank of X defined as follows:

$$\#sv(X) := \max\{k : \sigma_k(X) \geq \max\{10^{-8}, \tau\} \sigma_1(X)\}. \tag{70}$$

$p/q/\tau$	r	m; m/dr	it.	itsub	cg	R_p	R_D	relgap	MSE	#sv	time
1000/1000 /0.0	10	199104; 10	10.2	30.4	18.8	2.20e-7	8.05e-7	-1.57e-4	1.32e-3	10	1:41
	50	487314; 5	10.0	16.0	15.3	1.26e-7	7.07e-7	-3.94e-5	1.64e-3	50	1:04
	100	949927; 5	9.0	10.2	12.4	1.23e-7	4.38e-7	-8.96e-6	1.48e-3	100	43
1500/1500 /0.0	10	299272; 10	13.0	32.4	16.9	1.95e-7	1.92e-7	-1.70e-5	1.30e-3	10	5:33
	50	738078; 5	11.0	18.8	15.2	1.38e-7	6.46e-7	-3.54e-5	1.68e-3	50	3:45
	100	1449450; 5	10.0	15.2	18.7	1.27e-7	3.42e-7	-1.07e-5	1.60e-3	100	3:43
1000/1000 /0.1	10	199104; 10	20.0	46.4	10.5	4.97e-7	7.95e-7	-8.79e-5	7.75e-2	10	2:11
	50	487314; 5	23.0	44.4	11.0	1.67e-7	5.18e-7	-9.04e-6	9.64e-2	50	2:42
	100	949927; 5	21.0	25.2	9.7	3.68e-7	6.09e-7	-3.01e-7	9.66e-2	100	1:54
1500/1500 /0.1	10	299272; 10	21.4	48.6	10.7	1.17e-7	8.67e-7	-1.46e-4	7.50e-2	10	7:09
	50	738078; 5	22.8	44.8	11.7	1.59e-7	7.07e-7	-2.20e-5	9.72e-2	50	8:09
	100	1449450; 5	23.0	39.4	11.4	7.33e-7	6.63e-7	-2.95e-6	9.62e-2	100	7:57
100/10000 /0.0	10	504310; 5	14.2	23.4	13.4	5.73e-7	5.39e-7	-2.07e-5	1.66e-3	10	38
100/50000 /0.0	10	2504270; 5	14.4	21.6	16.3	4.05e-7	6.44e-7	-2.58e-5	1.67e-3	10	4:10
100/100000 /0.0	10	5004144; 5	14.4	22.4	18.4	2.70e-7	4.68e-7	-1.95e-5	1.67e-3	10	9:09
100/10000 /0.1	10	504310; 5	22.0	34.2	5.7	3.26e-7	6.49e-7	-4.07e-5	8.95e-2	10	31
100/50000 /0.1	10	2504270; 5	22.2	33.0	5.7	2.73e-7	7.22e-7	-4.57e-5	8.94e-2	10	3:29
100/100000 /0.1	10	5004144; 5	21.8	31.0	5.9	5.31e-7	7.04e-7	-4.49e-5	8.93e-2	10	6:47
200/10000 /0.0	10	510046; 5	13.4	31.4	18.6	4.66e-7	2.24e-7	-1.79e-5	1.76e-3	10	2:23
200/50000 /0.0	10	2509504; 5	13.6	31.2	22.3	4.23e-7	2.11e-7	-1.63e-5	1.78e-3	10	14:43
200/100000 /0.0	10	5010168; 5	13.8	29.2	22.8	2.30e-7	5.18e-7	-1.73e-5	1.78e-3	10	28:45
500/10000 /0.0	10	524511; 5	16.8	50.4	28.3	3.40e-7	2.75e-7	-2.00e-5	1.78e-3	10	17:21
200/10000 /0.1	10	510046; 5	19.0	36.0	7.6	5.40e-7	9.12e-7	-1.15e-4	8.78e-2	10	1:37
200/50000 /0.1	10	2509504; 5	19.0	34.0	8.0	4.68e-7	9.24e-7	-1.17e-4	8.67e-2	10	9:29
200/100000 /0.1	10	5010168; 5	19.6	35.4	8.1	3.46e-7	7.85e-7	-9.87e-5	8.65e-2	10	20:25
500/10000 /0.1	10	524511; 5	24.6	51.6	11.5	2.91e-7	7.56e-7	-1.62e-4	9.34e-2	10	11:44

Table 1 Numerical performance of the partial PPA on (69). In the table, $dr = r(p+q-r)$ is the degree of freedom in an $p \times q$ matrix of rank r.

In this example, we compare the performance of the SSNCG partial PPA with the ADMM method [8] which is applied to the dual problem (29) and the primal-dual splitting method [7]. We use the same stopping criterion (63) for ADMM. Table 2 reports the average results of ADMM for each instance of 5 runs. We may observe from the tables that our algorithm is overall more efficient than ADMM for solving (69). For the problem where p is moderate but q is large, e.g., $p = 100$, $q = 100000$ and $\tau = 0$, it takes the partial PPA less than half of the time needed by ADMM to achieve the tolerance of 10^{-6} while the MSE is reasonably small. Table 3 reports the average results of the primal-dual splitting method for each instance of 5 runs. We set the parameters $\lambda = 1.5$ and $\beta = 1/6$ after some tuning for good performance. The parameter μ_k is set to be 1 for all k as this choice gives the best performance. We can observe from the tables that the primal-dual splitting method is much slower than ADMM for solving (69). For $p = q = 1500, \tau = 0$ and $r = 10$, the primal-dual splitting method cannot achieve the tolerance of 10^{-6} within one hour and the obtained solution is of very high rank with relatively large MSE.

$p/q/\tau$	r	m; m/dr	it.	R_p	R_D	relgap	MSE	#sv	time
1000/1000 /0.0	10	199104; 10	360.6	9.91e-7	2.36e-7	1.03e-5	1.32e-3	10	4:01
	50	487314; 5	184.6	9.75e-7	3.24e-7	3.06e-6	1.64e-3	50	2:29
	100	949927; 5	147.8	9.68e-7	3.05e-7	1.57e-6	1.48e-3	100	2:24
1500/1500 /0.0	10	299272; 10	464.2	9.92e-7	2.59e-7	1.31e-5	1.30e-3	10	16:11
	50	738078; 5	330.2	9.63e-7	4.69e-7	8.56e-6	1.68e-3	50	12:43
	100	1449450; 5	169.8	9.83e-7	4.19e-7	1.88e-6	1.60e-3	100	7:22
1000/1000 /0.1	10	199104; 10	183.6	9.85e-7	5.94e-7	-5.02e-5	7.75e-2	10	2:02
	50	487314; 5	99.0	9.17e-7	5.87e-7	-1.79e-6	9.64e-2	50	1:22
	100	949927; 5	72.4	9.79e-7	4.98e-7	1.22e-7	9.66e-2	100	1:15
1500/1500 /0.1	10	299272; 10	198.6	9.69e-7	1.77e-7	-1.93e-5	7.50e-2	10	6:56
	50	738078; 5	93.0	9.61e-7	2.34e-7	-2.88e-6	9.72e-2	50	3:38
	100	1449450; 5	74.0	9.47e-7	4.36e-7	-2.11e-7	9.62e-2	100	3:20
100/10000 /0.0	10	504310; 5	276.6	9.78e-7	3.48e-7	4.31e-6	1.66e-3	10	1:48
100/100000 /0.0	10	5004144; 5	254.6	9.85e-7	3.30e-7	3.90e-6	1.67e-3	10	24:04
500/10000 /0.0	10	524511; 5	679.2	9.91e-7	2.90e-7	1.20e-5	1.78e-3	10	26:16
100/10000 /0.1	10	504310; 5	66.2	9.58e-7	5.27e-7	-1.71e-5	8.95e-2	10	27
100/100000 /0.1	10	5004144; 5	63.4	9.41e-7	4.28e-7	-1.34e-5	8.93e-2	10	6:05
500/10000 /0.1	10	524511; 5	329.2	9.91e-7	3.62e-7	-5.33e-5	9.33e-2	10	13:08

Table 2 Numerical performance of the ADMM method on (69).

$p/q/\tau$	r	m; m/dr	it.	R_p	R_D	relgap	MSE	#sv	time
1000/1000 /0.0	10	199104; 10	2000.0	2.10e-5	7.09e-5	-2.31e-3	2.57e-3	11	19:11
	50	487314; 5	806.4	9.83e-7	5.30e-8	-1.19e-7	1.64e-3	50	8:03
1500/1500 /0.0	10	299272; 10	2000.0	1.73e-5	1.79e-3	-5.26e-1	1.81e-1	302	1:04:46
	50	738078; 5	1379.6	9.83e-7	6.92e-8	-2.55e-7	1.68e-3	50	45:24
1000/1000 /0.1	10	199104; 10	2000.0	9.54e-6	3.64e-4	-7.78e-2	8.76e-2	10	19:09
	50	487314; 5	2000.0	2.19e-8	1.44e-6	-2.79e-5	9.64e-2	50	20:01
1500/1500 /0.1	10	299272; 10	2000.0	1.28e-5	1.41e-3	-3.71e-1	2.34e-1	10	1:04:47
	50	738078; 5	2000.0	1.38e-6	1.19e-4	-5.97e-3	9.84e-2	50	1:05:26
100/10000 /0.0	10	504310; 5	1292.8	9.93e-7	2.27e-8	-1.82e-8	1.66e-3	10	4:03
100/100000 /0.0	10	5004144; 5	1328.2	9.99e-7	2.34e-8	-1.71e-8	1.67e-3	10	1:21:59
100/10000 /0.1	10	504310; 5	1706.4	2.37e-8	9.98e-7	-4.91e-5	8.95e-2	10	5:29
100/100000 /0.1	10	5004144; 5	1711.0	2.49e-8	9.96e-7	-4.94e-5	8.93e-2	10	1:46:43

Table 3 Numerical performance of the primal-dual splitting method on (69).

5.2 Example 2

In the Euclidean metric embedding problem, we are given an incomplete, possibly noisy, dissimilarity matrix $B \in \mathscr{S}^n$ with $\mathrm{Diag}(B) = 0$ and sparsity pattern specified by the set of indices $\mathscr{E} = \{(i,j) \mid B_{ij} \neq 0, 1 \leq i < j \leq n\}$. The goal is to find an Euclidean distance matrix (EDM) [1] that is nearest to B. If the measure of nearness is in the Frobenius norm, then the mathematical formulation of the problem is as follows:

$$\min\left\{\frac{1}{2}\sum_{(i,j)\in\mathscr{E}}W_{ij}(D_{ij}-B_{ij})^2+\frac{\rho}{2n}\langle E,D\rangle \,:\, D \text{ is an EDM}\right\}, \qquad (71)$$

where $W_{ij}>0, (i,j)\in\mathscr{E}$, are given weights, $E\in\mathscr{S}^n$ is the matrix of all ones and $\rho>0$ is a regularization parameter. Here we add the term $\frac{\rho}{2n}\langle E,D\rangle$ to encourage a sparse solution. Recall that a standard characterization [1] of an EDM D is that $D=\text{Diag}(X)e^T+e\,\text{Diag}(X)^T-2X$ for some $X\succeq 0$ with $Xe=0$, where $e\in\mathfrak{R}^n$ is the vector of all ones. Thus the problem (71) can be rewritten as:

$$\min\left\{\frac{1}{2}\sum_{(i,j)\in\mathscr{E}}W_{ij}(\langle A_{ij},X\rangle-B_{ij})^2+\rho\langle I,X\rangle \,:\, \langle E,X\rangle=0,\ X\succeq 0\right\}, \qquad (72)$$

where $A_{ij}=(e_i-e_j)(e_i-e_j)^T$ and e_i is the i-th standard unit vector in $\mathfrak{R}^n$. Note that under the condition $X\succeq 0$, the constraint $Xe=0$ is equivalent to $\langle E,X\rangle=0$. It is interesting to note that desiring sparsity in the EDM D leads to the regularization term $\rho\langle I,X\rangle$, which is a proxy for desiring a low-rank X.

Let $m=|\mathscr{E}|$. The linear maps $\mathscr{A}:\mathscr{S}^n\to\mathfrak{R}^m$ and $\mathscr{B}:\mathscr{S}^n\to\mathfrak{R}$ for the problem (72) are given as follows:

$$(\mathscr{A}(X))_{(i,j)}=\langle\sqrt{W_{ij}}A_{ij},X\rangle,\ \forall\,(i,j)\in\mathscr{E},\quad \mathscr{B}(X)=\langle E,X\rangle.$$

Note that the components of a vector in $\mathfrak{R}^m$ are enumerated based on the elements in $\mathscr{E}$. And the operator $\mathscr{V}_t$ in (59) is given as follows:

$$\mathscr{V}_t=\sigma\left(\frac{1}{\sigma}T+\begin{bmatrix}\mathscr{A}\\\mathscr{B}\end{bmatrix}\Pi'_{\mathscr{S}^n_+}(W(y^t;X))\begin{bmatrix}\mathscr{A}^* & \mathscr{B}^*\end{bmatrix}\right). \qquad (73)$$

For the EDM problem (72), the condition number of $\mathscr{V}_t$ can be quite large and it is important to find a good preconditioner for $\mathscr{V}_t$ so that the CG method can have a reasonable convergence speed when solving the linear system of equations associated with $\mathscr{V}_t$. Let $\mathbf{A},\mathbf{B}$ and $\mathbf{S}$ be the matrix representations of $\mathscr{A},\mathscr{B}$ and $\Pi'_{\mathscr{S}^n_+}(W(y^t;X))$ with respect to the standard basis of $\mathscr{S}^n$ and $\mathfrak{R}^m$, respectively. Let $\mathbf{h}\in\mathfrak{R}^{n(n+1)/2}$ and $\Gamma=\{(i,j)\,|\,1\le i\le j\le n\}$. Suppose $\text{Diag}(\mathbf{h})$ is a positive definite diagonal approximation of $\mathbf{S}$. (In our implementation, we choose $\mathbf{h}$ to be the approximate diagonal of $\Pi'_{\mathscr{S}^n_+}(W(y^t;X))$ considered in [28].) Let $H\in\mathscr{S}^n$ be the matrix such that $H_{ij}=H_{ji}=\mathbf{h}_{(i,j)}$ for all $(i,j)\in\Gamma$. We consider the following approximation of $\frac{1}{\sigma}\mathscr{V}_t$:

$$\mathscr{M}=\begin{bmatrix}M & q\\q^T & \alpha\end{bmatrix}, \qquad (74)$$

where $q=\mathscr{A}(H)\in\mathfrak{R}^m$, $\alpha=\langle E,H\rangle$, and

$$M=\frac{1}{\sigma}I_m+\mathbf{A}\text{Diag}(\mathbf{h})\mathbf{A}^T\in\mathfrak{R}^{m\times m}. \qquad (75)$$

Note that the rows and columns of M are enumerated based on the elements of $\mathscr{E}$. We have that

$$M_{(i,j),(s,t)} = \begin{cases} 0 & \text{if } i \neq s, \, j \neq t, \\ \sqrt{W_{ij}W_{st}} \, H_{ss} & \text{if } i = s, \, j \neq t, \\ \sqrt{W_{ij}W_{st}} \, H_{tt} & \text{if } i \neq s, \, j = t, \\ 1/\sigma + \sqrt{W_{ij}W_{st}} (H_{ss} + H_{tt} + 2H_{st}) & \text{if } i = s, \, j = t. \end{cases}$$

Let $\bar{\mathbf{h}}_{(i,j)} = W_{ij}H_{ij}$ for all $(i,j) \in \mathscr{E}$. Then we know that M has the following structure

$$M = \mathbf{D} + JJ^T, \tag{76}$$

where $\mathbf{D} = \frac{1}{\sigma}I_m + 2\mathrm{Diag}(\bar{\mathbf{h}})$, and $J \in \Re^{m \times n}$ is the weighted arc-node incidence matrix for which the entry at the (s,t)-th row and k-th column is given by

$$J_{(s,t),k} = \begin{cases} \sqrt{W_{st}H_{ss}} & \text{if } k = s, \\ \sqrt{W_{st}H_{tt}} & \text{if } k = t, \\ 0 & \text{otherwise.} \end{cases}$$

To use $\mathscr{M}$ as a preconditioner for $\mathscr{V}_t$, we need the inverse of $\mathscr{M}$, which is given in the following expression:

$$\mathscr{M}^{-1} = \begin{bmatrix} S^{-1} & -\alpha^{-1}S^{-1}q \\ -\alpha^{-1}q^T S^{-1} & \alpha^{-1} + \alpha^{-2}q^T S^{-1}q \end{bmatrix}, \tag{77}$$

where

$$S = M - \alpha^{-1}qq^T = \mathbf{D} + \underbrace{[J, \, q]}_{\widehat{J}} \begin{bmatrix} I_n & 0 \\ 0 & -\alpha^{-1} \end{bmatrix} \begin{bmatrix} J^T \\ q^T \end{bmatrix}.$$

By using the Sherman-Morrison-Woodbury formula [14], we have that

$$S^{-1} = \mathbf{D}^{-1} - \mathbf{D}^{-1}\widehat{J}(\Lambda + \widehat{J}^T \mathbf{D}^{-1} \widehat{J})^{-1}\widehat{J}^T \mathbf{D}^{-1}, \tag{78}$$

where $\Lambda = [I_n, 0; 0, -\alpha]$. Here we assume that $\Lambda + \widehat{J}^T \mathbf{D}^{-1}\widehat{J}$ is nonsingular; otherwise we may consider the following block diagonal approximation of $\frac{1}{\sigma}\mathscr{V}_t$:

$$\mathscr{M}^d = \begin{bmatrix} M & 0 \\ 0 & \alpha \end{bmatrix}, \tag{79}$$

where the inverse of M can also be computed via the Sherman-Morrison-Woodbury formula.

The Euclidean metric problem arises in many applications. For the regularized kernel estimation (RKE) problem in statistics [21], we are given a set of n objects and dissimilarity measures d_{ij} for certain object pairs $(i,j) \in \mathscr{E}$. The goal is to estimate a positive semidefinite kernel matrix $X \in \mathscr{S}_+^n$ such that the fitted squared
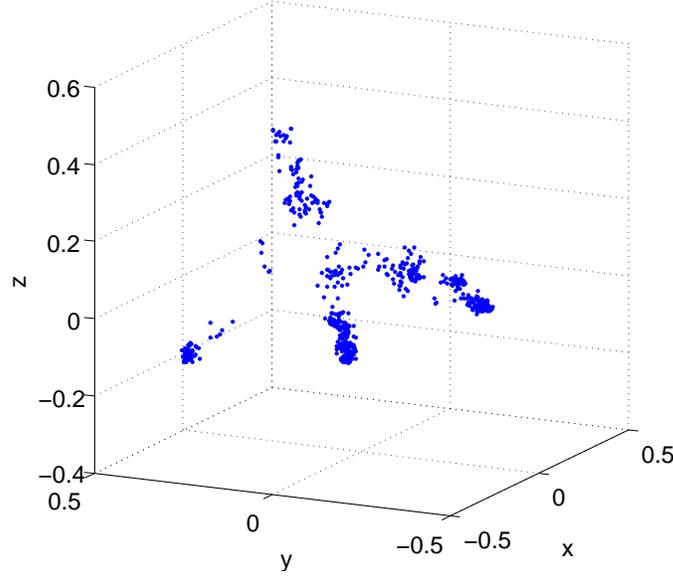
Fig. 1 A 3D representation of the sequence space for 630 proteins.

problem	n	$m+s$	ρ	it.	itsub	cg	R_p	R_D	relgap	#sv	time
RKE630-$\mathcal{M}$	630	198136	5.07e-1	6	36	10.3	2.67e-7	2.26e-8	-1.54e-6	388	36
PDB25-$\mathcal{M}$	1898	1646031	1.84e+0	23	68	22.3	1.89e-7	6.28e-7	-1.31e-6	1371	23:43
PDB25	1898	1646031	1.84e+0	23	80	76.7	9.60e-7	6.32e-7	-1.21e-6	1371	59:56

Table 4 Numerical results on the RKE problem arising from protein clustering.

distances induced by X between the objects satisfy the following condition:

$$X_{ii} + X_{jj} - 2X_{ij} = \langle A_{ij}, X \rangle \approx d_{ij}^2 \quad \forall \, (i,j) \in \mathcal{E}.$$

Formally, one version of the RKE problem proposed in [21] is the SDP problem (72).

In our numerical experiments, the data d_{ij} are normalized to be in the interval $[0, 1]$, and $\mathcal{E} = \{(i,j) : 1 \leq i < j \leq 630\}$. We set $W_{ij} = 1$ for all $(i,j) \in \mathcal{E}$. In [21], due to the prohibitive computational load encountered by the standard interior-point solver (such as SDPT3 or SeDuMi) used to solve (72), a subset of 280 globin proteins were selected from the entire set of 630 proteins for the numerical results reported in [21]. For each of the selected proteins, 55 dissimilarities were randomly selected out of the total of 279. Here we are able to consider the entire set of 630 proteins and the dissimilarities among all the pairs of proteins.

As mentioned in [21], the RKE methodology can provide an efficient way to represent each protein sequence by a feature vector in an appropriate coordinate system

using the pairwise dissimilarity between protein sequences. Specifically, we project the computed solution $\overline{X}$ onto a 3D space corresponding to the largest three eigen-values. Figure 1 displays a 3D representation of the sequence space for 630 proteins. There are at least 4 classes visually identifiable in the data set of 630 proteins, which is consistent with the observations in [21]. The numerical results for solving (72) are reported in Table 4, where #sv is the number of positive eigenvalues of $\overline{X}$. For the computed solution $\overline{X}$, we have $\langle \overline{X}, E \rangle = 4.46 \times 10^{-13}$ and $\langle \overline{X}, I \rangle = 1.85 \times 10^2$.

We also conducted numerical experiments on a much larger protein data set to evaluate the performance of our algorithm. We used the `PDB_SELECT 25` data set [17], a representative subset of the Protein Data Bank database, which contains 1898 protein chains. The numerical results for the `PDB_SELECT 25` data set are reported in Table 4. For the computed solution $\overline{X}$, we have $\langle \overline{X}, E \rangle = -1.94 \times 10^{-14}$ and $\langle \overline{X}, I \rangle = 8.76 \times 10^2$. To appreciate the usefulness of the preconditioner $\mathcal{M}$, we also report the numerical results for the PDB25 problem without using the preconditioner $\mathcal{M}$ in the last row of Table 4. We can observe that the CG solver without using the preconditioner $\mathcal{M}$ requires substantially more CG steps for computing the inexact Newton direction from the linear system (51).

5.3 Example 3: Molecular conformation problems

The molecular conformation problem for a molecule with n atoms is the problem of determining the positions $x_1, \ldots, x_n$ of the atoms, given estimated inter-atomic distances d_{ij} between some pairs of atoms. The estimated distances could be in-formation derived from covalent bond lengths or measured from nuclear magnetic resonance (NMR) experiments. Let $\mathcal{E}$ be the set of pairs of indices (i, j) $(i < j)$ for which estimates on the distances $\|x_i - x_j\|$ are available. The molecular conforma-tion problem can mathematically be formulated as follows:

$$\min \left\{ \frac{1}{2} \sum_{(i,j) \in \mathcal{E}} W_{ij} (\|x_i - x_j\|^2 - d_{ij}^2)^2 - \frac{\rho}{2n} \sum_{i,j=1}^n \|x_i - x_j\|^2 \mid \sum_{i=1}^n x_i = 0 \right\}, \quad (80)$$

where $W \in \mathcal{S}^n$ is a weight matrix with positive entries. The second term in the objective function is added to maximize the pairwise separations between the atoms. The equality constraint in (80) is included to set the center of mass of the molecule at the origin. The inclusion of weights is useful for differentiating data that are derived from different sources, and hence of different reliability. For example, distance data which are derived from covalent bond lengths are usually much more accurate than data which are derived from the NMR experiments.

Let $X = [x_1, \ldots, x_n] \in \mathfrak{R}^{3 \times n}$ and $A_{ij} = e_{ij} e_{ij}^T$, where $e_{ij} = e_i - e_j$. Then we have $x_i - x_j = X e_{ij}$ and hence $\|x_i - x_j\|^2 = \langle X^T X, A_{ij} \rangle$. Let $Y = X^T X$. The constraint $\sum_{i=1}^n x_i = 0$ can equivalently be replaced by $\langle E, Y \rangle = 0$. Note that under the latter constraint, it is easy to see that $\sum_{i,j=1}^n \|x_i - x_j\|^2 = 2n \langle I, Y \rangle$. By relaxing the non-convex constraint $Y = X^T X$ to $Y \succeq 0$ in (80), we get the following SDP problem:

$$\min\left\{\frac{1}{2}\sum_{(i,j)\in\mathscr{E}}W_{ij}(\langle A_{ij},Y\rangle-d_{ij}^2)^2-\rho\langle I,Y\rangle \mid \langle E,Y\rangle=0,Y\succeq 0\right\}. \quad (81)$$

Observe that under the constraints $\langle E,Y\rangle=0$ and $Y\succeq 0$, we have $\langle I,Y\rangle=\frac{1}{2n}\langle E,D\rangle$, where $D=\mathrm{Diag}(Y)e^T+e\,\mathrm{Diag}(Y)^T-2Y$ and $e\in\mathfrak{R}^n$ is a vector of all ones. Thus (81) seeks an Euclidean distance matrix D which is encouraged to have as many nonzero entries as possible. Note that in the maximum variance unfolding problem [30], one also consider a problem that has exactly the same form as (81).

In this example, we focus on molecular conformation problems with noisy and sparse distance data. In our numerical experiments, we set $W_{ij}=1/d_{ij}^2$ for all $(i,j)\in\mathscr{E}$ and $\rho=8\times 10^{-4}\|\mathscr{A}^*b\|_2$. For each molecule, we generated the partial inter-atomic distance matrix as follows. If the distance between two atoms is less than 6Å ($1\text{Å}=10^{-8}$cm), which is nearly the maximal distance that the NMR experiment can measure between two atoms, the distance is chosen; otherwise no distance information about the pair is known. Since not all the distances below 6Å are known from NMR experiments, we randomly choose 30% of all the distance below 6Å in our experiment. For realistic molecular conformation problems, in which the exact distances are not known and only the lower bounds $\underline{d}_{ij}$ and upper bounds $\bar{d}_{ij}$ on distances are provided, we use the mean $d_{ij}=(\bar{d}_{ij}+\underline{d}_{ij})/2$ as the estimated distances. After selecting 30% of inter-atomic distances, we add certain amount of normal noise or uniform noise to the distances to generate the lower and upper bounds. Suppose that $\hat{d}_{ij}$ is the exact distance between atom i and atom j, we set

$$\underline{d}_{ij}=\max(1,(1-|\underline{\varepsilon}_{ij}|)\hat{d}_{ij}),\quad \bar{d}_{ij}=(1+|\bar{\varepsilon}_{ij}|)\hat{d}_{ij}.$$

Let τ be a given noise level. In the normal noise model, $\underline{\varepsilon}_{ij},\bar{\varepsilon}_{ij}\sim\mathcal{N}(0,\pi\tau^2/2)$ are independent normal random variables. In the uniform noise model, $\underline{\varepsilon}_{ij},\bar{\varepsilon}_{ij}$ are independent uniform random variables in the interval $[0,2\tau]$. We said that the distances are corrupted by 20% noise if $\tau=0.2$.

Molecule	$n;m+s$	it.	itsub	cg	R_p	R_D	relgap	RMSD	time
1GM2	166; 1119	23	81	58.3	3.02e-7	7.46e-7	-4.92e-4	1.15	7
1PBM	388; 3145	29	113	89.5	6.25e-7	5.93e-7	-2.55e-4	1.20	52
1PTQ	402; 2182	28	108	155.8	1.04e-7	3.42e-7	-1.84e-4	1.51	1:24
1CTF	487; 2630	28	135	182.8	3.11e-7	3.65e-7	-2.88e-4	1.99	2:49
1AU6	506; 4767	24	105	168.7	2.88e-7	6.88e-7	-1.02e-3	0.96	2:24
1HOE	558; 3083	26	125	176.5	9.73e-7	6.70e-7	-4.01e-4	1.20	3:34
1PHT	814; 5239	31	169	204.8	2.90e-7	9.36e-7	-5.21e-4	2.65	13:05
1POA	914; 5045	31	192	224.4	3.29e-7	4.08e-7	-4.41e-4	2.57	20:40
1AX8	1003; 5563	30	184	207.3	2.67e-7	7.67e-7	-6.70e-4	2.05	22:49

Table 5 Numerical results on molecular conformation problems with 30% distances $\leq$ 6Å, which are corrupted by 20% normal noise.

Molecule	$n; m+s$	it.	itsub	cg	R_p	R_D	relgap	RMSD	time
1GM2	166; 1119	24	88	63.3	2.14e-7	5.19e-7	-1.51e-4	0.91	8
1PBM	388; 3145	24	105	106.6	1.33e-7	8.78e-7	-3.13e-4	1.02	57
1PTQ	402; 2182	26	112	145.1	1.03e-7	8.20e-7	-4.32e-4	1.31	1:22
1CTF	487; 2630	28	131	179.2	3.37e-7	3.18e-7	-2.38e-4	1.73	2:43
1AU6	506; 4767	24	131	162.7	3.32e-7	5.27e-7	-5.14e-4	0.79	2:54
1HOE	558; 3083	26	124	184.6	9.59e-8	6.92e-7	-3.94e-4	1.15	3:43
1PHT	814; 5239	31	180	205.8	6.22e-7	5.13e-7	-2.37e-4	2.47	13:57
1POA	914; 5045	30	185	209.5	6.80e-7	8.48e-7	-8.18e-4	2.25	18:43
1AX8	1003; 5563	30	175	214.4	6.99e-7	6.65e-7	-5.07e-4	1.84	22:13

Table 6 Numerical results on molecular conformation problems with 30% distances $\leq 6\mathring{A}$, which are corrupted by 20% uniform noise.

In Table 5 and Table 6, we report the numerical results on molecular conformation problems under the normal noise model and uniform noise model, respectively, where the root mean square deviation (RMSD) is used to measure the accuracy of the estimated positions. The RMSD is defined by the following formula:

$$\text{RMSD} := \frac{1}{\sqrt{n}} \left(\sum_{i=1}^{n} \|x_i - \hat{x}_i\|^2 \right)^{1/2}, \qquad (82)$$

where x_i is the estimated position and $\hat{x}_i$ is the actual position. We can observe from the tables that the estimated atomic positions via a simple projection of Y onto the 3-dimensional space are fairly accurate with RMSD $\approx 2\mathring{A}$.

6 Conclusion

In this paper, we introduced a partial PPA for solving nuclear norm regularized and semidefinite matrix least squares problems with linear equality constraints. The inner subproblems are solved inexactly by a semismooth Newton-CG method, whose convergence analysis is established under a constraint nondegeneracy condition, together with the strong semi-smoothness property of the soft-thresholding operator and the metric projector $\Pi_{\mathscr{S}_+^n}$. Numerical experiments conducted on nuclear norm regularized matrix least squares problems, regularized kernel estimation problems and molecular conformation problems demonstrated that our algorithm is efficient and robust. In [11], the graph visualization problem with applications in social network data analysis can be modeled as an optimization problem which is analogous to (80). It will be very interesting to investigate how to adapt our SSNCG partial PPA algorithm to solve large scale social network graph visualization problems.

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